Supplementary material for

Designing High-refractive Index Polymers using Materials Informatics

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Table S1: List of molecular descriptors used in this study.

Name	Description
CPSA_PPSA-1	partial positive surface area
CPSA_PPSA-2	partial positive surface area * total positive charge on the molecule
CPSA_PPSA-3	charge weighted partial positive surface area
CPSA_PNSA-1	partial negative surface area
CPSA_PNSA-2	partial negative surface area * total negative charge on the molecule
CPSA_PNSA-3	charge weighted partial negative surface area
CPSA_DPSA-1	difference of PPSA-1 and PNSA-1
CPSA_DPSA-2	difference of FPSA-2 and PNSA-2
CPSA_DPSA-3	difference of PPSA-3 and PNSA-3
CPSA_FPSA-1	PPSA-1/total molecular surface area
CPSA_FFSA-2	PPSA-2/total molecular surface area
CPSA_FPSA-3	PPSA-3/total molecular surface area
CPSA_FNSA-1	PNSA-1/total molecular surface area
CPSA_FNSA-2	PNSA-2/total molecular surface area
CPSA_FNSA-3	PNSA-3/total molecular surface area
CPSA_WPSA-1	PPSA-1 * total molecular surface area/1000
CPSA_WPSA-2	PPSA-2 * total molecular surface area /1000
CPSA_WPSA-3	PPSA-3 * total molecular surface area/1000
CPSA_WNSA-1	PNSA-1 * total molecular surface area /1000
CPSA_WNSA-2	PNSA-2 * total molecular surface area/1000
CPSA_WNSA-3	PNSA-3 * total molecular surface area/1000
CPSA_RPCG	relative positive charge
CPSA_RNCG	relative negative charge
CPSA_RPCS	relative positive charge surface area
CPSA_RNCS	relative negative charge surface area
CPSA_PPSA-4	additional CPSA descriptors [1]
CPSA_PPSA-5	additional CPSA descriptors
CPSA_PNSA-4	additional CPSA descriptors
CPSA_PNSA-5	additional CPSA descriptors
CPSA_SPMX	additional CPSA descriptors
CPSA_SNMX	additional CPSA descriptors
MOPAC_COSMO_AREA	Area of the solvent accessible surface
MOPAC_COSMO_VOLUME	Volume included in the COSMO surface
MOPAC_HOMO	Highest occupied molecular orbital
MOPAC_LUMO	Lowest unoccupied molecular orbital
MOPAC_HLGAP	Difference between HOMO-LUMO energies
MOPAC_HLFRACTION	ratio of HOMO/LUMO energies
MOPAC_CHARGE_DIPOLE	Dipole moment is calculated from the atomic charges
MOPAC_HYBRID_DIPOLE	hybrid dipole moment
MOPAC_TOTAL_DIPOLE	total dipole moment
MOPAC_HOF	Heat of formation
MOPAC_ABSOLUTE_HARDNESS	Parr and Pople absolute hardness
MOPAC_TOTAL_SOFTNESS	Inverse of the hardness
MOPAC_CORE-CORE_REPULSION	core-core repulsion energy
MOPAC_TOTAL_ENERGY	total energy
MOPAC_ELEC_NUC_ATTR	ELECTRON-NUCLEAR ATTRACTION
MOPAC_ELEC_ELEC_REPL	ELECTRON-ELECTRON REPULSION
MOPAC_ELEC_ENERGY	TOTAL OF ELECTRONIC AND NUCLEAR ENERGIES
MOPAC_RESONANCE_ENERGY	resonance energy
MOPAC_EXCHG_ENERGY	exchange energy
MOPAC_TOTAL_ELEC_INTRN	total electronic interaction
MOPAC_TOTAL_EPHIL_DELOC	total electrophilic delocalizability
MOPAC_TOTAL_NPHIL_DELOC	total neutrophilic delocalizability
MOPAC_TOTAL_SPOL	total self polarizability
MOPAC_ELECTROPHILICITY	electrophilicity
MOPAC_PIMX	Principal moments of inertia
MOPAC_PIMY	Principal moments of inertia
MOPAC_PIMZ	Principal moments of inertia
MOPAC_MW	Molecular Weight
MOPAC_FILLEDLEVELS	Number of filled levels
MOPAC_MIN_DNR	minimum nucleophilic delocalizability

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Table S1 – *Continued from previous page*

Name	Description
MOPAC_MIN_DER	minimum electrophilic delocalizability
MOPAC_MIN_SPOL	minimum self polarizability
MOPAC_MAX_DNR	maximum nucleophilic delocalizability
MOPAC_MAX_DER	maximum electrophilic delocalizability
MOPAC_MAX_SPOL	maximum self polarizability
MOPAC_AVG_POLARIZABILITY	average polarizability
MOPAC_POLARANISOTROPY	polar anisotropy
MOPAC_VIB_ENTHALPY	vibrational ENTHALPY
MOPAC_VIB_HEATCAP	vibrational HEATCAP
MOPAC_VIB_ENTROPY	vibrational ENTROPY
MOPAC_ROT_ENTHALPY	rotational ENTHALPY
MOPAC_ROT_HEATCAP	rotational HEATCAP
MOPAC_ROT_ENTROPY	rotational ENTROPY
MOPAC_TRANS_ENTHALPY	translational ENTHALPY
MOPAC_TRANS_HEATCAP	translational HEATCAP
MOPAC_TRANS_ENTROPY	translational ENTROPY
MOPAC_POL_ALPHA	ALPHA polarizability
MOPAC_POL_BETA	BETA polarizability
MOPAC_POL_GAMMA	GAMMA polarizability
CHG_MAXPOSCHG	maximum positive charge
CHG_MINNEGCHG	maximum negative charge
CHG_TOTABSCHG	Total absolute charge
CHG_TOTNEGCHG	Total negative charge
CHG_TOTPOSCHG	Total positive charge
CHG_TOTSQCHG	total squared charge
CHG_CHGPOL	charge polarization
CHG_LOCDIPOLEINDX	local dipole index
CHG_DP	second-order submolecular polarity Parameter
CHG_SPP	submolecular polarity Parameter
CHG_TEIATOMS	topological electronic index for atoms
CHG_TEIBONDS	topological electronic index for bonds
CHG_ECDCI	Electronic charge density connectivity index
GEOM_Wiener3D	3D Wiener index
GEOM_RadGyration	Radius of gyration
GEOM_InertialSF	inertial shape factor
GEOM_MolEccentricity	Molecular eccentricity
GEOM_Asphericity	Asphericity index
GEOM_Spherosity	Spherosity index
GEOM_Globularity	Globularity index
GEOM_Ovality	Ovality index
GRAPH_GEIGGE_PROPERTY	Graph energy from the weighted (charge,self-polarizability,delocalizability) adjacency matrix
Radial Distribution Function 1	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 1.1	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 1.2	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 1.3	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 1.4	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 1.5	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 1.6	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 1.7	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 1.8	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 1.9	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 2	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 2.1	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 2.2	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 2.3	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 2.4	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 2.5	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 2.6	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 2.7	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 2.8	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 2.9	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 3	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 3.1	weighted by charge, self-polarizability, delocalizability

Continued on next page

Table S1 – *Continued from previous page*

Name	Description
Radial Distribution Function 3.2	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 3.3	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 3.4	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 3.5	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 3.6	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 3.7	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 3.8	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 3.9	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 4	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 4.1	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 4.2	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 4.3	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 4.4	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 4.5	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 4.6	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 4.7	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 4.8	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 4.9	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 5	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 5.1	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 5.2	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 5.3	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 5.4	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 5.5	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 5.6	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 5.7	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 5.8	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 5.9	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 6	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 6.1	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 6.2	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 6.3	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 6.4	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 6.5	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 6.6	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 6.7	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 6.8	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 6.9	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 7	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 7.1	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 7.2	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 7.3	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 7.4	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 7.5	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 7.6	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 7.7	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 7.8	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 7.9	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 8	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 8.1	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 8.2	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 8.3	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 8.4	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 8.5	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 8.6	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 8.7	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 8.8	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 8.9	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 9	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 9.1	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 9.2	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 9.3	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 9.4	weighted by charge, self-polarizability, delocalizability

Continued on next page

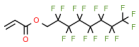
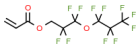
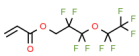
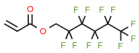
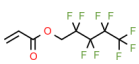
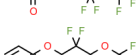
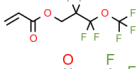
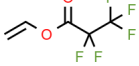
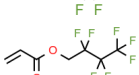
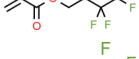
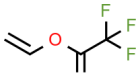
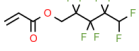
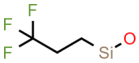
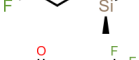
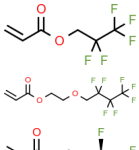
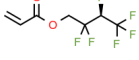
Table S1 – *Continued from previous page*

Name	Description
Radial Distribution Function 9.5	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 9.6	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 9.7	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 9.8	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 9.9	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 10	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 10.1	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 10.2	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 10.3	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 10.4	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 10.5	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 10.6	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 10.7	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 10.8	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 10.9	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 11	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 11.1	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 11.2	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 11.3	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 11.4	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 11.5	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 11.6	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 11.7	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 11.8	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 11.9	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 12	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 12.1	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 12.2	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 12.3	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 12.4	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 12.5	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 12.6	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 12.7	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 12.8	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 12.9	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 13	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 13.1	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 13.2	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 13.3	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 13.4	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 13.5	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 13.6	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 13.7	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 13.8	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 13.9	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 14	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 14.1	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 14.2	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 14.3	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 14.4	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 14.5	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 14.6	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 14.7	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 14.8	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 14.9	weighted by charge, self-polarizability, delocalizability
Radial Distribution Function 15	weighted by charge, self-polarizability, delocalizability

Table S2: Summary of the regression model performances for the refractive index (n), glass transition temperatures (T_g) and decomposition temperatures (T_d). Here, $NVAR$ is the number of variables used used in the model, N_{LV} the number of latent variables in the PLSR model, mtry the number of predictors sampled for splitting at each node in the RF model, MAE is the mean absolute error, $RMSE$ is the root mean squared error and R^2 the squared correlation between the observed and predicted values.

Model	**Property**	**NVAR**	$N_{LV}/mtry$	**Calibration**		**Testing**	
				R^2_{cv}	$RMSE$ (MAE)	R^2	$RMSE$ (MAE)
PLSR	n	61	4	0.79	0.04 (0.03)	0.79	0.04 (0.03)
	T_g (°C)	175	5	0.81	52 (34)	0.83	49 (38)
	T_d (°C)	218	4	0.61	49 (24)	0.62	51 (41)
RF	n	5	3	0.83	0.03 (0.01)	0.88	0.03 (0.02)
	T_g (°C)	16	4	0.86	44 (14)	0.88	40 (30)
	T_d (°C)	11	4	0.80	35 (12)	0.72	45 (30)
	ρ	7	3	0.64	0.13 (0.04)	0.66	0.14 (0.08)

Table S3: The table lists the experimental and predicted (± uncertainty) refractive indices for different polymers. Predictions for both PLSR and RF models are reported.

MONOMER	n^{exp}	n^{pred}_{PLSR}	n^{pred}_{RF}	Ref
	1.34	1.33 ± 0.02	1.36 ± 0.04	[6, 14, 4]
	1.35	1.36 ± 0.02	1.37 ± 0.03	[6, 14, 4]
	1.35	1.37 ± 0.02	1.36 ± 0.03	[6, 14, 4]
	1.35	1.44 ± 0.05	1.4 ± 0.05	[6, 14, 4]
	1.36	1.36 ± 0.02	1.36 ± 0.03	[6, 14, 4]
	1.36	1.38 ± 0.01	1.37 ± 0.03	[6, 14, 4]
	1.36	1.39 ± 0.02	1.37 ± 0.03	[6, 14, 4]
	1.36	1.41 ± 0.01	1.39 ± 0.05	[6, 14, 4]
	1.37	1.39 ± 0.01	1.37 ± 0.03	[6, 14, 4]
	1.38	1.42 ± 0.01	1.39 ± 0.04	[6, 14, 4]
	1.38	1.4 ± 0.01	1.38 ± 0.03	[6, 14, 4]
	1.38	1.38 ± 0.02	1.39 ± 0.03	[6, 14, 4]
	1.39	1.4 ± 0.01	1.38 ± 0.03	[6, 14, 4]
	1.39	1.38 ± 0.02	1.37 ± 0.04	[6, 14, 4]
	1.39	1.4 ± 0.01	1.4 ± 0.03	[6, 14, 4]
	1.4	1.35 ± 0.04	1.43 ± 0.06	[6, 14, 4]
	1.4	1.44 ± 0.03	1.42 ± 0.05	[6, 14, 4]
	1.41	1.42 ± 0.01	1.41 ± 0.04	[6, 14, 4]
	1.41	1.42 ± 0.01	1.41 ± 0.03	[6, 14, 4]
	1.42	1.45 ± 0.01	1.42 ± 0.03	[6, 14, 4]

Continued on next page

Table S3 – *Continued from previous page*

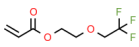
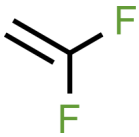
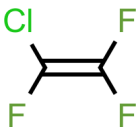
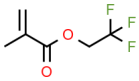
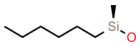
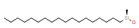
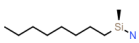
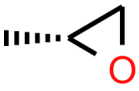
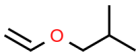
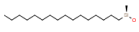
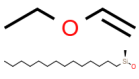
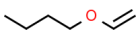
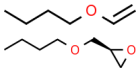
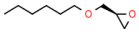
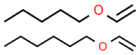
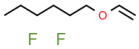
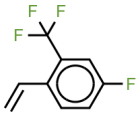
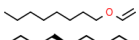
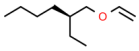
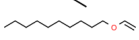
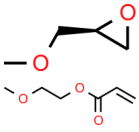
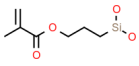
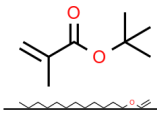
MONOMER	n^{exp}	n^{pred}_{PLSR}	n^{pred}_{RF}	Ref
	1.42	1.42 ± 0.01	1.41 ± 0.03	[6, 14, 4]
	1.42	1.48 ± 0.02	1.46 ± 0.07	[6, 14, 4]
	1.43	1.44 ± 0.05	1.46 ± 0.06	[6, 14, 4]
	1.44	1.44 ± 0.01	1.42 ± 0.03	[6, 14, 4]
	1.44	1.46 ± 0.02	1.45 ± 0.03	[6, 14, 4]
	1.44	1.47 ± 0.02	1.46 ± 0.03	[6, 14, 4]
	1.45	1.5 ± 0.02	1.48 ± 0.03	[6, 14, 4]
	1.45	1.42 ± 0.02	1.46 ± 0.03	[6, 14, 4]
	1.45	1.5 ± 0.01	1.46 ± 0.03	[6, 14, 4]
	1.45	1.45 ± 0.02	1.46 ± 0.03	[6, 14, 4]
	1.45	1.49 ± 0.01	1.46 ± 0.03	[6, 14, 4]
	1.46	1.46 ± 0.02	1.46 ± 0.03	[6, 14, 4]
	1.46	1.41 ± 0.03	1.46 ± 0.04	[6, 14, 4]
	1.46	1.48 ± 0.01	1.46 ± 0.02	[6, 14, 4]
	1.46	1.44 ± 0.01	1.47 ± 0.03	[6, 14, 4]
	1.46	1.43 ± 0.01	1.47 ± 0.03	[6, 14, 4]
	1.46	1.48 ± 0.01	1.46 ± 0.02	[6, 14, 4]
	1.46	1.48 ± 0.01	1.46 ± 0.02	[6, 14, 4]
	1.46	1.5 ± 0.02	1.52 ± 0.09	[6, 14, 4]
	1.46	1.48 ± 0.01	1.46 ± 0.02	[6, 14, 4]
	1.46	1.53 ± 0.01	1.46 ± 0.02	[6, 14, 4]
	1.46	1.49 ± 0.01	1.47 ± 0.03	[6, 14, 4]
	1.46	1.42 ± 0.02	1.47 ± 0.04	[6, 14, 4]
	1.46	1.49 ± 0.01	1.48 ± 0.03	[6, 14, 4]
	1.46	1.44 ± 0.02	1.45 ± 0.05	[6, 14, 4]
	1.46	1.53 ± 0.01	1.51 ± 0.04	[6, 14, 4]
	1.46	1.49 ± 0.01	1.48 ± 0.03	[6, 14, 4]

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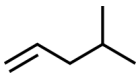
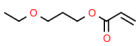
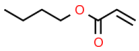
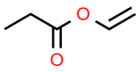
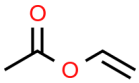
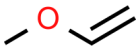
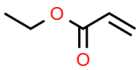
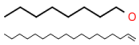
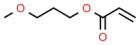
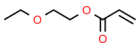
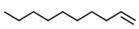
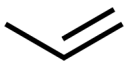
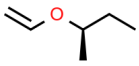
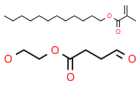
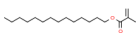
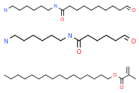
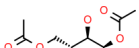
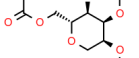
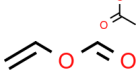
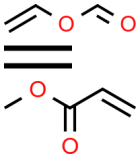
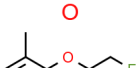
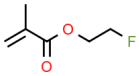
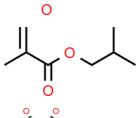
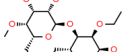
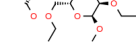
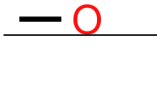
Table S3 – *Continued from previous page*

MONOMER	n^{exp}	n^{pred}_{PLSR}	n^{pred}_{RF}	Ref
	1.47	1.52 ± 0.02	1.48 ± 0.03	[6, 14, 4]
	1.47	1.48 ± 0.04	1.48 ± 0.02	[6, 14, 4]
	1.47	1.49 ± 0.01	1.47 ± 0.03	[6, 14, 4]
	1.47	1.5 ± 0.01	1.47 ± 0.03	[6, 14, 4]
	1.47	1.49 ± 0.01	1.47 ± 0.03	[6, 14, 4]
	1.47	1.5 ± 0.01	1.47 ± 0.02	[6, 14, 4]
	1.47	1.5 ± 0.01	1.48 ± 0.04	[6, 14, 4]
	1.47	1.43 ± 0.02	1.46 ± 0.02	[6, 14, 4]
	1.47	1.49 ± 0.02	1.49 ± 0.03	[6, 14, 4]
	1.47	1.48 ± 0.02	1.47 ± 0.02	[6, 14, 4]
	1.47	1.5 ± 0.01	1.47 ± 0.01	[6, 14, 4]
	1.47	1.49 ± 0.02	1.47 ± 0.01	[6, 14, 4]
	1.47	1.51 ± 0.02	1.49 ± 0.03	[6, 14, 4]
	1.47	1.53 ± 0.01	1.49 ± 0.06	[6, 14, 4]
	1.47	1.5 ± 0.01	1.48 ± 0.02	[6, 14, 4]
	1.47	1.45 ± 0.01	1.44 ± 0.05	[6, 14, 4]
	1.47	1.5 ± 0.01	1.48 ± 0.02	[6, 14, 4]
	1.48	1.54 ± 0.02	1.49 ± 0.03	[6, 14, 4]
	1.48	1.52 ± 0.01	1.51 ± 0.03	[6, 14, 4]
	1.48	1.5 ± 0.02	1.47 ± 0.03	[6, 14, 4]
	1.48	1.44 ± 0.01	1.47 ± 0.04	[6, 14, 4]
	1.48	1.49 ± 0.02	1.47 ± 0.03	[6, 14, 4]
	1.48	1.48 ± 0.04	1.51 ± 0.04	[6, 14, 4]
	1.48	1.49 ± 0.02	1.48 ± 0.04	[6, 14, 4]
	1.48	1.49 ± 0.01	1.46 ± 0.04	[6, 14, 4]
	1.48	1.52 ± 0.01	1.5 ± 0.03	[6, 14, 4]
	1.48	1.46 ± 0.02	1.47 ± 0.03	[6, 14, 4]
	1.48	1.35 ± 0.06	1.46 ± 0.04	[6, 14, 4]

Continued on next page

Table S3 – *Continued from previous page*

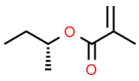
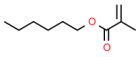
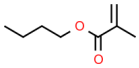
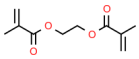
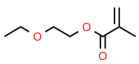
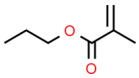
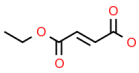
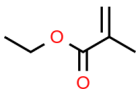
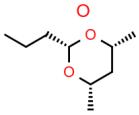
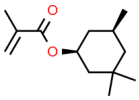
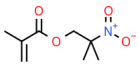
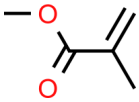
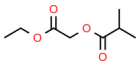
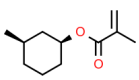
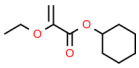
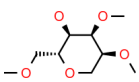
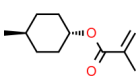
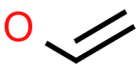
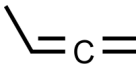
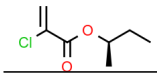
MONOMER	n^{exp}	n^{pred}_{PLSR}	n^{pred}_{RF}	Ref
	1.48	1.52 ± 0.01	1.49 ± 0.02	[6, 14, 4]
	1.48	1.5 ± 0.01	1.49 ± 0.02	[6, 14, 4]
	1.48	1.49 ± 0.01	1.5 ± 0.02	[6, 14, 4]
	1.48	1.5 ± 0.06	1.49 ± 0.03	[6, 14, 4]
	1.48	1.51 ± 0.01	1.48 ± 0.02	[6, 14, 4]
	1.48	1.5 ± 0.01	1.49 ± 0.03	[6, 14, 4]
	1.48	1.47 ± 0.02	1.48 ± 0.05	[6, 14, 4]
	1.49	1.51 ± 0.01	1.5 ± 0.03	[6, 14, 4]
	1.49	1.46 ± 0.02	1.48 ± 0.02	[6, 14, 4]
	1.49	1.53 ± 0.01	1.5 ± 0.03	[6, 14, 4]
	1.49	1.53 ± 0.01	1.5 ± 0.03	[6, 14, 4]
	1.49	1.51 ± 0.01	1.5 ± 0.03	[6, 14, 4]
	1.49	1.44 ± 0.01	1.45 ± 0.04	[6, 14, 4]
	1.49	1.52 ± 0.01	1.5 ± 0.02	[6, 14, 4]
	1.5	1.53 ± 0.01	1.49 ± 0.02	[6, 14, 4]
	1.5	1.47 ± 0.02	1.45 ± 0.04	[6, 14, 4]
	1.5	1.51 ± 0.01	1.5 ± 0.02	[6, 14, 4]
	1.5	1.46 ± 0.03	1.49 ± 0.03	[6, 14, 4]
	1.5	1.54 ± 0.02	1.5 ± 0.03	[6, 14, 4]
	1.5	1.52 ± 0.01	1.52 ± 0.03	[6, 14, 4]

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Table S3 – *Continued from previous page*

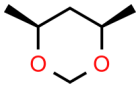
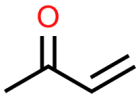
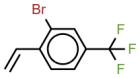
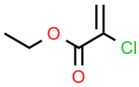
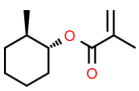
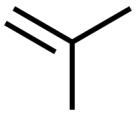
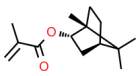
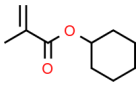
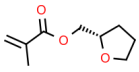
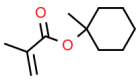
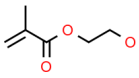
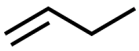
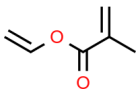
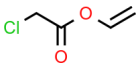
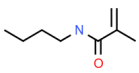
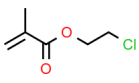
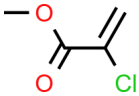
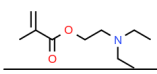
MONOMER	n^{exp}	n^{pred}_{PLSR}	n^{pred}_{RF}	Ref
	1.5	1.46 ± 0.02	1.48 ± 0.03	[6, 14, 4]
	1.5	1.51 ± 0.01	1.5 ± 0.03	[6, 14, 4]
	1.5	1.5 ± 0.02	1.48 ± 0.03	[6, 14, 4]
	1.5	1.55 ± 0.01	1.52 ± 0.07	[6, 14, 4]
	1.5	1.51 ± 0.01	1.51 ± 0.02	[6, 14, 4]
	1.5	1.53 ± 0.01	1.49 ± 0.02	[6, 14, 4]
	1.5	1.56 ± 0.02	1.5 ± 0.04	[6, 14, 4]
	1.51	1.53 ± 0.01	1.51 ± 0.03	[6, 14, 4]
	1.51	1.52 ± 0.01	1.51 ± 0.02	[6, 14, 4]
	1.51	1.51 ± 0.01	1.49 ± 0.03	[6, 14, 4]
	1.51	1.53 ± 0.01	1.52 ± 0.03	[6, 14, 4]
	1.51	1.5 ± 0.01	1.48 ± 0.03	[6, 14, 4]
	1.51	1.5 ± 0.02	1.5 ± 0.03	[6, 14, 4]
	1.51	1.54 ± 0.01	1.54 ± 0.04	[6, 14, 4]
	1.51	1.49 ± 0.01	1.52 ± 0.03	[6, 14, 4]
	1.51	1.54 ± 0.01	1.52 ± 0.03	[6, 14, 4]
	1.52	1.51 ± 0.01	1.5 ± 0.03	[6, 14, 4]
	1.52	1.52 ± 0.01	1.51 ± 0.03	[6, 14, 4]
	1.52	1.55 ± 0.01	1.57 ± 0.04	[6, 14, 4]
				

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Table S3 – *Continued from previous page*

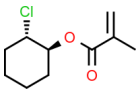
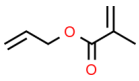
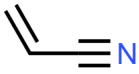
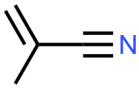
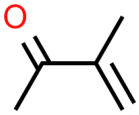
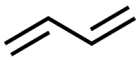
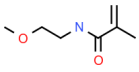
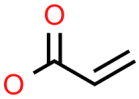
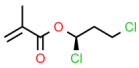
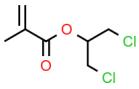
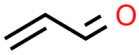
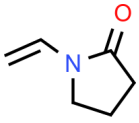
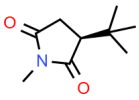
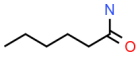
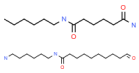
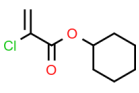
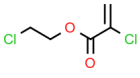
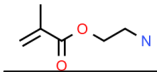
MONOMER	n^{exp}	n^{pred}_{PLSR}	n^{pred}_{RF}	Ref
	1.52	1.53 ± 0.01	1.48 ± 0.04	[6, 14, 4]
	1.52	1.52 ± 0.01	1.52 ± 0.02	[6, 14, 4]
	1.52	1.52 ± 0.02	1.51 ± 0.03	[6, 14, 4]
	1.52	1.57 ± 0.02	1.52 ± 0.03	[6, 14, 4]
	1.52	1.55 ± 0.01	1.52 ± 0.03	[6, 14, 4]
	1.52	1.56 ± 0.02	1.57 ± 0.07	[6, 14, 4]
	1.52	1.58 ± 0.02	1.55 ± 0.06	[6, 14, 4]
	1.52	1.53 ± 0.01	1.53 ± 0.03	[6, 14, 4]
	1.53	1.49 ± 0.01	1.5 ± 0.04	[6, 14, 4]
	1.53	1.52 ± 0.01	1.51 ± 0.03	[6, 14, 4]
	1.53	1.53 ± 0.02	1.51 ± 0.04	[6, 14, 4]
	1.53	1.51 ± 0.02	1.52 ± 0.03	[6, 14, 4]
	1.53	1.55 ± 0.01	1.55 ± 0.04	[6, 14, 4]
	1.53	1.5 ± 0.01	1.48 ± 0.03	[6, 14, 4]
	1.53	1.47 ± 0.01	1.51 ± 0.03	[6, 14, 4]
	1.53	1.46 ± 0.02	1.49 ± 0.02	[6, 14, 4]
	1.53	1.51 ± 0.01	1.51 ± 0.03	[6, 14, 4]
	1.53	1.53 ± 0.01	1.52 ± 0.02	[6, 14, 4]
	1.53	1.5 ± 0.01	1.52 ± 0.02	[6, 14, 4]
	1.54	1.53 ± 0.01	1.53 ± 0.03	[6, 14, 4]

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Table S3 – *Continued from previous page*

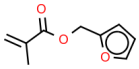
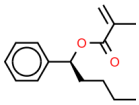
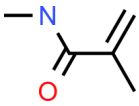
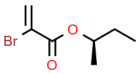
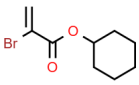
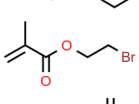
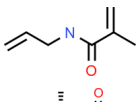
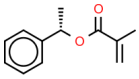
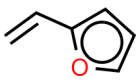
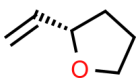
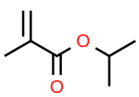
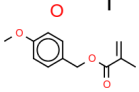
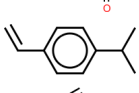
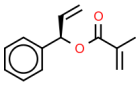
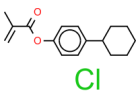
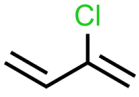
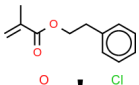
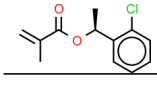
MONOMER	n^{exp}	n^{pred}_{PLSR}	n^{pred}_{RF}	Ref
	1.54	1.53 ± 0.01	1.57 ± 0.03	[6, 14, 4]
	1.54	1.49 ± 0.02	1.52 ± 0.04	[6, 14, 4]
	1.54	1.59 ± 0.01	1.57 ± 0.03	[6, 14, 4]
	1.54	1.55 ± 0.01	1.53 ± 0.02	[6, 14, 4]
	1.54	1.55 ± 0.01	1.52 ± 0.02	[6, 14, 4]
	1.54	1.55 ± 0.01	1.53 ± 0.02	[6, 14, 4]
	1.54	1.53 ± 0.01	1.51 ± 0.03	[6, 14, 4]
	1.55	1.55 ± 0.01	1.54 ± 0.03	[6, 14, 4]
	1.55	1.55 ± 0.01	1.56 ± 0.03	[6, 14, 4]
	1.55	1.57 ± 0.01	1.57 ± 0.03	[6, 14, 4]
	1.55	1.51 ± 0.01	1.5 ± 0.04	[6, 14, 4]
	1.55	1.52 ± 0.01	1.53 ± 0.03	[6, 14, 4]
	1.55	1.55 ± 0.01	1.57 ± 0.03	[6, 14, 4]
	1.55	1.58 ± 0.02	1.57 ± 0.03	[6, 14, 4]
	1.56	1.56 ± 0.01	1.57 ± 0.03	[6, 14, 4]
	1.56	1.54 ± 0.01	1.57 ± 0.03	[6, 14, 4]
	1.56	1.56 ± 0.02	1.57 ± 0.06	[6, 14, 4]
	1.56	1.53 ± 0.01	1.57 ± 0.03	[6, 14, 4]
	1.56	1.56 ± 0.01	1.58 ± 0.03	[6, 14, 4]

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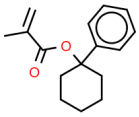
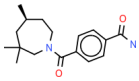
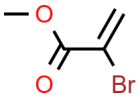
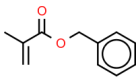
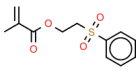
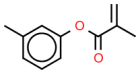
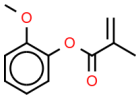
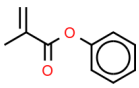
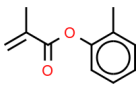
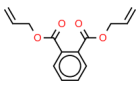
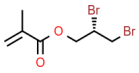
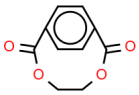
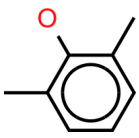
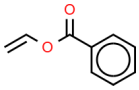
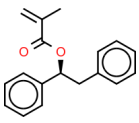
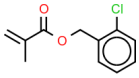
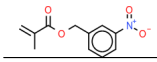
Table S3 – *Continued from previous page*

MONOMER	n^{exp}	n^{pred}_{PLSR}	n^{pred}_{RF}	Ref
	1.56	1.58 ± 0.01	1.56 ± 0.03	[6, 14, 4]
	1.57	1.58 ± 0.01	1.57 ± 0.02	[6, 14, 4]
	1.57	1.54 ± 0.01	1.52 ± 0.03	[6, 14, 4]
	1.57	1.53 ± 0.01	1.57 ± 0.03	[6, 14, 4]
	1.57	1.57 ± 0.06	1.55 ± 0.05	[6, 14, 4]
	1.57	1.55 ± 0.01	1.57 ± 0.02	[6, 14, 4]
	1.57	1.57 ± 0.01	1.57 ± 0.02	[6, 14, 4]
	1.57	1.55 ± 0.01	1.57 ± 0.02	[6, 14, 4]
	1.57	1.55 ± 0.01	1.57 ± 0.02	[6, 14, 4]
	1.57	1.54 ± 0.01	1.57 ± 0.04	[6, 14, 4]
	1.57	1.52 ± 0.01	1.51 ± 0.03	[6, 14, 4]
	1.57	1.54 ± 0.02	1.56 ± 0.06	[6, 14, 4]
	1.57	1.58 ± 0.02	1.58 ± 0.06	[6, 14, 4]
	1.58	1.55 ± 0.01	1.58 ± 0.02	[6, 14, 4]
	1.58	1.59 ± 0.01	1.58 ± 0.02	[6, 14, 4]
	1.58	1.54 ± 0.01	1.58 ± 0.03	[6, 14, 4]
	1.58	1.55 ± 0.01	1.56 ± 0.04	[6, 14, 4]

Continued on next page

Table S3 – *Continued from previous page*

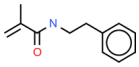
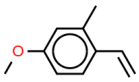
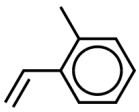
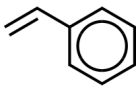
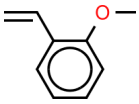
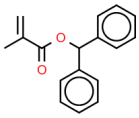
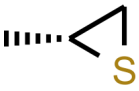
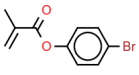
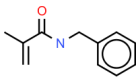
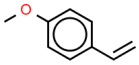
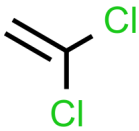
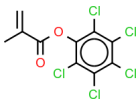
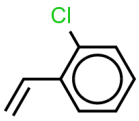
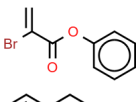
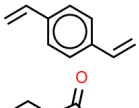
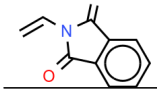
MONOMER	n^{exp}	n^{pred}_{PLSR}	n^{pred}_{RF}	Ref
	1.59	1.56 ± 0.01	1.58 ± 0.03	[6, 14, 4]
	1.59	1.57 ± 0.01	1.6 ± 0.03	[6, 14, 4]
	1.59	1.6 ± 0.02	1.59 ± 0.03	[6, 14, 4]
	1.59	1.6 ± 0.02	1.6 ± 0.03	[6, 14, 4]
	1.59	1.6 ± 0.01	1.59 ± 0.04	[6, 14, 4]
	1.59	1.59 ± 0.02	1.58 ± 0.05	[6, 14, 4]
	1.6	1.61 ± 0.02	1.57 ± 0.07	[6, 14, 4]
	1.6	1.58 ± 0.01	1.57 ± 0.02	[6, 14, 4]
	1.6	1.57 ± 0.01	1.57 ± 0.03	[6, 14, 4]
	1.6	1.57 ± 0.01	1.6 ± 0.03	[6, 14, 4]
	1.6	1.53 ± 0.03	1.57 ± 0.05	[6, 14, 4]
	1.61	1.56 ± 0.01	1.59 ± 0.04	[6, 14, 4]
	1.61	1.59 ± 0.02	1.6 ± 0.03	[6, 14, 4]
	1.61	1.56 ± 0.01	1.59 ± 0.03	[6, 14, 4]
	1.61	1.61 ± 0.02	1.62 ± 0.02	[6, 14, 4]
	1.62	1.59 ± 0.02	1.62 ± 0.04	[6, 14, 4]

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Table S3 – *Continued from previous page*

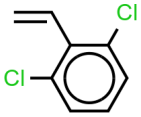
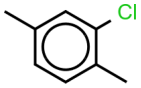
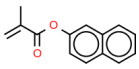
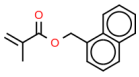
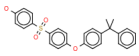
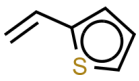
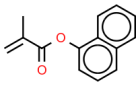
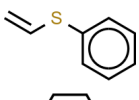
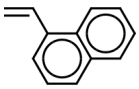
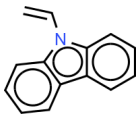
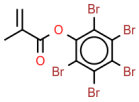
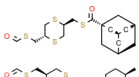
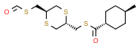
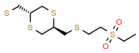
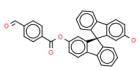
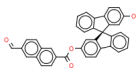
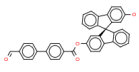
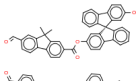
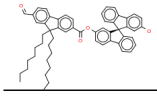
MONOMER	n^{exp}	n^{pred}_{PLSR}	n^{pred}_{RF}	Ref
	1.62	1.58 ± 0.02	1.61 ± 0.03	[6, 14, 4]
	1.63	1.56 ± 0.02	1.59 ± 0.06	[6, 14, 4]
	1.63	1.58 ± 0.01	1.62 ± 0.03	[6, 14, 4]
	1.63	1.58 ± 0.01	1.62 ± 0.04	[6, 14, 4]
	1.63	1.66 ± 0.06	1.62 ± 0.03	[6, 14, 4]
	1.64	1.65 ± 0.02	1.62 ± 0.03	[6, 14, 4]
	1.64	1.58 ± 0.01	1.63 ± 0.03	[6, 14, 4]
	1.66	1.7 ± 0.02	1.65 ± 0.02	[6, 14, 4]
	1.67	1.55 ± 0.02	1.6 ± 0.07	[6, 14, 4]
	1.68	1.63 ± 0.02	1.67 ± 0.02	[6, 14, 4]
	1.68	1.65 ± 0.01	1.67 ± 0.02	[6, 14, 4]
	1.71	1.62 ± 0.01	1.6 ± 0.05	[6, 14, 4]
	1.61	1.61 ± 0.02	1.63 ± 0.03	[60]
	1.63	1.59 ± 0.02	1.61 ± 0.03	[60]
	1.65	1.67 ± 0.05	1.65 ± 0.02	[60]
	1.68	1.65 ± 0.01	1.68 ± 0.02	[45]
	1.7	1.66 ± 0.01	1.68 ± 0.02	[45]
	1.68	1.67 ± 0.02	1.68 ± 0.01	[45]
	1.68	1.68 ± 0.01	1.68 ± 0.01	[45]
	1.68	1.7 ± 0.02	1.67 ± 0.02	[45]

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Table S3 – *Continued from previous page*

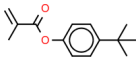
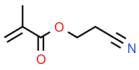
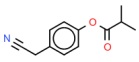
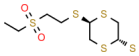
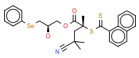
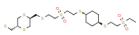
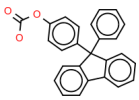
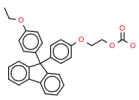
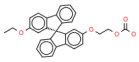
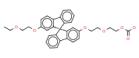
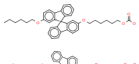
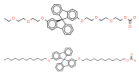
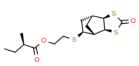
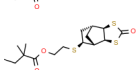
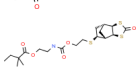
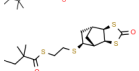
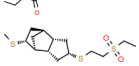
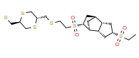
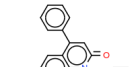
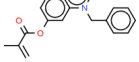
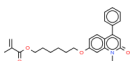
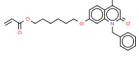
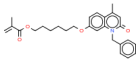
MONOMER	n^{exp}	n^{pred}_{PLSR}	n^{pred}_{RF}	Ref
	1.49	1.55 ± 0.01	1.56 ± 0.02	[29]
	1.51	1.52 ± 0.01	1.51 ± 0.03	[29]
	1.51	1.54 ± 0.01	1.57 ± 0.03	[29]
	1.69	1.64 ± 0.06	1.64 ± 0.02	[42]
	1.6	1.75 ± 0.03	1.67 ± 0.02	[46]
	1.65	1.69 ± 0.09	1.64 ± 0.05	[46]
	1.64	1.6 ± 0.02	1.63 ± 0.03	[46]
	1.64	1.61 ± 0.01	1.63 ± 0.02	[46]
	1.66	1.64 ± 0.02	1.66 ± 0.02	[46]
	1.64	1.64 ± 0.01	1.65 ± 0.04	[46]
	1.65	1.64 ± 0.01	1.65 ± 0.03	[46]
	1.62	1.61 ± 0.02	1.65 ± 0.04	[42]
	1.65	1.64 ± 0.02	1.65 ± 0.04	[42]
	1.62	1.61 ± 0.01	1.62 ± 0.04	[42]
	1.61	1.61 ± 0.02	1.61 ± 0.04	[42]
	1.59	1.6 ± 0.02	1.61 ± 0.06	[50]
	1.64	1.6 ± 0.02	1.63 ± 0.03	[50]
	1.61	1.65 ± 0.05	1.64 ± 0.04	[12]
	1.62	1.68 ± 0.1	1.65 ± 0.04	[12]
	1.69	1.64 ± 0.01	1.66 ± 0.03	[12]
	1.62	1.63 ± 0.01	1.62 ± 0.02	[12]
	1.62	1.65 ± 0.01	1.62 ± 0.02	[12]
	1.61	1.63 ± 0.01	1.61 ± 0.02	[12]
	1.63	1.65 ± 0.01	1.62 ± 0.02	[12]

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Table S3 – *Continued from previous page*

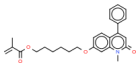
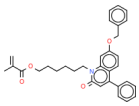
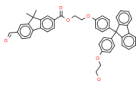
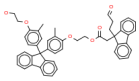
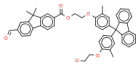
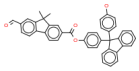
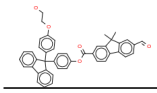
MONOMER	n^{exp}	n^{pred}_{PLSR}	n^{pred}_{RF}	Ref
	1.61	1.63 ± 0.01	1.63 ± 0.03	[44]
	1.62	1.64 ± 0.01	1.63 ± 0.02	[44]
	1.65	1.66 ± 0.01	1.65 ± 0.02	[44]
	1.66	1.6 ± 0.01	1.63 ± 0.03	[44]
	1.64	1.63 ± 0.01	1.65 ± 0.02	[44]
	1.66	1.66 ± 0.01	1.67 ± 0.02	[44]
	1.66	1.65 ± 0.01	1.66 ± 0.02	[44]

Table S4: The table lists the experimental and predicted (± uncertainty) glass transition temperatures for different monomers. Predictions for both PLSR and RF models are reported.

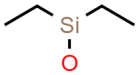
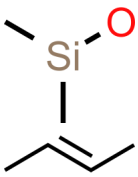
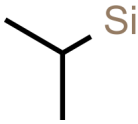
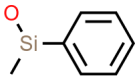
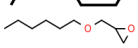
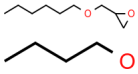
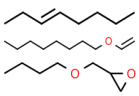
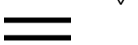
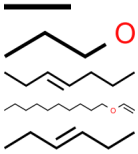
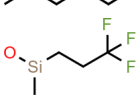
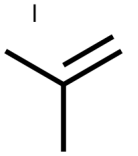
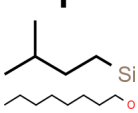
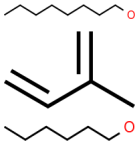
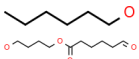
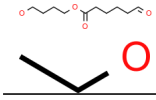
MONOMER	T_g^{exp}	$\widehat{T_g^{PLSR}}$	$\widehat{T_g^{RF}}$	Ref
	-143	-27± 32	15±76	[4]
	-121	-87± 30	1±79	[4]
	-102	-11± 10	-71±55	[4]
	-100	-27± 16	-65±46	[4]
	-86	-14± 21	-25±75	[4]
	-85	-61± 14	-71±37	[4]
	-83	-97± 15	-75±23	[4]
	-82	-53± 31	-14±79	[4]
	-81	-15± 12	-51±50	[4]
	-79	-31± 12	-46±36	[4]
	-79	-62± 13	-66±47	[4]
	-78	-16± 26	-16±59	[4]
	-78	-98± 17	-77±20	[4]
	-77	-10± 11	-49±57	[4]
	-76	-31± 12	-40±41	[4]
	-76	-7± 10	-44±58	[4]
	-74	-137± 35	13±81	[4]
	-74	9± 16	-59±65	[4]
	-70	-42± 13	-58±36	[4]
	-70	-92± 16	-72±33	[4]
	-70	57± 10	-40±61	[4]
	-69	-97± 15	-72±31	[4]
	-68	-10± 14	-47±59	[4]
	-67	-103± 27	-69±14	[4]

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Table S4 – *Continued from previous page*

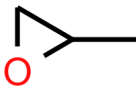
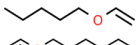
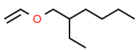
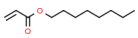
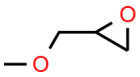
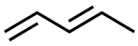
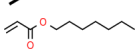
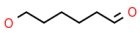
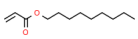
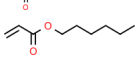
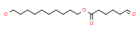
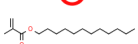
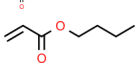
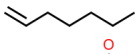
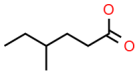
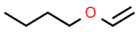
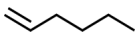
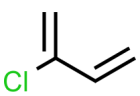
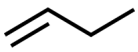
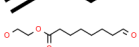
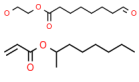
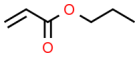
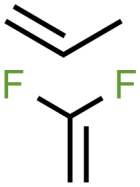
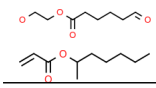
MONOMER	T_g^{exp}	$\widehat{T_g^{PLSR}}$	$\widehat{T_g^{RF}}$	Ref
	-67	-62± 19	-69±29	[4]
	-66	-29± 12	-52±30	[4]
	-66	20± 13	-33±60	[4]
	-65	-22± 10	-53±22	[4]
	-64	-30± 11	-55±27	[4]
	-62	-60± 12	-68±45	[4]
	-60	59± 11	-14±69	[4]
	-60	-19± 10	-55±15	[4]
	-60	-23± 11	-12±54	[4]
	-58	-24± 11	-49±28	[4]
	-57	-16± 9	-50±33	[4]
	-56	-9± 19	-35±57	[4]
	-55	-140± 49	-68±30	[4]
	-55	-31± 15	-23±53	[4]
	-54	-8± 7	-48±41	[4]
	-53	-20± 11	-18±47	[4]
	-53	-19± 9	-25±48	[4]
	-52	-28± 13	-44±35	[4]
	-50	-21± 10	-18±47	[4]
	-50	-19± 12	-28±47	[4]
	-48	80± 13	-38±62	[4]
	-47	19± 15	-35±66	[4]
	-45	-16± 15	-27±43	[4]
	-45	-11± 15	-43±57	[4]
	-45	-8± 11	-20±51	[4]
	-44	-3± 7	-42±48	[4]
	-7	-12± 20	-17±51	[4]
	-40	33± 27	-28±58	[4]
	-40	-14± 13	-47±57	[4]
	-38	2± 10	-26±47	[4]

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Table S4 – *Continued from previous page*

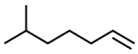
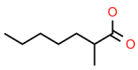
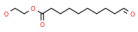
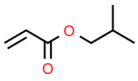
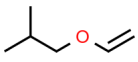
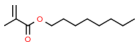
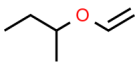
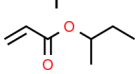
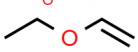
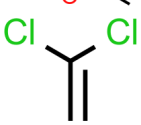
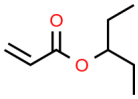
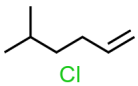
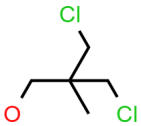
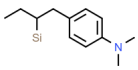
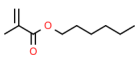
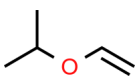
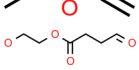
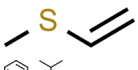
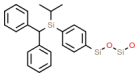
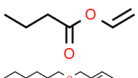
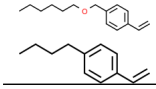
MONOMER	T_g^{exp}	$\widehat{T_g^{PLSR}}$	$\widehat{T_g^{RF}}$	Ref
	-34	-9± 10	-20±53	[4]
	-33	-23± 9	-26±47	[4]
	-30	-9± 16	-29±59	[4]
	-24	8± 9	-36±38	[4]
	-22	-11± 9	-17±43	[4]
	-22	10± 9	-25±62	[4]
	-20	-22± 11	-11±42	[4]
	-20	6± 10	-15±52	[4]
	-20	14± 11	-18±48	[4]
	-19	-18± 12	-30±38	[4]
	-17	-6± 33	-5±77	[4]
	-16	35± 13	-6±58	[4]
	-14	-12± 11	2±65	[4]
	-8	-5± 14	30±75	[4]
	-6	67± 9	23±56	[4]
	-5	-15± 9	-3±40	[4]
	-3	-5± 10	-27±45	[4]
	-1	-6± 13	-44±60	[4]
	-1	32± 17	-2±72	[4]
	0	87± 42	120±64	[4]
	5	-12± 7	38±52	[4]
	5	54± 9	40±34	[4]
	6	81± 8	35±45	[4]

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Table S4 – *Continued from previous page*

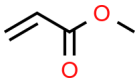
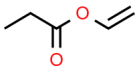
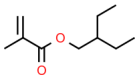
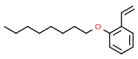
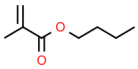
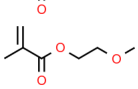
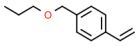
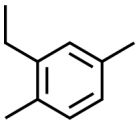
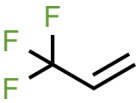
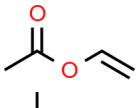
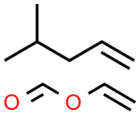
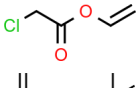
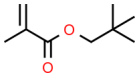
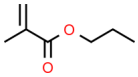
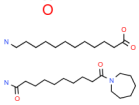
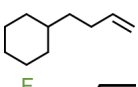
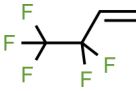
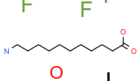
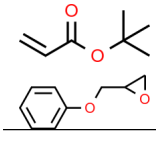
MONOMER	T_g^{exp}	$\widehat{T_g^{PLSR}}$	$\widehat{T_g^{RF}}$	Ref
	8	20± 10	2±64	[4]
	10	4± 8	22±46	[4]
	11	7± 10	26±42	[4]
	13	55± 9	32±32	[4]
	20	-10± 7	10±45	[4]
	20	-6± 8	11±67	[4]
	22	68± 8	34±31	[4]
	25	75± 10	68±45	[4]
	27	20± 13	-8±63	[4]
	28	0± 11	24±55	[4]
	29	-2± 10	6±65	[4]
	31	20± 18	32±69	[4]
	31	25± 9	30±50	[4]
	33	10± 9	42±51	[4]
	35	-5± 7	11±55	[4]
	37	-18± 14	36±35	[4]
	40	-18± 15	35±60	[4]
	40	0± 12	46±75	[4]
	41	29± 14	27±61	[4]
	42	-17± 13	36±36	[4]
	42	27± 11	24±60	[4]
	42	59± 7	53±42	[4]

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Table S4 – *Continued from previous page*

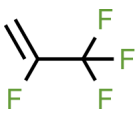
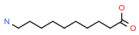
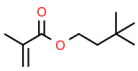
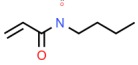
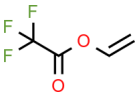
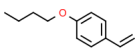
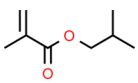
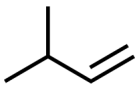
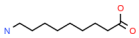
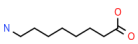
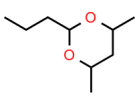
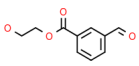
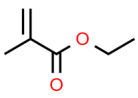
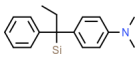
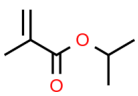
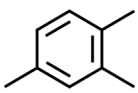
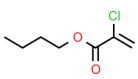
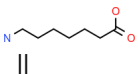
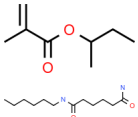
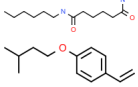
MONOMER	T_g^{exp}	$\widehat{T_g^{PLSR}}$	$\widehat{T_g^{RF}}$	Ref
	42	35± 13	43±41	[4]
	43	-14± 12	33±40	[4]
	45	1± 9	34±51	[4]
	46	20± 16	34±44	[4]
	46	-2± 8	47±42	[4]
	46	45± 14	54±56	[4]
	47	68± 8	54±33	[4]
	48	2± 8	33±41	[4]
	50	6± 13	23±63	[4]
	51	-18± 11	33±39	[4]
	51	-16± 11	34±41	[4]
	51	-37± 16	29±76	[4]
	51	96± 9	74±77	[4]
	51	5± 7	27±54	[4]
	52	139± 14	69±53	[4]
	54	6± 9	44±35	[4]
	55	70± 10	75±48	[4]
	57	19± 9	61±41	[4]
	57	-14± 11	39±41	[4]
	57	12± 10	53±43	[4]
	57	-10± 11	28±48	[4]
	57	70± 8	54±28	[4]
	58	40± 18	13±59	[4]

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Table S4 – *Continued from previous page*

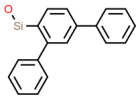
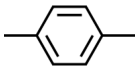
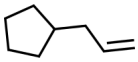
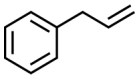
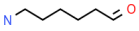
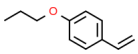
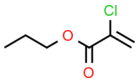
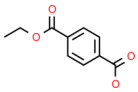
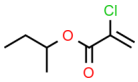
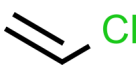
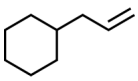
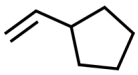
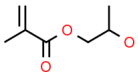
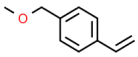
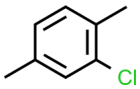
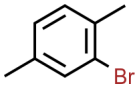
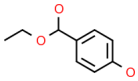
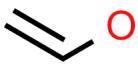
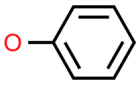
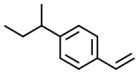
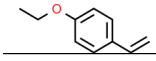
MONOMER	T_g^{exp}	$\widehat{T_g^{PLSR}}$	$\widehat{T_g^{RF}}$	Ref
	58	137± 13	89±42	[4]
	60	59± 10	64±50	[4]
	60	0± 10	31±63	[4]
	60	63± 7	64±36	[4]
	62	-13± 11	34±58	[4]
	70	73± 8	60±27	[4]
	71	21± 8	64±38	[4]
	72	90± 10	112±80	[4]
	74	33± 9	60±45	[4]
	75	-3± 22	33±63	[4]
	75	9± 11	50±75	[4]
	75	7± 12	4±67	[4]
	76	8± 7	47±58	[4]
	77	76± 7	66±48	[4]
	80	77± 9	62±62	[4]
	80	73± 10	76±60	[4]
	82	40± 7	50±57	[4]
	85	-18± 35	-30±64	[4]
	85	59± 13	53±66	[4]
	86	92± 9	61±51	[4]
	86	78± 8	70±36	[4]

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Table S4 – *Continued from previous page*

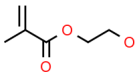
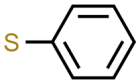
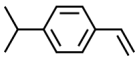
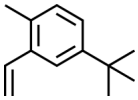
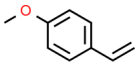
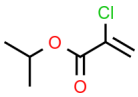
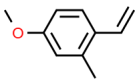
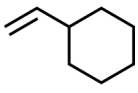
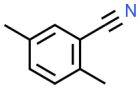
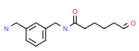
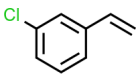
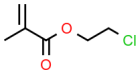
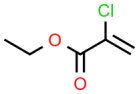
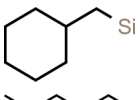
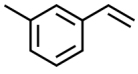
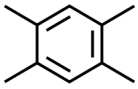
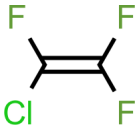
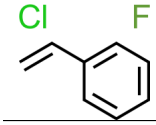
MONOMER	T_g^{exp}	$\widehat{T_g^{PLSR}}$	$\widehat{T_g^{RF}}$	Ref
	86	21± 8	47±59	[4]
	87	69± 9	74±69	[4]
	87	95± 8	80±44	[4]
	87	114± 13	69±43	[4]
	89	94± 8	90±28	[4]
	90	27± 9	54±48	[4]
	90	93± 7	85±43	[4]
	137	11± 14	80±71	[4]
	90	101± 19	102±46	[4]
	90	73± 11	82±46	[4]
	90	118± 10	114±32	[4]
	92	-1± 10	65±55	[4]
	93	26± 9	54±53	[4]
	93	-21± 13	52±73	[4]
	97	100± 11	107±36	[4]
	100	78± 11	90±43	[4]
	100	77± 12	76±54	[4]
	100	106± 11	104±40	[4]

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Table S4 – *Continued from previous page*

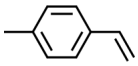
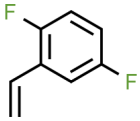
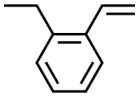
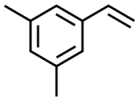
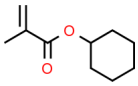
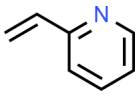
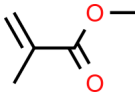
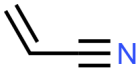
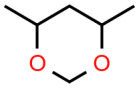
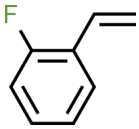
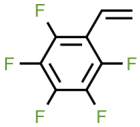
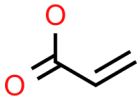
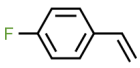
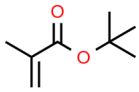
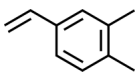
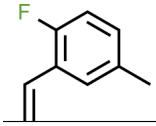
MONOMER	T_g^{exp}	$\widehat{T_g^{PLSR}}$	$\widehat{T_g^{RF}}$	Ref
	101	99± 9	100±33	[4]
	101	131± 10	126±41	[4]
	103	106± 12	107±38	[4]
	104	106± 11	105±41	[4]
	104	12± 10	89±48	[4]
	104	113± 11	104±26	[4]
	105	20± 8	70±64	[4]
	105	44± 24	14±62	[4]
	105	-43± 16	48±77	[4]
	105	123± 11	124±41	[4]
	105	168± 14	192±77	[4]
	106	34± 14	56±69	[4]
	106	109± 9	112±32	[4]
	107	24± 11	86±44	[4]
	111	101± 9	101±34	[4]
	111	118± 10	113±38	[4]

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Table S4 – *Continued from previous page*

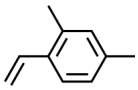
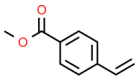
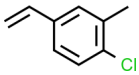
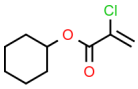
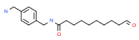
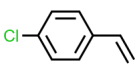
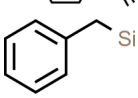
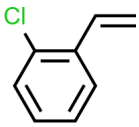
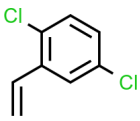
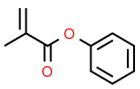
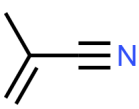
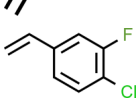
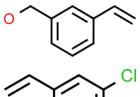
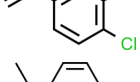
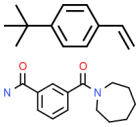
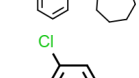
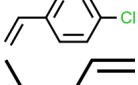
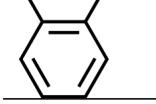
MONOMER	T_g^{exp}	$\widehat{T_g^{PLSR}}$	$\widehat{T_g^{RF}}$	Ref
	112	97± 10	105±41	[4]
	113	97± 8	90±40	[4]
	114	106± 8	120±51	[4]
	114	43± 11	61±46	[4]
	115	67± 12	95±38	[4]
	116	111± 11	123±32	[4]
	117	52± 10	25±67	[4]
	119	124± 11	122±31	[4]
	120	121± 10	124±30	[4]
	120	56± 8	104±36	[4]
	120	44± 20	25±66	[4]
	122	116± 9	124±31	[4]
	125	99± 11	109±41	[4]
	128	115± 10	120±31	[4]
	129	98± 9	76±47	[4]
	130	106± 12	113±41	[4]
	133	124± 11	128±33	[4]
	136	101± 11	126±34	[4]

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Table S4 – *Continued from previous page*

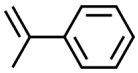
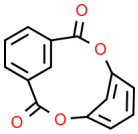
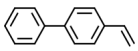
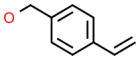
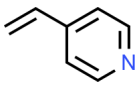
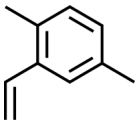
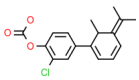
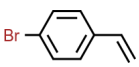
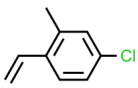
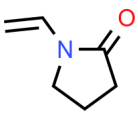
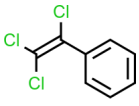
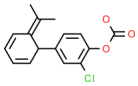
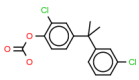
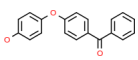
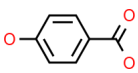
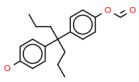
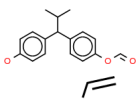
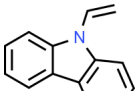
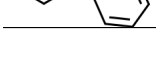
MONOMER	T_g^{exp}	$\widehat{T_g^{PLSR}}$	$\widehat{T_g^{RF}}$	Ref
	136	93± 9	112±38	[4]
	138	181± 18	139±66	[4]
	138	150± 11	135±42	[4]
	140	90± 8	100±45	[4]
	142	106± 11	126±37	[4]
	143	103± 11	118±40	[4]
	138	151± 12	115±54	[4]
	144	112± 10	125±33	[4]
	145	101± 9	123±48	[4]
	145	51± 13	33±62	[4]
	145	124± 12	141±35	[4]
	146	126± 13	111±58	[4]
	146	107± 9	116±39	[4]
	146	132± 8	157±61	[4]
	147	95± 11	124±53	[4]
	148	143± 15	134±51	[4]
	149	109± 10	117±63	[4]
	150	180± 14	141±45	[4]
				

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Table S4 – *Continued from previous page*

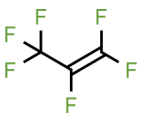
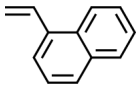
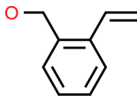
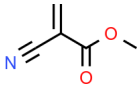
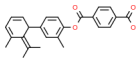
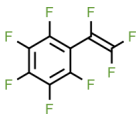
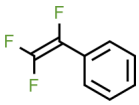
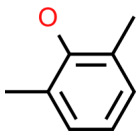
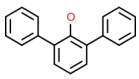
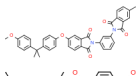
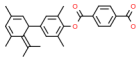
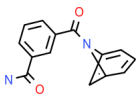
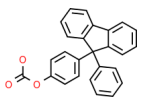
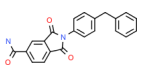
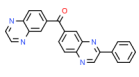
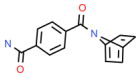
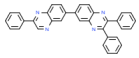
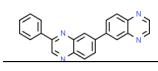
MONOMER	T_g^{exp}	$\widehat{T_g^{PLSR}}$	$\widehat{T_g^{RF}}$	Ref
	152	70± 18	126±62	[4]
	159	182± 13	144±30	[4]
	160	105± 12	116±35	[4]
	160	71± 21	104±69	[4]
	171	191± 14	257±99	[4]
	194	190± 19	214±96	[4]
	202	136± 12	169±53	[4]
	209	79± 11	89±56	[4]
	220	141± 9	178±74	[4]
	220	232± 13	248±69	[4]
	225	193± 13	257±94	[4]
	272	197± 20	197±98	[4]
	275	197± 20	190±89	[4]
	277	189± 10	296±58	[4]
	318	238± 17	299±62	[4]
	327	260± 59	192±106	[4]
	372	295± 21	332±68	[4]
	376	243± 17	306±82	[4]

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Table S4 – *Continued from previous page*

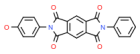
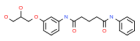
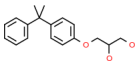
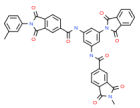
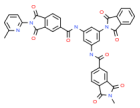
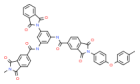
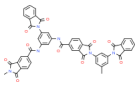
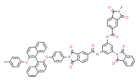
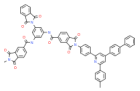
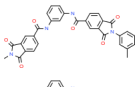
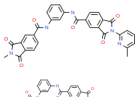
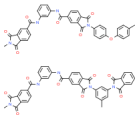
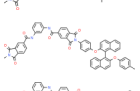
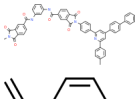
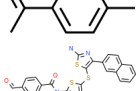
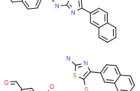
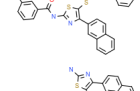
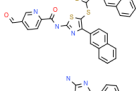
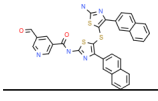
MONOMER	T_g^{exp}	$\widehat{T_g^{PLSR}}$	$\widehat{T_g^{RF}}$	Ref
	399	285± 13	360±61	[4]
	111	103± 10	147±92	[4]
	100	84± 9	89±36	[4]
	327	284± 23	333±25	[3]
	332	282± 22	332±23	[3]
	356	264± 37	332±35	[3]
	371	299± 32	334±29	[3]
	333	290± 37	331±19	[3]
	362	304± 42	336±32	[3]
	301	226± 25	317±40	[3]
	303	216± 25	315±44	[3]
	319	241± 30	318±34	[3]
	349	261± 28	339±34	[3]
	304	281± 33	323±33	[3]
	336	295± 41	328±35	[3]
	121	88± 8	97±44	[4]
	229	230± 17	226±22	[16]
	212	220± 18	225±26	[16]
	228	235± 20	230±28	[16]
	203	226± 20	213±27	[16]

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Table S4 – *Continued from previous page*

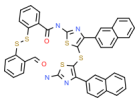
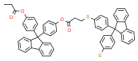
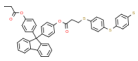
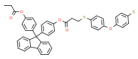
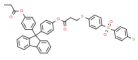
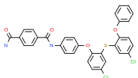
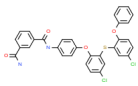
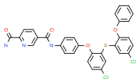
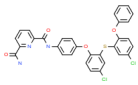
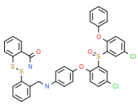
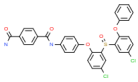
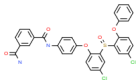
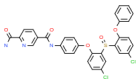
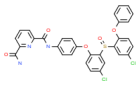
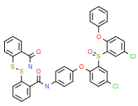
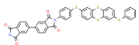
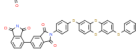
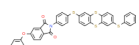
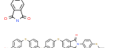
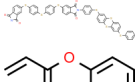
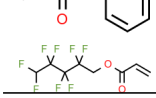
MONOMER	T_g^{exp}	$\widehat{T_g^{PLSR}}$	$\widehat{T_g^{RF}}$	Ref
	194	254± 46	238±38	[16]
	194	205± 33	193±34	[38]
	125	141± 19	165±48	[38]
	120	148± 17	181±53	[38]
	174	176± 19	214±33	[38]
	220	198± 11	216±30	[15]
	208	182± 12	211±40	[15]
	217	207± 11	216±38	[15]
	205	190± 12	217±34	[15]
	181	268± 28	196±25	[15]
	239	208± 18	206±26	[15]
	228	217± 14	205±29	[15]
	235	218± 12	216±29	[15]
	226	192± 16	218±24	[15]
	197	273± 29	200±28	[15]
	252	261± 11	243±21	[25]
	229	250± 10	233±22	[25]
	240	245± 11	232±23	[25]
	201	168± 17	211±31	[25]
	57	58± 9	75±63	[62]
	-35	45± 27	16±69	[62]

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Table S4 – *Continued from previous page*

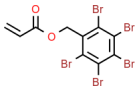
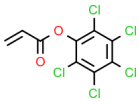
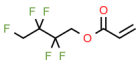
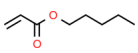
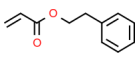
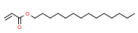
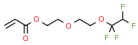
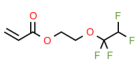
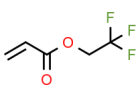
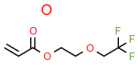
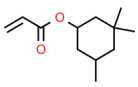
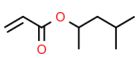
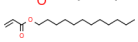
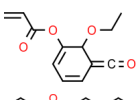
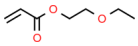
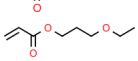
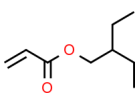
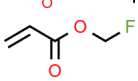
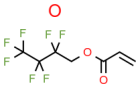
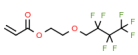
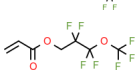
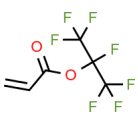
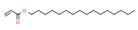
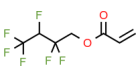
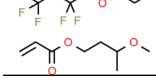
MONOMER	T_g^{exp}	$\widehat{T_g^{PLSR}}$	$\widehat{T_g^{RF}}$	Ref
	180	87± 25	138±93	[62]
	147	75± 15	129±55	[62]
	-26	48± 15	-9±47	[62]
	-57	-15± 8	-48±37	[62]
	-3	32± 9	24±38	[62]
	24	-37± 17	5±43	[62]
	-40	-24± 24	-15±58	[62]
	-22	-4± 23	5±55	[62]
	-10	23± 17	6±48	[62]
	-38	-11± 21	8±53	[62]
	15	42± 13	24±44	[62]
	-15	19± 12	-25±39	[62]
	-3	-31± 14	-16±39	[62]
	30	109± 18	86±64	[62]
	-50	-9± 8	-18±51	[62]
	-55	-12± 9	-22±50	[62]
	-50	10± 10	-36±46	[62]
	15	26± 11	18±55	[62]
	-30	43± 24	-8±52	[62]
	-45	6± 30	13±57	[62]
	-55	33± 39	21±58	[62]
	10	63± 33	11±53	[62]
	35	-42± 19	-18±47	[62]
	-22	24± 22	-19±50	[62]
	-56	1± 7	-38±43	[62]

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Table S4 – *Continued from previous page*

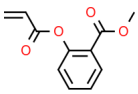
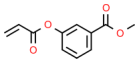
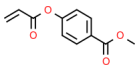
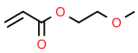
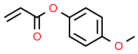
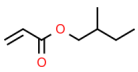
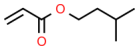
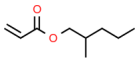
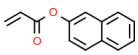
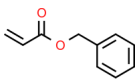
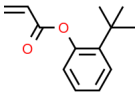
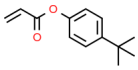
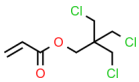
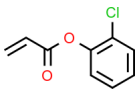
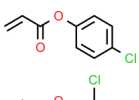
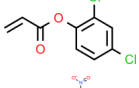
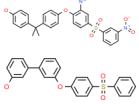
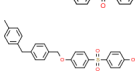
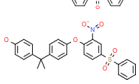
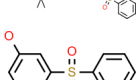
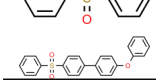
MONOMER	T_g^{exp}	$\widehat{T_g^{PLSR}}$	$\widehat{T_g^{RF}}$	Ref
	46	107± 12	86±52	[62]
	38	67± 10	68±51	[62]
	67	69± 10	73±50	[62]
	-50	-1± 8	-33±45	[62]
	51	64± 9	86±54	[62]
	-32	7± 9	-28±27	[62]
	-45	-6± 8	-43±34	[62]
	-38	6± 9	-34±40	[62]
	85	116± 9	96±48	[62]
	6	38± 7	28±44	[62]
	72	98± 14	89±36	[62]
	71	61± 7	75±29	[62]
	46	31± 16	23±60	[62]
	53	77± 9	66±34	[62]
	58	56± 12	78±48	[62]
	60	74± 8	72±43	[62]
	138	186± 26	234±26	[11]
	142	165± 13	201±43	[11]
	146	143± 12	189±47	[11]
	150	228± 17	208±28	[11]
	165	191± 21	100±64	[11]
	168	128± 25	194±43	[11]

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Table S4 – *Continued from previous page*

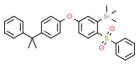
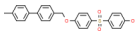
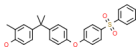
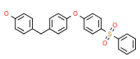
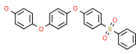
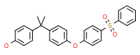
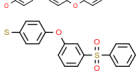
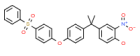
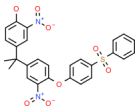
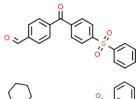
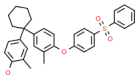
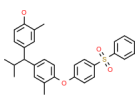
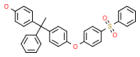
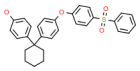
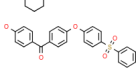
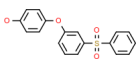
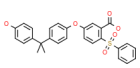
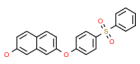
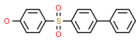
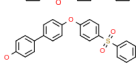
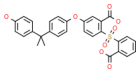
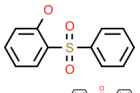
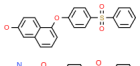
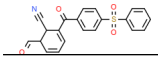
MONOMER	T_g^{exp}	$\widehat{T_g^{PLSR}}$	$\widehat{T_g^{RF}}$	Ref
	171	198± 31	178±34	[11]
	176	179± 12	184±56	[11]
	178	211± 13	186±50	[11]
	180	153± 15	196±45	[11]
	180	170± 11	202±46	[11]
	186	179± 15	195±42	[11]
	188	218± 28	186±51	[11]
	190	242± 15	210±33	[11]
	195	230± 24	226±25	[11]
	195	232± 18	207±37	[11]
	197	220± 16	185±36	[11]
	200	194± 13	194±28	[11]
	200	225± 14	200±30	[11]
	205	242± 14	201±34	[11]
	205	235± 18	204±29	[11]
	210	150± 18	181±56	[11]
	210	180± 12	200±40	[11]
	215	185± 10	200±51	[11]
	216	159± 15	180±65	[11]
	220	188± 11	194±44	[11]
	220	205± 16	213±21	[11]
	221	250± 41	112±65	[11]
	221	182± 10	200±47	[11]
	222	282± 39	223±29	[11]

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Table S4 – *Continued from previous page*

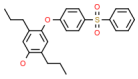
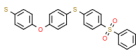
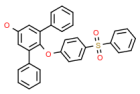
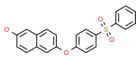
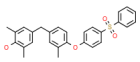
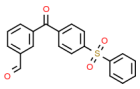
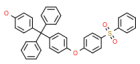
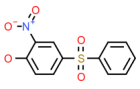
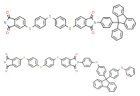
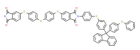
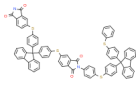
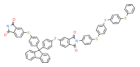
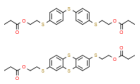
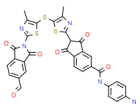
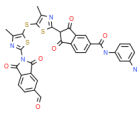
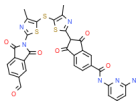
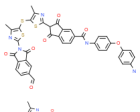
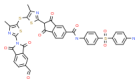
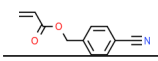
MONOMER	T_g^{exp}	$\widehat{T_g^{PLSR}}$	$\widehat{T_g^{RF}}$	Ref
	225	134± 15	194±45	[11]
	225	142± 21	205±38	[11]
	227	191± 19	210±36	[11]
	227	168± 12	200±50	[11]
	228	180± 12	187±48	[11]
	228	226± 15	207±41	[11]
	230	266± 21	208±33	[11]
	234	117± 26	206±64	[11]
	263	242± 19	244±27	[53]
	223	238± 25	234±27	[53]
	223	207± 21	230±37	[53]
	272	277± 31	251±31	[53]
	229	214± 21	234±34	[53]
	94	61± 21	117±40	[59]
	143	91± 27	134±30	[59]
	269	230± 16	250±22	[48]
	250	233± 14	252±13	[48]
	255	232± 15	251±18	[48]
	233	220± 17	241±17	[48]
	261	261± 17	253±19	[48]
	44	58± 16	81±52	[28]

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Table S4 – *Continued from previous page*

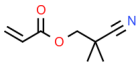
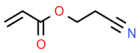
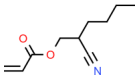
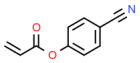
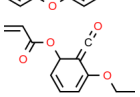
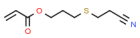
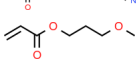
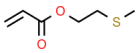
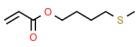
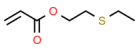
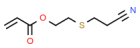
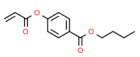
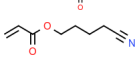
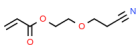
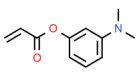
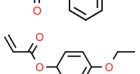
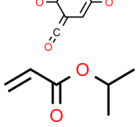
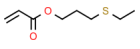
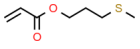
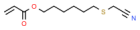
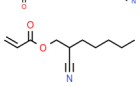
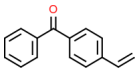
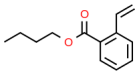
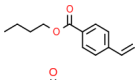
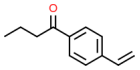
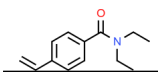
MONOMER	T_g^{exp}	$\widehat{T_g^{PLSR}}$	$\widehat{T_g^{RF}}$	Ref
	51	29± 17	42±53	[28]
	4	10± 16	15±62	[28]
	85	9± 17	79±57	[28]
	90	74± 19	78±52	[28]
	24	73± 18	51±66	[28]
	-58	-4± 20	15±73	[28]
	-75	-8± 8	-36±41	[28]
	-60	12± 12	-30±58	[28]
	-70	-1± 12	-16±58	[28]
	-71	-2± 12	-14±67	[28]
	-50	4± 20	29±74	[28]
	13	46± 11	80±55	[28]
	-40	-3± 16	-22±59	[28]
	-23	-6± 17	-11±55	[28]
	47	83± 10	90±55	[28]
	37	74± 16	52±49	[28]
	-3	11± 9	-24±47	[28]
	-76	-4± 13	-13±68	[28]
	-65	4± 12	-25±52	[28]
	-59	-17± 20	14±72	[28]
	116	-1± 17	82±56	[28]
	98	135± 8	100±36	[28]
	66	85± 6	86±29	[28]
	76	84± 7	81±36	[28]
	74	96± 7	73±35	[28]
	102	103± 9	96±28	[28]

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Table S4 – *Continued from previous page*

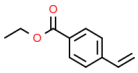
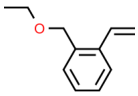
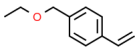
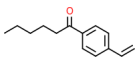
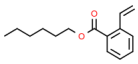
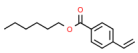
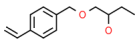
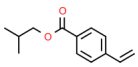
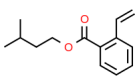
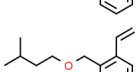
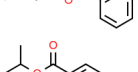
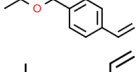
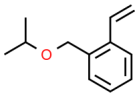
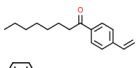
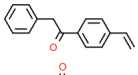
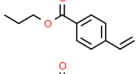
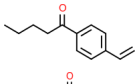
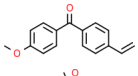
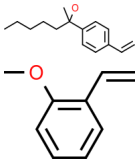
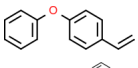
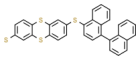
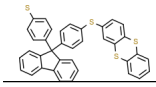
MONOMER	T_g^{exp}	$\widehat{T_g^{PLSR}}$	$\widehat{T_g^{RF}}$	Ref
	94	90± 8	84±38	[28]
	74	87± 9	74±29	[28]
	86	72± 7	49±43	[28]
	66	80± 8	69±28	[28]
	45	69± 7	79±28	[28]
	66	74± 8	77±33	[28]
	46	75± 8	54±39	[28]
	90	93± 6	91±43	[28]
	68	81± 6	81±28	[28]
	78	72± 7	70±32	[28]
	95	94± 7	78±35	[28]
	88	89± 9	80±25	[28]
	50	68± 10	72±22	[28]
	78	117± 8	108±54	[28]
	92	92± 7	85±20	[28]
	70	84± 7	72±36	[28]
	103	131± 8	109±41	[28]
	91	94± 13	91±34	[28]
	75	107± 10	94±42	[28]
	100	124± 9	115±52	[28]
	235	202± 17	208±51	[41]
	237	217± 23	185±56	[41]

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Table S4 – *Continued from previous page*

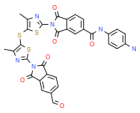
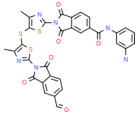
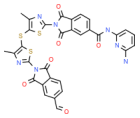
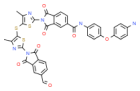
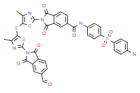
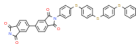
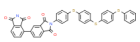
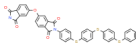
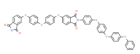
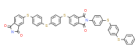
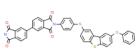
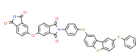
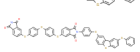
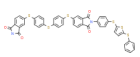
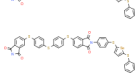
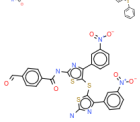
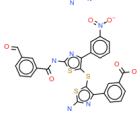
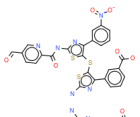
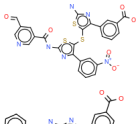
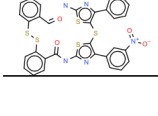
MONOMER	T_g^{exp}	$\widehat{T_g^{PLSR}}$	$\widehat{T_g^{RF}}$	Ref
	269	267± 15	261±17	[48]
	250	262± 14	254±15	[48]
	255	255± 16	252±14	[48]
	233	251± 15	244±25	[48]
	261	273± 17	260±21	[48]
	227	225± 13	234±17	[26]
	227	221± 11	233±24	[26]
	196	230± 16	234±23	[26]
	179	168± 18	211±31	[26]
	192	167± 15	210±35	[26]
	252	211± 13	249±16	[27]
	251	235± 10	246±16	[27]
	201	147± 21	204±27	[27]
	189	217± 20	189±23	[58]
	181	203± 18	190±27	[58]
	244	233± 25	245±23	[18]
	229	222± 22	231±23	[18]
	242	217± 24	243±20	[18]
	219	198± 24	227±20	[18]
	210	233± 31	229±28	[18]

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Table S4 – *Continued from previous page*

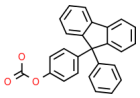
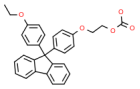
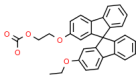
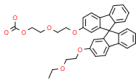
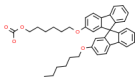
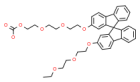
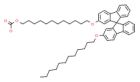
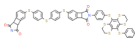
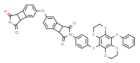
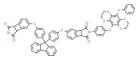
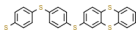
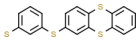
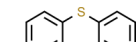
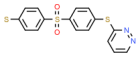
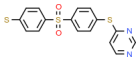
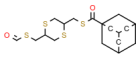
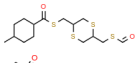
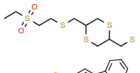
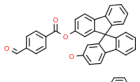
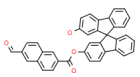
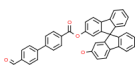
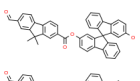
MONOMER	T_g^{exp}	$\widehat{T_g^{PLSR}}$	$\widehat{T_g^{RF}}$	Ref
	253	196± 20	188±91	[46]
	150	160± 17	169±92	[46]
	148	148± 26	120±81	[46]
	89	126± 26	124±73	[46]
	60	116± 26	91±52	[46]
	48	89± 29	125±60	[46]
	16	81± 39	106±56	[46]
	212	237± 78	200±40	[61]
	247	268± 79	215±41	[61]
	266	292± 82	224±41	[61]
	143	148± 20	144±46	[51]
	142	151± 17	127±44	[51]
	145	178± 18	133±30	[51]
	193	148± 18	187±29	[63]
	202	144± 20	197±32	[63]
	110	98± 31	107±53	[60]
	65	5± 35	60±47	[60]
	47	10± 56	58±48	[60]
	331	218± 23	300±74	[45]
	346	232± 23	325±52	[45]
	352	234± 25	288±72	[45]
	349	227± 23	322±64	[45]
	177	192± 36	203±46	[45]

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Table S4 – *Continued from previous page*

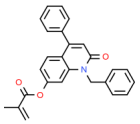
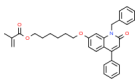
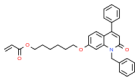
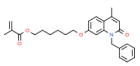
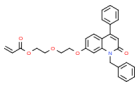
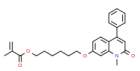
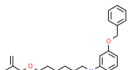
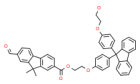
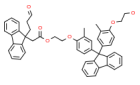
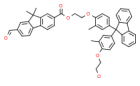
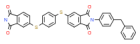
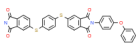
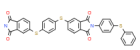
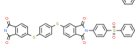
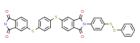
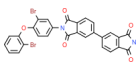
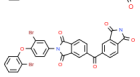
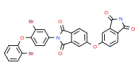
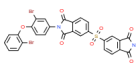
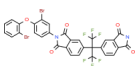
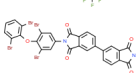
MONOMER	T_g^{exp}	$\widehat{T_g^{PLSR}}$	$\widehat{T_g^{RF}}$	Ref
	90	158± 16	125±84	[12]
	52	139± 15	171±93	[12]
	58	126± 16	151±88	[12]
	64	96± 17	89±52	[12]
	73	132± 14	180±107	[12]
	58	93± 15	124±91	[12]
	59	104± 16	168±92	[12]
	193	226± 21	200±51	[44]
	109	217± 30	187±47	[44]
	161	243± 23	184±43	[44]
	217	238± 19	215±69	[44]
	227	206± 10	234±19	[13]
	230	211± 11	232±20	[13]
	231	226± 11	230±27	[13]
	266	228± 21	235±22	[13]
	205	209± 16	236±26	[13]
	275	295± 11	287±31	[5]
	296	305± 13	283±30	[5]
	251	273± 12	282±40	[5]
	281	322± 16	271±41	[5]
	299	283± 24	283±43	[5]
	287	315± 15	286±30	[5]

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Table S4 – *Continued from previous page*

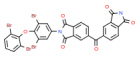
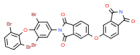
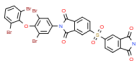
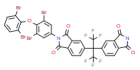
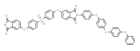
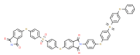
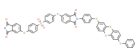
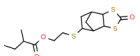
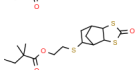
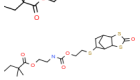
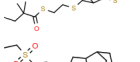
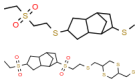
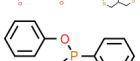
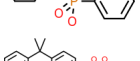
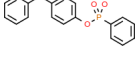
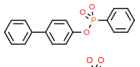
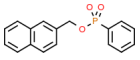
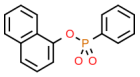
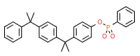
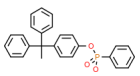
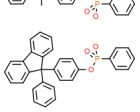
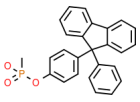
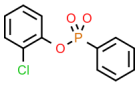
MONOMER	T_g^{exp}	$\widehat{T_g^{PLSR}}$	$\widehat{T_g^{RF}}$	Ref
	323	324± 17	287±38	[5]
	283	294± 14	278±37	[5]
	328	320± 21	289±47	[5]
	303	289± 23	285±40	[5]
	208	189± 20	214±20	[49]
	238	259± 86	249±38	[49]
	235	228± 19	224±24	[49]
	85	32± 28	89±37	[42]
	105	42± 28	100±48	[42]
	44	41± 28	99±70	[42]
	109	28± 35	93±28	[42]
	74	50± 46	82±55	[50]
	113	20± 85	109±69	[50]
	105	58± 23	95±29	[30]
	98	140± 14	109±30	[30]
	140	87± 27	126±37	[30]
	99	118± 22	110±30	[30]
	124	106± 24	121±38	[30]
	112	152± 22	139±59	[30]
	123	187± 12	166±48	[30]
	214	166± 34	199±42	[30]
	208	158± 39	164±55	[30]
	59	75± 20	75±42	[30]
	85	64± 21	88±48	[30]

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Table S4 – *Continued from previous page*

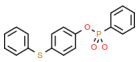
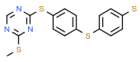
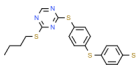
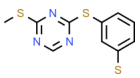
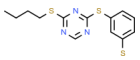
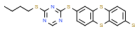
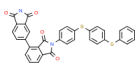
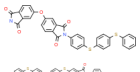
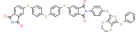
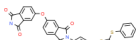
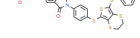
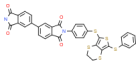
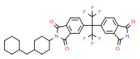
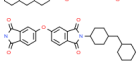
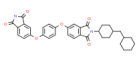
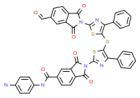
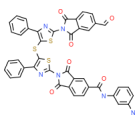
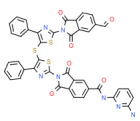
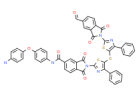
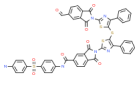
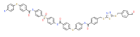
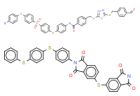
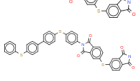
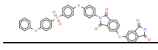
MONOMER	T_g^{exp}	$\widehat{T_g^{PLSR}}$	$\widehat{T_g^{RF}}$	Ref
	81	79± 24	130±50	[30]
	127	94± 17	121±61	[40]
	77	96± 17	98±52	[40]
	129	121± 13	123±36	[40]
	75	122± 16	98±42	[40]
	93	147± 19	105±56	[40]
	247	228± 11	238±20	[8]
	215	214± 10	224±19	[8]
	153	162± 18	176±32	[57]
	188	223± 15	230±33	[57]
	230	246± 15	242±29	[57]
	259	230± 24	247±35	[55]
	292	200± 18	272±53	[55]
	238	211± 19	246±28	[55]
	273	280± 20	256±19	[19]
	255	288± 17	256±18	[19]
	261	281± 18	258±14	[19]
	237	232± 34	263±32	[19]
	264	295± 25	263±22	[19]
	206	202± 24	245±36	[35]
	233	203± 21	233±26	[35]
	221	239± 12	233±37	[24]
	248	253± 12	248±30	[24]
	250	219± 14	243±20	[24]

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Table S4 – *Continued from previous page*

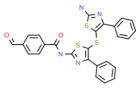
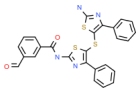
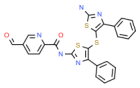
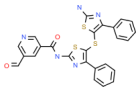
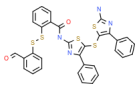
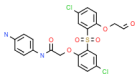
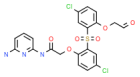
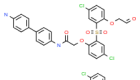
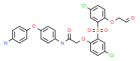
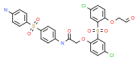
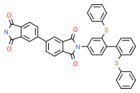
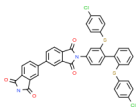
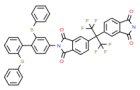
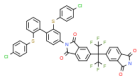
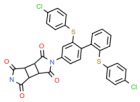
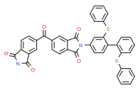
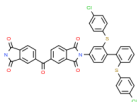
MONOMER	T_g^{exp}	$\widehat{T_g^{PLSR}}$	$\widehat{T_g^{RF}}$	Ref
	221	218± 17	228±46	[17]
	248	215± 18	215±45	[17]
	250	225± 18	245±36	[17]
	265	219± 19	245±39	[17]
	243	276± 29	228±45	[17]
	235	253± 25	207±33	[20]
	199	229± 17	203±33	[20]
	231	241± 15	210±28	[20]
	172	242± 19	194±28	[20]
	211	279± 23	213±23	[20]
	245	262± 12	247±14	[52]
	244	291± 19	245±25	[52]
	220	279± 20	240±25	[52]
	239	270± 28	248±34	[52]
	257	248± 28	230±38	[52]
	278	272± 14	269±27	[52]
	306	295± 19	259±32	[52]

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Table S4 – *Continued from previous page*

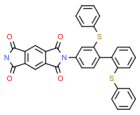
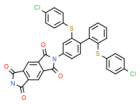
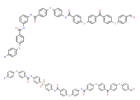
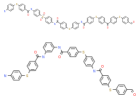
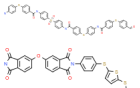
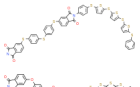
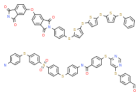
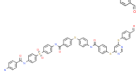
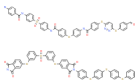
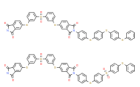
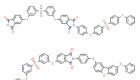
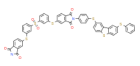
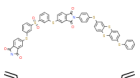
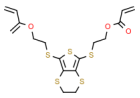
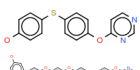
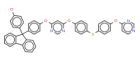
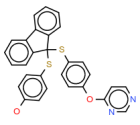
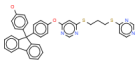
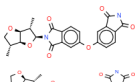
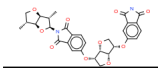
MONOMER	T_g^{exp}	$\widehat{T_g^{PLSR}}$	$\widehat{T_g^{RF}}$	Ref
	227	265± 15	235±17	[52]
	243	290± 21	245±39	[52]
	226	197± 26	237±21	[64]
	248	217± 34	253±19	[64]
	245	178± 26	241±22	[64]
	278	211± 21	261±28	[64]
	220	256± 13	224±19	[7]
	177	176± 29	189±25	[7]
	157	205± 25	223±35	[7]
	229	190± 14	223±16	[65]
	261	226± 19	254±28	[65]
	227	193± 15	228±16	[65]
	262	214± 20	259±30	[65]
	178	192± 15	192±32	[9]
	207	203± 30	242±33	[9]
	203	210± 19	218±35	[9]
	205	202± 20	207±20	[9]
	134	87± 28	119±58	[21]
	132	102± 12	122±39	[37]
	201	241± 24	193±46	[37]
	143	180± 24	192±63	[37]
	165	204± 22	177±43	[37]
	264	173± 14	244±56	[56]
	228	175± 24	221±29	[56]

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Table S4 – *Continued from previous page*

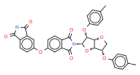
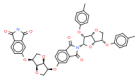
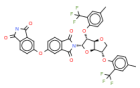
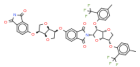
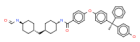
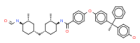
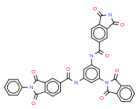
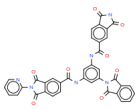
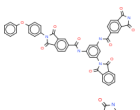
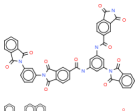
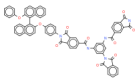
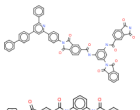
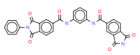
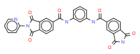
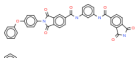
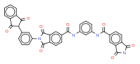
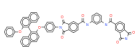
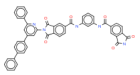
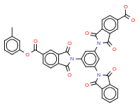
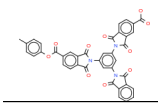
MONOMER	T_g^{exp}	$\widehat{T_g^{PLSR}}$	$\widehat{T_g^{RF}}$	Ref
	255	225± 17	250±34	[56]
	227	223± 27	228±22	[56]
	246	204± 27	245±35	[56]
	229	208± 26	234±32	[56]
	217	197± 20	204±38	[36]
	237	229± 23	199±45	[36]
	327	342± 21	327±23	[3]
	332	338± 22	334±28	[3]
	356	352± 21	343±27	[3]
	371	374± 25	351±25	[3]
	333	354± 52	337±28	[3]
	362	350± 48	350±26	[3]
	301	284± 14	314±35	[3]
	303	283± 14	311±39	[3]
	319	289± 17	310±32	[3]
	349	306± 29	313±39	[3]
	304	318± 32	313±32	[3]
	336	307± 33	316±32	[3]
	264	296± 17	314±27	[2]
	259	281± 17	318±28	[2]

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Table S4 – *Continued from previous page*

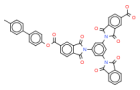
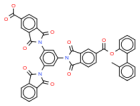
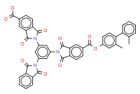
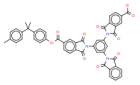
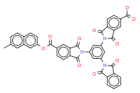
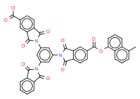
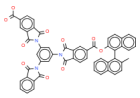
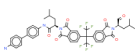
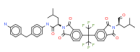
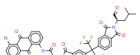
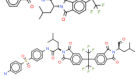
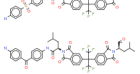
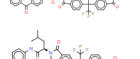
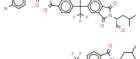
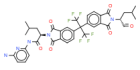
MONOMER	T_g^{exp}	$\widehat{T_g^{PLSR}}$	$\widehat{T_g^{RF}}$	Ref
	301	322± 19	310±24	[2]
	305	348± 17	324±31	[2]
	317	350± 16	319±32	[2]
	306	306± 20	307±28	[2]
	328	311± 18	320±26	[2]
	331	335± 18	325±27	[2]
	353	383± 21	344±22	[2]
	291	296± 15	255±30	[47]
	284	287± 17	256±29	[47]
	245	333± 23	261±34	[47]
	255	293± 23	258±38	[47]
	263	286± 19	268±34	[47]
	268	290± 21	256±32	[47]
	251	296± 21	256±36	[47]
	334	276± 45	263±88	[45]

Table S5: The table lists the experimental and predicted (± uncertainty) 10% thermal decomposition temperatures for different polymers. Predictions for only the RF model are reported.

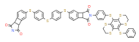
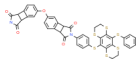
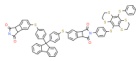
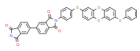
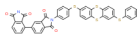
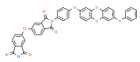
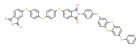
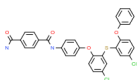
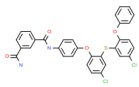
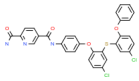
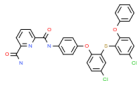
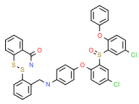
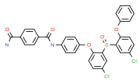
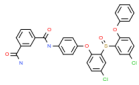
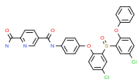
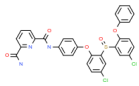
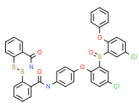
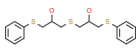
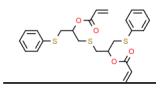
MONOMER	T_D^{exp}	T_D^{pred}	Ref
	443	415 ± 68	[61]
	391	401 ± 60	[61]
	424	410 ± 69	[61]
	563	546 ± 32	[25]
	546	536 ± 30	[25]
	527	531 ± 21	[25]
	508	489 ± 36	[25]
	442	453 ± 25	[15]
	435	451 ± 26	[15]
	436	468 ± 47	[15]
	430	460 ± 34	[15]
	415	477 ± 45	[15]
	450	453 ± 15	[15]
	447	448 ± 17	[15]
	448	457 ± 29	[15]
	445	448 ± 34	[15]
	426	458 ± 44	[15]
	125	300 ± 75	[22]
	235	273 ± 66	[22]

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Table S5 – *Continued from previous page*

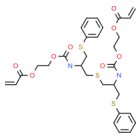
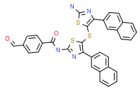
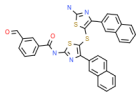
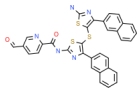
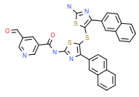
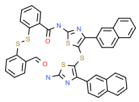
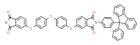
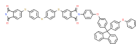
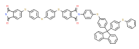
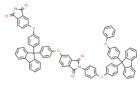
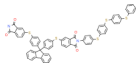
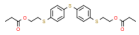
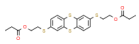
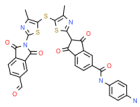
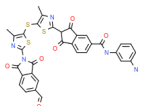
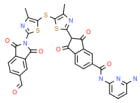
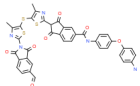
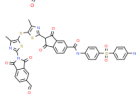
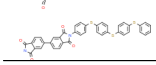
MONOMER	T_D^{exp}	T_D^{pred}	Ref
	237	284 ± 68	[22]
	513	499 ± 36	[16]
	501	489 ± 40	[16]
	507	495 ± 36	[16]
	496	493 ± 40	[16]
	478	475 ± 47	[16]
	497	499 ± 19	[53]
	494	487 ± 49	[53]
	496	501 ± 39	[53]
	532	516 ± 34	[53]
	513	491 ± 58	[53]
	365	380 ± 58	[59]
	365	355 ± 65	[59]
	510	506 ± 20	[48]
	496	499 ± 25	[48]
	503	502 ± 30	[48]
	482	491 ± 36	[48]
	507	441 ± 65	[48]
	529	528 ± 19	[26]

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Table S5 – *Continued from previous page*

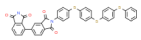
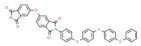
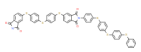
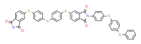
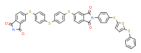
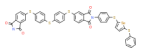
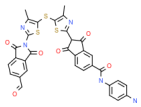
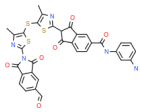
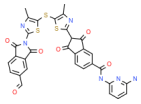
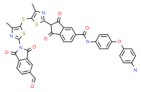
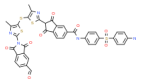
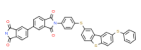
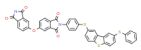
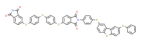
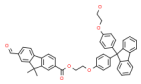
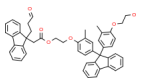
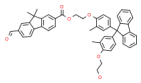
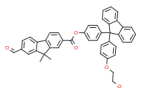
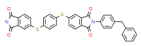
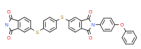
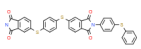
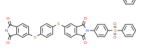
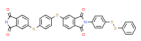
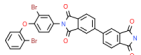
MONOMER	T_D^{exp}	T_D^{pred}	Ref
	536	521 ± 27	[26]
	532	534 ± 23	[26]
	500	497 ± 35	[26]
	504	510 ± 32	[26]
	456.2	504 ± 31	10.1002/pola.23497
	453.3	474 ± 61	10.1002/pola.23497
	510	506 ± 20	[48]
	496	499 ± 25	[48]
	503	502 ± 30	[48]
	482	491 ± 36	[48]
	507	441 ± 65	[48]
	557.6	528 ± 34	[27]
	549.7	539 ± 35	[27]
	506.3	497 ± 30	[27]
	429	436 ± 40	[44]
	407	411 ± 30	[44]
	408	418 ± 31	[44]
	486	442 ± 41	[44]
	533	520 ± 31	[13]
	543	519 ± 35	[13]
	540	527 ± 39	[13]
	508	491 ± 63	[13]
	503	518 ± 54	[13]
	552	540 ± 29	[5]

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Table S5 – *Continued from previous page*

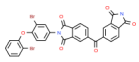
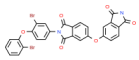
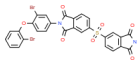
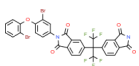
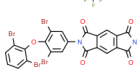
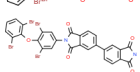
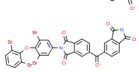
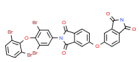
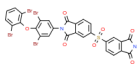
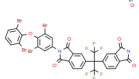
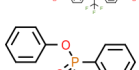
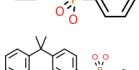
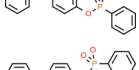
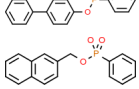
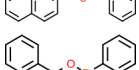
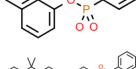
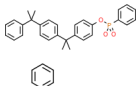
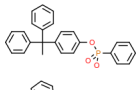
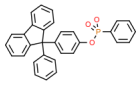
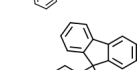
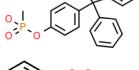
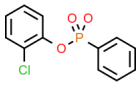
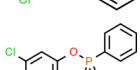
MONOMER	T_D^{exp}	T_D^{pred}	Ref
	500	507 ± 22	[5]
	554	539 ± 33	[5]
	523	513 ± 38	[5]
	517	505 ± 51	[5]
	539	512 ± 56	[5]
	563	550 ± 38	[5]
	484	500 ± 36	[5]
	537	536 ± 35	[5]
	531	510 ± 46	[5]
	549	523 ± 37	[5]
	357	421 ± 65	[30]
	433	430 ± 45	[30]
	327	423 ± 63	[30]
	242	391 ± 92	[30]
	241	422 ± 63	[30]
	430	430 ± 51	[30]
	471	405 ± 88	[30]
	484	465 ± 39	[30]
	414	428 ± 51	[30]
	405	422 ± 62	[30]
	433	425 ± 60	[30]
	443	422 ± 62	[30]
	540	527 ± 34	[8]

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Table S5 – *Continued from previous page*

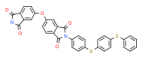
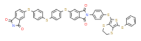
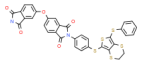
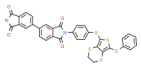
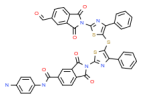
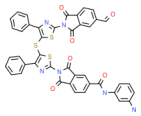
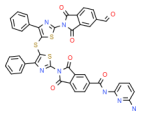
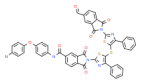
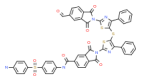
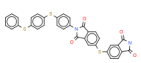
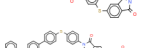
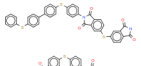
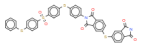
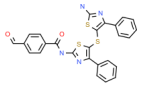
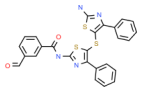
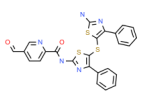
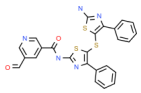
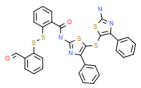
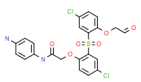
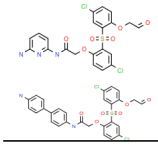
MONOMER	T_D^{exp}	T_D^{pred}	Ref
	529	524 ± 21	[8]
	478	448 ± 58	[57]
	409	477 ± 51	[57]
	521	480 ± 50	[57]
	522	502 ± 21	[19]
	507	501 ± 24	[19]
	510	503 ± 24	[19]
	490	489 ± 52	[19]
	518	495 ± 28	[19]
	542	540 ± 30	[24]
	545	516 ± 33	[24]
	521	512 ± 38	[24]
	542	479 ± 46	[17]
	545	478 ± 44	[17]
	521	488 ± 53	[17]
	556	481 ± 49	[17]
	536	507 ± 36	[17]
	423	445 ± 34	[20]
	404	417 ± 80	[20]
	421	450 ± 36	[20]

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Table S5 – *Continued from previous page*

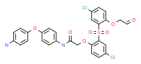
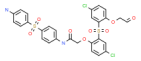
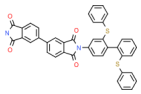
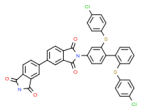
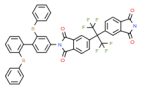
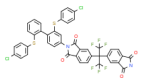
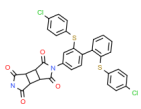
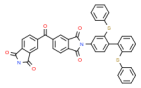
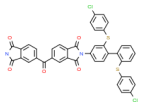
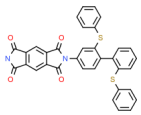
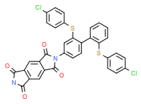
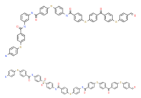
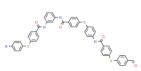
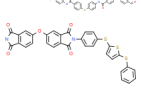
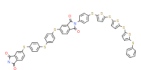
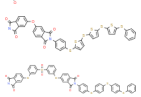
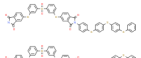
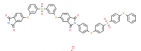
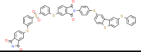
MONOMER	T_D^{exp}	T_D^{pred}	Ref
	401	428 ± 76	[20]
	410	465 ± 44	[20]
	498	506 ± 22	[52]
	507	519 ± 34	[52]
	495	497 ± 44	[52]
	506	503 ± 34	[52]
	467	459 ± 49	[52]
	509	513 ± 18	[52]
	512	513 ± 32	[52]
	501	510 ± 40	[52]
	505	516 ± 32	[52]
	427	440 ± 37	[64]
	439	477 ± 48	[64]
	431	438 ± 35	[64]
	439	473 ± 44	[64]
	443	469 ± 45	[7]
	374	432 ± 74	[7]
	354	419 ± 66	[7]
	511	473 ± 63	[9]
	494	500 ± 34	[9]
	506	494 ± 38	[9]

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Table S5 – *Continued from previous page*

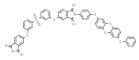
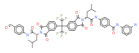
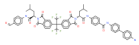
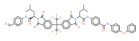
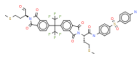
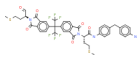
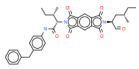
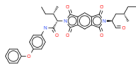
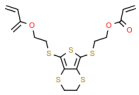
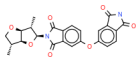
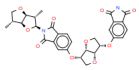
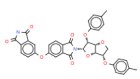
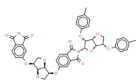
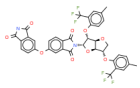
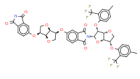
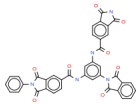
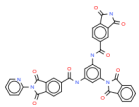
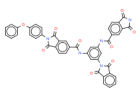
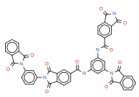
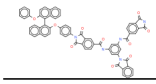
MONOMER	T_D^{exp}	T_D^{pred}	Ref
	498	459 ± 64	[9]
	363.9	372 ± 31	[33]
	369	372 ± 30	[33]
	363.2	380 ± 30	[33]
	357	406 ± 86	[31]
	350	362 ± 55	[31]
	350	376 ± 49	[32]
	340	385 ± 63	[32]
	312.5	365 ± 85	[21]
	460	442 ± 52	[56]
	445	436 ± 42	[56]
	439	466 ± 44	[56]
	433	440 ± 27	[56]
	450	461 ± 35	[56]
	440	446 ± 22	[56]
	516	512 ± 21	[3]
	520	508 ± 23	[3]
	528	510 ± 25	[3]
	529	501 ± 30	[3]
	543	524 ± 32	[3]

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Table S5 – *Continued from previous page*

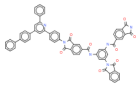
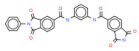
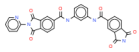
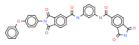
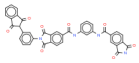
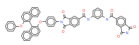
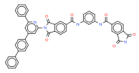
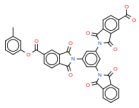
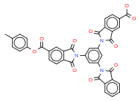
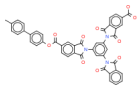
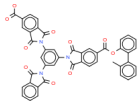
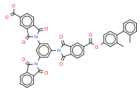
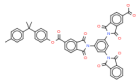
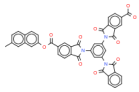
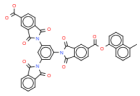
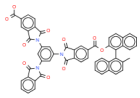
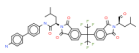
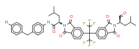
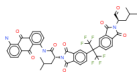
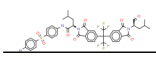
MONOMER	T_D^{exp}	T_D^{pred}	Ref
	539	514 ± 30	[3]
	506	506 ± 34	[3]
	508	509 ± 24	[3]
	513	503 ± 36	[3]
	516	502 ± 27	[3]
	522	514 ± 36	[3]
	518	515 ± 25	[3]
	455	466 ± 25	[2]
	461	465 ± 25	[2]
	473	466 ± 29	[2]
	477	464 ± 26	[2]
	458	464 ± 24	[2]
	451	454 ± 29	[2]
	460	464 ± 27	[2]
	468	465 ± 24	[2]
	482	474 ± 29	[2]
	396	415 ± 41	[47]
	440	423 ± 30	[47]
	383	406 ± 38	[47]
	412	425 ± 45	[47]

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Table S5 – *Continued from previous page*

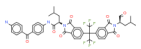
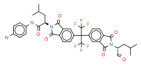
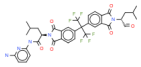
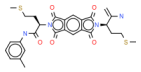
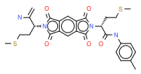
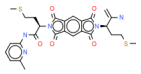
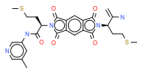
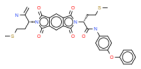
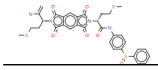
MONOMER	T_D^{exp}	T_D^{pred}	Ref
	425	408 ± 38	[47]
	389	398 ± 41	[47]
	375	390 ± 49	[47]
	250	270 ± 50	[10]
	255	268 ± 46	[10]
	300	290 ± 56	[10]
	318	298 ± 57	[10]
	300	299 ± 53	[10]
	280	311 ± 68	[10]

Table S6: The table lists the experimental and predicted (± uncertainty) densities for different polymers. Predictions for only the RF model are reported. The experimental values are taken from multiple references[23, 4, 34]

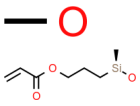
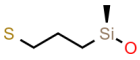
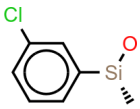
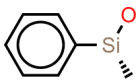
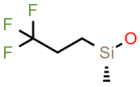
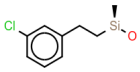
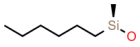
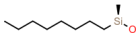
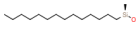
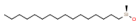
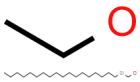
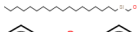
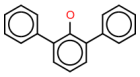
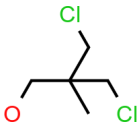
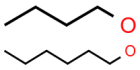
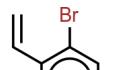
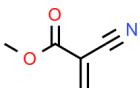
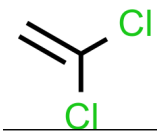
MONOMER	ρ_{exp}	ρ_{pred}
	1.42	1.22 ± 0.18
	1.11	1.09 ± 0.17
	1.06	1.14 ± 0.27
	1.10	1.17 ± 0.20
	1.11	1.09 ± 0.09
	1.30	1.30 ± 0.25
	1.09	1.15 ± 0.20
	0.91	0.93 ± 0.08
	0.91	0.98 ± 0.16
	0.89	0.92 ± 0.10
	0.88	0.93 ± 0.13
	1.12	1.14 ± 0.17
	0.89	0.98 ± 0.13
	1.14	1.18 ± 0.12
	1.39	1.38 ± 0.16
	0.98	1.03 ± 0.17
	0.93	1.01 ± 0.14
	2.10	1.93 ± 0.33
	1.20	1.18 ± 0.10
	1.30	1.25 ± 0.09
	1.66	1.48 ± 0.23

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Table S6 – *Continued from previous page*

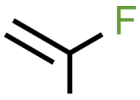
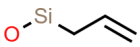
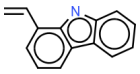
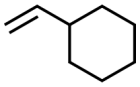
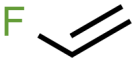
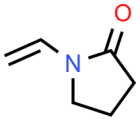
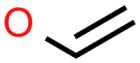
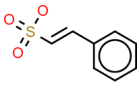
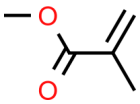
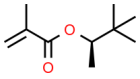
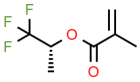
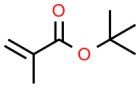
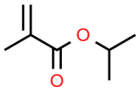
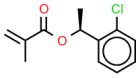
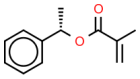
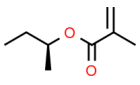
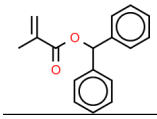
MONOMER	ρ_{exp}	ρ_{pred}
	1.60	1.46 ± 0.20
	0.98	1.01 ± 0.09
	1.20	1.17 ± 0.11
	0.95	0.95 ± 0.14
	1.38	1.40 ± 0.14
	1.38	1.39 ± 0.15
	1.25	1.18 ± 0.09
	1.26	1.02 ± 0.15
	1.10	1.17 ± 0.13
	1.17	1.13 ± 0.05
	0.99	1.01 ± 0.04
	1.34	1.37 ± 0.20
	1.02	1.03 ± 0.11
	1.03	1.05 ± 0.09
	1.27	1.33 ± 0.17
	1.13	1.12 ± 0.08
	1.05	1.05 ± 0.06
	1.17	1.19 ± 0.08

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Table S6 – *Continued from previous page*

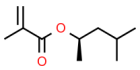
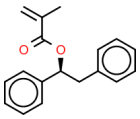
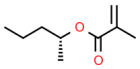
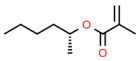
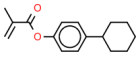
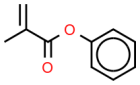
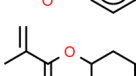
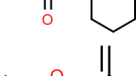
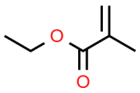
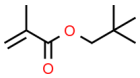
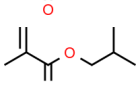
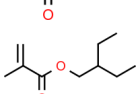
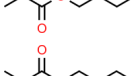
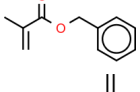
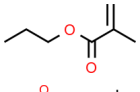
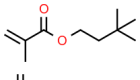
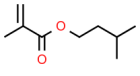
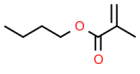
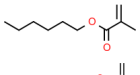
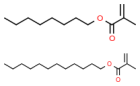
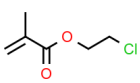
MONOMER	ρ_{exp}	ρ_{pred}
	1.00	1.02 ± 0.05
	1.15	1.16 ± 0.07
	1.03	1.04 ± 0.06
	1.01	1.02 ± 0.05
	1.12	1.14 ± 0.07
	1.21	1.17 ± 0.09
	1.10	1.03 ± 0.07
	1.11	1.10 ± 0.06
	0.99	1.04 ± 0.07
	1.04	1.05 ± 0.05
	1.04	1.03 ± 0.06
	1.18	1.10 ± 0.09
	1.08	1.06 ± 0.09
	1.00	1.02 ± 0.05
	1.03	1.04 ± 0.05
	1.05	1.03 ± 0.04
	1.01	1.03 ± 0.04
	0.97	1.01 ± 0.06
	0.93	1.02 ± 0.05
	1.32	1.30 ± 0.18
	1.15	1.11 ± 0.06

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Table S6 – *Continued from previous page*

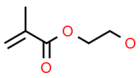
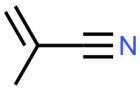
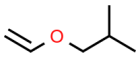
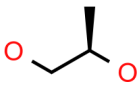
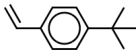
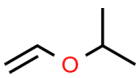
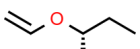
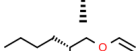
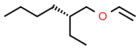
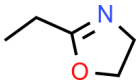
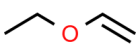
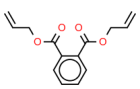
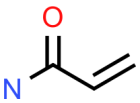
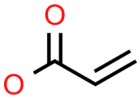
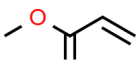
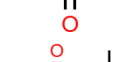
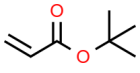
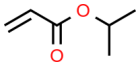
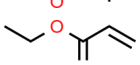
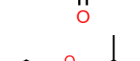
MONOMER	ρ_{exp}	ρ_{pred}
	1.15	1.15 ± 0.14
	1.10	1.06 ± 0.13
	0.93	0.99 ± 0.10
	1.00	1.10 ± 0.17
	1.19	1.12 ± 0.09
	0.95	1.05 ± 0.10
	0.92	0.98 ± 0.12
	0.92	0.96 ± 0.10
	0.90	0.96 ± 0.10
	1.14	1.11 ± 0.10
	0.95	0.99 ± 0.12
	1.27	1.26 ± 0.09
	1.30	1.25 ± 0.14
	1.41	1.20 ± 0.21
	1.22	1.18 ± 0.12
	1.00	1.07 ± 0.11
	1.08	1.09 ± 0.06
	1.12	1.10 ± 0.08
	1.06	1.09 ± 0.05
	1.11	1.04 ± 0.12
	1.09	1.09 ± 0.06

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Table S6 – *Continued from previous page*

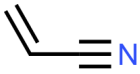
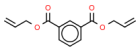
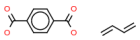
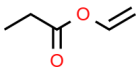
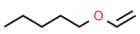
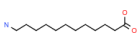
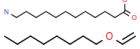
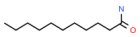
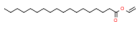
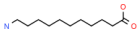
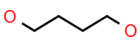
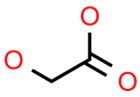
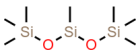
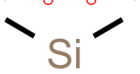
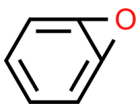
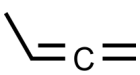
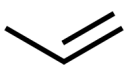
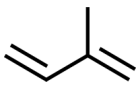
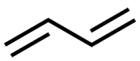
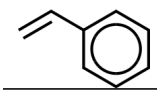
MONOMER	ρ_{exp}	ρ_{pred}
	1.18	1.17 ± 0.10
	1.26	1.25 ± 0.09
	1.31	1.26 ± 0.21
	1.02	1.06 ± 0.08
	0.93	0.96 ± 0.11
	0.98	1.09 ± 0.14
	1.04	0.98 ± 0.14
	0.92	0.94 ± 0.13
	0.99	1.05 ± 0.11
	0.91	0.95 ± 0.17
	0.88	0.98 ± 0.12
	1.04	1.08 ± 0.11
	0.89	0.95 ± 0.14
	1.00	1.12 ± 0.10
	1.01	1.04 ± 0.12
	0.97	1.03 ± 0.14
	1.36	1.33 ± 0.15
	1.60	1.22 ± 0.15
	0.99	1.12 ± 0.21
	0.91	0.92 ± 0.07
	1.06	1.16 ± 0.12
	1.36	1.22 ± 0.12
	0.85	0.91 ± 0.10
	0.91	0.94 ± 0.10
	0.85	0.88 ± 0.10
	0.91	0.95 ± 0.11
	0.89	0.98 ± 0.12
	1.05	1.02 ± 0.10

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Table S6 – *Continued from previous page*

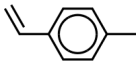
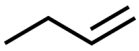
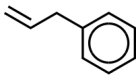
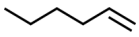
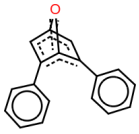
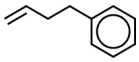
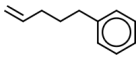
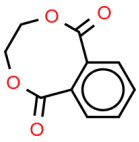
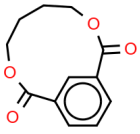
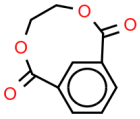
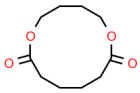
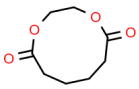
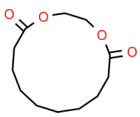
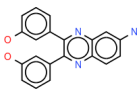
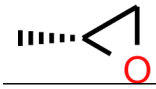
MONOMER	ρ_{exp}	ρ_{pred}
	1.04	1.03 ± 0.10
	0.86	0.90 ± 0.08
	0.89	0.92 ± 0.10
	1.05	1.04 ± 0.10
	0.85	0.90 ± 0.10
	0.86	0.90 ± 0.07
	0.86	0.93 ± 0.10
	1.14	1.25 ± 0.22
	1.04	1.06 ± 0.11
	1.05	1.05 ± 0.11
	1.34	1.26 ± 0.22
	1.27	1.23 ± 0.13
	1.34	1.25 ± 0.22
	1.02	1.03 ± 0.07
	1.18	1.13 ± 0.09
	1.18	1.07 ± 0.10
	1.08	1.07 ± 0.10
	1.07	1.21 ± 0.09
	1.00	1.23 ± 0.12

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Table S6 – *Continued from previous page*

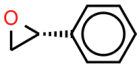
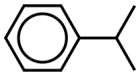
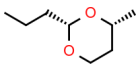
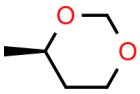
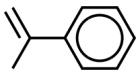
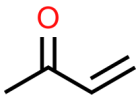
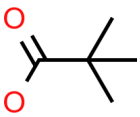
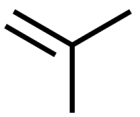
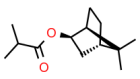
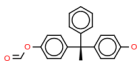
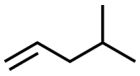
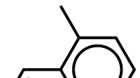
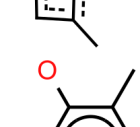
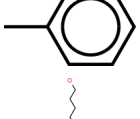
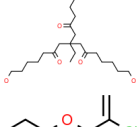
MONOMER	ρ_{exp}	ρ_{pred}
	1.15	1.20 ± 0.10
	1.06	1.04 ± 0.11
	1.21	1.21 ± 0.11
	1.08	1.13 ± 0.16
	1.23	1.11 ± 0.18
	1.07	1.03 ± 0.10
	1.12	1.13 ± 0.11
	1.10	1.04 ± 0.12
	0.84	0.89 ± 0.07
	1.06	1.03 ± 0.12
	1.20	1.20 ± 0.09
	0.84	0.91 ± 0.07
	1.03	1.02 ± 0.10
	1.06	1.10 ± 0.18
	1.07	1.08 ± 0.15
	1.07	1.14 ± 0.12
	1.30	1.26 ± 0.09

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Table S6 – *Continued from previous page*

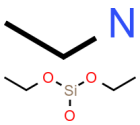
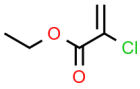
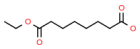
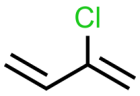
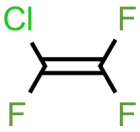
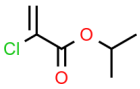
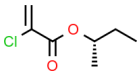
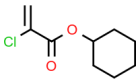
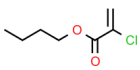
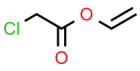
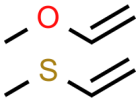
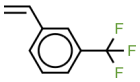
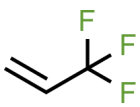
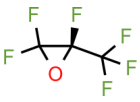
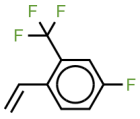
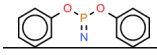
MONOMER	ρ_{exp}	ρ_{pred}
	1.07	1.11 ± 0.15
	1.06	1.07 ± 0.08
	1.39	1.35 ± 0.12
	1.15	1.07 ± 0.12
	1.24	1.43 ± 0.16
	1.92	1.37 ± 0.18
	1.27	1.28 ± 0.09
	1.24	1.28 ± 0.09
	1.25	1.29 ± 0.10
	1.24	1.29 ± 0.13
	1.45	1.40 ± 0.18
	1.05	1.03 ± 0.16
	1.18	1.17 ± 0.14
	2.00	1.38 ± 0.20
	1.32	1.37 ± 0.21
	1.58	1.44 ± 0.21
	1.91	1.38 ± 0.20
	1.43	1.38 ± 0.20
	1.20	1.27 ± 0.22

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Table S6 – *Continued from previous page*

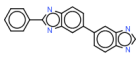
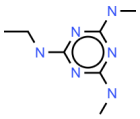
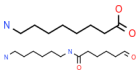
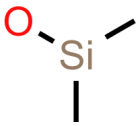
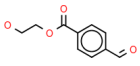
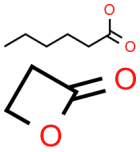
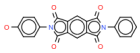
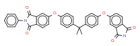
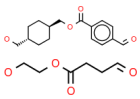
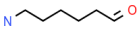
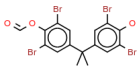
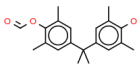
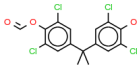
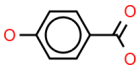
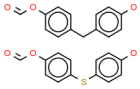
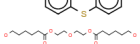
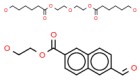
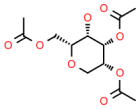
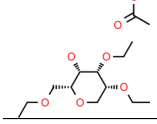
MONOMER	ρ_{exp}	ρ_{pred}
	1.30	1.27 ± 0.18
	1.48	1.14 ± 0.12
	1.04	1.09 ± 0.13
	1.14	1.14 ± 0.10
	0.98	0.96 ± 0.09
	1.46	1.17 ± 0.11
	1.14	1.10 ± 0.10
	1.36	1.37 ± 0.28
	1.42	1.21 ± 0.10
	1.27	1.23 ± 0.09
	1.20	1.18 ± 0.12
	1.18	1.13 ± 0.07
	1.12	1.14 ± 0.11
	1.99	1.96 ± 0.26
	1.95	1.88 ± 0.34
	1.08	1.12 ± 0.10
	1.42	1.35 ± 0.12
	1.44	1.34 ± 0.13
	1.24	1.21 ± 0.09
	1.36	1.32 ± 0.09
	1.07	1.20 ± 0.13
	1.33	1.21 ± 0.10
	1.31	1.15 ± 0.11
	1.14	1.20 ± 0.14

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Table S6 – *Continued from previous page*

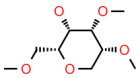
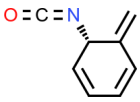
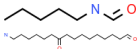
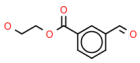
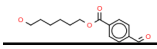
MONOMER	ρ_{exp}	ρ_{pred}
	1.39	1.27 ± 0.15
	1.24	1.20 ± 0.09
	1.19	1.17 ± 0.11
	1.23	1.16 ± 0.12
	1.16	1.16 ± 0.10
	1.36	1.22 ± 0.10
	1.13	1.18 ± 0.11

Table S7: Summary of the classification model performances for the polymer solubilities in different solvents (NMP, THF, $CHCl_3$, DMSO and DMAC). The solubility classes include: S - soluble, PS - partially soluble/swelling/soluble on heating and I - insoluble. Here, mtry is the number of predictors sampled for splitting at each node in the RF model, while accuracy and kappa coefficient are used as the performance metrics.

Solvent	I/PS/S	ACCURACY	KAPPA	*mtry*	I/PS/S	ACCURACY	KAPPA
$CHCl_3$	27/17/24	0.71	0.56	8	26/17/24	0.75	0.61
DMAC	4/21/28	0.74	0.52	15	4/20/28	0.73	0.48
DMSO	10/28/40	0.73	0.53	8	9/28/39	0.75	0.57
NMP	5/21/47	0.83	0.62	42	5/21/46	0.72	0.36
THF	8/30/23	0.72	0.49	51	7/29/23	0.78	0.62

Table S8: The table lists the experimental and predicted solubility classes (S - soluble, PS - partially soluble/swelling/soluble on heating, I - insoluble) for different polymers in $CHCl_3$. Predictions for the RF model are reported.

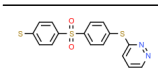
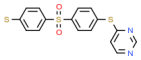
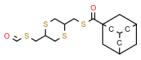
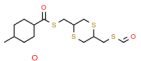
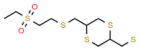
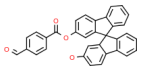
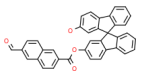
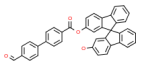
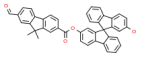
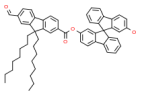
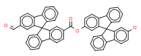
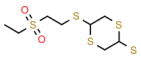
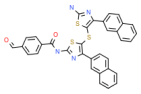
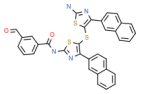
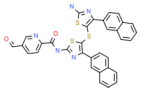
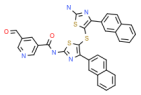
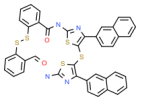
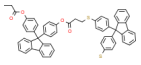
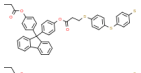
MONOMER	*Experimental*	*Predicted*	Ref
	PS	I	[63]
	I	I	[63]
	S	S	[60]
	S	S	[60]
	S	S	[60]
	S	S	[45]
	S	S	[45]
	S	S	[45]
	S	S	[45]
	S	S	[45]
	S	S	[45]
	S	I	[43]
	S	S	[16]
	PS	PS	[16]
	PS	PS	[16]
	PS	PS	[16]
	PS	PS	[16]
	S	S	[38]
	S	S	[38]
	S	S	[38]

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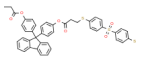
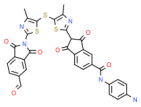
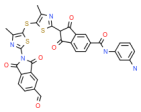
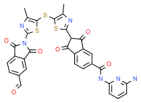
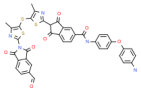
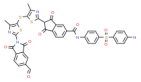
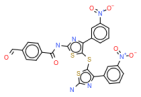
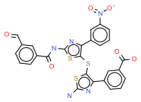
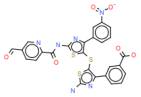
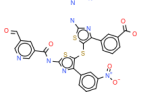
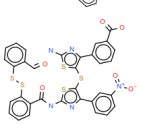
Table S8 – *Continued from previous page*

MONOMER	*Experimental*	*Predicted*	**Ref**
	S	I	[38]
	I	I	[48]
	I	I	[48]
	I	I	[48]
	PS	PS	[48]
	I	I	[48]
	I	PS	[18]
	PS	PS	[18]
	S	S	[18]
	PS	PS	[18]
	PS	PS	[18]
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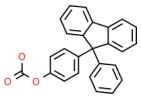
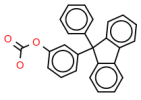
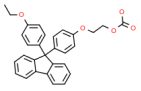
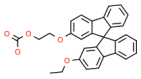
	S	S	[46]
	S	S	[46]
	S	S	[46]
	S	S	[46]

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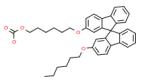
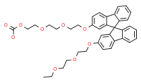
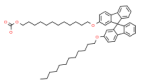
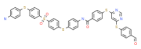
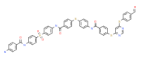
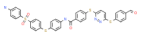
Table S8 – *Continued from previous page*

MONOMER	*Experimental*	*Predicted*	**Ref**
	S	S	[46]
	S	S	[46]
	S	S	[46]
	I	I	[65]
	I	I	[65]
	I	I	[65]
	I	I	[65]
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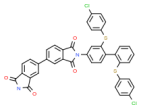
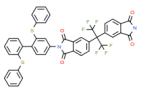
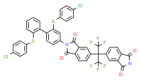
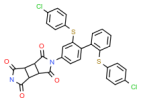
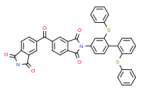
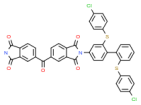
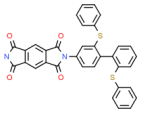
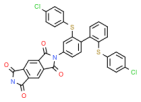
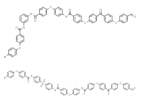
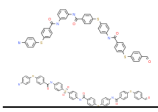
	PS	PS	[52]
	I	I	[52]
	I	I	[52]
	I	S	[52]
	I	I	[52]
	I	I	[52]
	I	PS	[52]
	I	PS	[52]
	I	I	[64]
	I	I	[64]
	I	I	[64]
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Table S8 – *Continued from previous page*

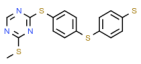
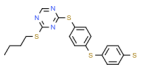
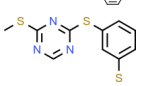
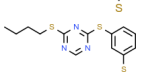
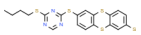
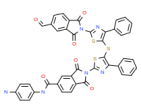
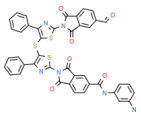
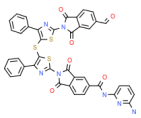
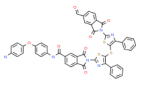
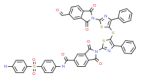
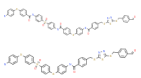
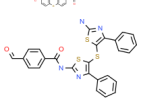
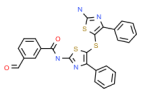
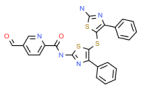
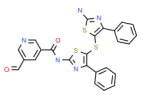
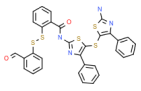
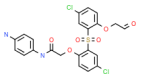
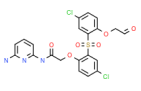
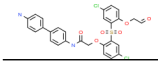
MONOMER	*Experimental*	*Predicted*	**Ref**
	S	S	[40]
	S	S	[40]
	S	S	[40]
	S	S	[40]
	I	I	[19]
	S	S	[19]
	PS	PS	[19]
	PS	I	[19]
	I	I	[19]
	I	I	[35]
	I	I	[35]
	I	I	[17]
	PS	I	[17]
	I	I	[17]
	PS	PS	[17]
	PS	PS	[17]
	I	I	[20]
	PS	PS	[20]
	I	I	[20]

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Table S8 – *Continued from previous page*

MONOMER	*Experimental*	*Predicted*	**Ref**
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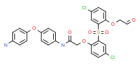
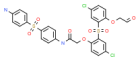
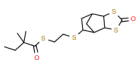
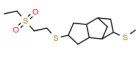
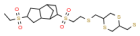
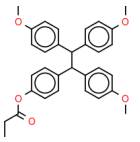
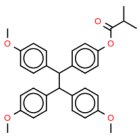
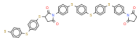
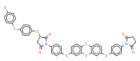
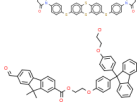
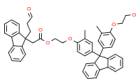
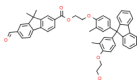
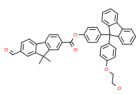
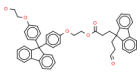
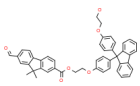
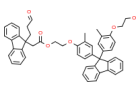
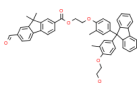
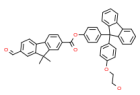
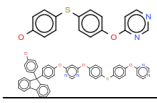
	I	I	[20]
	S	S	[42]
	I	I	[50]
	I	I	[50]
	S	S	[54]
	S	S	[54]
	S	S	[39]
	S	S	[39]
	S	S	[44]
	S	S	[44]
	S	S	[44]
	S	S	[44]
	S	S	[44]
	S	S	[44]
	S	S	[44]
	S	S	[44]
	S	S	[44]
	S	S	[37]
	S	S	[37]

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Table S8 – *Continued from previous page*

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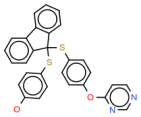
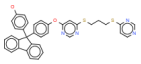
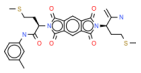
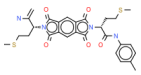
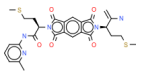
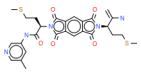
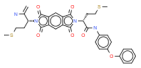
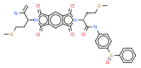
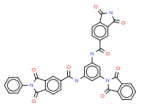
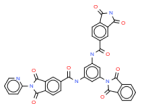
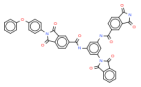
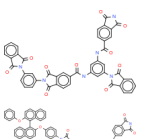
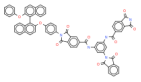
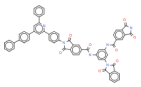
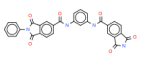
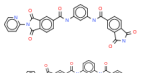
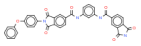
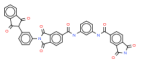
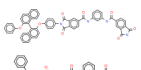
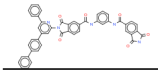
	S	S	[37]
	S	S	[37]
	I	I	[10]
	I	I	[10]
	I	I	[10]
	I	I	[10]
	I	I	[10]
	I	I	[10]
	PS	PS	[3]
	PS	PS	[3]
	I	I	[3]
	PS	PS	[3]
	PS	PS	[3]
	PS	PS	[3]
	PS	I	[3]
	I	I	[3]
	I	I	[3]
	PS	PS	[3]
	PS	I	[3]
	PS	PS	[3]
			

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Table S8 – *Continued from previous page*

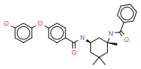
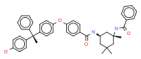
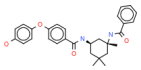
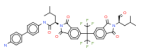
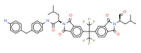
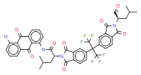
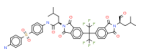
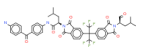
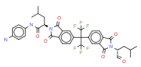
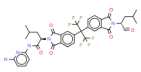
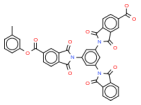
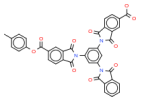
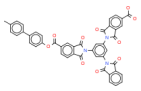
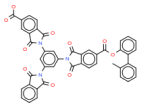
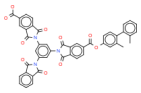
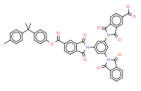
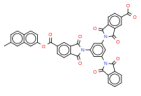
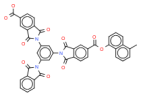
MONOMER	*Experimental*	*Predicted*	**Ref**
	I	S	[66]
	I	S	[66]
	I	I	[66]
	I	I	[47]
	I	I	[47]
	I	I	[47]
	I	I	[47]
	I	I	[47]
	I	I	[47]
	PS	PS	[2]
	I	PS	[2]
	I	PS	[2]
	PS	PS	[2]
	PS	PS	[2]
	PS	PS	[2]
	PS	PS	[2]
	PS	PS	[2]
	PS	PS	[2]

Table S9: The table lists the experimental and predicted solubility classes (S - soluble, PS - partially soluble/swelling/soluble on heating, I - insoluble) for different polymers in N-methylpyrrolidone (NMP). Predictions for the RF model are reported.

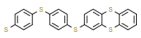
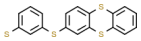
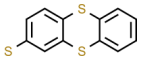
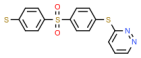
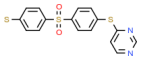
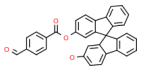
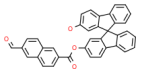
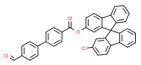
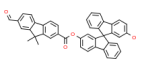
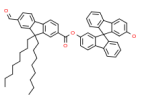
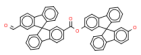
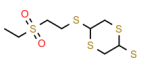
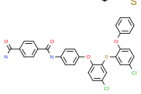
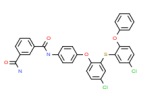
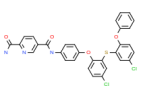
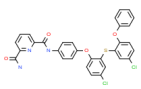
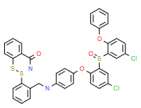
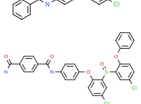
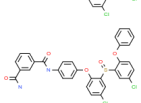
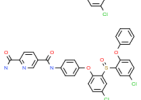
MONOMER	*Experimental*	*Predicted*	Ref
	I	S	[51]
	I	S	[51]
	I	S	[51]
	S	S	[63]
	S	S	[63]
	PS	PS	[45]
	PS	PS	[45]
	PS	PS	[45]
	S	S	[45]
	S	S	[45]
	PS	PS	[45]
	S	S	[43]
	PS	S	[15]
	S	S	[15]
	S	S	[15]
	S	S	[15]
	S	S	[15]
	PS	S	[15]
	S	S	[15]
	S	S	[15]

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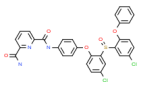
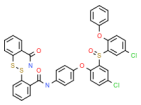
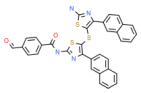
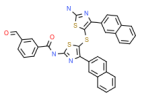
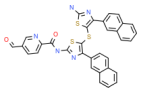
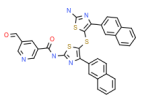
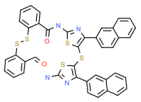
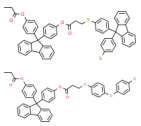
Table S9 – *Continued from previous page*

MONOMER	*Experimental*	*Predicted*	**Ref**
	S	S	[15]
	S	S	[15]
	S	S	[16]
	S	S	[16]
	S	S	[16]
	S	S	[16]
	S	S	[16]
	S	S	[38]
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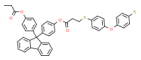
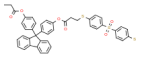
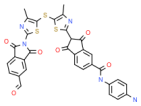
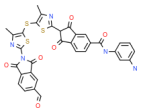
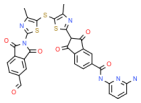
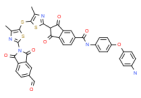
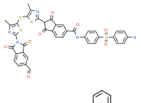
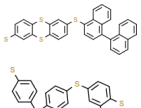
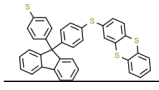
	S	S	[38]
	S	S	[38]
	PS	S	[48]
	S	S	[48]
	S	S	[48]
	S	S	[48]
	S	S	[48]
	S	S	[41]
	S	S	[41]

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Table S9 – *Continued from previous page*

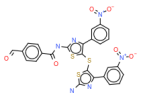
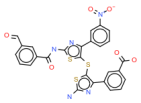
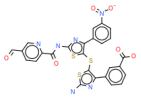
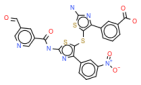
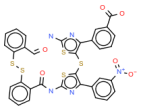
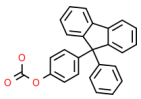
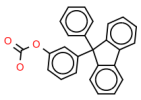
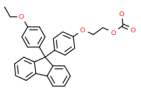
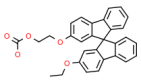
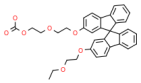
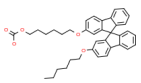
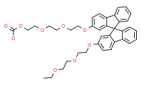
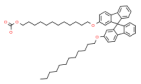
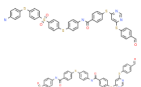
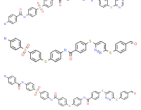
MONOMER	*Experimental*	*Predicted*	**Ref**
	S	S	[18]
	S	S	[18]
	S	S	[18]
	S	S	[18]
	S	S	[18]
	S	S	[46]
	PS	S	[46]
	S	S	[46]
	PS	S	[46]
	PS	PS	[46]
	PS	PS	[46]
	S	S	[65]
	S	S	[65]
	S	S	[65]
	PS	PS	[52]

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Table S9 – *Continued from previous page*

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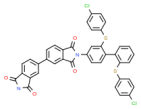
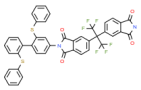
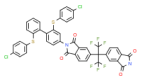
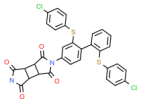
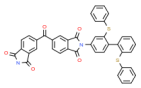
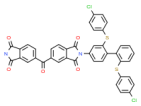
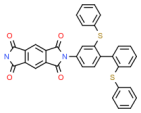
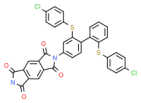
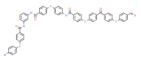
	PS	I	[52]
	I	I	[52]
	I	I	[52]
	I	I	[52]
	I	I	[52]
	I	I	[52]
	I	I	[52]
	I	I	[52]
	PS	S	[64]
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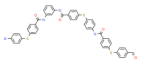
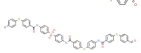
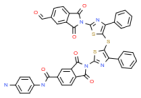
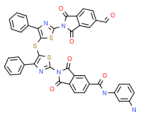
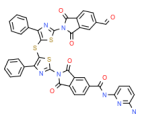
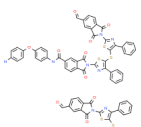
	PS	S	[64]
	PS	PS	[64]
	S	S	[19]
	S	S	[19]
	S	S	[19]
	S	S	[19]
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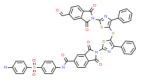
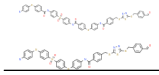
	S	PS	[35]
	S	S	[35]

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Table S9 – *Continued from previous page*

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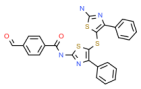
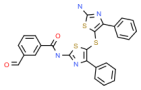
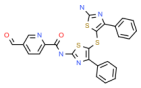
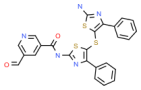
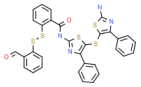
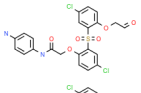
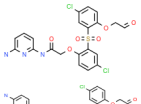
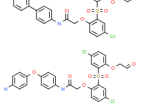
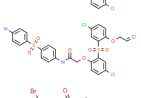
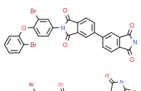
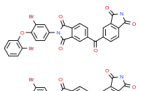
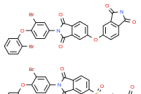
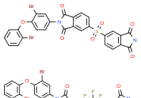
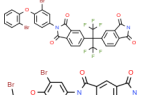
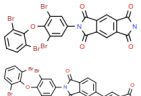
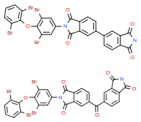
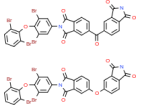
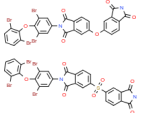
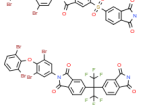
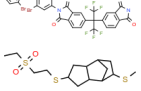
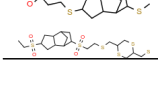
	S	S	[17]
	S	S	[17]
	S	S	[17]
	S	S	[17]
	S	S	[20]
	S	S	[20]
	S	S	[20]
	S	S	[20]
	S	S	[20]
	PS	S	[5]
	S	S	[5]
	S	S	[5]
	S	S	[5]
	S	S	[5]
	S	S	[5]
	S	S	[5]
	S	S	[5]
	S	S	[5]
	S	S	[5]
	S	S	[5]
	S	S	[50]
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Table S9 – *Continued from previous page*

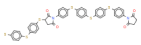
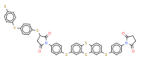
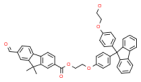
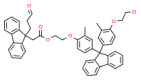
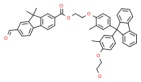
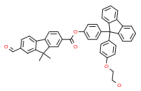
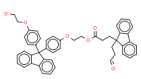
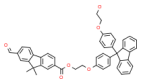
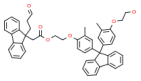
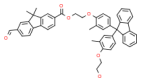
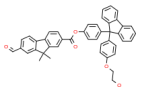
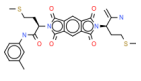
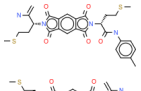
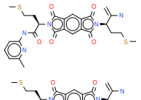
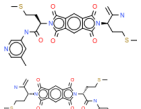
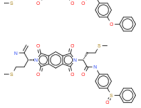
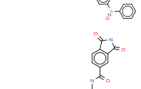
MONOMER	*Experimental*	*Predicted*	**Ref**
	S	S	[39]
	S	S	[39]
	S	S	[44]
	S	S	[44]
	S	S	[44]
	S	S	[44]
	S	S	[44]
	S	S	[44]
	S	S	[44]
	S	S	[44]
	PS	PS	[10]
	PS	PS	[10]
	PS	PS	[10]
	PS	PS	[10]
	PS	S	[10]
	S	S	[3]
	S	S	[3]

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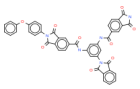
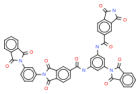
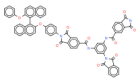
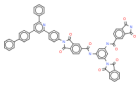
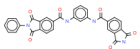
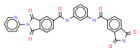
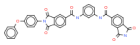
Table S9 – *Continued from previous page*

MONOMER	*Experimental*	*Predicted*	**Ref**
	PS	S	[3]
	S	S	[3]
	S	S	[3]
	S	S	[3]
	PS	S	[3]
	S	S	[3]
	PS	PS	[3]
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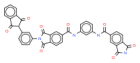
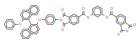
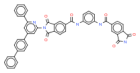
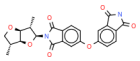
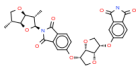
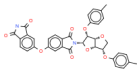
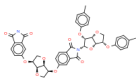
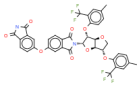
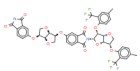
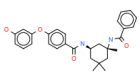
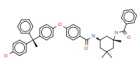
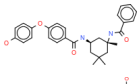
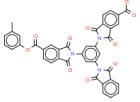
	PS	S	[3]
	S	S	[3]
	S	S	[56]
	PS	PS	[56]
	S	PS	[56]
	S	S	[56]
	S	S	[56]
	S	S	[56]
	PS	PS	[66]
	PS	S	[66]
	PS	PS	[66]
	PS	PS	[2]
	PS	PS	[2]

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Table S9 – *Continued from previous page*

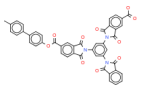
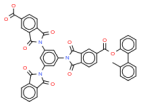
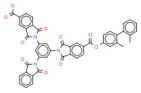
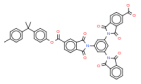
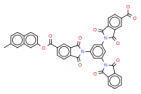
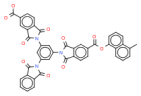
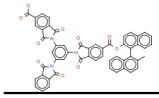
MONOMER	*Experimental*	*Predicted*	**Ref**
	PS	PS	[2]
	PS	PS	[2]
	PS	PS	[2]
	PS	PS	[2]
	PS	PS	[2]
	PS	PS	[2]
	PS	PS	[2]

Table S10: The table lists the experimental and predicted solubility classes (S - soluble, PS - partially soluble/swelling/soluble on heating, I - insoluble) for different polymers in THF. Predictions for the RF model are reported.

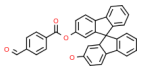
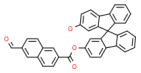
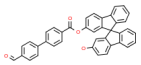
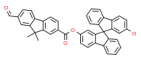
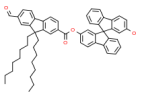
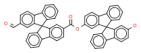
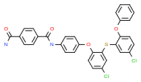
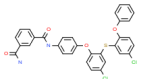
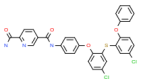
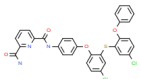
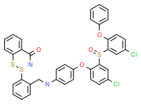
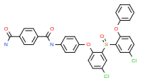
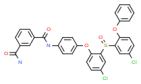
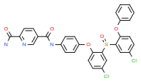
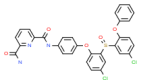
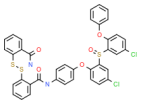
MONOMER	*Experimental*	*Predicted*	Ref
	S	S	[45]
	S	S	[45]
	S	S	[45]
	S	S	[45]
	S	S	[45]
	I	PS	[15]
	PS	PS	[15]
	PS	PS	[15]
	PS	PS	[15]
	S	S	[15]
	PS	PS	[15]
	PS	PS	[15]
	PS	PS	[15]
	PS	PS	[15]
	S	S	[15]
	PS	PS	[16]

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Table S10 – *Continued from previous page*

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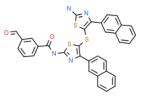
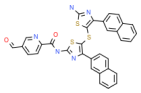
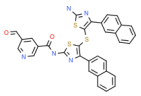
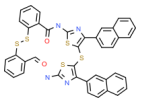
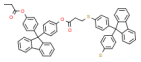
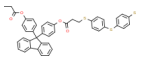
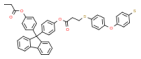
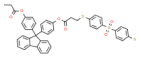
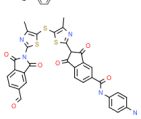
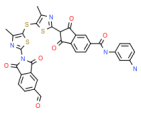
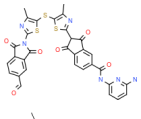
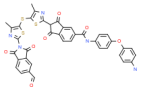
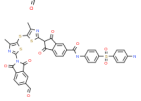
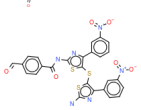
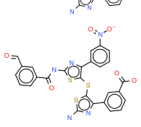
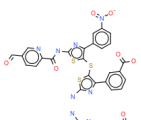
	PS	PS	[16]
	PS	PS	[16]
	S	S	[16]
	S	S	[16]
	S	S	[38]
	S	S	[38]
	S	S	[38]
	S	S	[38]
	PS	PS	[48]
	PS	PS	[48]
	PS	PS	[48]
	PS	PS	[48]
	PS	PS	[48]
	PS	PS	[18]
	PS	PS	[18]
	S	PS	[18]

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Table S10 – *Continued from previous page*

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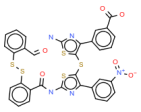
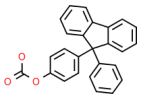
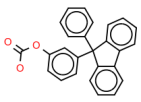
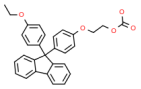
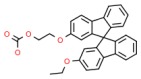
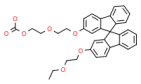
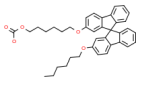
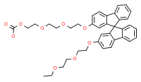
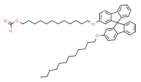
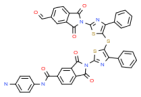
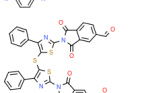
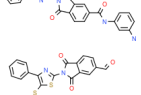
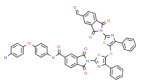
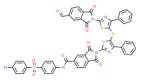
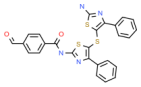
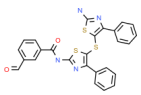
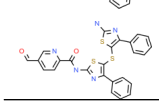
	S	S	[18]
	S	S	[46]
	S	S	[46]
	S	S	[46]
	S	S	[46]
	PS	S	[46]
	S	S	[46]
	S	S	[46]
	S	S	[46]
	PS	PS	[19]
	PS	PS	[19]
	PS	PS	[19]
	S	S	[19]
	PS	PS	[19]
	PS	PS	[17]
	PS	PS	[17]
	PS	S	[17]

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Table S10 – *Continued from previous page*

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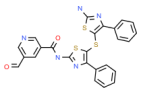
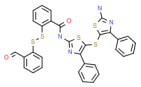
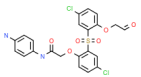
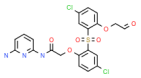
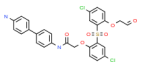
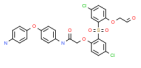
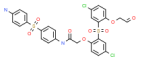
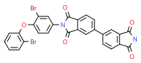
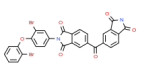
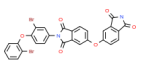
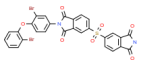
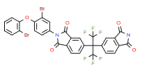
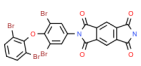
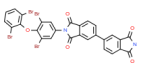
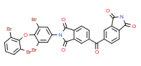
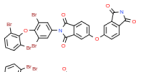
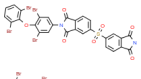
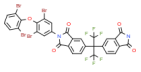
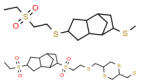
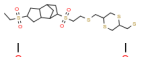
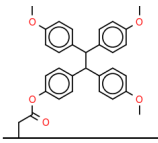
	PS	PS	[17]
	S	S	[17]
	PS	PS	[20]
	PS	PS	[20]
	PS	PS	[20]
	S	S	[20]
	PS	PS	[20]
	I	PS	[5]
	PS	PS	[5]
	PS	PS	[5]
	PS	PS	[5]
	S	PS	[5]
	S	S	[5]
	PS	S	[5]
	S	S	[5]
	S	S	[5]
	S	S	[5]
	S	S	[5]
	I	I	[50]
	I	I	[50]
	S	S	[54]

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Table S10 – *Continued from previous page*

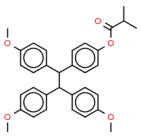
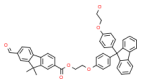
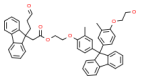
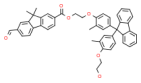
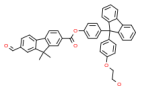
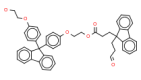
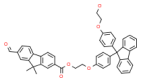
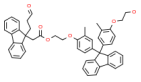
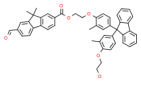
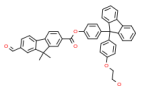
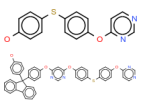
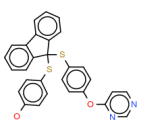
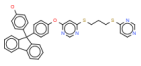
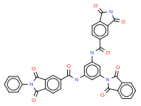
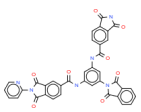
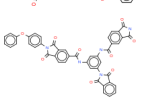
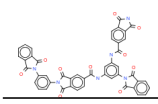
MONOMER	*Experimental*	*Predicted*	**Ref**
	S	S	[54]
	S	S	[44]
	S	S	[44]
	S	S	[44]
	S	S	[44]
	S	S	[44]
	S	S	[44]
	S	S	[44]
	S	S	[44]
	S	S	[44]
	I	I	[37]
	S	S	[37]
	S	S	[37]
	S	S	[37]
	PS	PS	[3]
	PS	PS	[3]
	I	I	[3]
	PS	PS	[3]

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Table S10 – *Continued from previous page*

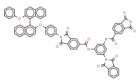
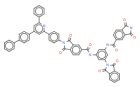
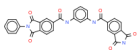
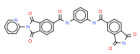
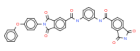
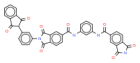
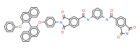
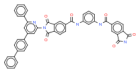
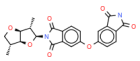
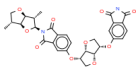
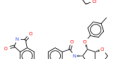
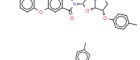
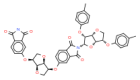
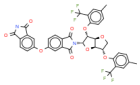
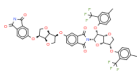
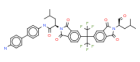
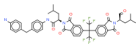
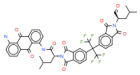
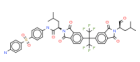
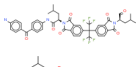
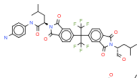
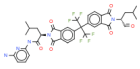
MONOMER	*Experimental*	*Predicted*	**Ref**
	PS	PS	[3]
	PS	PS	[3]
	PS	I	[3]
	PS	PS	[3]
	I	PS	[3]
	PS	PS	[3]
	PS	PS	[3]
	PS	PS	[3]
	PS	PS	[56]
	I	PS	[56]
	I	I	[56]
	I	I	[56]
	PS	PS	[56]
	PS	PS	[56]
	PS	PS	[47]
	PS	PS	[47]
	PS	PS	[47]
	PS	PS	[47]
	PS	PS	[47]
	PS	PS	[47]
	PS	PS	[47]
	PS	I	[2]

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Table S10 – *Continued from previous page*

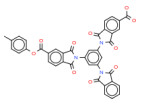
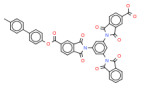
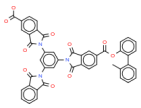
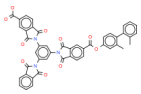
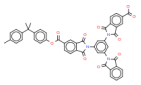
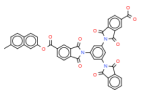
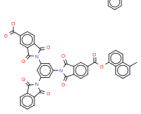
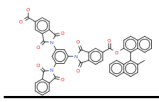
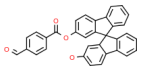
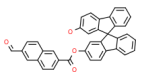
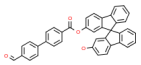
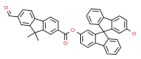
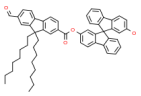
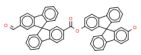
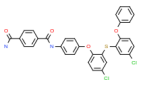
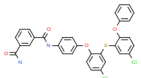
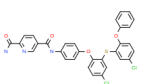
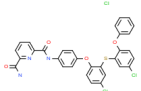
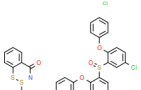
MONOMER	*Experimental*	*Predicted*	**Ref**
	I	PS	[2]
	I	I	[2]
	I	I	[2]
	PS	I	[2]
	PS	PS	[2]
	I	I	[2]
	I	I	[2]
	PS	PS	[2]

Table S11: The table lists the experimental and predicted solubility classes (S - soluble, PS - partially soluble/swelling/soluble on heating, I - insoluble) for different polymers in N,N-Dimethylacetamide (DMAc). Predictions for the RF model are reported.

MONOMER	*Experimental*	*Predicted*	**Ref**
	PS	PS	[45]
	PS	PS	[45]
	PS	PS	[45]
	PS	PS	[45]
	S	S	[45]
	PS	S	[45]
	S	S	[15]
	S	S	[15]
	S	S	[15]
	S	S	[15]
	S	S	[15]
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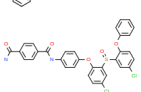
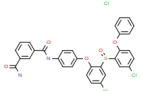
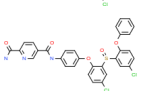
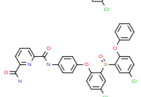
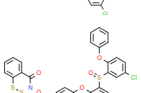
	S	S	[15]
	S	S	[15]
	S	S	[15]
	S	S	[15]
	S	S	[15]
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Table S11 – *Continued from previous page*

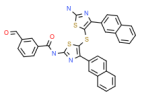
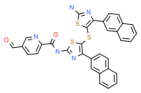
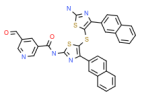
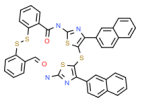
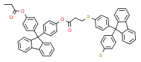
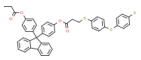
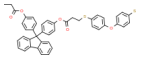
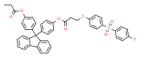
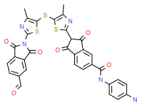
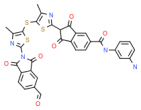
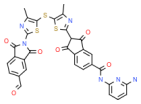
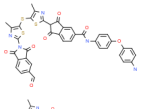
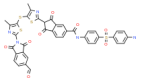
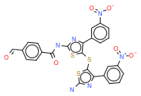
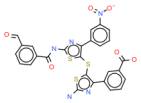
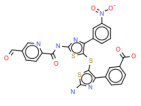
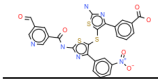
MONOMER	*Experimental*	*Predicted*	**Ref**
	S	S	[16]
	S	S	[16]
	S	S	[16]
	S	S	[16]
	S	S	[38]
	S	S	[38]
	S	S	[38]
	S	S	[38]
	PS	PS	[48]
	PS	S	[48]
	PS	S	[48]
	S	S	[48]
	PS	PS	[48]
	S	S	[18]
	S	S	[18]
	S	S	[18]
	S	S	[18]

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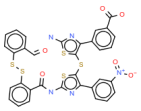
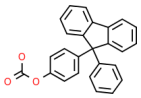
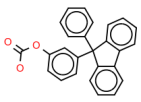
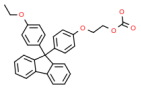
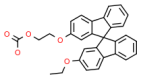
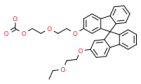
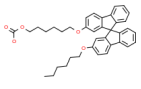
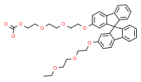
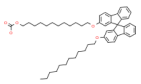
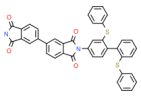
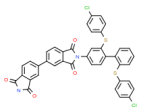
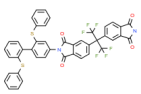
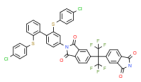
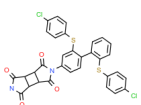
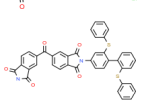
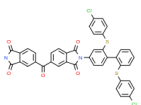
Table S11 – *Continued from previous page*

MONOMER	*Experimental*	*Predicted*	**Ref**
	S	S	[18]
	S	S	[46]
	S	S	[46]
	S	S	[46]
	S	S	[46]
	S	PS	[46]
	PS	PS	[46]
	PS	S	[46]
	PS	PS	[46]
	PS	PS	[52]
	PS	I	[52]
	I	PS	[52]
	I	I	[52]
	I	I	[52]
	I	PS	[52]
	I	PS	[52]

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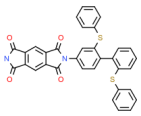
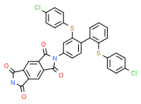
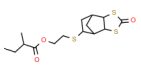
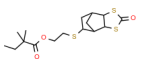
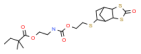
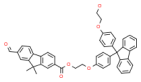
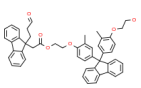
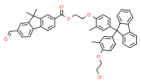
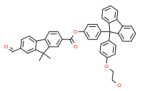
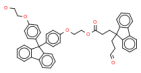
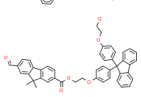
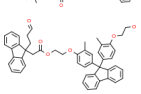
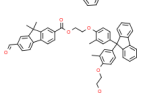
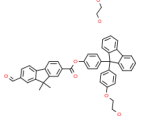
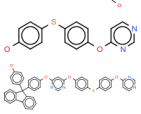
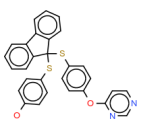
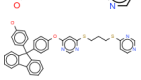
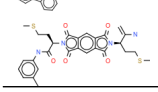
	I	S	[52]
	I	I	[52]
	S	PS	[42]
	S	S	[42]
	S	S	[42]
	S	S	[44]
	S	S	[44]
	S	S	[44]
	S	S	[44]
	S	S	[44]
	S	S	[44]
	S	S	[44]
	S	S	[44]
	S	S	[44]
	I	I	[37]
	S	S	[37]
	S	S	[37]
	S	S	[37]
	PS	PS	[10]

Continued on next page

Table S11 – *Continued from previous page*

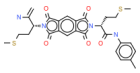
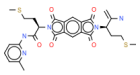
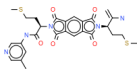
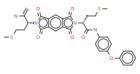
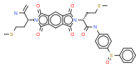
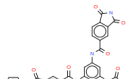
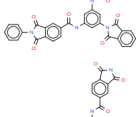
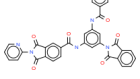
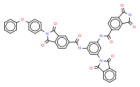
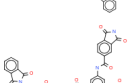
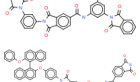
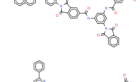
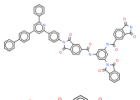
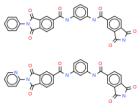
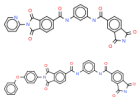
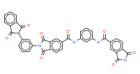
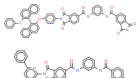
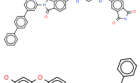
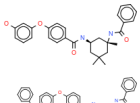
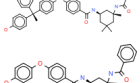
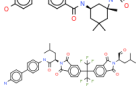
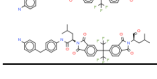
MONOMER	*Experimental*	*Predicted*	**Ref**
	PS	PS	[10]
	PS	PS	[10]
	PS	PS	[10]
	PS	PS	[10]
	PS	PS	[10]
	S	S	[3]
	S	S	[3]
	PS	S	[3]
	S	S	[3]
	S	S	[3]
	S	S	[3]
	S	S	[3]
	S	S	[3]
	S	S	[3]
	PS	S	[3]
	S	S	[3]
	S	S	[3]
	S	S	[3]
	PS	PS	[66]
	PS	S	[66]
	PS	PS	[66]
	PS	PS	[47]
	PS	PS	[47]

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Table S11 – *Continued from previous page*

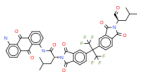
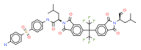
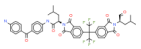
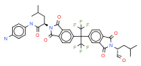
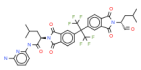
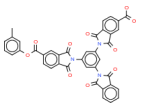
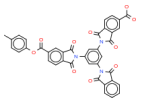
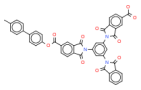
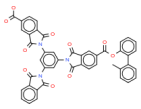
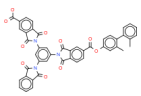
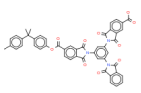
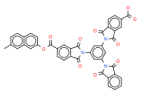
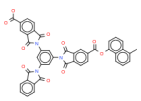
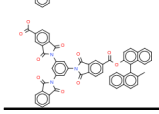
MONOMER	*Experimental*	*Predicted*	**Ref**
	PS	PS	[47]
	PS	PS	[47]
	PS	PS	[47]
	PS	PS	[47]
	PS	PS	[47]
	PS	PS	[2]
	PS	PS	[2]
	PS	PS	[2]
	PS	PS	[2]
	PS	PS	[2]
	PS	PS	[2]
	PS	PS	[2]
	PS	PS	[2]
	PS	PS	[2]
	PS	PS	[2]
	PS	PS	[2]

Table S12: The table lists the experimental and predicted solubility classes (S - soluble, PS - partially soluble/swelling/soluble on heating, I - insoluble) for different polymers in DMSO. Predictions for the RF model are reported.

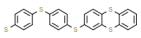
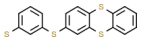
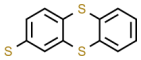
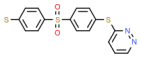
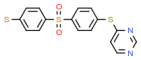
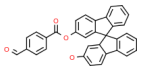
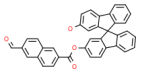
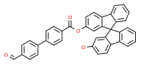
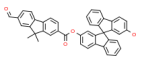
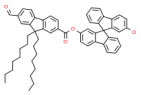
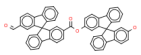
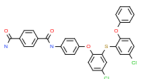
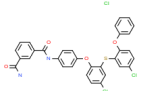
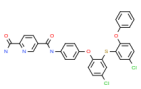
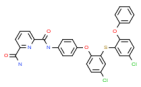
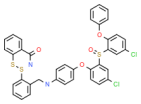
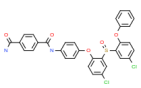
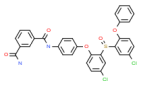
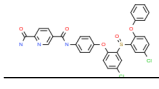
MONOMER	*Experimental*	*Predicted*	Ref
	I	I	[51]
	I	I	[51]
	I	I	[51]
	S	S	[63]
	S	S	[63]
	PS	PS	[45]
	PS	PS	[45]
	PS	PS	[45]
	PS	PS	[45]
	PS	PS	[45]
	PS	S	[45]
	S	S	[15]
	S	S	[15]
	S	S	[15]
	S	S	[15]
	S	S	[15]
	S	S	[15]
	S	S	[15]
	S	S	[15]

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Table S12 – *Continued from previous page*

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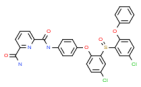
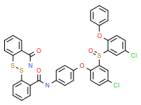
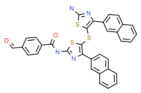
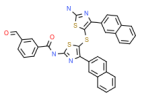
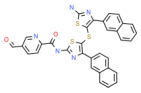
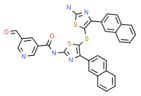
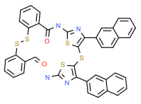
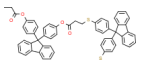
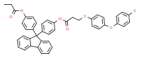
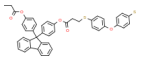
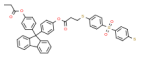
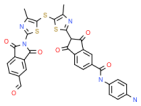
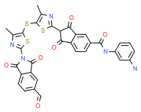
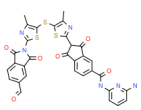
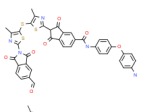
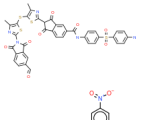
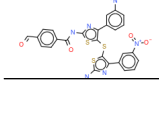
	S	S	[15]
	S	S	[15]
	S	S	[16]
	S	S	[16]
	S	S	[16]
	S	S	[16]
	S	S	[16]
	S	S	[38]
	PS	PS	[38]
	S	S	[38]
	S	S	[38]
	PS	S	[48]
	PS	S	[48]
	S	S	[48]
	S	S	[48]
	PS	S	[48]
	S	S	[18]

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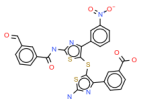
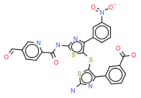
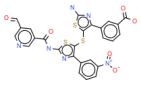
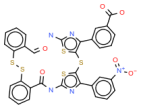
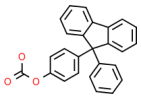
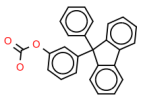
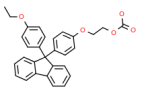
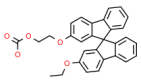
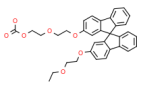
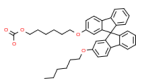
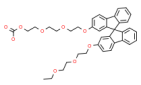
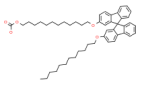
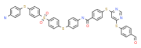
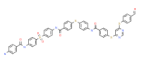
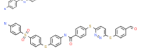
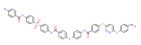
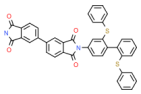
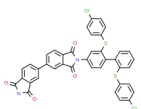
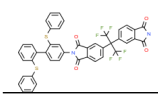
Table S12 – *Continued from previous page*

MONOMER	*Experimental*	*Predicted*	**Ref**
	S	S	[18]
	S	S	[18]
	S	S	[18]
	S	S	[18]
	S	S	[46]
	S	S	[46]
	PS	PS	[46]
	PS	S	[46]
	PS	PS	[46]
	PS	PS	[46]
	PS	PS	[46]
	PS	PS	[46]
	S	S	[65]
	S	S	[65]
	S	S	[65]
	S	S	[65]
	PS	PS	[52]
	PS	I	[52]
	I	PS	[52]

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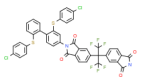
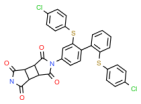
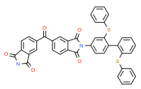
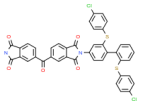
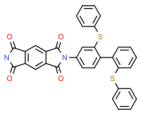
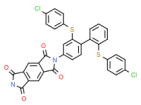
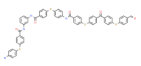
	I	I	[52]
	I	I	[52]
	I	I	[52]
	I	I	[52]
	I	I	[52]
	I	I	[52]
	PS	PS	[64]
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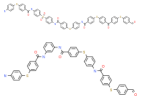
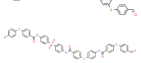
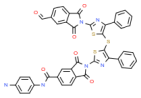
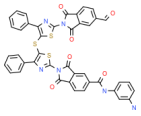
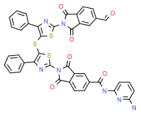
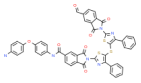
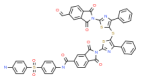
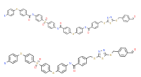
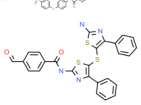
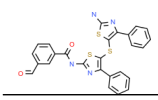
	PS	PS	[64]
	PS	PS	[19]
	S	S	[19]
	S	S	[19]
	S	S	[19]
	S	S	[19]
	S	PS	[35]
	S	S	[35]
	S	S	[17]
	S	S	[17]

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Table S12 – *Continued from previous page*

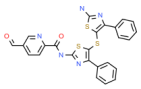
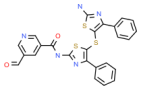
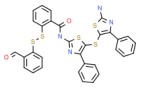
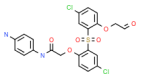
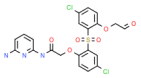
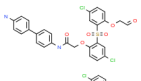
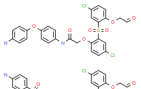
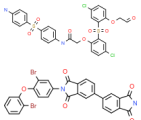
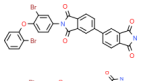
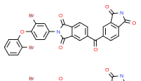
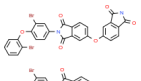
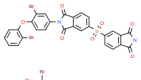
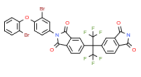
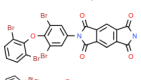
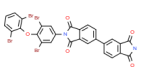
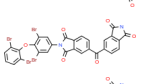
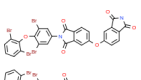
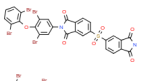
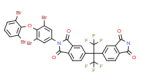
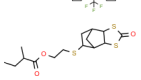
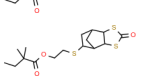
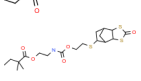
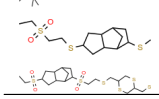
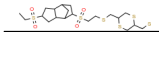
MONOMER	*Experimental*	*Predicted*	**Ref**
	S	S	[17]
	S	S	[17]
	S	S	[17]
	S	S	[20]
	S	S	[20]
	S	S	[20]
	S	S	[20]
	S	S	[20]
	I	S	[5]
	S	S	[5]
	S	S	[5]
	S	S	[5]
	S	S	[5]
	S	S	[5]
	I	I	[5]
	S	S	[5]
	S	S	[5]
	S	S	[5]
	S	S	[5]
	S	S	[42]
	S	S	[42]
	S	S	[42]
	S	S	[42]
	S	S	[50]

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Table S12 – *Continued from previous page*

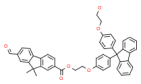
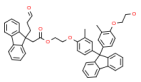
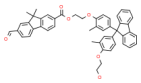
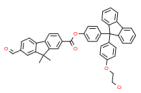
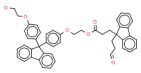
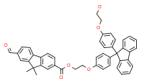
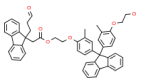
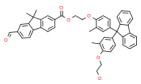
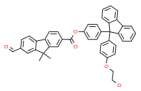
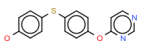
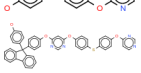
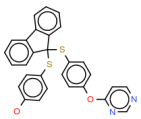
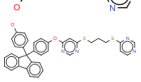
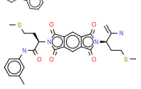
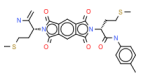
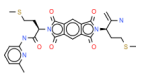
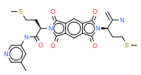
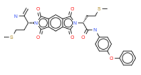
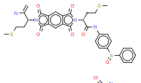
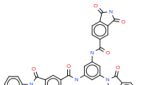
MONOMER	*Experimental*	*Predicted*	**Ref**
	I	I	[50]
	S	S	[44]
	I	I	[44]
	S	I	[44]
	S	S	[44]
	I	I	[44]
	S	S	[44]
	I	I	[44]
	S	I	[44]
	I	S	[44]
	I	PS	[37]
	I	I	[37]
	PS	I	[37]
	PS	PS	[37]
	PS	PS	[10]
	PS	PS	[10]
	PS	PS	[10]
	PS	PS	[10]
	PS	PS	[10]
	S	PS	[10]

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Table S12 – *Continued from previous page*

MONOMER	*Experimental*	*Predicted*	**Ref**
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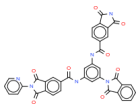
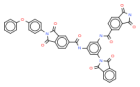
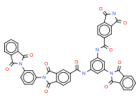
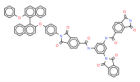
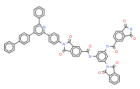
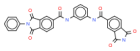
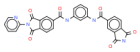
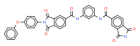
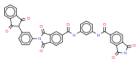
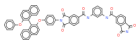
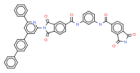
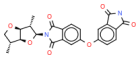
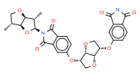
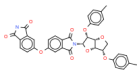
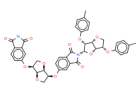
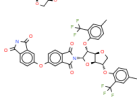
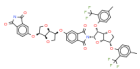
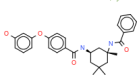
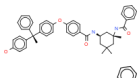
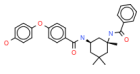
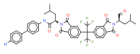
	PS	PS	[3]
	S	PS	[3]
	S	S	[3]
	S	S	[3]
	PS	PS	[3]
	PS	PS	[3]
	PS	PS	[3]
	PS	PS	[3]
	S	S	[3]
	S	PS	[3]
	S	S	[3]
	S	PS	[56]
	PS	PS	[56]
	S	S	[56]
	S	S	[56]
	S	S	[56]
	PS	PS	[56]
	PS	PS	[66]
	PS	PS	[66]
	PS	PS	[66]
	PS	PS	[47]

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Table S12 – *Continued from previous page*

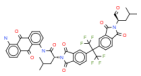
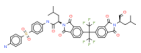
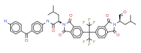
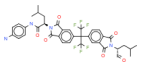
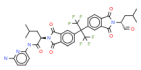
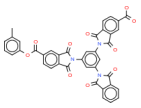
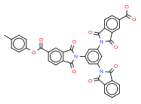
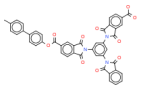
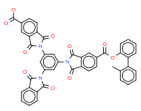
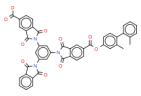
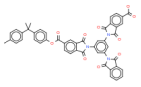
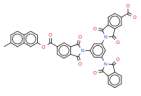
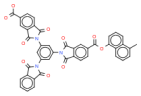
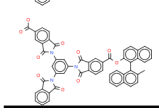
MONOMER	*Experimental*	*Predicted*	**Ref**
	PS	PS	[47]
	PS	S	[47]
	PS	PS	[47]
	PS	PS	[47]
	PS	PS	[47]
	PS	PS	[47]
	PS	PS	[2]
	PS	PS	[2]
	PS	PS	[2]
	PS	PS	[2]
	PS	PS	[2]
	PS	PS	[2]
	PS	PS	[2]
	PS	PS	[2]
	PS	PS	[2]

Table S13: The table lists the experimental and predicted refractive indices measured at given wavelengths for different polymers. Refractive indices for polymers at wavelengths other than 589 nm were taken from multiple references [51, 21, 16, 8, 57, 55, 19, 35, 42, 24, 54]. Here, the the refractive indices are predicted using the polarizabilities derived from DFT calculations and densities predicted using a QSPR model.

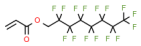
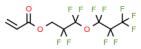
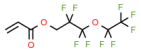
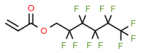
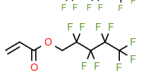
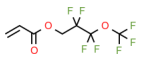
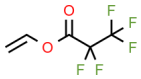
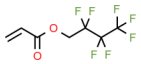
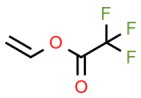
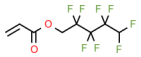
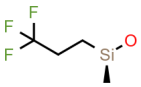
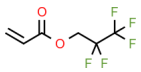
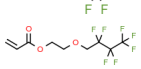
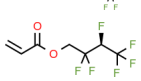
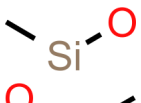
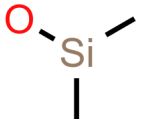
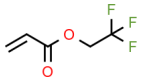
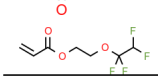
MONOMER	n_{DFT}	λ	n_{pred}
	1.34	589	1.27
	1.35	589	1.27
	1.35	589	1.29
	1.35	589	1.21
	1.36	589	1.28
	1.36	589	1.29
	1.36	589	1.30
	1.36	589	1.30
	1.37	589	1.31
	1.38	589	1.34
	1.38	589	1.31
	1.38	589	1.41
	1.39	589	1.34
	1.39	589	1.35
	1.39	589	1.33
	1.40	589	1.53
	1.40	589	1.42
	1.41	589	1.38
	1.41	589	1.38

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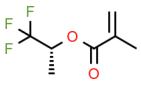
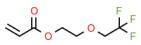
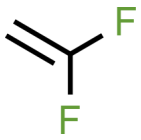
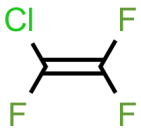
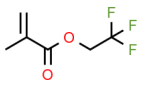
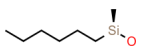
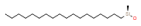
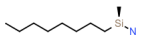
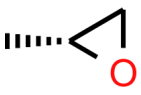
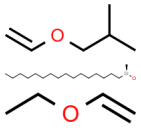
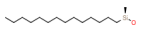
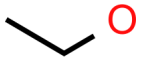
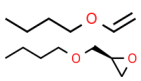
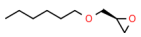
Table S13 – *Continued from previous page*

MONOMER	n_{DFT}	λ	n_{pred}
	1.42	589	1.44
	1.42	589	1.42
	1.42	589	1.36
	1.43	589	1.26
	1.44	589	1.41
	1.44	589	1.47
	1.44	589	1.51
	1.45	589	1.58
	1.45	589	1.55
	1.45	589	1.53
	1.45	589	1.52
	1.45	589	1.51
	1.46	589	1.51
	1.46	589	1.48
	1.46	589	1.59
	1.46	589	1.56
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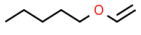	1.46	589	1.60
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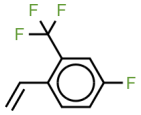	1.46	589	1.51
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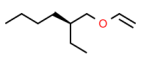
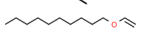
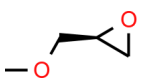
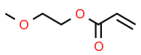
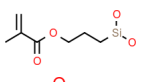
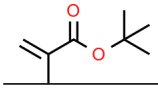
	1.46	589	1.54
	1.46	589	1.61
	1.46	589	1.48
	1.46	589	1.52
	1.46	589	1.48
	1.46	589	1.51

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Table S13 – *Continued from previous page*

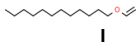
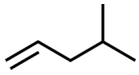
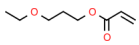
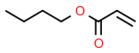
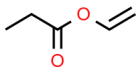
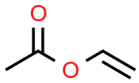
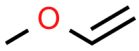
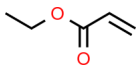
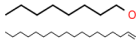
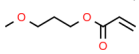
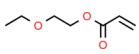
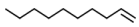
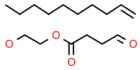
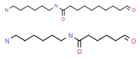
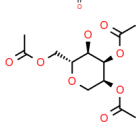
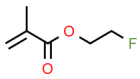
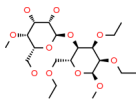
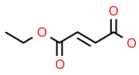
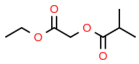
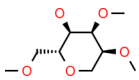
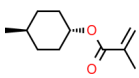
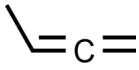
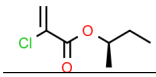
MONOMER	n_{DFT}	λ	n_{pred}
	1.46	589	1.61
	1.47	589	1.54
	1.47	589	1.56
	1.47	589	1.54
	1.47	589	1.49
	1.47	589	1.49
	1.47	589	1.48
	1.47	589	1.52
	1.47	589	1.55
	1.47	589	1.59
	1.47	589	1.51
	1.47	589	1.52
	1.47	589	1.59
	1.47	589	1.40
	1.48	589	1.58
	1.48	589	1.55
	1.48	589	1.44
	1.48	589	1.50
	1.48	589	1.47
	1.48	589	1.48
	1.49	589	1.41
	1.50	589	1.46
	1.50	589	1.49
	1.50	589	1.50
	1.50	589	1.70
	1.50	589	1.53

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Table S13 – *Continued from previous page*

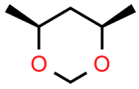
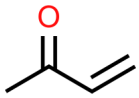
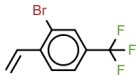
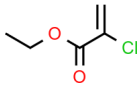
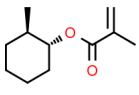
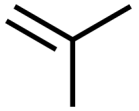
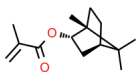
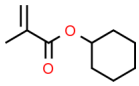
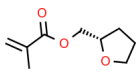
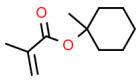
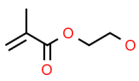
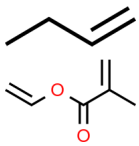
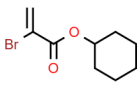
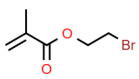
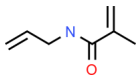
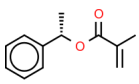
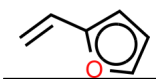
MONOMER	n_{DFT}	λ	n_{pred}
	1.50	589	1.48
	1.50	589	1.56
	1.50	589	1.54
	1.50	589	1.61
	1.50	589	1.52
	1.50	589	1.49
	1.51	589	1.56
	1.51	589	1.51
	1.51	589	1.47
	1.51	589	1.48
	1.51	589	1.50
	1.51	589	1.49
	1.51	589	1.56
	1.51	589	1.55
	1.54	589	1.58
	1.54	589	1.43
	1.55	589	1.61
	1.55	589	1.55
	1.55	589	1.60

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Table S13 – *Continued from previous page*

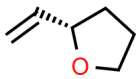
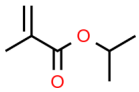
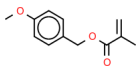
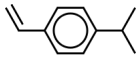
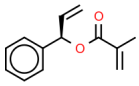
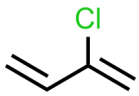
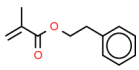
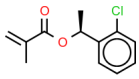
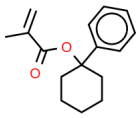
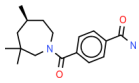
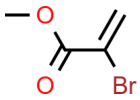
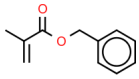
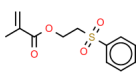
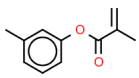
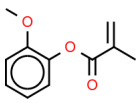
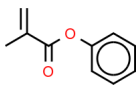
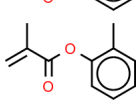
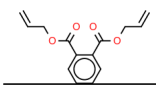
MONOMER	n_{DFT}	λ	n_{pred}
	1.55	589	1.53
	1.55	589	1.48
	1.55	589	1.55
	1.55	589	1.69
	1.56	589	1.63
	1.56	589	1.65
	1.56	589	1.62
	1.56	589	1.59
	1.56	589	1.55
	1.57	589	1.63
	1.57	589	1.46
	1.57	589	1.61
	1.57	589	1.56
	1.57	589	1.62
	1.57	589	1.59
	1.57	589	1.60
	1.57	589	1.60
	1.57	589	1.59

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Table S13 – *Continued from previous page*

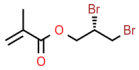
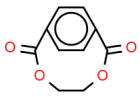
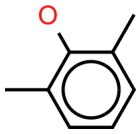
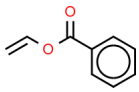
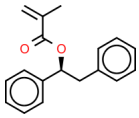
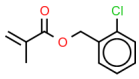
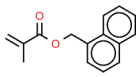
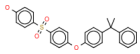
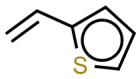
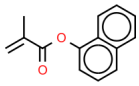
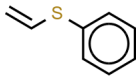
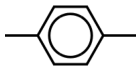
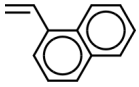
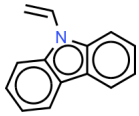
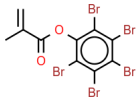
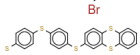
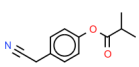
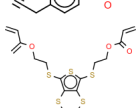
MONOMER	n_{DFT}	λ	n_{pred}
	1.57	589	1.52
	1.58	589	1.51
	1.58	589	1.56
	1.58	589	1.64
	1.58	589	1.64
	1.58	589	1.60
	1.63	589	1.69
	1.63	589	1.68
	1.64	589	1.72
	1.64	589	1.69
	1.66	589	1.73
	1.67	589	1.57
	1.68	589	1.81
	1.68	589	1.81
	1.71	589	1.52
	1.79	633	1.75
	1.51	589	1.60
	1.64	637	1.65

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Table S13 – *Continued from previous page*

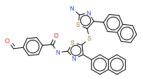
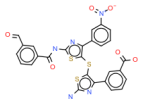
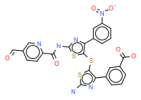
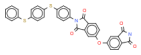
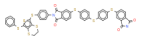
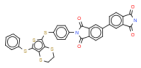
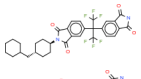
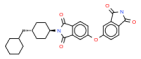
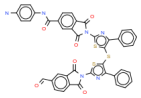
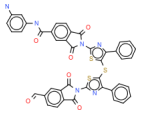
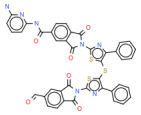
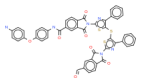
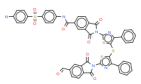
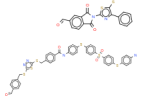
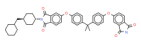
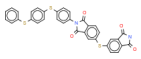
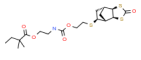
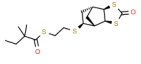
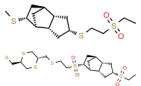
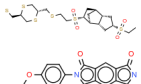
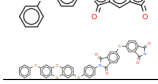
MONOMER	n_{DFT}	λ	n_{pred}
	1.76	633	1.85
	1.75	633	1.78
	1.76	633	1.81
	1.71	633	1.80
	1.76	633	1.81
	1.75	633	1.81
	1.58	1324	1.62
	1.51	1324	1.61
	1.74	633	1.78
	1.74	633	1.78
	1.74	633	1.78
	1.74	633	1.75
	1.75	633	1.74
	1.73	633	1.80
	1.57	1324	1.63
	1.70	1310	1.77
	1.59	589	1.58
	1.64	589	1.58
	1.61	589	1.61
	1.62	589	1.55
	1.65	1324	1.62
	1.72	1310	1.77

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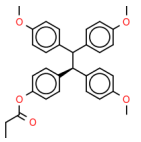
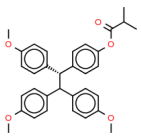
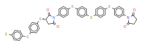
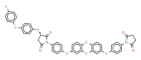
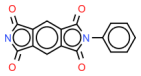
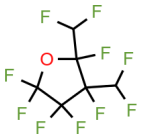
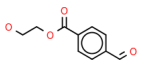
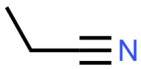
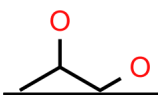
Table S13 – *Continued from previous page*

MONOMER	n_{DFT}	λ	n_{pred}
	1.60	633	1.66
	1.60	633	1.66
	1.71	633	1.75
	1.73	633	1.77
	1.69	1320	1.58
	1.52	589	1.33
	1.58	589	1.64
	1.52	589	1.56
	1.45	589	1.39

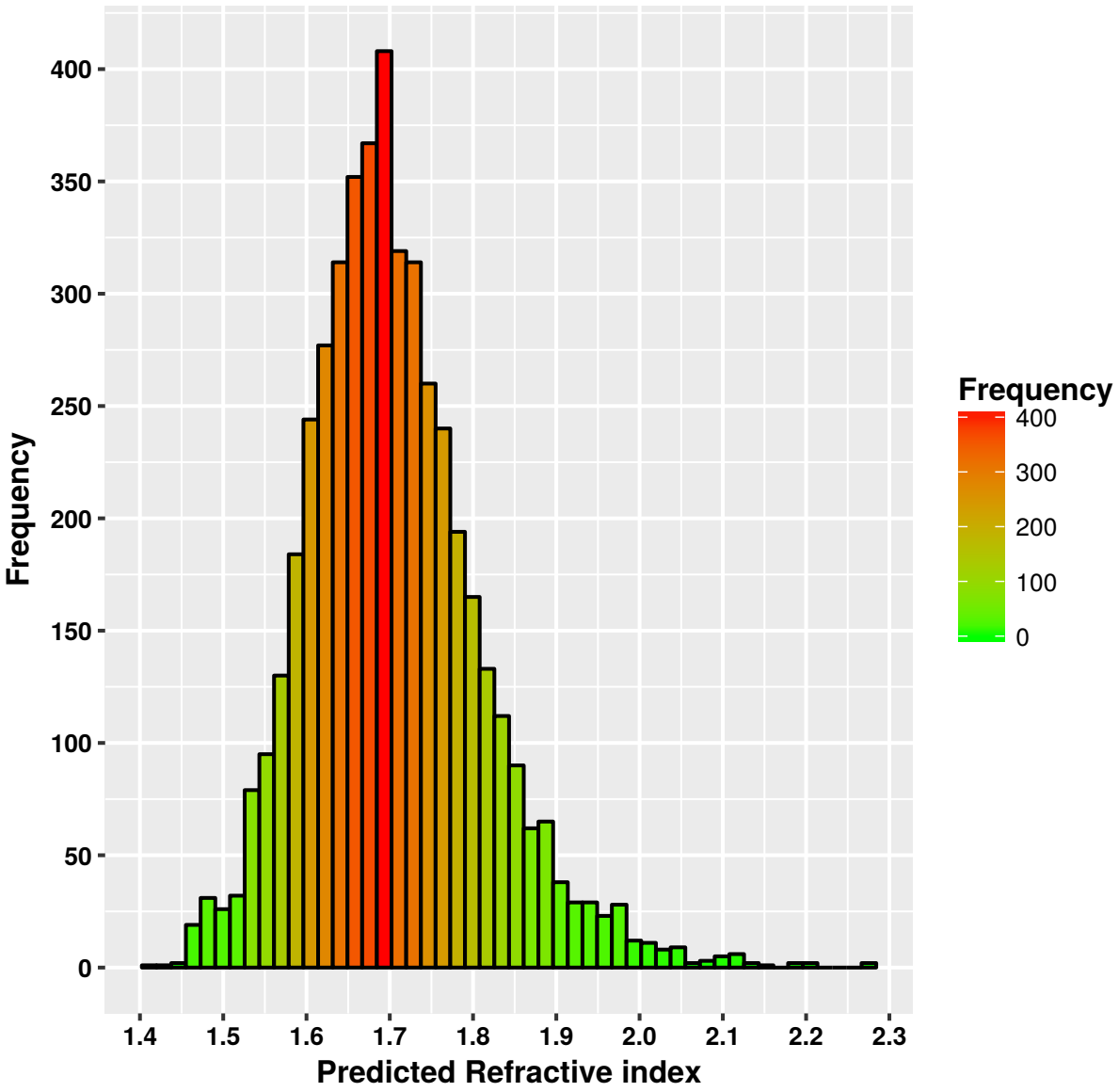


Figure S1: Plot shows the histogram of the predicted refractive indices for the different monomers emerging from the de novo runs.

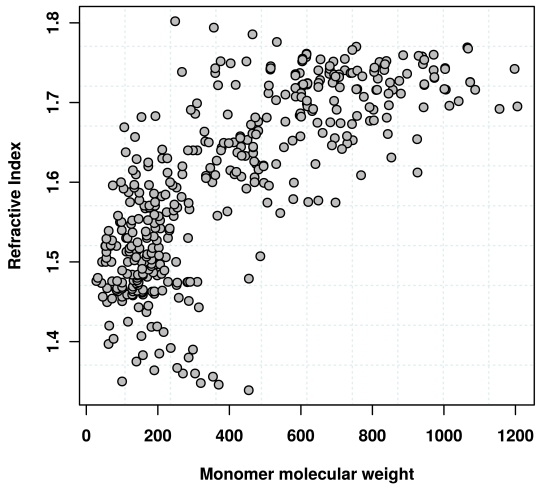


Figure S2: Plot shows the scatter plot of the molecular weights vs the experimental refractive indices (taken from literature) of various polymers.

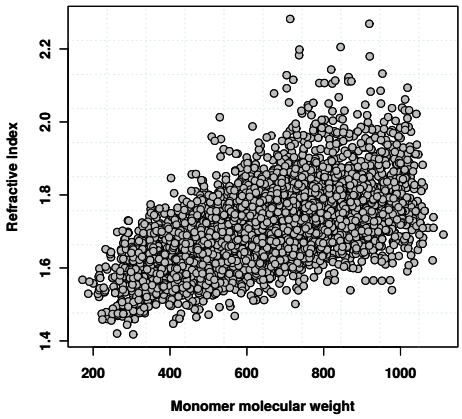


Figure S3: Plot shows the scatter plot of the molecular weights vs the predicted refractive indices of different monomers emerging from the de novo runs.

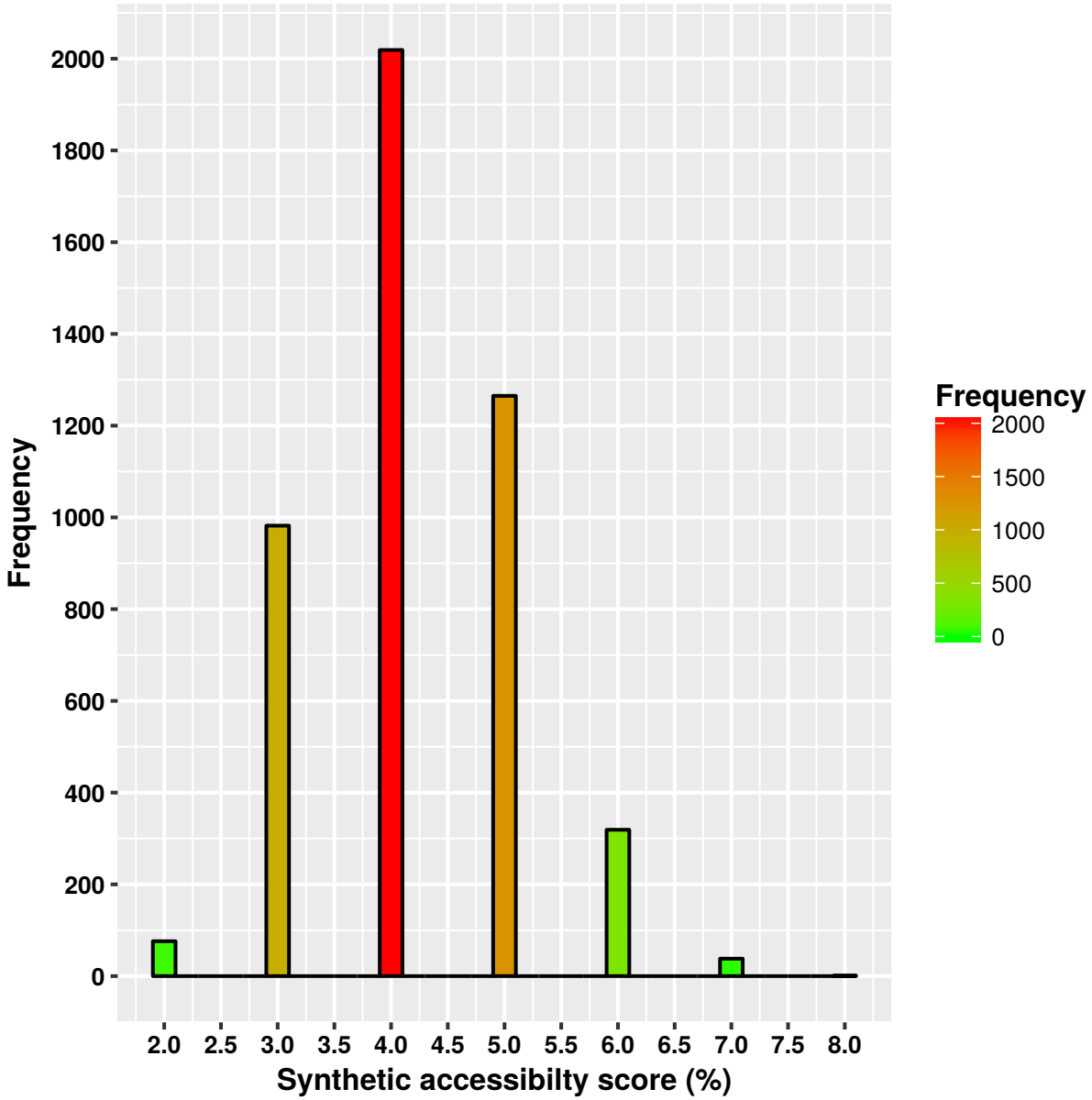
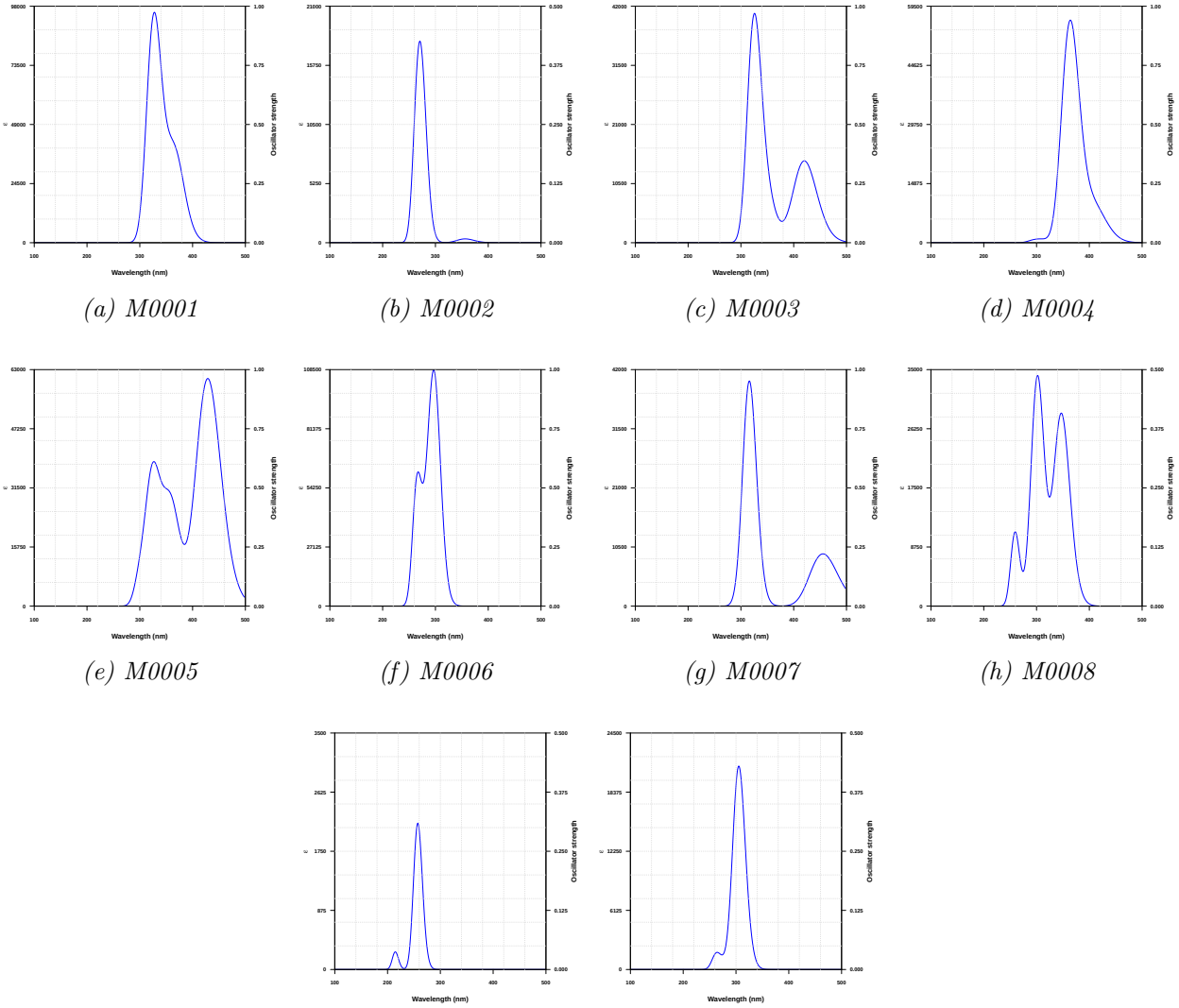


Figure S4: Plot shows the histogram of the synthetic accessibility scores for the different monomers emerging from the de novo *runs.*



(a) M0001 *(b) M0002* *(c) M0003* *(d) M0004*

(e) M0005 *(f) M0006* *(g) M0007* *(h) M0008*

(i) M0009 *(j) M0010*

Figure S5: Calculated UV-VIS spectra for different polymers (see main article).

Table S14: The table lists the experimental (n_{exp}) and predicted refractive indices (n_{pred}) for different polymers. The n were estimated using DFT-based polarizability values at 589 nm and reported experimental densities.

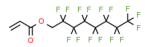
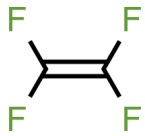
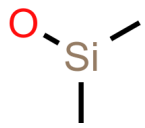
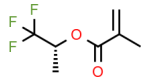
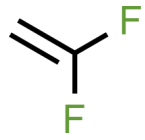
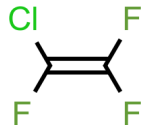
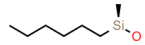
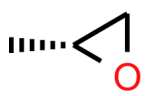
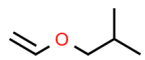
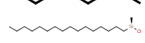
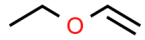
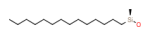
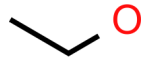
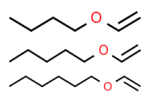
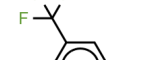
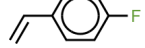
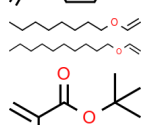
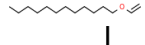
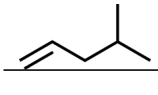
MONOMER	n_{exp}	ρ_{qspr}	ρ_{exp}	n_{pred}
	1.34	1.40	1.42	1.27
	1.35	1.37	0.91	1.14
	1.40	0.96	0.89	1.39
	1.42	1.38	0.88	1.27
	1.42	1.44	1.13	1.27
	1.43	1.36	1.66	1.32
	1.44	0.94	1.60	1.93
	1.45	1.25	1.39	1.62
	1.45	1.03	1.25	1.67
	1.45	0.97	1.26	1.73
	1.45	1.03	1.17	1.59
	1.46	0.95	1.34	1.79
	1.46	1.11	1.02	1.44
	1.46	1.13	1.03	1.53
	1.46	1.13	1.04	1.70
	1.46	1.13	1.13	1.61
	1.46	1.38	1.17	1.42
	1.46	1.13	1.15	1.63
	1.46	1.10	1.12	1.62
	1.46	1.09	1.21	1.58
	1.46	1.10	1.10	1.62
	1.47	0.93	1.11	1.68

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Table S14 – *Continued from previous page*

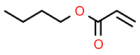
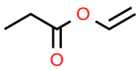
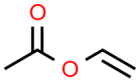
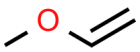
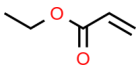
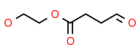
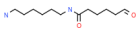
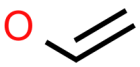
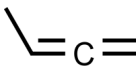
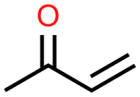
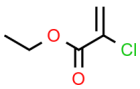
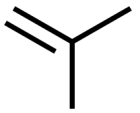
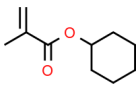
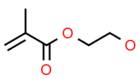
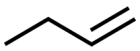
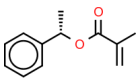
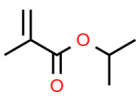
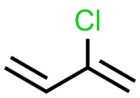
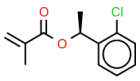
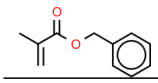
MONOMER	n_{exp}	ρ_{qspr}	ρ_{exp}	n_{pred}
	1.47	1.15	1.05	1.48
	1.47	1.13	1.18	1.51
	1.47	1.20	1.08	1.44
	1.47	1.03	1.06	1.50
	1.47	1.18	1.01	1.43
	1.47	0.99	0.93	1.54
	1.47	1.10	1.10	1.39
	1.48	1.14	0.93	1.43
	1.50	1.13	1.30	1.40
	1.50	1.07	1.04	1.68
	1.50	1.15	0.93	1.43
	1.50	1.37	0.91	1.33
	1.51	0.94	0.88	1.52
	1.51	1.01	0.89	1.41
	1.51	1.18	0.85	1.34
	1.51	0.93	0.91	1.54
	1.55	1.09	1.03	1.51
	1.55	1.04	1.07	1.49
	1.56	1.31	1.24	1.61
	1.56	1.26	1.92	2.04
	1.57	1.19	1.25	1.65

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Table S14 – *Continued from previous page*

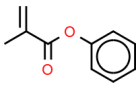
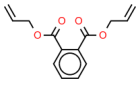
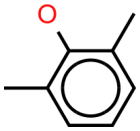
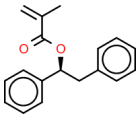
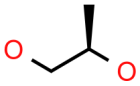
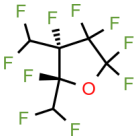
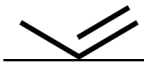
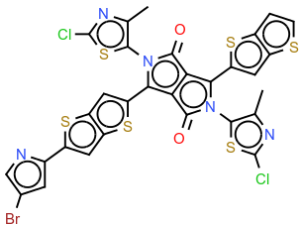
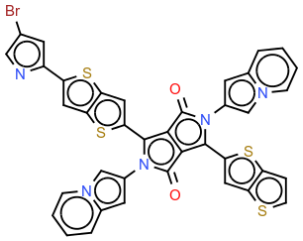
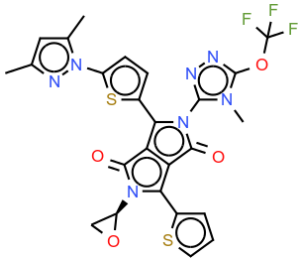
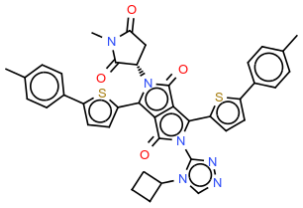
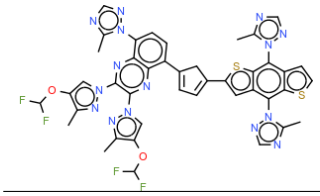
MONOMER	n_{exp}	ρ_{qspr}	ρ_{exp}	n_{pred}
	1.57	1.18	1.45	1.78
	1.57	1.23	1.05	1.49
	1.58	1.07	2.00	2.38
	1.58	1.19	1.43	1.82
	1.45	1.16	1.01	1.39
	1.34	1.45	2.03	1.33
	1.48	0.91	0.85	1.76
	1.47	0.91	0.85	1.88

Table S15: Cases where large deviations between QSPR and DFT estimates for n are observed.

Monomer	n_{qspr}	n_{DFT}
	2.14±0.15	5.79
	1.99±0.12	5.22
	1.89±0.08	2.37
	1.94±0.08	2.78
	1.93±0.09	2.38

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