SUPPORTING INFORMATION

Prediction of Partition Coefficients in SDS micelles by DFT Calculations

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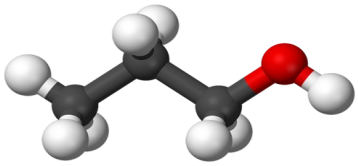
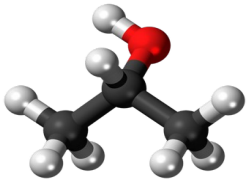
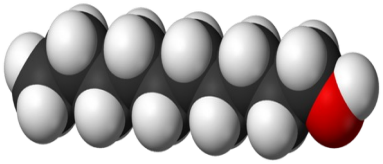
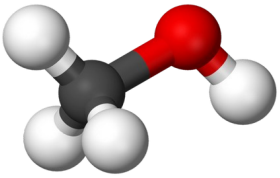
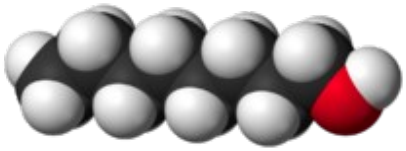
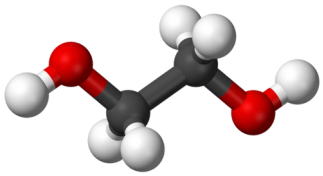
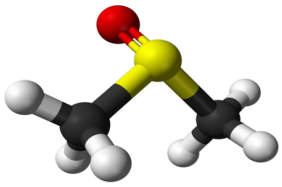
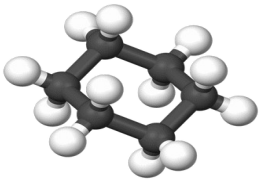
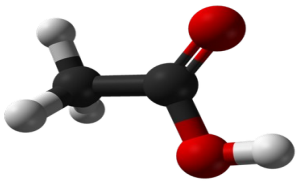
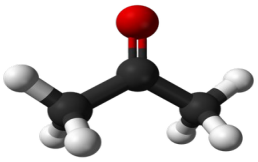
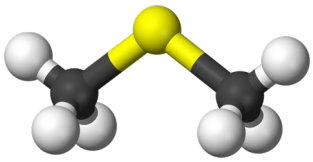
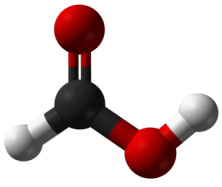
Iupac name	Cas number	Formula	Structure
Propan-1-ol	71-23-8	C_3H_8O	
Propan-2-ol	67-63-0	C_3H_8O	
Decan-1-ol	112-30-1	$C_{10}H_{21}OH$	
Methanol	67-56-1	CH_4O	

Octan-1-ol	111-87-5	$C_8H_{18}O$	
Ethane-1,2-diol	107-21-1	$C_2H_6O_2$	
(Methanesulfinyl)methane	67-68-5	C_2H_6OS	
Cyclohexane	110-82-7	C_6H_{12}	
Acetic acid	64-19-7	$C_2H_4O_2$	
Acetone	67-64-1	C_3H_6O	
(Ethylsulfanyl)ethane	352-93-2	$C_4H_{10}S$	
Formic acid	64-18-6	CH_2O_2	

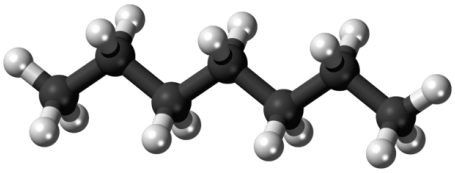
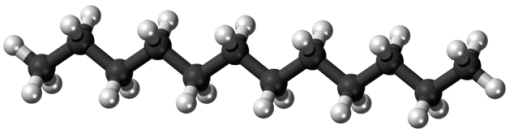
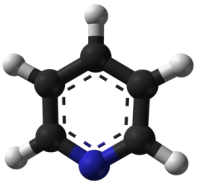
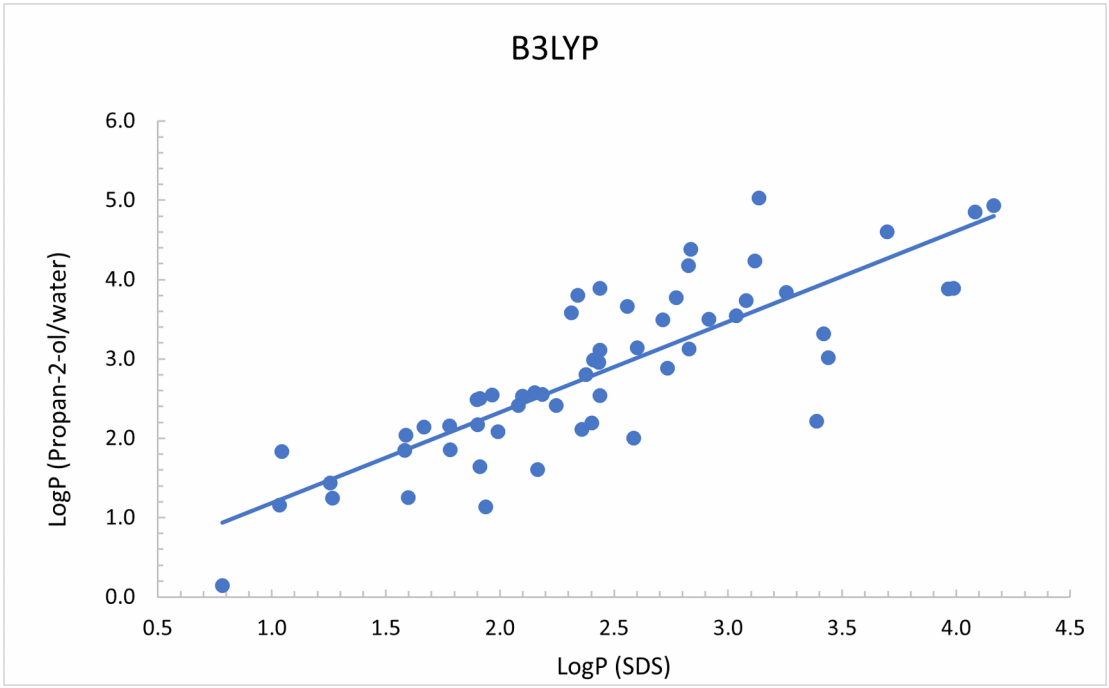
Heptane	142-82-5	C_7H_{16}	
Dodecane	112-40-3	$C_{12}H_{26}$	
Pyridine	110-86-1	C_5H_5N	

Figure S1. Chemical structures of the solvents used in DFT calculations.



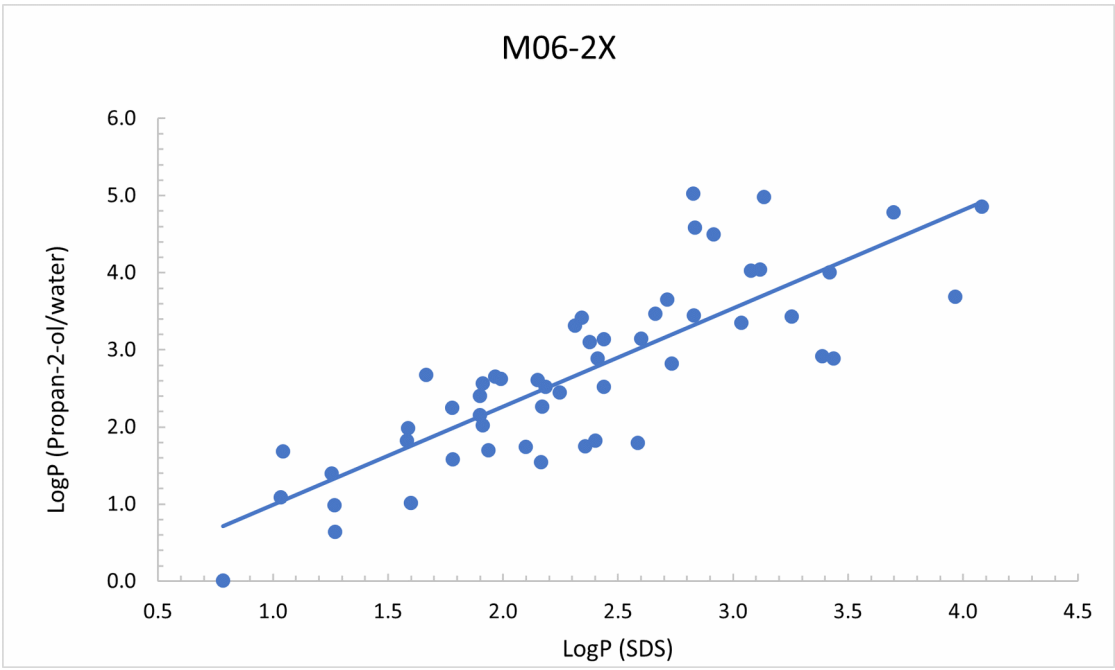
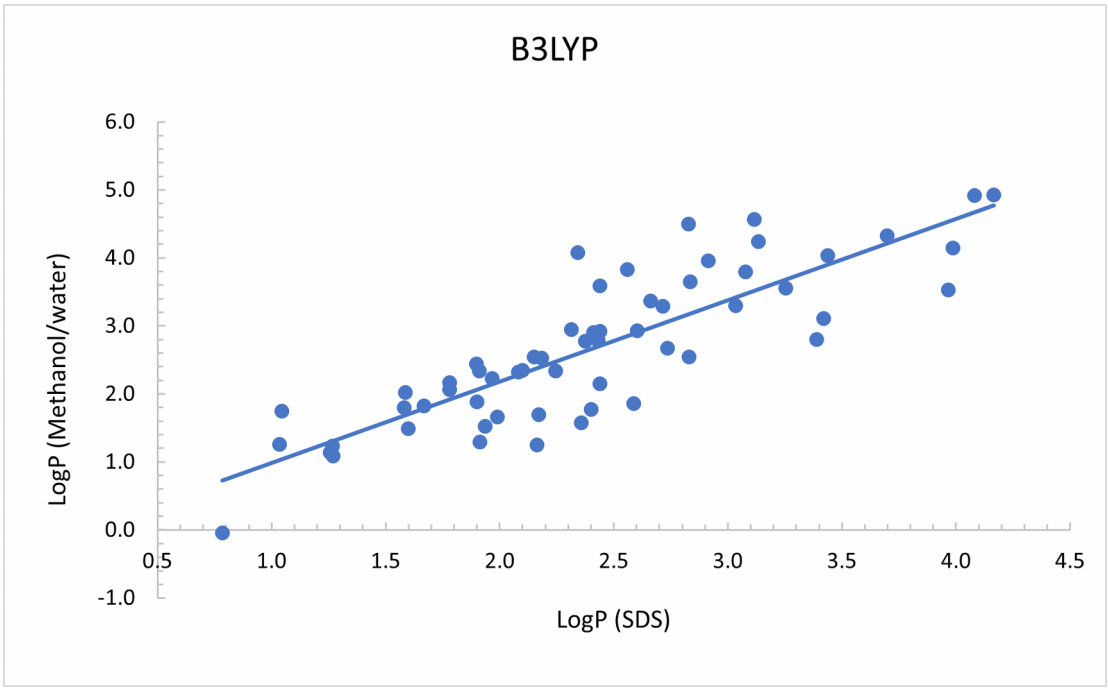


Figure S2. Comparison of the calculated logP in propan-2-ol/water with the experimental logP in SDS micelle system. The (a) shows the B3LYP model results and the (b) shows the M06-2X results.



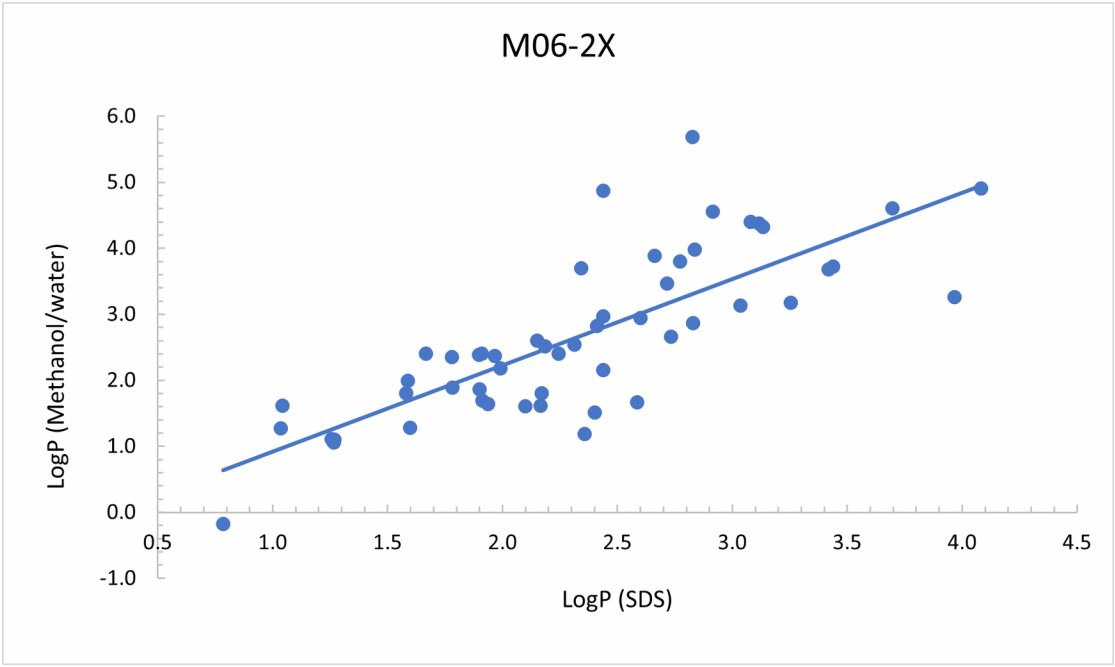


Figure S3. Comparison of the calculated logP in methanol/water with the experimental logP in SDS micelle system. The (a) shows the B3LYP model results and the (b) shows the M06-2X results.

Compound	Log P octanol/water	Log P Propan-1-ol/water	Log P Propan-2-ol/water	Log P Methanol/water
Ethylbenzene	3.03	3.40	3.49	3.28
Propylbenzene	NA	NA	NA	NA
Butylbenzene	4.02	4.48	4.60	4.32
1-phenylethanone	1.58	2.32	2.41	2.31
1-phenylpropan-1-one	2.22	2.95	2.98	2.90
1-phenylbutan-1-one	2.28	3.25	NA	NA
1-phenylpentan-1-one	NA	NA	NA	NA
1-phenylheptan-1-one	3.91	4.80	4.93	4.92
Furan	0.89	1.28	1.43	1.41
2-nitroaniline	0.54	1.43	1.60	1.25
2,3-benzofuran	1.90	2.37	2.54	2.14
Diphenylmethanone	2.88	3.70	3.83	3.55
Benzamide	0.16	1.23	1.25	1.49
4-chloroaniline	1.78	2.48	2.55	2.52
2,3-dimethylphenol	2.60	3.16	3.58	2.94
Naphthalen-2-ol	1.94	2.73	2.88	2.67
4-aminobenzamide	-0.87	0.63	NA	1.08
3-methylphenol	1.57	2.26	2.54	2.23
2,4-dimethylphenol	1.98	2.69	2.79	2.77
Naphthalene	3.01	3.47	3.54	3.29
Pyrimidine	-0.47	0.04	0.14	-0.04
Benzaldehyde	1.38	2.02	2.17	1.88
3-chloroaniline	1.81	2.50	2.57	2.54
Pyrrole	1.20	1.76	1.83	1.74
3-nitroaniline	0.47	1.44	1.64	1.29
4-chlorophenol	1.61	2.31	2.41	2.33
Phenol	1.10	1.77	1.84	1.79
Methylbenzoate	1.003	1.94	2.19	1.77
Bromobenzene	2.73	3.06	3.14	2.92
1,4-xylene	3.17	3.69	3.77	NA
Benzene-1,3-diol	0.16	1.17	1.24	1.23
2-methylaniline	1.73	2.41	2.48	2.43
1-methoxy-2-nitrobenzene	0.80	1.80	NA	1.69
N-4-chlorophenylacetamide	1.76	2.82	2.96	2.78

Aniline	1.32	1.98	2.04	2.022
Nitrobenzene	1.22	1.89	2.08	1.66
Chlorobenzene	2.68	3.03	3.10	2.92
N-phenylacetamide	0.89	2.02	2.15	1.16
4-nitroaniline	-0.22	1.09	1.13	1.52
Anisole	1.92	2.42	2.53	2.34
Benzonitrile	1.77	2.40	2.49	2.33
1-ethyl-4-nitrobenzene	2.13	2.87	3.12	2.54
1-methoxy-4-nitrobenzene	0.88	1.80	2.11	1.57
N,N-diethyl-4-nitroaniline	1.90	3.10	3.31	3.10
Benzyl benzoate	2.26	3.56	3.88	3.53
Caffeine	0.86	1.93	2.14	1.82
Corticosterone	1.49	3.88	3.88	4.14
Cortisone	-0.88	3.09	2.21	2.80
β-Estradiol	3.44	4.78	4.85	4.91
Estriol	2.40	4.03	4.23	4.56
Cortisol	0.48	3.01	3.01	4.03
Hydroquinone	0.05	1.07	1.15	1.28
Quinoline	1.36	1.94	2.004	1.85
Atrazine	3.12	4.06	4.38	3.64
Diuron	2.28	3.61	3.49	3.96
Fluometuron	2.56	3.54	3.66	3.82
Isoproturon	NA	4.54	4.17	4.50
Linuron	2.25	3.70	3.73	3.79
Metobromuron	NA	3.23	NA	3.36
Monuron	1.91	3.47	3.80	4.07
Metoxuron	1.88	3.59	3.89	3.59
Phenyl urea	0.47	1.86	1.85	2.06
Propazine	3.61	4.64	5.03	4.24

Table S1. Predicted partition coefficients for octanol/water, propan-1-ol/water, propan-2-ol/water and methanol/water with B3LYP calculations. NA indicates that partition coefficient could be not calculated because of ausence of true minimum.

Compound	Log P octanol/water	Log P Propan-1-ol/water	Log P Propan-2-ol/water	Log P Methanol/water
Ethylbenzene	2.95	3.39	3.65	3.46
Propylbenzene	3.35	3.82	NA	NA
Butylbenzene	3.92	4.44	4.78	4.60
1-phenylethanone	1.13	1.89	NA	NA
1-phenylpropan-1-one	2.25	2.99	2.88	2.82
1-phenylbutan-1-one	NA	NA	NA	NA
1-phenylpentan-1-one	3.42	4.39	NA	NA
1-phenylheptan-1-one	4.17	4.82	NA	NA
Furan	0.90	1.31	1.39	1.10
2-nitroaniline	0.40	1.33	1.54	1.61
2,3-benzofuran	1.83	2.34	2.52	2.15
Diphenylmethanone	2.57	3.28	3.42	3.17
Benzamide	-0.12	NA	1.01	1.27
4-chloroaniline	1.75	2.49	2.52	2.51
2,3-dimethylphenol	2.34	2.37	3.31	2.53
Naphthalen-2-ol	1.83	2.700	2.82	2.66
4-aminobenzamide	1.44	0.48	0.64	1.09
3-methylphenol	1.42	2.15	2.65	2.36
2,4-dimethylphenol	NA	NA	3.10	NA
Naphthalene	2.92	3.45	3.34	3.13
Pyrimidine	-0.49	0.01	0.01	-0.17
Benzaldehyde	1.34	2.005	2.15	1.26
3-chloroaniline	1.74	2.47	2.60	2.59
Pyrrole	1.21	1.82	1.68	1.61
3-nitroaniline	1.05	2.02	2.02	1.68
4-chlorophenol	1.53	2.27	2.44	2.40
Phenol	1.02	1.74	1.82	1.80
Methylbenzoate	0.82	1.81	1.82	1.51
Bromobenzene	2.75	3.08	3.14	2.94
1,4-xylene	3.70	3.56	NA	3.79
Benzene-1,3-diol	0.05	1.11	0.98	1.06
2-methylaniline	1.67	2.40	2.40	2.38
1-methoxy-2-nitrobenzene	1.01	NA	2.26	1.80

N-4-chlorophenylacetamide	NA	NA	NA	NA
Aniline	1.26	1.98	1.98	1.99
Nitrobenzene	1.54	2.18	2.62	2.17
Chlorobenzene	2.66	3.04	3.14	2.97
N-phenylacetamide	0.82	1.88	2.25	2.34
4-nitroaniline	0.28	1.44	1.69	1.63
Anisole	1.93	2.37	1.74	1.60
Benzonitrile	1.83	2.46	2.56	2.40
1-ethyl-4-nitrobenzene	2.27	3.04	3.44	2.86
1-methoxy-4-nitrobenzene	1.06	1.93	1.74	1.18
N,N-diethyl-4-nitroaniline	2.52	3.59	4.002	3.67
Benzyl benzoate	1.92	3.01	3.69	3.26
Caffeine	1.15	2.49	2.67	2.40
Corticosterone	NA	NA	NA	NA
Cortisone	NA	2.83	2.92	NA
β-Estradiol	3.27	4.64	4.85	4.90
Estriol	2.43	4.16	4.03	4.37
Cortisol	0.72	3.23	2.89	3.71
Hydroquinone	-0.12	0.96	1.09	1.26
Quinoline	1.27	1.89	1.79	1.66
Atrazine	3.37	4.31	4.58	3.97
Diuron	2.35	4.50	4.49	4.55
Fluometuron	NA	NA	NA	NA
Isoproturon	2.89	4.55	5.02	5.68
Linuron	2.35	3.96	4.02	4.39
Metobromuron	2.04	3.12	3.46	3.88
Monuron	2.22	3.63	3.41	3.69
Metoxuron	1.65	4.03	NA	4.87
Phenyl urea	0.38	1.56	1.58	1.88
Propazine	3.57	4.65	4.98	4.32

Table S2. Predicted partition coefficients for octanol/water, propan-1-ol/water, propan-2-ol/water and methanol/water with M06-2X calculations. NA indicates that partition coefficient could be not calculated because of ausence of true minimum.

	Coefficient	Standar Error	P-value	Lower 95%	Upper 95 %	F	Signific ance F	R^2
Calculated logP propan-1-ol/water vs Exp. logP of SDS micelles with B3LYP								
Intercept	-0.21	0.24	0.38	-0.68	0.27			
x	1.19	0.09	1.2E-18	1.01	1.38	163.6	1.2E-18	0.73
Calculated logP propan-1-ol/water vs Exp. logP of SDS micelles with M06-2X								
Intercept	-0.19	0.28	0.50	-0.74	0.37			
x	1.20	0.11	3.0E-15	0.98	1.42	120.3	3.0E-15	0.69
Calculated logP propan-2-ol/water vs Exp. logP of SDS micelles with B3LYP								
Intercept	0.04	0.27	0.87	-0.49	0.58			
x	1.14	0.10	2.1E-15	0.93	1.35	119.4	2.1E-15	0.68
Calculated logP propan-2-ol/water vs Exp. logP of SDS micelles with M06-2X								
Intercept	-0.28	0.30	0.35	-0.89	0.32			
x	1.27	0.12	2.9E-14	1.03	1.52	109.0	2.9E-14	0.68
Calculated logP methanol/water vs Exp. logP of SDS micelles with B3LYP								
Intercept	-0.21	0.25	0.41	-0.72	0.30			
x	1.20	0.10	4.1E-17	0.99	1.40	142.1	4.1E-17	0.71
Calculated logP methanol/water vs Exp. logP of SDS micelles with M06-2X								
Intercept	-0.39	0.35	0.27	-1.10	0.31			
x	1.31	0.14	2.6E-12	1.02	1.60	83.5	2.6E-12	0.62
Calculated logP heptane/water vs Exp. logP of SDS miclles with B3LYP								
Intercept	-1.32	1.15	0.26	-3.62	0.98			
x	0.67	0.45	0.15	-0.24	1.57	2.18	1.5E-01	0.04
Calculated logP heptane/water vs Exp. logP of SDS miclles with M06-2X								
Intercept	-1.99	1.21	0.11	-4.41	0.44			
x	0.92	0.47	0.06	-0.02	1.87	3.83	5.6E-02	0.07
Calculated logP cyclohexane/water vs Exp. logP of SDS miclles with B3LYP								
Intercept	-1.33	1.16	0.26	-3.66	1.00			
x	0.64	0.46	0.16	-0.27	1.55	1.99	1.6E-01	0.03
Calculated logP cyclohexane/water vs Exp. logP of SDS miclles with M06-2X								
Intercept	-1.78	1.19	0.14	-4.18	0.61			
x	0.85	0.46	0.07	-0.08	1.77	3.40	7.1E-02	0.06
Calculated logP N-dodecane/water vs Exp. logP of SDS miclles with B3LYP								
Intercept	-1.86	1.01	0.07	-3.87	0.15			
x	0.90	0.40	0.03	0.10	1.70	5.12	2.7E-02	0.08
Calculated logP N-dodecane/water vs Exp. logP of SDS miclles with M06-2X								
Intercept	-1.65	1.22	0.18	-4.11	0.81			

x	0.73	0.48	0.14	-0.24	1.70	2.28	1.4E-01	0.04
Calculated logP pyridine/water vs Exp. logP of SDS miclles with B3LYP								
Intercept	0.45	0.65	0.50	-0.85	1.75			
x	0.97	0.25	3.2E-04	0.46	1.48	14.57	3.2E-04	0.20
Calculated logP pyridine/water vs Exp. logP of SDS miclles with M06-2X								
Intercept	0.16	0.63	0.80	-1.10	1.43			
x	1.13	0.24	2.4E-05	0.64	1.62	21.65	2.4E-05	0.30
Calculated logP diethyl sulfide/water vs Exp. logP of SDS miclles with B3LYP								
Intercept	0.14	0.78	0.86	-1.41	1.70			
x	0.88	0.30	0.01	0.28	1.49	8.45	5.1E-03	0.12
Calculated logP diethyl sulfide/water vs Exp. logP of SDS miclles with M06-2SX								
Intercept	-0.48	0.81	0.56	-2.09	1.14			
x	1.18	0.31	3.7E-04	0.56	1.80	14.54	3.7E-04	0.22
Calculated logP acetic acid/water vs Exp. logP of SDS miclles with B3LYP								
Intercept	-1.80	0.86	0.04	-3.52	-0.08			
x	0.45	0.34	0.18	-0.22	1.13	1.84	1.8E-01	0.03
Calculated logP acetic acid/water vs Exp. logP of SDS miclles with M06-2X								
Intercept	-2.46	0.84	4.9E-03	-4.14	-0.78			
x	0.74	0.32	0.03	0.09	1.38	5.18	2.7E-02	0.09
Calculated logP decan-1-ol/water vs Exp. logP of SDS miclles with B3LYP								
Intercept	-0.87	0.47	0.07	-1.81	0.08			
x	0.83	0.18	3.1E-05	0.46	1.20	20.39	3.1E-05	0.26
Calculated logP decan-1-ol/water vs Exp. logP of SDS miclles with M06-2X								
Intercept	-1.19	0.48	0.02	-2.16	-0.23			
x	0.99	0.19	5.3E-06	0.60	1.38	25.85	5.3E-06	0.34
Calculated logP octanol/water vs Exp. logP of SDS miclles with B3LYP								
Intercept	-0.53	0.37	0.17	-1.28	0.22			
x	0.91	0.15	8.4E-08	0.61	1.20	37.72	8.4E-08	0.40
Calculated logP octanol/water vs Exp. logP of SDS miclles with M06-2X								
Intercept	-1.00	0.33	4.1E-03	-1.67	-0.33			
x	1.16	0.13	5.0E-12	0.90	1.42	77.57	5.0E-12	0.48
Calculated logP acetone/water vs Exp. logP of SDS miclles with B3LYP								
Intercept	0.94	0.60	0.13	-0.27	2.14			
x	0.88	0.24	4.1E-04	0.41	1.35	14.01	4.1E-04	0.19
Calculated logP acetone/water vs Exp. logP of SDS miclles with M06-2X								
Intercept	0.38	0.57	0.51	-0.77	1.52			
x	1.15	0.22	3.7E-06	0.71	1.59	27.07	3.7E-06	0.35
Calculated logP 1,2-ethane diol/water vs Exp. logP of SDS miclles with B3LYP								
Intercept	-1.33	0.38	9.4E-04	-2.10	-0.57			

x	0.41	0.15	0.01	0.12	0.71	7.71	7.4E-03	0.12
Calculated logP 1,2-ethane diol/water vs Exp. logP of SDS miclles with M06-2X								
Intercept	-1.99	0.43	3.1E-05	-2.87	-1.12			
x	0.73	0.18	1.4E-04	0.37	1.09	17.02	1.4E-04	0.26
Calculated logP dimethyl sulfoxide/water vs Exp. logP of SDS miclles with B3LYP								
Intercept	0.13	0.55	0.81	-0.97	1.24			
x	0.64	0.22	4.4E-03	0.21	1.07	8.79	4.4E-03	0.13
Calculated logP dimethyl sulfoxide/water vs Exp. logP of SDS miclles with M06-2X								
Intercept	-0.57	0.62	0.37	-1.82	0.68			
x	1.00	0.26	2.8E-04	0.49	1.52	15.31	2.8E-04	0.23
Calculated logP formic acid/water vs Exp. logP of SDS miclles with B3LYP								
Intercept	-1.29	0.62	0.04	-2.53	-0.05			
x	0.46	0.24	0.06	-0.03	0.94	3.57	6.4E-02	0.06
Calculated logP formic acid/water vs Exp. logP of SDS miclles with M06-2X								
Intercept	-1.85	0.71	0.01	-3.27	-0.44			
x	0.64	0.27	0.02	0.09	1.19	5.54	2.2E-02	0.10
Experimental logP octanol/water vs calculated logP octanol/water with B3LYP								
Intercept	1.00	0.15	1.4E-08	0.70	1.30			
x	0.67	0.07	1.3E-12	0.52	0.82	82.48	1.3E-12	0.60
Experimental logP octanol/water vs calculated logP octanol/water with M06-2X								
Intercept	0.90	0.15	3.3E-07	0.59	1.22			
x	0.71	0.07	1.3E-13	0.57	0.86	97.54	1.3E-13	0,65

Table S3. Statistical parameters obtained from the linear regressions for B3LYP and M06-2X calculations.

Molecule	Experimental $LogP_{o/w}$
Ethylbenzene	3.15[1]
Propylbenzene	3.69[2]
Butylbenzene	4.38[2]
1-phenylethanone	1.58[3]
1-phenylpropan-1-one	2.19[4]
1-phenylbutan-1-one	2.66[4]
1-phenylpentan-1-one	3.15[5]
1-phenylheptan-1-one	4.13[4]
Furan	1.34[6]
2-nitroaniline	1.85[2]
2,3-benzofuran	1.9[2]
Diphenylmethanone	3.18[7]
Benzamide	0.64[8]
4-chloroaniline	1.83[9]
2,3-dimethylphenol	2.48[10]
Naphthalen-2-ol	2.48[11]
3-methylphenol	1.96[12]
2,4-dimethylphenol	2.3[13]
Naphtalene	3.3[14]
Pyrimidine	1.37[15]
Benzaldehyde	1.48[16]
3-chloroaniline	1.88[17]
1H-pyrrole	0.75[18]
3-nitroaniline	1.37[2]
4-chlorophenol	2.39[19]
Phenol	1.46[20]
Methylbenzoate	2.12[21]
Bromobenzene	2.99[22]
1,4-xylene	3.15[23]
2-methylaniline	1.32[24]
1-methoxy-2-nitrobenzen	1.73[25]
***N*-4-chlorophenylacetamide**	2.41[26]
Aniline	1.24[27]
Nitrobenzene	1.85[28]
Chlorobenzene	2.84[29]
***N*-phenylacetamide**	2.84[9]
4-nitroaniline	1.39[2]
Anisole	2.11[28]
Benzonitrile	1.56[28]
1-ethyl-4-nitrobenzene	3.03[30]
1-methoxy-4-nitrobenzene	2.03[31]
***N,N*-diethyl-4-nitroaniline**	3.55[32]

Benzyl benzoate	3.97[33]
Caffeine	-0.07[34]
Corticosterone	0.94[35]
Cortisone	1.47[36]
b-estradiol	3.5[37]
Estriol	2.45[35]
Cortisol	1.61[38]
Hydroquinone	0.59[39]
Quinoline	2.03[28]
Atrazine	2.61[40]
Diuron	2.68[41]
Fluometuron	2.42[42]
Isoproturon	2.87[43]
Linuron	3.2[44]
Metobromuron	2.32[45]
Monuron	1.94[46]
Metoxuron	1.64[46]
Phenyl urea	0.83[47]
Propazine	2.93[48]

Table S4. List of experimental $LogP_{o/w}$ used in this study.

References of molecules of Table S4:

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Equations of the statistical measures used in the analysis: mean absolute error (**MAE**), mean square error (**MSE**), and root mean square error (**RMSE**) in Eq. S1, S2 and S3, respectively.

$$\mathrm{MAE} = \frac{\sum_{i=1}^{n} |y_i - x_i|}{n} \qquad \text{(S1)}$$

$$\mathrm{MSE} = \frac{\sum_{i=1}^{n} (y_i - x_i)^2}{n} \qquad \text{(S2)}$$

$$\mathrm{RMSE} = \sqrt{\frac{\sum_{i=1}^{n} (y_i - x_i)^2}{n}} \qquad \text{(S3)}$$

where y_i is the prediction, x_i the experimental value and n the number of observations.