

## Supplementary Material

### Designing Thiadiazoloquinoxaline-Based Conjugated Polymers for Efficient Organic Photovoltaics: A DFT/TDDFT Study

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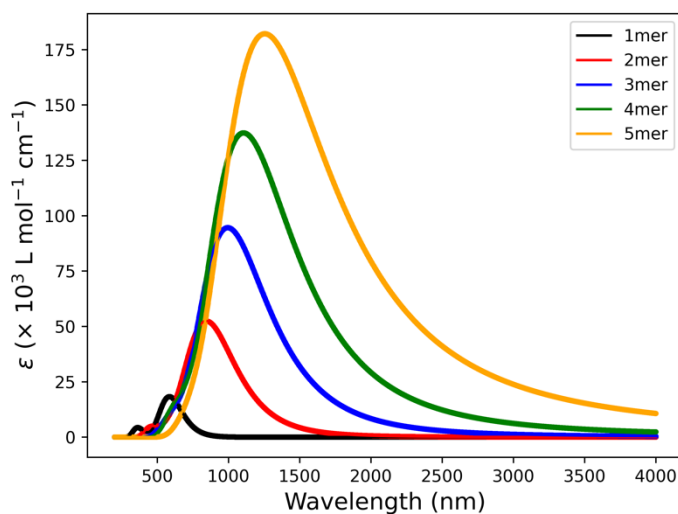
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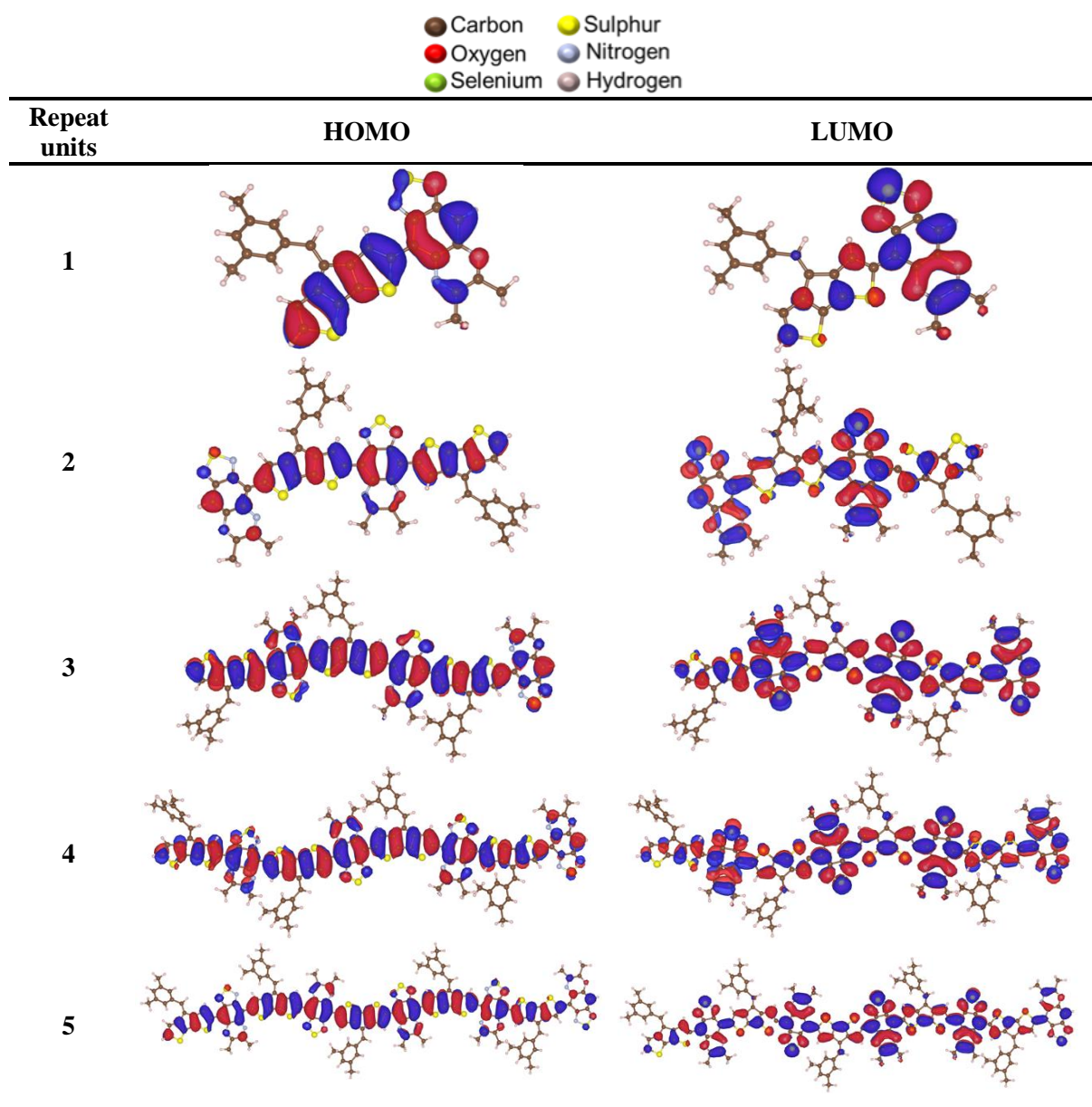
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**Table S1.** Computed at the level of theory B3LYP/6-311G(d,p) for ground state and B3LYP/6-311G(d,p)// CAM-B3LYP/6-311G(d,p) for TDDFT calculations. As we found that atactic and syndiotactic oligomers not affecting DFT and TDDFT results significantly (see Figure 1a), here we reported the results of syndiotactic oligomers.

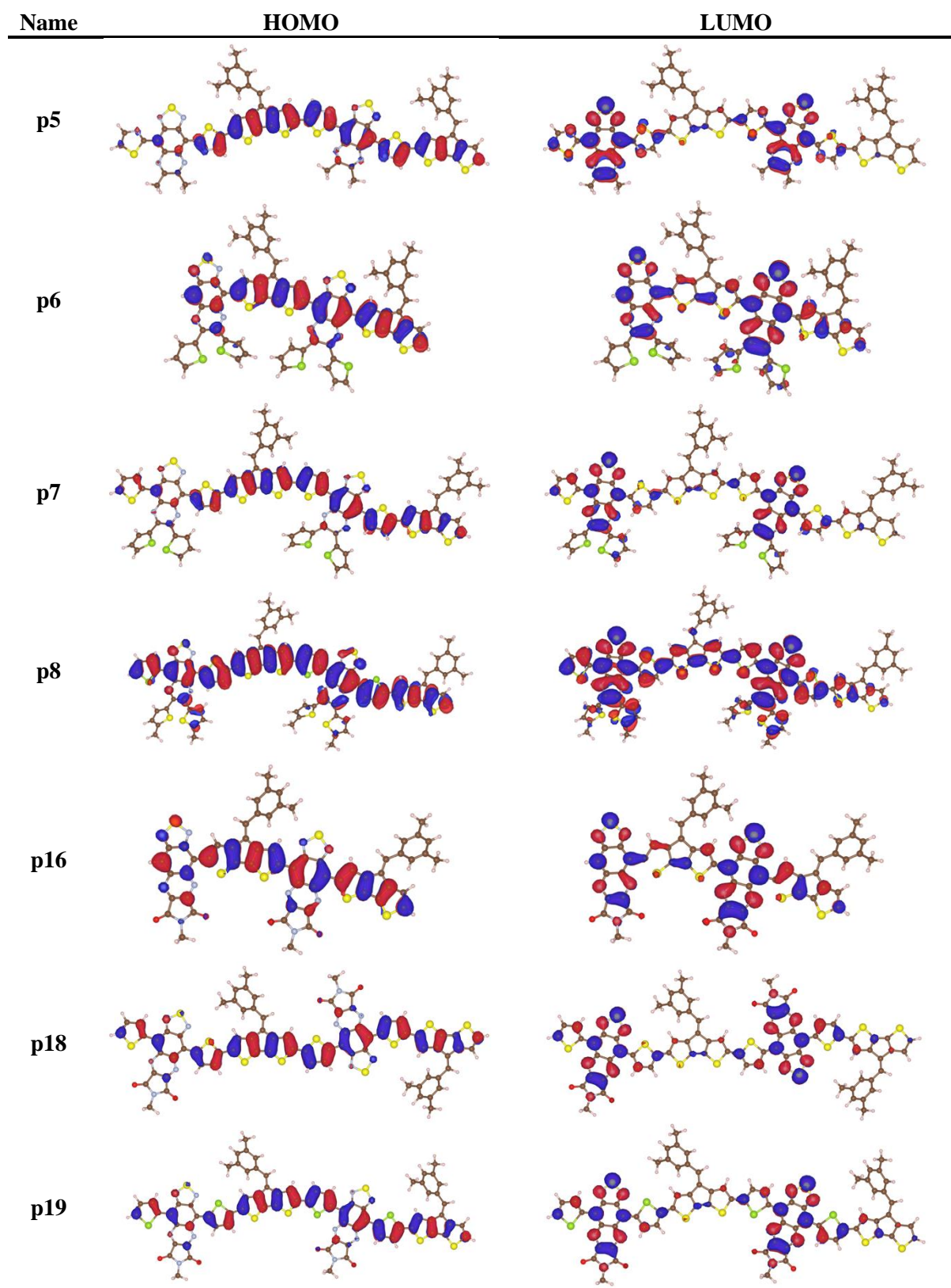
<i>Name</i>	<i>n</i>	$E_{HOMO}$ (eV)	$E_{LUMO}$ (eV)	$E_{gap}$ (eV)	$E_{abs}/\lambda_{max}$ (eV/nm)	$E_b$ (eV)	$\mu_D$ Debye	<i>f</i>	$S_0 \rightarrow S_1$ (major contributions)
<b>ref</b>	1	-5.09	-3.13	1.96	2.12/585.95	0.16	2.92	0.452	H $\rightarrow$ L (95.8%)
	2	-4.62	-3.35	1.27	1.46/851.69	0.19	6.87	1.267	H $\rightarrow$ L (90.1%)
	3	-4.44	-3.44	1.00	1.24/999.11	0.24	6.65	2.312	H $\rightarrow$ L (82.7%)
	4	-4.35	-3.49	0.86	1.12/1110.90	0.28	7.38	3.363	H $\rightarrow$ L (75.7%)
	5	-4.29	-3.55	0.74	0.98/1262.60	0.24	8.58	4.449	H $\rightarrow$ L (71.4%)
	$\infty$			0.52					



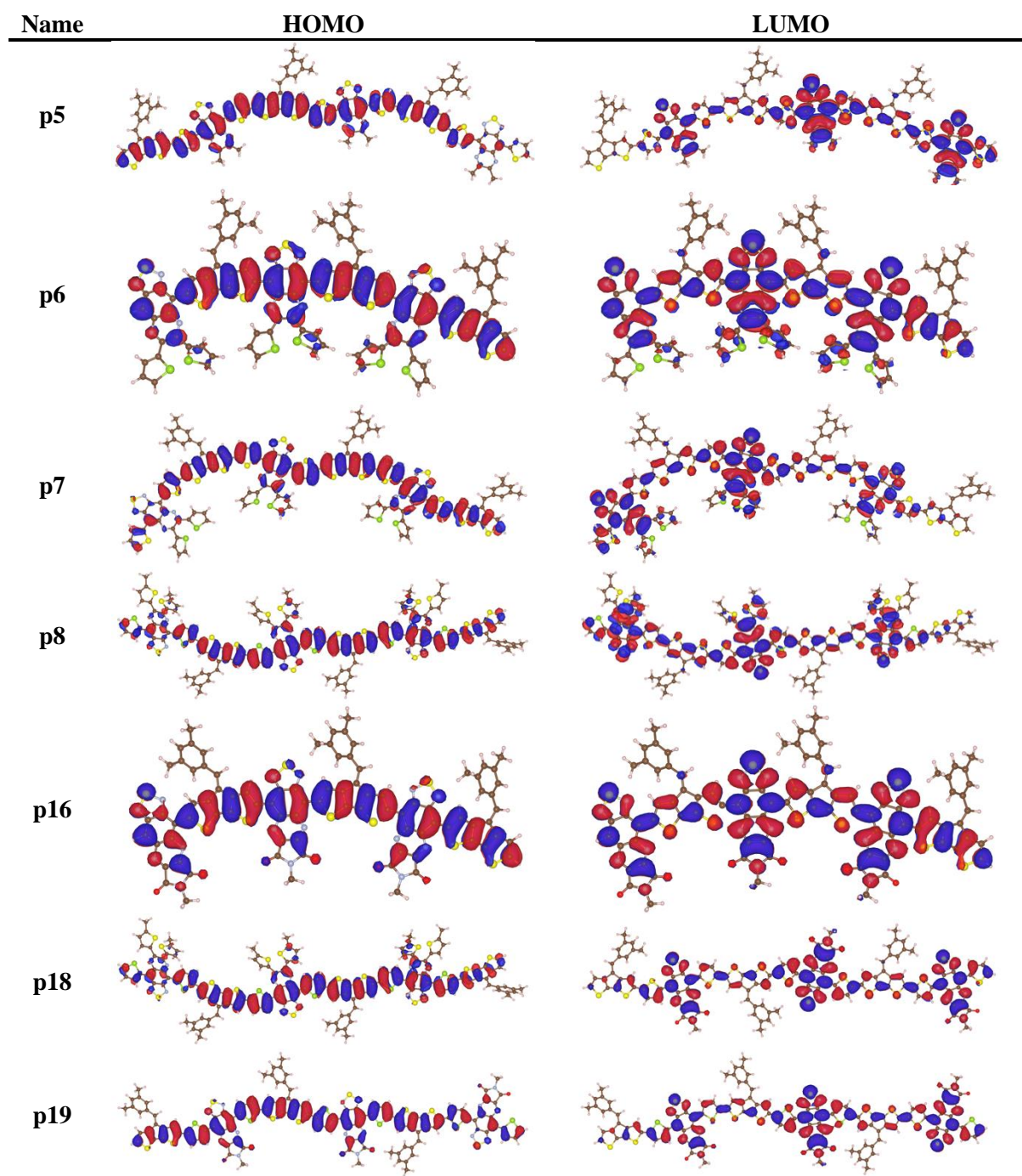
**Figure S1.** Simulated UV-vis absorption spectra of the reference oligomer.



**Figure S2.** Electron density distribution of the reference oilgomer with iso value= 0.01 au.

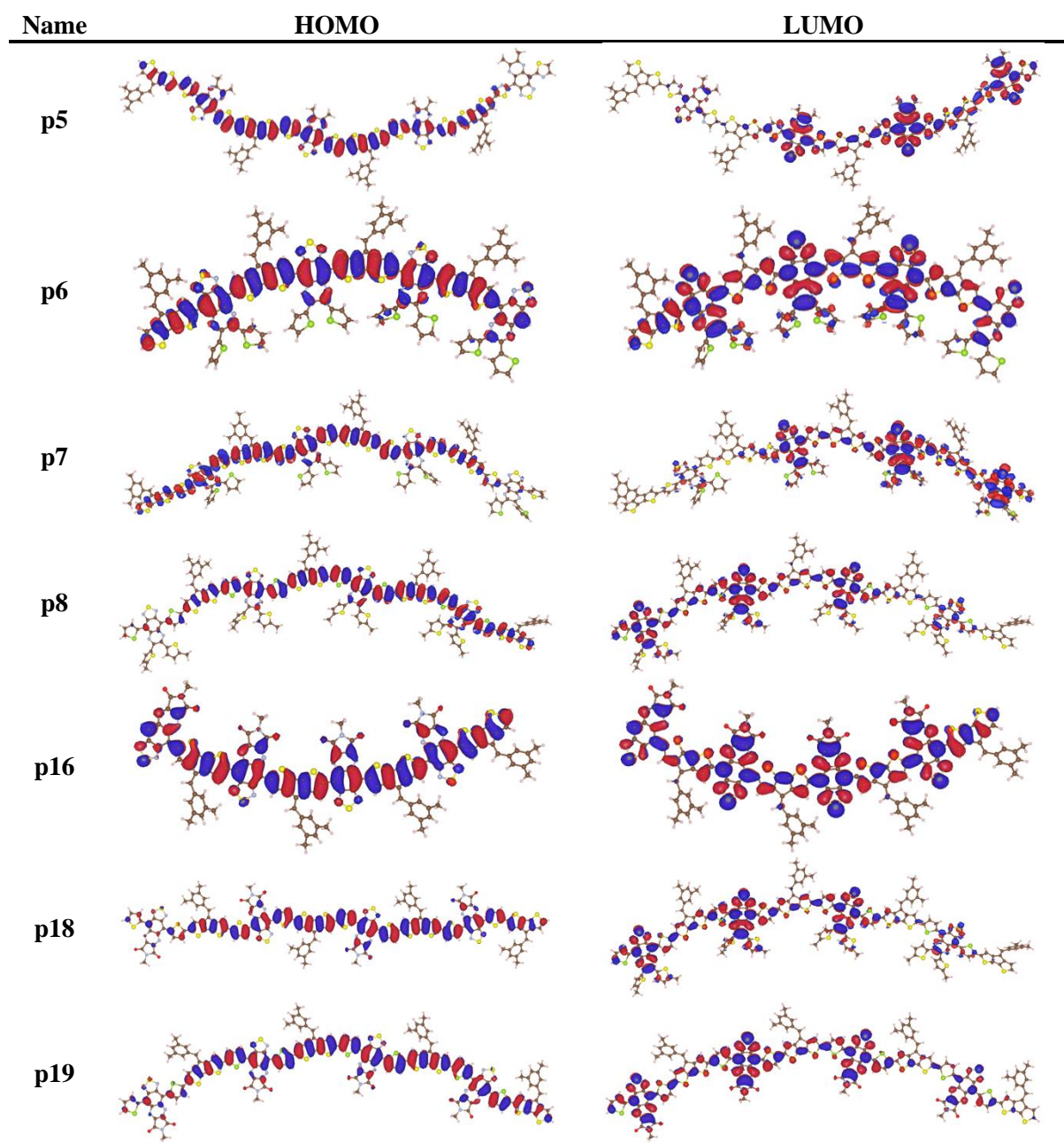


**Figure S3.** Electron density distribution of the designed oligomers, in this figure dimers are depicted.

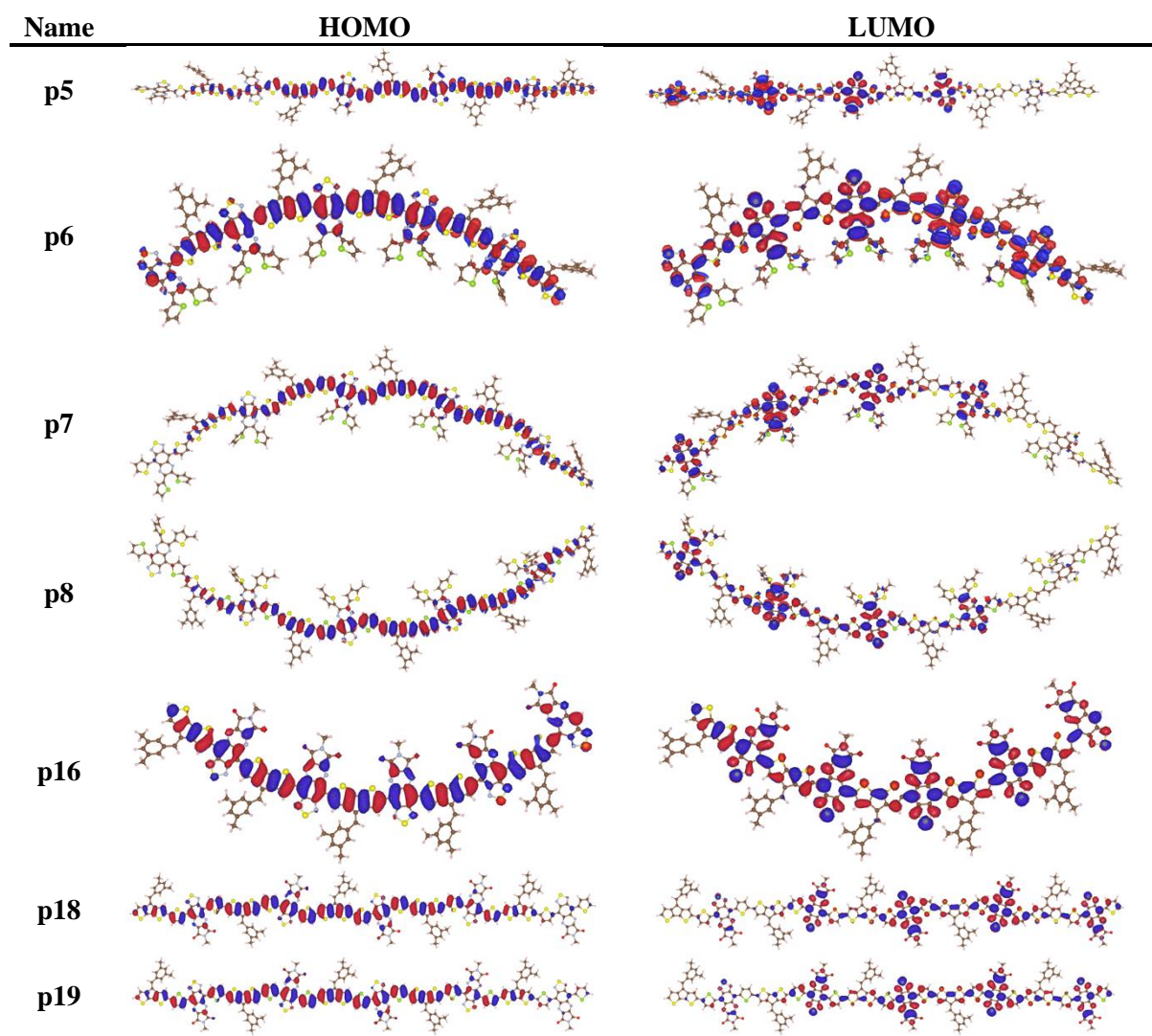


**Figure S4.** Electron density distribution of the designed oligomers, in this figure trimers are depicted.





**Figure S5.** Electron density distribution of the designed oligomers, in this figure tetramers are depicted.



**Figure S6.** Electron density distribution of the designed oligomers, in this figure pentamers are depicted.

Table S2. XYZ coordinates of the ground state geometry of the studied monomers.

p05			
Atom	X	Y	Z
C	-4.269547	1.517282	-0.20601
C	-2.922069	0.950391	-0.21287
C	-3.819559	-1.250518	0.085385
C	-5.155525	-0.697239	0.032432
C	-5.424072	0.676459	-0.1365
N	-1.961419	1.879539	-0.29618
N	-4.261461	2.856377	-0.2713
S	-2.708942	3.329619	-0.34096
N	-6.225112	-1.544667	0.140597
N	-3.658148	-2.574557	0.386661
C	-6.040491	-2.816734	0.349705
C	-4.699546	-3.342343	0.526869
C	3.387572	-0.4089	-0.08993
C	4.748668	-0.787714	-0.02859
C	4.914334	-2.171139	-0.11801
S	3.418342	-3.014823	-0.2362
C	6.315911	-2.480477	-0.16827
C	7.032428	-1.291525	-0.12096
C	6.089952	-0.157329	-0.01695
C	6.47792	1.137851	0.027378
S	7.34608	-3.862269	-0.25412
C	8.757141	-2.827602	-0.22579
C	8.436868	-1.499452	-0.14894
C	5.328909	4.708412	-0.2832
C	6.041918	3.523398	-0.4494
C	5.680991	2.350246	0.233474
C	4.611577	2.40228	1.13819
C	3.894031	3.582286	1.342106
C	4.25698	4.719305	0.615966
C	5.687414	5.948652	-1.06641
H	6.708798	5.897258	-1.44904
H	5.019494	6.07538	-1.92508
H	5.600222	6.84752	-0.45089
C	2.777126	3.638153	2.357545
H	2.251815	2.68318	2.428323
H	3.166861	3.872065	3.354179
H	2.046428	4.408608	2.102222
S	0.127797	-0.088708	0.137035
C	1.088123	-1.483565	-0.27498
C	-1.34096	-1.008053	-0.26347
C	0.240626	-2.493947	-0.69333
C	2.525757	-1.483101	-0.20107



C	-2.675967	-0.44955	-0.12746
C	-6.772669	1.225308	-0.24577
C	-9.174747	1.722219	-0.28563
C	-8.339583	2.766003	-0.56439
S	-8.264161	0.286747	0.012454
H	-8.656002	3.773521	-0.80031
H	-10.25369	1.715994	-0.257
H	9.185667	-0.718982	-0.11742
H	9.736151	-3.278667	-0.27046
H	3.030794	0.610789	-0.07962
H	0.577945	-3.459605	-1.04839
H	4.36422	1.520424	1.717282
H	6.883239	3.497857	-1.13518
H	3.700961	5.640657	0.764615
H	7.540709	1.319313	-0.11955
N	-1.082404	-2.225727	-0.67976
C	-4.469245	-4.780771	0.901219
H	-4.94482	-5.027041	1.856379
H	-4.888029	-5.458742	0.150598
H	-3.398087	-4.957512	0.979913
C	-7.245809	-3.711115	0.428883
H	-7.200867	-4.496955	-0.33195
H	-7.304098	-4.211754	1.400512
H	-8.149757	-3.123816	0.277761
N	-7.010105	2.480238	-0.53792
<b>p06</b>			
C	1.011304	4.368437	-0.33243
C	-0.050543	3.368063	-0.21675
C	0.248266	1.962656	-0.09533
C	1.635728	1.657513	-0.09365
C	2.671158	2.666819	-0.18472
C	2.36672	4.012145	-0.31253
N	-1.270576	3.920034	-0.24815
N	0.548492	5.625813	-0.44403
S	-1.07773	5.53388	-0.40655
N	3.986526	2.299306	-0.10117
N	2.008901	0.352174	-0.04939
C	4.311937	1.033455	0.001825
C	3.271127	0.00822	-0.0379
C	-0.788984	0.96031	0.002585
C	-2.167265	1.181072	0.020081
C	-2.920924	0.007502	0.139998
C	-2.126505	-1.134862	0.208704
S	-0.441989	-0.792727	0.124978
C	-2.990726	-2.273541	0.318448
C	-4.323665	-1.853785	0.311112

C	-4.348964	-0.379529	0.18188
C	-5.368251	0.508844	0.140248
S	-2.835575	-3.975106	0.557365
C	-4.573037	-4.130657	0.667824
C	-5.22284	-2.934948	0.526091
C	-8.749179	-0.924934	-0.80516
C	-7.368999	-0.753512	-0.71311
C	-6.813209	0.278465	0.059405
C	-7.68061	1.162525	0.718007
C	-9.065161	1.001453	0.661717
C	-9.582253	-0.047607	-0.10236
C	-9.338529	-2.009066	-1.67666
C	-9.981684	1.927357	1.425609
H	-10.16519	-2.518341	-1.17403
H	-9.73291	-1.591563	-2.60909
H	-8.590055	-2.758232	-1.94204
H	-7.261549	1.980127	1.296725
H	-6.712425	-1.401285	-1.28128
H	-6.297575	-2.846182	0.583268
H	-5.002712	-5.107468	0.827238
H	-2.574301	2.176717	-0.04937
H	3.150713	4.753072	-0.37479
H	-10.65933	-0.174863	-0.16636
H	-9.546802	2.924366	1.526168
H	-10.95023	2.027842	0.930572
H	-10.16765	1.548078	2.436282
H	-5.08198	1.557893	0.176203
C	5.742156	0.75501	0.188279
C	6.751131	1.62168	-0.15343
C	8.133735	0.063087	0.925776
C	8.062039	1.237672	0.235564
H	6.530149	2.544234	-0.67351
H	9.016758	-0.420534	1.316074
H	8.937102	1.832999	0.004919
C	3.551174	-1.440903	-0.08877
C	3.157539	-2.386601	0.815769
C	4.074454	-3.900839	-0.73195
C	3.459501	-3.738822	0.471391
H	2.651119	-2.112534	1.733168
H	4.389498	-4.82346	-1.19548
H	3.214369	-4.573138	1.117222
Se	4.359702	-2.264631	-1.59551
Se	6.455135	-0.732188	1.129366
<b>p07</b>			
C	-1.78953	3.3252	0.088399
C	-0.685785	2.370174	-0.01716

C	-2.231609	0.550896	0.034987
C	-3.326754	1.504252	0.028942
C	-3.160476	2.907046	0.069361
N	0.514765	2.960467	-0.01454
N	-1.357273	4.591099	0.166187
S	0.271441	4.567444	0.11287
N	-4.592576	1.013679	-0.08109
N	-2.519105	-0.757855	0.239312
C	-4.838688	-0.267502	-0.02633
C	-3.759276	-1.191772	0.294875
C	4.942737	-0.59672	-0.20383
C	6.1855	-1.266054	-0.14214
C	6.042837	-2.652042	-0.24011
S	4.397131	-3.144229	-0.3632
C	7.342275	-3.260858	-0.2891
C	8.302796	-2.258783	-0.22938
C	7.632419	-0.945775	-0.11972
C	8.296598	0.231459	-0.05851
S	8.044667	-4.834543	-0.3843
C	9.648709	-4.135341	-0.34299
C	9.627231	-2.769923	-0.25532
C	8.000906	3.972186	-0.33319
C	8.427132	2.658238	-0.50342
C	7.787713	1.589797	0.148967
C	6.732983	1.875121	1.025604
C	6.292042	3.185644	1.225643
C	6.929977	4.217561	0.53484
C	8.666435	5.109881	-1.07016
H	9.629559	4.80672	-1.48545
H	8.042766	5.457386	-1.90055
H	8.835594	5.965533	-0.41108
C	5.144611	3.471329	2.16557
H	4.185633	3.207603	1.70718
H	5.232078	2.890835	3.087535
H	5.103903	4.528852	2.434086
S	1.894275	0.45794	0.077637
C	2.46272	-1.132079	-0.3753
C	0.216686	0.033503	-0.27525
C	1.406619	-1.925097	-0.78884
C	0.163012	-1.277756	-0.73225
C	3.863297	-1.453526	-0.31753
C	-0.877586	0.958029	-0.09537
C	-4.263605	3.855779	0.072275
C	-6.4757	5.034422	-0.00806
C	-4.181552	5.235389	0.195219
C	-5.428988	5.898701	0.150976

S	-5.961958	3.388108	-0.10321
H	-3.239414	5.743698	0.313899
H	-5.539294	6.971994	0.233398
H	-7.527985	5.267728	-0.0784
H	10.528865	-2.173001	-0.21471
H	10.504978	-4.789965	-0.38898
H	4.820403	0.476399	-0.19391
H	1.5356	-2.935767	-1.15409
H	-0.762285	-1.737679	-1.03794
H	6.278931	1.068536	1.588714
H	9.263797	2.448906	-1.16282
H	6.598345	5.240517	0.688632
H	9.374629	0.173282	-0.19461
C	-6.223674	-0.684239	-0.31912
C	-7.362991	-0.272	0.31337
C	-8.451097	-1.507932	-1.36531
C	-8.587901	-0.738777	-0.25032
H	-7.32147	0.366929	1.186647
H	-9.231969	-1.96133	-1.95691
H	-9.554443	-0.49631	0.174222
C	-3.942663	-2.56728	0.765703
C	-2.915822	-3.456538	0.988044
C	-4.609034	-4.838976	1.83944
C	-3.279971	-4.702154	1.560874
H	-1.894082	-3.18775	0.757292
H	-5.108088	-5.69265	2.273278
H	-2.55685	-5.481599	1.7681
Se	-6.655009	-1.742766	-1.83521
Se	-5.585697	-3.323911	1.349743
<b>p08</b>			
C	-2.175324	3.114629	-0.19102
C	-0.995658	2.253132	-0.23893
C	-2.370714	0.313357	-0.02462
C	-3.545198	1.165552	-0.08315
C	-3.504661	2.577667	-0.1633
N	0.149104	2.941544	-0.28564
N	-1.853547	4.414989	-0.20639
S	-0.228587	4.52972	-0.26933
N	-4.765112	0.560452	-0.12408
N	-2.538606	-0.994092	0.287562
C	-4.897727	-0.728837	0.041822
C	-3.736159	-1.525301	0.407562
C	5.009686	-0.529879	-0.21478
C	6.261972	-1.176825	-0.29676
C	6.138725	-2.517342	-0.67118
S	4.501736	-2.998143	-0.89788

C	7.44568	-3.084899	-0.84123
C	8.392864	-2.101519	-0.58264
C	7.70473	-0.847861	-0.20845
C	8.353393	0.300969	0.090971
S	8.169146	-4.597442	-1.25161
C	9.763557	-3.897908	-1.07256
C	9.723805	-2.578152	-0.71252
C	7.988732	4.012953	0.595842
C	8.436609	2.769832	0.153585
C	7.827962	1.578424	0.580045
C	6.783649	1.655221	1.512704
C	6.329872	2.885449	1.990398
C	6.933389	4.052105	1.512884
C	8.611609	5.289963	0.084263
H	9.618192	5.115782	-0.3017
H	8.016238	5.716941	-0.72992
H	8.675801	6.045222	0.871437
C	5.239813	2.952362	3.033949
H	4.563684	2.097864	2.96257
H	5.665313	2.950843	4.043347
H	4.646168	3.86354	2.930989
C	2.536205	-1.057004	-0.48497
C	0.119597	0.010086	-0.35705
C	1.47633	-1.915299	-0.70507
C	0.193049	-1.345754	-0.63855
C	3.937689	-1.360059	-0.49613
C	-1.057479	0.826869	-0.21641
C	-4.687947	3.41383	-0.23567
C	-7.056705	4.497747	-0.44956
C	-4.740006	4.795574	-0.22507
C	-6.026465	5.383655	-0.33922
Se	1.89646	0.708657	-0.19707
Se	-6.465355	2.720184	-0.40616
H	1.620475	-2.967738	-0.92148
H	-0.701309	-1.925389	-0.80333
H	-3.843179	5.387829	-0.13515
H	-6.168299	6.458071	-0.33899
H	-8.107447	4.729539	-0.54974
H	4.87463	0.511705	0.038514
H	10.617539	-1.989091	-0.55407
H	10.628599	-4.517651	-1.24997
H	9.261531	2.718744	-0.55051
H	6.349257	0.740661	1.89837
H	6.583423	5.014551	1.875475
H	9.43135	0.28781	-0.05712
C	-3.791543	-2.869512	0.985292



C	-2.697802	-3.671633	1.230925
S	-5.238798	-3.623818	1.637255
C	-3.011387	-4.873248	1.906397
H	-1.699197	-3.372826	0.947628
C	-4.342921	-5.000844	2.209515
H	-2.276947	-5.623885	2.170186
C	-6.244058	-1.2922	-0.17307
C	-7.414046	-0.933909	0.440751
S	-6.552314	-2.464914	-1.43813
C	-8.551304	-1.616782	-0.07177
H	-7.448651	-0.207768	1.241573
C	-8.262028	-2.477835	-1.09499
H	-9.556842	-1.473386	0.303336
C	-5.029275	-6.128662	2.917144
H	-5.537194	-5.789579	3.824912
H	-5.778233	-6.611098	2.281804
H	-4.296074	-6.88438	3.205169
C	-9.20249	-3.342295	-1.87835
H	-9.195623	-3.088609	-2.94252
H	-8.950086	-4.40305	-1.79017
H	-10.22063	-3.20688	-1.50841
<b>p16</b>			
C	-2.943265	3.65388	0.123329
C	-1.771268	2.782665	0.073732
C	-1.897897	1.343879	0.029785
C	-3.242752	0.870358	0.038245
C	-4.400639	1.7688	0.087802
C	-4.249743	3.140511	0.130013
N	-0.626835	3.476594	0.07482
N	-2.635787	4.960604	0.160071
S	-1.010128	5.062619	0.133493
N	-5.692361	1.267442	0.09409
N	-3.43277	-0.477279	-0.00181
C	-5.78218	-0.022169	0.053568
C	-4.661388	-0.897508	0.005751
C	-5.155555	-2.307001	-0.03103
C	-7.028447	-0.865782	0.04806
N	-6.560635	-2.189749	-0.00282
O	-8.186624	-0.540564	0.078842
O	-4.541838	-3.342952	-0.07499
C	-7.45496	-3.335956	-0.02431
C	-0.751929	0.472058	-0.01756
C	0.593459	0.861551	-0.02138
C	1.485324	-0.209611	-0.08174
C	0.836047	-1.446325	-0.11535
S	-0.878015	-1.315658	-0.08002

C	1.832534	-2.470968	-0.16817
C	3.105412	-1.888797	-0.1579
C	2.949963	-0.419586	-0.09095
C	3.85266	0.588107	-0.08358
S	1.890764	-4.187427	-0.33384
C	3.634137	-4.130006	-0.40769
C	4.13315	-2.859035	-0.30864
C	7.373514	-0.369821	0.946097
C	5.983748	-0.374538	0.841277
C	5.313599	0.540954	0.014367
C	6.071252	1.49012	-0.68736
C	7.464647	1.502984	-0.61957
C	8.098605	0.566193	0.20022
C	8.08613	-1.329017	1.870297
C	8.268584	2.493075	-1.42812
H	-8.102682	-3.293493	-0.90191
H	-8.079983	-3.343728	0.870489
H	-6.839663	-4.233128	-0.05793
H	8.92934	-1.811526	1.368311
H	8.485671	-0.80695	2.745809
H	7.414081	-2.110539	2.229746
H	5.560174	2.21921	-1.30873
H	5.405967	-1.067448	1.44098
H	5.19021	-2.643162	-0.3515
H	4.183703	-5.052083	-0.51833
H	0.874503	1.901252	0.017398
H	-5.115179	3.786363	0.166447
H	9.182497	0.576074	0.27431
H	7.710475	3.416837	-1.5962
H	9.205654	2.748511	-0.92833
H	8.522757	2.080738	-2.41056
H	3.440523	1.59127	-0.17076
<b>p18</b>			
C	-3.40641	2.192734	-0.02131
C	-2.187157	1.385784	-0.01007
C	-3.478145	-0.625745	-0.02738
C	-4.70261	0.191222	-0.03693
C	-4.71414	1.606195	-0.03639
N	-1.078007	2.129503	0.00565
N	-3.143129	3.506436	-0.01455
S	-1.525839	3.695139	0.003934
N	-5.92739	-0.421806	-0.04772
N	-3.579751	-1.987364	-0.02893
C	-5.948251	-1.716042	-0.04901
C	-4.771666	-2.498456	-0.03952
C	-5.15863	-3.943874	-0.04339

C	-7.130649	-2.640195	-0.05912
N	-6.567801	-3.929898	-0.05502
O	-8.310103	-2.398884	-0.06871
O	-4.466228	-4.930102	-0.03844
C	-7.376891	-5.138071	-0.06261
C	3.830083	-0.534242	-0.01304
C	5.175191	-0.952815	0.031998
C	5.292658	-2.347068	0.05637
S	3.768698	-3.145188	0.05851
C	6.678863	-2.706841	-0.00738
C	7.435742	-1.542532	-0.08064
C	6.536111	-0.371034	-0.04464
C	6.967296	0.909541	-0.11434
S	7.660502	-4.126707	-0.00915
C	9.103432	-3.14263	-0.10905
C	8.830242	-1.801675	-0.13368
C	5.941819	4.486427	-0.67328
C	6.606285	3.266617	-0.76334
C	6.216221	2.161125	0.012113
C	5.168091	2.320693	0.927795
C	4.492419	3.537336	1.04972
C	4.885744	4.6035	0.238712
H	-8.003859	-5.167508	-0.95562
H	-8.021507	-5.166594	0.817756
H	-6.698034	-5.988853	-0.05551
C	6.339099	5.65695	-1.5405
H	7.32343	5.505873	-1.98789
H	5.623297	5.800654	-2.3567
H	6.367004	6.586347	-0.96563
C	3.357794	3.686278	2.035802
H	2.442874	3.218898	1.656229
H	3.593935	3.205948	2.988655
H	3.136384	4.7372	2.232313
S	0.649068	-0.0026	0.007413
C	1.493015	-1.532827	-0.00282
C	-0.939934	-0.798939	-0.01274
C	0.590567	-2.585774	-0.01942
C	-0.746579	-2.182493	-0.02446
C	2.925511	-1.583998	0.004613
C	-2.174952	-0.048549	-0.01656
C	-5.928857	2.407475	-0.04963
C	-8.269348	3.303024	-0.07358
C	-6.012235	3.794741	-0.0543
C	-7.331179	4.298148	-0.06784
S	-7.564988	1.72839	-0.06298
H	-5.137067	4.421779	-0.04804

H	-7.569236	5.353576	-0.07317
H	-9.344946	3.401693	-0.08377
H	9.60521	-1.048703	-0.18925
H	10.065502	-3.629622	-0.1445
H	3.508839	0.495594	-0.06645
H	0.891078	-3.625475	-0.03034
H	-1.574201	-2.87015	-0.03754
H	4.906006	1.497962	1.582383
H	7.436246	3.159804	-1.45497
H	4.37103	5.555632	0.331166
H	8.030861	1.041263	-0.30264
<b>p19</b>			
C	-3.31978	2.092269	-0.13461
C	-2.054615	1.363132	-0.11231
C	-3.213571	-0.725744	-0.02213
C	-4.486481	0.01325	-0.04365
C	-4.58896	1.424853	-0.10032
N	-0.993358	2.171582	-0.15037
N	-3.138109	3.418382	-0.18899
S	-1.535708	3.708424	-0.21
N	-5.669155	-0.676171	-0.0079
N	-3.228034	-2.088935	0.033352
C	-5.608756	-1.968897	0.044063
C	-4.385727	-2.674609	0.064652
C	-4.681619	-4.13983	0.126157
C	-6.731015	-2.963279	0.092101
N	-6.089889	-4.213774	0.13865
O	-7.923146	-2.79248	0.093299
O	-3.929882	-5.080782	0.159232
C	-6.821629	-5.469103	0.194586
C	4.254615	-0.470811	-0.00751
C	5.588431	-0.922505	0.009549
C	5.67231	-2.319713	-0.0277
S	4.130736	-3.081138	-0.05229
C	7.048616	-2.708679	-0.11685
C	7.8332	-1.560531	-0.14481
C	6.962635	-0.370686	-0.04986
C	7.424419	0.900821	-0.06386
S	7.995566	-4.150277	-0.18799
C	9.460975	-3.197439	-0.25559
C	9.220463	-1.850384	-0.21957
C	6.476813	4.522093	-0.44745
C	7.109413	3.292664	-0.60341
C	6.705462	2.162939	0.129754
C	5.677814	2.305703	1.070164
C	5.03733	3.533254	1.261622

C	5.44096	4.623799	0.490186
H	-7.460461	-5.573712	-0.68425
H	-7.448039	-5.502007	1.087858
H	-6.090572	-6.275041	0.222092
C	6.884518	5.719965	-1.27129
H	7.850938	5.561781	-1.75384
H	6.150668	5.92231	-2.0585
H	6.956463	6.620277	-0.65535
C	3.944615	3.669833	2.295799
H	3.102372	3.00718	2.074736
H	4.309992	3.405304	3.292528
H	3.564025	4.691947	2.33925
C	1.894162	-1.411172	-0.02758
C	-0.666012	-0.722428	-0.04054
C	0.978005	-2.448541	0.010345
C	-0.373677	-2.084062	0.004143
C	3.321201	-1.497048	-0.02973
C	-1.948653	-0.066335	-0.05681
C	-5.852938	2.137194	-0.12189
C	-8.321564	2.990674	-0.14096
C	-6.035307	3.509234	-0.17818
C	-7.374858	3.971833	-0.18854
Se	0.98997	0.256593	-0.086
Se	-7.566946	1.279159	-0.07457
H	1.280956	-3.488522	0.048526
H	-1.163644	-2.816328	0.034453
H	-5.196434	4.185553	-0.21233
H	-7.617733	5.02698	-0.23127
H	-9.394319	3.121599	-0.13928
H	3.961158	0.568961	-0.00746
H	10.013169	-1.114579	-0.24804
H	10.410773	-3.705211	-0.3195
H	7.922865	3.196363	-1.31586
H	5.404606	1.459473	1.689672
H	4.950607	5.582403	0.633313
H	8.489559	1.015767	-0.25433

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