Supporting Information

Machine Learning with Quantum Chemistry Descriptors: Predicting the Solubility of Small Molecular Optoelectronic Materials for Organic Solar Cells

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Table S1. Calculated surface descriptors of 473 substances. The geometries of these substances were optimized at the B3LYP/def2-TZVP level, and the single point energy was calculated with B3LYP/def2-TZVPD level. Multiwfn[1] was used to calculate the surface descriptors based on the wavefunction generated by the single point energy calculations

No.	Substance	Area	σ^2_+	σ^2_-	σ^2_{tot}	υ
1	xylenes	167.5671	9.52252	24.22332	33.74584	0.202556
2	Xanthene	219.9829	15.76467	16.18796	31.95263	0.249956
3	Water	46.24771	139.8836	89.23064	229.1143	0.237781
4	Undecanoicacid	286.9328	32.29905	136.5167	168.8157	0.154721
5	Undecane	275.7186	2.54883	0.78434	3.33317	0.179941
6	Triphenylene	258.7008	21.36884	12.09075	33.45959	0.230777
7	Triiodomethane	162.7789	63.65142	2.4463	66.09772	0.035641
8	Tridecanoicacid	329.4076	29.24068	129.0009	158.2416	0.15064
9	Tricosane	530.5632	2.1839	0.89766	3.08156	0.206444
10	Trichloromethane	119.4214	84.41003	3.93846	88.34849	0.042591
11	Trichlorofluoromethane	122.9943	25.91562	1.03724	26.95286	0.037002
12	Trichloroethene	132.2633	43.85065	3.35059	47.20124	0.065946
13	Tribromomethane	136.8341	71.19675	3.30629	74.50305	0.042409
14	Tribromofluoromethane	140.2042	38.44271	0.82206	39.26477	0.020498
15	trans-Decahydronaphthalene	199.1622	2.45242	0.77167	3.22409	0.182058
16	trans-1,3-Dichloro-1-propene	138.6781	66.0307	9.21349	75.24419	0.107454
17	trans-1,2-Diiodoethene	148.0084	48.83611	2.43506	51.27117	0.045238

18	trans-1,2-Dichloroethene	116.1938	53.23279	3.52379	56.75658	0.058231
19	toluene	146.9636	10.94329	20.81181	31.7551	0.225856
20	Thioxanthene	229.2353	18.82553	13.7566	32.58212	0.243949
21	Thianthrene	231.7227	22.81093	16.2768	39.08772	0.243014
22	Tetrahydrothiophene	131.8872	7.89461	46.69437	54.58898	0.123704
23	Tetradecanoicacid	350.7202	27.94884	124.7346	152.6834	0.149543
24	Tetradecanenitrile	341.8643	25.51845	194.1699	219.6883	0.102665
25	Tetradecanamine	355.1085	11.11269	65.12176	76.23445	0.124521
26	Tetradecafluorohexane	217.0567	12.38521	0.09143	12.47664	0.007274
27	Tetrachloromethane	134.6648	26.72788	0.6178	27.34568	0.022082
28	Tetrachloroethylene	147.7432	19.20889	1.0506	20.2595	0.049168
29	Tetrachloroethene	147.7432	19.20889	1.0506	20.2595	0.049168
30	Tetrabromomethane	156.0512	40.44613	1.03468	41.48081	0.024321
31	tert-Butylbenzene	195.7027	11.53264	24.30062	35.83326	0.21826
32	Sulfurdioxide	75.37469	80.2052	25.13472	105.3399	0.181673
33	Styrene	159.2175	17.12376	15.29542	32.41918	0.249205
34	Sodiumiodide	91.46274	2107.874	68.38591	2176.259	0.030436
35	Sodiumformate	84.71973	1701.21	182.689	1883.899	0.08757
36	Sodiumbromide	80.6697	2063.829	111.971	2175.8	0.048814
37	Silicontetrachloride	148.2244	12.30146	0.07102	12.37248	0.005707
38	sec-Butylbenzene	197.4407	9.51095	25.22685	34.7378	0.19883
39	Rubidiumiodide	110.5285	555.3587	119.0289	674.3876	0.145347
40	Rubidiumformate	102.8214	383.289	169.5756	552.8646	0.212644
41	Pyridine	121.5259	29.77913	103.1887	132.9679	0.1738
42	Pyrene	231.4533	18.17322	10.50097	28.67419	0.232102
43	p-Xylene	167.713	9.64311	24.20368	33.84678	0.203734
44	Propyloctadecanoate	502.8625	5.90862	117.7737	123.6823	0.04549
45	Propylenecarbonate	134.5647	46.50957	133.08	179.5895	0.191908
46	Propylbenzene	186.7148	8.0598	24.1858	32.2456	0.187475
47	Propanedioicacid	129.7756	155.1828	77.47602	232.6588	0.222112
48	Propane	105.7867	3.68359	0.59499	4.27858	0.119724
49	Potassiumiodide	103.7706	828.4055	107.6317	936.0372	0.101765
50	Potassiumformate	96.17518	580.1662	167.3752	747.5414	0.173769
51	Phenanthrene	217.8076	18.63301	12.52612	31.15913	0.240397

52	Perylene	272.5944	21.02177	10.50224	31.52402	0.222161
53	Pentanedioicacid	170.7559	95.49429	103.7912	199.2855	0.249567
54	Pentane	148.2807	3.20082	0.66582	3.86664	0.142544
55	Pentadecanoicacid	371.9111	26.80085	120.1779	146.9788	0.149095
56	Pentachlorophenol	213.356	54.47246	11.65763	66.13009	0.145208
57	Pentachloroethane	164.6553	56.37331	3.64163	60.01494	0.056997
58	Pentachlorobenzene	207.8474	24.4666	3.84555	28.31215	0.117378
59	p-Cymene	204.5741	9.54935	25.09293	34.64228	0.19967
60	o-Xylene	164.5714	9.23327	24.34173	33.575	0.199377
61	Octanoicacid	223.2084	38.69685	138.354	177.0508	0.170794
62	Octanedioicacid	234.4426	60.22214	114.2369	174.4591	0.226035
63	Octane	211.9679	2.77754	0.73948	3.51702	0.166049
64	Octanamide	227.1677	46.07957	251.7539	297.8334	0.130779
65	Octadecanoicacid	435.5993	23.89854	108.1914	132.0899	0.148192
66	Octadecanenitrile	426.8011	23.4375	183.9465	207.384	0.100243
67	Octadecanamine	440.0032	9.43319	54.77835	64.21154	0.125326
68	Octadecanamide	439.5877	31.20386	233.689	264.8929	0.103922
69	Octadecafluorooctane	268.3914	8.96435	0.0967	9.06105	0.010559
70	N-Phenyloctadecanamide	517.8784	22.79441	152.7141	175.5085	0.113009
71	N-Phenylhexadecanamide	475.908	23.97254	164.4871	188.4596	0.111022
72	N-Phenyldodecanamide	390.6979	27.5596	185.9547	213.5143	0.112415
73	N-Phenyldecanamide	348.1625	29.69544	196.9698	226.6653	0.113846
74	n-pentane	148.2612	3.20397	0.66412	3.86809	0.142214
75	Nonanoicacid	245.3899	32.97941	133.1272	166.1066	0.159124
76	Nonanedioicacid	256.9373	52.72979	109.7538	162.4836	0.219208
77	Nonane	233.2077	2.69009	0.75658	3.44667	0.171325
78	Nitromethane	91.36075	55.14286	55.0328	110.1757	0.25
79	Nitroethane	112.6247	33.93865	61.08463	95.02328	0.229597
80	nitrobenzene	155.7272	51.7722	87.87598	139.6482	0.23329
81	n-hexane	169.4894	3.04245	0.68689	3.72935	0.150261
82	n-Heptane	190.7576	2.90486	0.707	3.61186	0.157428
83	Neo-hexane	156.2084	4.59045	0.51848	5.10893	0.091186
84	n-Decane	254.4774	2.61748	0.7627	3.38018	0.174725
85	Naphthalene	173.544	16.03222	13.76949	29.8017	0.248559

86	Naphthacene	267.9128	19.1327	10.37349	29.50619	0.227969
87	N,N-Diphenyloctadecanamide	592.9685	14.93899	117.2689	132.2079	0.100228
88	N,N-Diphenylhexadecanamide	549.4413	15.63703	122.7705	138.4076	0.100214
89	N,N-Diphenyldodecanamide	465.088	17.35759	130.2785	147.6361	0.103747
90	N,N-Diphenyldecanamide	423.1291	18.94894	123.9672	142.9161	0.115008
91	N,N-Diethylethanamine	176.4216	6.18	30.98849	37.16849	0.138624
92	m-Xylene	167.5671	9.52251	24.22331	33.74583	0.202556
93	Methyltridecanoate	351.4641	9.92655	138.2463	148.1729	0.062505
94	Methyltetradecanoate	372.6851	9.64633	133.252	142.8983	0.062948
95	Methyloctanoate	245.2758	11.71699	158.5239	170.2409	0.064089
96	Methyloctadecanoate	457.6243	8.74917	115.53	124.2791	0.065443
97	Methylhexadecanoate	415.1567	9.17724	124.0988	133.276	0.064117
98	Methyldodecanoate	330.2209	10.2099	143.0709	153.2808	0.062172
99	Methylcyclopentane	148.7538	2.91149	0.62554	3.53703	0.145578
100	Methylcyclohexane	163.1546	2.86302	0.77455	3.63757	0.167591
101	Methylcis-9-octadecenoate	449.8425	9.6864	110.8493	120.5357	0.073903
102	Methylbenzene	146.9693	10.92086	20.77787	31.69873	0.225826
103	Methoxybenzene	156.2824	19.1379	27.09201	46.22992	0.242599
104	methanol	72.23025	73.03856	104.6667	177.7053	0.242081
105	Mesitylene	188.0649	8.39651	27.66893	36.06543	0.178611
106	Lithiumperchlorate	104.2803	4379.253	138.1381	4517.391	0.029644
107	Lithiumformate	80.59535	3518.506	213.3676	3731.874	0.053905
108	Lithiumbromide	73.4281	4293.012	76.42389	4369.436	0.017185
109	Isopropylcyclopentane	182.6477	3.01137	0.68516	3.69654	0.150997
110	Iodomethane	98.0909	26.2492	10.51137	36.76057	0.204179

111	Iodoethane	119.2262	19.72475	13.18949	32.91424	0.240144
112	Iodobenzene	160.0024	27.16172	7.14346	34.30518	0.164872
113	Indole	159.3654	102.6613	29.50371	132.165	0.173401
114	Hydrogenchloride	57.76131	159.1365	7.5967	166.7332	0.043486
115	Hexylcyclopentane	252.4481	2.53418	0.75061	3.2848	0.176294
116	Hexanedioicacid	191.9239	78.6152	109.8666	188.4818	0.243127
117	Hexane	169.523	3.03457	0.68447	3.71904	0.150172
118	Hexadecanoicacid	394.0574	23.53476	113.8911	137.4259	0.141926
119	Hexadecanenitrile	384.3518	24.41601	192.1859	216.6019	0.100017
120	Hexadecane	381.9158	2.32576	0.85621	3.18197	0.196677
121	Hexadecanamine	397.5193	10.1612	59.36208	69.52328	0.124794
122	Hexadecanamide	397.1447	33.37706	248.7561	282.1331	0.104307
123	Hexadecafluorooxoctane	253.6964	8.37332	1.56734	9.94066	0.13281
124	Hexadecafluoroheptane	242.6456	9.33192	0.09465	9.42657	0.00994
125	Hexacosafluorododecane	372.8337	11.67745	0.114	11.79145	0.009575
126	Hexachloroethane	175.6229	25.4852	1.10286	26.58806	0.039759
127	Hexachlorobenzene	220.1623	19.16149	2.28863	21.45012	0.095312
128	Heptanedioicacid	214.973	64.61728	103.3722	167.9895	0.236695
129	Heptane	190.7667	2.89416	0.71704	3.6112	0.159133
130	Heptadecanoicacid	414.4104	24.78289	112.4398	137.2227	0.147986
131	fluorobenzene	131.251	24.95719	23.94323	48.90042	0.249893
132	Fluorobenzene	131.2467	24.84239	23.97045	48.81284	0.24992
133	Fluorene	211.7882	14.15674	16.6672	30.82394	0.248342
134	Fluoranthene	237.6207	19.28605	12.78658	32.07263	0.239733
135	Ethyloctadecanoate	480.2207	7.48327	120.858	128.3413	0.054908
136	Ethylethanoate	141.3005	11.22896	134.2656	145.4945	0.071221
137	Ethylcyclopentane	167.5972	2.91864	0.66896	3.5876	0.151695
138	Ethylcyclohexane	181.8091	2.91667	0.69019	3.60685	0.154738
139	Ethylbenzene	166.4325	10.89852	22.79673	33.69525	0.218828
140	Ethene	76.00032	11.83997	17.08387	28.92383	0.241783
141	Ethanol	94.84158	63.23342	116.7575	179.9909	0.227893
142	Ethanedioicacid	108.4226	226.8681	66.77309	293.6412	0.175688
143	Ethane,1,2-Dichloro-	123.0775	42.25127	6.93652	49.18779	0.121134
144	Dodecanoicacid	308.9428	28.39677	129.415	157.8118	0.147562
145	Dodecanenitrile	299.3663	26.69466	181.6195	208.3141	0.111725
146	Dodecane	296.9045	2.49155	0.80474	3.2963	0.184533
147	Dodecanamine	312.594	12.22504	71.84508	84.07012	0.124269

148	Dodecanamide	312.1554	38.53007	272.2165	310.7466	0.108618
149	Dodecafluoropentane	190.8453	10.4947	0.08502	10.57971	0.007971
150	Docosafluorodecane	320.5885	13.7393	0.11731	13.85661	0.008394
151	d-Limonene	207.9424	6.29368	18.16762	24.4613	0.191093
152	Diiodomethene	132.6667	59.28394	4.70577	63.98972	0.068131
153	Diiodomethane	132.6616	59.45678	4.68119	64.13796	0.067659
154	Diethylbenzene	200.3197	7.90853	27.71017	35.6187	0.172734
155	Dichloromethane	101.7564	84.27146	9.18313	93.45459	0.088607
156	Dichloroethane	121.0902	43.04793	13.28647	56.3344	0.180225
157	Dibromomethane	114.1575	75.81304	7.22884	83.04188	0.079473
158	Dibromochloromethane	131.1302	75.00203	3.48712	78.48915	0.042454
159	Dibenzothiophene	212.8381	21.93229	10.08819	32.02047	0.215795
160	Dibenzofuran	203.6954	20.75619	14.67849	35.43468	0.242645
161	Decanoicacid	266.6828	31.11385	133.064	164.1779	0.153598
162	Decanenitrile	256.8811	27.56059	152.7791	180.3397	0.12947
163	Decanedioicacid	276.9726	50.9116	117.0401	167.9517	0.211243
164	Decane	254.463	2.60933	0.76819	3.37751	0.175712
165	Decanamine	270.1203	13.67562	79.60875	93.28437	0.125109
166	Decanamide	269.6451	41.82643	268.2102	310.0366	0.116708
167	decalin	199.1652	2.46047	0.77131	3.23178	0.181704
168	Cyclopentene	123.3395	5.88405	19.50092	25.38497	0.178065
169	Cyclopentane	129.3203	2.85969	0.56325	3.42294	0.137474
170	Cyclooctane	174.2949	2.93842	0.61276	3.55117	0.142777
171	Cyclohexene	139.8685	4.12679	21.57975	25.70654	0.134763
172	Cyclohexanol	153.3585	32.29193	123.102	155.394	0.164623
173	Cyclohexane	148.046	2.19547	0.9329	3.12837	0.209279
174	Cycloheptane	159.4468	2.95676	0.66142	3.61818	0.149387
175	Cumene	183.8346	11.39009	23.79758	35.18768	0.218917
176	cis-9-Octadecenoicacid	427.8687	25.05297	101.0745	126.1275	0.159177
177	cis-1,3-Dichloro-1-propene	135.979	43.45751	13.16029	56.61781	0.178412
178	cis-1,2-Diiodoethene	143.6452	55.82735	5.90099	61.72834	0.086458
179	cis-1,2-Dichloroethene	114.2052	74.08038	10.50186	84.58224	0.108745
180	cis,cis-9,12-Octadecadienoicacid	419.4618	25.93939	89.18988	115.1293	0.174544
181	Chrysene	262.016	20.61546	11.43476	32.05023	0.229487

182	Chloroethane	103.7706	18.3996	19.84371	38.24332	0.249644
183	Chlorobenzene	144.8888	27.37733	10.07795	37.45528	0.19667
184	Cesiumiodide	119.025	301.196	120.3832	421.5791	0.204012
185	Cesiumformate	117.4733	245.4096	357.0824	602.492	0.241411
186	Cesiumchloride	100.9379	216.0334	216.4337	432.4671	0.25
187	Carbondisulfide	98.04031	14.88442	0.09599	14.98041	0.006366
188	Carbondioxide	64.3409	75.86684	11.95485	87.82169	0.117596
189	Carbazole	207.1612	79.60373	20.73613	100.3399	0.163951
190	Calciumformate	152.1852	2128.649	144.3803	2273.029	0.059484
191	Butyloctadecanoate	524.1026	5.84942	117.7895	123.6389	0.045072
192	Butylcyclopentane	210.0166	2.69067	0.70791	3.39858	0.164909
193	Butylbenzene	207.9332	7.49505	25.41695	32.912	0.175869
194	Butanedioicacid	149.3621	121.1826	102.0457	223.2283	0.248163
195	Butane	127.0377	3.42476	0.61804	4.0428	0.129504
196	Buckminsterfullerene	402.2006	39.75489	0.00451	39.7594	0.000113
197	Bromotrichloromethane	140.1823	30.68873	0.80937	31.49811	0.025036
198	Bromoethane	109.9426	20.562	18.23064	38.79264	0.249097
199	Bromodichloromethane	125.3282	79.36596	3.69812	83.06409	0.042539
200	Bromochloromethane	108.0131	80.56974	8.09706	88.6668	0.082981
201	bromobenzene	150.9336	28.072	9.47542	37.54742	0.188674
202	Bromobenzene	150.9388	28.10805	9.45714	37.56519	0.188373
203	Biphenyl	205.9792	14.33194	14.54028	28.87222	0.249987
204	benzonitrile	149.547	53.26293	134.3606	187.6235	0.203293
205	Benzo[e]pyrene	272.4273	20.95484	10.48388	31.43872	0.222268
206	Benzo(ghi)perylene	286.2889	20.58099	9.17004	29.75102	0.213223
207	Benzo(a)pyrene	275.6662	20.29403	9.87466	30.16868	0.22018
208	Benzenemethanol	155.8683	69.52983	35.9566	105.4864	0.224676
209	Benzene	126.2944	13.5636	17.44576	31.00936	0.246082
210	Benz[a]anthracene	264.9765	20.22225	11.09207	31.31432	0.228747
211	Anthracene	220.7349	17.85961	11.64772	29.50733	0.23892
212	anisole	136.2152	73.10866	47.77587	120.8845	0.239021
213	Acridine	217.1591	26.87091	44.02279	70.89369	0.235367
214	Acetonitrile	85.00754	39.41957	111.5947	151.0143	0.192894
215	acetone	108.1297	26.24917	130.8373	157.0865	0.139178
216	Acenaphthene	198.18	9.25125	18.47636	27.72761	0.222327
217	7,8-Dimethyltetradeca	360.7883	3.08552	0.7551	3.84062	0.157954

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218	5-Methylindole	179.9061	92.74469	34.85774	127.6024	0.19855
219	5-Methyl-1-hexene	178.9599	5.61608	20.54904	26.16512	0.16857
220	4-Methyloctane	223.5647	3.1627	0.70182	3.86452	0.148625
221	4-Methylheptane	202.4281	3.27024	0.71162	3.98186	0.146776
222	4-Methyl-1-hexene	177.3702	6.41806	19.67009	26.08816	0.185491
223	4-Chlorophenol	154.472	132.824	18.81086	151.6349	0.108664
224	4-Chloro-3-methylphenol	171.8142	109.062	19.90752	128.9695	0.130532
225	4-Chloro-3-methyl-5-ethylphenol	207.1007	73.24574	23.383	96.62874	0.18343
226	4-Chloro-3,5-dimethylphenol	189.2072	90.42371	22.73024	113.1539	0.160527
227	4-Chloro-3,5-dimethyl-2-(phenylmethyl)-phenol	280.733	70.27213	19.15167	89.4238	0.1683
228	4-Chloro-2-methylphenol	173.4871	112.1648	17.05923	129.224	0.114585
229	4-Chloro-2,6-dimethylphenol	191.5369	67.76019	19.70887	87.46906	0.174553
230	4-Chloro-2,5-dimethylphenol	191.3483	93.64315	18.92	112.5632	0.139831
231	4-Bromotoluene	171.7256	19.35056	11.94877	31.29933	0.236019
232	4-Bromophenol	160.5155	132.3833	17.57447	149.9578	0.103461
233	4-Bromo-1-butene	146.0967	24.35937	17.79262	42.15199	0.243933
234	3-Methylpentane	160.2894	3.42774	0.64286	4.0706	0.132987
235	3-Methyloctane	223.7751	3.13312	0.70003	3.83315	0.149274
236	3-Methylheptane	202.6123	3.28741	0.67196	3.95937	0.140911
237	3-Methyl-1-hexene	178.9763	6.12866	17.60059	23.72925	0.191569
238	3-Methyl-1-butene	139.1427	7.77952	18.57998	26.3595	0.208029
239	3-Methyl-1-butanol	153.4678	41.74741	117.2972	159.0447	0.193588
240	3-Chlorophenol	154.353	134.6087	17.8481	152.4568	0.103365
241	3-Chloropentane	159.0331	10.1538	26.28338	36.43718	0.201011
242	3-Chloro-1-propene	118.547	30.39728	19.65511	50.05239	0.238485
243	3-Chloro-1,1,1-trifluoropropane	138.2507	52.51943	5.75021	58.26964	0.088944
244	3-Bromo-1-propene	124.6914	31.81351	16.20789	48.02139	0.223598
245	3,4-	181.5692	26.97141	17.5467	44.51812	0.238795

	Dichlorotoluene					
246	3,3-Dimethylpentane	172.5388	4.37551	0.56774	4.94325	0.101661
247	2-Undecylbenzothiazole	395.2612	10.80261	43.79607	54.59868	0.158708
248	2-Propyl-1,3,5-trimethylbenzene	238.3051	7.03684	32.23367	39.27051	0.14708
249	2-Propanone	108.4476	17.27248	133.7506	151.0231	0.101289
250	2-Propanol	114.3969	49.35495	121.1258	170.4808	0.205692
251	2-Octene	206.7569	4.16139	13.806	17.96739	0.177966
252	2-Nitropropane	131.1237	24.44968	66.87028	91.31996	0.196054
253	2-Methylthiophene	139.0959	14.78904	15.70076	30.4898	0.249776
254	2-Methylpentane	162.4276	3.5413	0.67975	4.22105	0.135104
255	2-Methyloctane	226.0468	3.01102	0.71865	3.72967	0.155557
256	2-Methylnaphthalene	194.1912	13.15817	16.62143	29.7796	0.246619
257	2-Methylhexane	183.5845	3.33058	0.66679	3.99736	0.138982
258	2-Methylheptane	204.8369	3.15519	0.69735	3.85253	0.148245
259	2-Methylbutane	142.9955	3.82717	0.60782	4.43499	0.118268
260	2-Methylanthracene	241.3483	14.84377	13.95559	28.79937	0.249762
261	2-Methyl-2-propanol	131.2543	37.28764	120.209	157.4966	0.1807
262	2-Methyl-2-butene	138.4081	5.86851	18.00957	23.87808	0.185367
263	2-Methyl-1-propanol	133.219	52.67119	80.57553	133.2467	0.239036
264	2-Methyl-1-pentene	158.9571	6.78752	21.70189	28.48941	0.181485
265	2-Methyl-1-hexene	180.2181	6.23945	21.10449	27.34394	0.176116
266	2-Methyl-1-heptene	201.4859	5.80956	20.29454	26.1041	0.173023
267	2-Methyl-1,3-butadiene	130.1652	11.41047	15.41739	26.82787	0.244423
268	2-Iodopropane	137.2928	16.84776	15.47832	32.32608	0.249551
269	2-Hydroxymethylbenzene	155.8532	69.45577	35.88539	105.3412	0.22461
270	2-Hexene	163.8327	5.36661	15.93187	21.29847	0.188482
271	2-Heptadecylbenzothiazole	522.5965	9.12059	39.63905	48.75964	0.152064
272	2-Ethyl-1,3,5-	217.6629	8.15867	30.51224	38.6709	0.166466

	trimethylbenzene					
273	2-Ethoxypropane	157.4881	8.17509	80.53265	88.70774	0.083665
274	2-Cyclopentyloctane	283.0239	2.86457	0.72927	3.59384	0.161745
275	2-Chloropropane	122.7964	16.0516	23.2292	39.28079	0.241653
276	2-Chlorophenol	152.9263	123.9266	36.8678	160.7944	0.176714
277	2-Chloropentane	162.9611	17.74084	29.36013	47.10097	0.234786
278	2-Chlorobutane	143.3906	17.12141	22.94499	40.0664	0.244718
279	2-Chloro-6-methylphenol	171.0461	66.30335	39.23326	105.5366	0.233552
280	2-Chloro-2-methylpropane	138.8179	13.94449	26.95304	40.89753	0.224707
281	2-Chloro-2-methylbutane	155.2828	14.63412	36.65094	51.28506	0.203925
282	2-Butanone	127.5688	13.30124	143.3711	156.6724	0.077691
283	2-Butanol	133.2499	38.80043	122.8329	161.6334	0.182427
284	2-Bromopropane	128.5353	16.86803	21.67756	38.54559	0.246108
285	2-Bromo-2-chloro-1,1,1-trifluoroethane	138.538	98.05553	3.31474	101.3703	0.03163
286	2-Allyl-1,3,5-trimethylbenzene	234.1775	9.52431	23.8872	33.41151	0.203801
287	2,7-Dimethyloctane	241.9353	3.24328	0.68058	3.92386	0.143363
288	2,6-Dimethylheptane	220.6672	3.48683	0.68728	4.17411	0.137543
289	2,6-Dichloro-4-methylphenol	189.9984	41.99441	40.38025	82.37465	0.249904
290	2,5-Norbornadiene	139.126	10.40641	22.13983	32.54624	0.217507
291	2,5-Dimethylhexane	199.4321	3.60985	0.66717	4.27702	0.131657
292	2,4-Dimethylpentane	176.238	4.00231	0.6752	4.67751	0.123514
293	2,4-Dimethylhexane	195.4322	4.10447	0.60841	4.71288	0.11243
294	2,4-Dichlorophenol	171.6741	170.5547	25.37148	195.9262	0.112726
295	2,4-Dichloro-6-propylphenol	229.3185	59.31822	27.4126	86.73082	0.216168
296	2,4-Dichloro-6-methylphenol	189.7983	97.10773	26.33156	123.4393	0.167812
297	2,4-Dichloro-6-ethylphenol	208.2239	72.536	27.05394	99.58994	0.197858

298	2,4-Dichloro-6-butylphenol	250.5698	53.88493	27.57446	81.45939	0.22392
299	2,4-Dichloro-6-(phenylmethyl)phenol	269.0774	76.35506	25.37602	101.7311	0.187221
300	2,4-Dibromophenol	183.4312	164.4321	21.78775	186.2199	0.103311
301	2,4,6-Trimethyl-2-phenylheptene	299.3552	8.95605	27.69078	36.64683	0.184663
302	2,4,6-Trichlorophenol	187.9819	55.20832	21.53121	76.73953	0.201853
303	2,4,6-Trichloro-3-methylphenol	202.0476	41.92536	27.46158	69.38694	0.239137
304	2,4,6-Trichloro-3,5-dimethylphenol	215.9072	31.87355	34.14519	66.01873	0.249704
305	2,4,6-Tribromophenol	205.37	50.02677	19.02968	69.05645	0.19963
306	2,4,5-Trichlorophenol	187.6404	167.1344	17.47443	184.6089	0.085697
307	2,4,5,6-Tetroachloro-3-methylphenol	214.6369	39.12392	18.99378	58.1177	0.220007
308	2,3-Dimethylbutane	158.053	4.33332	0.54912	4.88245	0.09982
309	2,3-Dimethyl-1-pentene	172.7966	6.71701	20.27624	26.99325	0.186919
310	2,3-Dimethyl-1-hexene	192.4328	6.6058	15.36359	21.96939	0.210272
311	2,3-Dimethyl-1-butene	153.1808	7.16833	19.80863	26.97696	0.195113
312	2,3-Dichloropentane	174.1845	33.06652	25.42058	58.4871	0.245728
313	2,3-Dichlorobutane	157.7354	25.76705	10.93217	36.69922	0.20915
314	2,3-Dichloro-2-methylbutane	167.7227	32.50268	25.56158	58.06426	0.246427
315	2,3,5-Trimethylhexane	211.5335	3.99828	0.63386	4.63214	0.118115
316	2,3,4-Trimethylpentane	187.512	4.26675	0.6023	4.86905	0.108398
317	2,3,4,6-Tetrachlorophenol	200.7557	56.83854	15.32122	72.15976	0.167242
318	2,2'-	164.8121	88.76259	93.65928	182.4219	0.24982

	Iminobisethanol					
319	2,2-Dimethylpentane	178.2568	4.2006	0.54976	4.75036	0.102337
320	2,2-Dimethylhexane	198.4438	3.94538	0.58272	4.5281	0.112128
321	2,2-Dimethylheptane	219.6595	3.70627	0.61627	4.32254	0.122244
322	2,2-Dimethylbutane	156.2111	4.5773	0.52147	5.09878	0.091814
323	2,2-Dichloro-1,1,1-trifluoroethane	133.0395	103.0722	3.11834	106.1906	0.028503
324	2,2,5-Trimethylhexane	214.1881	4.18733	0.55901	4.74633	0.103905
325	2,2,4-Trimethylpentane	190.0596	4.53158	0.56471	5.09629	0.09853
326	2,2,4-Trimethylhexane	210.1539	4.83217	0.52935	5.36152	0.088983
327	2,2,3-Trimethylbutane	169.5767	4.67833	0.5074	5.18573	0.088272
328	1-Undecanol	286.2278	23.59132	90.47727	114.0686	0.164044
329	1-Tridecanol	328.7158	20.99832	82.60664	103.605	0.161599
330	1-Tetradecanol	349.926	19.95116	79.16935	99.1205	0.160767
331	1-Propanol	116.1929	51.75223	116.3977	168.1499	0.213049
332	1-Pentene	141.8332	5.75157	21.49923	27.2508	0.166514
333	1-Pentanol	158.7658	39.07076	118.9456	158.0164	0.186121
334	1-Pentadecanol	371.1836	18.97288	75.77933	94.75221	0.160142
335	1-Octanol	222.4929	29.21217	104.3932	133.6053	0.17084
336	1-Octadecanol	434.8464	16.64928	67.11676	83.76604	0.159254
337	1-Nonanol	243.7443	27.03481	99.63296	126.6678	0.167878
338	1-Nitropropane	133.4703	32.09567	65.19756	97.29323	0.221061
339	1-Methylphenanthrene	235.2777	15.99045	14.65302	30.64347	0.249524
340	1-Methylnaphthalene	190.8025	13.32559	16.11388	29.43947	0.247757
341	1-methylnaphthalen	190.8081	13.37389	16.03396	29.40785	0.247955
342	1-Iodopropane	140.5687	15.4472	14.01268	29.45989	0.249407
343	1-Iodoheptane	225.6623	14.20086	18.86696	33.06782	0.245022
344	1-Iodobutane	161.8843	15.01126	14.78512	29.79639	0.249986
345	1-Hydropentadecaflu	239.527	65.45052	4.91267	70.36319	0.064944

	oroheptane					
346	1-Hexene	163.0816	5.41015	21.4142	26.82436	0.16101
347	1-Hexanol	180.0088	35.01919	113.9498	148.969	0.179816
348	1-Hexadecanol	392.3843	18.13365	72.92699	91.06064	0.159482
349	1-Heptene	184.3588	5.0966	20.97147	26.06807	0.157287
350	1-Heptanol	201.2559	31.8321	109.7184	141.5505	0.17431
351	1-Ethylnaphthalene	209.1659	11.35122	16.88273	28.23394	0.240404
352	1-Ethoxypropane	161.5969	5.89554	87.73932	93.63485	0.058999
353	1-Dodecanol	307.4481	22.23819	86.45474	108.6929	0.162737
354	1-Decene	248.0613	4.32691	18.2896	22.61651	0.154714
355	1-Decanol	264.9749	25.20188	94.96051	120.1624	0.165744
356	1-Chlorotetradecane	358.9682	11.14125	41.2338	52.37505	0.16747
357	1-Chloropropane	125.1816	13.82905	21.13613	34.96518	0.239082
358	1-Chloropentane	167.7804	14.20728	22.13497	36.34225	0.238104
359	1-Chlorooctane	231.5284	13.49565	34.36621	47.86186	0.202463
360	1-chloronaphthalen	189.3112	25.40129	8.06235	33.46363	0.182882
361	1-Chlorohexane	189.0362	14.64626	22.76075	37.40701	0.238236
362	1-Chloroheptane	210.2806	13.89044	30.27688	44.16732	0.215588
363	1-Chlorobutane	146.5174	14.30409	21.80415	36.10823	0.239214
364	1-Chloro-4-iodobenzene	178.6748	42.1036	5.78206	47.88566	0.106167
365	1-Chloro-3-iodobenzene	178.6346	41.90473	5.96384	47.86857	0.109066
366	1-Chloro-2-methylpropane	141.4404	18.00126	26.51072	44.51198	0.240863
367	1-Chloro-2-iodobenzene	174.6231	39.29864	11.46991	50.76856	0.174883
368	1-Chloro-2-fluoroethane	108.9813	31.73191	22.44665	54.17855	0.242657
369	1-Butanol	137.515	44.27873	119.3182	163.5969	0.197402
370	1-Bromopropane	131.325	15.35044	19.51995	34.87039	0.246426
371	1-Bromopentane	173.9248	15.09323	20.64236	35.73559	0.243972
372	1-Bromooctane	237.6887	14.3906	28.95395	43.34455	0.221778
373	1-Bromohexane	195.1924	15.4774	20.97711	36.45451	0.24431
374	1-Bromoheptane	216.4355	14.843	25.63104	40.47404	0.232239
375	1-Bromobutane	152.6628	15.34646	20.30301	35.64947	0.245167
376	1-Bromo-4-iodobenzene	184.7133	41.25378	5.63055	46.88433	0.105672
377	1-Bromo-4-chlorobenzene	169.6174	43.55274	7.02308	50.57582	0.11958

378	1-Bromo-3-methylbutane	168.6384	15.38278	20.50764	35.89043	0.244903
379	1-Bromo-3-chloropropane	150.824	59.61825	10.23074	69.84899	0.125016
380	1-Bromo-3-chlorobenzene	169.5721	43.19091	7.00652	50.19743	0.120097
381	1-Bromo-2-methylpropane	147.2109	19.77175	21.55725	41.329	0.249533
382	1-Bromo-2-chloroethane	129.1844	44.33127	6.3843	50.71557	0.110038
383	1-Bromo-2-chlorobenzene	166.2612	41.09667	14.69077	55.78745	0.19399
384	18-Pentatriacontanone	784.1968	8.60187	93.97653	102.5784	0.076825
385	16-Hentricontanone	699.2674	9.19448	104.4296	113.6241	0.074372
386	14-Heptacosanone	614.3053	9.92209	117.3674	127.2895	0.071873
387	12-Tricosanone	529.3778	10.83341	133.3438	144.1772	0.069494
388	10-Nonadecanone	444.4332	12.02116	152.8025	164.8237	0.067614
389	1,5-Hexadiene	156.6495	7.86335	15.94754	23.8109	0.221182
390	1,5-Dichloropentane	187.2944	27.10233	15.80493	42.90726	0.232669
391	1,4-Diphenylbenzene	293.5578	13.09932	12.87298	25.9723	0.249981
392	1,4-Dioxane	127.5687	13.38438	77.30333	90.68771	0.125806
393	1,4-Dimethylcyclohexane	181.6374	2.91777	0.74237	3.66014	0.161687
394	1,4-Dimethylbenzene	167.711	9.79491	23.84372	33.63863	0.206394
395	1,4-Diiodobenzene	193.7776	39.99767	4.30367	44.30135	0.087708
396	1,4-Difluorobenzene	136.2671	45.17542	26.22231	71.39773	0.232383
397	1,4-Dicyclopentylbutane	292.9608	2.36528	0.74472	3.11	0.182119
398	1,4-Dichlorobutane	165.9862	30.99373	13.1283	44.12202	0.209012
399	1,4-Dichlorobenzene	163.5733	44.5425	7.45443	51.99693	0.12281
400	1,4-Dibromobenzene	175.6562	42.7417	6.74305	49.48475	0.117697
401	1,4-	134.6001	5.75661	18.10969	23.8663	0.183024

	Cyclohexadiene					
402	1,4-Benzenediol	145.3355	151.2376	40.26266	191.5002	0.166044
403	1,3-Diphenylbenzene	293.4608	13.31225	13.29205	26.6043	0.25
404	1,3-Dimethylbenzene	167.5671	9.52252	24.22332	33.74584	0.202556
405	1,3-Diiodobenzene	193.7357	40.10436	4.55281	44.65717	0.091556
406	1,3-Difluorobenzene	136.2832	42.24515	22.48376	64.72891	0.226699
407	1,3-Dichloropropane	144.7117	56.76369	11.27206	68.03574	0.138229
408	1,3-Dichlorobenzene	163.5377	44.07127	7.23133	51.3026	0.121086
409	1,3-Dichloro-1-propene	138.6815	66.18447	9.15392	75.33839	0.106741
410	1,3-Dibromopropane	156.9051	61.96424	9.16623	71.13046	0.112259
411	1,3-Dibromobenzene	175.6259	42.52401	6.86967	49.39368	0.119737
412	1,3-Bis(trifluoromethyl)benzene	193.6401	51.77461	6.29272	58.06732	0.096625
413	1,3,5-Trimethylbenzene	188.0649	8.3965	27.66892	36.06543	0.178611
414	1,3,5-Trichlorobenzene	182.1791	28.57219	2.19873	30.77092	0.066349
415	1,3,5-Tribromobenzene	200.3178	29.30224	2.12888	31.43112	0.063144
416	1,3,5-Cycloheptatriene	143.7427	11.73583	18.64889	30.38473	0.237059
417	1,2-Ethanediol	105.3474	116.1253	82.18704	198.3123	0.242678
418	1,2-Diphenylbenzene	284.364	12.01706	21.83709	33.85415	0.228965
419	1,2-Dimethylbenzene	163.6158	10.40525	24.24784	34.65309	0.210108
420	1,2-Diiodobenzene	187.8858	37.50394	8.66761	46.17155	0.152485
421	1,2-Difluorobenzene	136.0471	41.78207	33.99525	75.77733	0.24736
422	1,2-Dichloropropane	139.9152	27.05735	8.63193	35.68928	0.183365
423	1,2-Dichloropentane	180.2891	23.22796	9.16375	32.3917	0.202869
424	1,2-Dichloroethane	123.0462	42.06179	6.97687	49.03866	0.122031

425	1,2-Dichlorobenzene	160.7584	42.19864	15.63634	57.83498	0.197266
426	1,2-Dichloro-1-propene	134.2681	39.02496	14.66276	53.68772	0.198522
427	1,2-Dichloro-1,1-difluoroethane	130.35	88.35993	6.85609	95.21602	0.066821
428	1,2-Dichloro-1,1,2,3,3,3-hexafluoropropane	160.2416	23.48674	0.64357	24.13031	0.025959
429	1,2-Dibromopropane	151.3521	30.33173	7.01461	37.34635	0.152547
430	1,2-Dibromoethane	135.3105	46.38395	5.55388	51.93784	0.095499
431	1,2-Dibromobenzene	171.6306	40.28946	13.77812	54.06758	0.189892
432	1,2-Dibromo-3-chloropropane	169.9426	65.66134	9.74018	75.40152	0.112491
433	1,2-Dibromo-1-chloroethane	147.9144	106.2927	14.62719	120.9199	0.106333
434	1,2-Dibromo-1,2-dichloroethane	164.9518	63.61058	4.94245	68.55303	0.066899
435	1,2-Dibromo-1,1,2,3,3,3-hexafluoropropane	170.332	35.33568	0.80086	36.13654	0.021671
436	1,2-Dibromo-1,1,2,2-tetrafluoroethane	148.4417	32.86734	0.55486	33.42219	0.016326
437	1,2,4-Trimethylbenzene	185.2549	8.65058	27.51488	36.16547	0.181981
438	1,2,4-Trichlorobenzene	179.4982	40.95711	6.64351	47.60062	0.120089
439	1,2,4-trichlorobenzen	179.4887	40.97775	6.62755	47.6053	0.119837
440	1,2,4-Tribromobenzene	196.3853	40.27925	5.76218	46.04143	0.109489
441	1,2,4,5-Tetrachlorobenzene	195.5011	27.63827	5.208	32.84628	0.133417
442	1,2,4,5-Tetrabromobenzene	217.2042	27.96207	4.29981	32.26188	0.115515
443	1,2,3-Trimethylbenzene	180.5886	9.03235	28.38369	37.41604	0.183128
444	1,2,3-	157.5154	63.70732	14.59401	78.30133	0.151644

	Trichloropropane					
445	1,2,3-Trichlorobenzene	176.4128	50.44366	9.8355	60.27916	0.136543
446	1,2,3-Propanetriol(glycerol)	216.5091	95.28211	111.3729	206.655	0.248484
447	1,2,3-Propanetriol	132.394	121.4445	81.11948	202.564	0.240093
448	1,2,3,5-Tetrachlorobenzene	195.1604	26.86144	5.26838	32.12982	0.137085
449	1,2,3,4-Tetrahydronaphthalene	187.1973	5.86712	26.39361	32.26073	0.148791
450	1,2,3,4-Tetrachlorobenzene	192.1232	40.81626	6.40776	47.22402	0.117277
451	1,1'-Oxybispentane	268.0531	4.05041	71.22519	75.2756	0.050913
452	1,1-Oxybisethane	140.276	6.43052	86.56779	92.99831	0.064365
453	1,1-Dichloroethene	114.4151	40.76675	5.8615	46.62825	0.109905
454	1,1-Dichloroethane	101.7621	84.4457	9.132	93.5777	0.088064
455	1,1-Dichlorobutane	159.694	32.42116	15.4789	47.90006	0.218724
456	1,1-Dichloro-1-fluoroethane	124.647	40.89506	10.80401	51.69907	0.165307
457	1,1,2-Trichloroethane	139.9651	63.89811	5.82149	69.7196	0.076527
458	1,1,2-Trichloro-1,2,2-trifluoroethane	147.6337	26.53859	1.38705	27.92563	0.047202
459	1,1,2-Tribromoethane	157.9467	54.34405	4.25326	58.59731	0.067316
460	1,1,2,3,4,5,5,5-Octachloro-1,3-pentadiene	254.7161	20.5447	2.27706	22.82176	0.089821
461	1,1,2,3,4,4-Hexachloro-1,3-butadiene	211.7285	19.49644	2.15135	21.64779	0.089503
462	1,1,2,3,3,3-Hexachloro-1-propene	191.9892	21.45142	3.15611	24.60753	0.111808
463	1,1,2,2-Tetrachloroethane	152.8015	72.84302	4.10193	76.94495	0.050468
464	1,1,2,2-	157.9039	27.06803	1.2252	28.29323	0.041428

	Tetrachloro-1,2-difluoroethane					
465	1,1,2,2-Tetrabromoethane	176.0333	57.85498	4.39749	62.25247	0.06565
466	1,1,1-Trichloroethane	136.0838	37.03997	8.44021	45.48018	0.15114
467	1,1,1-Trichloro-2,2,3,3,3-pentafluoropropane	170.198	26.78379	1.5544	28.33819	0.051843
468	1,1,1-Trichloro-2,2,2-trifluoroethane	146.6256	28.49646	1.79806	30.29452	0.05583
469	1,1,1,3-Tetrachloro-2,2,3,3-tetrafluoropropane	182.1574	27.15292	1.63489	28.78781	0.053566
470	1,1,1,2-Tetrachloroethane	151.6183	63.67439	7.15329	70.82768	0.090796
471	1,1,1,2,2,3,4,5,5,5-Decafluoro-3-[1,2,2,2-tetra-fluoro-1-(trifluoromethyl)ethyl]-4-(trifluoro-methyl)pentane	261.0721	11.45663	0.77814	12.23477	0.059555
472	1,1,1,2,2,3,3,4,5,5,5-Undecafluoro-4-(tri-fluoromethyl)-pentane	208.4813	10.40104	0.09846	10.4995	0.009289
473	(2-Ethylcyclopentyl)benzene	239.4784	9.47375	23.88371	33.35745	0.203347

Script S1. The python script use to obtain the model *g*.

```
# Using Python 3.7.3
import numpy as np
import pandas as pd
from sklearn.metrics import mean_squared_error
from sklearn.model_selection import train_test_split, GridSearchCV
from sklearn.preprocessing import StandardScaler
from sklearn.ensemble import RandomForestRegressor, RandomForestClassifier
from sklearn.metrics import r2_score

# Inputting data
df = pd.read_excel('input.xlsx')
fps = df.iloc[:, [1, 2, 3, 7, 8, 9]].values
solute_molWt = df['Solute-SMILEs'].apply(Chem.MolFromSmiles).apply(Descriptors.MolWt)
solvent_molWt = df['Solvent SMILEs'].apply(Chem.MolFromSmiles).apply(Descriptors.MolWt)
solute_molWt = np.asarray(solute_molWt).reshape(len(solvent_molWt), 1)
solvent_molWt = np.asarray(solvent_molWt).reshape(len(solvent_molWt), 1)
temperature = df[' Temperature (K)'].values.reshape(len(df[' Temperature (K)'].values), 1)
X = np.append(fps, temperature, axis=1)
X = np.append(X, solute_molWt, axis=1)
X = np.append(X, solvent_molWt, axis=1)
y = df['log(sol*1e4)'].values

# Standardizing data
sc = StandardScaler()
X_train_std = sc.fit_transform(X_train)
X_test_std = sc.transform(X_test)

# Building machine learning model.
model = RandomForestRegressor(n_estimators=90, oob_score=True, random_state=42, max_features=7)
model.fit(X_train_std, y_train)
y_train_pred = model.predict(X_train_std)
y_test_pred = model.predict(X_test_std)
RMSE_train = mean_squared_error(y_train, y_train_pred)
RMSE_test = mean_squared_error(y_test, y_test_pred)
r2_score_train = r2_score(y_train, y_train_pred)
r2_score_test = r2_score(y_test, y_test_pred)
print('RMSE_train:', RMSE_train, '\n', 'RMSE_test', RMSE_test, '\n',
        'r2_score_train ', r2_score_train, '\n', 'r2_score_test', r2_score_test)
col1 = y_test.reshape(len(y_test), 1)
```

```
col2 = y_test_pred.reshape(len(y_test_pred), 1)
col3 = y_train.reshape(len(y_train), 1)
col4 = y_train_pred.reshape(len(y_train_pred), 1)
data = np.column_stack((col1, col2))
data_train = np.column_stack((col3, col4))

# Saving data
np.savetxt('out-RandomForestR-input.txt', data)
f = open('out-RandomForestR-input.txt', 'r+')
content = f.read()
f.seek(0, 0)
f.writelines('RMSE_train:' + str(RMSE_train) + '\n' + 'RMSE_test' + str(RMSE_test) +
'\n' + 'r2_score_train ' +
                    str(r2_score_train) + '\n' + 'r2_score_test' + str(r2_score_test) + '\n' +
'\n' + 'y_test                y_test_pred\n'
                    + content + '\n')
f.close()
```

Script S2. The python script use to predict the solubility of PCBM and Y6.

```
# Using Python 3.7.3
import numpy as np
import pandas as pd
from rdkit.Chem import Descriptors
from rdkit import Chem
from sklearn.metrics import mean_squared_error
from sklearn.model_selection import train_test_split, GridSearchCV
from sklearn.preprocessing import StandardScaler
from sklearn.ensemble import RandomForestRegressor, RandomForestClassifier
from sklearn.metrics import r2_score
import pickle

def predict_fun(filename): # Define the predicting function.
    inputname = './input/' + filename + '.xlsx'
    df = pd.read_excel(inputname)
    fps = df.iloc[:, [1, 2, 3, 5, 6, 7]].values
    temperature = df['Temperature'].values.reshape(len(df['Temperature'].values), 1)
    X_pred = np.append(fps, temperature, axis=1)
    X_pred_std = sc.transform(X_pred)
    y_pred = model.predict(X_pred_std)
    # save data
    outputname = filename + '.txt'
    np.savetxt(outputname, y_pred)

# load standardscaler and model
sc = pickle.load(open('./model/sc.pkl', 'rb'))
model = pickle.load(open('./model/finalized_model.sav', 'rb'))

# predict PCBM in common 42 solvent
predict_fun('PCBM_common_solvent')
# predict PCBM in all solvent in dataset
predict_fun('PCBM_all_solvent')
# predict Y6 in common 42 solvent
predict_fun('Y6_common_solvent')
# predict Y6 in all solvent in dataset
predict_fun('Y6_all_solvent')
```

Table S2 Example of input dataset for the model used in this work

Solute Smile	Solute Area	Solute σ^2_+	Solute σ^2_-	Solvent Smile	Solvent Area	Solvent σ^2_+	Solvent σ^2_-	Temperature
CCCCCC	169.523	3.03457	0.68447	ClCCl	101.7564	84.27146	9.18313	298

Reference

1. T. Lu, F. Chen, *J. Comput. Chem.*, 2012, **33**, 580-592.