Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Easy and fast prediction of the green solvents for small molecule donor-based organic solar cells through machine learning

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Table S1. Data set used for machine learning

No	Solvent	δ_D	δ_P	δ_H	smiles	Ref
1	1,1,1-Trichloroethane	16.8	4.3	2	CC(Cl)(Cl)Cl	1
2	1,3-Butanediol	16.6	10	21.5	CC(O)CCO	1
3	1,4-Butandiol Diacrylate	16.8	9.1	4.2	C=CC(=O)OCCCCOC(=O)C=C	1
4	1,4-Dioxane	19	1.8	7.4	C1COCCO1	1
5	1-Bromonaphthalene	20.3	3.1	4.1	Brc1cccc2ccccc12	1
6	1-Butanol	16	5.7	15.8	CCCCO	1
7	1-Chlorobutane	16.2	5.5	2	CCCCCl	1
8	1-Pentanol	15.9	5.9	13.9	CCCCCO	1
9	1-Propanol	16	6.8	17.4	CCCO	1
10	2-Butanol	15.8	5.7	14.5	CCC(C)O	1
11	2-Ethyl Hexyl Acetate	15.8	2.9	5.1	CCCCC(CC)COC(C)=O	1
12	2-Ethyl Hexyl Acrylate	14.8	4.7	3.4	C=CC(=O)OCC(CC)CCCC	1
13	2-Ethyl-1-Butanol	15.8	4.3	13.5	CCC(CC)CO	1
14	2-Ethyl-Hexanol	15.9	3.3	11.8	CCCCC(CC)CO	1
15	2-Nitropropane	16.2	12.1	4.1	CC(C)[N+](=O)[O-]	1
16	2-Propanol	15.8	6.1	16.4	CC(C)O	1
17	2-Pyrrolidone	19.4	17.4	11.3	O=C1CCCN1	1
18	3-Chloro-1-Propanol	17.5	5.7	14.7	OCCCCl	1
19	Acetic Acid	14.5	8	13.5	CC(=O)O	1
20	Acetic Anhydride	16	11.7	10.2	CC(=O)OC(C)=O	1
21	Acetone	15.5	10.4	7	CC(C)=O	1
22	Acetonitrile	15.3	18	6.1	CC#N	1
23	Acetophenone	19.6	8.6	3.7	CC(=O)c1ccccc1	1
24	Acetylacetone	17.1	9	4.1	CC(=O)CC(C)=O	1
25	Acrylic Acid	17.7	6.4	14.9	C=CC(=O)O	1
26	Acrylonitrile	16	12.8	6.8	C=CC#N	1
27	Aniline	19.4	5.1	10.2	Nc1ccccc1	1
28	Anisole	17.8	4.1	6.7	COc1ccccc1	1
29	Benzaldehyde	19.4	7.4	5.3	O=Cc1ccccc1	1
30	Benzene	18.4	0	2	c1ccccc1	1

31	Benzyl Alcohol	18.4	6.3	13.7	OCc1ccccc1	1
32	Benzyl Butyl Phthalate	19	11.2	3.1	CCCCOC(=O)c1ccccc1C(=O)OCc1ccccc1	1
33	Benzyl Methacrylate	16.8	4.1	4.1	C=C(C)C(=O)OCc1ccccc1	1
34	Butoxy Ethoxy Propanol	15.5	6.5	10.2	CCCCOCC(O)COCC	1
35	Butyl Lactate	15.8	6.5	10.2	CCCCOC(=O)C(C)O	1
36	Butyric Acid	14.9	4.1	10.6	CCCC(=O)O	1
37	Butyronitrile	15.3	12.4	5.1	CCCC#N	1
38	Carbon Dioxide	15.7	6.3	5.7	O=C=O	1
39	Carbon Disulfide	20.5	0	0.6	S=C=S	1
40	Carbon Tetrachloride	17.8	0	0.6	ClC(Cl)(Cl)Cl	1
41	Chlorobenzene	19	4.3	2	Clc1ccccc1	1
42	Chloroform	17.8	3.1	5.7	ClC(Cl)Cl	1
43	Cyclohexane	16.8	0	0.2	C1CCCCC1	1
44	Cyclohexanol	17.4	4.1	13.5	OC1CCCCC1	1
45	Cyclohexanone	17.8	6.3	5.1	O=C1CCCCC1	1
46	Cyclohexylamine	17.2	3.1	6.5	NC1CCCCC1	1
47	Cyclohexylchloride	17.3	5.5	2	ClC1CCCCC1	1
48	Di-(2-Chloroethyl) Ether	18.8	9	5.7	ClCCOCCCl	1
49	Diacetone Alcohol	15.8	8.2	10.8	CC(=O)CC(C)(C)O	1
50	Dibutyl Phthalate	17.8	8.6	4.1	CCCCOC(=O)c1ccccc1C(=O)OCCCC	1
51	Diethyl Amine	14.9	2.3	6.1	CCNCC	1
52	Diethyl Ether	14.5	2.9	5.1	CCOCC	1
53	Diethyl Sulfide	16.8	3.1	2	CCSCC	1
54	Diethylene Glycol	16.6	12	20.7	OCCOCCO	1
55	Diethylene Glycol Butyl Ether Acetate	16	4.1	8.2	CCCCOCCOCCOC(C)=O	1
56	Diethylene Glycol Methyl t-Butyl Ether	16	7.2	7.2	COCCOCCOC(C)(C)C	1
57	Diethylene Glycol Monobutyl Ether	16	7	10.6	CCCCOCCOCCO	1
58	Diethylene Glycol Monoethyl Ether	16.1	9.2	12.2	CCOCCOCCO	1
59	Diethylene Glycol Monoethyl Ether Acetate	16.2	5.1	9.2	CCOCCOCCOC(C)=O	1
60	Diethylene Glycol Monomethyl Ether	16.2	7.8	12.6	COCCOCCO	1
61	Diethylenetriamine	16.7	13.3	14.3	NCCNCCN	1
62	Di-Isobutyl Carbinol	14.9	3.1	10.8	CC(C)CC(O)CC(C)C	1
63	Di-Isobutyl Ketone	16	3.7	4.1	CC(C)CC(=O)CC(C)C	1
64	Dimethoxymethane	15	1.8	8.6	COCOC	1
65	Dimethyl Ethanolamine	16.1	9.2	15.3	CN(C)CCO	1
66	Dimethyl Formamide	17.4	13.7	11.3	CN(C)C=O	1
67	Dimethyl Phthalate	18.6	10.8	4.9	COC(=O)c1ccccc1C(=O)OC	1
68	Dimethyl Sulfone	19	19.4	12.3	CS(C)(=O)=O	1
69	Dimethyl Sulfoxide	18.4	16.4	10.2	CS(C)=O	1
70	Dioctyl Adipate	16.7	2	5.1	CCCCCCCCOC(=O)CCCCC(=O)OC CCCCCCC	1
71	Dioctyl Phthalate	16.6	7	3.1	CCCCC(CC)COC(=O)c1ccccc1C(=O) OCC(CC)CCCC	1

72	Dipropyl Amine	15.3	1.4	4.1	CCCNCCC	1
73	Dipropylene Glycol	16.5	10.6	17.7	OCCCOCCCO	1
74	Dipropylene Glycol Methyl Ether	15.5	5.7	11.2	COCCCOCCCO	1
75	Epichlorohydrin	18.9	7.6	6.6	ClCC1CO1	1
76	Ethanol	15.8	8.8	19.4	CCO	1
77	Ethanolamine	17	15.5	21.2	NCCO	1
78	Ethyl Acetate	15.8	5.3	7.2	CCOC(C)=O	1
79	Ethyl Acrylate	15.5	7.1	5.5	C=CC(=O)OCC	1
80	Ethyl Benzene	17.8	0.6	1.4	CCc1ccccc1	1
81	Ethyl Lactate	16	7.6	12.5	CCOC(=O)C(C)O	1
82	Ethylene Carbonate	19.4	21.7	5.1	O=C1OCCO1	1
83	Ethylene Cyanohydrin	17.2	18.8	17.6	N#CCCO	1
84	Ethylene Dichloride	19	7.4	4.1	ClCCCl	1
85	Ethylene Glycol	17	11	26	OCCO	1
86	Ethylene Glycol Butyl Ethyl Ether	15.3	4.9	4.6	CCCCOCCOCC	1
87	Ethylene Glycol Di-t-Butyl Ether	14.7	4.1	8.2	CC(C)(C)OCCOC(C)(C)C	1
88	Ethylene Glycol Methyl t-Butyl Ether	15.3	5.1	8.2	COCCOC(C)(C)C	1
89	Ethylene Glycol Mono t-Butyl Ether	15.3	6.1	10.8	CC(C)(C)OCCO	1
90	Ethylene Glycol Monobutyl Ether	16	5.1	12.3	CCCCOCCO	1
91	Ethylene Glycol Monoethyl Ether	16.2	9.2	14.3	CCOCCO	1
92	Ethylene Glycol Monoethyl Ether Acetate	15.9	4.7	10.6	CCOCCOC(C)=O	1
93	Ethylene Glycol Monoisobutyl Ether	15.2	4.9	9.6	CC(C)COCCO	1
94	Ethylene Glycol Monomethyl Ether	16.2	9.2	16.4	COCCO	1
95	Formamide	17.2	26.2	19	NC=O	1
96	Formic Acid	14.3	11.9	16.6	O=CO	1
97	Furan	17.8	1.8	5.3	c1ccoc1	1
98	Furfuryl Alcohol	17.4	7.6	15.1	OCc1ccco1	1
99	gamma-Butyrolactone	19	16.6	7.4	O=C1CCCO1	1
100	Glycerol	17.4	12.1	29.3	OCC(O)CO	1
101	Glycidyl Methacrylate	16.3	8.5	5.7	C=C(C)C(=O)OCC1CO1	1
102	Hexafluoro Isopropanol	17.2	4.5	14.7	OC(C(F)(F)F)C(F)(F)F	1
103	Hexafluorohexanol	15.1	4.4	9.9	CCCC(F)(F)C(F)(F)C(O)(F)F	1
104	Hexamethylphosphoramide	18.5	8.6	11.3	CN(C)P(=O)(N(C)C)N(C)C	1
105	Hexane	14.9	0	0	CCCCCC	1
106	Hydroxyethyl Acrylate	16	13.2	13.4	C=CC(=O)OCCO	1
107	Isoamyl Acetate	15.3	3.1	7	CC(=O)OCCC(C)C	1
108	Isobutyl Acetate	15.1	3.7	6.3	CC(=O)OCC(C)C	1
109	Isobutyl Alcohol	15.1	5.7	15.9	CC(C)CO	1
110	Isobutyl Isobutyrate	15.1	2.9	5.9	CC(C)COC(=O)C(C)C	1
111	Isophorone	16.6	8.2	7.4	CC1=CC(=O)CC(C)(C)C1	1

112	Lauryl Methacrylate	14.4	2.2	5.1	C=C(C)C(=O)OCCCCCCCCCCCC	1
113	m-Cresol	18	5.1	12.9	Cc1cccc(O)c1	1
114	Mesityl Oxide	16.4	6.1	6.1	CC(=O)C=C(C)C	1
115	Methacrylic Acid	15.8	2.8	10.2	C=C(C)C(=O)O	1
116	Methacrylonitrile	15.8	15.1	5.4	C=C(C)C#N	1
117	Methanol	15.1	12.3	22.3	CO	1
118	Methyl Acetate	15.5	7.2	7.6	COC(C)=O	1
119	Methyl Acrylate	15.3	6.7	9.4	C=CC(=O)OC	1
120	Methyl Ethyl Ketone	16	9	5.1	CCC(C)=O	1
121	Methyl Ethyl Ketoxime	14.7	4.9	7.8	CCC(C)=NO	1
122	Methyl Isoamyl Ketone	16	5.7	4.1	CC(=O)CCC(C)C	1
123	Methyl Isobutyl Carbinol	15.4	3.3	12.3	CC(C)CC(C)O	1
124	Methyl Isobutyl Ketone	15.3	6.1	4.1	CC(=O)CC(C)C	1
125	Methyl Methacrylate	15.8	6.5	5.4	C=C(C)C(=O)OC	1
126	Methylene Dichloride	18.2	6.3	6.1	ClCCl	1
127	Morpholine	18.8	4.9	9.2	C1COCCN1	1
128	N,N-Dimethyl Acetamide	16.8	11.5	10.2	CC(=O)N(C)C	1
129	n-Butyl Acetate	15.8	3.7	6.3	CCCCOC(C)=O	1
130	n-Butyl Acrylate	15.6	6.2	4.9	C=CC(=O)OCCCC	1
131	Nitrobenzene	20	8.6	4.1	O=[N+]([O-])c1ccccc1	1
132	Nitroethane	16	15.5	4.5	CC[N+](=O)[O-]	1
133	Nitromethane	15.8	18.8	5.1	C[N+](=O)[O-]	1
134	N-Methyl-2-Pyrrolidone	18	12.3	7.2	CN1CCCC1=O	1
135	o-Dichlorobenzene	19.2	6.3	3.3	Clc1ccccc1Cl	1
136	Pentoxone	15.3	6	5.9	COC(C)(C)CC(C)=O	1
137	Propylene Carbonate	20	18	4.1	CC1COC(=O)O1	1
138	Propylene Glycol	16.8	9.4	23.3	CC(O)CO	1
139	Propylene Glycol Monomethyl Ether	15.6	6.3	11.6	COCC(C)O	1
140	p-Xylene	17.6	1	3.1	Cc1ccc(C)cc1	1
141	Pyridine	19	8.8	5.9	c1ccncc1	1
142	Styrene	18.6	1	4.1	C=Cc1ccccc1	1
143	t-Butyl Alcohol	15.2	5.1	14.7	CC(C)(C)O	1
144	Tetrahydrofuran	16.8	5.7	8	C1CCOC1	1
145	Tetrahydrofurfuryl Alcohol	17.8	8.2	10.2	OCC1CCCO1	1
146	Tetrahydronaphthalene	19.6	2	2.9	c1ccc2c(c1)CCCC2	1
147	Tetramethylurea	16.7	8.2	11	CN(C)C(=O)N(C)C	1
148	Toluene	18	1.4	2	Cc1ccccc1	1
149	Trichloroethylene	18	3.1	5.3	ClC=C(Cl)Cl	1
150	Tricresyl Phosphate	19	12.3	4.5	Cc1ccccc1OP(=O)(Oc1ccccc1C)Oc 1ccccc1C	1
151	Triethylamine	17.8	0.4	1	CCN(CC)CC	1
152	Triethylphosphate	16.7	11.4	9.2	CCOP(=O)(OCC)OCC	1
153	Trimethylphosphate	16.7	15.9	10.2	COP(=O)(OC)OC	1
154	Trioctyl Phosphate	16.2	5.9	4.2	CCCCCCCCOP(=O)(OCCCCCCCC)O CCCCCCCC	1

155	Tripropylene Glycol Monomethyl Ether	15.3	5.5	10.4	COCC(C)OCC(C)OCC(C)O	1
156	Urea	20.9	18.7	26.4	NC(N)=O	1
157	Benzoic Acid	17.63	10.1	10.74	O=C(O)c1ccccc1	2
158	Ibuprofen	16.44	6.39	8.89	CC(C)Cc1ccc(C(C)C(=O)O)cc1	2
159	Salicylic Acid	16.55	12.43	14.62	O=C(O)c1ccccc1O	3
160	Piroxicam	16.8	21.4	6.6	CN1C(=C(O)Nc2ccccn2)C(=O) c2ccccc2S1(=O)=O	4
161	Niflumic Acid	16.8	12.1	11.7	O=C(O)c1cccnc1Nc1cccc(C(F)(F)F)c1	4
162	Phenylbutazone	17.5	12.5	10.7	CCCCC1C(=O)N(c2ccccc2)N (c2ccccc2)C1=O	5
163	Theophylline	16.8	11.3	13.7	Cn1c(=O)[nH]c2nc(O)[nH]c2c1=O	5
164	Caffeine	17.3	13.7	13.4	Cn1c(=O)c2c(ncn2C)n(C)c1=O	5
165	Citric Acid	16.2	13.5	17.3	O=C(O)CC(O)(CC(=O)O)C(=O)O	6
166	Lorazepam	15.9	15.6	13.8	O=C1Nc2ccc(Cl)cc2C(c2ccccc2Cl)=NC1O	7
167	Oxazepam	15.6	16.2	13.6	O=C1Nc2ccc(Cl)cc2C(c2ccccc2)=NC1O	7
168	Diazepam	15.9	13.3	8.6	CN1C(=O)CN=C(c2ccccc2)c2cc(Cl)ccc21	7
169	Prazepam	15.7	12.6	6.8	O=C1CN=C(c2ccccc2)c2cc(Cl)ccc 2N1CC1CC1	7
170	Diclofenac	18.2	12.9	10.6	O=C(O)Cc1ccccc1Nc1c(Cl)cccc1Cl	2
171	p-Aminobenzoic Acid	17.3	14.3	14.4	Nc1ccc(C(=O)O)cc1	2
172	Haloperidol	17.2	9	10.8	O=C(CCCN1CCC(O)(c2ccc(Cl)cc2)CC1) c1ccc(F)cc1	8
173	Sucrose	17.1	18.5	13.1	OCC1OC(OC2(CO)OC(CO)C(O) C2O)C(O)C(O)C1O	9
174	Mannitol	16.2	24.5	14.6	OC[C@@H](O)[C@@H](O)[C@H] (O)[C@H](O)CO	9
175	Lactose	17.6	28.7	19	OCC1OC(OC2C(CO)OC(O)C (O)C2O)C(O)C(O)C1O	9
176	Meloxicam	19.2	13.2	5	Cc1cnc(NC(O)=C2C(=O)c3ccccc3S (=O)(=O)N2C)s1	9
177	Naphthalene	20.6	4	1.9	c1ccc2ccccc2c1	10
178	Naproxen	17.4	12.1	9.9	COc1ccc2cc(C(C)C(=O)O)ccc2c1	11
179	p-Hydroxybenzoic Acid	17	14.5	13.8	O=C(O)c1ccc(O)cc1	12
180	Pimozide	19.3	5.4	11.6	O=c1[nH]c2ccccc2n1C1CCN(CCCC(c2ccc (F)cc2)c2ccc(F)cc2)CC1	13
181	Temazepam	21.9	9.8	8.2	CN1C(=O)C(O)N=C(c2ccccc2)c2cc(Cl)ccc21	14
182	Trimethoprim	14.3	12.7	11.7	COc1cc(Cc2cnc(N)nc2N)cc(OC)c1OC	15
183	Cyclosporine	18.83	3.25	14.1	C/C=C/CC(C)C(O)C1C(O)=NC(CC) C(=O)N(C)CC(=O)N(C)C(CC(C)C)C(O) =NC(C(C)C)C(=O)N(C)C(CC(C)C)C(O)=NC (C)C(O)=NC(C)C(=O)N(C)C(CC(C)C)C (=O)N(C)C(CC(C)C)C(=O)N(C)C(C(C)C)C (=O)N1C	16
184	Digitoxine	20.73	3.69	17.61	C[C@H]1O[C@@H](O[C@H]2[C@@H] (O)C[C@H](O[C@H]3[C@@H](O)C[C@H] (O[C@H]4CC[C@]5(C)[C@H]6C[C@@H] (O)[C@]7(C)[C@@H](C8=CC(=O)OC8)CC [C@]7(O)[C@@H]6CC[C@@H]5C4)O [C@@H]3C)O[C@@H]2C)C[C@H](O) [C@@H]1O	16
185	Dicoumarol	26.25	5.57	17.83	O=C1OC2C=CC=CC2C(O)=C1Cc1c(O)c 2ccccc2oc1=O	16
186	Erythromycin	18.09	3.35	15.65	CC[C@H]1OC(=O)[C@H](C)[C@@H](O [C@H]2C[C@@](C)(OC)[C@@H](O) [C@H](C)O2)[C@H](C)[C@@H](O [C@@H]2O[C@H](C)C[C@H](N(C)C) [C@H]2O)[C@](C)(O)C[C@@H](C)C(=O) [C@H](C)[C@@H](O)[C@]1(C)O	16
187	Quinidine	20.72	5.53	11.97	C=C[C@H]1CN2CC[C@H]1C[C@@H]2	16

					[C@@H](O)c1ccnc2ccc(OC)cc12	
188	Chloramphenicol	23.06	9.5	18.68	O=C(N[C@H](CO)[C@H](O)c1ccc([N+](=O)[O-])cc1)C(Cl)Cl	[16]
189	Propranolol	19.57	3.35	11.04	C[C@]12C[C@H](O)[C@H]3[C@@H](CCC4=CC(=O)C=C[C@@]43C)[C@@H]1CC[C@]2(O)C(=O)CO	[16]
190	Tetracycline	24.99	8.53	22.25	CN(C)[C@@H]1C(O)=C(C(N)=O)C(=O)[C@@]2(O)C(O)=C3C(=O)c4c(O)cccc4[C@@](C)(O)[C@H]3C[C@@H]12	[16]
191	1,2,4-trichlorobenzene	20.2	4.2	3.2	Clc1c(Cl)ccc(Cl)c1	[17]
192	Iodobenzene	19.9	5.6	4.5	Ic1ccccc1	[17]
193	Bromobenzene	20.5	5.5	4.1	Brc1ccccc1	[17]
194	1-methyl naphthalene	20.6	0.8	4.7	c12c(cccc1C)cccc2	[17]
195	1,2,3,4-tetramethylbenzene	18.8	0.5	0.5	c1(c(c(ccc1C)C)C)C	[17]
196	1,2,3,5-tetramethylbenzene	18.6	0.5	0.5	c1(c(cc(cc1C)C)C)C	[17]
197	Quinoline	19.8	5.6	5.7	c1(c(cc(cc1C)C)C)C	[17]
198	1,2,4-trimethylbenzene	18	1	1	c1(c(ccc(c1)C)C)C	[17]
199	Fluorobenzene	18.7	6.1	2	Fc1ccccc1	[17]
200	1,1,2,2-tetrachloroethane	18.8	5.1	5.3	ClC(Cl)C(Cl)Cl	[17]
201	Isopropyl benzene	18.1	1.2	1.2	C(c1ccccc1)(C)C	[17]
202	cis-decahydronaphthalene	18.8	0	0	[C@H]12[C@@H](CCCC1)CCCC2	[17]
203	Benzyl chloride	18.8	7.1	2.6	ClCc1ccccc1	[17]
204	Tetrachloroethylene	18.3	5.7	0	ClC(=C(Cl)Cl)Cl	[17]
205	Methylene diiodide	17.8	3.9	5.5	ICI	[17]
206	Thiophene	18.9	2.4	7.8	s1cccc1	[17]
207	Bromochloromethane	17.3	5.7	3.5	BrCCl	[17]
208	n-butylbenzene	17.4	0.1	1.1	C(Cc1ccccc1)CC	[17]
209	1,3-dichloro propane	18.6	8.2	3	ClCCCCl	[17]
210	Tetrahydrothiophene	18.9	7.5	5.8	S1CCCC1	[17]
211	Ethylene dibromide	19.2	3.5	8.6	BrCCBr	[17]
212	Dibromomethane	17.8	6.4	7	BrCBr	[17]
213	Methyl iodide	17.5	7.7	5.3	IC	[17]
214	Cyclopentane	16.4	0	1.8	C1CCCC1	[17]
215	1-bromobutane	16.5	6	4.5	BrCCCC	[17]
216	Benzonitrile	17.4	9	3.3	N#Cc1ccccc1	[17]
217	n-tetradecane	16.2	0	0	C(CCCCCCC)CCCCCC	[17]
218	Methyl cyclohexane	16	0	1	C1(CCCCC1)C	[17]
219	Ethyl iodide	17.3	7.9	7.2	ICC	[17]
220	Dodecane	16	0	0	C(CCCCCC)CCCCC	[17]
221	Ethyl bromide	16.5	8.4	2.3	BrCC	[17]
222	1-bromopropane	16.4	7.9	4.8	BrCCC	[17]
223	Propyl chloride	16	7.8	2	ClCCC	[17]
224	n-butyl amine	16.2	4.5	8	NCCCC	[17]
225	Decane	15.7	0	0	C(CCCCC)CCCC	[17]
226	Nonane	15.7	0	0	C(CCCC)CCCC	[17]
227	Octane	15.5	0	0	C(CCCC)CCC	[17]
228	Heptane	15.3	0	0	C(CCC)CCC	[17]
229	1,2,3-trichloropropane	17.8	12.3	3.4	ClC(CCl)CCl	[17]
230	1,1,2-trichlorotrifluoroethane	14.7	1.6	0	ClC(Cl)(F)C(Cl)(F)F	[17]
231	Pentane	14.5	0	0	C(CC)CC	[17]
232	1-octanol	16	5	11.9	OCCCCCCCC	[17]
233	2-pentanol	15.6	6.4	13.3	O[C@H](CCC)C	[17]
234	1,4-butanediol	16.6	15.3	21.7	OCCCCO	[17]
235	2-chlorotoluene	19	4.9	2.3	Clc1c(cccc1)C	[18]
236	3-chlorotoluene	18.9	3.9	2.9	Clc1cc(ccc1)C	[18]
237	b-pinene	17.1	3	2.7	C1([C@@H]2C[C@H]1C(=C)CC2)(C)C	[18]
238	a-pinene	17.3	2.4	3.1	C1([C@@H]2C[C@H]1C(=CC2)C)(C)C	[18]
239	limonene	17.2	1.8	4.3	[C@@H]1(CCC(=CC1)C)C(=C)C	[18]
240	2-chlorophenol	19	5.5	13.9	Clc1c(O)cccc1	[18]

241	benzyl benzoate	20	5.1	5.2	O(Cc1ccccc1)C(=O)c1ccccc1	18
242	1,12-Dodecanethiol	17.3	5.7	4.1	OCCCCCCCCCCCCO	19
243	1,6-Hexanedithiol	17.4	7.6	6.4	SCCCCCCS	19
244	1,8-Octanedithiol	17.4	7.3	5.2	SCCCCCCCCS	19
245	4-Bromoanisole	19.8	7.7	7	Brc1ccc(OC)cc1	19
246	n-methyl-2-pyrrolidinone	18	12.3	7.2	O=C1N(CCC1)C	19
247	Triethylene glycol (TEG)	16	12.5	18.6	O(CCOCCO)CCO	20
248	1,8-diiodooctane (DIO)	17.6	4.8	4.6	ICCCCCCCCI	20
249	1-chloronaphthalene (CN)	19.9	4.9	2.5	Clc1c2c(ccc1)cccc2	20
250	2-Methylanisole	18.3	4.7	4.8	O(c1c(cccc1)C)C	21
251	3-Methylcyclohexanone	17.5	7.7	3.9	O=C1C[C@@H](CCC1)C	21
252	2-Methyl Tetrahydrofuran	16.9	5	4.3	O1[C@@H](CCC1)C	22

Major categories of descriptors

The descriptors are the languages that scientists use to communicate with machine learning models. Descriptors along the target property are used as input to trained machine models. Our studied materials are organic molecules. The molecular descriptors are suitable for machine leaning. Molecular descriptors are thousands in numbers. The major categories are given below:

Autocorrelation descriptors

Basak descriptors

BCUT descriptors

Burden descriptors

Connectivity descriptors

Constitutional descriptors

E-state descriptors

Kappa descriptors

Molecular property descriptors

Quantum chemical descriptors

Topological descriptors

CPSA descriptors

RDF descriptors

Geometrical descriptors

WHIM descriptors

Autocorrelation (2D and 3D) descriptors

Constitutional indices

Ring descriptors

matrix-based descriptors (2D and 3D)

MoRSE descriptors

GETAWAY descriptors

These categories also have sub categories.

Table S2. R^2 (test) of various models calculated using fingerprints as input.

δ_D		δ_P		δ_H	
Model	R^2	Model	R^2	Model	R^2
BaggingRegressor	0.40	XGBRegressor	0.40	AdaBoostRegressor	0.52
RandomForestRegressor	0.35	MLPRegressor	0.36	GradientBoostingRegressor	0.48
LarsCV	0.35	GradientBoostingRegressor	0.34	RandomForestRegressor	0.46
LassoLarsIC	0.34	RandomForestRegressor	0.33	XGBRegressor	0.45
HistGradientBoostingRegressor	0.31	AdaBoostRegressor	0.28	Lasso	0.4
LGBMRegressor	0.31	LGBMRegressor	0.22	BaggingRegressor	0.34
LassoLarsCV	0.28	HistGradientBoostingRegressor	0.22	LGBMRegressor	0.34
GradientBoostingRegressor	0.28	BaggingRegressor	0.22	HistGradientBoostingRegressor	0.34
AdaBoostRegressor	0.26	PoissonRegressor	0.21	ExtraTreeRegressor	0.33
ElasticNetCV	0.25	ExtraTreesRegressor	0.19	ExtraTreesRegressor	0.31
LassoCV	0.24	RidgeCV	0.17	SVR	0.29
GammaRegressor	0.24	BayesianRidge	0.17	NuSVR	0.29
KNeighborsRegressor	0.23	ExtraTreeRegressor	0.11	KNeighborsRegressor	0.23
GeneralizedLinearRegressor	0.23	DecisionTreeRegressor	0.09	ElasticNet	0.21
TweedieRegressor	0.23	Ridge	0	LassoLarsIC	0.2
OrthogonalMatchingPursuitCV	0.23	ElasticNetCV	0	DecisionTreeRegressor	0.19
NuSVR	0.19	LassoCV	0	MLPRegressor	0.18
SVR	0.19	GeneralizedLinearRegressor	0	GeneralizedLinearRegressor	0.17
XGBRegressor	0.13	TweedieRegressor	0	TweedieRegressor	0.17
ExtraTreeRegressor	0.1	PassiveAggressiveRegressor	0	LarsCV	0.15
BayesianRidge	0.05	KNeighborsRegressor	0	ElasticNetCV	0.15
ExtraTreesRegressor	0.05	LassoLarsCV	0	LassoLarsCV	0.08
ElasticNet	0	LassoLarsIC	0	DummyRegressor	0.08
PoissonRegressor	0	LinearSVR	0	LassoLars	0.06
RidgeCV	0	LarsCV	0	LassoCV	0.05
DecisionTreeRegressor	0	ElasticNet	0	OrthogonalMatchingPursuitCV	0.05
OrthogonalMatchingPursuit	0	SVR	0	BayesianRidge	0.05
PassiveAggressiveRegressor	0	NuSVR	0	OrthogonalMatchingPursuit	0.03
Ridge	0	HuberRegressor	0	SGDRegressor	0.01
Lasso	0	OrthogonalMatchingPursuit	0	RidgeCV	0
DummyRegressor	0	Lasso	0	PoissonRegressor	0
LassoLars	0	OrthogonalMatchingPursuitCV	0	LinearSVR	0
LinearSVR	0	DummyRegressor	0	Ridge	0
HuberRegressor	0	LassoLars	0	HuberRegressor	0
MLPRegressor	0	KernelRidge	0	PassiveAggressiveRegressor	0
GaussianProcessRegressor	0	GaussianProcessRegressor	0	GaussianProcessRegressor	0
KernelRidge	0	SGDRegressor	0	KernelRidge	0
SGDRegressor	0	LinearRegression	0	LinearRegression	0
RANSACRegressor	0	TransformedTargetRegressor	0	TransformedTargetRegressor	0
TransformedTargetRegressor	0	RANSACRegressor	0	RANSACRegressor	0
LinearRegression	0	Lars	0	Lars	0
Lars	0				

Note: GammaRegressor is failed to execute for the prediction of δ_P and δ_H.

Table S3. Hansen solubility parameters for 30 small molecule donors (SMDs)

No.	SMD	δ_D	δ_P	δ_H

1	DMPh (DPP-Py)2	20.98	9.97	5.24
2	DFPh(DPP-Py)2	21.56	8.57	5.63
3	CP3	21.63	9.99	10.2
4	CP4	18.38	9.5	2.75
5	RTh-BSe-ThR	17.93	9.72	6.67
6	SM1	21.19	10.5	4.89
7	SM2	20.98	10.7	4.89
8	BDT-TITRh	18.29	9.81	4.2
9	BDT-TI2TRh	18.29	9.81	4.2
10	DTTFB(PyDPP-T)2	20.98	13.9	4.93
11	DTTFB(TDPP-T)2	17.04	13.9	5.68
12	DTTFB(IID-T)2	20.98	10.3	6.08
13	An(DTDPPA)2	17.04	10.5	6.51
14	2D-NDT(TPD)2	17.04	10.5	6.27
15	2D-NDT(Ester)2	17.04	10.5	6.51
16	2D-NDT(Amide)2	17.04	10.5	9.89
17	CP1	20.34	10.7	4.93
18	CP2	20.98	9.97	5.17
19	ZnPTDPP	21.24	10.8	6.89
20	ZnPTDPPCN	21.56	10.8	6.33
21	ZnPTDPPO	21.56	10.8	6.89
22	BTI(2T-DCV-Hex)3	20.34	8.7	5.75
23	BTI(2T-CNA-EHex)3	20.34	10.5	5.24
24	N(Ph-2T-DCV-Hex)3	17.04	8.7	5.51
25	flu(3TRD)2	18.16	9.81	4.2
26	flu(3TCN)2	17.04	8.17	5.31
27	flu(3TIN)2	20.34	8.45	4.1
28	DR3TSBDT	18.29	9.81	4.92
29	D(CATBTzT)BDT	16.47	10	8.34
30	DCAO3TBDT	18.13	10.8	6.41

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