Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Application of Classification Models to Identify Solvents for Single-Walled Carbon Nanotubes Dispersion

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Table S1. Names, SMILES of organic solvents dataset exploited for developing and validating the classification models.

No.	**Chemical Name**	**SMILES**	**Class**
1	N-Cyclohexyl-pyrrolidinone	C1CCC(CC1)N2CCCC2=O	solvent
2	1,3-Dimethyltetrahydro-2(1H)-pyrimidinone	O=C1N(C)CCCN1C	solvent
3	1-Butylpyrrolidin-2-one	CCCCN1CCCC1=O	solvent
4	1-Benzylpyrrolidin-2-one	C1CC(=O)N(C1)CC2=CC=CC=C2	solvent
5	1-Methylpyrrolidin-2-one (NMP)	CN1CCCC1=O	solvent
6	3-(2-Oxo-1-pyrrolidinyl) propanenitrile	O=C1CCCN1CCC#N	solvent
7	N-Ethyl-pyrrolidinone	CCN1CCCC1=O	solvent
8	N-Octyl-pyrrolidone	CCCCCCCCN1CCCC1=O	solvent
9	N-Vinyl-pyrrolidinone	N1(C(CCC1)=O)C=C	solvent
10	Dimethyl-imidazolidinone	CN1CCN(C1=O)C	solvent
11	Dimethylacetamide	O=C(C)N(C)C	solvent
12	N-Formyl-piperidine	O=CN1CCCCC1	solvent
13	N-Dodecyl-pyrrolidone	CCCCCCCCCCCCN1CCCC1=O	solvent
14	Dimethylformamide	O=CN(C)C	solvent
15	Benzyl acetate	CC(=O)OCc1ccccc1	solvent
16	Propionitrile	CCC#N	solvent
17	Acrylic acid	C=CC(=O)O	solvent
18	2,2'-thiodiethanol	OCCSCCO	solvent
19	Ethanol amine	NCCO	solvent
20	Cyclopentanone	C1CCC(=O)C1	solvent
21	Chlorophenol	Oc1ccccc1Cl	solvent
22	Acetone	CC(=O)C	solvent
23	Benzyl benzoate	O=C(OCc1ccccc1)c2ccccc2	solvent
24	Isopropyl alcohol	CC(C)O	solvent
25	Cyclohexanone	C1CCC(=O)CC1	solvent
26	Toluene	Cc1ccccc1	solvent
27	Triethyleneglycol	OCCOCCOCCO	solvent
28	Formamide	O=CN	solvent
29	Benzyl alcohol	OCC1=CC=CC=C1	solvent
30	Nitropropane	O=[N+]([O-])CCC	nonsolvent
31	Ethylene glycol	OCCO	nonsolvent
32	Tetraethylene glycol	O(CCOCCO)CCOCCO	nonsolvent
33	Triethylenephosphate	P(OCC)(OCC)(OCC)=O	nonsolvent
34	Diethylenetriamine	N(CCN)CCN	nonsolvent
35	Tetrahydrofuran(THF)	O1CCCC1	nonsolvent
36	2-Methoxy-1,3-Dioxolane	O1CCOC1OC	nonsolvent
37	2-Pyrrolidone	O=C1NCCC1	nonsolvent
38	Acrylonitrile	N#CC=C	nonsolvent
39	Dichloroacetonitrile	ClC(Cl)C#N	nonsolvent

40	Pulegone	O=C1CC(CCC1=C(C)C)C	nonsolvent
41	Dibenzyl ether	O(Cc1ccccc1)Cc1ccccc1	nonsolvent
42	Dioxane	O1CCOCC1	nonsolvent
43	Benzophenone	O=C(c1ccccc1)c1ccccc1	nonsolvent
44	Dioxolane	O1CCOC1	nonsolvent
45	Benzaldehyde	O=Cc1ccccc1	nonsolvent
46	Morpholine	O1CCNCC1	nonsolvent
47	Diethyleneglycol	O(CCO)CCO	nonsolvent
48	1,3-Butanediol	OC(CCO)C	nonsolvent
49	1,1-Dichloroethane	ClC(Cl)C	nonsolvent
50	Dimethylsulphate	S(OC)(OC)(=O)=O	nonsolvent
51	Ethyl-Chloroformate	ClC(OCC)=O	nonsolvent
52	2-Nitropropane	O=[N+]([O-])C(C)C	nonsolvent
53	Dichloromethane	ClCCl	nonsolvent
54	Bromotrichloromethane	BrC(Cl)(Cl)Cl	nonsolvent
55	Furfural	o1cccc1C=O	nonsolvent
56	Heptane	C(CCC)CCC	nonsolvent
57	Aniline	Nc1ccccc1	nonsolvent
58	Acetonitrile	N#CC	nonsolvent
59	Tert-butylchloride	ClC(C)(C)C	nonsolvent
60*	1,1,3,3-tetramethylguanidine (TMG)	CN(C)C(=N)N(C)C	nonsolvent
61*	1,8-diazabicycloundec-7-ene (DBU)	N1=C2N(CCCCC2)CCC1	solvent
62*	1,5-diazabicyclo(4.3.0)non-5-ene (DBN)	N\2=C1\N(CCC1)CCC/2	nonsolvent