Electronic Supplementary Material for CrystEngComm

Crystal Structure Prediction with the Supramolecular Synthon Approach: Experimental Structures of 2-Amino-4-ethylphenol and 3-Amino-2-naphthol and Comparison with Prediction

Archan Dey, Narendra Nath Pati and Gautam R. Desiraju*

School of Chemistry, University of Hyderabad, Hyderabad 500 046, India.

E-mail: gautam_desiraju@yahoo.com

Supporting Information
(13 pages)

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Scheme SI1

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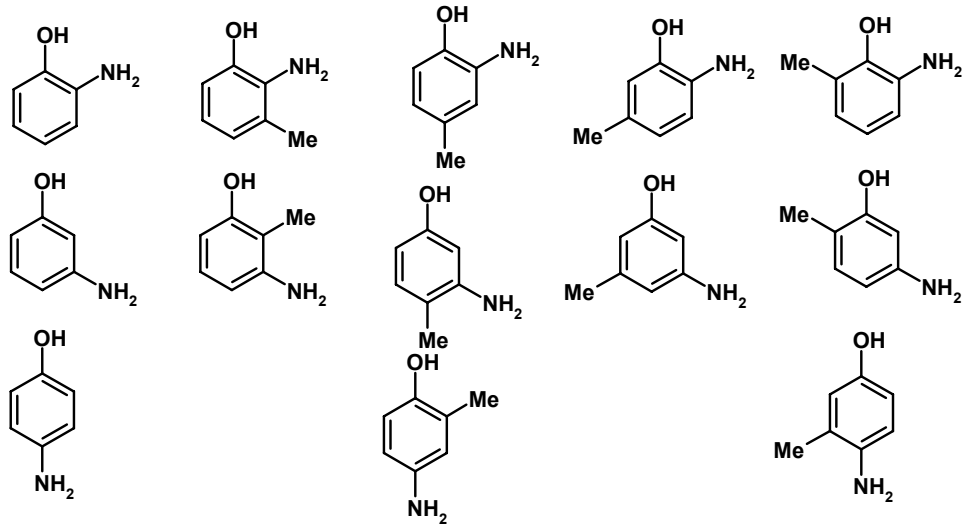
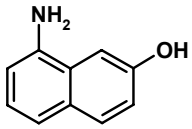
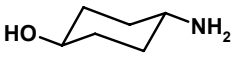
Training set compounds



Test set compounds



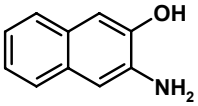
Correct prediction



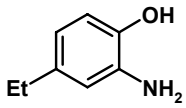
Correct prediction

(J. Am. Chem. Soc., 2005, 127, 10545)

Experimental structures determined after prediction



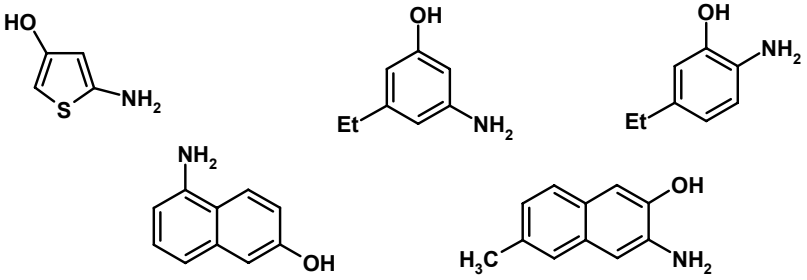
Correct prediction



Incorrect prediction

(From this paper)

Experimental structures determined after prediction



No experimental work has been carried out on these compounds

Table SI1: Polymorph prediction results: ten lowest energy crystal structures for **1** and **2**[a]

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Aminol	Rank	Re-rank	Space Group	Energy kcal/mol	Net Vol. Å^3	Cell Parameters Å	Structural Description
1	**1**	**1**	***C*2/*c***	**–36.620**	**183.84**	**30.788,5.604,8.528, 88.17**	**Synthons I, II and II, variation of C–H···O for synthon IV.**
	2	–	*C*2/*c*	–36.607	180.06	35.935, 5.195, 8.812, 118.88	Distorted dimer herringbone arrangement with O–H···O, therefore rejected.
	3	–	*C*2/*c*	–36.598	183.35	31.007,5.617, 8.446, 94.37	Variation of structure 2.
	4	–	*Pbca*	–36.061	180.34	30.181, 5.246, 8.998	Variation of structure 2.
	5	3	*C*2/*c*	–36.043	170.08	32.919, 4.352, 10.273, 112.39	Synthon **I**. Synthon **III** distorted.
	6	4	*C*2/*c*	–35.844	171.64	10.240, 4.344, 33.199, 68.41	Variation of structure 5.
	7	2	*C*2/*c*	–35.820	177.69	33.031, 5.649, 8.596, 62.410	Variation of structure 1.
	8	–	*C*2/*c*	–35.806	180.07	35.364, 5.229, 8.902, 60.47	Variation of structure 2.
	9	–	*Pbca*	–35.773	180.78	4.985, 9.663 30.024	Rejected because small synthons not found.
	10	–	*Pbca*	–35.742	182.58	31.530, 4.772, 9.708	Rejected because small synthons not found.
2	**1**	**1**	***C*2/*c***	**68.744**	**188.35**	**31.575, 5.850, 8.889, 66.58**	**Synthons I, II, III and IV with distorted C–H···O.**
	2	2	*C*2/*c*	69.084	190.52	30.198, 5.847, 8.765, 99.99	Variation of structure 1.
	3	1	Pbca	69.389	193.90	29.879, 5.844, 8.883	Variation of structure 1.
	4	–	Pbca	70.249	185.82	9.630, 32.780, 4.709	Rejected because small synthons not found.
	5	–	*Iba*2	70.692	197.24	31.680, 9.944, 5.009	Rejected because small synthons not found.
	6	–	$Pna2_1$	70.850	188.23	5.437, 27.969, 4.951	Rejected because small synthons not found.
	7	4	*Pbca*	70.865	187.00	9.188, 32.919, 4.946	Synthon **I** without large synthons.
	8	3	*C*2/*c*	71.044	186.59	34.354, 4.515, 10.054	Synthons **I**, **III**. Unusual conformation of hydroxyl group.
	9	3	$P2_1/c$	71.166	187.65	5.328, 4.457, 32.541	Variation of structure 8.
	10	3	$P2_1/c$	71.193	187.69	4.462, 5.302, 31.752	Variation of structure 9.

[a]The structures in bold font are the predicted ones.

Table SI2: Pairs of compounds with both methyl and ethyl derivatives, which have crystal structures in the CSD

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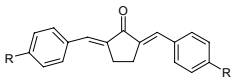
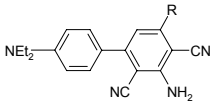
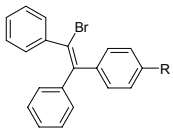
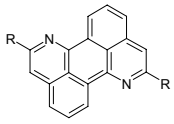
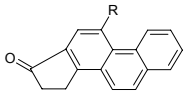
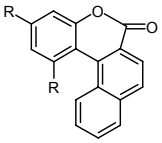
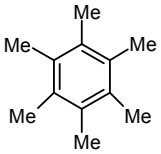
Sl No	Compounds	Refcode	Reduced cells	Structural Description	Remarks
1		Me **QADYUP** Et **QADZIE**	*Pca*2$_1$ 5.998 14.899, 18.152, V = 1622.1 *C*2/*c* 6.093, 15.633, 19.861, 97.39, 90.00, 101.24 V = 1839.6	Trifurcated C—H….O interactions. For Et molecules it two interactions come form same molecule.	Not homologous
2		Me **FACSEI** Me **FACSEI01** Et **QOGLIH**	*P2$_1$/c*, 9.293, 10.865, 10.865, 90.37, V =1688.4 *Fdd2* 7.749, 12.152, 19.007, 86.27, 78.24, 71.41, V = 1660.9 *P2$_1$/c* 10.346, 10.892, 16.571, 101.50, V = 1829.8	Et derivative and one of the polymorph form dimer with, N—H···N interactions. In case of methyl derivative the dimer is discreet and other polymorph of methyl have only N—H···N interaction	Not homologous
3		Me **FABSIK10** Et **ZIZYIQ**	*P2$_1$/c* 5.762, 8.653, 33.365, 96.85, V = 1651.7 *P*2$_1$/*c* 7.989, 12.977, 13.909, 97.89, V = 1428.3	Br···Br interaction is present in case of methyl but in case of case of ethyl it is absent.	Not homologous
4		Me **WUGGEK** Et **VADJAM**	*P*2$_1$/*c* 6.849,9.113, 11.449, 104.63, V=691.4 *P*2$_1$/*c* 8.611, 12.948, 14.361 90.93, V = 1601.0	No characteristic short contacts.	Not homologous
5		Me **VEFVUX** Et **VEFWOS01**	*Pbca* 7.526, 14.355, 23.153, V = 2501.4 *Pbca* 7.647, 17.012, 21.042, V = 2737.2	In case of Me chain structure but in Et it is dimer through C—H···O interaction.	Not homologous
6		Me **YADRIE** Et **YADROK**	*P*-1 8.204, 8.547, 11.450, 76.21, 72.69, 61.58, V = 669.6 *P2$_1$/n* 10.318, 11.528, 14.278, 114.48, V =1545.6	Two types of C—H···O interaction are present in case of Me but in Et one type is present.	Not homologous
7		Me **HMBENZ04** Et **ZZZEMS01**	*P*-1 5.260, 6.199, 8.004, 103.82, 98.72,100.19, V = 244.3 *P*-1 6.013, 8.405, 9.286, 109.14, 107.99, 95.59, V = 411.3	No characteristic short contacts.	Not homologous

Table SI3: Pairs of compounds with both phenyl and naphthyl derivatives, which have

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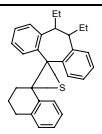
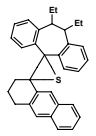
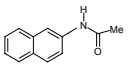
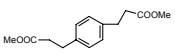
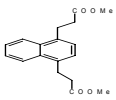
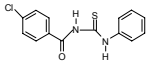
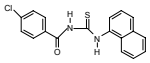
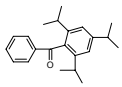
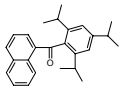
crystal structures in the CSD

Sl. No.	Compounds	Refcode	Reduced cell	Structural description	Remarks
1		**ABEKAT** ($P3_12_1$)	8.888, 8.888, 48.492, 120.00, V=3317.2	C–H(sp2)···S and C–H···π interactions are present.	Not homologous
		**ABEKEX** ($P2_1$)	8.601, 9.682, 15.196, 91.66, V=1264.9	C–H(sp3)···S present but no C–H···π interaction.	
2		**ACANIL03** (*Pbca*)	7.980, 9.474, 19.615, V=1482.9	Molecules propagate with N–H···O interaction and C–H···O acts as supporting interaction.	Homologous
		**ACACTB** (*Pbca*)	7.518, 9.651, 28.230 V=2048.0	Molecules propagate in similar fashion. It gains C–H···π in expense of C–H···O	
3		**PPDACR** (*P*-1)	5.844, 6.893, 8.382, 98.11, 94.97, 112.30, V=305.6	Forms planar dimer through C–H···O interactions.	Not homologous
		**ACAYAE** ($P2_1/c$)	5.645, 11.934, 22.253, 90.76, V=1499.0	There is absence of this type of synthon.	
4		**GACXEN10** ($P2_1/c$)	8.667, 11.851, 13.456, 90.60, V=1382.	It contains only N–H···S (non-planar) dimer	Not homologous
		**AMEBOJ** (*P*-1)	6.962, 10.770, 11.738, 65.76, 80.03, 84.86, V=790.2	Propagate through alternative N–H···S (non-planar) dimer and N–H···O (planar) dimer.	
5		**BAZZAD01** ($P2_1/n$)	8.944, 13.293, 16.657, 93.09, V=1977.5	Chain structure through C–H(sp2)···O intermolecular interaction	Not homologous
		**BAZZIL** ($P2_1/c$)	11.07,17.36, 11.96, 111.2, V=2142.87 (From Hg)	Forms C–H···π interaction in expense of C–H(sp2)···O.	
6		**HEYJOK** ($P2_12_12_1$) Z'= 5	3.901,23.00, 35.368, V=3174.4	Forms C–H···N interaction.	Not homologous

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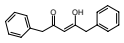
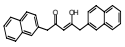
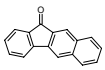
		**BEZSAA** ($P2_1/a$) $Z' = 2$	15.078, 9.122, 13.591, 108.08, V=1777.03 (From Hg)	Forms dimer through C–H···N & C–H···π.	
7		**BIPHEN04** ($P2_1/a$)	5.630, 8.120, 9.510, 95.10, V= 433.0	No specific interaction	Not homologous
		**BINAPH01** ($C2/c$)	6.342, 10.218, 11.029, 75.47, 73.29, 90.00, V=660.6	No specific interaction	
8		**NUTSUQ** ($P2_1/c$)	7.392, 8.965, 14.925, 102.90, V=964.1	It forms helical O–H···O interactions through intra and intermolecular interactions.	Not homologous
		**BIRKOC** ($Iba2$)	15.691, 21.617, 8.628, V=2926.55 (From Hg)	Isolated O–H···O present.	
9		**BOLZAD** ($C2/c$)	5.519,8.601,4.716, 84.84, 79.19, 90.00, V= 683.3	Forms intrarmolecular O–H···O.	Homologous
		**BOLZEH** ($C2/c$)	5.805, 8.313, 18.974, 89.91, 81.20, 90.00, V= 904.8	Similar packing with additional C–H···π interaction	
10		**HEHLAH** ($P2_1/n$)	9.966, 10.007, 13.053, 96.74, V=1292.8	Br···Br and C–H···π interaction are present.	Not homologous
		**BRMBNP** ($P2_12_12_1$)	10.360, 13.052, 13.187, V=1783.13 (From Hg)	Br···Br interaction is absent. But C–H···Br & C–H···π interactions are present.	
11		**FLURON** ($Pbca$)	12.550, 16.068, 18.650, V=3760.8	Forms trifurcated C–H···O interaction forms between different molecules.	Not homologous
		**BZFLRN** ($P2_1/c$)	6.103, 11.867, 16.405, 108.32, V=1127.9	Forms bifurcated C–H···O interaction between same molecules and become forms a dimer.	
12		**THBZPS10** ($P2_1/n$)	5.863, 13.403, 14.042, 106.40, V=1058.6	No significant short contact is present.	Not homologous
		**CELDUS** ($P2_12_12_1$)	5.873, 13.677, 15.668, V=1258.5	C–H···S and C–H···π interactions are present.	

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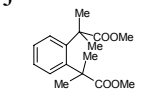
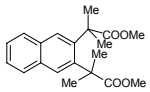
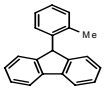
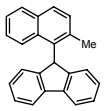
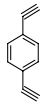
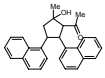
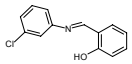
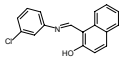
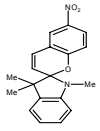
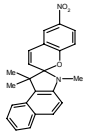
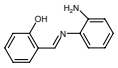
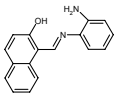
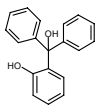
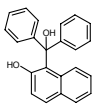
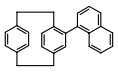
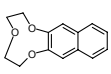
13		**CIXGIZ** (*A*2/*a*)	8.467, 9.585, 10.66, 104.26, 90.00, 116.1, V=746.7	Carbonyl O is bifurcated acceptor and OCH_3 takes part in packing.	Not homologous
		**CIXGOF** ($P2_1/c$)	9.099, 11.293, 18.849, 113.58, V=1775.1	Carbonyl O is not bifurcated acceptor and OCH_3 has no role in packing.	
14		**INOHOI** ($P2_1/c$)	6.075, 12.989, 18.790, 104.70, V=1434.1	One benzene ring attracts one H by C–H···π· interaction.	Not homologous
		**COTYUF** ($P2_1/n$)	9.264, 8.621, 21.083, 91.53, V=1683.19	Different packing with C–H···π· interactions. Packing is different.	
15		**DCLBEN03** ($P2_1/c$)	6.021, 7.175, 7.414 107.54, V=305.4	C–H···π· interaction is present.	Not homologous
		**DCLNAQ** ($P2_1/c$)	3.939, 13.386, 16.693, 103.20, V=857.0	No specific interaction is present.	
16		**ETYNBZ01** ($P2_1/c$)	3.887, 5.931, 15.114, 90.84, V=348.4	Alkyne π bond bifurcated acceptor.	Not homologous
		**DEYNAP** ($Pca2_1$) Z'=2	4.024, 15.638, 31.065, V=1954.8	Alkyne π bond trifurcated acceptor.	
17		**NPURET** (*Pbca*)	8.56, 9.67, 22.44, V=1857.48 (From Hg)	Benzenes are *trans* with respect to the main chain. OCH_3 group is act as bifurcated acceptor.	Not homologous
		**DODGAE** ($P2_1/c$)	7.618, 8.451, 17.388, 95.34, V=1114.6	Naphthalene rings are in *cis* with respect to the main chain.	
18		**ESIBAJ** (*P*-1)	5.726, 9.535, 16.038, 82.25, 89.04, 76.96, V=845.2	Forms intramolecular O–H···O·	Not homologous
		**ESIBIR** (*Pbca*)	10.953, 13.392, 28.412, V=4167.5	Forms intermolecular O–H···O	

19		**NADZUO** ($Pca2_1$)	3.898, 10.806, 25.499, V=1074.1	No specific interaction	Not homologous
		**FADBUI** ($C2/c$)	4.786, 15.538, 18.994, 107.91, 90.00, 98.86, V=1326.3	C–H···π· interaction is present.	
20		**BEXLUL01** ($P2_1/n$) Z'=2	10.979, 16.146, 19.728, 105.83, V=3364.6	O is trifurcated acceptor. C–H···O interaction.	Not homologous
		**FAFSEK** ($P2_12_12_1$)	11.227, 11.242, 15.393, V=1942.8	C–H···π interaction in expense of C–H···O interaction.	
21		**YORFIU** ($Pna2_1$)	11.501, 6.833, 14.232, V=1118.44	Intramolecular O–H···N and intermolecular N–H···O	Not homologous
		**HOFNEV** ($P2_1$)	7.203, 7.670, 12.197, 99.10, V= 665.4	Intramolecular O–H···N, no intermolecular N–H···O but C–H···π and C–H···O interaction are present.	
22		**HNPHMB** ($C2/c$)	8.630, 12.006, 15.989, 106.65, 90.00, 111.06, V=1471.3	C–H···O interaction is present, trifurcated in nature.	Not homologous
		**HNPHMA** ($P2_1/c$)	8.402, 13.097, 16.400, 111.25, V=1682.1	C–H···π interaction in expense of C–H···O interaction.	
23		**CAHHAV** ($P2_1/c$)	7.850, 14.717, 15.177, 118.10, V=1546.8	Aromatic C–H···π· interaction is only present.	Not homologous
		**HOQLOO** ($Pca2_1$)	7.287, 15.860, 30.95 V=3577.5	Aliphatic & aromatic both C–H···π interactions are present.	
24		LENYOS ($Pbca$)	8.268, 8.535, 25.005, V=1764.5	O is bifurcated, trifurcated acceptor.	Not homologous
		**HUGHUM** ($P2_1/c$)	8.866, 6.451, 20.110, 91.055, V=1149.99	O is not bi or trifurcated acceptor.	

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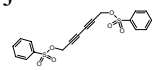
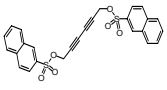
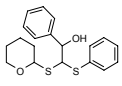
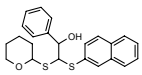
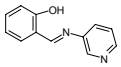
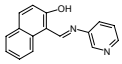
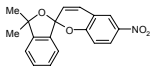
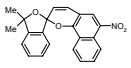
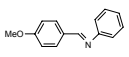
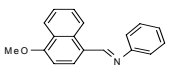
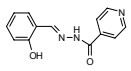
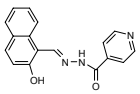
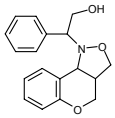
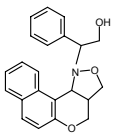
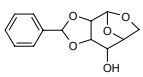
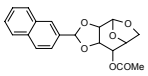
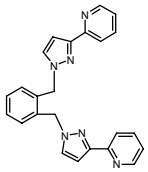
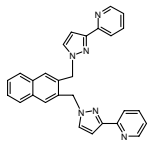
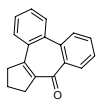
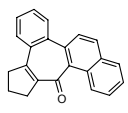
25		**COYMAE** ($P2_1/c$)	5.280,13.079, 13.977, 111.19, V=900.0	C–H···O interaction is absent.	Not homologous
		**HXYNPS** ($P2_1/n$)	5.421, 13.446, 15.903, 100.96, V=1138.1	C–H···O interaction is present	
26		**ALAFEY** ($P2_1/c$)	9.172, 9.614, 19.734, 93.45, V=1737.0	C–H···O H bond.	Not homologous
		**IFAKOP** ($P2_1$)	9.903, 10.201, 10.564, 107.79, V=1016.2	O–H···O intermolecular H bond.	
27		**SLCPYA** ($P2_1/n$)	4.692, 14.316, 15.233, 98.19, V=1012.8	Packing is not planar. C–H···N bifurcated interaction.	Not homologous
		**IHAREO** ($P2_1/a$)	7.010, 12.764, 13.669, 101.23, V=1199.6	Packing is almost planar due to C–H···π· & C–H···N interaction.	
28		**PHESAZ01** (*Pnma*)	5.894, 7.916, 20.974, V= 978.6	Forms zigzag chain.	Not homologous
		**JUKYOD** ($P2_1/a$)	8.306, 23.347, 25.269, 91.71, V=4898.0	Herringbone type due to C–H···π· interaction.	
29		**BEJBUN** ($P112_1/b$)	10.857, 11.978, 24.481, 96.97, V=3160.1	O of NO_2 forms bifurcated C–H···O synthon with only aromatic H atom.	Not homologous
		**KAJSOD** ($P2_1/b$)	11.037, 12.612, 13.627, 106.97, V=1814.3	O of NO_2 forms bifurcated C–H···O synthon with both aliphatic & aromatic H atom.	
30		**YAHDER** ($P2_1/n$) Z′=2	10.067, 12.637, 17.732, 95.23, V=2246.4	C–H···N & C–H···π interactions are present.	Not homologous
		**KAPDIO** ($P2_1/c$)	8.027, 10.280, 16.731, 90.33, V=1380.6	C–H···π interaction is only present.	
31		**WEHFEU** ($P2_1/n$)	8.133, 9.534, 15.548, 105.67, V=1160.8	Carbonyl O takes part in packing through C–H···O interaction.	Not homologous
		**KAVSEF** ($P2_1/c$)	8.790, 10.228, 15.797, 99.36, V=1401.3	Carbonyl O doesn't take part in packing.	

32		**QQQGMJ01** ($P2_1/c$)	7.218, 7.838, 12.366, 106.30, V=671.5	Forms tetramer through C–H···O synthon. C–H···π interaction is absent.	Not homologous
		**LEQJAS** ($Pna2_1$)	7.700, 15.400, 15.695, V=1861.1	Not forms tetramer. C–H···π interaction is present.	
33		**RIYFAG** ($P2_12_12_1$)	4.036, 11.806, 15.695, V=747.9	Not forms zigzag chain. C–H···O bifurcated interaction is present.	Not homologous
		**LOVBON** ($P2_1/c$)	8.590, 10.330, 11.757, 109.02, V=986.4	Forms zigzag chain.	
34		**LOXNUH** ($P2_12_12_1$)	5.202, 13.860, 20.039, V=1444.8	Forms zigzag chain. C–H···O bifurcated interaction is present.	Not homologous
		**LOXMUG** ($P2_12_12_1$) $Z'=2$	5.568, 16.754, 36.597, V=3414.1	Not forms zigzag chain. C–H···π interaction is main factor in packing.	
35		**QIJCER** ($P2_1$)	6.338, 7.067, 13.027, 96.43, V=579.8	Forms chain trough O–H···O interaction.	Not homologous
		**LUMNIQ** ($P2_12_12_1$) $Z'=2$	5.723, 17.232, 33.173, V=3271.3	C–H···π interaction in expense of O–H···O interaction.	
36		**NUSJIU** ($P2_1/c$)	8.103, 10.183, 24.930, 102.11, V=2011.4	C–H···N interaction is present.	Not homologous
		**LUZHOD** ($C2/c$)	7.778, 12.219, 12.219, 69.25, 82.68, 82.68, V=1072.9	C–H···N interaction is absent. C–H···π interaction is main factor in packing.	
37		**MATBOY** ($Pbca$)	8.055, 17.378, 17.919, V=2508.2	O interacts with three moieties by trifurcated C–H···O interactions.	Not homologous
		**MATBUE** ($Pbca$)	11.847, 12.489, 20.703, V=3063.1	O interacts with two moieties by bifurcated C–H···O interactions.	
38		**PIPROV** ($Pbca$)	7.668, 14.123, 22.122, V=2395.7	Forms dimer through I···I interaction.	Not homologous

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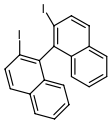
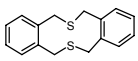
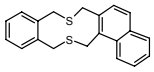
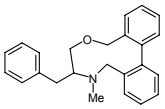
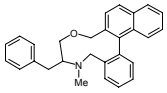
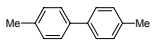
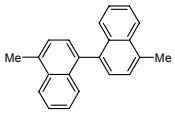
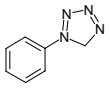
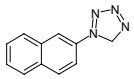
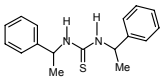
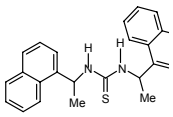
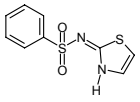
		**MEBCOL** ($P2_12_12_1$)	10.439, 12.054, 13.318, V=1675.8	I···I interaction is absent here.	
39		**VAKXAG01** ($P2_1/c$)	4.933, 8.274, 16.550 100.37, V=664.5	Forms chain structure through C–H···S interaction.	Not homologous
		**MEKHEP** ($C2/c$)	9.470, 12.913, 14.530, 108.52, 90.00, 111.51, V=1553.7	Forms dimer through C–H···S interaction.	
40		**MELTUS** ($P2_12_12_1$) Z'=2	10.044, 10.765, 35.262,V=3812.5	Forms dimer through C–H···O & C–H···π· interaction.	Not homologous
		**MELWAB** ($P2_12_12_1$)	10.357, 10.680, 19.388,V=2144.7	Forms chain structure through C–H···O interaction.	
41		**BTOLYL** ($P2_1/c$) Z'=2	9.770, 13.670, 16.108, 93.98, V=2146.0	Aromatic H atom acts as a bifurcated donor.	Not homologous
		**MEPPHA** ($C2/c$)	8.527, 8.527, 11.572, 71.58, 71.58,78.31, V=752.5	Aromatic H atom acts as a single donor. Herringbone type.	
42		**PHTETZ01** ($P2_1/a$)	4.328, 10.936, 15.146, 97.50, V=710.7	C–H(five membered H)···N interaction.	Not homologous
		**QALQIE** ($P2_1/n$)	4.525, 11.323, 18.469, 91.96 V=945.7	C–H(six membered H)···N interaction.	
43		**TIQGEF** ($P3_1$)	10.314, 10.314, 13.177,120.00, V=1214.0	C–H···π interaction is absent.	Not homologous
		**HAMFOR** (P1) Z'=4	10.093, 14.215, 15.991, 84.79, 73.84, 77.36, V=2149.2	C–H···π interaction is present.	
44		**BESNUI** ($P2_1/n$)	5.510, 8.766, 20.681, 96.23, V =993.0	S···S interaction is observed.	Homologous

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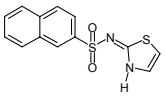
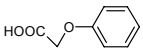
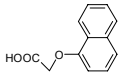
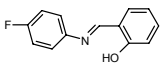
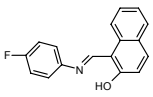
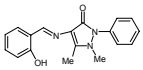
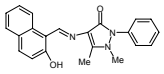
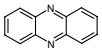
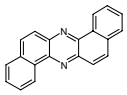
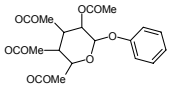
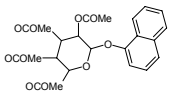
		**GAFPEJ** ($P2_1/c$)	9.125, 11.033, 12.818, 90.99, V=1290.2	S···S interaction is absent.	
45		**BEFTEL** ($P2_1/c$)	5.114, 11.710, 12.390,91.36, V=741.8	. Forms dimer through C–H···O in one dimension.	Not homologous
		**DAKXOD** ($C2/c$)	5.845, 7.712, 23.484, 86.08, 82.85, 67.73, V=971.8	Forms dimer through C–H···O bifurcated interactions in two dimensions.	
46		**CAVQAR** ($P2_1/c$)	5.787, 12.820, 14.817, 107.93, V=1045.9	No C–H···F interaction.	Not homologous
		**MUDGAT** ($P2_1/a$)	6.988, 13.998, 13.050, 92.850, V=1274.95 (From Hg)	C–H···F interaction is present.	
47		**WOVYUB01** ($P2_1/n$)	7.527,7.554, 26.961, 95.42, V=1526.1	Trifurcated C–H···O interaction	Not homologous
		**MUDHIC** ($P\ 2_12_12_1$)	8.717, 14.561, 14.690, V= 1864.58 (From Hg)	C–H···π interaction is expense of C–H···O.	
48		**PHENAZ04** ($P2_1/n$)	5.072,7.083, 12.794,102.34, V=449.0	No specific interaction.	Not homologous
		**NAAZAS** ($P2_1/c$)	10.970, 4.710, 14.100, 113.90, V=666.06	C–H···π & C–H···N interactions are present.	
49		**ZUTPIN** ($P2_1$)	9.882, 10.494, 10.802, 103.01, V=1091.4	C–H···π interaction is absent.	Not homologous
		**NAPAGQ** ($P2_12_12_1$)	16.423, 21.83, 26.876, V=2465.37	C–H···π interaction is present.	
50		**GOHWAB** (P-1)	6.369,7.359,7.382, 85.41, 66.72, 66.12, V=289.3	No specific interaction.	Not homologous

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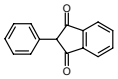
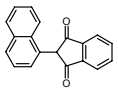
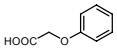
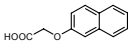
		**NAPCBU** ($P2_1/c$)	5.796, 8.291, 18.015, 106.50, V=830.1	No specific interaction.	
51		**GESNIB** ($P\ 2_12_12_1$)	5.772, 7.505, 11.565, V=501.0	C–H···π interaction is absent.	Not homologous
		**NAPCPR** (*Pnma*)	6.390,10.398,11.391, V=756.9	C–H···π interaction is present.	
52		**TEPHTH13** ($C2/m$)	3.790, 6.873, 6.873, 98.86, 90.79, 90.79, V = 176.9	One dimensional chain structure through C–H···O dimer interaction.	Not homologous
		**NAPDCX** (P-1)	3.709, 9.591, 13.217, 87.60, 83.37, 82.62, V=463.0	Three dimensions packing through C–H···O trifurcated interaction.	
53		**PINDON** ($Pca2_1$)	6.206, 10.205, 17.923, V=1135.1	C–H···O synthon is not planar.	Not homologous
		**NAPINO** ($P2_1/c$)	8.700, 10.792, 14.305, 101.96, V=1313.9	C–H···O synthon is planar.	
54		**BEFTEL** ($P2_1/c$)	5.114, 11.710, 12.390, 91.36, V=741.8	C–H···π interaction is present.	Not homologous
		**NAPXAC01** ($P2_1/n$)	6.840, 12.311, 13.166, 116.51, V=992.1	C–H···π interaction is absent.	
55		**ZZZUCY01** Z'=2 ($P2_1/c$)	11.952, 13.616, 14.032, 91.46, V=2282.8	C–H··π interaction is absent.	Not homologous
		**NATMAW**01 (P-1)	9.932, 11.320, 15.733, 81.75, 80.57, 89.34, V=1726.8	C–H···π interaction is present.	