

Optimization and comparison of statistical tools for the prediction of multicomponent forms of a molecule: the antiretroviral Nevirapine as a case study

Rogeria Nunes Costa,^{*a} Duane Choquesillo-Lazarte,^b Silvia Lucía Cuffini,^a Elna Pidcock,^c and Lourdes Infantes^{*d}

^a Instituto de Ciência e Tecnologia, Universidade Federal de São Paulo, 12331-280 São José dos Campos, Brazil.

^b Laboratorio de Estudios Cristalográficos, IACT, CSIC-Universidad de Granada, Avda. de las Palmeras 4, 18100 Armilla, Granada, Spain.

^c Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge, UK.

^d Instituto de Química Física Rocasolano, Consejo Superior de Investigaciones Científicas, 28006, Madrid, Spain.

Supplementary information

Content:

Table S1 – List of all compounds with the 2D diagram tested with NVP to form multicomponents, grouping in G1 (green), G2 (yellow) and G3 (red). Ranking positions obtained through the techniques used for all of them are shown. Each group has been sorted by the consensus C score.

Table S2 – Experimental methods used in the trials to form NVP multicomponents for compounds in the groups G2 and G3. A description of each method is given below.

Table S3 – H-Bond Propensity results for a multicomponent analysis of 450 co-formers against NVP molecule. Molecules are ordered by HBP ranking position. In bold are represented the 76 molecules for which experimental multicomponent results are available. Black-italic letter identify the positive results; ^{CSD} means molecules reported in the CSD database. Red-underline letter identify the negative results.

Table S4 – Coordination value results for a multicomponent analysis of 450 co-formers against NVP molecule. Molecules are ordered by CV ranking position. In bold are represented the 76 molecules for which experimental multicomponent results are available. Black-italic letter identify the positive results; ^{CSD} means molecules reported in the CSD database. Red-underline letter identify the negative results.

Table S5 – Molecular complementarity results for a multicomponent analysis of 450 co-formers against NVP molecule. Molecules are ordered by MC ranking position. In bold are represented the 76 molecules for which experimental multicomponent results are available. Black-italic letter identify the positive results; ^{CSD} means molecules reported in the CSD database. Red-underline letter identify the negative results.

Table S56 – COSMOQuick results for a multicomponent analysis of 450 co-formers against NVP molecule. Molecules are ordered by COSMO ranking position. In bold are represented the 76 molecules for which experimental multicomponent results are available. Black-italic letter identify the positive results; ^{CSD} means molecules reported in the CSD database. Red-underline letter identify the negative results.

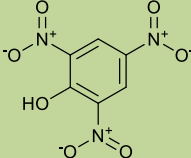
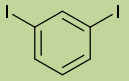

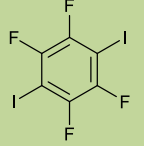

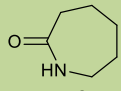
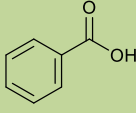
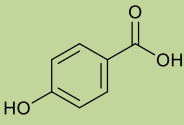
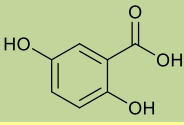
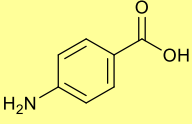
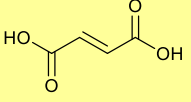
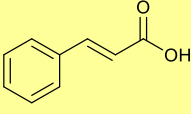
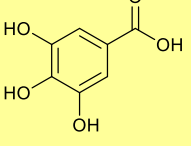
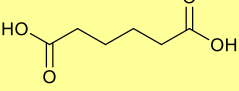
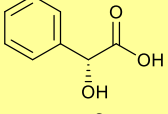
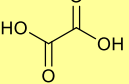
Table S7 – Scores and Ranking obtained for CV, MC, HBP, COSMOQuick and the three consensus ranking A, B and C for the multicomponent analysis of 450 co-formers against NVP molecule. The co-formers were ordered by the consensus ranking C, obtained from the sum of ranking positions obtained for MC, HBP analysis, and CosmoQuick prediction. In bold are represented the 76 molecules for which experimental multicomponent results are available. Black-italic letter identify the positive results; ^{CSD} means molecules reported in the CSD database. Red-underline letter identify the negative results.

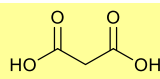
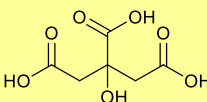
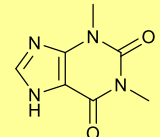
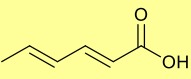
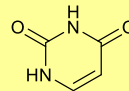
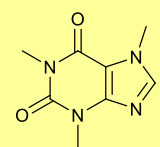
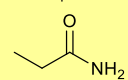
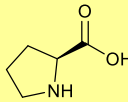
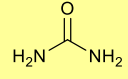
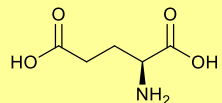
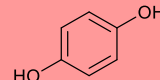
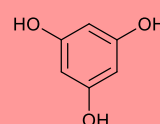
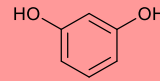
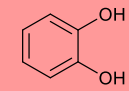
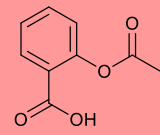
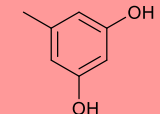
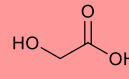
Table S8 – Distribution of some frequent chemical groups in the database of 450 structures used in the theoretical screening and in the 76 molecules tested to form multicomponent with NVP.

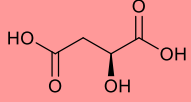
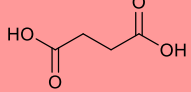
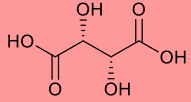
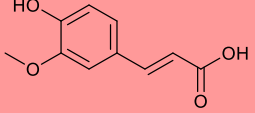
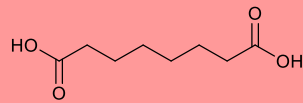
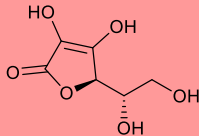
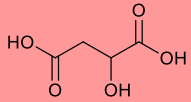
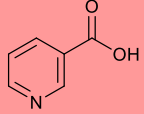
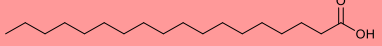
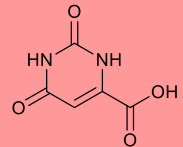
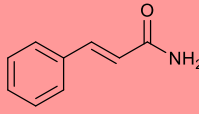
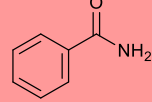
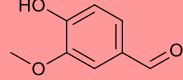
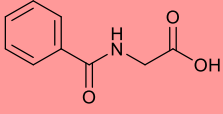
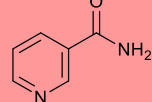
Figure S1 –ROC curves and AUC values obtained for each method: CV, MC, HBP, COSMOQuick, and the three consensus A, B and C.

Table S1 – List of all compounds with the 2D diagram tested with NVP to form multicomponents, grouping in G1 (green), G2 (yellow) and G3 (red). Ranking positions obtained through the techniques used for all of them are shown. Each group has been sorted by the consensus C score.

Co-former	CV ranking	MC ranking	HBP ranking	Consensus Ranking A	COSMO ranking	Consensus ranking B	Consensus ranking C	2D diagram
Maleic Acid	73	158	33	29	42	5	10	
4-Hydroxybenzoic acid	56	85	117	24	32	4	11	
Salicylic acid	109	121	90	44	30	11	13	
Ethanol	222	234	65	126	134	97	61	
Glutaric acid	84	93	67	21	279	51	66	
Trichloroacetic acid**	235	372	69	201	10	113	76	
Naphthalene-1,5-disulfonic acid**	317	201	225	252	26	155	77	
3,5-Dinitrosalicylic acid**	364	272	206	328	22	180	98	
n-Butanol	170	83	153	78	291	120	122	
Tartaric acid	75	348	110	132	72	74	126	
Ethyl acetate	339	124	185	183	246	198	149	
Hexanol	155	40	164	60	365	138	158	
1,4-Dioxane	371	323	97	292	150	223	161	
Heptanol	147	29	163	54	386	139	163	
Octanol	140	21	168	48	395	137	167	
Saccharin	406	337	202	388	71	274	185	

Picric acid**	435	293	262	410	69	300	193	
1,3-Diiodobenzene	264	51	427	251	156	202	197	
Dichloromethane	226	115	444	285	98	190	215	
1,2,4,5-Tetrafluoro-3,6-diiodobenzene	248	39	434	231	249	238	255	
Toluene*	224	75	450	257	212	233	267	
ε-Caprolactam	230	336	328	363	126	276	306	
Benzoic acid	161	72	51	35	57	9	2	
3-Hydroxybenzoic acid	52	128	75	23	29	3	9	
Gentisic acid	64	136	162	62	20	21	27	
4-Aminobenzoic acid	108	81	38	16	97	7	5	
Fumaric acid	181	123	66	67	40	26	8	
Cinnamic acid	190	44	76	40	175	43	23	
Gallic acid	276	233	138	181	16	101	44	
Adipic acid	66	69	32	8	330	44	59	
L-Mandelic acid	88	270	141	119	47	60	78	
Oxalic acid	153	248	305	222	4	130	150	

Malonic acid	114	257	189	140	133	116	164	
Citric acid	96	301	63	98	229	114	174	
Theophylline	389	249	229	347	147	272	195	
Sorbic acid	174	55	384	165	187	160	196	
Uracil	296	275	236	299	164	241	227	
Caffeine	436	225	365	422	155	382	272	
Propionamide	8	247	242	116	264	152	279	
L-Proline	203	296	318	310	228	291	344	
Urea	145	350	279	280	236	269	357	
Glutamic acid	85	442	326	335	378	396	448	
Hydroquinone	115	90	165	68	17	23	18	
Phloroglucinol	213	188	143	134	3	61	32	
Resorcinol	116	173	181	106	5	38	37	
Catechol	137	197	160	113	9	45	39	
Acetylsalicylic acid	271	231	31	131	137	104	48	
Orcinol	113	230	169	122	12	52	50	
Glycolic acid	124	313	86	128	64	73	81	

L-Malic acid	49	291	102	91	75	48	84	
Succinic acid	141	312	68	127	94	81	87	
L-Tartaric acid	71	384	18	107	73	59	89	
Ferulic acid	45	138	100	34	255	58	96	
Suberic acid	47	35	78	7	391	64	102	
L-Ascorbic acid	177	342	77	157	88	110	108	
DL-Malic acid	16	297	147	99	76	56	120	
Nicotinic acid	358	112	320	290	100	196	130	
Stearic acid	106	1	92	11	444	93	138	
Orotic acid	260	212	277	256	54	162	144	
Cinnamamide	4	80	252	51	287	83	190	
Benzamide	58	117	259	88	243	107	191	
Vanillin	243	215	297	265	139	199	209	
Hippuric acid	55	171	187	82	301	131	216	
Nicotinamide	312	113	296	228	265	251	226	

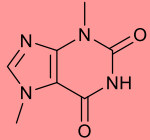
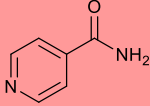
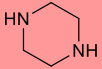
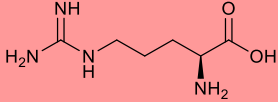
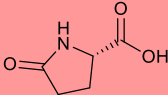
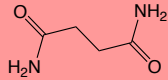
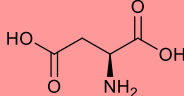
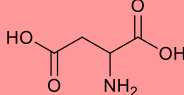
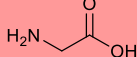
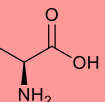
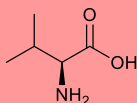
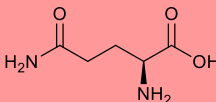
Theobromine	423	220	311	395	168	346	241	
Isonicotinamide	319	131	337	287	257	290	260	
Piperazine	274	318	263	337	160	273	269	
L-Arginine	408	203	150	268	413	377	286	
Pyroglutamic acid	225	277	364	346	140	266	297	
Succinamide	83	160	270	123	358	186	304	
L-Aspartic acid	14	263	317	156	238	169	326	
DL-Aspartic acid	130	411	325	344	239	327	403	
Glycine	301	430	302	423	293	427	416	
L-Alanine	232	448	338	419	289	422	424	
L-Valine	217	433	354	413	323	428	437	
L-Glutamine	22	429	340	293	394	384	449	

Table S2 – Experimental methods used in the trials to form NVP multicomponents for compounds in the groups G2 and G3. A description of each method is given below.

Co-formers	Experimental techniques used
G2	
4-Aminobenzoic acid	LAG method using magnetic stirrer. LAG method using manual grinding. ¹ Nalte et al. has obtained the co-crystal by using the neat grinding method.
Fumaric acid	LAG method using magnetic stirrer. ² Caira et al. has employed dry co-grinding and LAG methods, and obtained the co-crystal.
Cinnamic acid	¹ Nalte et al. has obtained the co-crystal by using the neat grinding method.
Gallic acid	LAG method applying high energy. ¹ Nalte et al. has obtained the co-crystal by using the neat grinding method.

Adipic acid	LAG method using magnetic stirrer. LAG method using manual grinding. ² Caira et al. has obtained the co-crystal by using the LAG method.
L-Mandelic acid	¹ Nalte et al. has obtained the co-crystal by using the neat grinding method.
Oxalic acid	LAG method applying high energy. LAG method applying low energy. LAG method using magnetic stirrer. LAG method using manual grinding. ³ Gujar et al. has obtained the co-crystal by using the solution crystallization method, dissolving equimolar quantities of NVP and oxalic acid in acetone. ¹ Nalte et al. has obtained the co-crystal by using the neat grinding method. ² Caira et al. has employed slow evaporation, neat grinding, solvent-drop grinding, and LAG methods.
Malonic acid	LAG method using magnetic stirrer. LAG method using manual grinding. ¹ Nalte et al. has obtained the co-crystal by using the neat grinding method. ² Caira et al. has employed LAG method.
Citric acid	LAG method applying high energy. LAG method applying low energy. LAG method using manual grinding. ¹ Nalte et al. has obtained the co-crystal by using the neat grinding method. ² Caira et al. has employed slow-evaporation and solvent-drop grinding methods.
Theophylline	LAG method applying low energy. An eutectic was obtained.
Sorbic acid	² Caira et al. obtained the co-crystal by using dry co-grinding and LAG methods.
Uracil	² Caira et al. has obtained the co-crystal by using the LAG method.
Caffeine	LAG method applying low energy. An eutectic was obtained.
Propionamide	² Caira et al. has obtained the co-crystal by using the LAG method.
L-Proline	² Caira et al. has obtained the co-crystal by using the LAG method.
Urea	LAG method applying low energy. LAG method using manual grinding. ¹ Nalte et al. has obtained the co-crystal by using the neat grinding method.
Glutamic acid	LAG method using manual grinding. ² Caira et al. has obtained the co-crystal by using dry co-grinding and LAG methods.
G3	
Hydroquinone	LAG method applying high energy.
Phloroglucinol	LAG method applying high energy.
Resorcinol	LAG method applying high energy.
Catechol	LAG method applying high energy.
Acetylsalicylic acid	LAG method using magnetic stirrer. LAG method using manual grinding.
Orcinol	LAG method applying high energy.
Glycolic acid	LAG method using manual grinding.
L-Malic acid	LAG method applying low energy. ² Caira et al. has employed dry co-grinding and LAG methods.
Succinic acid	LAG method using magnetic stirrer. ² Caira et al. has employed slow-evaporation, neat grinding, solvent-drop grinding, and LAG methods.
L-Tartaric acid	LAG method using magnetic stirrer. LAG method using manual grinding. ¹ Nalte et al. has employed the neat grinding method. ² Caira et al. has employed slow-evaporation, neat grinding, solvent-drop grinding and LAG methods.
Ferulic acid	¹ Nalte et al. has employed the neat grinding method.
Suberic acid	² Caira et al. has employed the LAG method.
L-Ascorbic acid	LAG method using magnetic stirrer. ² Caira et al. has employed the LAG method.

DL-Malic acid	LAG method using magnetic stirrer. LAG method using manual grinding.
Nicotinic acid	LAG method using magnetic stirrer. LAG method using manual grinding. ² Caira et al. has employed the LAG method.
Stearic acid	² Caira et al. has employed slow-evaporation, neat grinding, and solvent-drop grinding methods.
Orotic acid	² Caira et al. has employed the LAG method.
Cinnamamide	² Caira et al. has employed the LAG method.
Benzamide	LAG method using manual grinding. ² Caira et al. has employed the LAG method.
Vanillin	LAG method using manual grinding.
Hippuric acid	LAG method using magnetic stirrer. LAG method using manual grinding. ¹ Nalte et al. has employed the neat grinding method. ² Caira et al. has employed the LAG method.
Nicotinamide	LAG method using manual grinding. ² Caira et al. has employed slow-evaporation, neat grinding, solvent-drop grinding, and LAG methods.
Theobromine	LAG method applying low energy.
Isonicotinamide	LAG method using manual grinding. ² Caira et al. has employed slow-evaporation, neat grinding, solvent-drop grinding, and LAG methods.
Piperazine	² Caira et al. has employed the LAG method.
L-Arginine	LAG method using manual grinding. ² Caira et al. has employed the LAG method.
Pyroglutamic acid	² Caira et al. has employed the LAG method.
Succinamide	² Caira et al. has employed the LAG method.
L-Aspartic acid	LAG method using manual grinding. ² Caira et al. has employed slow-evaporation and solvent-drop grinding methods.
DL-Aspartic acid	² Caira et al. has employed slow-evaporation and solvent-drop grinding methods.
Glycine	² Caira et al. has employed the LAG method.
L-Alanine	LAG method using manual grinding.
L-Valine	² Caira et al. has employed the LAG method.
L-Glutamine	LAG method using manual grinding.

Techniques that we have used for the liquid assisted grinding (LAG):

- 1) **LAG method applying high energy:** By using the mixer mill MM200 (Retsch), 150 mg of stoichiometric (1:1) amounts of NVP and coformer were ground in the presence of 4 or 5 drops of chloroform. The sample mixture and the solvent were placed in an agate jar with two steel balls ($\Phi = 5$ mm) and maintained under 25 HZ of vibrational frequency, during 30 minutes, and at room temperature. The solvent was evaporated at room temperature.
- 2) **LAG method applying low energy:** 3 mmol of NVP and 3 mmol of coformer were ground in the presence of 1000 μ L of chloroform. The sample mixture and the solvent were placed in a glass tube with 4 steel balls ($\Phi = 5$ mm) and 8 steel balls ($\Phi = 3$ mm). The glass tubes were mounted in a system using a PVC tube and polystyrene foam to keep the tubes immobilized. The system (PVC tube + polystyrene foam + tubes) was put in a roller mill and it was maintained under rotation frequency of 270 rpm, during 24 hours, and at room temperature. The solvent was evaporated at room temperature.
- 3) **LAG method using magnetic stirrer:** 0.3 mmol of NVP and 0.3 mmol of coformer were ground in the presence of 300 μ L of solvent (acetone or chloroform). The sample mixture and the solvent were placed in a glass tube with a magnetic bar. The system was let under agitation in a magnetic stirrer, at low agitation, during 2 hours, and at room temperature. The solvent was evaporated at room temperature.
- 4) **LAG method using manual grinding:** 150 mg of stoichiometric (1:1) amounts of NVP and coformer were manually ground in the presence of 4 or 5 drops of chloroform in an agate mortar.

Techniques used by other authors:

- 5) ¹Nalte et al. has applied the **neat grinding method**. Stoichiometric ratios of NVP and co-former were ground in a mortar pestle by manual grinding during 20 minutes.
- 6) ²Caira et al. has employed a series of experiments using different methods:
 - a. **Slow-evaporation method** using stoichiometric ratios (1:1 and 1:2) and various solvents.
 - b. **Neat-grinding** (manual grinding) method using NVP-co-former stoichiometric ratios 1:1 and 2:1.
 - c. **Solvent-drop grinding** (manual grinding) method using NVP-co-former stoichiometric ratios 1:1 and 2:1, and different solvents.
 - d. **Dry co-grinding** method using 1:1 stoichiometric ratio.
 - e. **Liquid-assisted grinding (LAG)** method using various solvents and different stoichiometric ratios (1:1, 2:1, and 1:3).
- 7) ³Gujar et al. has applied the **solution crystallization method**. Equimolar quantities of NVP and co-former were dissolved in 110 ml of acetone and were kept in a warm bath (40 °C). After, the solution was let to crystallize for 1 hour.

References:

- 1 Y. K. Nalte, V. A. Arsul, S. G. Shep and S. B. Bothara, *J. Pharm. Res.*, 2015, **9**, 556–561.
- 2 M. R. Caira, S. A. Bourne, H. Samsodien, E. Engel, W. Liebenberg, N. Stieger and M. Aucamp, *CrystEngComm*, 2012, **14**, 2541–2551.
- 3 P. P. Gujar, A. A. Kokil, P. S. Karekar, Y. A. Gurav and A. V. Yadav, *Int. J. Pharm. Technol.*, 2013, **4**, 4831–4842.

Table S3 –H-Bond Propensity results for a multicomponent analysis of 450 co-formers against NVP molecule. Molecules are ordered by HBP ranking position. In bold are represented the 76 molecules for which experimental multicomponent results are available. Black-italic letter identify the positive results; CSD means molecules reported in the CSD database. Red-underline letter identify the negative results.

Co-former	Molecular formula	HBP Multicomponent Score	Max Interaction	Max A:B or B:A propensity	Max A:A propensity	Max B:B propensity	HBP ranking
1,2-Ethanedithiol	C2H6S2	0.48	B:A	0.93	0.46	0.43	1
1,8-Octanedithiol	C8H18S2	0.47	B:A	0.93	0.46	0.34	2
1,3-Propanedithiol	C3H8S2	0.46	B:A	0.91	0.45	0.36	3
1,6-Hexanedithiol	C6H14S2	0.44	B:A	0.91	0.46	0.30	4
1,9-Nonanedithiol	C9H20S2	0.44	B:A	0.90	0.46	0.30	5
D-(+)-chiro-Inositol	C6H12O6	0.43	B:A	0.88	0.46	0.44	6
Pyrrole	C4H5N	0.43	B:A	0.86	0.43		7
cis-Inositol	C6H12O6	0.42	B:A	0.87	0.45	0.45	8
L-chiro-Inositol	C6H12O6	0.41	B:A	0.85	0.43	0.44	9
Betaine	C5H10NO2	0.39	A:B	0.81	0.42		10
Scyllo-inositol	C6H12O6	0.38	B:A	0.85	0.47	0.45	11
epi-Inositol	C6H12O6	0.38	B:A	0.86	0.48	0.44	12
neo-Inositol	C6H12O6	0.37	B:A	0.82	0.45	0.44	13
2,4-Dihydroxybenzoic acid	C7H6O4	0.35	B:A	0.72	0.38	0.23	14
Cyclohexane-1,2,3,4,5,6-hexol	C6H12O6	0.35	B:A	0.80	0.44	0.45	15
1,7,7-Trimethyltricyclo(2.2.1.0 ^{2,6})heptan-4-ol	C10H16O	0.33	B:A	0.82	0.49	0.27	16
Isocaryolan-9 α -ol	C15H26O	0.33	B:A	0.79	0.46	0.34	17
L-Tartaric acid	C4H6O6	0.31	B:A	0.76	0.38	0.44	18
Meso-Tartaric acid	C4H6O6	0.31	B:A	0.76	0.37	0.45	19
N,N-Dimethylformamide	C3H7NO	0.31	A:B	0.71	0.40		20
2-Amino-5-methylbenzoic acid	C8H9NO2	0.30	B:A	0.76	0.43	0.46	21
2-Amino-5-picolinic acid	C6H6N2O2	0.30	B:A	0.82	0.40	0.52	22

2-Acetylpyrrole	C6H7NO	0.29	B:A	0.72	0.42	0.44	23
3-Methylbut-2-enoic acid	C5H8O2	0.29	B:A	0.78	0.49	0.48	24
DL-Ribose	C5H10O5	0.29	B:A	0.83	0.52	0.54	25
2,6-Dimethylpyrazine	C6H8N2	0.28	A:B	0.65	0.37		26
Anthranilic acid	C7H7NO2	0.28	B:A	0.78	0.39	0.50	27
cis-Aconitic acid	C6H6O6	0.28	B:A	0.70	0.42	0.42	28
o-Anisic acid	C8H8O3	0.28	B:A	0.64	0.36	0.30	29
Tramadol	C16H25NO2	0.28	B:A	0.70	0.42	0.17	30
Acetylsalicylic acid	C9H8O4	0.27	B:A	0.70	0.43	0.31	31
Adipic acid	C10H18	0.27	B:A	0.73	0.47	0.41	32
Maleic Acid^{CSD}	C4H4O4	0.27	B:A	0.69	0.43	0.41	33
Tetrahydrofuran	C4H8O	0.27	A:B	0.67	0.40		34
1,4-Phenylenediamine	C6H8N2	0.26	B:A	0.73	0.46	0.10	35
Allocinnamic acid	C9H8O2	0.26	B:A	0.75	0.50	0.40	36
D-Glucitol	C6H14O6	0.26	B:A	0.72	0.42	0.46	37
4-Aminobenzoic acid	C7H7NO2	0.26	B:A	0.81	0.38	0.55	38
Phenoxyacetic acid	C8H8O3	0.26	B:A	0.72	0.46	0.47	39
Cyclohexane-1,4-diamine	C6H14N2	0.25	B:A	0.71	0.41	0.46	40
3,3'-Thiodipropionic acid	C6H10O4S	0.25	B:A	0.75	0.43	0.49	41
D-Glucono-1,5-lactone	C6H10O6	0.25	B:A	0.72	0.47	0.43	42
Formic acid	CH2O2	0.25	B:A	0.67	0.36	0.42	43
Lactic acid	C3H6O3	0.25	B:A	0.80	0.44	0.55	44
Linoleic acid	C18H32O2	0.25	B:A	0.75	0.44	0.49	45
Ribitol	C5H12O5	0.25	B:A	0.76	0.51	0.50	46
(1R,2R)-Cyclohexane-1,2-Diamine	C6H14N2	0.25	B:A	0.78	0.53	0.50	47
DL-Mannitol	C6H14O6	0.24	B:A	0.68	0.38	0.43	48
4-Methoxybenzoic acid	C8H8O3	0.24	B:A	0.71	0.47	0.45	49
Pyrazine-1,4-dioxide	C4H4N2O2	0.24	A:B	0.65	0.41		50
Benzoic acid^{CSD}	C7H6O2	0.23	B:A	0.71	0.45	0.48	51
D-Iditol	C6H14O6	0.23	B:A	0.69	0.46	0.46	52
DL-Arabinitol	C5H12O5	0.23	B:A	0.71	0.44	0.48	53
Methyl paraben	C8H8O3	0.23	B:A	0.65	0.43	0.35	54
Pyrimethamine	C12H13ClN4	0.23	B:A	0.83	0.48	0.60	55
Tromethamine	C4H11NO3	0.23	B:A	0.69	0.44	0.46	56
Xylitol	C5H12O5	0.23	B:A	0.72	0.49	0.49	57
α-D-Tagatopyranose	C5H6O3	0.23	B:A	0.79	0.49	0.55	58
α-L-Sorbopyranose	C6H12O6	0.23	B:A	0.83	0.51	0.59	59
Acetic acid	C2H4O2	0.22	B:A	0.75	0.47	0.54	60
Allitol	C6H14O6	0.22	B:A	0.68	0.43	0.46	61
Cholic acid	C24H40O5	0.22	B:A	0.77	0.43	0.55	62
Citric acid	C6H8O7	0.22	B:A	0.61	0.40	0.36	63
l-Iditol	C6H14O6	0.22	B:A	0.72	0.50	0.47	64
Ethanol^{CSD}	C2H5OH	0.22	B:A	0.57	0.41	0.35	65
Fumaric acid	C4H4O4	0.22	B:A	0.76	0.48	0.53	66
Glutaric acid^{CSD}	C5H8O4	0.22	B:A	0.79	0.51	0.57	67
Succinic acid	C4H6O4	0.22	B:A	0.77	0.49	0.55	68

Trichloroacetic acid^{CSD}	C2HCl3O2	0.22	B:A	0.70	0.42	0.48	69
Tridecanoic Acid	C13H26O2	0.22	B:A	0.64	0.42	0.37	70
α-D-Galactose	C6H12O6	0.22	B:A	0.77	0.47	0.54	71
α-L-Xylopyranose	C5H10O5	0.22	B:A	0.84	0.49	0.62	72
β-D-Glucose	C6H12O6	0.22	B:A	0.76	0.47	0.54	73
13-epi-Sclareol	C20H36O2	0.21	B:A	0.75	0.54	0.24	74
3-Hydroxybenzoic acid^{CSD}	C7H6O3	0.21	B:A	0.62	0.40	0.41	75
Cinnamic acid	C9H8O2	0.21	B:A	0.64	0.43	0.35	76
L-Ascorbic acid	C6H8O6	0.21	B:A	0.73	0.52	0.51	77
Suberic acid	C8H14O4	0.21	B:A	0.80	0.51	0.59	78
Tryphenylphosphine oxide	C18H15OP	0.21	A:B	0.75	0.53		79
Undecanoic Acid	C11H22O2	0.21	B:A	0.80	0.50	0.60	80
Vanillic acid	C8H8O4	0.21	B:A	0.64	0.43	0.33	81
α-D-Talose	C6H12O6	0.21	B:A	0.76	0.49	0.54	82
1-Hydroxydiamantane	C14H20O	0.20	B:A	0.65	0.45	0.12	83
Butyric acid	C4H8O2	0.20	B:A	0.67	0.47	0.38	84
Cyclobutanol	C4H8O	0.20	B:A	0.89	0.50	0.69	85
Glycolic acid	C2H4O3	0.20	B:A	0.65	0.42	0.45	86
Palmitic Acid	C16H32O2	0.20	B:A	0.81	0.50	0.61	87
Pentadecanoic acid	C15H30O2	0.20	B:A	0.81	0.50	0.61	88
2-Phenylacetic acid	C8H8O2	0.20	B:A	0.70	0.50	0.39	89
Salicylic acid^{CSD}	C7H6O3	0.20	B:A	0.66	0.46	0.30	90
Sebacic acid	C10H18O4	0.20	B:A	0.80	0.51	0.60	91
Stearic acid	C18H36O2	0.20	B:A	0.81	0.50	0.61	92
Tetradecanoic acid	C14H28O2	0.20	B:A	0.81	0.49	0.61	93
β-D-Altropyranose	C6H12O6	0.20	B:A	0.81	0.51	0.61	94
(-)-Epicedrol	C15H26O	0.19	B:A	0.69	0.50	0.31	95
Cyclohexane-1,2,3,4,5,6-hexaol	C6H12O6	0.19	B:A	0.67	0.47	0.38	96
1,4-Dioxane^{CSD}	C4H8O2	0.19	B:A	0.59	0.40		97
4-(Hydroxymethyl)phenol	C7H8O2	0.19	B:A	0.65	0.46	0.24	98
D-Glucuronic acid	C6H10O7	0.19	B:A	0.77	0.43	0.58	99
Ferulic acid	C10H10O4	0.19	B:A	0.59	0.40	0.35	100
Lauric acid	C12H24O2	0.19	B:A	0.82	0.52	0.63	101
L-Malic acid	C4H6O5	0.19	B:A	0.62	0.38	0.43	102
D-Lysine	C6H14N2O2	0.19	B:A	0.75	0.42	0.56	103
L-Lysine	C6H14N2O2	0.19	B:A	0.75	0.44	0.56	104
Sucrose	C12H22O11	0.19	B:A	0.80	0.50	0.61	105
1,4,8,11-Tetra-azacyclotetradecane	C10H24N4	0.18	B:A	0.57	0.39	0.34	106
3β,12β-Dihydroxy-5β-cholan-24-oic acid	C24H40O4	0.18	B:A	0.74	0.42	0.56	107
D-Altritol	C6H14O6	0.18	B:A	0.62	0.40	0.44	108
Quinoxaline-N,N'-dioxide	C8H6N2O2	0.18	A:B	0.58	0.40		109
Tartaric acid^{CSD}	C4H6O6	0.18	B:A	0.64	0.46	0.36	110
Terephthalic acid	C8H6O4	0.18	B:A	0.68	0.51	0.42	111
Thiourea	CH4N2S	0.18	B:A	0.77	0.44	0.59	112
Trimethylamine	C3H9N	0.18	A:B	0.69	0.51		113
α,α-Galacto-trehalose	C12H22O11	0.18	B:A	0.75	0.51	0.58	114

2,2,2-Trifluoroethanol	C2H3F3O	0.17	B:A	0.60	0.42	0.43	115
2,2'-Dihydroxy-5,5'-diallyl-biphenyl	C18H18O2	0.17	B:A	0.62	0.45	0.15	116
4-Hydroxybenzoic acid^{CSD}	C7H6O3	0.17	B:A	0.62	0.44	0.26	117
Benzoin	C14H12O2	0.17	B:A	0.56	0.40	0.25	118
Butan-2-ol	C4H10O	0.17	B:A	0.82	0.44	0.65	119
Galactitol	C6H14O6	0.17	B:A	0.66	0.43	0.49	120
Hexan-1-amine	C6H15N	0.17	B:A	0.77	0.48	0.60	121
Pentan-1-amine	C5H13N	0.17	B:A	0.77	0.48	0.60	122
Trimesic acid	C9H6O6	0.17	B:A	0.56	0.39	0.36	123
α -D-Glucose	C6H12O6	0.17	B:A	0.71	0.46	0.55	124
β -D-Galactose	C6H12O6	0.17	B:A	0.72	0.41	0.55	125
β -DL-Arabinose	C5H10O5	0.17	B:A	0.80	0.47	0.62	126
2,5,5,8 α -Tetramethyloctahydro-2H-2,4 α -methanonaphthalen-1-ol	C15H26O	0.16	B:A	0.66	0.50	0.23	127
2-Coumaric acid	C9H8O3	0.16	B:A	0.58	0.42	0.34	128
4'-Hydroxyacetophenone	C8H8O2	0.16	B:A	0.65	0.49	0.41	129
Ibuprofen	C13H18O2	0.16	B:A	0.56	0.40	0.21	130
Butan-1-amine	C4H11N	0.16	B:A	0.79	0.48	0.63	131
Pterostilbene	C16H16O3	0.16	B:A	0.56	0.40	0.14	132
Pyrazine	C4H4N2	0.16	A:B	0.57	0.41		133
4-(4-Hydroxyphenyl)butan-2-one	C10H12O2	0.16	B:A	0.62	0.46	0.26	134
3-Oxocyclobutanecarboxylic acid	C5H6O3	0.15	B:A	0.79	0.51	0.64	135
Crotonic acid	C4H6O2	0.15	B:A	0.56	0.40	0.30	136
Cyclodecanol	C10H20O	0.15	B:A	0.70	0.44	0.55	137
Gallic acid	C7H6O5	0.15	B:A	0.56	0.41	0.24	138
Glycerol	C3H8O3	0.15	B:A	0.75	0.45	0.60	139
iso-Deoxycholic acid	C24H40O4	0.15	B:A	0.76	0.37	0.61	140
L-Mandelic acid	C8H8O3	0.15	B:A	0.57	0.42	0.28	141
N,N-Dimethylacetamide	C4H9NO	0.15	A:B	0.58	0.43		142
Phloroglucinol	C6H6O3	0.15	B:A	0.61	0.46	0.12	143
Trifluoroacetic acid	C2HF3O2	0.15	B:A	0.71	0.47	0.56	144
α -Lactose	C12H22O11	0.15	B:A	0.81	0.48	0.66	145
(+)-Camphoric acid	C10H16O4	0.14	B:A	0.55	0.41	0.15	146
DL-Malic acid	C4H6O5	0.14	B:A	0.64	0.38	0.51	147
(E)-4,4'-Diazastilbene	C12H10N2	0.14	A:B	0.60	0.46		148
4-(Hydroxymethyl)-2-methoxyphenol	C8H10O3	0.14	B:A	0.58	0.44	0.23	149
L-Arginine	C6H14N4O2	0.14	B:A	0.84	0.44	0.70	150
L-Ribose	C5H10O5	0.14	B:A	0.82	0.43	0.68	151
Myricetin	C15H10O8	0.14	B:A	0.68	0.50	0.54	152
n-Butanol^{CSD}	C4H10O	0.14	B:A	0.56	0.42	0.34	153
Salicylaldehyde	C7H6O2	0.14	B:A	0.61	0.47	0.27	154
(1R,2S)-2-Methyl-4-oxocyclohexane-1-carboxylic acid	C8H12O3	0.13	B:A	0.59	0.39	0.46	155
(R,S)-Hesperetin	C16H14O6	0.13	B:A	0.61	0.47	0.29	156
2,5-bis(4-Pyridyl)-1,3,4-oxadiazole	C12H8N4O	0.13	A:B	0.52	0.39		157
Sucralose	C12H19Cl3O8	0.13	B:A	0.80	0.47	0.67	158
Propan-2-one	C3H6O	0.13	A:B	0.59	0.46		159

Catechol	C6H6O2	0.13	B:A	0.59	0.46	0.14	160
Ethylene glycol	C2H6O2	0.13	B:A	0.61	0.37	0.48	161
Gentisic acid^{CSD}	C7H6O4	0.13	B:A	0.54	0.41	0.23	162
Heptanol^{CSD}	C7H16O	0.13	B:A	0.55	0.42	0.33	163
Hexanol^{CSD}	C6H14O	0.13	B:A	0.55	0.42	0.33	164
Hydroquinone	C6H6O2	0.13	B:A	0.62	0.49	0.18	165
Levulinic acid	C5H8O3	0.13	B:A	0.53	0.37	0.40	166
Propan-1-amine	C3H9N	0.13	B:A	0.79	0.47	0.67	167
Octanol^{CSD}	C8H18O	0.13	B:A	0.55	0.42	0.34	168
Orcinol	C7H8O2	0.13	B:A	0.59	0.46	0.11	169
α,α-Trehalose	C12H22O11	0.13	B:A	0.76	0.49	0.63	170
4-Acetamidobenzoic acid	C9H9NO3	0.12	B:A	0.55	0.43	0.40	171
5-Nitroisophthalic acid	C8H5NO6	0.12	B:A	0.56	0.44	0.30	172
D-Arabinitol	C5H12O5	0.12	B:A	0.55	0.43	0.31	173
D-Mannitol	C6H14O6	0.12	B:A	0.63	0.35	0.51	174
Melamine	C3H6N6	0.12	B:A	0.84	0.46	0.72	175
Methanol	CH4O	0.12	B:A	0.62	0.50	0.50	176
2-Chloroacetic acid	C2H3ClO2	0.12	B:A	0.69	0.41	0.57	177
Acetylmethionine	C7H13NO3S	0.12	B:A	0.66	0.49	0.54	178
Phenyl 2-Hydroxybenzoate	C13H10O3	0.12	B:A	0.55	0.43	0.16	179
Pyridine	C5H5N	0.12	A:B	0.61	0.49		180
Resorcinol	C6H6O2	0.12	B:A	0.61	0.49	0.18	181
2-Methylpropan-2-ol	C4H10O	0.12	B:A	0.54	0.42	0.30	182
1,13-Tridecanediol	C13H28O2	0.11	B:A	0.56	0.45	0.26	183
Biotin	C10H16N2O3S	0.11	B:A	0.69	0.42	0.58	184
Ethyl acetate^{CSD}	C4H8O2	0.11	A:B	0.54	0.43		185
Ethylenediamine	C2H8N2	0.11	B:A	0.79	0.48	0.68	186
Hippuric acid	C9H9NO3	0.11	B:A	0.59	0.48	0.39	187
Indomethacin	C19H16ClNO4	0.11	B:A	0.56	0.45	0.34	188
Malonic acid	C3H4O4	0.11	B:A	0.64	0.53	0.43	189
n-Methyl-D-glucamine	C7H17NO5	0.11	B:A	0.58	0.43	0.47	190
o-β-D-Mannopyranosyl-(1-4)-α-D-mannopyranose	C12H22O11	0.11	B:A	0.75	0.44	0.63	191
4,4,7-Trimethyldecahydro-1H-cyclopenta[cd]inden-7-ol	C14H24O	0.11	B:A	0.62	0.50	0.28	192
β-Maltose	C12H22O11	0.11	B:A	0.78	0.49	0.67	193
Muco-inositol	C6H12O6	0.10	B:A	0.71	0.36	0.62	194
1-Hydroxy-2-naphthoic acid	C11H8O3	0.10	B:A	0.51	0.41	0.21	195
4-Ethoxyphenol	C8H10O2	0.10	B:A	0.54	0.44	0.20	196
Adamantane-1,3,5,7-tetracarboxylic acid	C14H16O8	0.10	B:A	0.53	0.43	0.12	197
cis,cis-1,3,5-Cyclohexanetricarboxylic acid	C9H12O6	0.10	B:A	0.53	0.43	0.26	198
1,1-Dihydroxypropan-2-one	C3H6O3	0.10	B:A	0.59	0.39	0.49	199
Hexanoic acid	C6H12O2	0.10	B:A	0.60	0.49	0.32	200
Octanoic acid	C8H16O2	0.10	B:A	0.59	0.49	0.32	201
Saccharin^{CSD}	C7H5NO3S	0.10	B:A	0.56	0.46	0.21	202

(2R,3R)-2,3-Dimethylcyclopropane-1-carboxylic acid	C6H10O2	0.10	B:A	0.54	0.43	0.38	203
β-D-Fructopyranose	C6H12O6	0.10	B:A	0.76	0.45	0.66	204
2,4,6-Trimethylphenol	C9H12O	0.09	B:A	0.58	0.49	0.12	205
3,5-Dinitrosalicylic acid^{CSD}	C7H4N2O7	0.09	B:A	0.53	0.44	0.28	206
β-D-Psicose	C6H12O6	0.09	B:A	0.76	0.42	0.67	207
Decanoic acid	C10H20O2	0.09	B:A	0.59	0.49	0.33	208
Heptanoic acid	C7H14O2	0.09	B:A	0.58	0.49	0.32	209
myo-Inositol	C6H12O6	0.09	B:A	0.71	0.36	0.62	210
Nonanoic acid	C9H18O2	0.09	B:A	0.59	0.50	0.33	211
β-D-Allose	C6H12O6	0.09	B:A	0.71	0.36	0.62	212
β-Lactose	C12H22O11	0.09	B:A	0.72	0.38	0.63	213
1-Amino-1-methylcyclopropane	C4H9N	0.08	B:A	0.71	0.46	0.63	214
1-Hydroxypropan-2-one	C3H6O2	0.08	B:A	0.57	0.49	0.38	215
2,6-Pyridinedicarboxylic acid	C7H5NO4	0.08	B:A	0.63	0.48	0.55	216
3,5-Dinitrobenzoic acid	C7H4N2O6	0.08	B:A	0.41	0.32	0.30	217
Ethylamine	C2H7N	0.08	B:A	0.80	0.48	0.72	218
n-Hexadecanol	C16H34O	0.08	B:A	0.60	0.52	0.36	219
Dihydrofuran-2,5-dione	C4H4O3	0.08	A:B	0.48	0.40		220
β-D-Gulose	C6H12O6	0.08	B:A	0.71	0.35	0.62	221
2-Isopropyl-5-methylphenol	C10H14O	0.07	B:A	0.57	0.51	0.07	222
2-(Tert-butyl)-4-methoxyphenol	C11H16O2	0.07	B:A	0.51	0.44	0.14	223
Lidocaine	C18H32O2	0.07	B:A	0.49	0.42	0.28	224
Naphthalene-1,5-disulfonic acid^{CSD}	C10H8S2O6	0.07	B:A	0.54	0.44	0.47	225
o-Cresol	C7H8O	0.07	B:A	0.50	0.43	0.13	226
Phenol	C6H6O	0.07	B:A	0.57	0.51	0.20	227
Phenylmethanol	C7H8O	0.07	B:A	0.57	0.50	0.19	228
Theophylline	C7H8N4O2	0.07	B:A	0.53	0.39	0.46	229
1-Naphthalenesulfonic acid	C10H8O3S	0.06	B:A	0.52	0.44	0.46	230
1-Naphthol	C10H8O	0.06	B:A	0.52	0.46	0.08	231
4-Nitrobenzoic acid	C7H5NO4	0.06	B:A	0.63	0.57	0.37	232
2-Ethyl-3-hydroxy-4H-pyran-4-one	C7H8O3	0.06	B:A	0.67	0.46	0.61	233
L-Cysteine	C3H7NO2S	0.06	B:A	0.97	0.44	0.91	234
Acrylaldehyde	C3H4O	0.06	A:B	0.53	0.47		235
Uracil	C4H4N2O2	0.06	A:B	0.62	0.49	0.56	236
β-L-Lyxopyranose	C5H10O5	0.06	B:A	0.68	0.36	0.62	237
1,11-Undecanediol	C11H24O2	0.05	B:A	0.58	0.53	0.35	238
4-Aminobenzamide	C7H8N2O	0.05	B:A	0.76	0.42	0.71	239
N-Methylpyrrolidone	C5H9NO	0.05	A:B	0.52	0.47		240
4-Hydroxybenzaldehyde	C7H6O2	0.05	B:A	0.50	0.45	0.35	241
Propionamide	C3H7NO	0.05	B:A	0.85	0.52	0.79	242
(S)-2-Hydroxypropanamide	C3H7NO2	0.05	B:A	0.79	0.44	0.74	243
α-8'-β-Apocarotenal	C30H40O	0.05	A:B	0.56	0.51		244
α-Maltose	C12H22O11	0.05	B:A	0.67	0.38	0.63	245
(E)-4-(4-Hydroxy-3-methoxyphenyl)but-3-en-2-one	C11H12O3	0.04	B:A	0.44	0.40	0.33	246
1,3-Di(pyridin-4-yl)propane	C13H14N2	0.04	A:B	0.56	0.52		247

1-Pentanol	C5H12O	0.04	B:A	0.58	0.54	0.38	248
2,2',2''-Nitrilotriethanol	C6H15NO3	0.04	B:A	0.55	0.50	0.30	249
2,4-Pyridinedicarboxylic acid	C7H5NO4	0.04	B:A	0.63	0.48	0.59	250
2,5-Dimethylphenol	C8H10O	0.04	B:A	0.47	0.43	0.13	251
Cinnamide	C9H9NO	0.04	B:A	0.80	0.52	0.75	252
2-Aminoethan-1-ol	C2H7NO	0.04	B:A	0.72	0.51	0.68	253
Pyruvic acid	C3H4O3	0.04	A:B	0.61	0.46	0.57	254
β -8'- β -Apocarotenal	C30H40O	0.04	A:B	0.55	0.51		255
1,1'-Azo-bis(carbamide)	C2H4N4O2	0.03	B:A	0.89	0.39	0.86	256
1,2-bis(4-Pyridyl)ethane	C12H10N2	0.03	A:B	0.55	0.52		257
4,4'-Bipyridine	C10H8N2	0.03	A:B	0.55	0.52		258
Benzamide	C7H7NO	0.03	B:A	0.68	0.42	0.65	259
2,8,16,20-Tetramethylcalix(4)resorcinarene	C32H32O8	0.03	B:A	0.53	0.50	0.10	260
2-Hydroxyacetamide	C2H5NO2	0.03	B:A	0.81	0.44	0.78	261
Picric acid^{CSO}	C6H3N3O7	0.03	B:A	0.52	0.50	0.17	262
Piperazine	C4H10N2	0.03	B:A	0.62	0.51	0.59	263
(R)-2-Hydroxypropanamide	C3H7NO2	0.03	B:A	0.78	0.44	0.75	264
2-Aminopyrimidine	C4H5N3	0.02	B:A	0.84	0.42	0.82	265
Phenylmethanethiol	C7H8S	0.02	B:A	0.46	0.44	0.03	266
Piperidine	C5H11N	0.02	B:A	0.61	0.51	0.60	267
4-Methylbenzenesulfonic acid	C7H8O3S	0.02	B:A	0.56	0.43	0.54	268
S(+)-Camphor-10-sulfonic acid	C10H16O4S	0.02	B:A	0.59	0.45	0.57	269
Succinamide	C4H8N2O2	0.02	B:A	0.80	0.43	0.78	270
2,3,5,6-Tetrachlorocyclohexa-2,5-diene-1,4-dione	C6Cl4O2	0.02	A:B	0.52	0.50		271
α -Ketoglutaric acid	C5H6O5	0.02	B:A	0.61	0.39	0.59	272
2,2-Dibromo-2-cyanoacetamide	C3H2Br2N2O	0.01	B:A	0.81	0.48	0.80	273
[1,1'-Biphenyl]-4,4'-diol	C12H10O2	0.01	B:A	0.34	0.33	0.06	274
4-Hydroxy-3,5-dimethoxybenzaldehyde	C9H10O4	0.01	B:A	0.50	0.49	0.42	275
4-Nitrophenol	C6H5NO3	0.01	B:A	0.55	0.54	0.28	276
Orotic acid	C5H4N2O4	0.01	B:A	0.54	0.54	0.51	277
(5-Hydroxy-6-methylpyridine-3,4-diyl)dimethanol	C8H11NO3	0.01	B:A	0.48	0.47	0.33	278
Urea	CH4N2O	0.01	B:A	0.91	0.54	0.91	279
Butyramide	C4H9NO	0.00	B:B	0.79	0.37	0.79	280
Imidazole	C3H4N2	0.00	B:B	0.70	0.44	0.70	281
Piperine	C17H19NO3	0.00	A:B	0.37	0.37		282
Chloranilic acid	C6H2Cl2O4	-0.01	B:B	0.52	0.37	0.54	283
Furfural	C6H12O2	-0.01	A:A	0.38	0.39		284
β -Cellobiose	C12H22O11	-0.01	B:B	0.68	0.34	0.70	285
DL-Valine	C5H11NO2	-0.02	B:B	0.96	0.54	0.98	286
β -galabiose	C12H22O11	-0.02	B:B	0.67	0.34	0.70	287
1,1-bis(4-Hydroxyphenyl)cyclohexane	C18H20O2	-0.03	A:A	0.57	0.60	0.20	288
2-Pyridone	C5H5NO	-0.03	B:B	0.83	0.43	0.87	289
5,5-Diethylbarbituric acid	C8H12N2O3	-0.03	B:B	0.61	0.33	0.64	290
Acetamide	C2H5NO	-0.03	B:B	0.83	0.44	0.86	291

4,4'-Ethene-1,2-diyl dipyridine	C12H10N2	-0.03	A:A	0.41	0.44		292
DL-Isoleucine	C6H13NO2	-0.03	B:B	0.95	0.54	0.98	293
DL-Leucine	C6H13NO2	-0.03	B:B	0.95	0.54	0.98	294
L-Leucine	C6H13NO2	-0.03	B:B	0.95	0.54	0.98	295
Nicotinamide	C6H6N2O	-0.03	B:B	0.74	0.51	0.78	296
Vanillin	C8H8O3	-0.03	A:A	0.58	0.61	0.41	297
1,2,4,5-Tetracyanobenzene	C10H2N4	-0.04	A:A	0.44	0.48		298
Cinnamaldehyde	C9H8O	-0.04	A:A	0.39	0.42		299
D-Alanine	C3H7NO2	-0.04	B:B	0.95	0.55	0.99	300
Formamide	CH3NO	-0.04	B:B	0.83	0.41	0.87	301
Glycine	C2H5NO2	-0.04	B:B	0.95	0.54	0.99	302
L-Methionine	C5H11NO2S	-0.04	B:B	0.93	0.69	0.97	303
Neotame	C20H30N2O5	-0.04	B:B	0.92	0.54	0.96	304
Oxalic acid	C2H2O4	-0.04	A:A	0.47	0.52	0.41	305
1,4-Diazabicyclo[2.2.2]octane	C6H12N2	-0.05	A:A	0.47	0.51		306
DL-Glutamic acid	C5H9NO4	-0.05	B:B	0.93	0.48	0.98	307
DL-Glutamine	C5H10N2O3	-0.05	B:B	0.93	0.46	0.98	308
4-Aminobutanoic acid	C4H9NO2	-0.05	B:B	0.93	0.48	0.98	309
Methyl acetate	C3H6O2	-0.05	A:A	0.44	0.48		310
Theobromine	C7H8N4O2	-0.05	B:B	0.43	0.36	0.48	311
1,2-Ethanedisulfonic acid	C2H6O6S2	-0.06	B:B	0.61	0.45	0.67	312
3S-cis-3,6-Dimethyl-1,4-dioxane-2,5-dione	C6H8O4	-0.06	A:A	0.39	0.45		313
DL-Arginine	C6H14N4O2	-0.06	B:B	0.93	0.43	0.98	314
DL-Methionine	C5H11NO2S	-0.06	B:B	0.91	0.54	0.97	315
L-Asparagine	C4H8N2O3	-0.06	B:B	0.91	0.49	0.97	316
L-Aspartic acid	C4H7NO4	-0.06	B:B	0.92	0.46	0.98	317
L-Proline	C5H9NO2	-0.06	B:B	0.87	0.54	0.94	318
L-Tryptophan	C11H12N2O2	-0.06	B:B	0.90	0.50	0.96	319
Nicotinic acid	C6H5NO2	-0.06	B:B	0.61	0.53	0.67	320
1,1,6,6-Tetraphenylhexa-2,4-diyne-1,6-diol	C30H22O2	-0.07	A:A	0.43	0.50	0.09	321
2,4-Dimethylpyridine	C7H9N	-0.07	A:A	0.40	0.47		322
2,6-Dimethylpyridine	C7H9N	-0.07	A:A	0.41	0.48		323
Cyclamic acid	C6H13NO3S	-0.07	B:B	0.69	0.45	0.76	324
DL-Aspartic acid	C4H7NO4	-0.07	B:B	0.91	0.50	0.98	325
Glutamic acid	C5H9NO4	-0.07	B:B	0.90	0.51	0.97	326
D-Threonine	C4H9NO3	-0.07	B:B	0.90	0.45	0.97	327
<i>ε</i>-Caprolactam^{CSD}	C6H11NO	-0.07	B:B	0.69	0.46	0.76	328
Formaldehyde	CH2O	-0.07	A:A	0.39	0.46		329
L-Cystine	C6H12N2O4S2	-0.07	B:B	0.90	0.47	0.98	330
Pyromellitic	C10H2O6	-0.07	A:A	0.40	0.47		331
[1,1'-Binaphthalene]-2,2'-diol	C20H14O2	-0.08	A:A	0.31	0.39	0.05	332
2,6-Di-tert-butyl-4-methylphenol	C15H24O	-0.08	A:A	0.39	0.47	0.05	333
D-Asparagine	C4H8N2O3	-0.08	B:B	0.88	0.45	0.96	334
Dimethylsulfoxide	C2H6OS	-0.08	A:A	0.32	0.40		335
D-Isoleucine	C6H13NO2	-0.08	B:B	0.88	0.43	0.96	336

<u>Isonicotinamide</u>	<u>C6H6N2O</u>	<u>-0.08</u>	<u>B:B</u>	<u>0.64</u>	<u>0.39</u>	<u>0.72</u>	<u>337</u>
<u>L-Alanine</u>	<u>C3H7NO2</u>	<u>-0.08</u>	<u>B:B</u>	<u>0.89</u>	<u>0.52</u>	<u>0.97</u>	<u>338</u>
L-Cysteine	C3H7NO2S	-0.08	B:B	0.89	0.44	0.97	339
<u>L-Glutamine</u>	<u>C5H10N2O3</u>	<u>-0.08</u>	<u>B:B</u>	<u>0.89</u>	<u>0.55</u>	<u>0.97</u>	<u>340</u>
L- α -Leucine	C6H13NO2	-0.08	B:B	0.88	0.44	0.96	341
Nitromethane	CH3NO2	-0.08	A:A	0.34	0.42		342
β -Alanine	C3H7NO2	-0.08	B:B	0.91	0.49	0.99	343
2,2'-Bipyridine	C10H8N2	-0.09	A:A	0.39	0.48		344
Cyclohexanone	C4H8	-0.09	A:A	0.36	0.45		345
DL-Cysteine	C3H7NO2S	-0.09	B:B	0.89	0.49	0.98	346
Tetramethylpyrazine	C8H12N2	-0.09	A:A	0.30	0.39		347
4-Hydroxy-L-proline	C5H9NO3	-0.10	B:B	0.87	0.52	0.96	348
Chloro(methoxy)methane	C2H5ClO	-0.10	A:A	0.31	0.41		349
Proline	C5H9NO2	-0.10	B:B	0.76	0.42	0.87	350
DL-Tryptophan	C11H12N2O2	-0.10	B:B	0.85	0.43	0.95	351
DL-Tyrosine	C9H11NO3	-0.10	B:B	0.86	0.47	0.96	352
L-Threonine	C4H9NO3	-0.10	B:B	0.89	0.40	0.98	353
<u>L-Valine</u>	<u>C5H11NO2</u>	<u>-0.10</u>	<u>B:B</u>	<u>0.87</u>	<u>0.55</u>	<u>0.97</u>	<u>354</u>
Terephthalaldehyde	C8H6O2	-0.10	A:A	0.29	0.39		355
3-Isochromanone	C9H8O2	-0.11	A:A	0.33	0.44		356
DL-Serine	C3H7NO3	-0.11	B:B	0.87	0.50	0.98	357
Morpholine	C4H9NO	-0.11	B:B	0.56	0.36	0.67	358
Trimethylamine oxide	C3H9NO	-0.11	A:A	0.34	0.45		359
1,3-Distearoyl-2-oleoylglycerol	C57H108O6	-0.12	A:A	0.33	0.45		360
2,3-Dimethylpyrazine	C6H8N2	-0.12	A:A	0.35	0.47		361
2,5-Dimethylpyrazine	C6H8N2	-0.12	A:A	0.35	0.47		362
Phthalide	C8H6O2	-0.12	A:A	0.37	0.49		363
<u>Pyroglutamic acid</u>	<u>C5H7NO3</u>	<u>-0.12</u>	<u>B:B</u>	<u>0.65</u>	<u>0.48</u>	<u>0.77</u>	<u>364</u>
<i>Caffeine</i>	<i>C8H10N4O2</i>	<i>-0.13</i>	<i>A:A</i>	<i>0.35</i>	<i>0.48</i>		<i>365</i>
Hexamethylenetetramine	C6H12N4	-0.13	A:A	0.37	0.50		366
L-Tyrosine	C9H11NO3	-0.13	B:B	0.84	0.37	0.98	367
4-Benzoquinone	C6H4O2	-0.14	A:A	0.32	0.46		368
Tetracyanoethylene	C6N4	-0.14	A:A	0.33	0.47		369
2,5-Piperazinedione	C4H6N2O2	-0.15	B:B	0.67	0.34	0.82	370
Benzalacetone	C10H10O	-0.15	A:A	0.35	0.50		371
Carbamazepine	C15H12N2O	-0.15	B:B	0.77	0.46	0.93	372
2-(Oleoyloxy)propane-1,3-diyl distearate	C57H108O6	-0.15	A:A	0.31	0.46		373
(3 α R,4R,6 α S,10 α S)-3 α ,4,7,7-Tetramethylperhydronaphtho(8 α ,1- β)furan-2-one	C16H26O2	-0.16	A:A	0.31	0.48		374
1,3-Distearoyl-2-elaidoylglycerol	C57H108O6	-0.16	A:A	0.31	0.46		375
Sucrose octa-acetate	C28H38O19	-0.16	A:A	0.21	0.37		376
2,2'-(cyclohexa-2,5-diene-1,4-diylidene)dimalononitrile	C12H4N4	-0.16	A:A	0.32	0.48		377
2,3-Butanedione	C4H6O2	-0.17	A:A	0.30	0.47		378
Cyclodecanone	C10H18O	-0.17	A:A	0.31	0.48		379
Vitamin A acetate	C22H32O2	-0.17	A:A	0.31	0.49		380

Acetophenone	C8H8O	-0.18	A:A	0.33	0.51		381
1,10-Phenanthroline	C12H8N2	-0.19	A:A	0.34	0.53		382
Coumarin	C9H6O2	-0.19	A:A	0.25	0.43		383
Sorbic acid	C6H8O2	-0.19	A:A	0.33	0.51	0.08	384
(-)-1,3,3-Trimethyl-2-norbornanone	C10H16O	-0.20	A:A	0.28	0.48		385
1,2-Dicyclopropylethane-1,2-dione	C8H10O2	-0.20	A:A	0.27	0.47		386
n-Butyl acetate	C6H12O2	-0.20	A:A	0.23	0.43		387
Benzophenone	C13H10O	-0.21	A:A	0.27	0.48		388
4-Methylmorpholine	C5H11NO	-0.21	A:A	0.19	0.40		389
1,2-Distearoyl-3-elaidoylglycerol	C57H108O6	-0.22	A:A	0.25	0.48		390
3 α ,4,7,7-Tetramethyl-(3 α R,4S,6 α R,10 α S)-perhydronaphtho(8 α ,1- β)furan-2-one	C16H26O2	-0.22	A:A	0.30	0.51		391
Acridine	C13H9N	-0.22	A:A	0.24	0.46		392
Cycloundecanone	C11H20O	-0.22	A:A	0.23	0.45		393
Tricyclopropylamine	C9H15N	-0.22	A:A	0.23	0.45		394
(3 α R,4S,6 α S,10 α S)-3 α ,4,7,7-Tetramethylperhydronaphtho(8 α ,1- β)furan-2-one	C16H26O2	-0.23	A:A	0.22	0.45		395
2,3,5,6-Tetrafluoro-7,7,8,8-tetracyanoquinodimethane	C12F4N4	-0.24	A:A	0.24	0.48		396
Dimethyl succinate	C6H10O4	-0.24	A:A	0.22	0.46		397
1,4-Dimethylpiperazine	C6H14N2	-0.24	A:A	0.19	0.43		398
Phenazine	C12H8N2	-0.26	A:A	0.25	0.52		399
Ethyl Propionate	C5H10O2	-0.27	A:A	0.22	0.48		400
Oxetane	C3H6O	-0.27	A:A	0.08	0.35		401
1-(4-Methoxyphenyl)ethan-1-one	C9H10O2	-0.27	A:A	0.16	0.42		402
1,3,5-Trinitrobenzene	C6H3N3O6	-0.28	A:A	0.22	0.50		403
3,4-(Methylenedioxy)benzaldehyde	C8H6O3	-0.28	A:A	0.14	0.42		404
Dibenzoyl peroxide	C14H10O4	-0.28	A:A	0.17	0.44		405
(Z)-Ethyl 2-benzylidene-3-oxobutanoate	C13H14O3	-0.29	A:A	0.16	0.44		406
4-tert-Butyl-3-methoxy-2,6-dinitrotoluene	C12H16N2O5	-0.29	A:A	0.20	0.49		407
1-(Naphthalen-2-yl)Ethan-1-One	C12H10O	-0.30	A:A	0.15	0.45		408
β -Tristearin	C57H110O6	-0.30	A:A	0.12	0.42		409
1,3-Diphenylpropan-2-one	C15H14O	-0.31	A:A	0.19	0.50		410
4-Methoxybenzaldehyde	C8H8O2	-0.31	A:A	0.11	0.43		411
cis-anti-cis-Dicyclohexano-18-crown-6	C20H36O6	-0.31	A:A	0.04	0.35		412
Nootkatone	C15H22O	-0.31	A:A	0.13	0.44		413
(1S,6R,10R)-(+)-6-Methyl-4-oxabicyclo(8.4.1)pentadecan-3-one	C15H26O2	-0.32	A:A	0.13	0.44		414
(4R,7S)-7-Isopropyl-4-methyloxepan-2-one	C10H18O2	-0.32	A:A	0.23	0.55		415
2-Methoxy-4-(1-(E)-propenyl)phenyl acetate	C12H14O3	-0.32	A:A	0.10	0.42		416
4-Allyl-2-methoxyphenyl benzoate	C17H16O3	-0.32	A:A	0.21	0.53		417
Methyl benzoate	C8H8O2	-0.32	A:A	0.17	0.49		418
L-Carvone	C10H14O	-0.33	A:A	0.13	0.46		419
Methyl cubane-1-carboxylate	C10H10O2	-0.33	A:A	0.14	0.47		420

Phenyl acetate	C8H8O2	-0.34	A:A	0.16	0.50	421
Tetraiodoethene	C2I4	-0.34	A:A	0.17	0.51	422
Tetrabromomethane	CBr4	-0.35	A:A	0.02	0.37	423
Dichlorodifluoromethane	CCl2F2	-0.36	A:A	0.03	0.39	424
2-Methoxynaphthalene	C11H10O	-0.38	A:A	0.08	0.46	425
1,2-Dimethoxybenzene	C8H10O2	-0.39	A:A	0.05	0.45	426
<i>1,3-Diiodobenzene^{CSD}</i>	<i>C6H4I2</i>	<i>-0.40</i>	<i>A:A</i>	<i>0.03</i>	<i>0.43</i>	<i>427</i>
1-Chloro-1,1,2,2,2-pentafluoroethane	C2ClF5	-0.40	A:A	0.05	0.45	428
bis(Methylthio)methane	C3H8S2	-0.40	A:A	0.06	0.46	429
Chlorine	Cl2	-0.40	A:A	0.03	0.43	430
Ethyl(methyl)sulfane	C3H8S	-0.40	A:A	0.07	0.47	431
Ethylene oxide	C2H4O	-0.40	A:A	0.04	0.44	432
Eucalyptol	C10H18O	-0.40	A:A	0.06	0.46	433
<i>1,2,4,5-Tetrafluoro-3,6-diiodobenzene^{CSD}</i>	<i>C6F4I2</i>	<i>-0.41</i>	<i>A:A</i>	<i>0.12</i>	<i>0.53</i>	<i>434</i>
1,4-Dimethoxybenzene	C8H10O2	-0.41	A:A	0.09	0.50	435
Dimethylsulfide	C2H6S	-0.41	A:A	0.06	0.47	436
1,2-Dichloroethane	C2H4Cl2	-0.42	A:A	0.05	0.47	437
1,4-Dithiane	C4H8S2	-0.43	A:A	0.04	0.47	438
Tetrathiafulvalene	C6H4S4	-0.43	A:A	0.01	0.44	439
1,2-bis(Methylthio)ethane	C4H10S2	-0.44	A:A	0.05	0.49	440
Diallyldisulfide	C6H10S2	-0.44	A:A	0.01	0.45	441
Diallylsulfide	C6H10S	-0.44	A:A	0.01	0.45	442
1,2-Dibenzylsulfane	C14H14S2	-0.45	A:A	0.01	0.46	443
<i>Dichloromethane^{CSD}</i>	<i>CH2Cl2</i>	<i>-0.46</i>	<i>A:A</i>	<i>0.06</i>	<i>0.51</i>	<i>444</i>
1,2-Dimethyldisulfane	C2H6S2	-0.46	A:A	0.04	0.50	445
Diphenyl ether	C12H10O	-0.46	A:A	0.01	0.48	446
Caryophyllen- α -oxide	C15H24O	-0.47	A:A	0.02	0.49	447
1,2-Diphenyldisulfane	C12H10S2	-0.47	A:A	0.01	0.48	448
Chloroform	CHCl3	-0.48	A:A	0.00	0.48	449
<i>Toluene^{CSD}</i>	<i>C7H8</i>	<i>*</i>	<i>A:A</i>		<i>0.44</i>	<i>*</i>

*Toluene does not exhibit donor or acceptor groups and, so, it is not possible to calculate the HBP score.

Table S4 – Coordination value results for a multicomponent analysis of 450 co-formers against NVP molecule. Molecules are ordered by CV ranking position. In bold are represented the 76 molecules for which experimental multicomponent results are available. Black-italic letter identify the positive results; CSD means molecules reported in the CSD database. Red-underline letter identify the negative results.

Co-former	Molecular formula	CV score	CV ranking
Cyclohexane-1,4-diamine	C6H14N2	-1.143	1
(+)-Camphoric acid	C10H16O4	-1.139	2
4-Ethoxyphenol	C8H10O2	-1.134	3
<i>Cinnamide</i>	<i>C9H9NO</i>	<i>-1.134</i>	<i>4</i>
1-Hydroxydiamantane	C14H20O	-1.129	5
DL-Glutamine	C5H10N2O3	-1.129	6
2,6-Di-tert-butyl-4-methylphenol	C15H24O	-1.126	7
<i>Propionamide</i>	<i>C3H7NO</i>	<i>-1.126</i>	<i>8</i>
L-Lysine	C6H14N2O2	-1.100	9
1,2-Ethanedithiol	C2H6S2	-1.099	10

2,5,5,8α-Tetramethyloctahydro-2H-2,4α-methanonaphthalen-1-ol	C15H26O	-1.099	11
Butyramide	C4H9NO	-1.093	12
D-Threonine	C4H9NO3	-1.079	13
<u>L-Aspartic acid</u>	<u>C4H7NO4</u>	<u>-1.076</u>	<u>14</u>
1,11-Undecanediol	C11H24O2	-1.073	15
<u>DL-Malic acid</u>	<u>C4H6O5</u>	<u>-1.069</u>	<u>16</u>
Phenol	C6H6O	-1.064	17
2-(Tert-butyl)-4-methoxyphenol	C11H16O2	-1.062	18
Glycerol	C3H8O3	-1.059	19
1,13-Tridecanediol	C13H28O2	-1.019	20
DL-Tyrosine	C9H11NO3	-1.018	21
<u>L-Glutamine</u>	<u>C5H10N2O3</u>	<u>-1.014</u>	<u>22</u>
L-Threonine	C4H9NO3	-1.013	23
L-Tyrosine	C9H11NO3	-1.010	24
Trimesic acid	C9H6O6	-1.001	25
cis,cis-1,3,5-Cyclohexanetricarboxylic acid	C9H12O6	-0.996	26
2,2'-Dihydroxy-5,5'-diallyl-biphenyl	C18H18O2	-0.990	27
13-epi-Sclareol	C20H36O2	-0.987	28
cis-Aconitic acid	C6H6O6	-0.985	29
(R)-2-Hydroxypropanamide	C3H7NO2	-0.974	30
(S)-2-Hydroxypropanamide	C3H7NO2	-0.969	31
1,3-Propanedithiol	C3H8S2	-0.968	32
1,1'-Azo-bis(carbamide)	C2H4N4O2	-0.968	33
Lactic acid	C3H6O3	-0.962	34
1-Naphthol	C10H8O	-0.959	35
2,4,6-Trimethylphenol	C9H12O	-0.955	36
4-(Hydroxymethyl)-2-methoxyphenol	C8H10O3	-0.950	37
Sebacic acid	C10H18O4	-0.942	38
2-Isopropyl-5-methylphenol	C10H14O	-0.935	39
2,5-Dimethylphenol	C8H10O	-0.935	40
Cyclamic acid	C6H13NO3S	-0.932	41
o-Cresol	C7H8O	-0.930	42
D-Lysine	C6H14N2O2	-0.919	43
Vanillic acid	C8H8O4	-0.914	44
<u>Ferulic acid</u>	<u>C10H10O4</u>	<u>-0.885</u>	<u>45</u>
Tromethamine	C4H11NO3	-0.883	46
<u>Suberic acid</u>	<u>C8H14O4</u>	<u>-0.862</u>	<u>47</u>
D-Asparagine	C4H8N2O3	-0.858	48
<u>L-Malic acid</u>	<u>C4H6O5</u>	<u>-0.851</u>	<u>49</u>
D-Glucono-1,5-lactone	C6H10O6	-0.846	50
Pterostilbene	C16H16O3	-0.843	51
<i>3-Hydroxybenzoic acid</i>^{CSD}	<i>C7H6O3</i>	<i>-0.841</i>	<i>52</i>
Biotin	C10H16N2O3S	-0.827	53
4-(Hydroxymethyl)phenol	C7H8O2	-0.809	54
<u>Hippuric acid</u>	<u>C9H9NO3</u>	<u>-0.808</u>	<u>55</u>
<i>4-Hydroxybenzoic acid</i>^{CSD}	<i>C7H6O3</i>	<i>-0.808</i>	<i>56</i>

L-Cystine	C6H12N2O4S2	-0.793	57
<u>Benzamide</u>	<u>C7H7NO</u>	<u>-0.782</u>	<u>58</u>
2,2',2''-Nitrilotriethanol	C6H15NO3	-0.777	59
2-Hydroxyacetamide	C2H5NO2	-0.763	60
Terephthalic acid	C8H6O4	-0.741	61
2-Coumaric acid	C9H8O3	-0.738	62
Ethylene glycol	C2H6O2	-0.726	63
<i>Gentisic acid</i>^{CSD}	<i>C7H6O4</i>	<i>-0.718</i>	<i>64</i>
2,4-Dihydroxybenzoic acid	C7H6O4	-0.710	65
<i>Adipic acid</i>	<i>C10H18</i>	<i>-0.703</i>	<i>66</i>
L-Tryptophan	C11H12N2O2	-0.698	67
1,7,7-Trimethyltricyclo(2.2.1.0 ^{2,6})heptan-4-ol	C10H16O	-0.689	68
L-Asparagine	C4H8N2O3	-0.672	69
4,4,7-Trimethyldecahydro-1H-cyclopenta[cd]inden-7-ol	C14H24O	-0.625	70
<u>L-Tartaric acid</u>	<u>C4H6O6</u>	<u>-0.616</u>	<u>71</u>
1,6-Hexanedithiol	C6H14S2	-0.615	72
<i>Maleic Acid</i>^{CSD}	<i>C4H4O4</i>	<i>-0.609</i>	<i>73</i>
Pyrrrole	C4H5N	-0.604	74
<i>Tartaric acid</i>^{CSD}	<i>C4H6O6</i>	<i>-0.590</i>	<i>75</i>
(1R,2R)-Cyclohexane-1,2-Diamine	C6H14N2	-0.585	76
DL-Tryptophan	C11H12N2O2	-0.569	77
3,3'-Thiodipropionic acid	C6H10O4S	-0.543	78
Adamantane-1,3,5,7-tetracarboxylic acid	C14H16O8	-0.542	79
4-Aminobenzamide	C7H8N2O	-0.536	80
Acetamide	C2H5NO	-0.527	81
Cyclodecanol	C10H20O	-0.523	82
<u>Succinamide</u>	<u>C4H8N2O2</u>	<u>-0.517</u>	<u>83</u>
<i>Glutaric acid</i>^{CSD}	<i>C5H8O4</i>	<i>-0.505</i>	<i>84</i>
<i>Glutamic acid</i>	<i>C5H9NO4</i>	<i>-0.504</i>	<i>85</i>
Isocaryolan-9 α -ol	C15H26O	-0.494	86
Ethylenediamine	C2H8N2	-0.490	87
<i>L-Mandelic acid</i>	<i>C8H8O3</i>	<i>-0.455</i>	<i>88</i>
2-Methylpropan-2-ol	C4H10O	-0.438	89
1-Hydroxy-2-naphthoic acid	C11H8O3	-0.435	90
L-Cysteine	C3H7NO2S	-0.425	91
L-Cysteine	C3H7NO2S	-0.425	92
α -D-Talose	C6H12O6	-0.415	93
1,8-Octanedithiol	C8H18S2	-0.413	94
1,1,6,6-Tetraphenylhexa-2,4-diyne-1,6-diol	C30H22O2	-0.400	95
<i>Citric acid</i>	<i>C6H8O7</i>	<i>-0.400</i>	<i>96</i>
3 β ,12 β -Dihydroxy-5 β -cholan-24-oic acid	C24H40O4	-0.393	97
4-Acetamidobenzoic acid	C9H9NO3	-0.373	98
DL-Valine	C5H11NO2	-0.362	99
Formamide	CH3NO	-0.357	100
Meso-Tartaric acid	C4H6O6	-0.355	101
Ibuprofen	C13H18O2	-0.349	102

Phenyl 2-Hydroxybenzoate	C13H10O3	-0.344	103
Linoleic acid	C18H32O2	-0.337	104
Butan-2-ol	C4H10O	-0.333	105
<u>Stearic acid</u>	<u>C18H36O2</u>	<u>-0.322</u>	<u>106</u>
1,9-Nonanedithiol	C9H20S2	-0.322	107
4-Aminobenzoic acid	C7H7NO2	-0.311	108
Salicylic acid^{CSD}	C7H6O3	-0.309	109
n-Hexadecanol	C16H34O	-0.303	110
(R,S)-Hesperetin	C16H14O6	-0.299	111
[1,1'-Biphenyl]-4,4'-diol	C12H10O2	-0.296	112
<u>Orcinol</u>	<u>C7H8O2</u>	<u>-0.295</u>	<u>113</u>
Malonic acid	C3H4O4	-0.293	114
<u>Hydroquinone</u>	<u>C6H6O2</u>	<u>-0.286</u>	<u>115</u>
<u>Resorcinol</u>	<u>C6H6O2</u>	<u>-0.285</u>	<u>116</u>
Palmitic Acid	C16H32O2	-0.283	117
2-Aminoethan-1-ol	C2H7NO	-0.282	118
2-Acetylpyrrole	C6H7NO	-0.280	119
[1,1'-Binaphthalene]-2,2'-diol	C20H14O2	-0.276	120
DL-Serine	C3H7NO3	-0.269	121
D-Isoleucine	C6H13NO2	-0.268	122
Allocinnamic acid	C9H8O2	-0.267	123
<u>Glycolic acid</u>	<u>C2H4O3</u>	<u>-0.260</u>	<u>124</u>
Anthranilic acid	C7H7NO2	-0.259	125
Tetradecanoic acid	C14H28O2	-0.257	126
1,1-bis(4-Hydroxyphenyl)cyclohexane	C18H20O2	-0.253	127
Carbamazepine	C15H12N2O	-0.250	128
(-)-Epicedrol	C15H26O	-0.244	129
<u>DL-Aspartic acid</u>	<u>C4H7NO4</u>	<u>-0.241</u>	<u>130</u>
Sucralose	C12H19Cl3O8	-0.224	131
Chloranilic acid	C6H2Cl2O4	-0.222	132
iso-Deoxycholic acid	C24H40O4	-0.218	133
Methyl paraben	C8H8O3	-0.216	134
2-Amino-5-methylbenzoic acid	C8H9NO2	-0.212	135
(5-Hydroxy-6-methylpyridine-3,4-diy)dimethanol	C8H11NO3	-0.194	136
<u>Catechol</u>	<u>C6H6O2</u>	<u>-0.180</u>	<u>137</u>
Decanoic acid	C10H20O2	-0.177	138
Undecanoic Acid	C11H22O2	-0.176	139
Octanol^{CSD}	C8H18O	-0.165	140
<u>Succinic acid</u>	<u>C4H6O4</u>	<u>-0.165</u>	<u>141</u>
Cholic acid	C24H40O5	-0.151	142
3-Methylbut-2-enoic acid	C5H8O2	-0.150	143
β -D-Psicose	C6H12O6	-0.148	144
Urea	CH4N2O	-0.137	145
Phenylmethanethiol	C7H8S	-0.134	146
Heptanol^{CSD}	C7H16O	-0.128	147
Nonanoic acid	C9H18O2	-0.124	148

Tramadol	C16H25NO2	-0.120	149
Octanoic acid	C8H16O2	-0.117	150
2-Phenylacetic acid	C8H8O2	-0.103	151
Pentadecanoic acid	C15H30O2	-0.097	152
Oxalic acid	C2H2O4	-0.093	153
β-DL-Arabinose	C5H10O5	-0.091	154
Hexanol^{CSD}	C6H14O	-0.090	155
1-Amino-1-methylcyclopropane	C4H9N	-0.089	156
(2R,3R)-2,3-Dimethylcyclopropane-1-carboxylic acid	C6H10O2	-0.081	157
Heptanoic acid	C7H14O2	-0.081	158
Hexan-1-amine	C6H15N	-0.080	159
Pentan-1-amine	C5H13N	-0.079	160
Benzoic acid^{CSD}	C7H6O2	-0.058	161
Tridecanoic Acid	C13H26O2	-0.053	162
Phenylmethanol	C7H8O	-0.033	163
DL-Glutamic acid	C5H9NO4	-0.031	164
Cyclobutanol	C4H8O	-0.030	165
β-L-Lyxopyranose	C5H10O5	-0.019	166
Hexanoic acid	C6H12O2	-0.017	167
DL-Cysteine	C3H7NO2S	-0.015	168
Lauric acid	C12H24O2	-0.012	169
n-Butanol^{CSD}	C4H10O	-0.009	170
Methanol	CH4O	0.002	171
Butan-1-amine	C4H11N	0.009	172
DL-Isoleucine	C6H13NO2	0.020	173
Sorbic acid	C6H8O2	0.027	174
Propan-1-amine	C3H9N	0.032	175
DL-Ribose	C5H10O5	0.046	176
L-Ascorbic acid	C6H8O6	0.056	177
L-Ribose	C5H10O5	0.056	178
o-Anisic acid	C8H8O3	0.093	179
β-D-Gulose	C6H12O6	0.097	180
Fumaric acid	C4H4O4	0.103	181
Butyric acid	C4H8O2	0.117	182
Lidocaine	C18H32O2	0.117	183
Thiourea	CH4N2S	0.123	184
β-D-Glucose	C6H12O6	0.124	185
2,2,2-Trifluoroethanol	C2H3F3O	0.126	186
Crotonic acid	C4H6O2	0.130	187
α-L-Xylopyranose	C5H10O5	0.140	188
D-Glucuronic acid	C6H10O7	0.147	189
Cinnamic acid	C9H8O2	0.156	190
Ethylamine	C2H7N	0.164	191
Acetylmethionine	C7H13NO3S	0.189	192
Pyrimethamine	C12H13ClN4	0.190	193
β-D-Galactose	C6H12O6	0.193	194

α -D-Glucose	C6H12O6	0.224	195
2,6-Pyridinedicarboxylic acid	C7H5NO4	0.230	196
Proline	C5H9NO2	0.233	197
Xylitol	C5H12O5	0.246	198
Imidazole	C3H4N2	0.259	199
Trifluoroacetic acid	C2HF3O2	0.281	200
DL-Arabinitol	C5H12O5	0.293	201
Acetic acid	C2H4O2	0.293	202
L-Proline	C5H9NO2	0.296	203
4-(4-Hydroxyphenyl)butan-2-one	C10H12O2	0.298	204
α -D-Galactose	C6H12O6	0.312	205
D-Arabinitol	C5H12O5	0.313	206
o- β -D-Mannopyranosyl-(1-4)- α -D-mannopyranose	C12H22O11	0.330	207
β -D-Altropyranose	C6H12O6	0.332	208
4-Methoxybenzoic acid	C8H8O3	0.333	209
Phenoxyacetic acid	C8H8O3	0.371	210
1-Pentanol	C5H12O	0.382	211
4-Nitrophenol	C6H5NO3	0.382	212
<u>Phloroglucinol</u>	<u>C6H6O3</u>	<u>0.397</u>	<u>213</u>
n-Methyl-D-glucamine	C7H17NO5	0.398	214
β -D-Allose	C6H12O6	0.400	215
2-Chloroacetic acid	C2H3ClO2	0.419	216
<u>L-Valine</u>	<u>C5H11NO2</u>	<u>0.426</u>	<u>217</u>
4'-Hydroxyacetophenone	C8H8O2	0.442	218
β -D-Fructopyranose	C6H12O6	0.465	219
Ribitol	C5H12O5	0.501	220
DL-Leucine	C6H13NO2	0.535	221
<i>Ethanol</i>^{CSD}	<i>C2H5OH</i>	<i>0.538</i>	<i>222</i>
Sucrose	C12H22O11	0.544	223
<i>Toluene</i>^{CSD}	<i>C7H8</i>	<i>0.575**</i>	<i>224**</i>
<u>Pyroglutamic acid</u>	<u>C5H7NO3</u>	<u>0.579</u>	<u>225</u>
<i>Dichloromethane</i>^{CSD}	<i>CH2Cl2</i>	<i>0.593</i>	<i>226</i>
L-Leucine	C6H13NO2	0.598	227
L- α -Leucine	C6H13NO2	0.598	228
Chloroform	CHCl3	0.604	229
<i>ϵ-Caprolactam</i>^{CSD}	<i>C6H11NO</i>	<i>0.606</i>	<i>230</i>
Benzoin	C14H12O2	0.608	231
<u>L-Alanine</u>	<u>C3H7NO2</u>	<u>0.612</u>	<u>232</u>
L-Methionine	C5H11NO2S	0.619	233
Tricyclopropylamine	C9H15N	0.623	234
<i>Trichloroacetic acid</i>^{CSD}	<i>C2HCl3O2</i>	<i>0.623</i>	<i>235</i>
Diallylsulfide	C6H10S	0.624	236
5-Nitroisophthalic acid	C8H5NO6	0.628	237
Ethyl(methyl)sulfane	C3H8S	0.633	238
D-Alanine	C3H7NO2	0.634	239
Dimethylsulfide	C2H6S	0.638	240

2-Ethyl-3-hydroxy-4H-pyran-4-one	C7H8O3	0.641	241
4-Hydroxybenzaldehyde	C7H6O2	0.646	242
Vanillin	C8H8O3	0.668	243
1-Chloro-1,1,2,2,2-pentafluoroethane	C2ClF5	0.670	244
DL-Methionine	C5H11NO2S	0.675	245
1,2-bis(Methylthio)ethane	C4H10S2	0.676	246
L-chiro-Inositol	C6H12O6	0.682	247
1,2,4,5-Tetrafluoro-3,6-di-iodobenzene^{CS}	C6F4I2	0.682	248
bis(Methylthio)methane	C3H8S2	0.686	249
1,2-Dichloroethane	C2H4Cl2	0.690	250
Formic acid	CH2O2	0.692	251
cis-Inositol	C6H12O6	0.699	252
1,4-Dithiane	C4H8S2	0.699	253
1,2-Dibenzyldisulfane	C14H14S2	0.704	254
Diphenyl ether	C12H10O	0.704	255
Tetrathiafulvalene	C6H4S4	0.708	256
1,2-Diphenyldisulfane	C12H10S2	0.712	257
2-Pyridone	C5H5NO	0.714	258
Allitol	C6H14O6	0.718	259
Orotic acid	C5H4N2O4	0.718	260
Diallyldisulfide	C6H10S2	0.719	261
2-Methoxynaphthalene	C11H10O	0.720	262
2-Aminopyrimidine	C4H5N3	0.727	263
1,3-Diiodobenzene^{CS}	C6H4I2	0.727	264
1,2-Dimethyldisulfane	C2H6S2	0.731	265
1-Naphthalenesulfonic acid	C10H8O3S	0.732	266
Piperidine	C5H11N	0.735	267
α -L-Sorbopyranose	C6H12O6	0.746	268
Tetraiodoethene	C2I4	0.747	269
1,4-Phenylenediamine	C6H8N2	0.755	270
Acetylsalicylic acid	C9H8O4	0.759	271
4-Hydroxy-3,5-dimethoxybenzaldehyde	C9H10O4	0.764	272
2,5-Piperazinedione	C4H6N2O2	0.769	273
Piperazine	C4H10N2	0.769	274
(E)-4-(4-Hydroxy-3-methoxyphenyl)but-3-en-2-one	C11H12O3	0.770	275
Gallic acid	C7H6O5	0.773	276
1,4,8,11-Tetra-azacyclotetradecane	C10H24N4	0.786	277
1,3-Distearoyl-2-oleoylglycerol	C57H108O6	0.808	278
β -Tristearin	C57H110O6	0.815	279
2-(Oleoyloxy)propane-1,3-diyl distearate	C57H108O6	0.816	280
α -Ketoglutaric acid	C5H6O5	0.817	281
Dichlorodifluoromethane	CCl2F2	0.819	282
1,3-Distearoyl-2-elaidoylglycerol	C57H108O6	0.820	283
2,4-Pyridinedicarboxylic acid	C7H5NO4	0.831	284
1,2-Dimethoxybenzene	C8H10O2	0.832	285
4-Hydroxy-L-proline	C5H9NO3	0.839	286

2,2-Dibromo-2-cyanoacetamide	C3H2Br2N2O	0.839	287
1,1-Dihydroxypropan-2-one	C3H6O3	0.841	288
1,2-Distearoyl-3-elaidoylglycerol	C57H108O6	0.847	289
α-D-Tagatopyranose	C5H6O3	0.850	290
D-Iditol	C6H14O6	0.851	291
Vitamin A acetate	C22H32O2	0.861	292
β-Alanine	C3H7NO2	0.869	293
1,4-Dimethoxybenzene	C8H10O2	0.870	294
Caryophyllen-α-oxide	C15H24O	0.875	295
Uracil	C4H4N2O2	0.877	296
4-Aminobutanoic acid	C4H9NO2	0.879	297
D-Altritol	C6H14O6	0.880	298
D-Mannitol	C6H14O6	0.891	299
myo-Inositol	C6H12O6	0.914	300
Glycine	C2H5NO2	0.914	301
α-8'-β-Apocarotenal	C30H40O	0.929	302
4-Methylbenzenesulfonic acid	C7H8O3S	0.933	303
4-Nitrobenzoic acid	C7H5NO4	0.934	304
Tetrabromomethane	CBr4	0.935	305
Eucalyptol	C10H18O	0.936	306
β-8'-β-Apocarotenal	C30H40O	0.946	307
Scyllo-inositol	C6H12O6	0.951	308
α-Maltose	C12H22O11	0.954	309
D-Glucitol	C6H14O6	0.959	310
Galactitol	C6H14O6	0.963	311
Nicotinamide	C6H6N2O	0.978	312
I-Iditol	C6H14O6	0.984	313
Ethyl Propionate	C5H10O2	0.995	314
Chlorine	Cl2	1.001	315
DL-Mannitol	C6H14O6	1.008	316
Naphthalene-1,5-disulfonic acid^{CS}	C10H8S2O6	1.009	317
Methyl cubane-1-carboxylate	C10H10O2	1.027	318
Isonicotinamide	C6H6N2O	1.034	319
Cycloundecanone	C11H20O	1.042	320
Ethylene oxide	C2H4O	1.043	321
Levulinic acid	C5H8O3	1.062	322
Neotame	C20H30N2O5	1.062	323
epi-Inositol	C6H12O6	1.067	324
n-Butyl acetate	C6H12O2	1.070	325
β-Lactose	C12H22O11	1.073	326
Oxetane	C3H6O	1.075	327
Methyl benzoate	C8H8O2	1.081	328
(1R,2S)-2-Methyl-4-oxocyclohexane-1-carboxylic acid	C8H12O3	1.092	329
1,3-Diphenylpropan-2-one	C15H14O	1.095	330
Indomethacin	C19H16ClNO4	1.096	331
β-Cellobiose	C12H22O11	1.102	332

Morpholine	C4H9NO	1.110	333
(1S,6R,10R)-(+)-6-Methyl-4-oxabicyclo(8.4.1)pentadecan-3-one	C15H26O2	1.115	334
4-Allyl-2-methoxyphenyl benzoate	C17H16O3	1.117	335
2,6-Dimethylpyridine	C7H9N	1.126	336
Benzophenone	C13H10O	1.128	337
Cyclohexane-1,2,3,4,5,6-hexaol	C6H12O6	1.132	338
Ethyl acetate^{CSD}	C4H8O2	1.144	339
Methyl acetate	C3H6O2	1.144	340
Cyclodecanone	C10H18O	1.144	341
Acridine	C13H9N	1.156	342
β -galabiose	C12H22O11	1.157	343
(-)-1,3,3-Trimethyl-2-norbornanone	C10H16O	1.162	344
Tetrahydrofuran	C4H8O	1.163	345
1-Hydroxypropan-2-one	C3H6O2	1.170	346
Salicylaldehyde	C7H6O2	1.171	347
Chloro(methoxy)methane	C2H5ClO	1.173	348
S(+)-Camphor-10-sulfonic acid	C10H16O4S	1.176	349
Phenyl acetate	C8H8O2	1.177	350
2-Methoxy-4-(1-(E)-propenyl)phenyl acetate	C12H14O3	1.208	351
(3 α R,4R,6 α S,10 α S)-3 α ,4,7,7-Tetramethylperhydronaphtho(8 α ,1- β)furan-2-one	C16H26O2	1.220	352
1-(Naphthalen-2-yl)Ethan-1-One	C12H10O	1.236	353
Pyruvic acid	C3H4O3	1.242	354
(3 α R,4S,6 α S,10 α S)-3 α ,4,7,7-Tetramethylperhydronaphtho(8 α ,1- β)furan-2-one	C16H26O2	1.244	355
3 α ,4,7,7-Tetramethyl-(3 α R,4S,6 α R,10 α S)-perhydronaphtho(8 α ,1- β)furan-2-one	C16H26O2	1.252	356
Benzalacetone	C10H10O	1.259	357
Nicotinic acid	C6H5NO2	1.261	358
4-tert-Butyl-3-methoxy-2,6-dinitrotoluene	C12H16N2O5	1.265	359
(4R,7S)-7-Isopropyl-4-methyloxepan-2-one	C10H18O2	1.268	360
Acetophenone	C8H8O	1.271	361
Melamine	C3H6N6	1.283	362
Cyclohexane-1,2,3,4,5,6-hexol	C6H12O6	1.289	363
3,5-Dinitrosalicylic acid^{CSD}	C7H4N2O7	1.293	364
L-Carvone	C10H14O	1.300	365
1,2-Ethanedisulfonic acid	C2H6O6S2	1.315	366
3-Isochromanone	C9H8O2	1.329	367
Propan-2-one	C3H6O	1.334	368
Phthalide	C8H6O2	1.342	369
2,4-Dimethylpyridine	C7H9N	1.356	370
1,4-Dioxane^{CSD}	C4H8O2	1.357	371
1-(4-Methoxyphenyl)ethan-1-one	C9H10O2	1.361	372
Muco-inositol	C6H12O6	1.367	373
Coumarin	C9H6O2	1.371	374
Nootkatone	C15H22O	1.397	375
α -Lactose	C12H22O11	1.398	376
N,N-Dimethylacetamide	C4H9NO	1.409	377
5,5-Diethylbarbituric acid	C8H12N2O3	1.413	378

N-Methylpyrrolidone	C5H9NO	1.416	379
neo-Inositol	C6H12O6	1.418	380
Dimethyl succinate	C6H10O4	1.420	381
4-Methoxybenzaldehyde	C8H8O2	1.449	382
Cinnamaldehyde	C9H8O	1.451	383
3,5-Dinitrobenzoic acid	C7H4N2O6	1.453	384
Piperine	C17H19NO3	1.458	385
α,α -Galacto-trehalose	C12H22O11	1.463	386
1,2-Dicyclopropylethane-1,2-dione	C8H10O2	1.469	387
Myricetin	C15H10O8	1.476	388
Theophylline	C7H8N4O2	1.486	389
Pyridine	C5H5N	1.486	390
2,2'-Bipyridine	C10H8N2	1.496	391
Tetramethylpyrazine	C8H12N2	1.496	392
Nitromethane	CH3NO2	1.515	393
Cyclohexanone	C4H8	1.525	394
D-(+)-chiro-Inositol	C6H12O6	1.526	395
3-Oxocyclobutanecarboxylic acid	C5H6O3	1.538	396
(Z)-Ethyl 2-benzylidene-3-oxobutanoate	C13H14O3	1.540	397
Acrylaldehyde	C3H4O	1.543	398
Furfural	C6H12O2	1.545	399
3,4-(Methylenedioxy)benzaldehyde	C8H6O3	1.560	400
Trimethylamine	C3H9N	1.562	401
Dibenzoyl peroxide	C14H10O4	1.563	402
Formaldehyde	CH2O	1.566	403
2-Amino-5-picolinic acid	C6H6N2O2	1.647	404
4-Methylmorpholine	C5H11NO	1.668	405
Saccharin^{CSD}	C7H5NO3S	1.674	406
DL-Arginine	C6H14N4O2	1.693	407
<u>L-Arginine</u>	<u>C6H14N4O2</u>	<u>1.693</u>	<u>408</u>
Tryphenylphosphine oxide	C18H15OP	1.719	409
1,10-Phenanthroline	C12H8N2	1.722	410
N,N-Dimethylformamide	C3H7NO	1.739	411
α,α -Trehalose	C12H22O11	1.746	412
Phenazine	C12H8N2	1.750	413
Trimethylamine oxide	C3H9NO	1.777	414
β -Maltose	C12H22O11	1.858	415
1,4-Dimethylpiperazine	C6H14N2	1.910	416
2,3-Butanedione	C4H6O2	1.992	417
3S-cis-3,6-Dimethyl-1,4-dioxane-2,5-dione	C6H8O4	1.994	418
Dimethylsulfoxide	C2H6OS	2.003	419
2,6-Dimethylpyrazine	C6H8N2	2.008	420
Terephthalaldehyde	C8H6O2	2.021	421
2,3-Dimethylpyrazine	C6H8N2	2.044	422
<u>Theobromine</u>	<u>C7H8N4O2</u>	<u>2.079</u>	<u>423</u>
Dihydrofuran-2,5-dione	C4H4O3	2.124	424

2,5-Dimethylpyrazine	C6H8N2	2.130	425
1,3-Di(pyridin-4-yl)propane	C13H14N2	2.183	426
(E)-4,4'-Diaza stilbene	C12H10N2	2.224	427
cis-anti-cis-Dicyclohexano-18-crown-6	C20H36O6	2.241	428
4,4'-Ethene-1,2-diyl dipyridine	C12H10N2	2.241	429
2,3,5,6-Tetrachlorocyclohexa-2,5-diene-1,4-dione	C6Cl4O2	2.255	430
1,2-bis(4-Pyridyl)ethane	C12H10N2	2.272	431
1,3,5-Trinitrobenzene	C6H3N3O6	2.279	432
1,4-Diazabicyclo[2.2.2]octane	C6H12N2	2.301	433
4,4'-Bipyridine	C10H8N2	2.319	434
Picric acid^{CSD}	C6H3N3O7	2.341	435
Caffeine	C8H10N4O2	2.353	436
Sucrose octa-acetate	C28H38O19	2.384	437
Pyrazine	C4H4N2	2.451	438
2,2'-(cyclohexa-2,5-diene-1,4-diylidene)dimalononitrile	C12H4N4	2.505	439
2,3,5,6-Tetrafluoro-7,7,8,8-tetracyanoquinodimethane	C12F4N4	2.505	440
1,2,4,5-Tetracyanobenzene	C10H2N4	2.616	441
4-Benzoquinone	C6H4O2	2.639	442
2,8,16,20-Tetramethylcalix(4)resorcinarene	C32H32O8	2.693	443
Tetracyanoethylene	C6N4	2.818	444
Quinoxaline-N,N'-dioxide	C8H6N2O2	2.874	445
Pyrazine-1,4-dioxide	C4H4N2O2	2.993	446
2,5-bis(4-Pyridyl)-1,3,4-oxadiazole	C12H8N4O	3.383	447
Hexamethylenetetramine	C6H12N4	3.427	448
Betaine	C5H10NO2	3.558	449
Pyromellitic	C10H2O6	3.566	450

**Toluene does not exhibit donor or acceptor groups. Thus, the CV score value obtained reflects only the CV for NVP molecule.

Table S5– Molecular complementarity results for a multicomponent analysis of 450 co-formers against NVP molecule. Molecules are ordered by MC ranking position. In bold are represented the 76 molecules for which experimental multicomponent results are available. Black-italic letter identify the positive results; CSD means molecules reported in the CSD database. Red-underline letter identify the negative results.

API	M/L axis ratio	S axis (Å)	S/L axis ratio	dipole moment magnitude (Debye)	fraction of Nitrogen and Oxygen
Nevirapine	0.895	6.667	0.611	1.972	0.250

Co-former	M/L axis ratio	M/L axis ratio Delta (pass < 0.31)	S axis (Å)	S axis (Å) Delta (pass < 3.23)	S/L axis ratio	S/L axis ratio Delta (pass < 0.275)	dipole moment magnitude (Debye)	dipole moment magnitude (Debye) Delta (pass < 5.94)	fraction of Nitrogen and Oxygen	fraction of Nitrogen and Oxygen Delta (pass < 0.294)	PASS/FAIL	MC score	MC ranking
<i>Stearic acid</i>	<i>0.196</i>	<i>0.699</i>	<i>4.452</i>	<i>2.215</i>	<i>0.166</i>	<i>0.445</i>	<i>0.690</i>	<i>1.282</i>	<i>0.100</i>	<i>0.150</i>	<i>FAIL</i>	<i>3.071</i>	<i>1</i>
n-Hexadecanol	0.200	0.695	4.404	2.263	0.185	0.426	2.269	0.297	0.059	0.191	FAIL	3.264	2
Palmitic Acid	0.215	0.680	4.635	2.032	0.190	0.421	0.763	1.209	0.111	0.139	FAIL	3.325	3
1,9-Nonanedithiol	0.280	0.615	4.417	2.250	0.263	0.348	0.676	1.296	0.000	0.250	FAIL	3.341	4
1,8-Octanedithiol	0.327	0.568	4.393	2.274	0.283	0.328	0.000	1.972	0.000	0.250	FAIL	3.444	5
Tetradecanoic acid	0.239	0.656	4.681	1.986	0.215	0.396	0.722	1.250	0.125	0.125	FAIL	3.549	6
Pentadecanoic acid	0.239	0.656	4.774	1.893	0.212	0.399	0.760	1.212	0.118	0.132	FAIL	3.549	7
Tridecanoic Acid	0.271	0.624	4.479	2.188	0.225	0.386	0.744	1.228	0.133	0.117	FAIL	3.657	8
β-Tristearin	0.190	0.705	7.157	0.490	0.135	0.476	0.332	1.640	0.095	0.155	FAIL	3.699	9
1,2-Distearoyl-3-elaidoylglycerol	0.199	0.696	6.801	0.134	0.130	0.481	1.341	0.631	0.095	0.155	FAIL	3.769	10
1,6-Hexanedithiol	0.385	0.510	4.403	2.264	0.336	0.275	0.000	1.972	0.000	0.250	FAIL	3.827	11
Lauric acid	0.280	0.615	4.662	2.005	0.251	0.360	0.819	1.153	0.143	0.107	FAIL	3.884	12
Undecanoic Acid	0.301	0.594	4.476	2.191	0.254	0.357	0.802	1.170	0.154	0.096	FAIL	3.939	13
1,3-Distearoyl-2-elaidoylglycerol	0.197	0.698	6.853	0.186	0.132	0.479	2.498	0.526	0.095	0.155	FAIL	3.981	14
Decanoic acid	0.314	0.581	4.403	2.264	0.264	0.347	0.754	1.218	0.167	0.083	FAIL	4.031	15
2-(Oleoyloxy)propane-1,3-diyl distearate	0.323	0.572	6.894	0.227	0.146	0.465	0.395	1.577	0.095	0.155	FAIL	4.097	16
1,13-Tridecanediol	0.268	0.627	5.410	1.257	0.265	0.346	0.962	1.010	0.133	0.117	FAIL	4.117	17
[1,1'-Biphenyl]-4,4'-diol	0.521	0.374	3.433	3.234	0.266	0.345	0.000	1.972	0.143	0.107	FAIL	4.197	18
Sebacic acid	0.317	0.578	4.353	2.314	0.247	0.364	0.000	1.972	0.286	0.036	FAIL	4.241	19
Nonanoic acid	0.350	0.545	4.358	2.309	0.286	0.325	0.706	1.266	0.182	0.068	FAIL	4.256	20
<i>Octano^{CSD}</i>	<i>0.329</i>	<i>0.566</i>	<i>4.310</i>	<i>2.357</i>	<i>0.306</i>	<i>0.305</i>	<i>2.217</i>	<i>0.245</i>	<i>0.111</i>	<i>0.139</i>	<i>FAIL</i>	<i>4.259</i>	<i>21</i>
1,3-Distearoyl-2-oleoylglycerol	0.315	0.580	7.105	0.438	0.148	0.463	1.469	0.503	0.095	0.155	FAIL	4.324	22
4,4'-Ethene-1,2-diylpyridine	0.562	0.333	3.402	3.265	0.273	0.338	0.003	1.969	0.143	0.107	FAIL	4.346	23

(E)-4,4'-Diazastilbene	0.557	0.338	3.517	3.150	0.281	0.330	0.000	1.972	0.143	0.107	FAIL	4.394	24
Tetrathiafulvalene	0.625	0.270	3.635	3.032	0.346	0.265	0.000	1.972	0.000	0.250	PASS	4.400	25
1,11-Undecanediol	0.316	0.579	5.358	1.309	0.301	0.310	0.928	1.044	0.154	0.096	FAIL	4.453	26
β -8'- β -Apocarotenal	0.346	0.549	6.637	0.030	0.241	0.370	1.858	0.114	0.032	0.218	FAIL	4.469	27
Octanoic acid	0.374	0.521	4.479	2.188	0.319	0.292	0.735	1.237	0.200	0.050	FAIL	4.557	28
Heptano^{CSD}	0.373	0.522	4.312	2.355	0.337	0.274	2.224	0.252	0.125	0.125	FAIL	4.563	29
α -8'- β -Apocarotenal	0.323	0.572	7.126	0.459	0.258	0.353	1.710	0.262	0.032	0.218	FAIL	4.583	30
2,2'-Bipyridine	0.585	0.310	3.419	3.248	0.297	0.314	0.000	1.972	0.167	0.083	FAIL	4.594	31
Hexan-1-amine	0.405	0.490	4.238	2.429	0.376	0.235	0.756	1.216	0.143	0.107	FAIL	4.599	32
1,2-bis(4-Pyridyl)ethane	0.551	0.344	4.040	2.627	0.324	0.287	0.112	1.860	0.143	0.107	FAIL	4.712	33
Linoleic acid	0.503	0.392	5.502	1.165	0.256	0.355	0.704	1.268	0.100	0.150	FAIL	4.716	34
Suberic acid	0.370	0.525	4.370	2.297	0.290	0.321	0.000	1.972	0.333	0.083	FAIL	4.734	35
Acridine	0.643	0.252	3.510	3.157	0.304	0.307	1.354	0.618	0.071	0.179	FAIL	4.736	36
Phenazine	0.648	0.247	3.459	3.208	0.304	0.307	0.027	1.945	0.143	0.107	FAIL	4.758	37
Heptanoic acid	0.419	0.476	4.305	2.362	0.337	0.274	0.746	1.226	0.222	0.028	FAIL	4.791	38
1,2,4,5-Tetrafluoro-3,6-di-iodobenzene^{CSD}	0.704	0.191	3.961	2.706	0.363	0.248	0.000	1.972	0.000	0.250	PASS	4.817	39
Hexanol^{CSD}	0.400	0.495	4.308	2.359	0.373	0.238	2.216	0.244	0.143	0.107	FAIL	4.840	40
Cinnamaldehyde	0.626	0.269	3.527	3.140	0.311	0.300	1.737	0.235	0.100	0.150	FAIL	4.875	41
2,3,5,6-Tetrafluoro-7,7,8,8-tetracyanoquinodimethane	0.653	0.242	3.457	3.210	0.293	0.318	0.000	1.972	0.200	0.050	FAIL	4.922	42
2,5-bis(4-Pyridyl)-1,3,4-oxadiazole	0.539	0.356	3.575	3.092	0.263	0.348	0.744	1.228	0.294	0.044	FAIL	4.927	43
Cinnamic acid	0.620	0.275	3.514	3.153	0.310	0.301	0.687	1.285	0.182	0.068	FAIL	4.950	44
1,2-Dibenzylsulfane	0.445	0.450	6.000	0.667	0.400	0.211	1.445	0.527	0.000	0.250	FAIL	4.991	45
Benzalacetone	0.579	0.316	4.170	2.497	0.344	0.267	1.802	0.170	0.091	0.159	FAIL	5.023	46
Terephthalaldehyde	0.676	0.219	3.401	3.266	0.326	0.285	0.001	1.971	0.200	0.050	FAIL	5.099	47
2,2'-(cyclohexa-2,5-diene-1,4-diylidene)dimalononitrile	0.655	0.240	3.418	3.249	0.299	0.312	0.000	1.972	0.250	0.000	FAIL	5.109	48
Pentan-1-amine	0.482	0.413	4.293	2.374	0.432	0.179	0.688	1.284	0.167	0.083	FAIL	5.139	49
Hexanoic acid	0.459	0.436	4.327	2.340	0.378	0.233	0.745	1.227	0.250	0.000	FAIL	5.171	50
1,3-Diiodobenzene^{CSD}	0.741	0.154	3.960	2.707	0.397	0.214	0.884	1.088	0.000	0.250	PASS	5.209	51
1-Hydroxy-2-naphthoic acid	0.669	0.226	3.412	3.255	0.291	0.320	1.481	0.491	0.214	0.036	FAIL	5.250	52
Terephthalic acid	0.598	0.297	3.463	3.204	0.307	0.304	0.000	1.972	0.333	0.083	FAIL	5.250	53
1,2-Dichloroethane	0.618	0.277	4.202	2.465	0.539	0.072	0.000	1.972	0.000	0.250	PASS	5.254	54
Sorbic acid	0.506	0.389	4.173	2.494	0.376	0.235	0.753	1.219	0.250	0.000	FAIL	5.269	55
1,4-Dimethoxybenzene	0.605	0.290	4.284	2.383	0.367	0.244	0.000	1.972	0.200	0.050	PASS	5.293	56

1,10-Phenanthroline	0.692	0.203	3.494	3.173	0.304	0.307	2.372	0.400	0.143	0.107	FAIL	5.305	57
1-Pentanol	0.486	0.409	4.191	2.476	0.425	0.186	2.278	0.306	0.167	0.083	FAIL	5.362	58
Vitamin A acetate	0.461	0.434	7.045	0.378	0.370	0.241	0.484	1.488	0.083	0.167	FAIL	5.377	59
1-(Naphthalen-2-yl)Ethan-1-One	0.684	0.211	4.171	2.496	0.362	0.249	1.811	0.161	0.077	0.173	PASS	5.381	60
1,2-bis(Methylthio)ethane	0.573	0.322	5.347	1.320	0.531	0.080	0.000	1.972	0.000	0.250	FAIL	5.435	61
1,2-Ethanedithiol	0.618	0.277	4.532	2.135	0.565	0.046	0.000	1.972	0.000	0.250	PASS	5.451	62
4,4'-Bipyridine	0.633	0.262	4.255	2.412	0.418	0.193	0.038	1.934	0.167	0.083	PASS	5.454	63
Chlorine	0.638	0.257	3.500	3.167	0.638	0.027	0.000	1.972	0.000	0.250	PASS	5.462	64
Benzophenone	0.625	0.270	4.764	1.903	0.397	0.214	1.710	0.262	0.071	0.179	PASS	5.464	65
Piperine	0.501	0.394	5.747	0.920	0.340	0.271	1.216	0.756	0.190	0.060	FAIL	5.483	66
2-Methoxynaphthalene	0.688	0.207	4.175	2.492	0.362	0.249	2.226	0.254	0.083	0.167	PASS	5.485	67
Dimethyl succinate	0.472	0.423	4.288	2.379	0.351	0.260	0.000	1.972	0.400	0.150	FAIL	5.487	68
Adipic acid	0.447	0.448	4.512	2.155	0.363	0.248	0.000	1.972	0.400	0.150	FAIL	5.519	69
Butan-1-amine	0.525	0.370	4.174	2.493	0.480	0.131	0.800	1.172	0.200	0.050	FAIL	5.546	70
2-Coumaric acid	0.677	0.218	3.400	3.267	0.287	0.324	2.504	0.532	0.250	0.000	FAIL	5.552	71
Benzoic acid^{CSD}	0.718	0.177	3.423	3.244	0.366	0.245	0.598	1.374	0.222	0.028	FAIL	5.563	72
Phenyl 2-Hydroxybenzoate	0.564	0.331	4.907	1.760	0.358	0.253	1.858	0.114	0.188	0.062	FAIL	5.593	73
4-Hydroxybenzaldehyde	0.732	0.163	3.424	3.243	0.362	0.249	0.593	1.379	0.222	0.028	FAIL	5.593	74
Toluene^{CSD}	0.804	0.091	4.028	2.639	0.487	0.124	0.117	1.855	0.000	0.250	PASS	5.631	75
1,2,4,5-Tetracyanobenzene	0.730	0.165	3.431	3.236	0.340	0.271	0.153	1.819	0.286	0.036	FAIL	5.652	76
1-Naphthol	0.821	0.074	3.411	3.256	0.357	0.254	2.068	0.096	0.091	0.159	FAIL	5.660	77
Ethyl Propionate	0.552	0.343	4.265	2.402	0.423	0.188	0.313	1.659	0.286	0.036	FAIL	5.665	78
1,4-Phenylenediamine	0.741	0.154	3.420	3.247	0.379	0.232	0.000	1.972	0.250	0.000	FAIL	5.678	79
Cinnamide	0.567	0.328	4.805	1.862	0.403	0.208	1.692	0.280	0.182	0.068	FAIL	5.686	80
4-Aminobenzoic acid	0.663	0.232	3.535	3.132	0.352	0.259	0.999	0.973	0.300	0.050	PASS	5.702	81
Dibenzoyl peroxide	0.415	0.480	6.320	0.347	0.406	0.205	1.245	0.727	0.222	0.028	FAIL	5.736	82
n-Butanol^{CSD}	0.514	0.381	4.272	2.395	0.475	0.136	2.216	0.244	0.200	0.050	FAIL	5.761	83
Allocinnamic acid	0.666	0.229	4.485	2.182	0.415	0.196	0.670	1.302	0.182	0.068	PASS	5.778	84
4-Hydroxybenzoic acid^{CSD}	0.672	0.223	3.470	3.197	0.349	0.262	1.563	0.409	0.300	0.050	PASS	5.795	85
4-Methoxybenzoic acid	0.606	0.289	4.207	2.460	0.371	0.240	1.587	0.385	0.273	0.023	PASS	5.802	86
Acetophenone	0.699	0.196	4.167	2.500	0.433	0.178	1.823	0.149	0.111	0.139	PASS	5.804	87
1-(4-Methoxyphenyl)ethan-1-one	0.588	0.307	4.299	2.368	0.368	0.243	3.681	1.709	0.182	0.068	PASS	5.805	88
Phenoxyacetic acid	0.601	0.294	4.159	2.508	0.355	0.256	2.264	0.292	0.273	0.023	PASS	5.827	89
Hydroquinone	0.772	0.123	3.426	3.241	0.394	0.217	0.000	1.972	0.250	0.000	FAIL	5.834	90

Ibuprofen	0.530	0.365	5.925	0.742	0.467	0.144	0.872	1.100	0.133	0.117	FAIL	5.841	91
Myricetin	0.684	0.211	3.526	3.141	0.246	0.365	2.849	0.877	0.348	0.098	FAIL	5.856	92
Glutaric acid^{CSD}	0.465	0.430	4.496	2.171	0.400	0.211	0.115	1.857	0.444	0.194	FAIL	5.876	93
Pterostilbene	0.770	0.125	4.164	2.503	0.287	0.324	3.149	1.177	0.158	0.092	FAIL	5.884	94
Dimethylsulfide	0.689	0.206	4.183	2.484	0.600	0.011	1.168	0.804	0.000	0.250	PASS	5.896	95
4-Acetamidobenzoic acid	0.552	0.343	4.478	2.189	0.359	0.252	2.309	0.337	0.308	0.058	FAIL	5.909	96
4-Methoxybenzaldehyde	0.635	0.260	4.172	2.495	0.377	0.234	3.390	1.418	0.200	0.050	PASS	5.962	97
Methyl paraben	0.627	0.268	4.175	2.492	0.381	0.230	2.055	0.083	0.273	0.023	PASS	5.975	98
4-Ethoxyphenol	0.620	0.275	4.284	2.383	0.382	0.229	3.447	1.475	0.200	0.050	PASS	5.976	99
1,3-Propanedithiol	0.629	0.266	5.245	1.422	0.611	0.000	0.620	1.352	0.000	0.250	PASS	5.979	100
1,2-Diphenyldisulfane	0.577	0.318	6.499	0.168	0.527	0.084	1.224	0.748	0.000	0.250	FAIL	5.996	101
Methyl benzoate	0.646	0.249	4.786	1.881	0.462	0.149	0.486	1.486	0.200	0.050	PASS	6.008	102
4-Nitrobenzoic acid	0.636	0.259	3.538	3.129	0.335	0.276	1.422	0.550	0.417	0.167	FAIL	6.023	103
4-Benzoquinone	0.819	0.076	3.415	3.252	0.409	0.202	0.000	1.972	0.250	0.000	FAIL	6.037	104
1,2-Dicyclopropylethane-1,2-dione	0.620	0.275	4.972	1.695	0.503	0.108	0.000	1.972	0.200	0.050	PASS	6.049	105
Coumarin	0.788	0.107	3.423	3.244	0.348	0.263	3.466	1.494	0.182	0.068	FAIL	6.070	106
4-Aminobenzamide	0.661	0.234	4.014	2.653	0.400	0.211	1.353	0.619	0.300	0.050	PASS	6.078	107
cis-anti-cis-Dicyclohexano-18-crown-6	0.619	0.276	6.235	0.432	0.378	0.233	0.000	1.972	0.231	0.019	PASS	6.087	108
Pyromellitic	0.766	0.129	3.447	3.220	0.352	0.259	0.000	1.972	0.375	0.125	PASS	6.094	109
4'-Hydroxyacetophenone	0.661	0.234	4.142	2.525	0.405	0.206	3.138	1.166	0.200	0.050	PASS	6.096	110
2-Methoxy-4-(1-(E)-propenyl)phenyl acetate	0.629	0.266	5.226	1.441	0.378	0.233	2.404	0.432	0.200	0.050	PASS	6.107	111
Nicotinic acid	0.723	0.172	3.463	3.204	0.373	0.238	1.357	0.615	0.333	0.083	PASS	6.122	112
Nicotinamide	0.709	0.186	3.726	2.941	0.397	0.214	0.666	1.306	0.333	0.083	PASS	6.129	113
2,4-Dihydroxybenzoic acid	0.735	0.160	3.401	3.266	0.344	0.267	1.390	0.582	0.364	0.114	FAIL	6.147	114
Dichloromethane^{CSD}	0.720	0.175	4.098	2.569	0.638	0.027	1.443	0.529	0.000	0.250	PASS	6.154	115
1,3-Di(pyridin-4-yl)propane	0.539	0.356	6.130	0.537	0.489	0.122	1.734	0.238	0.133	0.117	FAIL	6.159	116
Benzamide	0.714	0.181	4.073	2.594	0.436	0.175	1.562	0.410	0.222	0.028	PASS	6.168	117
2,3,5,6-Tetrachlorocyclohexa-2,5-diene-1,4-dione	0.938	0.043	3.595	3.072	0.403	0.208	0.000	1.972	0.167	0.083	PASS	6.172	118
2,5-Dimethylpyrazine	0.730	0.165	4.193	2.474	0.461	0.150	0.000	1.972	0.250	0.000	PASS	6.180	119
Phenol	0.846	0.049	3.410	3.257	0.429	0.182	2.254	0.282	0.143	0.107	FAIL	6.211	120
Salicylic acid^{CSD}	0.788	0.107	3.414	3.253	0.367	0.244	1.572	0.400	0.300	0.050	FAIL	6.219	121
(E)-4-(4-Hydroxy-3-methoxyphenyl)but-3-en-2-one	0.700	0.195	4.146	2.521	0.343	0.268	4.247	2.275	0.214	0.036	PASS	6.232	122
Fumaric acid	0.630	0.265	3.423	3.244	0.396	0.215	0.000	1.972	0.500	0.250	FAIL	6.233	123

Ethyl acetate^{CSD}	0.634	0.261	4.251	2.416	0.475	0.136	0.275	1.697	0.333	0.083	PASS	6.267	124
Phenyl acetate	0.653	0.242	5.263	1.404	0.499	0.112	0.310	1.662	0.200	0.050	PASS	6.283	125
4-(4-Hydroxyphenyl)butan-2-one	0.535	0.360	6.041	0.626	0.485	0.126	2.203	0.231	0.167	0.083	FAIL	6.299	126
Tetraiodoethene	0.988	0.093	3.960	2.707	0.519	0.092	0.000	1.972	0.000	0.250	PASS	6.300	127
3-Hydroxybenzoic acid^{CSD}	0.815	0.080	3.470	3.197	0.373	0.238	1.428	0.544	0.300	0.050	PASS	6.321	128
Anthranilic acid	0.851	0.044	3.460	3.207	0.373	0.238	0.759	1.213	0.300	0.050	PASS	6.321	129
Acrylaldehyde	0.746	0.149	3.404	3.263	0.476	0.135	1.749	0.223	0.250	0.000	FAIL	6.336	130
Isonicotinamide	0.702	0.193	4.020	2.647	0.428	0.183	0.856	1.116	0.333	0.083	PASS	6.342	131
bis(Methylthio)methane	0.678	0.217	5.414	1.253	0.674	0.063	0.183	1.789	0.000	0.250	PASS	6.345	132
4-Nitrophenol	0.726	0.169	3.444	3.223	0.371	0.240	1.397	0.575	0.400	0.150	PASS	6.353	133
Chloranilic acid	0.880	0.015	3.500	3.167	0.357	0.254	0.000	1.972	0.333	0.083	PASS	6.353	134
2,6-Dimethylpyrazine	0.761	0.134	4.185	2.482	0.476	0.135	0.189	1.783	0.250	0.000	PASS	6.364	135
Gentisic acid^{CSD}	0.810	0.085	3.446	3.221	0.365	0.246	0.737	1.235	0.364	0.114	PASS	6.369	136
iso-Deoxycholic acid	0.459	0.436	7.972	1.305	0.429	0.182	2.229	0.257	0.143	0.107	FAIL	6.370	137
Ferulic acid	0.714	0.181	4.207	2.460	0.341	0.270	3.307	1.335	0.286	0.036	PASS	6.375	138
(1S,6R,10R)-(+)-6-Methyl-4-oxabicyclo(8.4.1)pentadecan-3-one	0.684	0.211	6.187	0.480	0.498	0.113	0.266	1.706	0.118	0.132	PASS	6.379	139
2,5-Dimethylphenol	0.811	0.084	4.415	2.252	0.467	0.144	1.987	0.015	0.111	0.139	PASS	6.393	140
3,3'-Thiodipropionic acid	0.556	0.339	5.322	1.345	0.442	0.169	0.697	1.275	0.364	0.114	FAIL	6.404	141
1,2-Dimethyldisulfane	0.669	0.226	5.287	1.380	0.652	0.041	1.458	0.514	0.000	0.250	PASS	6.411	142
Crotonic acid	0.640	0.255	4.263	2.404	0.495	0.116	0.628	1.344	0.333	0.083	PASS	6.423	143
2,4-Pyridinedicarboxylic acid	0.784	0.111	3.401	3.266	0.334	0.277	1.299	0.673	0.417	0.167	FAIL	6.434	144
2,4-Dimethylpyridine	0.841	0.054	4.200	2.467	0.484	0.127	1.413	0.559	0.125	0.125	PASS	6.436	145
n-Butyl acetate	0.619	0.276	5.331	1.336	0.518	0.093	0.333	1.639	0.250	0.000	PASS	6.437	146
Propan-1-amine	0.640	0.255	4.239	2.428	0.574	0.037	0.754	1.218	0.250	0.000	PASS	6.441	147
3,4-(Methylenedioxy)benzaldehyde	0.725	0.170	4.167	2.500	0.426	0.185	2.044	0.072	0.273	0.023	PASS	6.451	148
L-Lysine	0.525	0.370	5.336	1.331	0.442	0.169	0.860	1.112	0.400	0.150	FAIL	6.458	149
1,3-Diphenylpropan-2-one	0.593	0.302	6.685	0.018	0.538	0.073	1.889	0.083	0.063	0.187	PASS	6.471	150
2-Amino-5-methylbenzoic acid	0.835	0.060	3.956	2.711	0.413	0.198	0.751	1.221	0.273	0.023	PASS	6.475	151
Levulinic acid	0.567	0.328	4.500	2.167	0.443	0.168	2.191	0.219	0.375	0.125	FAIL	6.477	152
2,6-Dimethylpyridine	0.828	0.067	4.460	2.207	0.504	0.107	1.150	0.822	0.125	0.125	PASS	6.503	153
Phenylmethanethiol	0.754	0.141	5.586	1.081	0.601	0.010	0.933	1.039	0.000	0.250	PASS	6.504	154
Lidocaine	0.644	0.251	6.024	0.643	0.430	0.181	2.528	0.556	0.176	0.074	PASS	6.530	155
D-Lysine	0.528	0.367	5.342	1.325	0.443	0.168	1.251	0.721	0.400	0.150	FAIL	6.539	156

4-Methylbenzenesulfonic acid	0.645	0.250	5.127	1.540	0.494	0.117	0.929	1.043	0.273	0.023	PASS	6.549	157
Maleic Acid^{CS}	0.696	0.199	3.400	3.267	0.373	0.238	1.168	0.804	0.500	0.250	FAIL	6.551	158
Salicylaldehyde	0.834	0.061	3.412	3.255	0.391	0.220	3.746	1.774	0.222	0.028	FAIL	6.554	159
Succinamide	0.597	0.298	4.402	2.265	0.433	0.178	0.000	1.972	0.500	0.250	PASS	6.564	160
3-Methylbut-2-enoic acid	0.727	0.168	4.261	2.406	0.495	0.116	0.893	1.079	0.286	0.036	PASS	6.587	161
4-Allyl-2-methoxyphenyl benzoate	0.562	0.333	7.226	0.559	0.444	0.167	2.536	0.564	0.150	0.100	FAIL	6.602	162
Quinoxaline-N,N'-dioxide	0.920	0.025	3.503	3.164	0.383	0.228	0.151	1.821	0.333	0.083	PASS	6.603	163
Trimesic acid	0.907	0.012	3.404	3.263	0.310	0.301	0.868	1.104	0.400	0.150	FAIL	6.614	164
2-Phenylacetic acid	0.646	0.249	5.672	0.995	0.548	0.063	0.613	1.359	0.200	0.050	PASS	6.616	165
Ethyl(methyl)sulfane	0.725	0.170	5.219	1.448	0.683	0.072	1.179	0.793	0.000	0.250	PASS	6.637	166
1,1,6,6-Tetraphenylhexa-2,4-diyne-1,6-diol	0.698	0.197	7.723	1.056	0.479	0.132	0.274	1.698	0.063	0.187	PASS	6.645	167
Indomethacin	0.650	0.245	6.973	0.306	0.418	0.193	1.187	0.785	0.200	0.050	PASS	6.656	168
Tetramethylpyrazine	0.857	0.038	4.426	2.241	0.507	0.104	0.000	1.972	0.200	0.050	PASS	6.659	169
2-Acetylpyrrole	0.758	0.137	4.160	2.507	0.475	0.136	2.154	0.182	0.250	0.000	PASS	6.673	170
Hippuric acid	0.564	0.331	5.850	0.817	0.465	0.146	1.862	0.110	0.308	0.058	FAIL	6.682	171
2-Pyridone	0.847	0.048	3.448	3.219	0.437	0.174	1.908	0.064	0.286	0.036	PASS	6.683	172
Resorcinol	0.844	0.051	3.410	3.257	0.391	0.220	3.867	1.895	0.250	0.000	FAIL	6.701	173
1,4-Dimethylpiperazine	0.728	0.167	4.933	1.734	0.547	0.064	0.000	1.972	0.250	0.000	PASS	6.715	174
4-(Hydroxymethyl)phenol	0.679	0.216	4.762	1.905	0.473	0.138	3.531	1.559	0.222	0.028	PASS	6.734	175
2,6-Pyridinedicarboxylic acid	0.809	0.086	3.404	3.263	0.338	0.273	2.614	0.642	0.417	0.167	FAIL	6.751	176
Furfural	0.782	0.113	3.400	3.267	0.414	0.197	4.208	2.236	0.286	0.036	FAIL	6.762	177
α -Ketoglutaric acid	0.568	0.327	4.557	2.110	0.412	0.199	1.994	0.022	0.500	0.250	FAIL	6.778	178
3 β ,12 β -Dihydroxy-5 β -cholan-24-oic acid	0.478	0.417	8.375	1.708	0.457	0.154	3.080	1.108	0.143	0.107	FAIL	6.802	179
Diphenyl ether	0.633	0.262	6.652	0.015	0.575	0.036	2.169	0.197	0.077	0.173	PASS	6.819	180
2,3-Butanedione	0.740	0.155	4.312	2.355	0.550	0.061	0.000	1.972	0.333	0.083	PASS	6.855	181
Pyrrole	0.984	0.089	3.417	3.250	0.529	0.082	0.189	1.783	0.200	0.050	FAIL	6.868	182
Nootkatone	0.731	0.164	6.467	0.200	0.543	0.068	2.011	0.039	0.063	0.187	PASS	6.888	183
Pyridine	0.990	0.095	3.400	3.267	0.509	0.102	1.341	0.631	0.167	0.083	FAIL	6.891	184
2,4,6-Trimethylphenol	0.990	0.095	4.256	2.411	0.468	0.143	2.014	0.042	0.100	0.150	PASS	6.892	185
Cyclohexane-1,4-diamine	0.735	0.160	5.150	1.517	0.571	0.040	0.028	1.944	0.250	0.000	PASS	6.897	186
1-Chloro-1,1,2,2,2-pentafluoroethane	0.765	0.130	5.106	1.561	0.745	0.134	0.852	1.120	0.000	0.250	PASS	6.901	187
Phloroglucinol	0.966	0.071	3.414	3.253	0.412	0.199	0.596	1.376	0.333	0.083	FAIL	6.904	188
1,4,8,11-Tetra-azacyclotetradecane	0.845	0.050	5.126	1.541	0.454	0.157	0.000	1.972	0.286	0.036	PASS	6.937	189
1,1'-Azo-bis(carbamide)	0.631	0.264	3.438	3.229	0.355	0.256	0.000	1.972	0.750	0.500	FAIL	6.942	190

Pyrazine-1,4-dioxide	0.818	0.077	3.401	3.266	0.420	0.191	0.188	1.784	0.500	0.250	FAIL	6.951	191
L-Carvone	0.666	0.229	6.459	0.208	0.609	0.002	1.876	0.096	0.091	0.159	PASS	6.988	192
L-Cystine	0.561	0.334	6.114	0.553	0.476	0.135	0.567	1.405	0.429	0.179	FAIL	6.988	193
(R,S)-Hesperetin	0.565	0.330	6.819	0.152	0.441	0.170	3.272	1.300	0.273	0.023	FAIL	7.017	194
Pyrazine	0.907	0.012	3.413	3.254	0.525	0.086	0.000	1.972	0.333	0.083	FAIL	7.024	195
o-Cresol	0.942	0.047	4.170	2.497	0.534	0.077	2.025	0.053	0.125	0.125	PASS	7.038	196
Catechol	0.937	0.042	3.428	3.239	0.437	0.174	3.112	1.140	0.250	0.000	FAIL	7.047	197
2-Aminopyrimidine	0.835	0.060	3.440	3.227	0.429	0.182	1.630	0.342	0.429	0.179	PASS	7.052	198
Galactitol	0.510	0.385	5.855	0.812	0.485	0.126	0.857	1.115	0.500	0.250	FAIL	7.066	199
Phthalide	0.842	0.053	4.172	2.495	0.483	0.128	3.721	1.749	0.200	0.050	PASS	7.071	200
Naphthalene-1,5-disulfonic acid^{CSD}	0.776	0.119	5.519	1.148	0.447	0.164	0.701	1.271	0.333	0.083	PASS	7.088	201
DL-Arginine	0.501	0.394	5.879	0.788	0.470	0.141	1.457	0.515	0.500	0.250	FAIL	7.091	202
L-Arginine	0.501	0.394	5.879	0.788	0.470	0.141	1.457	0.515	0.500	0.250	FAIL	7.091	203
Tetracyanoethylene	0.942	0.047	3.405	3.262	0.451	0.160	0.000	1.972	0.400	0.150	FAIL	7.093	204
Butyramide	0.646	0.249	5.020	1.647	0.558	0.053	1.783	0.189	0.333	0.083	PASS	7.100	205
Allitol	0.585	0.310	5.562	1.105	0.493	0.118	0.000	1.972	0.500	0.250	PASS	7.102	206
Dichlorodifluoromethane	0.796	0.099	4.986	1.681	0.779	0.168	1.010	0.962	0.000	0.250	PASS	7.114	207
Pyrimethamine	0.733	0.162	6.666	0.001	0.494	0.117	0.637	1.335	0.235	0.015	PASS	7.131	208
Cyclamic acid	0.642	0.253	5.673	0.994	0.549	0.062	0.563	1.409	0.364	0.114	PASS	7.157	209
Phenylmethanol	0.808	0.087	5.193	1.474	0.598	0.013	2.134	0.162	0.125	0.125	PASS	7.173	210
Methyl cubane-1-carboxylate	0.709	0.186	6.397	0.270	0.629	0.018	0.334	1.638	0.167	0.083	PASS	7.179	211
Orotic acid	0.825	0.070	3.436	3.231	0.375	0.236	1.418	0.554	0.545	0.295	FAIL	7.181	212
2,6-Di-tert-butyl-4-methylphenol	0.788	0.107	6.781	0.114	0.578	0.033	1.506	0.466	0.063	0.187	PASS	7.211	213
2-Chloroacetic acid	0.762	0.133	4.120	2.547	0.546	0.065	0.834	1.138	0.400	0.150	PASS	7.220	214
Vanillin	0.925	0.030	4.128	2.539	0.444	0.167	2.583	0.611	0.273	0.023	PASS	7.240	215
1,2-Dimethoxybenzene	0.907	0.012	4.214	2.453	0.473	0.138	3.655	1.683	0.200	0.050	PASS	7.246	216
3-Isochromanone	0.783	0.112	5.052	1.615	0.529	0.082	3.665	1.693	0.182	0.068	PASS	7.250	217
Diallylsulfide	0.879	0.016	5.442	1.225	0.703	0.092	1.034	0.938	0.000	0.250	PASS	7.251	218
1,2-Ethanedisulfonic acid	0.525	0.370	5.333	1.334	0.514	0.097	0.000	1.972	0.600	0.350	FAIL	7.255	219
Theobromine	0.801	0.094	4.281	2.386	0.426	0.185	1.386	0.586	0.462	0.212	PASS	7.263	220
Cyclodecanol	0.902	0.007	5.204	1.463	0.568	0.043	2.186	0.214	0.091	0.159	PASS	7.264	221
Chloroform	0.944	0.049	4.592	2.075	0.720	0.109	1.129	0.843	0.000	0.250	PASS	7.275	222
2,5-Piperazinedione	0.764	0.131	4.199	2.468	0.499	0.112	0.000	1.972	0.500	0.250	PASS	7.280	223
2-Isopropyl-5-methylphenol	0.742	0.153	6.446	0.221	0.613	0.002	2.124	0.152	0.091	0.159	PASS	7.285	224

<i>Caffeine</i>	0.864	0.031	4.261	2.406	0.423	0.188	1.123	0.849	0.429	0.179	PASS	7.293	225
Tricyclopropylamine	0.954	0.059	5.324	1.343	0.585	0.026	0.632	1.340	0.100	0.150	PASS	7.300	226
Benzoïn	0.689	0.206	6.499	0.168	0.560	0.051	3.742	1.770	0.125	0.125	PASS	7.326	227
Ethylenediamine	0.675	0.220	4.159	2.508	0.599	0.012	0.000	1.972	0.500	0.250	PASS	7.344	228
3,5-Dinitrobenzoic acid	0.888	0.007	3.726	2.941	0.353	0.258	1.466	0.506	0.533	0.283	PASS	7.361	229
<u>Orcinol</u>	<u>0.998</u>	<u>0.103</u>	<u>4.054</u>	<u>2.613</u>	<u>0.490</u>	<u>0.121</u>	<u>2.172</u>	<u>0.200</u>	<u>0.222</u>	<u>0.028</u>	<u>PASS</u>	<u>7.377</u>	<u>230</u>
<u>Acetylsalicylic acid</u>	<u>0.834</u>	<u>0.061</u>	<u>5.556</u>	<u>1.111</u>	<u>0.519</u>	<u>0.092</u>	<u>0.296</u>	<u>1.676</u>	<u>0.308</u>	<u>0.058</u>	<u>PASS</u>	<u>7.395</u>	<u>231</u>
Propan-2-one	0.822	0.073	4.179	2.488	0.630	0.019	1.888	0.084	0.250	0.000	PASS	7.405	232
<i>Gallic acid</i>	0.864	0.031	3.483	3.184	0.346	0.265	5.181	3.209	0.417	0.167	PASS	7.414	233
<i>Ethanol</i>^{CS_D}	0.708	0.187	4.176	2.491	0.643	0.032	2.209	0.237	0.333	0.083	PASS	7.419	234
Cycloundecanone	0.886	0.009	5.644	1.023	0.611	0.000	1.859	0.113	0.083	0.167	PASS	7.423	235
o-Anisic acid	0.956	0.061	4.224	2.443	0.448	0.163	2.825	0.853	0.273	0.023	PASS	7.425	236
Ethylamine	0.738	0.157	4.183	2.484	0.683	0.072	0.797	1.175	0.333	0.083	PASS	7.426	237
Vanillic acid	0.885	0.010	4.123	2.544	0.432	0.179	3.521	1.549	0.333	0.083	PASS	7.428	238
Cyclodecanone	0.866	0.029	5.595	1.072	0.627	0.016	1.860	0.112	0.091	0.159	PASS	7.428	239
Isocaryolan-9 α -ol	0.774	0.121	6.691	0.024	0.613	0.002	2.497	0.525	0.063	0.187	PASS	7.432	240
Butan-2-ol	0.770	0.125	5.075	1.592	0.647	0.036	2.110	0.138	0.200	0.050	PASS	7.443	241
1,3,5-Trinitrobenzene	0.950	0.055	3.437	3.230	0.346	0.265	0.094	1.878	0.600	0.350	FAIL	7.443	242
N,N-Dimethylacetamide	0.822	0.073	4.164	2.503	0.564	0.047	1.942	0.030	0.333	0.083	PASS	7.451	243
Methyl acetate	0.765	0.130	4.427	2.240	0.604	0.007	0.361	1.611	0.400	0.150	PASS	7.456	244
1-Naphthalenesulfonic acid	0.941	0.046	5.275	1.392	0.529	0.082	0.814	1.158	0.214	0.036	PASS	7.457	245
[1,1'-Binaphthalene]-2,2'-diol	0.678	0.217	7.282	0.615	0.589	0.022	3.358	1.386	0.091	0.159	PASS	7.458	246
<i>Propionamide</i>	0.724	0.171	4.497	2.170	0.576	0.035	1.780	0.192	0.400	0.150	PASS	7.482	247
<i>Oxalic acid</i>	0.763	0.132	3.408	3.259	0.475	0.136	0.000	1.972	0.667	0.417	FAIL	7.512	248
<i>Theophylline</i>	0.879	0.016	4.404	2.263	0.442	0.169	0.829	1.143	0.462	0.212	PASS	7.517	249
5-Nitroisophthalic acid	0.826	0.069	3.400	3.267	0.304	0.307	6.578	4.606	0.467	0.217	FAIL	7.518	250
2,3-Dimethylpyrazine	0.993	0.098	4.332	2.335	0.574	0.037	0.287	1.685	0.250	0.000	PASS	7.530	251
1,4-Dithiane	0.986	0.091	5.277	1.390	0.747	0.136	0.000	1.972	0.000	0.250	PASS	7.531	252
2-Ethyl-3-hydroxy-4H-pyran-4-one	0.863	0.032	4.881	1.786	0.526	0.085	1.936	0.036	0.300	0.050	PASS	7.554	253
13-epi-Sclareol	0.700	0.195	7.731	1.064	0.567	0.044	3.288	1.316	0.091	0.159	PASS	7.576	254
Cholic acid	0.487	0.408	8.254	1.587	0.483	0.128	6.596	4.624	0.172	0.078	FAIL	7.578	255
Chloro(methoxy)methane	0.825	0.070	4.488	2.179	0.636	0.025	2.165	0.193	0.250	0.000	PASS	7.578	256
<i>Malonic acid</i>	0.607	0.288	4.907	1.760	0.582	0.029	0.259	1.713	0.571	0.321	FAIL	7.579	257
Carbamazepine	0.724	0.171	7.021	0.354	0.608	0.003	1.756	0.216	0.167	0.083	PASS	7.584	258

Biotin	0.594	0.301	6.826	0.159	0.549	0.062	2.973	1.001	0.313	0.063	PASS	7.591	259
4-Hydroxy-3,5-dimethoxybenzaldehyde	0.903	0.008	4.232	2.435	0.412	0.199	4.908	2.936	0.308	0.058	PASS	7.595	260
N-Methylpyrrolidone	0.871	0.024	4.307	2.360	0.590	0.021	2.019	0.047	0.286	0.036	PASS	7.601	261
DL-Mannitol	0.522	0.373	5.874	0.793	0.483	0.128	3.833	1.861	0.500	0.250	FAIL	7.605	262
L-Aspartic acid	0.638	0.257	5.235	1.432	0.549	0.062	0.383	1.589	0.556	0.306	FAIL	7.631	263
(4R,7S)-7-Isopropyl-4-methyloxepan-2-one	0.715	0.180	6.421	0.246	0.591	0.020	3.702	1.730	0.167	0.083	PASS	7.635	264
(2R,3R)-2,3-Dimethylcyclopropane-1-carboxylic acid	0.861	0.034	5.288	1.379	0.618	0.007	0.745	1.227	0.250	0.000	PASS	7.638	265
Cyclohexanone	0.860	0.035	5.217	1.450	0.672	0.061	1.913	0.059	0.143	0.107	PASS	7.641	266
4,4,7-Trimethyldecahydro-1H-cyclopenta[cd]inden-7-ol	0.855	0.040	6.618	0.049	0.631	0.020	2.084	0.112	0.067	0.183	PASS	7.680	267
2-(Tert-butyl)-4-methoxyphenol	0.736	0.159	6.686	0.019	0.603	0.008	3.227	1.255	0.154	0.096	PASS	7.704	268
Diallyldisulfide	0.845	0.050	6.301	0.366	0.771	0.160	1.334	0.638	0.000	0.250	PASS	7.705	269
L-Mandelic acid	0.714	0.181	5.986	0.681	0.633	0.022	2.133	0.161	0.273	0.023	PASS	7.746	270
Imidazole	0.982	0.087	3.423	3.244	0.529	0.082	1.415	0.557	0.400	0.150	FAIL	7.750	271
3,5-Dinitrosalicylic acid^{CSD}	0.979	0.084	3.404	3.263	0.336	0.275	2.386	0.414	0.563	0.313	FAIL	7.750	272
(5-Hydroxy-6-methylpyridine-3,4-diyl)dimethanol	0.896	0.001	4.532	2.135	0.461	0.150	3.866	1.894	0.333	0.083	PASS	7.753	273
(-)-Epicedrol	0.880	0.015	6.569	0.098	0.614	0.003	2.581	0.609	0.063	0.187	PASS	7.754	274
Uracil	0.946	0.051	3.406	3.261	0.450	0.161	1.919	0.053	0.500	0.250	FAIL	7.766	275
Piperidine	0.926	0.031	5.035	1.632	0.699	0.088	0.863	1.109	0.167	0.083	PASS	7.801	276
Pyroglutamic acid	0.735	0.160	5.107	1.560	0.569	0.042	1.607	0.365	0.444	0.194	PASS	7.802	277
2,5,5,8α-Tetramethyloctahydro-2H-2,4α-methanonaphthalen-1-ol	0.797	0.098	6.935	0.268	0.692	0.081	2.106	0.134	0.063	0.187	PASS	7.803	278
1-Hydroxypropan-2-one	0.768	0.127	4.168	2.499	0.557	0.054	3.924	1.952	0.400	0.150	PASS	7.814	279
3-Oxocyclobutanecarboxylic acid	0.680	0.215	5.808	0.859	0.640	0.029	1.326	0.646	0.375	0.125	PASS	7.818	280
1,1-Dihydroxypropan-2-one	0.625	0.270	4.352	2.315	0.494	0.117	5.864	3.892	0.500	0.250	PASS	7.848	281
D-Altritol	0.608	0.287	6.015	0.652	0.530	0.081	2.513	0.541	0.500	0.250	PASS	7.875	282
1,1-bis(4-Hydroxyphenyl)cyclohexane	0.873	0.022	6.818	0.151	0.564	0.047	3.335	1.363	0.100	0.150	PASS	7.879	283
2-Aminoethan-1-ol	0.678	0.217	4.360	2.307	0.625	0.014	2.238	0.266	0.500	0.250	PASS	7.887	284
(1R,2R)-Cyclohexane-1,2-Diamine	0.922	0.027	5.146	1.521	0.651	0.040	0.623	1.349	0.250	0.000	PASS	7.890	285
β-Cellobiose	0.718	0.177	5.817	0.850	0.412	0.199	3.864	1.892	0.478	0.228	PASS	7.892	286
Dihydrofuran-2,5-dione	0.731	0.164	4.269	2.398	0.571	0.040	4.305	2.333	0.429	0.179	PASS	7.940	287
3S-cis-3,6-Dimethyl-1,4-dioxane-2,5-dione	0.785	0.110	5.030	1.637	0.560	0.051	2.743	0.771	0.400	0.150	PASS	7.948	288
Butyric acid	0.744	0.151	5.332	1.335	0.724	0.113	0.806	1.166	0.333	0.083	PASS	7.952	289
Trimethylamine	0.996	0.101	4.289	2.378	0.665	0.054	0.904	1.068	0.250	0.000	PASS	7.961	290

L-Malic acid	0.661	0.234	5.200	1.467	0.564	0.047	1.693	0.279	0.556	0.306	FAIL	7.969	291
Melamine	0.990	0.095	3.419	3.248	0.398	0.213	0.022	1.950	0.667	0.417	FAIL	7.972	292
Picric acid^{CSD}	0.928	0.033	3.722	2.945	0.372	0.239	2.121	0.149	0.625	0.375	FAIL	7.982	293
cis,cis-1,3,5-Cyclohexanetricarboxylic acid	0.923	0.028	5.480	1.187	0.524	0.087	0.424	1.548	0.400	0.150	PASS	8.011	294
2,2'-Dihydroxy-5,5'-diallyl-biphenyl	0.886	0.009	6.779	0.112	0.581	0.030	3.610	1.638	0.100	0.150	PASS	8.017	295
L-Proline	0.740	0.155	5.696	0.971	0.678	0.067	0.892	1.080	0.375	0.125	PASS	8.042	296
DL-Malic acid	0.652	0.243	5.254	1.413	0.576	0.035	2.119	0.147	0.556	0.306	FAIL	8.072	297
2,2,2-Trifluoroethanol	0.831	0.064	5.147	1.520	0.798	0.187	2.038	0.066	0.167	0.083	PASS	8.087	298
N,N-Dimethylformamide	0.903	0.008	4.164	2.503	0.610	0.001	1.825	0.147	0.400	0.150	PASS	8.088	299
(Z)-Ethyl 2-benzylidene-3-oxobutanoate	0.957	0.062	6.436	0.231	0.579	0.032	1.605	0.367	0.188	0.062	PASS	8.095	300
Citric acid	0.643	0.252	6.050	0.617	0.552	0.059	1.953	0.019	0.538	0.288	PASS	8.113	301
Proline	0.759	0.136	5.722	0.945	0.691	0.080	0.818	1.154	0.375	0.125	PASS	8.146	302
Xylitol	0.687	0.208	5.859	0.808	0.591	0.020	1.605	0.367	0.500	0.250	PASS	8.150	303
Dimethylsulfoxide	0.901	0.006	4.753	1.914	0.695	0.084	2.352	0.380	0.250	0.000	PASS	8.152	304
cis-Aconitic acid	0.694	0.201	6.167	0.500	0.592	0.019	0.903	1.069	0.500	0.250	PASS	8.153	305
4-(Hydroxymethyl)-2-methoxyphenol	0.951	0.056	5.238	1.429	0.582	0.029	2.512	0.540	0.273	0.023	PASS	8.157	306
4-Methylmorpholine	0.877	0.018	4.992	1.675	0.668	0.057	2.302	0.330	0.286	0.036	PASS	8.164	307
Thiourea	0.994	0.099	3.600	3.067	0.559	0.052	0.655	1.317	0.500	0.250	PASS	8.165	308
Acetylmethionine	0.796	0.099	6.212	0.455	0.606	0.005	2.007	0.035	0.333	0.083	PASS	8.165	309
Eucalyptol	0.808	0.087	6.662	0.005	0.774	0.163	2.433	0.461	0.091	0.159	PASS	8.203	310
1-Hydroxydiamantane	0.896	0.001	6.676	0.009	0.727	0.116	2.234	0.262	0.067	0.183	PASS	8.205	311
Succinic acid	0.706	0.189	5.327	1.340	0.647	0.036	1.338	0.634	0.500	0.250	PASS	8.205	312
Glycolic acid	0.767	0.128	4.159	2.508	0.590	0.021	1.607	0.365	0.600	0.350	FAIL	8.219	313
Cyclobutanol	0.906	0.011	4.976	1.691	0.738	0.127	2.379	0.407	0.200	0.050	PASS	8.228	314
Pyruvic acid	0.872	0.023	4.164	2.503	0.610	0.001	1.260	0.712	0.500	0.250	PASS	8.233	315
1-Amino-1-methylcyclopropane	0.927	0.032	4.938	1.729	0.798	0.187	0.793	1.179	0.200	0.050	PASS	8.235	316
(+)-Camphoric acid	0.719	0.176	7.101	0.434	0.702	0.091	1.137	0.835	0.286	0.036	PASS	8.235	317
Piperazine	0.924	0.029	5.025	1.642	0.708	0.097	0.000	1.972	0.333	0.083	PASS	8.244	318
3 α ,4,7,7-Tetramethyl-(3 α R,4S,6 α R,10 α S)-perhydronaphtho(8 α ,1- β)furan-2-one	0.766	0.129	7.248	0.581	0.679	0.068	4.072	2.100	0.111	0.139	PASS	8.247	319
Trifluoroacetic acid	0.843	0.052	4.822	1.845	0.767	0.156	1.770	0.202	0.286	0.036	PASS	8.272	320
(-)-1,3,3-Trimethyl-2-norbornanone	0.888	0.007	6.521	0.146	0.756	0.145	1.965	0.007	0.091	0.159	PASS	8.273	321
2,8,16,20-Tetramethylcalix(4)resorcinarene	0.734	0.161	8.705	2.038	0.600	0.011	2.153	0.181	0.200	0.050	PASS	8.287	322
1,4-Dioxane^{CSD}	0.882	0.013	5.023	1.644	0.761	0.150	0.000	1.972	0.333	0.083	PASS	8.300	323

Acetic acid	0.864	0.031	4.099	2.568	0.674	0.063	0.699	1.273	0.500	0.250	PASS	8.325	324
1,7,7-Trimethyltricyclo(2.2.1.0 ^{2,6})heptan-4-ol	0.829	0.066	6.688	0.021	0.795	0.184	2.302	0.330	0.091	0.159	PASS	8.333	325
(1R,2S)-2-Methyl-4-oxocyclohexane-1-carboxylic acid	0.865	0.030	6.213	0.454	0.680	0.069	1.334	0.638	0.273	0.023	PASS	8.340	326
D-Iditol	0.710	0.185	6.151	0.516	0.583	0.028	1.977	0.005	0.500	0.250	PASS	8.348	327
Caryophyllen- α -oxide	0.874	0.021	7.084	0.417	0.699	0.088	3.581	1.609	0.063	0.187	PASS	8.372	328
Scyllo-inositol	0.968	0.073	5.082	1.585	0.549	0.062	0.000	1.972	0.500	0.250	PASS	8.393	329
Glycerol	0.728	0.167	5.092	1.575	0.614	0.003	3.222	1.250	0.500	0.250	PASS	8.401	330
DL-Tyrosine	0.581	0.314	5.712	0.955	0.492	0.119	11.456	9.484	0.308	0.058	FAIL	8.408	331
o- β -D-Mannopyranosyl-(1-4)- α -D-mannopyranose	0.741	0.154	6.375	0.292	0.490	0.121	3.799	1.827	0.478	0.228	PASS	8.411	332
D-Glucuronic acid	0.818	0.077	5.213	1.454	0.516	0.095	2.720	0.748	0.538	0.288	PASS	8.417	333
Ribitol	0.692	0.203	5.797	0.870	0.586	0.025	3.498	1.526	0.500	0.250	PASS	8.447	334
Tryphenylphosphine oxide	0.972	0.077	7.819	1.152	0.654	0.043	2.140	0.168	0.050	0.200	PASS	8.465	335
<i>E-Caprolactam</i>^{CSD}	0.953	0.058	5.457	1.210	0.689	0.078	2.106	0.134	0.250	0.000	PASS	8.474	336
<i>Saccharin</i>^{CSD}	0.947	0.052	5.475	1.192	0.618	0.007	2.048	0.076	0.333	0.083	PASS	8.475	337
Tetrabromomethane	0.997	0.102	6.172	0.495	0.920	0.309	0.019	1.953	0.000	0.250	FAIL	8.476	338
Formamide	0.860	0.035	3.400	3.267	0.579	0.032	1.659	0.313	0.667	0.417	FAIL	8.480	339
D-Glucitol	0.605	0.290	6.136	0.531	0.552	0.059	5.473	3.501	0.500	0.250	PASS	8.481	340
β -D-Allose	0.830	0.065	5.636	1.031	0.617	0.006	0.802	1.170	0.500	0.250	PASS	8.502	341
<u>L-Ascorbic acid</u>	<u>0.782</u>	<u>0.113</u>	<u>6.017</u>	<u>0.650</u>	<u>0.616</u>	<u>0.005</u>	<u>1.142</u>	<u>0.830</u>	<u>0.500</u>	<u>0.250</u>	<u>PASS</u>	<u>8.518</u>	<u>342</u>
Oxetane	0.955	0.060	4.422	2.245	0.751	0.140	3.156	1.184	0.250	0.000	PASS	8.562	343
D-Arabinitol	0.597	0.298	5.823	0.844	0.534	0.077	7.155	5.183	0.500	0.250	PASS	8.576	344
DL-Arabinitol	0.597	0.298	5.821	0.846	0.534	0.077	7.159	5.187	0.500	0.250	PASS	8.576	345
α -Lactose	0.817	0.078	5.638	1.029	0.444	0.167	5.751	3.779	0.478	0.228	PASS	8.590	346
Acetamide	0.944	0.049	3.969	2.698	0.636	0.025	1.804	0.168	0.500	0.250	PASS	8.591	347
<i>Tartaric acid</i>^{CSD}	0.674	0.221	5.858	0.809	0.672	0.061	0.744	1.228	0.600	0.350	FAIL	8.598	348
α -D-Glucose	0.842	0.053	5.353	1.314	0.546	0.065	3.250	1.278	0.500	0.250	PASS	8.607	349
<i>Urea</i>	0.880	0.015	3.400	3.267	0.526	0.085	1.544	0.428	0.750	0.500	FAIL	8.615	350
n-Methyl-D-glucamine	0.702	0.193	6.975	0.308	0.603	0.008	2.565	0.593	0.462	0.212	PASS	8.620	351
Tetrahydrofuran	0.943	0.048	5.018	1.649	0.792	0.181	2.773	0.801	0.200	0.050	PASS	8.623	352
2-Hydroxyacetamide	0.871	0.024	4.159	2.508	0.637	0.026	1.124	0.848	0.600	0.350	FAIL	8.644	353
2,2',2''-Nitrilotriethanol	0.789	0.106	5.756	0.911	0.593	0.018	4.792	2.820	0.400	0.150	PASS	8.651	354
D-Mannitol	0.669	0.226	6.359	0.308	0.618	0.007	3.426	1.454	0.500	0.250	PASS	8.652	355
D-Glucono-1,5-lactone	0.895	0.000	5.575	1.092	0.607	0.004	1.021	0.951	0.500	0.250	PASS	8.693	356

1,4-Diazabicyclo[2.2.2]octane	0.916	0.021	5.673	0.994	0.862	0.251	0.001	1.971	0.250	0.000	PASS	8.696	357
β-Maltose	0.663	0.232	6.536	0.131	0.490	0.121	7.016	5.044	0.478	0.228	PASS	8.751	358
L-Tyrosine	0.579	0.316	5.724	0.943	0.492	0.119	13.540	11.568	0.308	0.058	FAIL	8.756	359
DL-Ribose	0.813	0.082	5.428	1.239	0.623	0.012	3.030	1.058	0.500	0.250	PASS	8.779	360
L-Ribose	0.813	0.082	5.428	1.239	0.623	0.012	3.030	1.058	0.500	0.250	PASS	8.779	361
α-L-Xylopyranose	0.862	0.033	5.336	1.331	0.632	0.021	2.069	0.097	0.500	0.250	PASS	8.780	362
Formaldehyde	0.945	0.050	3.400	3.267	0.756	0.145	1.675	0.297	0.500	0.250	FAIL	8.833	363
Formic acid	0.953	0.058	3.400	3.267	0.645	0.034	0.579	1.393	0.667	0.417	FAIL	8.838	364
β-D-Galactose	0.867	0.028	5.585	1.082	0.593	0.018	2.793	0.821	0.500	0.250	PASS	8.853	365
β-galabiose	0.832	0.063	6.650	0.017	0.549	0.062	2.943	0.971	0.478	0.228	PASS	8.860	366
S(+)-Camphor-10-sulfonic acid	0.764	0.131	7.665	0.998	0.739	0.128	2.613	0.641	0.267	0.017	PASS	8.873	367
α-D-Galactose	0.777	0.118	5.673	0.994	0.564	0.047	5.122	3.150	0.500	0.250	PASS	8.877	368
Sucralose	0.789	0.106	8.295	1.628	0.665	0.054	0.973	0.999	0.348	0.098	PASS	8.879	369
(3αR,4R,6αS,10αS)-3α,4,7,7-Tetramethylperhydronaphtho(8α,1-β)furan-2-one	0.857	0.038	7.791	1.124	0.734	0.123	3.912	1.940	0.111	0.139	PASS	8.882	370
neo-Inositol	0.979	0.084	5.483	1.184	0.643	0.032	0.000	1.972	0.500	0.250	PASS	8.894	371
Trichloroacetic acid^{CSD}	0.875	0.020	6.149	0.518	0.849	0.238	0.860	1.112	0.286	0.036	PASS	8.931	372
α-D-Tagatopyranose	0.713	0.182	5.917	0.750	0.627	0.016	4.917	2.945	0.500	0.250	PASS	8.940	373
β-L-Lyxopyranose	0.823	0.072	5.344	1.323	0.609	0.002	4.395	2.423	0.500	0.250	PASS	8.964	374
Morpholine	0.984	0.089	5.034	1.633	0.765	0.154	2.006	0.034	0.333	0.083	PASS	8.985	375
α-L-Sorbopyranose	0.815	0.080	5.879	0.788	0.604	0.007	4.170	2.198	0.500	0.250	PASS	9.048	376
l-Iditol	0.757	0.138	6.205	0.462	0.629	0.018	4.181	2.209	0.500	0.250	PASS	9.055	377
β-D-Glucose	0.921	0.026	5.371	1.296	0.587	0.024	3.562	1.590	0.500	0.250	PASS	9.069	378
Ethylene oxide	0.905	0.010	4.266	2.401	0.862	0.251	3.427	1.455	0.333	0.083	PASS	9.084	379
Lactic acid	0.851	0.044	5.284	1.383	0.738	0.127	1.999	0.027	0.500	0.250	PASS	9.102	380
Neotame	0.633	0.262	6.683	0.016	0.381	0.230	16.190	14.218	0.259	0.009	FAIL	9.103	381
β-Lactose	0.748	0.147	6.335	0.332	0.477	0.134	8.164	6.192	0.478	0.228	FAIL	9.109	382
4-tert-Butyl-3-methoxy-2,6-dinitrotoluene	0.946	0.051	6.713	0.046	0.654	0.043	2.112	0.140	0.368	0.118	PASS	9.115	383
L-Tartaric acid	0.711	0.184	5.887	0.780	0.692	0.081	2.656	0.684	0.600	0.350	FAIL	9.120	384
2-Amino-5-picolinic acid	0.664	0.231	3.451	3.216	0.343	0.268	20.025	18.053	0.400	0.150	FAIL	9.189	385
Methanol	0.876	0.019	3.996	2.671	0.848	0.237	2.099	0.127	0.500	0.250	PASS	9.201	386
myo-Inositol	0.990	0.095	5.535	1.132	0.665	0.054	1.463	0.509	0.500	0.250	PASS	9.272	387
(R)-2-Hydroxypropanamide	0.920	0.025	5.361	1.306	0.761	0.150	1.288	0.684	0.500	0.250	PASS	9.312	388
(S)-2-Hydroxypropanamide	0.920	0.025	5.361	1.306	0.761	0.150	1.288	0.684	0.500	0.250	PASS	9.312	389

DL-Methionine	0.587	0.308	5.471	1.196	0.510	0.101	16.415	14.443	0.333	0.083	FAIL	9.338	390
(3αR,4S,6αS,10αS)-3α,4,7,7-Tetramethylperhydronaphtho(8α,1-β)furan-2-one	0.925	0.030	8.015	1.348	0.774	0.163	4.049	2.077	0.111	0.139	PASS	9.339	391
Tromethamine	0.905	0.010	5.686	0.981	0.724	0.113	1.940	0.032	0.500	0.250	PASS	9.340	392
β-D-Psicose	0.806	0.089	6.080	0.587	0.699	0.088	3.770	1.798	0.500	0.250	PASS	9.360	393
2-Methylpropan-2-ol	0.985	0.090	5.927	0.740	0.911	0.300	2.172	0.200	0.200	0.050	FAIL	9.371	394
epi-Inositol	0.904	0.009	5.762	0.905	0.656	0.045	3.573	1.601	0.500	0.250	PASS	9.388	395
Sucrose	0.835	0.060	6.829	0.162	0.605	0.006	4.564	2.592	0.478	0.228	PASS	9.402	396
L-Tryptophan	0.716	0.179	5.801	0.866	0.491	0.120	15.484	13.512	0.267	0.017	FAIL	9.406	397
α,α-Galacto-trehalose	0.684	0.211	7.958	1.291	0.613	0.002	5.476	3.504	0.478	0.228	PASS	9.447	398
α-D-Talose	0.883	0.012	5.992	0.675	0.657	0.046	4.085	2.113	0.500	0.250	PASS	9.481	399
Ethylene glycol	0.866	0.029	5.143	1.524	0.845	0.234	2.053	0.081	0.500	0.250	PASS	9.505	400
2,2-Dibromo-2-cyanoacetamide	0.840	0.055	6.843	0.176	0.836	0.225	2.552	0.580	0.375	0.125	PASS	9.573	401
β-D-Gulose	0.825	0.070	6.135	0.532	0.659	0.048	5.942	3.970	0.500	0.250	PASS	9.658	402
DL-Tryptophan	0.713	0.182	6.073	0.594	0.532	0.079	15.881	13.909	0.267	0.017	FAIL	9.696	403
Cyclohexane-1,2,3,4,5,6-hexol	0.878	0.017	6.156	0.511	0.699	0.088	4.407	2.435	0.500	0.250	PASS	9.723	404
Hexamethylenetetramine	0.929	0.034	6.526	0.141	0.929	0.318	0.000	1.972	0.400	0.150	FAIL	9.756	405
DL-Glutamine	0.638	0.257	5.433	1.234	0.535	0.076	14.333	12.361	0.500	0.250	FAIL	9.799	406
Cyclohexane-1,2,3,4,5,6-hexaol	0.958	0.063	6.243	0.424	0.738	0.127	2.381	0.409	0.500	0.250	PASS	9.808	407
β-DL-Arabinose	0.992	0.097	5.438	1.229	0.702	0.091	4.047	2.075	0.500	0.250	PASS	9.818	408
D-Asparagine	0.700	0.195	5.209	1.458	0.572	0.039	11.779	9.807	0.556	0.306	FAIL	9.825	409
Sucrose octa-acetate	0.884	0.011	10.344	3.677	0.620	0.009	1.230	0.742	0.404	0.154	FAIL	9.890	410
DL-Aspartic acid	0.689	0.206	5.222	1.445	0.565	0.046	12.555	10.583	0.556	0.306	FAIL	9.899	411
α-Maltose	0.857	0.038	7.106	0.439	0.597	0.014	7.144	5.172	0.478	0.228	PASS	9.964	412
5,5-Diethylbarbituric acid	0.964	0.069	7.697	1.030	0.859	0.248	0.664	1.308	0.385	0.135	PASS	10.038	413
Meso-Tartaric acid	0.912	0.017	6.233	0.434	0.777	0.166	1.881	0.091	0.600	0.350	FAIL	10.055	414
Nitromethane	0.993	0.098	4.007	2.660	0.759	0.148	2.009	0.037	0.750	0.500	FAIL	10.093	415
D-Isoleucine	0.779	0.116	6.195	0.472	0.677	0.066	13.007	11.035	0.333	0.083	FAIL	10.215	416
β-D-Fructopyranose	0.929	0.034	6.596	0.071	0.794	0.183	3.657	1.685	0.500	0.250	PASS	10.242	417
L-chiro-Inositol	0.895	0.000	6.157	0.510	0.700	0.089	7.420	5.448	0.500	0.250	PASS	10.289	418
D-(+)-chiro-Inositol	0.902	0.007	6.190	0.477	0.706	0.095	7.232	5.260	0.500	0.250	PASS	10.312	419
β-D-Altropyranose	0.919	0.024	6.046	0.621	0.703	0.092	7.339	5.367	0.500	0.250	PASS	10.329	420
L-Methionine	0.686	0.209	6.249	0.418	0.670	0.059	15.629	13.657	0.333	0.083	FAIL	10.348	421
DL-Cysteine	0.743	0.152	5.362	1.305	0.651	0.040	14.987	13.015	0.429	0.179	FAIL	10.406	422

Adamantane-1,3,5,7-tetracarboxylic acid	0.950	0.055	9.143	2.476	0.874	0.263	0.737	1.235	0.364	0.114	PASS	10.436	423
cis-Inositol	0.974	0.079	5.803	0.864	0.730	0.119	6.899	4.927	0.500	0.250	PASS	10.455	424
Muco-inositol	0.989	0.094	6.271	0.396	0.757	0.146	5.203	3.231	0.500	0.250	PASS	10.461	425
Trimethylamine oxide	0.922	0.027	5.713	0.954	0.876	0.265	7.407	5.435	0.400	0.150	PASS	10.536	426
4-Hydroxy-L-proline	0.715	0.180	5.497	1.170	0.626	0.015	16.425	14.453	0.444	0.194	FAIL	10.560	427
α,α -Trehalose	0.786	0.109	8.903	2.236	0.727	0.116	6.228	4.256	0.478	0.228	PASS	10.610	428
<u>L-Glutamine</u>	<u>0.765</u>	<u>0.130</u>	<u>6.121</u>	<u>0.546</u>	<u>0.666</u>	<u>0.055</u>	<u>13.035</u>	<u>11.063</u>	<u>0.500</u>	<u>0.250</u>	<u>FAIL</u>	<u>10.680</u>	<u>429</u>
<u>Glycine</u>	<u>0.791</u>	<u>0.104</u>	<u>4.669</u>	<u>1.998</u>	<u>0.655</u>	<u>0.044</u>	<u>13.479</u>	<u>11.507</u>	<u>0.600</u>	<u>0.350</u>	<u>FAIL</u>	<u>10.689</u>	<u>430</u>
DL-Isoleucine	0.781	0.114	6.171	0.496	0.688	0.077	15.767	13.795	0.333	0.083	FAIL	10.719	431
L-Asparagine	0.769	0.126	5.469	1.198	0.642	0.031	13.992	12.020	0.556	0.306	FAIL	10.755	432
<u>L-Valine</u>	<u>0.882</u>	<u>0.013</u>	<u>5.354</u>	<u>1.313</u>	<u>0.674</u>	<u>0.063</u>	<u>15.588</u>	<u>13.616</u>	<u>0.375</u>	<u>0.125</u>	<u>FAIL</u>	<u>10.853</u>	<u>433</u>
Betaine	0.786	0.109	5.600	1.067	0.667	0.056	17.236	15.264	0.375	0.125	FAIL	10.872	434
D-Threonine	0.792	0.103	5.745	0.922	0.712	0.101	14.099	12.127	0.500	0.250	FAIL	10.997	435
DL-Valine	0.883	0.012	6.182	0.485	0.768	0.157	12.988	11.016	0.375	0.125	FAIL	11.017	436
L-Threonine	0.886	0.009	5.343	1.324	0.681	0.070	13.917	11.945	0.500	0.250	FAIL	11.032	437
DL-Glutamic acid	0.786	0.109	5.628	1.039	0.631	0.020	16.393	14.421	0.500	0.250	FAIL	11.033	438
L-Leucine	0.846	0.049	6.609	0.058	0.800	0.189	13.205	11.233	0.333	0.083	FAIL	11.040	439
L- α -Leucine	0.846	0.049	6.609	0.058	0.800	0.189	13.205	11.233	0.333	0.083	FAIL	11.040	440
β -Alanine	0.724	0.171	4.971	1.696	0.649	0.038	19.495	17.523	0.500	0.250	FAIL	11.217	441
<i>Glutamic acid</i>	<i>0.803</i>	<i>0.092</i>	<i>5.828</i>	<i>0.839</i>	<i>0.681</i>	<i>0.070</i>	<i>15.757</i>	<i>13.785</i>	<i>0.500</i>	<i>0.250</i>	<i>FAIL</i>	<i>11.224</i>	<i>442</i>
4-Aminobutanoic acid	0.599	0.296	5.081	1.586	0.577	0.034	24.969	22.997	0.429	0.179	FAIL	11.266	443
DL-Leucine	0.833	0.062	6.534	0.133	0.774	0.163	15.552	13.580	0.333	0.083	FAIL	11.275	444
Tramadol	0.844	0.051	7.290	0.623	0.575	0.036	23.243	21.271	0.158	0.092	FAIL	11.521	445
L-Cysteine	0.996	0.101	5.768	0.899	0.849	0.238	12.986	11.014	0.429	0.179	FAIL	11.731	446
L-Cysteine	0.996	0.101	5.768	0.899	0.849	0.238	12.986	11.014	0.429	0.179	FAIL	11.731	447
<u>L-Alanine</u>	<u>0.916</u>	<u>0.021</u>	<u>5.388</u>	<u>1.279</u>	<u>0.789</u>	<u>0.178</u>	<u>15.788</u>	<u>13.816</u>	<u>0.500</u>	<u>0.250</u>	<u>FAIL</u>	<u>11.851</u>	<u>448</u>
D-Alanine	0.917	0.022	5.394	1.273	0.791	0.180	15.791	13.819	0.500	0.250	FAIL	11.863	449
DL-Serine	0.951	0.056	5.729	0.938	0.844	0.233	14.628	12.656	0.571	0.321	FAIL	12.315	450

Table S6 – COSMOQuick results for a multicomponent analysis of 450 co-formers against NVP molecule. Molecules are ordered by COSMO ranking position. In bold are represented the 76 molecules for which experimental multicomponent results are available. Black-italic letter identify the positive results; CSD means molecules reported in the CSD database. Red-underline letter identify the negative results.

Co-former	Molecular formula	f_{fit}	H_{ex} (kcal.mol ⁻¹)	COSMO ranking
[1,1'-Binaphthalene]-2,2'-diol	C20H14O2	-4.436	-6.477	1
Trifluoroacetic acid	C2HF3O2	-3.951	-4.971	2
<u>Phloroglucinol</u>	<u>C6H6O3</u>	<u>-3.654</u>	<u>-5.695</u>	<u>3</u>
<i>Oxalic acid</i>	<i>C2H2O4</i>	<i>-3.469</i>	<i>-5.509</i>	<i>4</i>
<u>Resorcinol</u>	<u>C6H6O2</u>	<u>-3.215</u>	<u>-4.745</u>	<u>5</u>
Myricetin	C15H10O8	-3.176	-7.258	6
2,8,16,20-Tetramethylcalix(4)resorcinarene	C32H32O8	-3.163	-7.755	7
Chloranilic acid	C6H2Cl2O4	-3.084	-4.615	8
<u>Catechol</u>	<u>C6H6O2</u>	<u>-3.049</u>	<u>-4.579</u>	<u>9</u>
<i>Trichloroacetic acid</i> ^{CSD}	<i>C2HCl3O2</i>	<i>-2.918</i>	<i>-3.938</i>	<i>10</i>
1,2-Ethanedisulfonic acid	C2H6O6S2	-2.853	-5.914	11
<u>Orcinol</u>	<u>C7H8O2</u>	<u>-2.806</u>	<u>-4.336</u>	<u>12</u>
1-Naphthol	C10H8O	-2.741	-3.762	13
[1,1'-Biphenyl]-4,4'-diol	C12H10O2	-2.688	-4.728	14
2,4-Dihydroxybenzoic acid	C7H6O4	-2.421	-4.972	15
<i>Gallic acid</i>	<i>C7H6O5</i>	<i>-2.402</i>	<i>-5.463</i>	<i>16</i>
<u>Hydroquinone</u>	<u>C6H6O2</u>	<u>-2.288</u>	<u>-3.819</u>	<u>17</u>
4-Nitrophenol	C6H5NO3	-2.268	-3.799	18
o-Cresol	C7H8O	-2.097	-3.117	19
<i>Gentisic acid</i> ^{CSD}	<i>C7H6O4</i>	<i>-1.985</i>	<i>-4.536</i>	<i>20</i>
2,5-Dimethylphenol	C8H10O	-1.871	-2.891	21
<i>3,5-Dinitrosalicylic acid</i> ^{CSD}	<i>C7H4N2O7</i>	<i>-1.861</i>	<i>-4.922</i>	<i>22</i>
Phenol	C6H6O	-1.853	-2.873	23
1,1-bis(4-Hydroxyphenyl)cyclohexane	C18H20O2	-1.665	-4.216	24
2-Isopropyl-5-methylphenol	C10H14O	-1.521	-3.052	25
<i>Naphthalene-1,5-disulfonic acid</i> ^{CSD}	<i>C10H8S2O6</i>	<i>-1.381</i>	<i>-3.932</i>	<i>26</i>
1-Hydroxy-2-naphthoic acid	C11H8O3	-1.373	-3.414	27
2-(Tert-butyl)-4-methoxyphenol	C11H16O2	-1.349	-2.879	28
<i>3-Hydroxybenzoic acid</i> ^{CSD}	<i>C7H6O3</i>	<i>-1.271</i>	<i>-3.311</i>	<i>29</i>
<i>Salicylic acid</i> ^{CSD}	<i>C7H6O3</i>	<i>-1.170</i>	<i>-3.211</i>	<i>30</i>
1-Naphthalenesulfonic acid	C10H8O3S	-1.166	-2.697	31
<i>4-Hydroxybenzoic acid</i> ^{CSD}	<i>C7H6O3</i>	<i>-0.868</i>	<i>-2.909</i>	<i>32</i>
Formic acid	CH2O2	-0.864	-1.885	33
2,4,6-Trimethylphenol	C9H12O	-0.820	-1.841	34
cis-Aconitic acid	C6H6O6	-0.762	-4.843	35
2,2,2-Trifluoroethanol	C2H3F3O	-0.755	-1.775	36
4-Methylbenzenesulfonic acid	C7H8O3S	-0.748	-2.278	37
3,5-Dinitrobenzoic acid	C7H4N2O6	-0.738	-3.289	38
5-Nitroisophthalic acid	C8H5NO6	-0.727	-3.788	39
<i>Fumaric acid</i>	<i>C4H4O4</i>	<i>-0.707</i>	<i>-3.258</i>	<i>40</i>
2-Chloroacetic acid	C2H3ClO2	-0.639	-2.169	41
<i>Maleic Acid</i> ^{CSD}	<i>C4H4O4</i>	<i>-0.568</i>	<i>-3.119</i>	<i>42</i>

Trimesic acid	C9H6O6	-0.567	-4.139	43
4-Nitrobenzoic acid	C7H5NO4	-0.500	-2.541	44
Trimethylamine oxide	C3H9NO	-0.473	-1.493	45
Terephthalic acid	C8H6O4	-0.423	-2.974	46
<i>L-Mandelic acid</i>	<i>C8H8O3</i>	<i>-0.361</i>	<i>-2.912</i>	<i>47</i>
4-Hydroxybenzaldehyde	C7H6O2	-0.279	-1.810	48
Pyruvic acid	C3H4O3	-0.237	-1.768	49
Anthranilic acid	C7H7NO2	-0.174	-2.215	50
2,4-Pyridinedicarboxylic acid	C7H5NO4	-0.148	-2.699	51
Acetic acid	C2H4O2	-0.111	-1.132	52
2-Amino-5-methylbenzoic acid	C8H9NO2	-0.096	-2.137	53
<u>Orotic acid</u>	<u>C5H4N2O4</u>	<u>-0.071</u>	<u>-1.602</u>	<u>54</u>
2,6-Di-tert-butyl-4-methylphenol	C15H24O	-0.052	-1.072	55
4-Ethoxyphenol	C8H10O2	-0.027	-2.068	56
<i>Benzoic acid</i>^{CSD}	<i>C7H6O2</i>	<i>-0.019</i>	<i>-1.549</i>	<i>57</i>
2-Coumaric acid	C9H8O3	0.013	-2.538	58
1,7,7-Trimethyltricyclo(2.2.1.0 ^{2,6})heptan-4-ol	C10H16O	0.106	-0.914	59
1,4-Diazabicyclo[2.2.2]octane	C6H12N2	0.134	-0.886	60
Cyclamic acid	C6H13NO3S	0.189	-1.851	61
Betaine	C5H10NO2	0.192	-0.828	62
Lactic acid	C3H6O3	0.216	-1.825	63
<u>Glycolic acid</u>	<u>C2H4O3</u>	<u>0.234</u>	<u>-1.807</u>	<u>64</u>
4'-Hydroxyacetophenone	C8H8O2	0.236	-1.295	65
S(+)-Camphor-10-sulfonic acid	C10H16O4S	0.250	-1.791	66
(+)-Camphoric acid	C10H16O4	0.260	-2.291	67
Vanillic acid	C8H8O4	0.265	-2.286	68
<i>Picric acid</i>^{CSD}	<i>C6H3N3O7</i>	<i>0.276</i>	<i>-2.275</i>	<i>69</i>
α -Ketoglutaric acid	C5H6O5	0.279	-3.292	70
<i>Saccharin</i>^{CSD}	<i>C7H5NO3S</i>	<i>0.286</i>	<i>-0.734</i>	<i>71</i>
<i>Tartaric acid</i>^{CSD}	<i>C4H6O6</i>	<i>0.334</i>	<i>-3.747</i>	<i>72</i>
<u>L-Tartaric acid</u>	<u>C4H6O6</u>	<u>0.334</u>	<u>-3.747</u>	<u>73</u>
Meso-Tartaric acid	C4H6O6	0.334	-3.747	74
<u>L-Malic acid</u>	<u>C4H6O5</u>	<u>0.388</u>	<u>-3.183</u>	<u>75</u>
<u>DL-Malic acid</u>	<u>C4H6O5</u>	<u>0.388</u>	<u>-3.183</u>	<u>76</u>
1,10-Phenanthroline	C12H8N2	0.412	-0.609	77
2-Phenylacetic acid	C8H8O2	0.417	-1.624	78
Pterostilbene	C16H16O3	0.435	-2.626	79
4-(Hydroxymethyl)-2-methoxyphenol	C8H10O3	0.439	-2.112	80
(2R,3R)-2,3-Dimethylcyclopropane-1-carboxylic acid	C6H10O2	0.451	-1.079	81
4-(Hydroxymethyl)phenol	C7H8O2	0.474	-1.567	82
Hexamethylenetetramine	C6H12N4	0.479	-0.541	83
Methyl paraben	C8H8O3	0.480	-1.561	84
Chloroform	CHCl3	0.481	-0.539	85
3-Oxocyclobutanecarboxylic acid	C5H6O3	0.487	-1.043	86
Crotonic acid	C4H6O2	0.495	-1.035	87
<u>L-Ascorbic acid</u>	<u>C6H8O6</u>	<u>0.546</u>	<u>-3.026</u>	<u>88</u>

N,N-Dimethylacetamide	C4H9NO	0.560	-0.460	89
Dimethylsulfoxide	C2H6OS	0.572	-0.448	90
N-Methylpyrrolidone	C5H9NO	0.595	-0.426	91
3-Methylbut-2-enoic acid	C5H8O2	0.597	-0.934	92
Pyrrrole	C4H5N	0.608	-0.412	93
<u>Succinic acid</u>	<u>C4H6O4</u>	<u>0.617</u>	<u>-2.444</u>	<u>94</u>
Tetramethylpyrazine	C8H12N2	0.625	-0.396	95
2,2'-Dihydroxy-5,5'-diallyl-biphenyl	C18H18O2	0.636	-3.446	96
<i>4-Aminobenzoic acid</i>	<i>C7H7NO2</i>	<i>0.680</i>	<i>-1.361</i>	<i>97</i>
<i>Dichloromethane^{CSD}</i>	<i>CH2Cl2</i>	<i>0.683</i>	<i>-0.337</i>	<i>98</i>
2-Amino-5-picolinic acid	C6H6N2O2	0.690	-1.351	99
<u>Nicotinic acid</u>	<u>C6H5NO2</u>	<u>0.690</u>	<u>-0.840</u>	<u>100</u>
Allocinnamic acid	C9H8O2	0.691	-1.349	101
2,4-Dimethylpyridine	C7H9N	0.693	-0.328	102
Oxetane	C3H6O	0.701	-0.319	103
1,4-Dimethylpiperazine	C6H14N2	0.715	-0.306	104
N,N-Dimethylformamide	C3H7NO	0.723	-0.297	105
1-Amino-1-methylcyclopropane	C4H9N	0.727	-0.293	106
Ethylamine	C2H7N	0.744	-0.277	107
cis,cis-1,3,5-Cyclohexanetricarboxylic acid	C9H12O6	0.748	-2.824	108
2,6-Dimethylpyridine	C7H9N	0.762	-0.258	109
2,5,5,8 α -Tetramethyloctahydro-2H-2,4 α -methanonaphthalen-1-ol	C15H26O	0.763	-0.257	110
2,3-Dimethylpyrazine	C6H8N2	0.771	-0.250	111
4-Methoxybenzoic acid	C8H8O3	0.773	-1.267	112
2,6-Dimethylpyrazine	C6H8N2	0.777	-0.243	113
2,5-Dimethylpyrazine	C6H8N2	0.780	-0.241	114
4,4'-Bipyridine	C10H8N2	0.801	-0.219	115
Cyclobutanol	C4H8O	0.802	-0.219	116
Pyridine	C5H5N	0.807	-0.213	117
Methanol	CH4O	0.810	-0.210	118
(R,S)-Hesperetin	C16H14O6	0.817	-2.244	119
Tetrahydrofuran	C4H8O	0.819	-0.201	120
Tetrathiafulvalene	C6H4S4	0.819	-0.201	121
4-Methylmorpholine	C5H11NO	0.855	-0.165	122
Ethylenediamine	C2H8N2	0.857	-0.673	123
Phenoxyacetic acid	C8H8O3	0.860	-1.691	124
Trimethylamine	C3H9N	0.865	-0.156	125
<i>ϵ-Caprolactam^{CSD}</i>	<i>C6H11NO</i>	<i>0.870</i>	<i>-0.150</i>	<i>126</i>
Pyromellitic	C10H2O6	0.872	-0.148	127
Tetraiodoethene	C2I4	0.897	-0.123	128
2,2-Dibromo-2-cyanoacetamide	C3H2Br2N2O	0.900	-0.631	129
Butyric acid	C4H8O2	0.910	-1.131	130
Phenylmethanol	C7H8O	0.912	-0.619	131
Acridine	C13H9N	0.912	-0.108	132
<i>Malonic acid</i>	<i>C3H4O4</i>	<i>0.914</i>	<i>-1.637</i>	<i>133</i>
<i>Ethanol^{CSD}</i>	<i>C2H5OH</i>	<i>0.914</i>	<i>-0.106</i>	<i>134</i>

2-Acetylpyrrole	C6H7NO	0.915	-0.105	135
Morpholine	C4H9NO	0.929	-0.091	136
<u>Acetylsalicylic acid</u>	<u>C9H8O4</u>	<u>0.936</u>	<u>-1.615</u>	<u>137</u>
Isocaryolan-9 α -ol	C15H26O	0.936	-0.084	138
<u>Vanillin</u>	<u>C8H8O3</u>	<u>0.937</u>	<u>-1.104</u>	<u>139</u>
<u>Pyroglutamic acid</u>	<u>C5H7NO3</u>	<u>0.937</u>	<u>-0.593</u>	<u>140</u>
2-Aminopyrimidine	C4H5N3	0.938	-0.083	141
Piperidine	C5H11N	0.939	-0.081	142
2-Methylpropan-2-ol	C4H10O	0.940	-0.080	143
2,6-Pyridinedicarboxylic acid	C7H5NO4	0.941	-1.610	144
1,4,8,11-Tetra-azacyclotetradecane	C10H24N4	0.941	-0.079	145
Thiourea	CH4N2S	0.947	-0.584	146
<i>Theophylline</i>	<i>C7H8N4O2</i>	<i>0.948</i>	<i>-0.072</i>	<i>147</i>
Pyrazine	C4H4N2	0.955	-0.066	148
Cyclohexanone	C6H10O	0.958	-0.062	149
<i>1,4-Dioxane</i>^{CSD}	<i>C4H8O2</i>	<i>0.960</i>	<i>-0.060</i>	<i>150</i>
Phenazine	C12H8N2	0.961	-0.059	151
Furfural	C6H12O2	0.969	-0.051	152
Nootkatone	C15H22O	0.969	-0.051	153
Salicylaldehyde	C7H6O2	0.970	-0.561	154
<i>Caffeine</i>	<i>C8H10N4O2</i>	<i>0.971</i>	<i>-0.050</i>	<i>155</i>
<i>1,3-Diiodobenzene</i>^{CSD}	<i>C6H4I2</i>	<i>0.971</i>	<i>-0.050</i>	<i>156</i>
1-Hydroxydiamantane	C14H20O	0.974	-0.047	157
Propan-2-one	C3H6O	0.983	-0.038	158
5,5-Diethylbarbituric acid	C8H12N2O3	0.996	-0.534	159
<u>Piperazine</u>	<u>C4H10N2</u>	<u>0.998</u>	<u>-0.022</u>	<u>160</u>
1,2-Dichloroethane	C2H4Cl2	1.011	-0.010	161
Methyl acetate	C3H6O2	1.020	0.000	162
Ethylene oxide	C2H4O	1.030	0.010	163
<i>Uracil</i>	<i>C4H4N2O2</i>	<i>1.031</i>	<i>0.010</i>	<i>164</i>
4-Benzoquinone	C6H4O2	1.034	0.013	165
2,2'-Bipyridine	C10H8N2	1.034	0.014	166
3,4-(Methylenedioxy)benzaldehyde	C8H6O3	1.035	0.014	167
<u>Theobromine</u>	<u>C7H8N4O2</u>	<u>1.041</u>	<u>0.020</u>	<u>168</u>
1,1-Dihydroxypropan-2-one	C3H6O3	1.045	-0.996	169
Imidazole	C3H4N2	1.050	0.030	170
Cyclodecanol	C10H20O	1.054	0.034	171
Quinoxaline-N,N'-dioxide	C8H6N2O2	1.056	0.036	172
Coumarin	C9H6O2	1.066	0.046	173
Acrylaldehyde	C3H4O	1.071	0.051	174
<i>Cinnamic acid</i>	<i>C9H8O2</i>	<i>1.076</i>	<i>-0.965</i>	<i>175</i>
2-Pyridone	C5H5NO	1.091	0.071	176
Acetophenone	C8H8O	1.094	0.073	177
Eucalyptol	C10H18O	1.094	0.074	178
Chloro(methoxy)methane	C2H5ClO	1.095	0.074	179
Cycloundecanone	C11H20O	1.100	0.079	180

Formaldehyde	CH2O	1.100	0.080	181
Methyl cubane-1-carboxylate	C10H10O2	1.100	0.080	182
Pyrazine-1,4-dioxide	C4H4N2O2	1.108	0.087	183
Phthalide	C8H6O2	1.109	0.089	184
3-Isochromanone	C9H8O2	1.111	0.091	185
1-(Naphthalen-2-yl)Ethan-1-One	C12H10O	1.114	0.093	186
Sorbic acid	C6H8O2	1.115	-0.925	187
3S-cis-3,6-Dimethyl-1,4-dioxane-2,5-dione	C6H8O4	1.118	0.098	188
2,3-Butanedione	C4H6O2	1.120	0.100	189
4,4,7-Trimethyldecahydro-1H-cyclopenta[cd]inden-7-ol	C14H24O	1.132	0.111	190
1,2-Dimethyldisulfane	C2H6S2	1.137	0.117	191
Adamantane-1,3,5,7-tetracarboxylic acid	C14H16O8	1.138	-2.944	192
2-Methoxynaphthalene	C11H10O	1.144	0.123	193
Acetamide	C2H5NO	1.145	0.125	194
Dimethylsulfide	C2H6S	1.149	0.129	195
(4R,7S)-7-Isopropyl-4-methyloxepan-2-one	C10H18O2	1.150	0.129	196
cis-anti-cis-Dicyclohexano-18-crown-6	C20H36O6	1.152	0.131	197
3 α ,4,7,7-Tetramethyl-(3 α R,4S,6 α R,10 α S)-perhydronaphtho(8 α ,1- β)furan-2-one	C16H26O2	1.160	0.139	198
(3 α R,4R,6 α S,10 α S)-3 α ,4,7,7-Tetramethylperhydronaphtho(8 α ,1- β)furan-2-one	C16H26O2	1.160	0.139	199
(3 α R,4S,6 α S,10 α S)-3 α ,4,7,7-Tetramethylperhydronaphtho(8 α ,1- β)furan-2-one	C16H26O2	1.160	0.139	200
Nitromethane	CH3NO2	1.163	0.143	201
Cyclodecanone	C10H18O	1.164	0.143	202
2,5-Piperazinedione	C4H6N2O2	1.173	0.153	203
(1R,2R)-Cyclohexane-1,2-Diamine	C6H14N2	1.183	-0.348	204
Ethyl(methyl)sulfane	C3H8S	1.185	0.164	205
(-)-1,3,3-Trimethyl-2-norbornanone	C10H16O	1.185	0.165	206
(-)-Epicedrol	C15H26O	1.189	0.169	207
1,4-Dithiane	C4H8S2	1.190	0.169	208
Formamide	CH3NO	1.190	0.170	209
Cyclohexane-1,4-diamine	C6H14N2	1.208	-0.323	210
L-Carvone	C10H14O	1.230	0.209	211
Toluene^{CSD}	C7H8	1.230	0.210	212
2,3,5,6-Tetrachlorocyclohexa-2,5-diene-1,4-dione	C6Cl4O2	1.234	0.214	213
2-Ethyl-3-hydroxy-4H-pyran-4-one	C7H8O3	1.245	-0.286	214
Dihydrofuran-2,5-dione	C4H4O3	1.255	0.234	215
Caryophyllen- α -oxide	C15H24O	1.265	0.244	216
Propan-1-amine	C3H9N	1.268	-0.263	217
(E)-4,4'-Diazastilbene	C12H10N2	1.285	-0.246	218
4,4'-Ethene-1,2-diylpyridine	C12H10N2	1.285	-0.246	219
Chlorine	Cl2	1.289	0.268	220
4-Acetamidobenzoic acid	C9H9NO3	1.334	-1.217	221
1,4-Phenylenediamine	C6H8N2	1.361	-0.170	222
(1S,6R,10R)-(+)-6-Methyl-4-oxabicyclo(8.4.1)pentadecan-3-one	C15H26O2	1.373	0.353	223
1,1,6,6-Tetraphenylhexa-2,4-diyne-1,6-diol	C30H22O2	1.380	-2.191	224
1,2,4,5-Tetracyanobenzene	C10H2N4	1.390	0.369	225
Ibuprofen	C13H18O2	1.410	-1.651	226

Proline	C5H9NO2	1.411	-0.119	227
L-Proline	C5H9NO2	1.411	-0.119	228
Citric acid	C6H8O7	1.427	-3.675	229
2,2'-(cyclohexa-2,5-diene-1,4-diylidene)dimalononitrile	C12H4N4	1.428	0.408	230
Butan-2-ol	C4H10O	1.433	-0.097	231
D-Threonine	C4H9NO3	1.452	-1.610	232
L-Threonine	C4H9NO3	1.452	-1.610	233
1-Hydroxypropan-2-one	C3H6O2	1.453	-0.078	234
(5-Hydroxy-6-methylpyridine-3,4-diyl)dimethanol	C8H11NO3	1.467	-1.594	235
Urea	CH4N2O	1.477	-0.054	236
Ethylene glycol	C2H6O2	1.480	-0.560	237
L-Aspartic acid	C4H7NO4	1.490	-2.081	238
DL-Aspartic acid	C4H7NO4	1.490	-2.081	239
2,5-bis(4-Pyridyl)-1,3,4-oxadiazole	C12H8N4O	1.491	-0.040	240
Phenylmethanethiol	C7H8S	1.495	-0.036	241
Dichlorodifluoromethane	CCl2F2	1.498	0.478	242
Benzamide	C7H7NO	1.518	-0.013	243
Carbamazepine	C15H12N2O	1.520	-0.010	244
4-(4-Hydroxyphenyl)butan-2-one	C10H12O2	1.522	-1.029	245
Ethyl acetate^{CSD}	C4H8O2	1.523	-0.007	246
β -L-Lyxopyranose	C5H10O5	1.524	-1.027	247
α -L-Xylopyranose	C5H10O5	1.524	-1.027	248
1,2,4,5-Tetrafluoro-3,6-di-iodobenzene^{CSD}	C6F4I2	1.525	0.505	249
Levulinic acid	C5H8O3	1.526	-1.025	250
Tryphenylphosphine oxide	C18H15OP	1.547	-0.494	251
β -DL-Arabinose	C5H10O5	1.569	-1.492	252
(1R,2S)-2-Methyl-4-oxocyclohexane-1-carboxylic acid	C8H12O3	1.581	0.050	253
Benzalacetone	C10H10O	1.586	0.056	254
Ferulic acid	C10H10O4	1.595	-1.467	255
Cinnamaldehyde	C9H8O	1.602	0.071	256
Isonicotinamide	C6H6N2O	1.603	0.072	257
1-(4-Methoxyphenyl)ethan-1-one	C9H10O2	1.604	0.073	258
Terephthalaldehyde	C8H6O2	1.608	0.078	259
Melamine	C3H6N6	1.609	-0.432	260
Methyl benzoate	C8H8O2	1.617	0.087	261
4-Hydroxy-3,5-dimethoxybenzaldehyde	C9H10O4	1.621	-0.930	262
4-Methoxybenzaldehyde	C8H8O2	1.625	0.094	263
Propionamide	C3H7NO	1.625	0.095	264
Nicotinamide	C6H6N2O	1.626	0.096	265
Benzophenone	C13H10O	1.639	0.108	266
β -D-Fructopyranose	C6H12O6	1.639	-1.933	267
α -L-Sorbopyranose	C6H12O6	1.639	-1.933	268
α -D-Tagatopyranose	C5H6O3	1.639	-1.933	269
1,2-Dimethoxybenzene	C8H10O2	1.639	0.109	270
Phenyl acetate	C8H8O2	1.640	0.110	271
bis(Methylthio)methane	C3H8S2	1.647	0.116	272

Tetracyanoethylene	C6N4	1.664	0.644	273
Diphenyl ether	C12H10O	1.675	0.145	274
1,2-bis(4-Pyridyl)ethane	C12H10N2	1.687	-0.354	275
4-Hydroxy-L-proline	C5H9NO3	1.701	-0.340	276
1,4-Dimethoxybenzene	C8H10O2	1.704	0.173	277
4-Aminobenzamide	C7H8N2O	1.781	-0.260	278
Glutaric acid^{CSD}	C5H8O4	1.783	-1.788	279
Butan-1-amine	C4H11N	1.804	-0.237	280
1-Chloro-1,1,2,2,2-pentafluoroethane	C2ClF5	1.832	0.812	281
Phenyl 2-Hydroxybenzoate	C13H10O3	1.855	-0.696	282
1,2-Ethanedithiol	C2H6S2	1.856	-0.185	283
(E)-4-(4-Hydroxy-3-methoxyphenyl)but-3-en-2-one	C11H12O3	1.873	-0.678	284
o-Anisic acid	C8H8O3	1.883	-0.158	285
Indomethacin	C19H16ClNO4	1.931	-1.640	286
Cinnamide	C9H9NO	1.939	-0.101	287
D-Alanine	C3H7NO2	1.945	-0.096	288
L-Alanine	C3H7NO2	1.945	-0.096	289
Tetrabromomethane	CBr4	1.950	0.930	290
n-Butanol^{CSD}	C4H10O	1.961	-0.080	291
Hexanoic acid	C6H12O2	1.996	-1.065	292
Glycine	C2H5NO2	2.050	0.010	293
D-Glucono-1,5-lactone	C6H10O6	2.053	-1.008	294
Tricyclopropylamine	C9H15N	2.060	0.019	295
Ethyl Propionate	C5H10O2	2.061	0.020	296
Benzoin	C14H12O2	2.062	-0.489	297
1,3,5-Trinitrobenzene	C6H3N3O6	2.069	0.028	298
2,3,5,6-Tetrafluoro-7,7,8,8-tetracyanoquinodimethane	C12F4N4	2.075	1.054	299
Pyrimethamine	C12H13ClN4	2.085	-0.466	300
Hippuric acid	C9H9NO3	2.087	-0.975	301
DL-Cysteine	C3H7NO2S	2.091	-0.970	302
L-Cysteine	C3H7NO2S	2.091	-0.970	303
L-Cysteine	C3H7NO2S	2.091	-0.970	304
1,3-Di(pyridin-4-yl)propane	C13H14N2	2.116	-0.435	305
2-Hydroxyacetamide	C2H5NO2	2.129	0.088	306
(R)-2-Hydroxypropanamide	C3H7NO2	2.130	0.089	307
(S)-2-Hydroxypropanamide	C3H7NO2	2.130	0.089	308
2-Aminoethan-1-ol	C2H7NO	2.136	0.095	309
Butyramide	C4H9NO	2.140	0.100	310
1,2-Dicyclopropylethane-1,2-dione	C8H10O2	2.200	0.159	311
1,2-Diphenyldisulfane	C12H10S2	2.210	0.169	312
1,2-bis(Methylthio)ethane	C4H10S2	2.222	0.181	313
α -D-Talose	C6H12O6	2.232	-1.340	314
β -D-Gulose	C6H12O6	2.232	-1.340	315
β -D-Allose	C6H12O6	2.232	-1.340	316
β -D-Altropyranose	C6H12O6	2.232	-1.340	317
α -D-Galactose	C6H12O6	2.232	-1.340	318

β-D-Galactose	C6H12O6	2.232	-1.340	319
α-D-Glucose	C6H12O6	2.232	-1.340	320
β-D-Glucose	C6H12O6	2.232	-1.340	321
DL-Valine	C5H11NO2	2.269	-0.282	322
<u>L-Valine</u>	<u>C5H11NO2</u>	<u>2.269</u>	<u>-0.282</u>	<u>323</u>
4-tert-Butyl-3-methoxy-2,6-dinitrotoluene	C12H16N2O5	2.285	0.244	324
3,3'-Thiodipropionic acid	C6H10O4S	2.332	-2.260	325
Pentan-1-amine	C5H13N	2.345	-0.206	326
DL-Tyrosine	C9H11NO3	2.378	-1.193	327
L-Tyrosine	C9H11NO3	2.378	-1.193	328
DL-Serine	C3H7NO3	2.386	-0.675	329
<i>Adipic acid</i>	<i>C10H18</i>	<i>2.418</i>	<i>-1.664</i>	<i>330</i>
DL-Tryptophan	C11H12N2O2	2.421	-0.640	331
L-Tryptophan	C11H12N2O2	2.421	-0.640	332
1,3-Propanedithiol	C3H8S2	2.438	-0.113	333
Piperine	C17H19NO3	2.528	-0.023	334
1-Pentanol	C5H12O	2.532	-0.019	335
Heptanoic acid	C7H14O2	2.534	-1.037	336
Scyllo-inositol	C6H12O6	2.551	-1.020	337
Cyclohexane-1,2,3,4,5,6-hexaol	C6H12O6	2.551	-1.020	338
epi-Inositol	C6H12O6	2.551	-1.020	339
L-chiro-Inositol	C6H12O6	2.551	-1.020	340
myo-Inositol	C6H12O6	2.551	-1.020	341
cis-Inositol	C6H12O6	2.551	-1.020	342
D-(+)-chiro-Inositol	C6H12O6	2.551	-1.020	343
neo-Inositol	C6H12O6	2.551	-1.020	344
Muco-inositol	C6H12O6	2.551	-1.020	345
Cyclohexane-1,2,3,4,5,6-hexol	C6H12O6	2.551	-1.020	346
Glycerol	C3H8O3	2.584	-0.478	347
n-Butyl acetate	C6H12O2	2.591	0.040	348
β-D- Psicose	C6H12O6	2.627	-1.454	349
β-Alanine	C3H7NO2	2.642	0.091	350
D-Glucuronic acid	C6H10O7	2.674	-2.939	351
1,3-Diphenylpropan-2-one	C15H14O	2.679	0.128	352
2-Methoxy-4-(1-(E)-propenyl)phenyl acetate	C12H14O3	2.716	0.165	353
Diallylsulfide	C6H10S	2.763	0.212	354
DL-Leucine	C6H13NO2	2.794	-0.267	355
L-α-Leucine	C6H13NO2	2.794	-0.267	356
L-Leucine	C6H13NO2	2.794	-0.267	357
<u>Succinamide</u>	<u>C4H8N2O2</u>	<u>2.813</u>	<u>-0.248</u>	<u>358</u>
Hexan-1-amine	C6H15N	2.878	-0.183	359
4-Aminobutanoic acid	C4H9NO2	2.880	-0.182	360
D-Isoleucine	C6H13NO2	2.887	-0.175	361
DL-Isoleucine	C6H13NO2	2.887	-0.175	362
13-epi-Sclareol	C20H36O2	2.957	-0.614	363
Octanoic acid	C8H16O2	3.053	-1.029	364

Hexanol^{CSD}	C6H14O	3.078	0.017	365
DL-Ribose	C5H10O5	3.083	-1.509	366
L-Ribose	C5H10O5	3.083	-1.509	367
3 β ,12 β -Dihydroxy-5 β -cholan-24-oic acid	C24H40O4	3.127	-0.955	368
iso-Deoxycholic acid	C24H40O4	3.127	-0.955	369
Diallyldisulfide	C6H10S2	3.146	0.084	370
Dimethyl succinate	C6H10O4	3.159	0.098	371
Dibenzoyl peroxide	C14H10O4	3.176	0.115	372
(Z)-Ethyl 2-benzylidene-3-oxobutanoate	C13H14O3	3.185	0.123	373
D-Asparagine	C4H8N2O3	3.189	-0.383	374
L-Asparagine	C4H8N2O3	3.189	-0.383	375
1,2-Dibenzylsulfane	C14H14S2	3.199	0.138	376
DL-Glutamic acid	C5H9NO4	3.235	-0.846	377
Glutamic acid	C5H9NO4	3.235	-0.846	378
Tramadol	C16H25NO2	3.240	0.179	379
Biotin	C10H16N2O3S	3.259	-0.312	380
DL-Methionine	C5H11NO2S	3.291	-0.281	381
L-Methionine	C5H11NO2S	3.291	-0.281	382
Acetylmethionine	C7H13NO3S	3.347	-0.735	383
1,1'-Azo-bis(carbamide)	C2H4N4O2	3.446	-0.126	384
Cholic acid	C24H40O5	3.538	-1.053	385
Heptanol^{CSD}	C7H16O	3.569	-0.003	386
Nonanoic acid	C9H18O2	3.598	-0.994	387
Lidocaine	C18H32O2	3.640	0.068	388
4-Allyl-2-methoxyphenyl benzoate	C17H16O3	3.750	0.178	389
Tromethamine	C4H11NO3	3.921	-0.161	390
Suberic acid	C8H14O4	3.932	-1.170	391
Sucralose	C12H19Cl3O8	4.008	-1.604	392
DL-Glutamine	C5H10N2O3	4.029	-0.052	393
L-Glutamine	C5H10N2O3	4.029	-0.052	394
Octanol^{CSD}	C8H18O	4.074	-0.008	395
1,6-Hexanedithiol	C6H14S2	4.095	0.013	396
Decanoic acid	C10H20O2	4.160	-0.942	397
Vitamin A acetate	C22H32O2	4.441	0.360	398
D-Arabinitol	C5H12O5	4.590	-0.512	399
DL-Arabinitol	C5H12O5	4.590	-0.512	400
Ribitol	C5H12O5	4.590	-0.512	401
Xylitol	C5H12O5	4.590	-0.512	402
L-Cystine	C6H12N2O4S2	4.591	-1.531	403
Sebacic acid	C10H18O4	4.613	-1.509	404
D-Lysine	C6H14N2O2	4.615	0.023	405
L-Lysine	C6H14N2O2	4.615	0.023	406
Undecanoic Acid	C11H22O2	4.695	-0.917	407
2,2',2''-Nitrilotriethanol	C6H15NO3	4.985	-0.117	408
α,α -Trehalose	C12H22O11	5.154	-1.478	409
α,α -Galacto-trehalose	C12H22O11	5.154	-1.478	410

1,8-Octanedithiol	C8H18S2	5.173	0.071	411
DL-Arginine	C6H14N4O2	5.192	0.090	412
L-Arginine	C6H14N4O2	5.192	0.090	413
Lauric acid	C12H24O2	5.217	-0.905	414
α -8'- β -Apocarotenal	C30H40O	5.519	0.417	415
β -8'- β -Apocarotenal	C30H40O	5.519	0.417	416
β -Cellobiose	C12H22O11	5.660	-0.973	417
o- β -D-Mannopyranosyl-(1-4)- α -D-mannopyranose	C12H22O11	5.660	-0.973	418
α -Lactose	C12H22O11	5.660	-0.973	419
β -Lactose	C12H22O11	5.660	-0.973	420
β -Maltose	C12H22O11	5.660	-0.973	421
α -Maltose	C12H22O11	5.660	-0.973	422
β -galabiose	C12H22O11	5.665	-2.498	423
Allitol	C6H14O6	5.678	-0.445	424
Galactitol	C6H14O6	5.678	-0.445	425
D-Glucitol	C6H14O6	5.678	-0.445	426
D-Iditol	C6H14O6	5.678	-0.445	427
I-Iditol	C6H14O6	5.678	-0.445	428
D-Altritol	C6H14O6	5.678	-0.445	429
D-Mannitol	C6H14O6	5.678	-0.445	430
DL-Mannitol	C6H14O6	5.678	-0.445	431
1,9-Nonanedithiol	C9H20S2	5.712	0.100	432
Tridecanoic Acid	C13H26O2	5.744	-0.889	433
n-Methyl-D-glucamine	C7H17NO5	5.812	-0.310	434
Sucrose	C12H22O11	6.173	-0.969	435
Tetradecanoic acid	C14H28O2	6.280	-0.863	436
1,11-Undecanediol	C11H24O2	6.559	-0.074	437
Neotame	C20H30N2O5	6.689	-0.454	438
Pentadecanoic acid	C15H30O2	6.815	-0.838	439
Linoleic acid	C18H32O2	7.301	-0.862	440
Palmitic Acid	C16H32O2	7.350	-0.813	441
1,13-Tridecanediol	C13H28O2	7.620	-0.033	442
n-Hexadecanol	C16H34O	8.401	0.237	443
Stearic acid	C18H36O2	8.418	-0.765	444
Sucrose octa-acetate	C28H38O19	11.476	0.251	445
1,2-Distearoyl-3-elaidoylglycerol	C57H108O6	29.408	0.837	446
1,3-Distearoyl-2-oleoylglycerol	C57H108O6	29.490	0.919	447
2-(Oleoyloxy)propane-1,3-diyl distearate	C57H108O6	29.490	0.919	448
1,3-Distearoyl-2-elaidoylglycerol	C57H108O6	29.492	0.921	449
β -Tristearin	C57H110O6	30.039	0.958	450

Table S7 – Scores and Ranking obtained for CV, MC, HBP, COSMOQuick and the three consensus ranking A, B and C for the multicomponent analysis of 450 co-formers against NVP molecule. The co-formers were ordered by the consensus ranking C, obtained from the sum of ranking positions obtained for MC, HBP analysis, and CosmoQuick prediction. In bold are represented the 76 molecules for which experimental multicomponent results are available. Black-italic letter identify the positive results; CSD means molecules reported in the CSD database. Red-underline letter identify the negative results.

Co-former	Molecular formula	CV score	CV ranking	MC score	MC ranking	HBP score	HBP ranking	Consensus A	Consensus Ranking A	f_{fit}	H_{ex} (kcal.mol ⁻¹)	COSMOQuick ranking	Consensus B	Consensus ranking B	Consensus C	Consensus ranking C
2,4-Dihydroxybenzoic acid	C7H6O4	-0.710	65	6.147	114	0.35	14	193	10	-2.421	-4.972	15	208	1	143	1
<i>Benzoic acid</i> ^{CSD}	<i>C7H6O2</i>	<i>-0.058</i>	<i>161</i>	<i>5.563</i>	<i>72</i>	<i>0.23</i>	<i>51</i>	<i>284</i>	<i>35</i>	<i>-0.019</i>	<i>-1.549</i>	<i>57</i>	<i>341</i>	<i>9</i>	<i>180</i>	<i>2</i>
Anthranilic acid	C7H7NO2	-0.259	125	6.321	129	0.28	27	281	32	-0.174	-2.215	50	331	8	206	3
Terephthalic acid	C8H6O4	-0.741	61	5.250	53	0.18	111	225	14	-0.423	-2.974	46	271	2	210	4
<i>4-Aminobenzoic acid</i>	<i>C7H7NO2</i>	<i>-0.311</i>	<i>108</i>	<i>5.702</i>	<i>81</i>	<i>0.26</i>	<i>38</i>	<i>227</i>	<i>16</i>	<i>0.680</i>	<i>-1.361</i>	<i>97</i>	<i>324</i>	<i>7</i>	<i>216</i>	<i>5</i>
Allocinnamic acid	C9H8O2	-0.267	123	5.778	84	0.26	36	243	20	0.691	-1.349	101	344	10	221	6
2-Amino-5-methylbenzoic acid	C8H9NO2	-0.212	135	6.475	151	0.30	21	307	39	-0.096	-2.137	53	360	18	225	7
<i>Fumaric acid</i>	<i>C4H4O4</i>	<i>0.103</i>	<i>181</i>	<i>6.233</i>	<i>123</i>	<i>0.22</i>	<i>66</i>	<i>370</i>	<i>67</i>	<i>-0.707</i>	<i>-3.258</i>	<i>40</i>	<i>410</i>	<i>26</i>	<i>229</i>	<i>8</i>
<i>3-Hydroxybenzoic acid</i> ^{CSD}	<i>C7H6O3</i>	<i>-0.841</i>	<i>52</i>	<i>6.321</i>	<i>128</i>	<i>0.21</i>	<i>75</i>	<i>255</i>	<i>23</i>	<i>-1.271</i>	<i>-3.311</i>	<i>29</i>	<i>284</i>	<i>3</i>	<i>232</i>	<i>9</i>
<i>Maleic Acid</i> ^{CSD}	<i>C4H4O4</i>	<i>-0.609</i>	<i>73</i>	<i>6.551</i>	<i>158</i>	<i>0.27</i>	<i>33</i>	<i>264</i>	<i>29</i>	<i>-0.568</i>	<i>-3.119</i>	<i>42</i>	<i>306</i>	<i>5</i>	<i>233</i>	<i>10</i>
<i>4-Hydroxybenzoic acid</i> ^{CSD}	<i>C7H6O3</i>	<i>-0.808</i>	<i>56</i>	<i>5.795</i>	<i>85</i>	<i>0.17</i>	<i>117</i>	<i>258</i>	<i>24</i>	<i>-0.868</i>	<i>-2.909</i>	<i>32</i>	<i>290</i>	<i>4</i>	<i>234</i>	<i>11</i>
Methyl paraben	C8H8O3	-0.216	134	5.975	98	0.23	54	286	36	0.480	-1.561	84	370	20	236	12
<i>Salicylic acid</i> ^{CSD}	<i>C7H6O3</i>	<i>-0.309</i>	<i>109</i>	<i>6.219</i>	<i>121</i>	<i>0.20</i>	<i>90</i>	<i>320</i>	<i>44</i>	<i>-1.170</i>	<i>-3.211</i>	<i>30</i>	<i>350</i>	<i>11</i>	<i>241</i>	<i>13</i>
4-Methoxybenzoic acid	C8H8O3	0.333	209	5.802	86	0.24	49	344	57	0.773	-1.267	112	456	33	247	14
Myricetin	C15H10O8	1.476	388	5.856	92	0.14	152	632	174	-3.176	-7.258	6	638	90	250	15
Phenoxyacetic acid	C8H8O3	0.371	210	5.827	89	0.26	39	338	53	0.860	-1.691	124	462	35	252	16
2-Coumaric acid	C9H8O3	-0.738	62	5.552	71	0.16	128	261	26	0.013	-2.538	58	319	6	257	17
<u>Hydroquinone</u>	<u>C6H6O2</u>	<u>-0.286</u>	<u>115</u>	<u>5.834</u>	<u>90</u>	<u>0.13</u>	<u>165</u>	<u>370</u>	<u>68</u>	<u>-2.288</u>	<u>-3.819</u>	<u>17</u>	<u>387</u>	<u>23</u>	<u>272</u>	<u>18</u>
1-Hydroxy-2-naphthoic acid	C11H8O3	-0.435	90	5.250	52	0.10	195	337	52	-1.373	-3.414	27	364	19	274	19
2,6-Dimethylpyrazine	C6H8N2	2.008	420	6.364	135	0.28	26	581	151	0.777	-0.243	113	694	117	274	20
3-Methylbut-2-enoic acid	C5H8O2	-0.150	143	6.587	161	0.29	24	328	47	0.597	-0.934	92	420	28	277	21
Pyrrole	C4H5N	-0.604	74	6.868	182	0.43	7	263	28	0.608	-0.412	93	356	15	282	22
<i>Cinnamic acid</i>	<i>C9H8O2</i>	<i>0.156</i>	<i>190</i>	<i>4.950</i>	<i>44</i>	<i>0.21</i>	<i>76</i>	<i>310</i>	<i>40</i>	<i>1.076</i>	<i>-0.965</i>	<i>175</i>	<i>485</i>	<i>43</i>	<i>295</i>	<i>23</i>
4'-Hydroxyacetophenone	C8H8O2	0.442	218	6.096	110	0.16	129	457	95	0.236	-1.295	65	522	50	304	24
Pterostilbene	C16H16O3	-0.843	51	5.884	94	0.16	132	277	30	0.435	-2.626	79	356	16	305	25
[1,1'-Biphenyl]-4,4'-diol	C12H10O2	-0.296	112	4.197	18	0.01	274	404	75	-2.688	-4.728	14	418	27	306	26
<i>Gentisic acid</i> ^{CSD}	<i>C7H6O4</i>	<i>-0.718</i>	<i>64</i>	<i>6.369</i>	<i>136</i>	<i>0.13</i>	<i>162</i>	<i>362</i>	<i>62</i>	<i>-1.985</i>	<i>-4.536</i>	<i>20</i>	<i>382</i>	<i>21</i>	<i>318</i>	<i>27</i>
1-Naphthol	C10H8O	-0.959	35	5.660	77	0.06	231	343	55	-2.741	-3.762	13	356	17	321	28

2-Acetylpyrrole	C6H7NO	-0.280	119	6.673	170	0.29	23	312	43	0.915	-0.105	135	447	31	328	29
Trimesic acid	C9H6O6	-1.001	25	6.614	164	0.17	123	312	41	-0.567	-4.139	43	355	13	330	30
2-Phenylacetic acid	C8H8O2	-0.103	151	6.616	165	0.20	89	405	77	0.417	-1.624	78	483	41	332	31
Phloroglucinol	C6H6O3	0.397	213	6.904	188	0.15	143	544	134	-3.654	-5.695	3	547	61	334	32
1,4-Phenylenediamine	C6H8N2	0.755	270	5.678	79	0.26	35	384	73	1.361	-0.170	222	606	76	336	33
1,2-Ethanedithiol	C2H6S2	-1.099	10	5.451	62	0.48	1	73	1	1.856	-0.185	283	356	14	346	34
4-Ethoxyphenol	C8H10O2	-1.134	3	5.976	99	0.10	196	298	37	-0.027	-2.068	56	354	12	351	35
4-(Hydroxymethyl)phenol	C7H8O2	-0.809	54	6.734	175	0.19	98	327	46	0.474	-1.567	82	409	25	355	36
Resorcinol	C6H6O2	-0.285	116	6.701	173	0.12	181	470	106	-3.215	-4.745	5	475	38	359	37
4-Hydroxybenzaldehyde	C7H6O2	0.646	242	5.593	74	0.05	241	557	138	-0.279	-1.810	48	605	75	363	38
Catechol	C6H6O2	-0.180	137	7.047	197	0.13	160	494	113	-3.049	-4.579	9	503	45	366	39
Crotonic acid	C4H6O2	0.130	187	6.423	143	0.15	136	466	105	0.495	-1.035	87	553	66	366	40
cis-Aconitic acid	C6H6O6	-0.985	29	8.153	305	0.28	28	362	63	-0.762	-4.843	35	397	24	368	41
Phenol	C6H6O	-1.064	17	6.211	120	0.07	227	364	65	-1.853	-2.873	23	387	22	370	42
4-Nitrobenzoic acid	C7H5NO4	0.934	304	6.023	103	0.06	232	639	176	-0.500	-2.541	44	683	109	379	43
Gallic acid	C7H6O5	0.773	276	7.414	233	0.15	138	647	181	-2.402	-5.463	16	663	101	387	44
Vanillic acid	C8H8O4	-0.914	44	7.428	238	0.21	81	363	64	0.265	-2.286	68	431	29	387	45
(E)-4,4'-Diazastilbene	C12H10N2	2.224	427	4.394	24	0.14	148	599	159	1.285	-0.246	218	817	168	390	46
Isocaryolan-9 α -ol	C15H26O	-0.494	86	7.432	240	0.33	17	343	56	0.936	-0.084	138	481	39	395	47
Acetylsalicylic acid	C9H8O4	0.759	271	7.395	231	0.27	31	533	131	0.936	-1.615	137	670	104	399	48
1,7,7-Trimethyltricyclo(2.2.1.0 ^{2,6})heptan-4-ol	C10H16O	-0.689	68	8.333	325	0.33	16	409	80	0.106	-0.914	59	468	37	400	49
Orcinol	C7H8O2	-0.295	113	7.377	230	0.13	169	512	122	-2.806	-4.336	12	524	52	411	50
1,6-Hexanedithiol	C6H14S2	-0.615	72	3.827	11	0.44	4	87	2	4.095	0.013	396	483	40	411	51
2,5-Dimethylphenol	C8H10O	-0.935	40	6.393	140	0.04	251	431	87	-1.871	-2.891	21	452	32	412	52
1,8-Octanedithiol	C8H18S2	-0.413	94	3.444	5	0.47	2	101	3	5.173	0.071	411	512	47	418	53
2,4,6-Trimethylphenol	C9H12O	-0.955	36	6.892	185	0.09	205	426	86	-0.820	-1.841	34	460	34	424	54
Pyrazine-1,4-dioxide	C4H4N2O2	2.993	446	6.951	191	0.24	50	687	211	1.108	0.087	183	870	184	424	55
N,N-Dimethylformamide	C3H7NO	1.739	411	8.088	299	0.31	20	730	240	0.723	-0.297	105	835	171	424	56
Chloranilic acid	C6H2Cl2O4	-0.222	132	6.353	134	-0.01	283	549	135	-3.084	-4.615	8	557	68	425	57
4-Nitrophenol	C6H5NO3	0.382	212	6.353	133	0.01	276	621	167	-2.268	-3.799	18	639	92	427	58
Adipic acid	C10H18	-0.703	66	5.519	69	0.27	32	167	8	2.418	-1.664	330	497	44	431	59
2-Chloroacetic acid	C2H3ClO2	0.419	216	7.220	214	0.12	177	607	164	-0.639	-2.169	41	648	95	432	60
Ethanol^{CSD}	C2H5OH	0.538	222	7.419	234	0.22	65	521	126	0.914	-0.106	134	655	97	433	61

4,4'-Bipyridine	C10H8N2	2.319	434	5.454	63	0.03	258	755	264	0.801	-0.219	115	870	185	436	62
1,3-Propanedithiol	C3H8S2	-0.968	32	5.979	100	0.46	3	135	5	2.438	-0.113	333	468	36	436	63
Cyclohexane-1,4-diamine	C6H14N2	-1.143	1	6.897	186	0.25	40	227	17	1.208	-0.323	210	437	30	436	64
Acetic acid	C2H4O2	0.293	202	8.325	324	0.22	60	586	153	-0.111	-1.132	52	638	89	436	65
Glutaric acid^{CSD}	C5H8O4	-0.505	84	5.876	93	0.22	67	244	21	1.783	-1.788	279	523	51	439	66
2,5-bis(4-Pyridyl)-1,3,4-oxadiazole	C12H8N4O	3.383	447	4.927	43	0.13	157	647	182	1.491	-0.040	240	887	192	440	67
1,4,8,11-Tetra-azacyclotetradecane	C10H24N4	0.786	277	6.937	189	0.18	106	572	145	0.941	-0.079	145	717	133	440	68
Formic acid	CH2O2	0.692	251	8.838	364	0.25	43	658	186	-0.864	-1.885	33	691	115	440	69
1,9-Nonanedithiol	C9H20S2	-0.322	107	3.341	4	0.44	5	116	4	5.712	0.100	432	548	62	441	70
o-Cresol	C7H8O	-0.930	42	7.038	196	0.07	226	464	102	-2.097	-3.117	19	483	42	441	71
Quinoxaline-N,N'-dioxide	C8H6N2O2	2.874	445	6.603	163	0.18	109	717	223	1.056	0.036	172	889	194	444	72
2,4-Pyridinedicarboxylic acid	C7H5NO4	0.831	284	6.434	144	0.04	250	678	202	-0.148	-2.699	51	729	141	445	73
Ibuprofen	C13H18O2	-0.349	102	5.841	91	0.16	130	323	45	1.410	-1.651	226	549	63	447	74
2,2,2-Trifluoroethanol	C2H3F3O	0.126	186	8.087	298	0.17	115	599	160	-0.755	-1.775	36	635	87	449	75
Trichloroacetic acid^{CSD}	C2HCl3O2	0.623	235	8.931	372	0.22	69	676	201	-2.918	-3.938	10	686	113	451	76
Naphthalene-1,5-disulfonic acid^{CSD}	C10H8S2O6	1.009	317	7.088	201	0.07	225	743	252	-1.381	-3.932	26	769	155	452	77
L-Mandelic acid	C8H8O3	-0.455	88	7.746	270	0.15	141	499	119	-0.361	-2.912	47	546	60	458	78
5-Nitroisophthalic acid	C8H5NO6	0.628	237	7.518	250	0.12	172	659	188	-0.727	-3.788	39	698	121	461	79
4-Methylbenzenesulfonic acid	C7H8O3S	0.933	303	6.549	157	0.02	268	728	238	-0.748	-2.278	37	765	153	462	80
Glycolic acid	C2H4O3	-0.260	124	8.219	313	0.20	86	523	128	0.234	-1.807	64	587	73	463	81
Trifluoroacetic acid	C2HF3O2	0.281	200	8.272	320	0.15	144	664	193	-3.951	-4.971	2	666	102	466	82
Salicylaldehyde	C7H6O2	1.171	347	6.554	159	0.14	154	660	190	0.970	-0.561	154	814	167	467	83
L-Malic acid	C4H6O5	-0.851	49	7.969	291	0.19	102	442	91	0.388	-3.183	75	517	48	468	84
(R,S)-Hesperetin	C16H14O6	-0.299	111	7.017	194	0.13	156	461	100	0.817	-2.244	119	580	70	469	85
2-Isopropyl-5-methylphenol	C10H14O	-0.935	39	7.285	224	0.07	222	485	109	-1.521	-3.052	25	510	46	471	86
Succinic acid	C4H6O4	-0.165	141	8.205	312	0.22	68	521	127	0.617	-2.444	94	615	81	474	87
N,N-Dimethylacetamide	C4H9NO	1.409	377	7.451	243	0.15	142	762	269	0.560	-0.460	89	851	176	474	88
L-Tartaric acid	C4H6O6	-0.616	71	9.120	384	0.31	18	473	107	0.334	-3.747	73	546	59	475	89
Pyrazine	C4H4N2	2.451	438	7.024	195	0.16	133	766	273	0.955	-0.066	148	914	208	476	90
Butan-1-amine	C4H11N	0.009	172	5.546	70	0.16	131	373	69	1.804	-0.237	280	653	96	481	91
Pyridine	C5H5N	1.486	390	6.891	184	0.12	180	754	261	0.807	-0.213	117	871	187	481	92
3,5-Dinitrobenzoic acid	C7H4N2O6	1.453	384	7.361	229	0.08	217	830	321	-0.738	-3.289	38	868	182	484	93
Lactic acid	C3H6O3	-0.962	34	9.102	380	0.25	44	458	96	0.216	-1.825	63	521	49	487	94
4-Acetamidobenzoic acid	C9H9NO3	-0.373	98	5.909	96	0.12	171	365	66	1.334	-1.217	221	586	72	488	95

Ferulic acid	C10H10O4	-0.885	45	6.375	138	0.19	100	283	34	1.595	-1.467	255	538	58	493	96
Pentan-1-amine	C5H13N	-0.079	160	5.139	49	0.17	122	331	50	2.345	-0.206	326	657	98	497	97
3,5-Dinitrosalicylic acid^{CSD}	C7H4N2O7	1.293	364	7.750	272	0.09	206	842	328	-1.861	-4.922	22	864	180	500	98
Undecanoic Acid	C11H22O2	-0.176	139	3.939	13	0.21	80	232	18	4.695	-0.917	407	639	91	500	99
3-Oxocyclobutanecarboxylic acid	C5H6O3	1.538	396	7.818	280	0.15	135	811	305	0.487	-1.043	86	897	201	501	100
Butyric acid	C4H8O2	0.117	182	7.952	289	0.20	84	555	137	0.910	-1.131	130	685	111	503	101
Suberic acid	C8H14O4	-0.862	47	4.734	35	0.21	78	160	7	3.932	-1.170	391	551	64	504	102
4-(4-Hydroxyphenyl)butan-2-one	C10H12O2	0.298	204	6.299	126	0.16	134	464	101	1.522	-1.029	245	709	129	505	103
1-Naphthalenesulfonic acid	C10H8O3S	0.732	266	7.457	245	0.06	230	741	249	-1.166	-2.697	31	772	156	506	104
Tetrahydrofuran	C4H8O	1.163	345	8.623	352	0.27	34	731	243	0.819	-0.201	120	851	174	506	105
2-Amino-5-picolinic acid	C6H6N2O2	1.647	404	9.189	385	0.30	22	811	304	0.690	-1.351	99	910	206	506	106
Betaine	C5H10NO2	3.558	449	10.872	434	0.39	10	893	361	0.192	-0.828	62	955	230	506	107
L-Ascorbic acid	C6H8O6	0.056	177	8.518	342	0.21	77	596	157	0.546	-3.026	88	684	110	507	108
3,3'-Thiodipropionic acid	C6H10O4S	-0.543	78	6.404	141	0.25	41	260	25	2.332	-2.260	325	585	71	507	109
2,2'-Dihydroxy-5,5'-diallyl-biphenyl	C18H18O2	-0.990	27	8.017	295	0.17	116	438	89	0.636	-3.446	96	534	55	507	110
Meso-Tartaric acid	C4H6O6	-0.355	101	10.055	414	0.31	19	534	133	0.334	-3.747	74	608	77	507	111
Tridecanoic Acid	C13H26O2	-0.053	162	3.657	8	0.22	70	240	19	5.744	-0.889	433	673	106	511	112
Hexan-1-amine	C6H15N	-0.080	159	4.599	32	0.17	121	312	42	2.878	-0.183	359	671	105	512	113
Sebacic acid	C10H18O4	-0.942	38	4.241	19	0.20	91	148	6	4.613	-1.509	404	552	65	514	114
2,5,5,8α-Tetramethyloctahydro-2H-2,4α-methanonaphthalen-1-ol	C15H26O	-1.099	11	7.803	278	0.16	127	416	83	0.763	-0.257	110	526	53	515	115
Cyclobutanol	C4H8O	-0.030	165	8.228	314	0.20	85	564	143	0.802	-0.219	116	680	108	515	116
1,10-Phenanthroline	C12H8N2	1.722	410	5.305	57	-0.19	382	849	331	0.412	-0.609	77	926	213	516	117
Linoleic acid	C18H32O2	-0.337	104	4.716	34	0.25	45	183	9	7.301	-0.862	440	623	82	519	118
2-(Tert-butyl)-4-methoxyphenol	C11H16O2	-1.062	18	7.704	268	0.07	223	509	121	-1.349	-2.879	28	537	57	519	119
DL-Malic acid	C4H6O5	-1.069	16	8.072	297	0.14	147	460	99	0.388	-3.183	76	536	56	520	120
α-Ketoglutaric acid	C5H6O5	0.817	281	6.778	178	0.02	272	731	241	0.279	-3.292	70	801	161	520	121
n-Butanol^{CSD}	C4H10O	-0.009	170	5.761	83	0.14	153	406	78	1.961	-0.080	291	697	120	527	122
Lauric acid	C12H24O2	-0.012	169	3.884	12	0.19	101	282	33	5.217	-0.905	414	696	118	527	123
Trimethylamine	C3H9N	1.562	401	7.961	290	0.18	113	804	296	0.865	-0.156	125	929	216	528	124
Cyclodecanol	C10H20O	-0.523	82	7.264	221	0.15	137	440	90	1.054	0.034	171	611	79	529	125
Tartaric acid^{CSD}	C4H6O6	-0.590	75	8.598	348	0.18	110	533	132	0.334	-3.747	72	605	74	530	126
(+)-Camphoric acid	C10H16O4	-1.139	2	8.235	317	0.14	146	465	103	0.260	-2.291	67	532	54	530	127
Palmitic Acid	C16H32O2	-0.283	117	3.325	3	0.20	87	207	12	7.350	-0.813	441	648	94	531	128

Propan-1-amine	C3H9N	0.032	175	6.441	147	0.13	167	489	111	1.268	-0.263	217	706	125	531	129
Nicotinic acid	C6H5NO2	1.261	358	6.122	112	-0.06	320	790	290	0.690	-0.840	100	890	196	532	130
Pentadecanoic acid	C15H30O2	-0.097	152	3.549	7	0.20	88	247	22	6.815	-0.838	439	686	112	534	131
4,4'-Ethene-1,2-diylidipyridine	C12H10N2	2.241	429	4.346	23	-0.03	292	744	253	1.285	-0.246	219	963	235	534	132
Phenyl 2-Hydroxybenzoate	C13H10O3	-0.344	103	5.593	73	0.12	179	355	58	1.855	-0.696	282	637	88	534	133
Tetradecanoic acid	C14H28O2	-0.257	126	3.549	6	0.20	93	225	15	6.280	-0.863	436	661	99	535	134
4-(Hydroxymethyl)-2-methoxyphenol	C8H10O3	-0.950	37	8.157	306	0.14	149	492	112	0.439	-2.112	80	572	69	535	135
2,6-Pyridinedicarboxylic acid	C7H5NO4	0.230	196	6.751	176	0.08	216	588	154	0.941	-1.610	144	732	142	536	136
(1R,2R)-Cyclohexane-1,2-Diamine	C6H14N2	-0.585	76	7.890	285	0.25	47	408	79	1.183	-0.348	204	612	80	536	137
Stearic acid	C18H36O2	-0.322	106	3.071	1	0.20	92	199	11	8.418	-0.765	444	643	93	537	138
Ethylenediamine	C2H8N2	-0.490	87	7.344	228	0.11	186	501	120	0.857	-0.673	123	624	84	537	139
Acrylaldehyde	C3H4O	1.543	398	6.336	130	0.06	235	763	270	1.071	0.051	174	937	218	539	140
2,2'-Bipyridine	C10H8N2	1.496	391	4.594	31	-0.09	344	766	272	1.034	0.014	166	932	217	541	141
Hexanoic acid	C6H12O2	-0.017	167	5.171	50	0.10	200	417	84	1.996	-1.065	292	709	128	542	142
1,2-Ethanedisulfonic acid	C2H6O6S2	1.315	366	7.255	219	-0.06	312	897	366	-2.853	-5.914	11	908	205	542	143
Orotic acid	CSH4N2O4	0.718	260	7.181	212	0.01	277	749	256	-0.071	-1.602	54	803	162	543	144
Propan-2-one	C3H6O	1.334	368	7.405	232	0.13	159	759	267	0.983	-0.038	158	917	209	549	145
(2R,3R)-2,3-Dimethylcyclopropane-1-carboxylic acid	C6H10O2	-0.081	157	7.638	265	0.10	203	625	171	0.451	-1.079	81	706	126	549	146
o-Anisic acid	C8H8O3	0.093	179	7.425	236	0.28	29	444	92	1.883	-0.158	285	729	140	550	147
1-Hydroxydiamantane	C14H20O	-1.129	5	8.205	311	0.20	83	399	74	0.974	-0.047	157	556	67	551	148
Ethyl acetate^{CSD}	C4H8O2	1.144	339	6.267	124	0.11	185	648	183	1.523	-0.007	246	894	198	555	149
Oxalic acid	C2H2O4	-0.093	153	7.512	248	-0.04	305	706	222	-3.469	-5.509	4	710	130	557	150
Acridine	C13H9N	1.156	342	4.736	36	-0.22	392	770	276	0.912	-0.108	132	902	204	560	151
Ethylamine	C2H7N	0.164	191	7.426	237	0.08	218	646	180	0.744	-0.277	107	753	149	562	152
Pyrimethamine	C12H13ClN4	0.190	193	7.131	208	0.23	55	456	94	2.085	-0.466	300	756	150	563	153
1,2-bis(4-Pyridyl)ethane	C12H10N2	2.272	431	4.712	33	0.03	257	721	230	1.687	-0.354	275	996	256	565	154
Thiourea	CH4N2S	0.123	184	8.165	308	0.18	112	604	163	0.947	-0.584	146	750	147	566	155
Pyromellitic	C10H2O6	3.566	450	6.094	109	-0.07	331	890	358	0.872	-0.148	127	1017	275	567	156
Levulinic acid	C5H8O3	1.062	322	6.477	152	0.13	166	640	177	1.526	-1.025	250	890	195	568	157
Hexano^{CSD}	C6H14O	-0.090	155	4.840	40	0.13	164	359	60	3.078	0.017	365	724	138	569	158
2,4-Dimethylpyridine	C7H9N	1.356	370	6.436	145	-0.07	322	837	324	0.693	-0.328	102	939	220	569	159
Phenylmethanol	C7H8O	-0.033	163	7.173	210	0.07	228	601	162	0.912	-0.619	131	732	143	569	160
1,4-Dioxane^{CSD}	C4H8O2	1.357	371	8.300	323	0.19	97	791	292	0.960	-0.060	150	941	223	570	161

(-)-Epicedrol	C15H26O	-0.244	129	7.754	274	0.19	95	498	118	1.189	0.169	207	705	124	576	162
Heptano^{CSD}	C7H16O	-0.128	147	4.563	29	0.13	163	339	54	3.569	-0.003	386	725	139	578	163
Malonic acid	C3H4O4	-0.293	114	7.579	257	0.11	189	560	140	0.914	-1.637	133	693	116	579	164
[1,1'-Binaphthalene]-2,2'-diol	C20H14O2	-0.276	120	7.458	246	-0.08	332	698	217	-4.436	-6.477	1	699	122	579	165
Heptanoic acid	C7H14O2	-0.081	158	4.791	38	0.09	209	405	76	2.534	-1.037	336	741	144	583	166
Octano^{CSD}	C8H18O	-0.165	140	4.259	21	0.13	168	329	48	4.074	-0.008	395	724	137	584	167
Tetrathiafulvalene	C6H4S4	0.708	256	4.400	25	-0.43	439	720	226	0.819	-0.201	121	841	172	585	168
2,6-Dimethylpyridine	C7H9N	1.126	336	6.503	153	-0.07	323	812	306	0.762	-0.258	109	921	211	585	169
Phenazine	C12H8N2	1.750	413	4.758	37	-0.26	399	849	332	0.961	-0.059	151	1000	258	587	170
2,8,16,20-Tetramethylcalix(4)resorcinarene	C32H32O8	2.693	443	8.287	322	0.03	260	1025	421	-3.163	-7.755	7	1032	284	589	171
Butan-2-ol	C4H10O	-0.333	105	7.443	241	0.17	119	465	104	1.433	-0.097	231	696	119	591	172
N-Methylpyrrolidone	C5H9NO	1.416	379	7.601	261	0.05	240	880	354	0.595	-0.426	91	971	242	592	173
Citric acid	C6H8O7	-0.400	96	8.113	301	0.22	63	460	98	1.427	-3.675	229	689	114	593	174
Octanoic acid	C8H16O2	-0.117	150	4.557	28	0.10	201	379	70	3.053	-1.029	364	743	146	593	175
Cyclamic acid	C6H13NO3S	-0.932	41	7.157	209	-0.07	324	574	147	0.189	-1.851	61	635	86	594	176
2,5-Dimethylpyrazine	C6H8N2	2.130	425	6.180	119	-0.12	362	906	372	0.780	-0.241	114	1020	277	595	177
1,1-bis(4-Hydroxyphenyl)cyclohexane	C18H20O2	-0.253	127	7.879	283	-0.03	288	698	218	-1.665	-4.216	24	722	136	595	178
Cinnamaldehyde	C9H8O	1.451	383	4.875	41	-0.04	299	723	234	1.602	0.071	256	979	246	596	179
1,2,4,5-Tetracyanobenzene	C10H2N4	2.616	441	5.652	76	-0.04	298	815	308	1.390	0.369	225	1040	287	599	180
cis,cis-1,3,5-Cyclohexanetricarboxylic acid	C9H12O6	-0.996	26	8.011	294	0.10	198	518	125	0.748	-2.824	108	626	85	600	181
2,6-Di-tert-butyl-4-methylphenol	C15H24O	-1.126	7	7.211	213	-0.08	333	553	136	-0.052	-1.072	55	608	78	601	182
2,3,5,6-Tetrachlorocyclohexa-2,5-diene-1,4-dione	C6Cl4O2	2.255	430	6.172	118	0.02	271	819	312	1.234	0.214	213	1032	283	602	183
2-Aminopyrimidine	C4H5N3	0.727	263	7.052	198	0.02	265	726	236	0.938	-0.083	141	867	181	604	184
Saccharin^{CSD}	C7H5NO3S	1.674	406	8.475	337	0.10	202	945	388	0.286	-0.734	71	1016	274	610	185
Tetramethylpyrazine	C8H12N2	1.496	392	6.659	169	-0.09	347	908	373	0.625	-0.396	95	1003	263	611	186
Furfural	C6H12O2	1.545	399	6.762	177	-0.01	284	860	340	0.969	-0.051	152	1012	270	613	187
Nonanoic acid	C9H18O2	-0.124	148	4.256	20	0.09	211	379	71	3.598	-0.994	387	766	154	618	188
Pyruvic acid	C3H4O3	1.242	354	8.233	315	0.04	254	923	380	-0.237	-1.768	49	972	244	618	189
Cinnamide	C9H9NO	-1.134	4	5.686	80	0.04	252	336	51	1.939	-0.101	287	623	83	619	190
Benzamide	C7H7NO	-0.782	58	6.168	117	0.03	259	434	88	1.518	-0.013	243	677	107	619	191
Decanoic acid	C10H20O2	-0.177	138	4.031	15	0.09	208	361	61	4.160	-0.942	397	758	151	620	192
Picric acid^{CSD}	C6H3N3O7	2.341	435	7.982	293	0.03	262	990	410	0.276	-2.275	69	1059	300	624	193

4-Aminobenzamide	C7H8N2O	-0.536	80	6.078	107	0.05	239	426	85	1.781	-0.260	278	704	123	624	194
Theophylline	C7H8N4O2	1.486	389	7.517	249	0.07	229	867	347	0.948	-0.072	147	1014	272	625	195
Sorbic acid	C6H8O2	0.027	174	5.269	55	-0.19	384	613	165	1.115	-0.925	187	800	160	626	196
1,3-Diiodobenzene^{CSD}	C6H4I2	0.727	264	5.209	51	-0.40	427	742	251	0.971	-0.050	156	898	202	634	197
1-Amino-1-methylcyclopropane	C4H9N	-0.089	156	8.235	316	0.08	214	686	207	0.727	-0.293	106	792	159	636	198
4-Benzoquinone	C6H4O2	2.639	442	6.037	104	-0.14	368	914	377	1.034	0.013	165	1079	315	637	199
2-Pyridone	C5H5NO	0.714	258	6.683	172	-0.03	289	719	225	1.091	0.071	176	895	200	637	200
1-Pentanol	C5H12O	0.382	211	5.362	58	0.04	248	517	124	2.532	-0.019	335	852	177	641	201
1,13-Tridecanediol	C13H28O2	-1.019	20	4.117	17	0.11	183	220	13	7.620	-0.033	442	662	100	642	202
Indomethacin	C19H16ClNO4	1.096	331	6.656	168	0.11	188	687	210	1.931	-1.640	286	973	245	642	203
Benzoin	C14H12O2	0.608	231	7.326	227	0.17	118	576	149	2.062	-0.489	297	873	188	642	204
Acetophenone	C8H8O	1.271	361	5.804	87	-0.18	381	829	319	1.094	0.073	177	1006	265	645	205
iso-Deoxycholic acid	C24H40O4	-0.218	133	6.370	137	0.15	140	410	81	3.127	-0.955	369	779	158	646	206
4,4,7-Trimethyldecahydro-1H-cyclopenta[cd]inden-7-ol	C14H24O	-0.625	70	7.680	267	0.11	192	529	130	1.132	0.111	190	719	135	649	207
1,1-Dihydroxypropan-2-one	C3H6O3	0.841	288	7.848	281	0.10	199	768	275	1.045	-0.996	169	937	219	649	208
Vanillin	C8H8O3	0.668	243	7.240	215	-0.03	297	755	265	0.937	-1.104	139	894	199	651	209
1,2-Dichloroethane	C2H4Cl2	0.690	250	5.254	54	-0.42	437	741	248	1.011	-0.010	161	902	203	652	210
(E)-4-(4-Hydroxy-3-methoxyphenyl)but-3-en-2-one	C11H12O3	0.770	275	6.232	122	0.04	246	643	178	1.873	-0.678	284	927	215	652	211
1-(Naphthalen-2-yl)Ethan-1-One	C12H10O	1.236	353	5.381	60	-0.30	408	821	314	1.114	0.093	186	1007	268	654	212
3β,12β-Dihydroxy-5β-cholan-24-oic acid	C24H40O4	-0.393	97	6.802	179	0.18	107	383	72	3.127	-0.955	368	751	148	654	213
2,2'-(cyclohexa-2,5-diene-1,4-diylidene)dimalononitrile	C12H4N4	2.505	439	5.109	48	-0.16	377	864	343	1.428	0.408	230	1094	325	655	214
Dichloromethane^{CSD}	CH2Cl2	0.593	226	6.154	115	-0.46	444	785	285	0.683	-0.337	98	883	190	657	215
Hippuric acid	C9H9NO3	-0.808	55	6.682	171	0.11	187	413	82	2.087	-0.975	301	714	131	659	216
L-Lysine	C6H14N2O2	-1.100	9	6.458	149	0.19	104	262	27	4.615	0.023	406	668	103	659	217
Terephthalaldehyde	C8H6O2	2.021	421	5.099	47	-0.10	355	823	316	1.608	0.078	259	1082	317	661	218
Phenylmethanethiol	C7H8S	-0.134	146	6.504	154	0.02	266	566	144	1.495	-0.036	241	807	164	661	219
Coumarin	C9H6O2	1.371	374	6.070	106	-0.19	383	863	342	1.066	0.046	173	1036	285	662	220
n-Hexadecanol	C16H34O	-0.303	110	3.264	2	0.08	219	331	49	8.401	0.237	443	774	157	664	221
D-Lysine	C6H14N2O2	-0.919	43	6.539	156	0.19	103	302	38	4.615	0.023	405	707	127	664	222
Tryphenylphosphine oxide	C18H15OP	1.719	409	8.465	335	0.21	79	823	317	1.547	-0.494	251	1074	310	665	223
1,3-Di(pyridin-4-yl)propane	C13H14N2	2.183	426	6.159	116	0.04	247	789	288	2.116	-0.435	305	1094	324	668	224
Benzalacetone	C10H10O	1.259	357	5.023	46	-0.15	371	774	279	1.586	0.056	254	1028	280	671	225

Nicotinamide	C6H6N2O	0.978	312	6.129	113	-0.03	296	721	228	1.626	0.096	265	986	251	674	226
Uracil	C4H4N2O2	0.877	296	7.766	275	0.06	236	807	299	1.031	0.010	164	971	241	675	227
1,4-Dimethylpiperazine	C6H14N2	1.910	416	6.715	174	-0.24	398	988	409	0.715	-0.306	104	1092	322	676	228
Tetraiodoethene	C2I4	0.747	269	6.300	127	-0.34	422	818	311	0.897	-0.123	128	946	224	677	229
Scyllo-inositol	C6H12O6	0.951	308	8.393	329	0.38	11	648	184	2.551	-1.020	337	985	249	677	230
Methanol	CH4O	0.002	171	9.201	386	0.12	176	733	245	0.810	-0.210	118	851	175	680	231
Piperine	C17H19NO3	1.458	385	5.483	66	0.00	282	733	246	2.528	-0.023	334	1067	305	682	232
α -L-Xylopyranose	C5H10O5	0.140	188	8.780	362	0.22	72	622	168	1.524	-1.027	248	870	183	682	233
2-Methoxynaphthalene	C11H10O	0.720	262	5.485	67	-0.38	425	754	262	1.144	0.123	193	947	225	685	234
Piperidine	C5H11N	0.735	267	7.801	276	0.02	267	810	302	0.939	-0.081	142	952	229	685	235
α -8'- β -Apocarotenal	C30H40O	0.929	302	4.583	30	0.05	244	576	148	5.519	0.417	415	991	255	689	236
Allitol	C6H14O6	0.718	259	7.102	206	0.22	61	526	129	5.678	-0.445	424	950	227	691	237
13-epi-Sclareol	C20H36O2	-0.987	28	7.576	254	0.21	74	356	59	2.957	-0.614	363	719	134	691	238
D-Glucono-1,5-lactone	C6H10O6	-0.846	50	8.693	356	0.25	42	448	93	2.053	-1.008	294	742	145	692	239
β -8'- β -Apocarotenal	C30H40O	0.946	307	4.469	27	0.04	255	589	155	5.519	0.417	416	1005	264	698	240
Theobromine	C7H8N4O2	2.079	423	7.263	220	-0.05	311	954	395	1.041	0.020	168	1122	346	699	241
2-Ethyl-3-hydroxy-4H-pyran-4-one	C7H8O3	0.641	241	7.554	253	0.06	233	727	237	1.245	-0.286	214	941	222	700	242
α -D-Tagatopyranose	C5H6O3	0.850	290	8.940	373	0.23	58	721	229	1.639	-1.933	269	990	254	700	243
1,11-Undecanediol	C11H24O2	-1.073	15	4.453	26	0.05	238	279	31	6.559	-0.074	437	716	132	701	244
Cholic acid	C24H40O5	-0.151	142	7.578	255	0.22	62	459	97	3.538	-1.053	385	844	173	702	245
S(+)-Camphor-10-sulfonic acid	C10H16O4S	1.176	349	8.873	367	0.02	269	985	407	0.250	-1.791	66	1051	294	702	246
α -L-Sorbopyranose	C6H12O6	0.746	268	9.048	376	0.23	59	703	220	1.639	-1.933	268	971	240	703	247
1,1,6,6-Tetraphenylhexa-2,4-diyne-1,6-diol	C30H22O2	-0.400	95	6.645	167	-0.07	321	583	152	1.380	-2.191	224	807	165	712	248
Chlorine	Cl2	1.001	315	5.462	64	-0.40	430	809	300	1.289	0.268	220	1029	281	714	249
Methyl acetate	C3H6O2	1.144	340	7.456	244	-0.05	310	894	362	1.020	0.000	162	1056	297	716	250
cis-anti-cis-Dicyclohexano-18-crown-6	C20H36O6	2.241	428	6.087	108	-0.31	412	948	389	1.152	0.131	197	1145	357	717	251
Benzophenone	C13H10O	1.128	337	5.464	65	-0.21	388	790	289	1.639	0.108	266	1056	296	719	252
3,4-(Methylenedioxy)benzaldehyde	C8H6O3	1.560	400	6.451	148	-0.28	404	952	393	1.035	0.014	167	1119	342	719	253
2-Methylpropan-2-ol	C4H10O	-0.438	89	9.371	394	0.12	182	665	194	0.940	-0.080	143	808	166	719	254
1,2,4,5-Tetrafluoro-3,6-di-iodobenzene^{CSP}	C6F4I2	0.682	248	4.817	39	-0.41	434	721	231	1.525	0.505	249	970	238	722	255
Imidazole	C3H4N2	0.259	199	7.750	271	0.00	281	751	259	1.050	0.030	170	921	210	722	256
Dihydrofuran-2,5-dione	C4H4O3	2.124	424	7.940	287	0.08	220	931	383	1.255	0.234	215	1146	359	722	257
2,3-Dimethylpyrazine	C6H8N2	2.044	422	7.530	251	-0.12	361	1034	424	0.771	-0.250	111	1145	358	723	258

1,4-Diazabicyclo[2.2.2]octane	C6H12N2	2.301	433	8.696	357	-0.05	306	1096	441	0.134	-0.886	60	1156	369	723	259
Isonicotinamide	C6H6N2O	1.034	319	6.342	131	-0.08	337	787	287	1.603	0.072	257	1044	290	725	260
Dimethylsulfide	C2H6S	0.638	240	5.896	95	-0.41	436	771	278	1.149	0.129	195	966	237	726	261
Melamine	C3H6N6	1.283	362	7.972	292	0.12	175	829	320	1.609	-0.432	260	1089	320	727	262
1-Hydroxypropan-2-one	C3H6O2	1.170	346	7.814	279	0.08	215	840	326	1.453	-0.078	234	1074	311	728	263
neo-Inositol	C6H12O6	1.418	380	8.894	371	0.37	13	764	271	2.551	-1.020	344	1108	330	728	264
Dimethylsulfoxide	C2H6OS	2.003	419	8.152	304	-0.08	335	1058	429	0.572	-0.448	90	1148	362	729	265
(1R,2S)-2-Methyl-4-oxocyclohexane-1-carboxylic acid	C8H12O3	1.092	329	8.340	326	0.13	155	810	301	1.581	0.050	253	1063	304	734	266
Toluene^{CSD}	C7H8	0.575	224	5.631	75		450	749	257	1.230	0.210	212	961	233	737	267
2,3,5,6-Tetrafluoro-7,7,8,8-tetracyanoquinodimethane	C12F4N4	2.505	440	4.922	42	-0.24	396	878	350	2.075	1.054	299	1177	379	737	268
Piperazine	C4H10N2	0.769	274	8.244	318	0.03	263	855	337	0.998	-0.022	160	1015	273	741	269
DL-Mannitol	C6H14O6	1.008	316	7.605	262	0.24	48	626	172	5.678	-0.445	431	1057	298	741	270
Galactitol	C6H14O6	0.963	311	7.066	199	0.17	120	630	173	5.678	-0.445	425	1055	295	744	271
Caffeine	C8H10N4O2	2.353	436	7.293	225	-0.13	365	1026	422	0.971	-0.050	155	1181	382	745	272
epi-Inositol	C6H12O6	1.067	324	9.388	395	0.38	12	731	242	2.551	-1.020	339	1070	309	746	273
Phthalide	C8H6O2	1.342	369	7.071	200	-0.12	363	932	384	1.109	0.089	184	1116	336	747	274
1-(4-Methoxyphenyl)ethan-1-one	C9H10O2	1.361	372	5.805	88	-0.27	402	862	341	1.604	0.073	258	1120	343	748	275
2,3-Butanedione	C4H6O2	1.992	417	6.855	181	-0.17	378	976	405	1.120	0.100	189	1165	375	748	276
Nootkatone	C15H22O	1.397	375	6.888	183	-0.31	413	971	403	0.969	-0.051	153	1124	347	749	277
DL-Ribose	C5H10O5	0.046	176	8.779	360	0.29	25	561	141	3.083	-1.509	366	927	214	751	278
Propionamide	C3H7NO	-1.126	8	7.482	247	0.05	242	497	116	1.625	0.095	264	761	152	753	279
Chloroform	CHCl3	0.604	229	7.275	222	-0.48	449	900	370	0.481	-0.539	85	985	250	756	280
α -D-Galactose	C6H12O6	0.312	205	8.877	368	0.22	71	644	179	2.232	-1.340	318	962	234	757	281
3-Isochromanone	C9H8O2	1.329	367	7.250	217	-0.11	356	940	386	1.111	0.091	185	1125	348	758	282
Cyclohexanone	C4H8	1.525	394	7.641	266	-0.09	345	1005	414	0.958	-0.062	149	1154	366	760	283
Xylitol	C5H12O5	0.246	198	8.150	303	0.23	57	558	139	4.590	-0.512	402	960	232	762	284
Cyclohexane-1,2,3,4,5,6-hexol	C6H12O6	1.289	363	9.723	404	0.35	15	782	283	2.551	-1.020	346	1128	349	765	285
L-Arginine	C6H14N4O2	1.693	408	7.091	203	0.14	150	761	268	5.192	0.090	413	1174	377	766	286
Lidocaine	C18H32O2	0.117	183	6.530	155	0.07	224	562	142	3.640	0.068	388	950	228	767	287
L-chiro-Inositol	C6H12O6	0.682	247	10.289	418	0.41	9	674	200	2.551	-1.020	340	1014	271	767	288
1,4-Dimethoxybenzene	C8H10O2	0.870	294	5.293	56	-0.41	435	785	286	1.704	0.173	277	1062	303	768	289
D-(+)-chiro-Inositol	C6H12O6	1.526	395	10.312	419	0.43	6	820	313	2.551	-1.020	343	1163	373	768	290
4-Methoxybenzaldehyde	C8H8O2	1.449	382	5.962	97	-0.31	411	890	360	1.625	0.094	263	1153	365	771	291

β -D-Glucose	C6H12O6	0.124	185	9.069	378	0.22	73	636	175	2.232	-1.340	321	957	231	772	292
Ethyl Propionate	C5H10O2	0.995	314	5.665	78	-0.27	400	792	294	2.061	0.020	296	1088	319	774	293
cis-Inositol	C6H12O6	0.699	252	10.455	424	0.42	8	684	206	2.551	-1.020	342	1026	279	774	294
(1S,6R,10R)-(+)-6-Methyl-4-oxabicyclo[8.4.1]pentadecan-3-one	C15H26O2	1.115	334	6.379	139	-0.32	414	887	356	1.373	0.353	223	1110	332	776	295
1,2-Dimethyldisulfane	C2H6S2	0.731	265	6.411	142	-0.46	445	852	334	1.137	0.117	191	1043	289	778	296
Pyroglutamic acid	C5H7NO3	0.579	225	7.802	277	-0.12	364	866	346	0.937	-0.593	140	1006	266	781	297
Methyl benzoate	C8H8O2	1.081	328	6.008	102	-0.32	418	848	330	1.617	0.087	261	1109	331	781	298
Ribitol	C5H12O5	0.501	220	8.447	334	0.25	46	600	161	4.590	-0.512	401	1001	259	781	299
D-Glucuronic acid	C6H10O7	0.147	189	8.417	333	0.19	99	621	166	2.674	-2.939	351	972	243	783	300
Chloro(methoxy)methane	C2H5ClO	1.173	348	7.578	256	-0.10	349	953	394	1.095	0.074	179	1132	353	784	301
(5-Hydroxy-6-methylpyridine-3,4-diy)dimethanol	C8H11NO3	-0.194	136	7.753	273	0.01	278	687	208	1.467	-1.594	235	922	212	786	302
β -DL-Arabinose	C5H10O5	-0.091	154	9.818	408	0.17	126	688	212	1.569	-1.492	252	940	221	786	303
Succinamide	C4H8N2O2	-0.517	83	6.564	160	0.02	270	513	123	2.813	-0.248	358	871	186	788	304
3S-cis-3,6-Dimethyl-1,4-dioxane-2,5-dione	C6H8O4	1.994	418	7.948	288	-0.06	313	1019	420	1.118	0.098	188	1207	392	789	305
<i>ϵ-Caprolactam</i>^{CSD}	C6H11NO	0.606	230	8.474	336	-0.07	328	894	363	0.870	-0.150	126	1020	276	790	306
α -D-Glucose	C6H12O6	0.224	195	8.607	349	0.17	124	668	195	2.232	-1.340	320	988	252	793	307
Butyramide	C4H9NO	-1.093	12	7.100	205	0.00	280	497	117	2.140	0.100	310	807	163	795	308
α -D-Talose	C6H12O6	-0.415	93	9.481	399	0.21	82	574	146	2.232	-1.340	314	888	193	795	309
2,5-Piperazinedione	C4H6N2O2	0.769	273	7.280	223	-0.15	370	866	345	1.173	0.153	203	1069	307	796	310
4-Hydroxy-3,5-dimethoxybenzaldehyde	C9H10O4	0.764	272	7.595	260	0.01	275	807	298	1.621	-0.930	262	1069	306	797	311
DL-Arabinitol	C5H12O5	0.293	201	8.576	345	0.23	53	599	158	4.590	-0.512	400	999	257	798	312
Ethylene glycol	C2H6O2	-0.726	63	9.505	400	0.13	161	624	170	1.480	-0.560	237	861	178	798	313
1,2-Dicyclopropylethane-1,2-dione	C8H10O2	1.469	387	6.049	105	-0.20	386	878	352	2.200	0.159	311	1189	387	802	314
Ethyl(methyl)sulfane	C3H8S	0.633	238	6.637	166	-0.40	431	835	323	1.185	0.164	205	1040	288	802	315
D-Glucitol	C6H14O6	0.959	310	8.481	340	0.26	37	687	209	5.678	-0.445	426	1113	333	803	316
2,2-Dibromo-2-cyanoacetamide	C3H2Br2N2O	0.839	287	9.573	401	0.01	273	961	400	0.900	-0.631	129	1090	321	803	317
D-Iditol	C6H14O6	0.851	291	8.348	327	0.23	52	670	197	5.678	-0.445	427	1097	326	806	318
Cycloundecanone	C11H20O	1.042	320	7.423	235	-0.22	393	948	390	1.100	0.079	180	1128	350	808	319
β -D-Galactose	C6H12O6	0.193	194	8.853	365	0.17	125	684	205	2.232	-1.340	319	1003	262	809	320
Adamantane-1,3,5,7-tetracarboxylic acid	C14H16O8	-0.542	79	10.436	423	0.10	197	699	219	1.138	-2.944	192	891	197	812	321
Methyl cubane-1-carboxylate	C10H10O2	1.027	318	7.179	211	-0.33	420	949	391	1.100	0.080	182	1131	352	813	322
1,2-bis(Methylthio)ethane	C4H10S2	0.676	246	5.435	61	-0.44	440	747	255	2.222	0.181	313	1060	301	814	323

Glycerol	C3H8O3	-1.059	19	8.401	330	0.15	139	488	110	2.584	-0.478	347	835	170	816	324
Phenyl acetate	C8H8O2	1.177	350	6.283	125	-0.34	421	896	364	1.640	0.110	271	1167	376	817	325
L-Aspartic acid	C4H7NO4	-1.076	14	7.631	263	-0.06	317	594	156	1.490	-2.081	238	832	169	818	326
4-Methylmorpholine	C5H11NO	1.668	405	8.164	307	-0.21	389	1101	442	0.855	-0.165	122	1223	394	818	327
D-Altritol	C6H14O6	0.880	298	7.875	282	0.18	108	688	213	5.678	-0.445	429	1117	338	819	328
Cyclodecanone	C10H18O	1.144	341	7.428	239	-0.17	379	959	397	1.164	0.143	202	1161	371	820	329
L-Carvone	C10H14O	1.300	365	6.988	192	-0.33	419	976	406	1.230	0.209	211	1187	385	822	330
Biotin	C10H16N2O3S	-0.827	53	7.591	259	0.11	184	496	115	3.259	-0.312	380	876	189	823	331
1,3-Distearoyl-2-oleoylglycerol	C57H108O6	0.808	278	4.324	22	-0.12	360	660	189	29.490	0.919	447	1107	328	829	332
1,1'-Azo-bis(carbamide)	C2H4N4O2	-0.968	33	6.942	190	0.03	256	479	108	3.446	-0.126	384	863	179	830	333
Trimethylamine oxide	C3H9NO	1.777	414	10.536	426	-0.11	359	1199	448	-0.473	-1.493	45	1244	404	830	334
β -D-Altropyranose	C6H12O6	0.332	208	10.329	420	0.20	94	722	232	2.232	-1.340	317	1039	286	831	335
Acetamide	C2H5NO	-0.527	81	8.591	347	-0.03	291	719	224	1.145	0.125	194	913	207	832	336
bis(Methylthio)methane	C3H8S2	0.686	249	6.345	132	-0.40	429	810	303	1.647	0.116	272	1082	316	833	337
Dimethyl succinate	C6H10O4	1.420	381	5.487	68	-0.24	397	846	329	3.159	0.098	371	1217	393	836	338
2-(Oleoyloxy)propane-1,3-diyl distearate	C57H108O6	0.816	280	4.097	16	-0.15	373	669	196	29.490	0.919	448	1117	337	837	339
Vitamin A acetate	C22H32O2	0.861	292	5.377	59	-0.17	380	731	244	4.441	0.360	398	1129	351	837	340
1,3-Distearoyl-2-elaidoylglycerol	C57H108O6	0.820	283	3.981	14	-0.16	375	672	198	29.492	0.921	449	1121	344	838	341
Tromethamine	C4H11NO3	-0.883	46	9.340	392	0.23	56	494	114	3.921	-0.161	390	884	191	838	342
Cyclohexane-1,2,3,4,5,6-hexaol	C6H12O6	1.132	338	9.808	407	0.19	96	841	327	2.551	-1.020	338	1179	380	841	343
L-Proline	C5H9NO2	0.296	203	8.042	296	-0.06	318	817	310	1.411	-0.119	228	1045	291	842	344
1,2-Distearoyl-3-elaidoylglycerol	C57H108O6	0.847	289	3.769	10	-0.22	390	689	214	29.408	0.837	446	1135	354	846	345
Tetracyanoethylene	C6N4	2.818	444	7.093	204	-0.14	369	1017	418	1.664	0.644	273	1290	417	846	346
2-Aminoethan-1-ol	C2H7NO	-0.282	118	7.887	284	0.04	253	655	185	2.136	0.095	309	964	236	846	347
Oxetane	C3H6O	1.075	327	8.562	343	-0.27	401	1071	435	0.701	-0.319	103	1174	378	847	348
Formamide	CH3NO	-0.357	100	8.480	339	-0.04	301	740	247	1.190	0.170	209	949	226	849	349
Hexamethylenetetramine	C6H12N4	3.427	448	9.756	405	-0.13	366	1219	449	0.479	-0.541	83	1302	420	854	350
Tramadol	C16H25NO2	-0.120	149	11.521	445	0.28	30	624	169	3.240	0.179	379	1003	261	854	351
β -L-Lyxopyranose	C5H10O5	-0.019	166	8.964	374	0.06	237	777	282	1.524	-1.027	247	1024	278	858	352
Dibenzoyl peroxide	C14H10O4	1.563	402	5.736	82	-0.28	405	889	357	3.176	0.115	372	1261	410	859	353
1,2-Diphenyldisulfane	C12H10S2	0.712	257	5.996	101	-0.47	448	806	297	2.210	0.169	312	1118	341	861	354
5,5-Diethylbarbituric acid	C8H12N2O3	1.413	378	10.038	413	-0.03	290	1081	438	0.996	-0.534	159	1240	402	862	355
1,2-Dibenzylsulfane	C14H14S2	0.704	254	4.991	45	-0.45	443	742	250	3.199	0.138	376	1118	339	864	356

Urea	CH4N2O	-0.137	145	8.615	350	0.01	279	774	280	1.477	-0.054	236	1010	269	865	357
β-Tristearin	C57H110O6	0.815	279	3.699	9	-0.30	409	697	216	30.039	0.958	450	1147	360	868	358
β-D-Allose	C6H12O6	0.400	215	8.502	341	0.09	212	768	274	2.232	-1.340	316	1084	318	869	359
Morpholine	C4H9NO	1.110	333	8.985	375	-0.11	358	1066	433	0.929	-0.091	136	1202	390	869	360
l-Iditol	C6H14O6	0.984	313	9.055	377	0.22	64	754	260	5.678	-0.445	428	1182	383	869	361
Acetylmethionine	C7H13NO3S	0.189	192	8.165	309	0.12	178	679	203	3.347	-0.735	383	1062	302	870	362
Dichlorodifluoromethane	CCl2F2	0.819	282	7.114	207	-0.36	424	913	375	1.498	0.478	242	1155	368	873	363
Formaldehyde	CH2O	1.566	403	8.833	363	-0.07	329	1095	439	1.100	0.080	181	1276	413	873	364
Carbamazepine	C15H12N2O	-0.250	128	7.584	258	-0.15	372	758	266	1.520	-0.010	244	1002	260	874	365
(4R,7S)-7-Isopropyl-4-methylxepan-2-one	C10H18O2	1.268	360	7.635	264	-0.32	415	1039	425	1.150	0.129	196	1235	399	875	366
Proline	C5H9NO2	0.233	197	8.146	302	-0.10	350	849	333	1.411	-0.119	227	1076	313	879	367
L-Ribose	C5H10O5	0.056	178	8.779	361	0.14	151	690	215	3.083	-1.509	367	1057	299	879	368
2-Methoxy-4-(1-(E)-propenyl)phenyl acetate	C12H14O3	1.208	351	6.107	111	-0.32	416	878	353	2.716	0.165	353	1231	397	880	369
n-Butyl acetate	C6H12O2	1.070	325	6.437	146	-0.20	387	858	338	2.591	0.040	348	1206	391	881	370
β-D-Fructopyranose	C6H12O6	0.465	219	10.242	417	0.10	204	840	325	1.639	-1.933	267	1107	329	888	371
1-Chloro-1,1,2,2,2-pentafluoroethane	C2ClF5	0.670	244	6.901	187	-0.40	428	859	339	1.832	0.812	281	1140	355	896	372
1,4-Dithiane	C4H8S2	0.699	253	7.531	252	-0.43	438	943	387	1.190	0.169	208	1151	364	898	373
Diphenyl ether	C12H10O	0.704	255	6.819	180	-0.46	446	881	355	1.675	0.145	274	1155	367	900	374
3α,4,7,7-Tetramethyl-(3αR,4S,6αR,10αS)-perhydronaphtho(8α,1-β)furan-2-one	C16H26O2	1.252	356	8.247	319	-0.22	391	1066	432	1.160	0.139	198	1264	411	908	375
α-Lactose	C12H22O11	1.398	376	8.590	346	0.15	145	867	348	5.660	-0.973	419	1286	414	910	376
1,3-Diphenylpropan-2-one	C15H14O	1.095	330	6.471	150	-0.31	410	890	359	2.679	0.128	352	1242	403	912	377
1,2-Dimethoxybenzene	C8H10O2	0.832	285	7.246	216	-0.39	426	927	381	1.639	0.109	270	1197	389	912	378
(-)-1,3,3-Trimethyl-2-norbornanone	C10H16O	1.162	344	8.273	321	-0.20	385	1050	428	1.185	0.165	206	1256	406	912	379
Tricyclopropylamine	C9H15N	0.623	234	7.300	226	-0.22	394	854	336	2.060	0.019	295	1149	363	915	380
D-Arabinitol	C5H12O5	0.313	206	8.576	344	0.12	173	723	233	4.590	-0.512	399	1122	345	916	381
Sucralose	C12H19Cl3O8	-0.224	131	8.879	369	0.13	158	658	187	4.008	-1.604	392	1050	293	919	382
2-Hydroxyacetamide	C2H5NO2	-0.763	60	8.644	353	0.03	261	674	199	2.129	0.088	306	980	247	920	383
Eucalyptol	C10H18O	0.936	306	8.203	310	-0.40	433	1049	427	1.094	0.074	178	1227	395	921	384
α,α-Galacto-trehalose	C12H22O11	1.463	386	9.447	398	0.18	114	898	369	5.154	-1.478	410	1308	423	922	385
L-Cystine	C6H12N2O4S2	-0.793	57	6.988	193	-0.07	330	580	150	4.591	-1.531	403	983	248	926	386
DL-Arginine	C6H14N4O2	1.693	407	7.091	202	-0.06	314	923	379	5.192	0.090	412	1335	430	928	387

Sucrose	C12H22O11	0.544	223	9.402	396	0.19	105	724	235	6.173	-0.969	435	1159	370	936	388
myo-Inositol	C6H12O6	0.914	300	9.272	387	0.09	210	897	367	2.551	-1.020	341	1238	400	938	389
β-D-Gulose	C6H12O6	0.097	180	9.658	402	0.08	221	803	295	2.232	-1.340	315	1118	340	938	390
(S)-2-Hydroxypropanamide	C3H7NO2	-0.969	31	9.312	389	0.05	243	663	192	2.130	0.089	308	971	239	940	391
o-β-D-Mannopyranosyl-(1-4)-α-D-mannopyranose	C12H22O11	0.330	207	8.411	332	0.11	191	730	239	5.660	-0.973	418	1148	361	941	392
1,3,5-Trinitrobenzene	C6H3N3O6	2.279	432	7.443	242	-0.28	403	1077	437	2.069	0.028	298	1375	440	943	393
(3αR,4R,6αS,10αS)-3α,4,7,7-Tetramethylperhydronaphtho(8α,1-β)furan-2-one	C16H26O2	1.220	352	8.882	370	-0.16	374	1096	440	1.160	0.139	199	1295	418	943	394
β-D-Psicose	C6H12O6	-0.148	144	9.360	393	0.09	207	744	254	2.627	-1.454	349	1093	323	949	395
Nitromethane	CH3NO2	1.515	393	10.093	415	-0.08	342	1150	447	1.163	0.143	201	1351	437	958	396
D-Mannitol	C6H14O6	0.891	299	8.652	355	0.12	174	828	318	5.678	-0.445	430	1258	408	959	397
(R)-2-Hydroxypropanamide	C3H7NO2	-0.974	30	9.312	388	0.03	264	682	204	2.130	0.089	307	989	253	959	398
Muco-inositol	C6H12O6	1.367	373	10.461	425	0.10	194	992	411	2.551	-1.020	345	1337	431	964	399
4-Allyl-2-methoxyphenyl benzoate	C17H16O3	1.117	335	6.602	162	-0.32	417	914	376	3.750	0.178	389	1303	421	968	400
β-Maltose	C12H22O11	1.858	415	8.751	358	0.11	193	966	401	5.660	-0.973	421	1387	441	972	401
Ethylene oxide	C2H4O	1.043	321	9.084	379	-0.40	432	1132	444	1.030	0.010	163	1295	419	974	402
DL-Aspartic acid	C4H7NO4	-0.241	130	9.899	411	-0.07	325	866	344	1.490	-2.081	239	1105	327	975	403
n-Methyl-D-glucamine	C7H17NO5	0.398	214	8.620	351	0.11	190	755	263	5.812	-0.310	434	1189	386	975	404
L-Cysteine	C3H7NO2S	-0.425	91	11.731	446	0.06	234	771	277	2.091	-0.970	304	1075	312	984	405
(3αR,4S,6αS,10αS)-3α,4,7,7-Tetramethylperhydronaphtho(8α,1-β)furan-2-one	C16H26O2	1.244	355	9.339	391	-0.23	395	1141	445	1.160	0.139	200	1341	436	986	406
β-Cellobiose	C12H22O11	1.102	332	7.892	286	-0.01	285	903	371	5.660	-0.973	417	1320	426	988	407
Caryophyllen-α-oxide	C15H24O	0.875	295	8.372	328	-0.47	447	1070	434	1.265	0.244	216	1286	416	991	408
D-Threonine	C4H9NO3	-1.079	13	10.997	435	-0.07	327	775	281	1.452	-1.610	232	1007	267	994	409
α,α-Trehalose	C12H22O11	1.746	412	10.610	428	0.13	170	1010	417	5.154	-1.478	409	1419	445	1007	410
DL-Tyrosine	C9H11NO3	-1.018	21	8.408	331	-0.10	352	704	221	2.378	-1.193	327	1031	282	1010	411
2,2',2''-Nitrilotriethanol	C6H15NO3	-0.777	59	8.651	354	0.04	249	662	191	4.985	-0.117	408	1070	308	1011	412
Diallylsulfide	C6H10S	0.624	236	7.251	218	-0.44	442	896	365	2.763	0.212	354	1250	405	1014	413
β-Lactose	C12H22O11	1.073	326	9.109	382	0.09	213	921	378	5.660	-0.973	420	1341	434	1015	414
L-Threonine	C4H9NO3	-1.013	23	11.032	437	-0.10	353	813	307	1.452	-1.610	233	1046	292	1023	415
Glycine	C2H5NO2	0.914	301	10.689	430	-0.04	302	1033	423	2.050	0.010	293	1326	427	1025	416
D-Alanine	C3H7NO2	0.634	239	11.863	449	-0.04	300	988	408	1.945	-0.096	288	1276	412	1037	417
DL-Valine	C5H11NO2	-0.362	99	11.017	436	-0.02	286	821	315	2.269	-0.282	322	1143	356	1044	418

L-Tryptophan	C11H12N2O2	-0.698	67	9.406	397	-0.06	319	783	284	2.421	-0.640	332	1115	335	1048	419
Tetrabromomethane	CBr4	0.935	305	8.476	338	-0.35	423	1066	431	1.950	0.930	290	1356	438	1051	420
4-Hydroxy-L-proline	C5H9NO3	0.839	286	10.560	427	-0.10	348	1061	430	1.701	-0.340	276	1337	432	1051	421
L-Tyrosine	C9H11NO3	-1.010	24	8.756	359	-0.13	367	750	258	2.378	-1.193	328	1078	314	1054	422
DL-Cysteine	C3H7NO2S	-0.015	168	10.406	422	-0.09	346	936	385	2.091	-0.970	302	1238	401	1070	423
L-Alanine	C3H7NO2	0.612	232	11.851	448	-0.08	338	1018	419	1.945	-0.096	289	1307	422	1075	424
β-galactose	C12H22O11	1.157	343	8.860	366	-0.02	287	996	412	5.665	-2.498	423	1419	444	1076	425
(Z)-Ethyl 2-benzylidene-3-oxobutanoate	C13H14O3	1.540	397	8.095	300	-0.29	406	1103	443	3.185	0.123	373	1476	449	1079	426
α-Maltose	C12H22O11	0.954	309	9.964	412	0.05	245	966	402	5.660	-0.973	422	1388	442	1079	427
Diallyldisulfide	C6H10S2	0.719	261	7.705	269	-0.44	441	971	404	3.146	0.084	370	1341	435	1080	428
DL-Tryptophan	C11H12N2O2	-0.569	77	9.696	403	-0.10	351	831	322	2.421	-0.640	331	1162	372	1085	429
DL-Methionine	C5H11NO2S	0.675	245	9.338	390	-0.06	315	950	392	3.291	-0.281	381	1331	429	1086	430
DL-Isoleucine	C6H13NO2	0.020	173	10.719	431	-0.03	293	897	368	2.887	-0.175	362	1259	409	1086	431
L-Cysteine	C3H7NO2S	-0.425	92	11.731	447	-0.08	339	878	351	2.091	-0.970	303	1181	381	1089	432
L-Leucine	C6H13NO2	0.598	227	11.040	439	-0.03	295	961	399	2.794	-0.267	357	1318	425	1091	433
DL-Leucine	C6H13NO2	0.535	221	11.275	444	-0.03	294	959	398	2.794	-0.267	355	1314	424	1093	434
L-Methionine	C5H11NO2S	0.619	233	10.348	421	-0.04	303	957	396	3.291	-0.281	382	1339	433	1106	435
DL-Glutamine	C5H10N2O3	-1.129	6	9.799	406	-0.05	308	720	227	4.029	-0.052	393	1113	334	1107	436
L-Valine	C5H11NO2	0.426	217	10.853	433	-0.10	354	1004	413	2.269	-0.282	323	1327	428	1110	437
4-Aminobutanoic acid	C4H9NO2	0.879	297	11.266	443	-0.05	309	1049	426	2.880	-0.182	360	1409	443	1112	438
D-Isoleucine	C6H13NO2	-0.268	122	10.215	416	-0.08	336	874	349	2.887	-0.175	361	1235	398	1113	439
4-tert-Butyl-3-methoxy-2,6-dinitrotoluene	C12H16N2O5	1.265	359	9.115	383	-0.29	407	1149	446	2.285	0.244	324	1473	448	1114	440
D-Asparagine	C4H8N2O3	-0.858	48	9.825	409	-0.08	334	791	291	3.189	-0.383	374	1165	374	1117	441
DL-Glutamic acid	C5H9NO4	-0.031	164	11.033	438	-0.05	307	909	374	3.235	-0.846	377	1286	415	1122	442
Neotame	C20H30N2O5	1.062	323	9.103	381	-0.04	304	1008	415	6.689	-0.454	438	1446	447	1123	443
L-Asparagine	C4H8N2O3	-0.672	69	10.755	432	-0.06	316	817	309	3.189	-0.383	375	1192	388	1123	444
β-Alanine	C3H7NO2	0.869	293	11.217	441	-0.08	343	1077	436	2.642	0.091	350	1427	446	1134	445
DL-Serine	C3H7NO3	-0.269	121	12.315	450	-0.11	357	928	382	2.386	-0.675	329	1257	407	1136	446
L-α-Leucine	C6H13NO2	0.598	228	11.040	440	-0.08	341	1009	416	2.794	-0.267	356	1365	439	1137	447
Glutamic acid	C5H9NO4	-0.504	85	11.224	442	-0.07	326	853	335	3.235	-0.846	378	1231	396	1146	448
L-Glutamine	C5H10N2O3	-1.014	22	10.680	429	-0.08	340	791	293	4.029	-0.052	394	1185	384	1163	449
Sucrose octa-acetate	C28H38O19	2.384	437	9.890	410	-0.16	376	1223	450	11.476	0.251	445	1668	450	1231	450

Table S8 – Distribution of some frequent chemical groups in the database of 450 structures used in the theoretical screening and in the 76 molecules tested to form multicomponent with NVP.

Chemical Groups	<chem>NC(=O)O</chem>		<chem>NC(=O)C</chem>		<chem>NC(=O)N</chem>		<chem>N</chem>		<chem>OC(=O)C</chem>		<chem>O</chem>		<chem>c1ccccc1</chem>		<chem>c1ccncc1</chem>	
	N ^o mol.	%	N ^o mol.	%	N ^o mol.	%	N ^o mol.	%	N ^o mol.	%	N ^o mol.	%	N ^o mol.	%	N ^o mol.	%
Total sample of 450 co-formers	34	7.6	17	3.8	13	2.9	25	5.6	97	21.6	161	35.8	126	28	18	4
76 co-formers experimentally tested	7	9.2	8	10.5	6	7.9	0	0	32	42.1	26	34.2	27	35.5	2	2.6

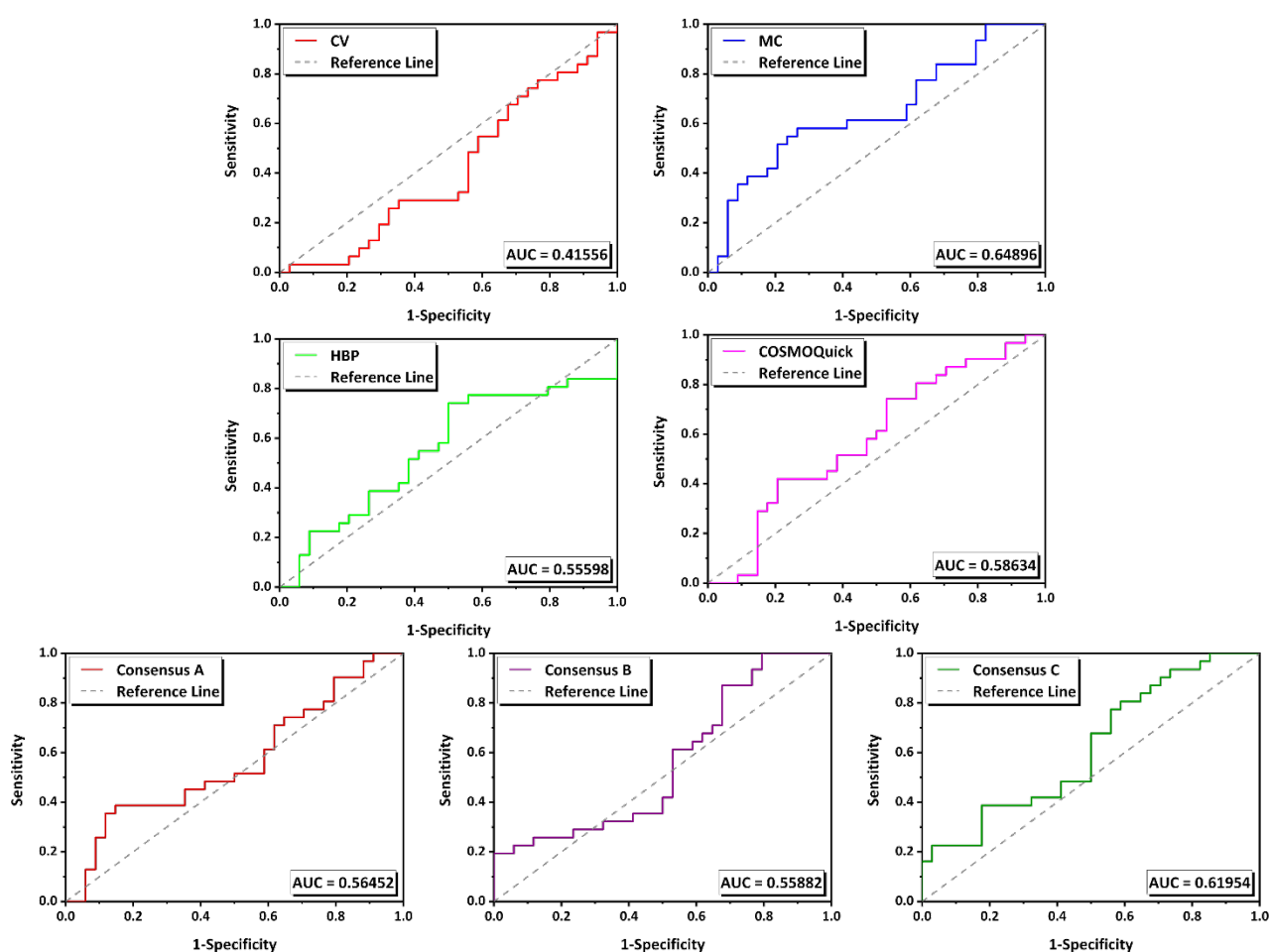


Figure S1 –ROC curves and AUC values obtained for each method: CV, MC, HBP, COSMOQuick, and the three consensus A, B and C.