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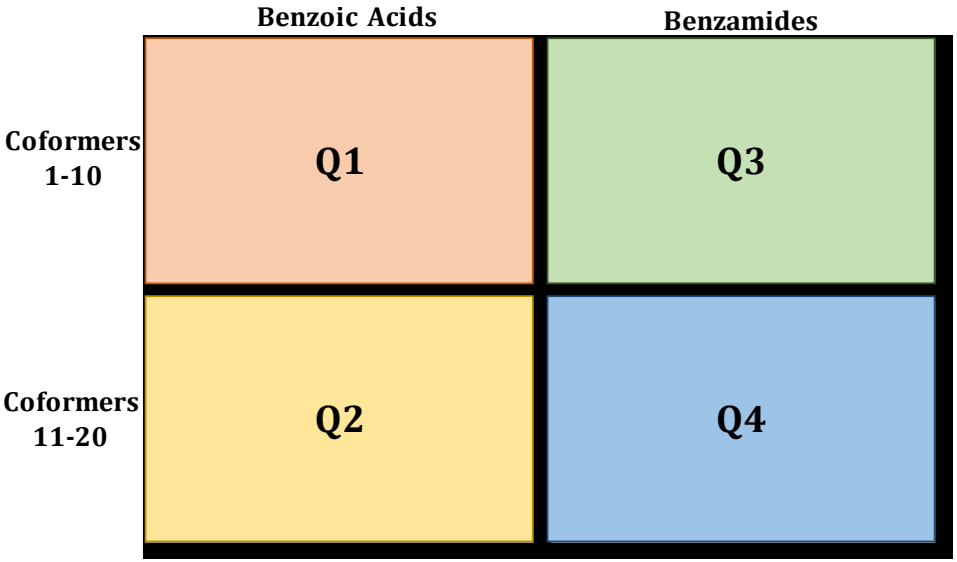
Supplementary Information for Will They Co-crystallize?

J. G. P. Wicker, L. M. Crowley, O. Robshaw, E. J. Little, S. P. Stokes, R. I. Cooper, S. E. Lawrence



Complete Data Matrix Acids and Amides

	2-Nitrobenzoic Acid	3-Nitrobenzoic Acid	4-Nitrobenzoic Acid	2-Hydroxybenzoic Acid	3-Hydroxybenzoic Acid	4-Hydroxybenzoic Acid	2-Fluorobenzoic Acid	3-Fluorobenzoic Acid	4-Fluorobenzoic Acid	2-Aminobenzoic Acid	3-Aminobenzoic Acid	4-Aminobenzoic Acid	2-Methoxybenzoic Acid	3-Methoxybenzoic Acid	4-Methoxybenzoic Acid	2-Methylbenzoic Acid	3-Methylbenzoic Acid	4-Methylbenzoic Acid	2-Nitrobenzamide	3-Nitrobenzamide	4-Nitrobenzamide	2-Hydroxybenzamide	4-Hydroxybenzamide	3-Fluorobenzamide	4-Fluorobenzamide	2-Aminobenzamide	3-Aminobenzamide	4-Aminobenzamide	2-Methoxybenzamide	3-Methoxybenzamide	4-Methoxybenzamide	2-Methylbenzamide	3-Methylbenzamide	4-Methylbenzamide
Nicotinamide	1	0	1	1	1	1	1	0	1	1	0	1	0	1	1	1	1	1	0	1	1	1	1	0	0	0	0	1	0	0	0	0	0	0
Isonicotinamide	1	1	1	1	1	1	1	1	1	1	1	1	0	1	0	1	1	1	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2
4,4'-Bipyridine	1	1	1	1	1	1	1	0	0	1	1	1	1	1	1	0	1	1	1	1	1	1	1	1	1	1	1	1	1	0	1	0	1	0
Fumaric Acid	0	0	0	0	1	0	0	0	0	0	1	0	0	0	0	0	1	0	0	1	0	1	1	1	1	1	1	1	1	1	1	0	1	1
Salicylic Acid	0	0	0	2	0	0	0	0	0	1	0	0	0	0	0	1	0	0	0	1	1	1	1	0	1	1	1	0	1	0	1	0	1	1
Urea	1	1	1	1	1	1	1	0	0	0	0	1	0	0	0	1	0	0	0	1	0	0	0	0	0	1	1	0	0	0	0	0	0	0
Benzamide	1	1	1	1	0	0	1	1	1	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	1	0	1
Oxalic Acid	0	0	0	0	1	0	0	0	0	1	1	1	0	0	0	1	0	0	1	0	1	1	1	1	1	1	1	1	1	1	1	1	1	1
Hydroquinone	0	0	0	0	1	0	0	0	0	0	0	0	1	0	1	1	0	1	0	1	0	0	1	1	0	0	1	0	1	0	1	0	1	1
2-Pyrrolidinone	1	1	1	1	1	1	0	1	1	1	1	1	2	2	2	0	0	1	2	1	1	1	1	1	2	1	2	1	1	1	1	1	1	1
Caffeine	1	1	0	1	1	1	1	1	0	1	0	0	1	1	0	1	1	0	0	1	1	1	1	0	1	0	0	0	0	1	0	0	0	0
Caprylic Acid	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	1
L-Glutamic Acid	0	1	1	0	1	0	1	0	1	0	0	0	1	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
Nicotinic Acid	1	0	0	0	2	0	1	0	0	1	0	1	0	0	0	1	0	0	0	1	0	0	1	0	0	0	0	0	0	0	1	0	0	0
Pyridoxine	0	0	1	0	0	1	1	1	0	0	0	1	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
3,3'-Thiodipropionic Acid	0	0	0	0	1	0	1	0	0	0	0	0	0	0	0	1	0	0	0	0	1	0	0	0	0	1	1	0	0	1	1	0	1	1
Malic Acid	0	0	0	0	1	0	0	0	0	0	0	1	0	0	0	1	0	0	0	1	1	0	1	1	1	1	0	1	0	1	1	0	1	1
Trans-Aconitic Acid	0	1	0	0	1	0	0	0	0	0	0	1	0	0	0	1	0	0	0	0	0	1	1	0	1	0	1	0	1	0	1	1	1	1
L-Ascorbic Acid	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	1	0	0	0	0	0	1	0	0	0	1	0	0	0	0
Riboflavin	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Acids Matrix (Quadrant 1 orange, Quadrant 2 yellow)

	2-Nitrobenzoic Acid	3-Nitrobenzoic Acid	4-Nitrobenzoic Acid	2-Hydroxybenzoic Acid	3-Hydroxybenzoic Acid	4-Hydroxybenzoic Acid	2-Fluorobenzoic Acid	3-Fluorobenzoic Acid	4-Fluorobenzoic Acid	2-Aminobenzoic Acid	3-Aminobenzoic Acid	4-Aminobenzoic Acid	2-Methoxybenzoic Acid	3-Methoxybenzoic Acid	4-Methoxybenzoic Acid	2-Methylbenzoic Acid	3-Methylbenzoic Acid	4-Methylbenzoic Acid
Nictotinamide	1	0	1	1	1	1	1	0	1	1	0	1	0	1	0	1	1	1
Isonicotinamide	1	1	1	1	1	1	1	1	1	1	1	1	0	1	0	1	1	1
4,4'-Bipyridine	1	1	1	1	1	1	1	0	0	1	1	1	1	1	1	0	1	1
Fumaric Acid	0	0	0	0	1	0	0	0	0	0	1	0	0	0	0	1	0	0
Sailcylic Acid	0	0	0	2	0	0	0	0	0	1	0	0	0	0	0	1	0	0
Urea	1	1	1	1	1	1	1	0	0	0	0	1	0	0	0	1	0	0
Benzamide	1	1	1	1	0	0	1	1	1	0	0	0	0	0	0	0	0	0
Oxalic Acid	0	0	0	0	1	0	0	0	0	1	1	1	0	0	0	1	0	0
Hydroquinone	0	0	0	0	1	0	0	0	0	0	0	0	1	0	1	1	0	1
2-Pyrrolidinone	1	1	1	1	1	1	0	0	1	1	0	1	2	2	0	0	0	1
Caffeine	1	1	0	1	1	1	1	1	0	1	0	0	1	1	0	1	1	0
Capryllic Acid	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
L-Glutamic Acid	0	1	1	0	1	0	1	0	1	0	0	0	1	0	0	1	0	0
Nicotinic Acid	1	0	0	0	2	0	1	0	0	1	0	1	0	0	0	1	0	0
Pyridoxine	0	0	1	0	0	1	1	1	0	0	0	1	0	0	0	1	0	0
3,3'-Thiodipropionic Acid	0	0	0	0	1	0	1	0	0	0	0	0	0	0	0	1	0	0
Malic Acid	0	0	0	0	1	0	0	0	0	0	0	1	0	0	0	1	0	0
Trans-Aconitic Acid	0	1	0	0	1	0	0	0	0	0	0	1	0	0	0	1	0	0
L-Ascorbic Acid	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
Riboflavin	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0

Amides Matrix (Quadrant 3 green, Quadrant 4 blue)

	2-Nitrobenzamide	3-Nitrobenzamide	4-Nitrobenzamide	2-Hydroxybenzamide	4-Hydroxybenzamide	3-Fluorobenzamide	4-Fluorobenzamide	2-Aminobenzamide	3-Aminobenzamide	4-Aminobenzamide	2-Methoxybenzamide	3-Methoxybenzamide	4-Methoxybenzamide	2-Methylbenzamide	3-Methylbenzamide	4-Methylbenzamide
Nictotinamide	0	1	1	1	1	0	0	0	0	1	0	0	0	0	0	0
Isonicotinamide	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2
4,4'-Bipyridine	1	1	1	1	1	1	1	1	1	1	1	0	1	0	1	0
Fumaric Acid	0	1	0	0	1	1	1	1	1	1	1	1	1	0	1	1
Sailcylic Acid	0	1	1	1	1	0	1	1	1	0	1	0	1	0	1	1
Urea	0	1	0	0	1	0	0	0	0	1	1	0	0	0	0	0
Benzamide	0	0	1	0	0	0	0	0	0	0	0	0	0	1	0	1
Oxalic Acid	1	0	1	1	1	1	1	1	1	1	1	1	1	1	1	1
Hydroquinone	0	1	0	0	1	1	0	0	1	0	1	0	1	0	1	1
2-Pyrrolidinone	2	1	1	1	1	1	1	1	2	1	2	1	1	1	1	1
Caffeine	0	1	1	1	1	1	0	1	0	0	0	0	1	0	0	0
Capryllic Acid	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	1
L-Glutamic Acid	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
Nicotinic Acid	0	1	0	0	1	0	0	0	0	0	0	0	1	0	0	0
Pyridoxine	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
3,3'-Thiodipropionic Acid	0	0	1	0	0	0	1	1	0	0	0	1	1	0	1	1
Malic Acid	0	1	1	0	1	1	1	1	0	1	0	1	1	0	1	1
Trans-Aconitic Acid	0	0	0	0	0	1	1	0	1	0	1	0	1	1	1	1
L-Ascorbic Acid	0	1	0	0	0	0	0	0	1	0	0	0	1	0	0	0
Riboflavin	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Paracetamol Test Set Output

	Label	Probability	Predictions	Rank	Co-crystal
Phenazine	1	0.90	1	1	yes
Piperazine	1	0.83	1	2	yes
N,N-dimethyl-piperazine	1	0.79	1	3	yes
Morpholine	1	0.78	1	4	yes
N-Methylmorpholine	1	0.76	1	5	yes
4,4'-Bipyridine	1	0.73	1	6	yes
1,4-dioxane	1	0.73	1	7	yes
Oxalic acid	1	0.69	1	8	yes
Pyrazine	0	0.66	1	9	no
Imidazole	0	0.62	1	10	no
1,4-di-4-pyridyl-ethylene	1	0.62	1	11	yes
Malonic acid	0	0.59	1	12	no
1,2-bis-4-pyridyl-ethane	1	0.57	1	13	yes
Fumaric acid	0	0.56	1	14	no
Maleic acid	0	0.56	1	15	no
Resorcinol	0	0.51	1	16	no
Malic acid	0	0.51	1	17	no
Theobromine	0	0.50	1	18	no
Citric acid	1	0.49	1	19	yes
Caffeine	0	0.47	1	20	no
Isonicotinamide	0	0.47	1	21	no
Theophylline	1	0.44	1	22	yes
Nicotinamide	0	0.43	1	23	no
2,5-dihydroxybenzoic acid	0	0.39	0	24	no
Succinic acid	0	0.38	0	25	no
Melamine	0	0.35	0	26	no
Saccharin	0	0.34	0	27	no
1-naphthol	0	0.33	0	28	no
3S-cis-3,6-dimethyl-1,4-dioane-2,5-dione	0	0.31	0	29	no
Adipic acid	0	0.29	0	30	no
1,4-diaminocyclohexane	1	0.20	0	31	yes
Ascorbic acid	0	0.16	0	32	no
Benzoic acid	0	0.13	0	33	no
3-isochromanone	0	0.10	0	34	no

Training Set – SMILES Data [1]

Compound	SMILES
Nicotinamide	c1cc(cnc1)C(=O)N
Isonicotinamide	c1cnccc1C(=O)N
4,4'-Bipyridine	c1cnccc1c2ccncc2
Fumaric Acid	C(=C/C(=O)O)\C(=O)O
Salicylic Acid	c1ccc(c(c1)C(=O)O)O
Urea	C(=O)(N)N
Benzamide	c1ccc(cc1)C(=O)N
Oxalic Acid	C(=O)(C(=O)O)O
Hydroquinone	c1cc(ccc1O)O
2-Pyrrolidinone	C1CC(=O)NC1
Caffeine	CN1C=NC2=C1C(=O)N(C(=O)N2C)C
Capryllic Acid	CCCCCCCC(=O)O
L-Glutamic Acid	C(CC(=O)O)C(C(=O)O)N
Nicotinic Acid	C1=CC(=CN=C1)C(=O)O
Pyridoxine	CC1=NC=C(C(=C1O)CO)CO
3,3'-Thiodipropionic Acid	C(CSCCC(=O)O)C(=O)O
Malic Acid	C(C(C(=O)O)O)C(=O)O
Trans-Aconitic Acid	C(/C(=C\C(=O)O)/C(=O)O)C(=O)O
L-Ascorbic Acid	C(C(C1C(=C(C(=O)O1)O)O)O)O
Riboflavin	CC1=CC2=C(C=C1C)N(C3=NC(=O)NC(=O)C3=N2)CC(C(C(CO)O)O)O
2-Nitrobenzoic Acid	c1ccc(c(c1)C(=O)O)[N+](=O)[O-]
3-Nitrobenzoic Acid	c1cc(cc(c1)[N+](=O)[O-])C(=O)O
4-Nitrobenzoic Acid	c1cc(ccc1C(=O)O)[N+](=O)[O-]
2-Hydroxybenzoic Acid	c1ccc(c(c1)C(=O)O)O
3-Hydroxybenzoic Acid	c1cc(cc(c1)O)C(=O)O
4-Hydroxybenzoic Acid	c1cc(ccc1C(=O)O)O
2-Fluorobenzoic Acid	c1ccc(c(c1)C(=O)O)F
3-Fluorobenzoic Acid	c1cc(cc(c1)F)C(=O)O
4-Fluorobenzoic Acid	c1cc(ccc1C(=O)O)F
2-Aminobenzoic Acid	c1ccc(c(c1)C(=O)O)N
3-Aminobenzoic Acid	c1cc(cc(c1)N)C(=O)O
4-Aminobenzoic Acid	c1cc(ccc1C(=O)O)N
2-Methoxybenzoic Acid	COc1ccccc1C(=O)O
3-Methoxybenzoic Acid	COc1cccc(c1)C(=O)O
4-Methoxybenzoic Acid	COc1ccc(cc1)C(=O)O
2-Methylbenzoic Acid	Cc1ccccc1C(=O)O
3-Methylbenzoic Acid	Cc1cccc(c1)C(=O)O

4-Methylbenzoic Acid	Cc1ccc(cc1)C(=O)O
2-Nitrobenzamide	C1=CC=C(C(=C1)C(=O)N)[N+](=O)[O-]
3-Nitrobenzamide	C1=CC(=CC(=C1)[N+](=O)[O-])C(=O)N
4-Nitrobenzamide	C1=CC(=CC=C1C(=O)N)[N+](=O)[O-]
2-Hydroxybenzamide	C1=CC=C(C(=C1)C(=O)N)O
4-Hydroxybenzamide	C1=CC(=CC=C1C(=O)N)O
3-Fluorobenzamide	C1=CC(=CC(=C1)F)C(=O)N
4-Fluorobenzamide	C1=CC(=CC=C1C(=O)N)F
2-Aminobenzamide	C1=CC=C(C(=C1)C(=O)N)N
3-Aminobenzamide	C1=CC(=CC(=C1)N)C(=O)N
4-Aminobenzamide	C1=CC(=CC=C1C(=O)N)N
2-Methoxybenzamide	COC1=CC=CC=C1C(=O)N
3-Methoxybenzamide	COC1=CC=CC(=C1)C(=O)N
4-Methoxybenzamide	COC1=CC=C(C=C1)C(=O)N
2-Methylbenzamide	CC1=CC=CC=C1C(=O)N
3-Methylbenzamide	CC1=CC=CC(=C1)C(=O)N
4-Methylbenzamide	CC1=CC=C(C=C1)C(=O)N

Paracetamol Test Set - SMILES Data [1]

Compound	SMILES
Paracetamol	CC(NC1=CC=C(O)C=C1)=O
Caffeine	CN1C=NC2=C1C(=O)N(C(=O)N2C)C
Pyrazine	c1cnccn1
1,2-bis-4-pyridyl-ethane	c1cc(CCc2ccncc2)ccn1
4,4'-Bipyridine	c1cnccc1c2ccncc2
1,4-di-4-pyridyl-ethylene	C1=CN=CC=C1C=CC2=CC=NC=C2
Phenazine	n1c3c(nc2c1cccc2)cccc3
Citric acid	OC(=O)CC(O)(C(=O)O)CC(=O)O
Malic acid	C(C(C(=O)O)O)C(=O)O
Malonic acid	O=C(O)CC(O)=O
N-Methylmorpholine	O1CCN(C)CC1
Adipic acid	O=C(O)CCCCC(=O)O
2,5-dihydroxybenzoic acid	O=C(O)c1cc(O)ccc1O
Benzoic acid	O=C(O)c1ccccc1
Piperazine	C1CNCCN1
1,4-diaminocyclohexane	C1CC(CCC1N)N
Theobromine	Cn1cnc2c1c(=O)[nH]c(=O)n2C
Succinic acid	C(CC(=O)O)C(=O)O
Fumaric acid	C(=C/C(=O)O)\C(=O)O
Maleic acid	O=C(O)\C=C/C(=O)O
Morpholine	C1CNCCO1
N,N-dimethyl-piperazine	CN1CCN(CC1)C
Saccharin	O=C2c1ccccc1S(=O)(=O)N2
Melamine	c1(nc(nc(n1)N)N)N
Resorcinol	c1cc(cc(c1)O)O
Theophylline	Cn1c2c(c(=O)n(c1=O)C)[nH]cn2
Ascorbic acid	C(C(C1C(=C(C(=O)O1)O)O)O)O
Imidazole	c1cnc[nH]1
Oxalic acid	C(=O)(C(=O)O)O
1,4-dioxane	O1CCOCC1
1-naphthol	Oc2cccc1ccccc12
Nicotinamide	c1cc(cnc1)C(=O)N
Isonicotinamide	c1cnccc1C(=O)N
3S-cis-3,6-dimethyl-1,4-dioane-2,5-dione	C[C@@H]1OC(=O)[C@H](C)OC1=O
3-isochromanone	C1C2=CC=CC=C2COC1=O

Values of hydrogen-bond parameters, α and β, as described by Hunter [2]

Compound	Donor	Acceptor
fr_pyridine	0	7
fr_NH0	0	7.8
fr_NH1	1.5	7.8
fr_NH2	1.5	7.8
fr_nitro	0	3.7
fr_amide	2.9	8.3
fr_urea	3	8.3
fr_COO	3.6	5.3
fr_phenol	3.8	2.7
fr_aniline	2.1	5.3
fr_methoxy	0	3.7
fr_Al_OH	2.7	5.8
fr_imidazole	3.7	0
fr_Ar_F	1.4	1.6
fr_Ar_Cl	1.3	1.6
fr_Ar_X	0	1.6
fr_tert_amide	0	8.3
fr_ester	0	5.3
fr_ether	0	5.3

Experimental

Materials and reagents

All reagents were of standard laboratory grade, as purchased from fine chemical suppliers, and were used without further purification.

Neat grinding

Solid state grinding in all cases was performed using a Retsch MM400 Mixer Mill, equipped with two stainless steel grinding vessels and one stainless steel grinding ball per vessel. All grinds were carried out at a rate of 30 Hz for 20 min using a 1:1 molar ratio of materials. Where an alternative ratio was determined from analysis, neat grinding was repeated in 1:2 or 2:1 molar ratio, as appropriate.

Infrared Spectra [University College Cork, Q1 and 2]

Infrared spectra were recorded on a Bruker Tensor 37 FT-IR spectrophotometer interfaced with Opus version 7.2.139.1294 over a range of 400 – 4000 cm^{-1}. An average of 16 scans were taken for each spectrum obtained with a resolution of 4 cm^{-1}. Values are given to the nearest whole number.

Infrared Spectra [University of Oxford, Q3 and 4]

Infrared spectra were recorded on a Shimadzu IR Affinity- 1S FTIR spectrophotometer in the range 4000 - 480 cm^{-1}.

Powder X-ray Diffraction (PXRD) [University College Cork, Q1 and 2]

PXRD data were collected using a Bruker D2-Phaser bench-top powder X-ray diffractometer with Cu Kα radiation, using a LYNXEYE detector over the 2θ range of 3.5 – 45.5° with a step size of 0.075°. Samples were analysed neat in reflectance mode with no further sample preparation. Data collection parameters were defined using DIFFRAC.SUITE™ software and data were analysed using DIFFRAC.EVA™ software.

Powder X-ray Diffraction (PXRD) [University of Oxford, Q3 and 4]

PXRD data were collected on the flat spinner stage of a Rigaku Miniflex II desktop diffractometer with a Cu Kα source (λ = 1.5406 Å) and scans conducted in the range 10° to 60° 2θ at a 0.02° step size.

Differential Scanning Calorimetry (DSC) [University College Cork]

DSC were collected using a DSC Q1000 in conjunction with a refrigerated cooling system. The samples were equilibrated at 20 °C and ramped up to the required temperature at 2 °C per minute at a N_2 flow rate of 50 mL min^{-1}. The samples were prepared on aluminium pans and the data were viewed via Universal Analysis software.

Single Crystal X-Ray Diffraction (SCXRD) [University College Cork]

Single crystal X-ray data were collected at University College Cork on a Bruker APEX II DUO diffractometer or a Bruker SMART X2S diffractometer[3] at temperatures between 100-300 K using graphite monochromatic Mo Kα (λ = 0.7107 Å) radiation. Calculations were performed using the APEX2 software suite,[4] incorporating the SHELX suite of programs[5] and refined on F^2. All non-hydrogen atoms were located and refined with anisotropic thermal parameters. Hydrogen atoms were found and refined where possible; alternatively, hydrogens were included in calculated positions and allowed to ride on the parent atom for refinement.

Experimental DSC, IR and PXRD data.

These are available at http://www.xtl.ox.ac.uk/will-it-co-crystallize-supplementary-information.html.

ORTEP plots.

All ORTEP plots have been drawn with 40% probability and show the atomic numbering.

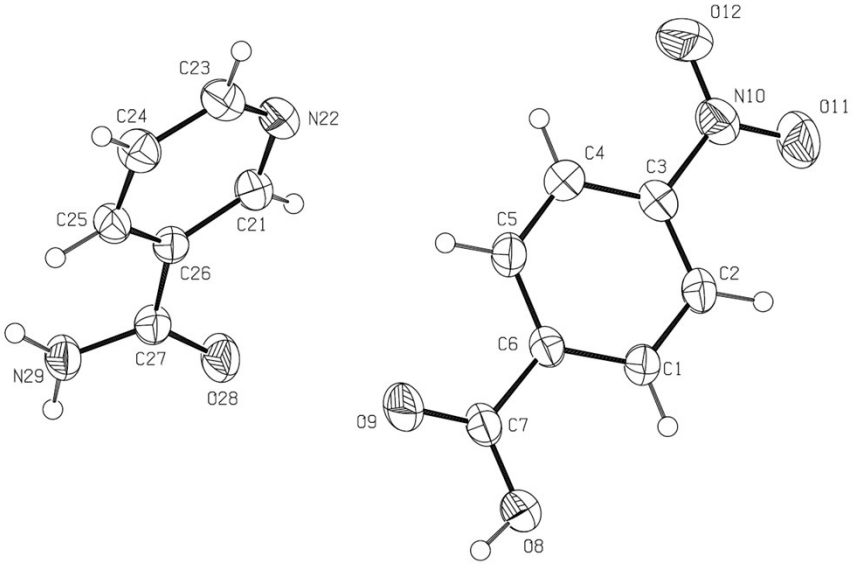


Figure 1 CCDC code 1538729: nicotinamide and 4-nitrobenzoic acid cocrystal

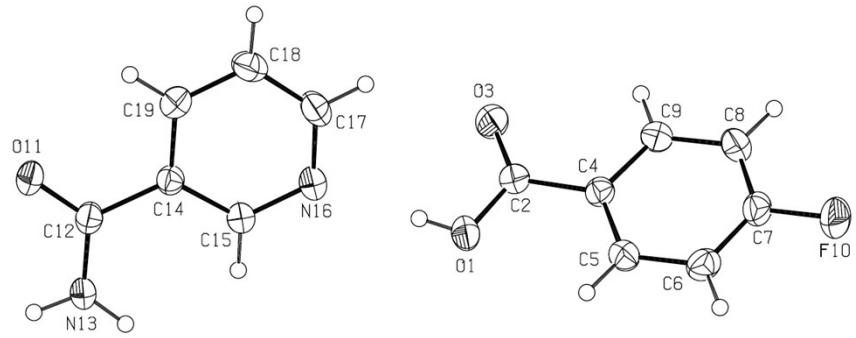


Figure 2 CCDC code 1538730: nicotinamide and 4-fluorobenzoic acid cocrystal

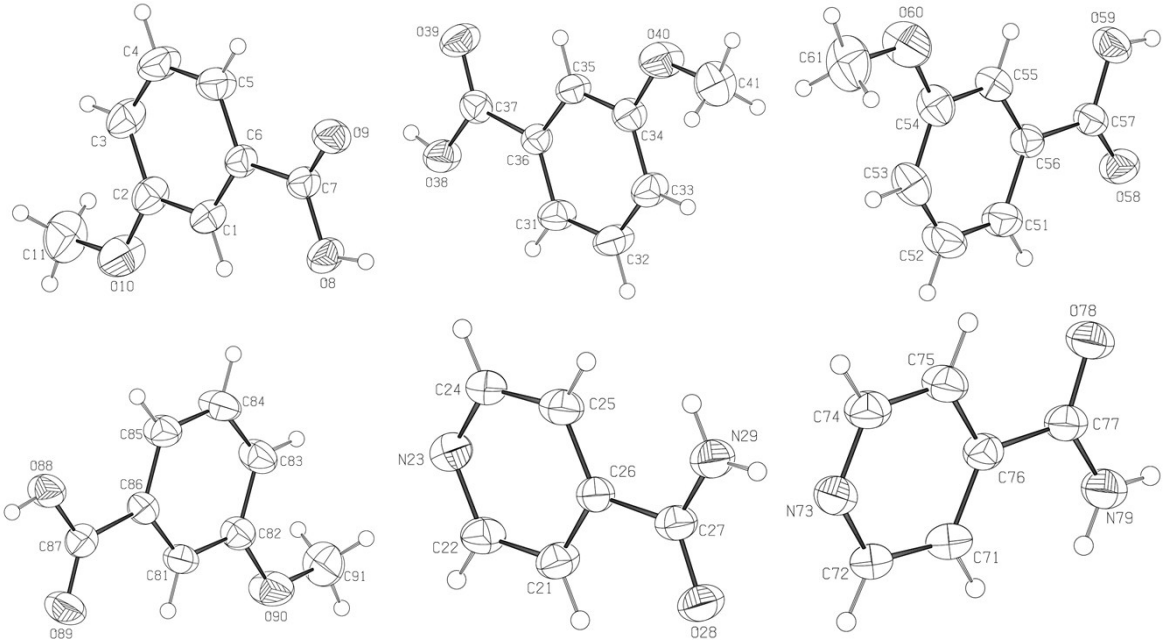


Figure 3 CCDC code 1538731: isonicotinamide and 3-methyoxybenzoic acid cocrystal

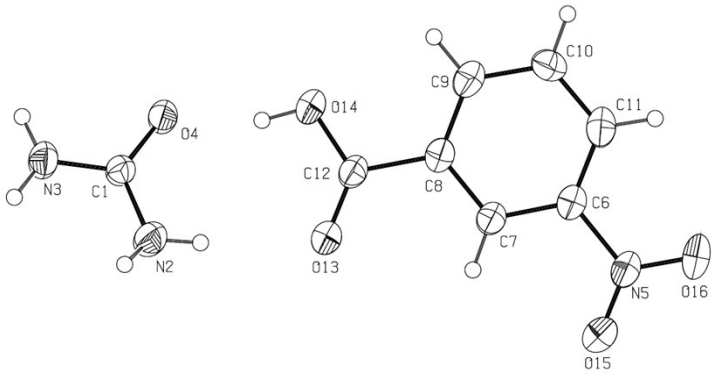


Figure 4 CCDC code 1538732: urea and 3-nitrobenzoic acid cocrystal

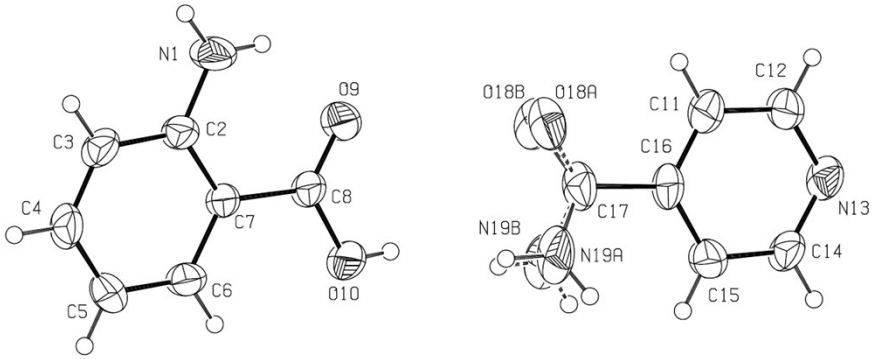


Figure 5 CCDC code 1538733: isonicotinamide and 2-aminobenzoic acid cocrystal (showing disorder)

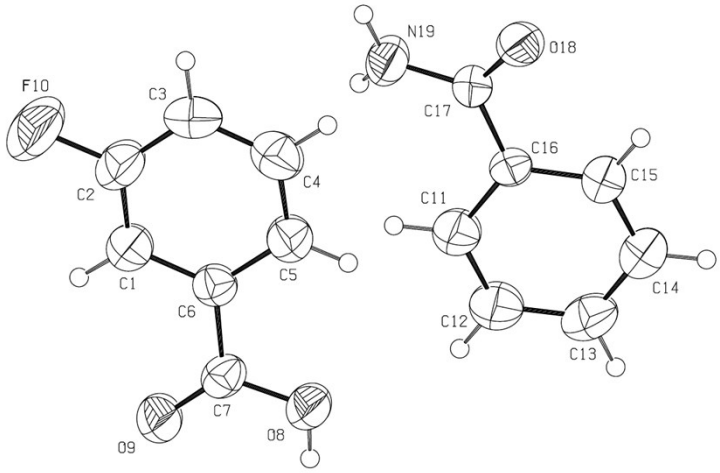


Figure 6 CCDC code 1538734: benzamide and 3-fluorobenzoic acid cocrystal

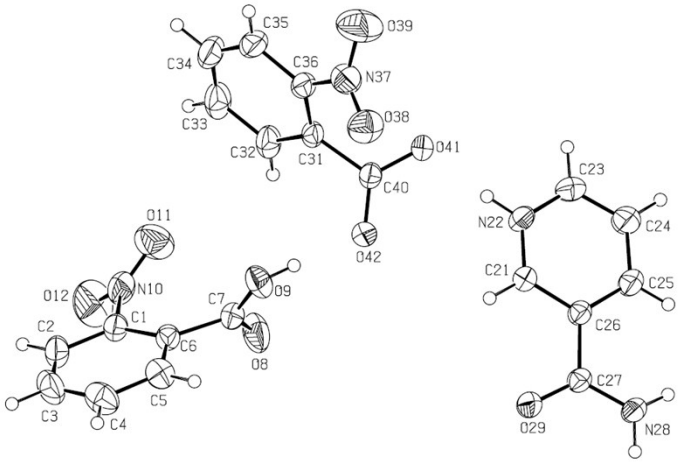


Figure 7 CCDC code 1538735: nicotinamide and 2-nitrobenzoic acid salt cocrystal

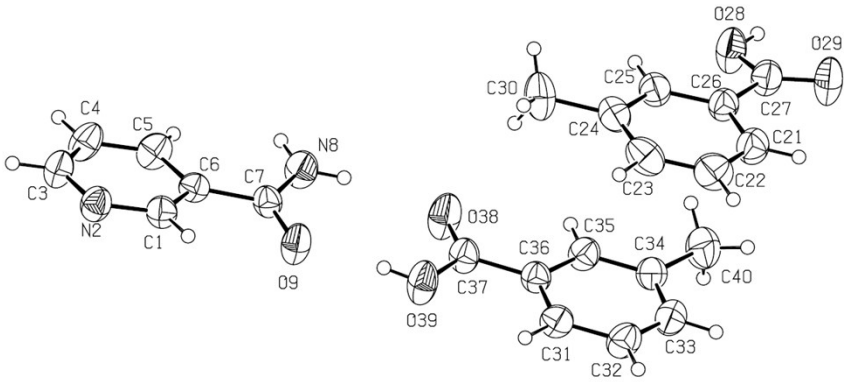


Figure 8 CCDC code 1538736: nicotinamide and 3-methylbenzoic acid cocrystal

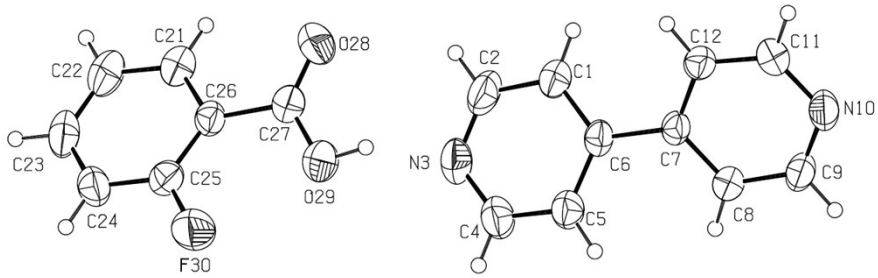


Figure 9 CCDC code 1538737: 4,4'-bipyridyl and 2-fluorobenzoic acid cocrystal

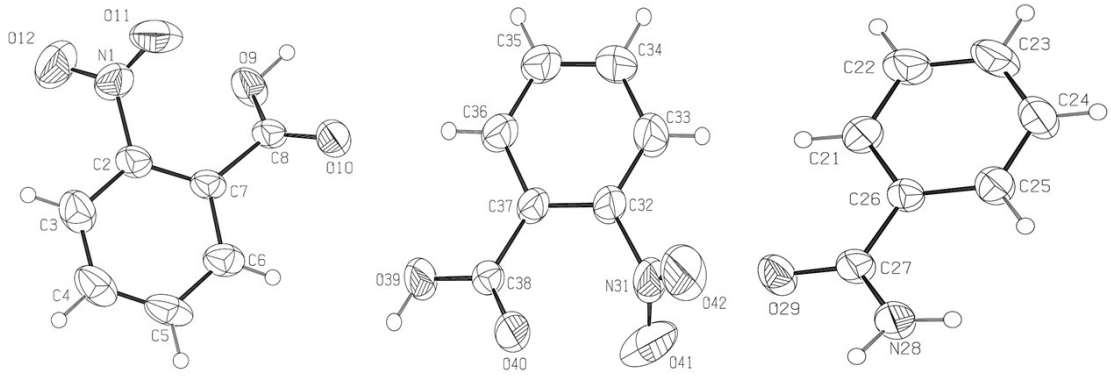


Figure 10 CCDC code 1538738: benzamide and 2-nitrobenzoic acid cocrystal

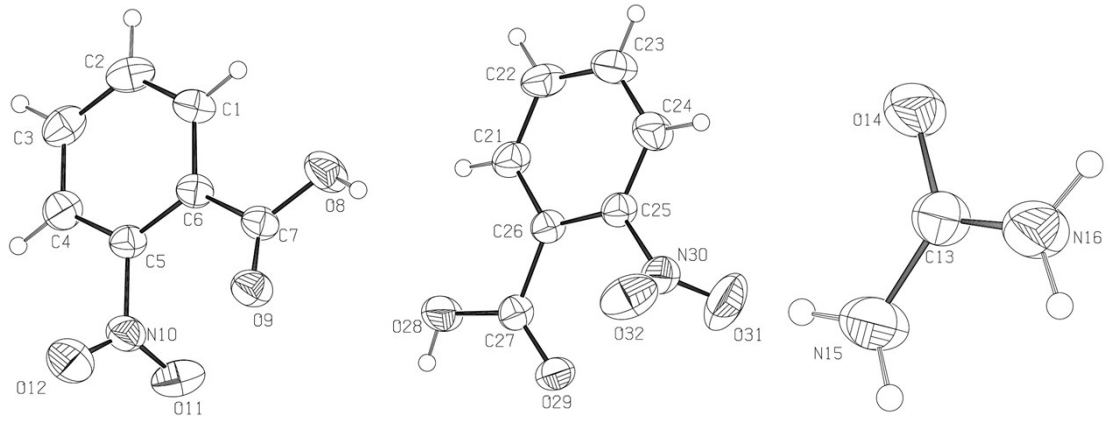


Figure 11 CCDC code 1538739: urea and 2-nitrobenzoic acid cocrystal

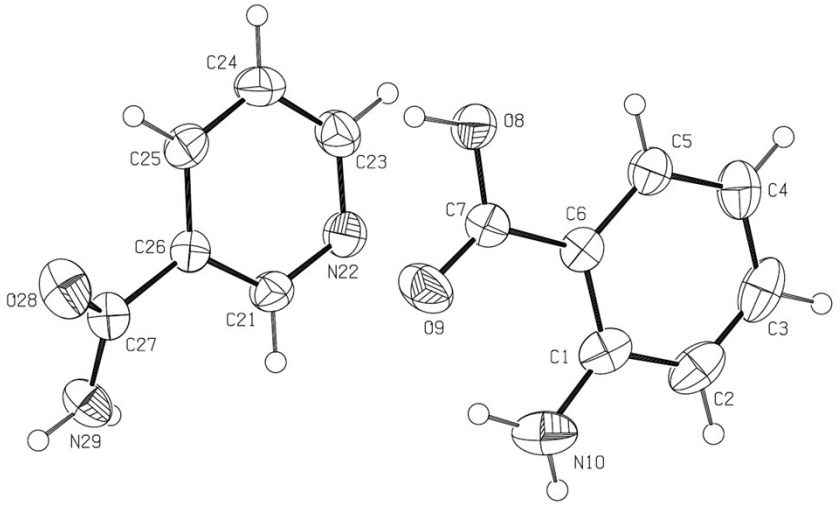


Figure 12 CCDC code 1538740: nicotinamide and 2-aminobenzoic acid cocrystal

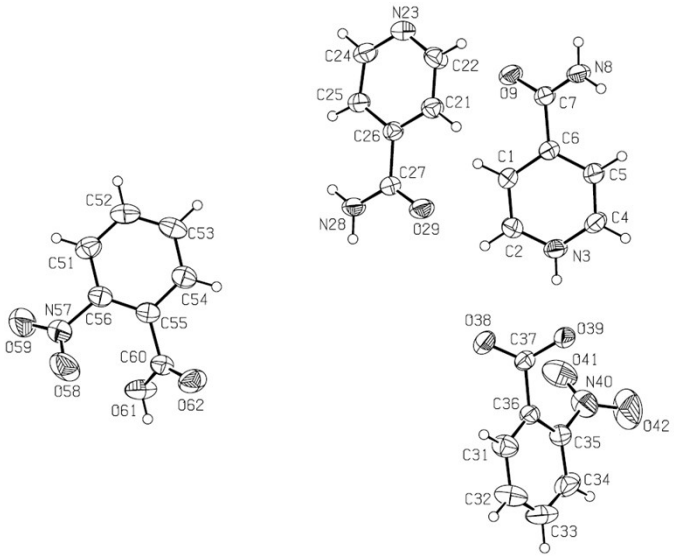


Figure 13 CCDC code 1538741: isonicotinamide and 2-nitrobenzoic acid salt cocrystal

References.

1 SMILES (Simplified Molecular Input Line Entry System) is a chemical language and information system that converts chemical diagrams into a computer readable format, see D. Weininger, *J. Chem. Info. Comp. Sci.* **1988**, 28, 31–36.

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4 APEX2 v2009.3-0; Bruker AXS: Madison, WI, **2009**.

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