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The principles underlying the use of powder diffraction data in solving pharmaceutical crystal structures
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Name	Fig. 6	Formula	SMILES string (generated using MarvinSketch v6.0.0)
Salicylic acid	a	$C_7H_6O_3$	OC(=O)C1=CC=CC=C1O
Chlorothiazide	b	$C_7H_6Cl_1N_3O_4S_2$	NS(=O)(=O)C1=CC2=C(NC=NS2(=O)=O)C=C1Cl
Ibuprofen	c	$C_{13}H_{18}O_2$	CC(C)CC1=CC=C(C=C1)C(C)C(O)=O
L-glutamic acid	d	$C_5H_9N_1O_4$	[NH3+][C@@H](CCC(O)=O)C([O-])=O
Remacemide nitrate	e	$C_{17}H_{21}N_3O_4$	[O-]N(=O)=O.CC(CC1=CC=CC=C1)(NC(=O)C[NH3+])C1=CC=CC=C1
Tri-β-peptide	f	$C_{32}H_{53}N_3O_6$	CC(C)C[C@H](NC(=O)[C@H](C)[C@H](C)NC(=O)[C@H](C)[C@@H](NC(=O)OC(C)(C)C)C(C)C)[C@@H](C)C(=O)OCC1=CC=CC=C1
Capsaicin	g	$C_{18}H_{27}N_1O_3$	COC1=CC(CNC(=O)CCCC\C=C\C(C)C)=CC=C1O
Baicalein	h	$C_{15}H_{10}O_5$	OC1=CC2=C(C(O)=C1O)C(=O)C=C(O2)C1=CC=CC=C1
Famotidine	i	$C_8H_{15}N_7O_2S_3$	NC(N)=NC1=NC(CSCC\C(N)=N\S(N)(=O)=O)=CS1
Caffeine	j	$C_8H_{10}N_4O_2$	CN1C=NC2=C1C(=O)N(C)C(=O)N2C
Captopril	k	$C_9H_{15}N_1O_3S_1$	C[C@H](CS)C(=O)N1CCC[C@H]1C(O)=O
Cyheptamide	l	$C_{16}H_{15}N_1O_1$	NC(=O)C1C2=CC=CC=C2CCC2=CC=CC=C12
Tolbutamide	m	$C_{12}H_{18}N_2O_3S_1$	CCCCNC(=O)NS(=O)(=O)C1=CC=C(C)C=C1
Nifedipine	n	$C_{17}H_{18}N_2O_6$	COC(=O)C1=C(C)NC(C)=C(C1C1=CC=CC=C1N(=O)=O)C(=O)OC
L-arginine	o	$C_6H_{14}N_4O_2$	N[C@@H](CCCNC(N)=[NH2+])C([O-])=O
Amodiaquinium dichloride dihydrate	p	$C_{20}H_{28}Cl_3N_3O_3$	O.[Cl-].CC[NH+](CC)CC1=CC(NC2=C3C=CC(Cl)=CC3=[NH+]C=C2)=CC=C1O
Vorinostat	q	$C_{14}H_{20}N_2O_3$	ONC(=O)CCCCCCC(=O)NC1=CC=CC=C1
Amcinonide	r	$C_{28}H_{35}F_1O_7$	CC(=O)OCC(=O)[C@@]12OC3(CCCC3)O[C@@H]1C[C@H]1[C@@H]3CCC4=CC(=O)C=C[C@]4(C)[C@@]3(F)[C@@H](O)C[C@]21C
Diphenhydramine hydrochloride	s	$C_{17}H_{22}Cl_1N_1O_1$	[Cl-].C[NH+](C)CCOC(C1=CC=CC=C1)C1=CC=CC=C1
Verapamil hydrochloride	t	$C_{27}H_{39}Cl_1N_2O_4$	[Cl-].COC1=CC=C(CC[NH+](C)CCCC(C#N)(C(C)C)C2=CC=C(OC)C(OC)=C2)C=C1OC
Zopiclone dihydrate	u	$C_{17}H_{21}Cl_1N_6O_5$	O.CN1CCN(CC1)C(=O)OC1N(C(=O)C2=NC=CN=C12)C1=CC=C(Cl)C=N1
Prilocaine	v	$C_{13}H_{20}N_2O_1$	CCCNC(C)C(=O)NC1=CC=CC=C1C

(i) To produce a 2D structure, copy-&-paste the SMILES string into MarvinSketch;

(ii) to produce a 3D structure, copy-&-paste the SMILES string into MarvinSketch and click ‘Clean in 3D’;
(iii) to search for a corresponding CSD refcode, copy-&-paste the following into ConQuest: (a) the MarvinSketch 2D structure; (b) the formula, as shown above, checking the box for ‘Formula applies to all molecules in structure added together’ – then, combine the queries and search.