

Supporting information

Crystal structure of 3-bromo-2-hydroxybenzoic acid

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S1. Results of XPac comparisons

Table S1. Overview of the investigated substituted derivatives of salicylic acid and results of an XPac study aimed at identifying common packing motifs with the reference structure of 3-Br.

Compound	Short notation	Refcode ^a	SC ^b	x_{10} ^c	d (Å) ^d
3-Bromo-2-hydroxybenzoic acid	3-Br	–	<i>reference</i>		3.80
Salicylic acid	SalAc	SALIAC17	A0	9.7	.
3,4-difluoro-2-hydroxybenzoic acid	3,4-F	HIXPAH	A0	6.1	.
2,3,4-Trihydroxybenzoic acid hydrate	3,4-OH · 0.25H ₂ O	LAPZUZ	A11	5.6	3.73
2,3,4-Trihydroxybenzoic acid dihydrate	3,4-OH · 2H ₂ O	MUQHOU	none	.	.
2,3,5-Trichloro-6-hydroxybenzoic acid	3,5,6-Cl	MIQKEE02	A0	10.1	.
3,5-Dibromo-2-hydroxybenzoic acid	3,5-Br	XISGEM	S2	11.8	.
3,5-Dichloro-2-hydroxybenzoic acid	3,5-Cl	WECXAE	S2	12.4	.
3,5-Dichloro-2-hydroxy-4-methoxy-6- <i>n</i> -propylbenzoic acid	3,5-Cl, 4-OMe, 6- <i>n</i> Pr	COPIAS	A0	10.3	.
2-Hydroxy-3,5-diisopropylbenzoic acid	3,5- <i>i</i> Pr	NEQTAF	A0	7.0	.
3,5-Dinitrosalicylic acid monohydrate	3,5-NO ₂ · H ₂ O (E)	ZAJGUM	none	.	.
3,5-Dinitrosalicylic acid monohydrate	3,5-NO ₂ · H ₂ O (F)	ZAJGUM01	none	.	.
3,5-Di- <i>t</i> -butyl-2-hydroxybenzoic acid	3,5- <i>t</i> Bu	ELIDUY	A0	4.3	.
3-Butyl-2-hydroxybenzoic acid	3-Bu	HEWLUS	A0	6.9	.
3-(Ethoxycarbonyl)-2-hydroxy-6-methoxy-4-methylbenzoic acid	3-COOEt, 4-Me, 6-OMe	ZAPYEW	X11	11.1	3.72
2-Hydroxy-1,3-dicarboxybenzene	3-COOH	IBUMAT	none	.	.
3-Carboxysalicylaldehyde monohydrate	3-CHO · H ₂ O	JOHXEJ	none	.	.
2-Hydroxybenzene-1,2-dioic acid monohydrate	3-COOH · H ₂ O	TOLCAY02	X11	16.4	3.67
2-Hydroxy-3-methylbenzoic acid	3-Me	CRESOT10	A11	16.7	4.11
2-Hydroxy-6-isopropyl-3-methylbenzoic acid	3-Me, 6- <i>i</i> Pr	URAKUU	A0	7.9	.
2-Hydroxy-3-nitrobenzoic acid monohydrate	3-NO ₂ · H ₂ O	VAXXID	X11	15.9	3.59
2,3-Dihydroxybenzoic acid	3-OH (triclinic)	CACDAM01	A0	8.0	.
2,3-Dihydroxybenzoic acid	3-OH (monoclinic)	CACDAM	none	.	.
2-Hydroxy-3-methoxybenzoic acid	3-OMe	PIDJES01	A11	16.1	3.79
2-Hydroxy-3-methoxybenzoic acid monohydrate	3-OMe · H ₂ O	DIWNON01	none	.	.
5-Methyl-3-sulfosalicylic acid dihydrate	3-SO ₃ , 5-Me · 2H ₂ O	MSUSAL	A0	3.8	.
2,4,6-Trihydroxybenzoic acid monohydrate	4,6-OH · H ₂ O	XIPVEY	none	.	.
4-Acetamido-2-hydroxybenzoic acid	4-ACM	VAXXOJ	none	.	.
4-Chloro-2-hydroxybenzoic acid	4-Cl	VAXYAW	A11	9.2	3.72
2,5-Dihydroxybenzene-1,4-dicarboxylic acid dihydrate	4-COOH, 5-OH · 2H ₂ O	DUSJUX	none	.	.
2-Hydroxy-4-methylbenzoic acid	4-Me	VAXYIE	A11	11.5	3.87
4-Amino-2-hydroxybenzoic acid	4-NH ₂	AMSALA02	A11	10.3	3.73
5-Carboxy-2,4-dihydroxyanilinium chloride	4-NH ₃ ⁺ , 5-COOH · Cl ⁻	SUZTAJ	A0	8.3	.
2,4-Dihydroxybenzoic acid	4-OH (I)	ZZZEEU08	A0	4.0	.
2,4-Dihydroxybenzoic acid	4-OH (II)	ZZZEEU04	A11	10.7	3.69
2,4-Dihydroxybenzoic acid hemihydrate	4-OH · 0.5H ₂ O	QIVTUK01	A0	7.6	.
6- <i>n</i> -Pentadecyl-2,4-dihydroxybenzoic acid	4-OH, 6- <i>n</i> Pentadecyl	PDCHBZ10	A0	9.7	.
2-Hydroxy-4-methoxybenzoic acid	4-OMe	VAXYEA	A0	4.3	.
5-Acetamido-2-hydroxybenzoic acid monohydrate	5-ACM · H ₂ O	VAXYOK	X11	2.2	3.75
5-Bromo-2-hydroxybenzoic acid	5-Br (α)	IYAWIO01	A0	7.7	.
5-Bromo-2-hydroxybenzoic acid	5-Br (β)	IYAWIO02	A0	11.4	.
5-Formyl-2-hydroxybenzoic acid	5-CHO	UJOFEF	X11	5.6	3.78
5-Chloro-2-hydroxybenzoic acid	5-Cl	VABVAX01	A11	7.1	3.71
5-Chloro-2-hydroxybenzoic acid monohydrate	5-Cl · H ₂ O	VAYBOO	X11	13.1	3.73
4-Hydroxyisophthalic acid	5-COOH	OJICEP	A11	4.8	3.68
5-Fluorosalicylic acid	5-F	ABENEB	A11	4.2	3.82
2-Hydroxy-5-iodobenzoic acid	5-I (α)	VAXZIF	A11	14.8	4.58
2-Hydroxy-5-iodobenzoic acid	5-I (β)	VAXZIF01	A0	7.7	.
2-Hydroxy-5-methylbenzoic acid	5-Me	BESKEP01	A0	6.0	.
5-Ammonio-2-hydroxybenzoate	5-NH ₃ ⁺	SAQJAV01	X11	20.5	3.72
5-Nitrososalicylic acid	5-NO	NTSALA	A11	9.5	3.67
2-Hydroxy-5-nitrobenzoic acid	5-NO ₂	GUTNIS01	A0	5.9	.
2,5-Dihydroxybenzoic acid	5-OH (I)	BESKAL02	A0	4.4	.
2,5-Dihydroxybenzoic acid	5-OH (II)	BESKAL03	A0	5.2	.
2-Hydroxy-5-methoxybenzoic acid	5-OMe	VAXZUR	A11	5.6	3.98
2-Fluoro-6-hydroxybenzoic acid	6-F	VAYBUU	A0	5.5	.
2,6-Dihydroxybenzoic acid	6-OH (orthorhombic)	LEZJAB	X11	13.8	3.83
2,6-Dihydroxybenzoic acid	6-OH (monoclinic)	LEZJAB01	A0	6.6	.
2,6-Dihydroxybenzoic acid monohydrate	6-OH · H ₂ O	LEZJEF	none	.	.
2-Hydroxy-6-methoxybenzoic acid	6-OMe	VAYCAB	none	.	.

^a CSD Refcode. ^b Largest supramolecular construct shared with 3-Br. ^c Dissimilarity index x_{10} for the largest supramolecular construct shared with 3-Br. ^d Length of the stacking vector of the SCs **X11** / **A11**.

Table S2. Crystallographic parameters associated with the occurrence of the two-periodic SC **S2** (Figure 3a) in three crystal structures.

Crystal structure	Refcode ^a	Corresponding lattice parameters ^b					plane	x_{10} ^c
		\mathbf{t}_1	d_1 (Å)	\mathbf{t}_2	d_2 (Å)	$\angle(\mathbf{t}_1, \mathbf{t}_2)$		
3-Br	–	010	10.56	301	21.30	90	(10 $\bar{3}$)	–
3,5-Br	XISGEM	010	11.08	201	22.65	90	(10 $\bar{2}$)	11.8
3,5-Cl	WECXAE	101	10.93	0 $\bar{1}$ 0	21.63	90	(10 $\bar{1}$)	12.4

^a CSD Refcode. ^b $\mathbf{t}_1, \mathbf{t}_2$ = lattice directions; d_1, d_2 = length of translation along \mathbf{t}_1 and \mathbf{t}_2 , respectively; $\angle(\mathbf{t}_1, \mathbf{t}_2)$ = angle between \mathbf{t}_1 and \mathbf{t}_2 ; plane = plane defined by \mathbf{t}_1 and \mathbf{t}_2 . ^c Dissimilarity index x_{10} for supramolecular construct S2 for the comparison with 3-Br.