

Further Relationships and Associations in the Crystal Structures of a Family of Substituted Aspirin Molecules

Michael B Hursthouse*, Riccardo Montis and Graham J Tizzard

School of Chemistry, University of Southampton, Southampton SO17 1BJ, UK

Electronic Supplementary Information

Synthesis and crystallisation of functionalized 2-acetoxybenzoic acids.

The functionalized salicylic acid (10.8 mmol) was mixed with acetic anhydride (2mL, 21 mmol) and 1 drop of 85% phosphoric acid solution. The mixture was stirred under reflux for 2 hours at 80° C whereupon water (2 mL) was added. The reaction continued for 5 minutes and the mixture was cooled with an ice water bath. The precipitate formed was filtered off and washed with water.

XPac: Supramolecular Constructs and Translational Vectors.

SC	D	Description	#	Base	Dependencies
A1	0	Carboxylic acid dimer	14	-	-
B1	0	CarboxylicO...5sub dimer	4	-	-
C1	0	Acetyl-Acetyl dimer	9	-	-
C2	1	Row of Acetyl-Acetyl dimers > translation	3	<i>t1</i>	C1 → C2
E1	1	Row of single molecules > translation	3	<i>t2</i>	COSP (CP) → E1
D1	1	Stack of single molecules > translation	11	<i>t3</i>	COSP (CP) → D1
AB1	1	Tape- chain of A1 and B1 dimers > translation	4	<i>t4</i>	A1, B1 → AB1
A8	1	Sheet-A1 dimer stacks > translation	2	<i>t5</i>	A1 → A8
Isostructural		4MeO, 4F			

Table S1: Supramolecular Construct descriptions. SC = Supramolecular Construct; D = dimensionality; Description, '>' = is related by; # = Number of structures in which construct occurs; Base = base vector of SC (see Table 2); Dependencies show lower dimensionality SCs present in given SC.

Structures	<i>t1</i>	d1	<i>t2</i>	d2	<i>t3</i>	d3	<i>t4</i>	d4	<i>t5</i>	d5
3-MeO	-	-	-	-	-	-	-	-	001	7.381
4-MeO	-	-	-	-	100	5.069	-	-	-	-
5-MeO	-	-	-	-	-	-	-10-1	11.563	-	-
4-F	-	-	-	-	100	4.908	-	-	-	-
6-F	010	7.095	010	7.095	-	-	-	-	-	-
4-CF ₃	-	-	-	-	1-10	5.752	-	-	-	-
5-Cl	-	-	-	-	-	-	100	10.086	-	-
5-Br	-	-	-	-	-	-	100	10.391	-	-
5-I	-	-	-	-	-	-	-100	10.784	-	-
6-Me	-	-	-	-	-	-	-	-	010	7.238
Asp 1	0-10	6.552	0-10	6.552	-	-	-	-	-	-
Asp 2	-	-	0-10	6.506	-	-	-	-	-	-

Table S2: Translational vectors with lengths (Å). Grey colour is used to indicate structures involved in the previous paper.