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

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Electronic Supplementary Information

SC	D	Description	#	Base	Dependencies
A1	0	Carboxylic acid dimer	11		
A2	1	Zig-zag row of acetyl H-bonded A1 dimers > translation	7	t1	A1→A2
A3	1	Stack of A1 dimers > translation	8	t2	A1→A3
A4	1	Row of A1 dimers > translation	4	t3	A1→A4
A5	2	Sheet – A3 dimer stacks > 2_1 screw axes	6	t2, t4	A1xA3→A5
A6	2	Sheet – A3 dimer stacks > 2_1 screw axes	5	t2, t5	A1xA2xA3→A6
A7	2	Sheet – A1 dimer stacks > 2-fold rotation	2	t6, t7	A1→A7
Isostructural		**1/2/4, 3/5/6**			

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	t1	d1	t2	d2	t3	d3	t4	d4	t5	d5	t6	d6	t7	d7	∠ (t2, t4)	∠ (t2, t5)	∠ (t6, t7)
5-F Asp	-110	10.9223	0-10	4.8919			-101	22.8044	100	9.7655					90	90	
5-Cl Asp			010	4.7144	110	11.1337	10-1	22.8603							90		
5-Br Asp			010	4.7265	110	11.4156	-101	23.1033							90		
5-I Asp			010	4.7168	1-10	11.7702	-101	23.3919							90		
5-NO2 Asp	-110	11.1259	0-10	5.0444			10-1	22.5754	100	9.9166					90	90	
3-Me Asp	-110	12.6903	100	4.91					0-10	11.702						90	
4-Me Asp	-1-10	11.3221	100	4.6363					010	10.3293						90	
5-Me Asp	1-10	11.2456	0-10	4.8831			-101	23.1027	-100	10.1301					90	90	
6-Me Asp					-100	10.164											
Asp form 1	-100	11.2776									010	6.5517	00-1	11.2741			90
Asp form 2											0-10	6.5064	00-1	11.3677			90

Table S2: Translation vectors with lengths (Å) and angle relationships (°)