Electronic supplementary information

Melting point–solubility–structure correlations in multicomponent crystals containing fumaric or adipic acid

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1 Powder X-ray diffraction

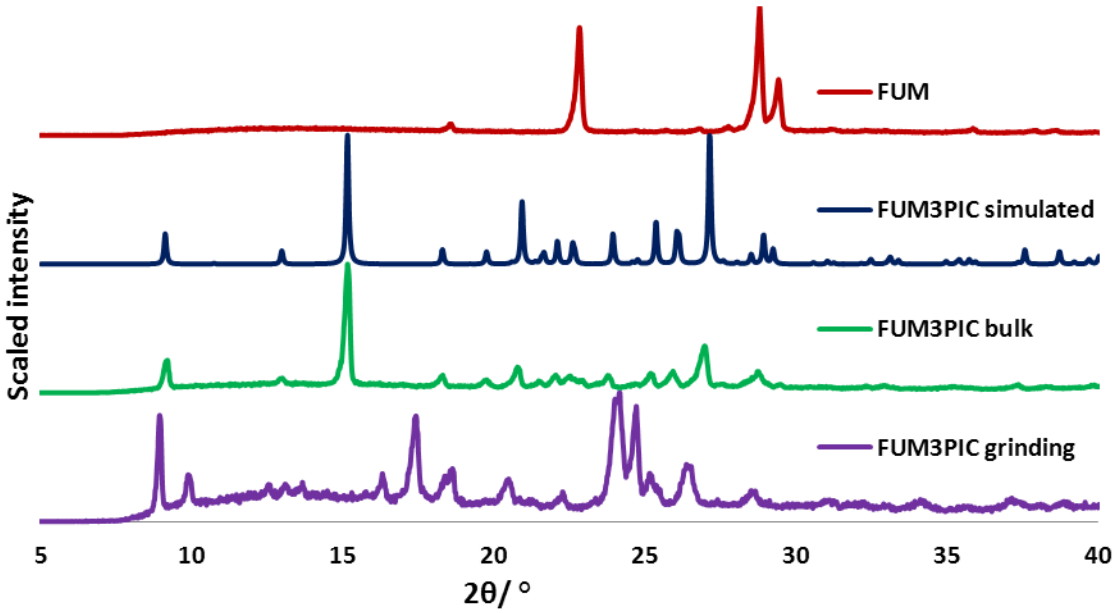

Fig. S1 The PXRD patterns for **FUM** (red), **FUM3PIC** simulated (dark blue), **FUM3PIC** bulk (green) and **FUM3PIC** grinding (purple)

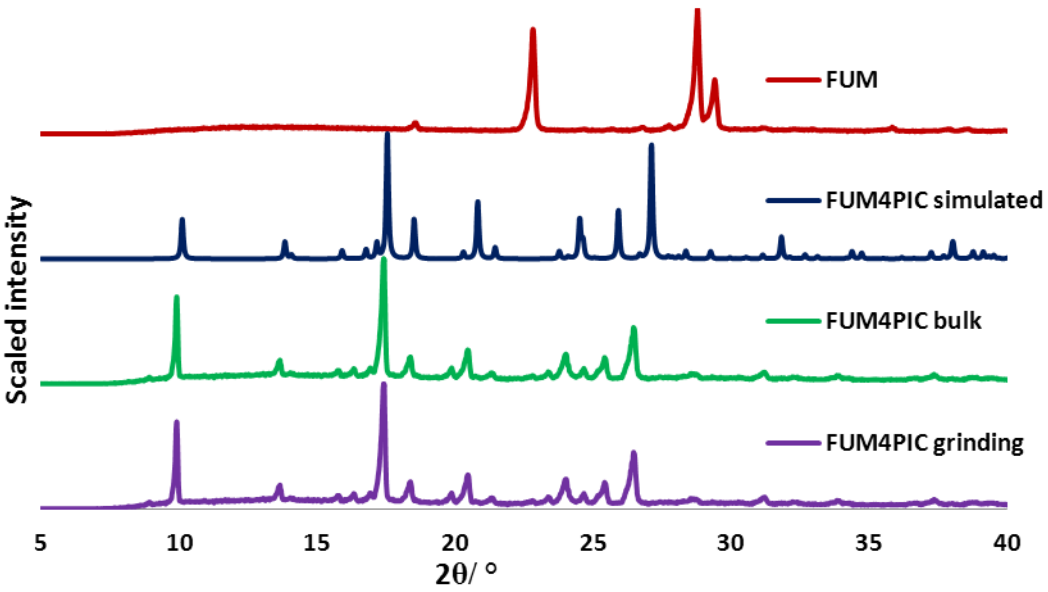

Fig. S2 The PXRD patterns for **FUM** (red), **FUM4PIC** simulated (dark blue), **FUM4PIC** bulk (green) and **FUM4PIC** grinding (purple)

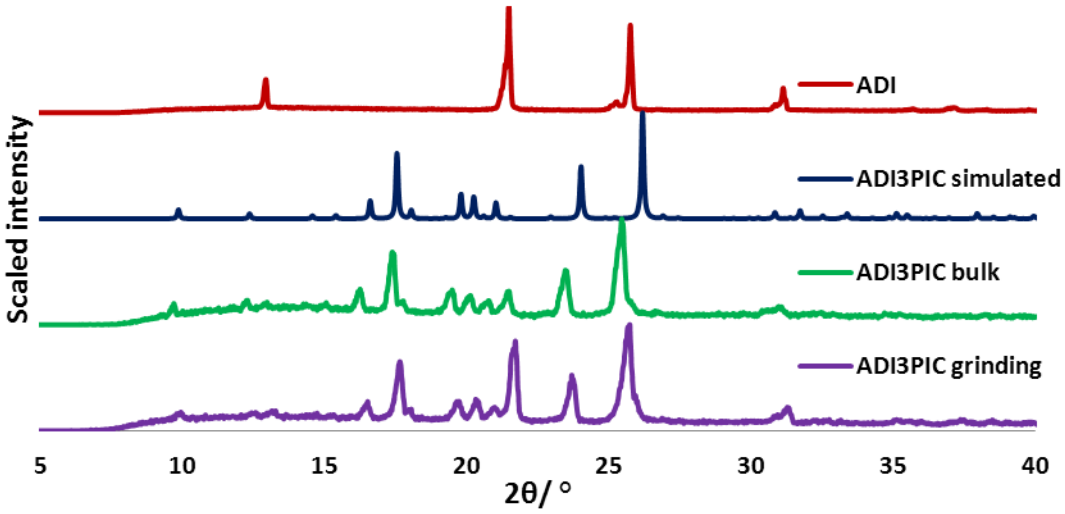

Fig. S3 The PXRD patterns for **ADI** (red), **ADI3PIC** simulated (dark blue), **ADI3PIC** bulk (green) and **ADI3PIC** grinding (purple)

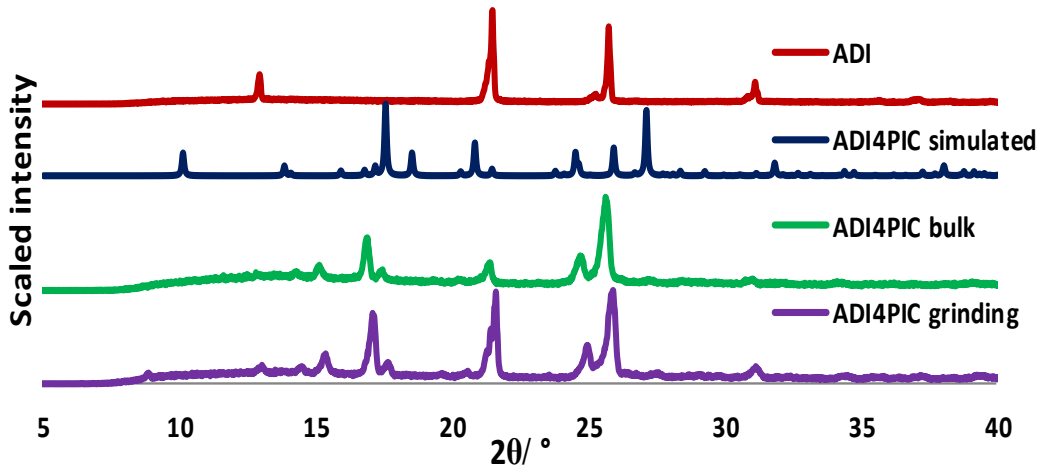

Fig. S4 The PXRD patterns for **ADI** (red), **ADI4PIC** simulated (dark blue), **ADI4PIC** bulk (green) and **ADI4PIC** grinding (purple)

2 Solubility measurements

The solubility for each compound was measured in water and in ethanol. Each experiment was conducted in three parallel measurements, the occasionally obtained out of range results were excluded from the final average solubility calculation.

	solvent	mass of vial (g)	mass of vial+ solvent (g)	mass of vial+ solvent+ compund (g)	mass comp (g)	mass of solvent (g)	mass of paper (g)	mass of paper+ mass of undissolved (g)	mass of undissolved (g)	mass of dissolved (g)	volume of solvent (mL)	solubility (g/g)	average (g/g)	solubility (mg/mL)	average (mg/mL)
FUM	ethanol	16.6701	20.6011	21.5552	0.9541	3.9310	0.3252	1.1321	0.8069	0.1472	4.9759	0.0374		**29.58**	
		15.1358	18.8558	19.7316	0.8758	3.7200	0.3413	1.0327	0.6914	0.1844	4.7089	0.0496		**39.16**	
		16.9641	20.8201	21.6190	0.7989	3.8560	0.3615	0.9829	0.6214	0.1775	4.8810	0.0460	0.04	**36.37**	35.04
	water	16.6609	19.6706	20.0710	0.4004	3.0097	0.3294	0.6105	0.2811	0.1193	3.0097	0.0396		**39.64**	
		15.2010	18.1124	18.5180	0.4056	2.9114	0.3292	0.6480	0.3188	0.0868	2.9114	0.0298		**29.81**	
		17.0229	19.8653	20.2652	0.3999	2.8424	0.3151	0.5530	0.2379	0.1620	2.8424	0.0570	0.04	**56.99**	42.15
FUMDABCO	ethanol	13.8510	15.5649	16.6464	1.0815	1.7139	0.3432	0.8856	0.5424	0.5391	2.1695	0.4985		**248.49**	
		14.1673	15.6614	16.7461	1.0847	1.4941	0.3011	0.8341	0.5330	0.5517	1.8913	0.5086		**291.71**	
		13.8510	15.1281	16.2425	1.1144	1.2771	0.3076	0.8123	0.5047	0.6097	1.6166	0.5471	1.19	**377.15**	305.78
	water	13.7665	14.7767	14.9289	0.1522	1.0102	0.3166	0.3918	0.0752	0.0770	1.0102	0.0762		**76.22**	
		13.7524	14.6618	14.7691	0.1073	0.9094	0.3211	0.3885	0.0674	0.0399	~~0.9094~~	~~0.0439~~			
		13.9509	14.5545	14.6974	0.1429	0.6036	0.3188	0.3925	0.0737	0.0692	0.6036	0.1146	0.10	**114.65**	95.43
FUM3PIC	ethanol	15.4212	17.0053	17.0851	0.0798	1.5841	0.3178	0.3711	0.0533	0.0265	2.0052	0.0167		**13.22**	
		16.2370	17.6657	17.7460	0.0803	1.4287	0.3212	0.3711	0.0499	0.0304	1.8085	0.0213		**16.81**	
		16.8957	18.1901	18.2578	0.0677	1.2944	0.3211	0.3611	0.0400	0.0277	1.6385	0.0214	0.02	**16.91**	15.64
	water	13.9674	14.6003	14.6917	0.0914	0.6329	0.3218	0.3956	0.0738	0.0176	0.6329	0.0278		**27.81**	
		14.0713	14.8703	14.9532	0.0829	0.7990	0.3216	0.3723	0.0507	0.0322	0.7990	0.0403		**40.30**	
		14.0714	15.0228	15.1492	0.1264	0.9514	0.3207	0.4120	0.0913	0.0351	0.9514	0.0369	0.04	**36.89**	35.00
FUM4PIC	ethanol	13.7017	14.1990	14.4066	0.2076	0.4973	0.3208	0.3392	0.0184	0.1892	0.6295	0.3805		**300.56**	
		14.0104	14.6093	14.7338	0.1245	0.5989	0.3143	0.3357	0.0214	0.1031	~~0.7581~~	~~0.1721~~			
		13.7647	14.1732	14.3356	0.1624	0.4085	0.3186	0.3554	0.0368	0.1256	0.5171	0.3075	0.34	**242.90**	271.73
	water	14.1051	14.9759	15.4473	0.4714	0.8708	0.3187	0.6856	0.3669	0.1045	0.8708	0.1200		**120.00**	
		13.7886	14.5708	15.2328	0.6620	0.7823	0.3235	0.8123	0.4888	0.1732	~~0.7823~~	~~0.2214~~			
		14.1020	14.7718	15.2940	0.5222	0.6698	0.3225	0.7423	0.4198	0.1024	0.6698	0.1529	0.14	**152.88**	136.44

Fig. S5 A summary of the aqueous and ethanol solubility measurements of the **FUM** series

	solvent	mass of vial (g)	mass of vial+ solvent (g)	mass of vial+ solvent+ compund (g)	mass of compound (g)	mass of solvent (g)	mass of paper (g)	mass of paper+ mass of undissolved (g)	mass of undissolved (g)	mass of dissolved (g)	volume of solvent (mL)	solubility (g/g)	average (g/g)	solubility (mg/mL)	average (mg/mL)
ADI	ethanol	13.8279	17.6718	18.4694	0.7976	3.8439	0.3428	0.7933	0.4505	0.3471	4.8657	0.0903		**71.34**	
		13.7623	17.6136	18.6775	1.0639	3.8513	0.332	0.8724	0.5404	0.5235	4.8751	0.1359		**107.38**	
		13.1592	17.5597	18.1167	0.5570	4.4005	0.3344	0.7544	0.4200	0.1370	~~5.5703~~	~~0.0311~~	0.11		**89.36**
	water	13.2500	15.1695	18.8760	1.0526	1.9195	0.8113	1.9418	0.8523	0.2003	1.9195	0.1044		**104.35**	
		14.6989	16.4273	18.9050	1.0231	1.7284	0.8214	1.8909	0.7251	0.2980	1.7284	0.1724		**172.41**	
		14.6989	17.1695	19.2750	2.1055	2.4706	0.8077	1.9777	1.1700	0.9355	~~2.4706~~	~~0.3786~~	0.14		**138.38**
ADIDABCO	ethanol	13.9460	17.9403	18.4288	0.4885	3.9943	0.3247	0.6771	0.3524	0.1361	5.0561	0.0341		**26.92**	
		14.3047	18.0278	18.5487	0.5209	3.7231	0.3236	0.6392	0.3156	0.2053	4.7128	0.0551		**43.56**	
		14.5342	18.5342	18.9763	0.4421	4.0000	0.3238	0.6634	0.3396	0.1025	5.0633	0.0256	0.04	**20.24**	**30.24**
	water	13.9309	14.3775	14.5302	0.1527	0.4466	0.321	0.3912	0.0702	0.0825	0.4466	0.1847		**184.73**	
		14.2037	14.7670	14.9019	0.1349	0.5633	0.319	0.3821	0.0631	0.0718	0.5633	0.1275		**127.46**	
		13.7810	14.5563	14.7152	0.1589	0.7753	0.3181	0.4012	0.0831	0.0758	~~0.7753~~	~~0.0978~~	0.16		**156.10**
ADI3PIC	ethanol	13.7546	14.7094	15.0236	0.3142	0.9548	0.3232	0.4458	0.1226	0.1916	1.2086	0.2007		**158.53**	
		13.7868	14.5405	14.8323	0.2918	0.7537	0.3245	0.4674	0.1429	0.1489	0.9541	0.1976		**156.07**	
		14.0075	14.8819	15.1340	0.2521	0.8744	0.3105	0.4185	0.1080	0.1441	1.1068	0.1648	0.19	**130.19**	**148.26**
	water	13.9671	14.4596	14.5083	0.0487	0.4925	0.3207	0.358	0.0373	0.0114	0.4925	0.0231		**23.15**	
		14.1052	14.7866	14.8332	0.0466	0.6814	0.3176	0.3525	0.0349	0.0117	0.6814	0.0172		**17.17**	
		13.9509	14.6403	14.6923	0.0520	0.6894	0.3157	0.3552	0.0395	0.0125	0.6894	0.0181	0.02	**18.13**	**19.48**
ADI4PIC	ethanol	13.7022	16.7818	16.8909	0.1091	3.0796	0.4992	0.5192	0.0200	0.0891	3.8982	0.0289		**22.86**	
		14.0764	17.5565	17.6059	0.0494	3.4801	0.3904	0.4062	0.0158	0.0336	~~4.4052~~	~~0.0097~~			
		13.8939	17.0270	17.1112	0.0842	3.1331	0.5107	0.5259	0.0152	0.0690	3.9659	0.0220	0.03	**17.40**	**20.13**
	water	13.8883	14.2268	14.4631	0.2363	0.3385	0.3185	0.3959	0.0774	0.1589	~~0.3395~~	~~0.4694~~			
		14.3016	14.9576	15.1790	0.2214	0.6560	0.3218	0.397	0.0752	0.1462	0.6560	0.2229		**222.87**	
		13.8386	14.2597	14.4497	0.1900	0.4211	0.3183	0.3899	0.0716	0.1184	0.4211	0.2812	0.25	**281.17**	**252.02**

Fig. S6 A summary of the aqueous and ethanol solubility measurements of the **ADI** series

3 Differential scanning calorimetry

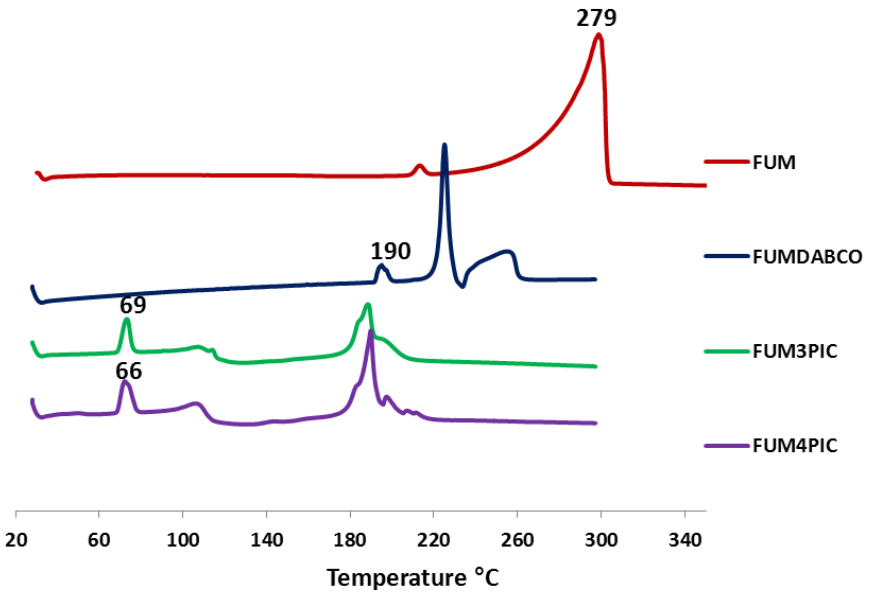

Fig. S7 The DSC thermograms (endo up) for **FUM** (red), **FUMDABCO** (dark blue), **FUM3PIC** (green) and **FUM4PIC** (purple)

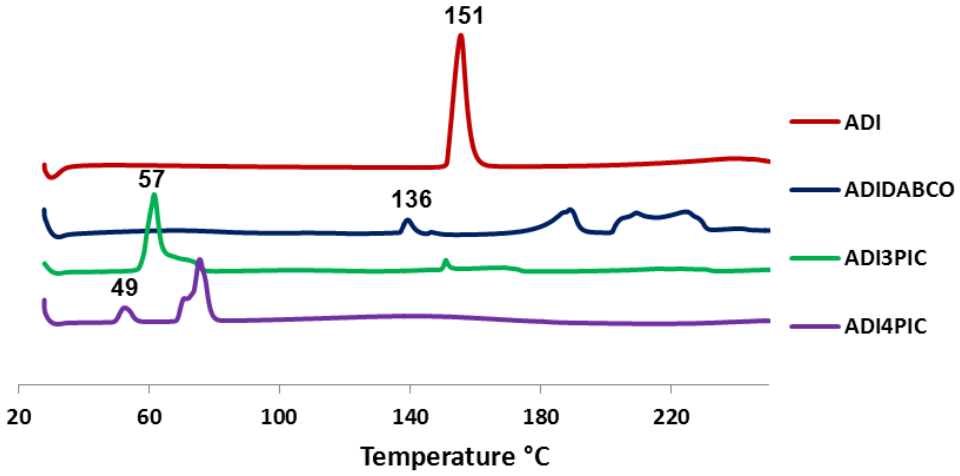

Fig. S8 The DSC thermograms (endo up) for **ADI** (red), **ADIDABCO** (dark blue), **ADI3PIC** (green) and **ADI4PIC** (purple)

4 Hirshfeld surface analysis

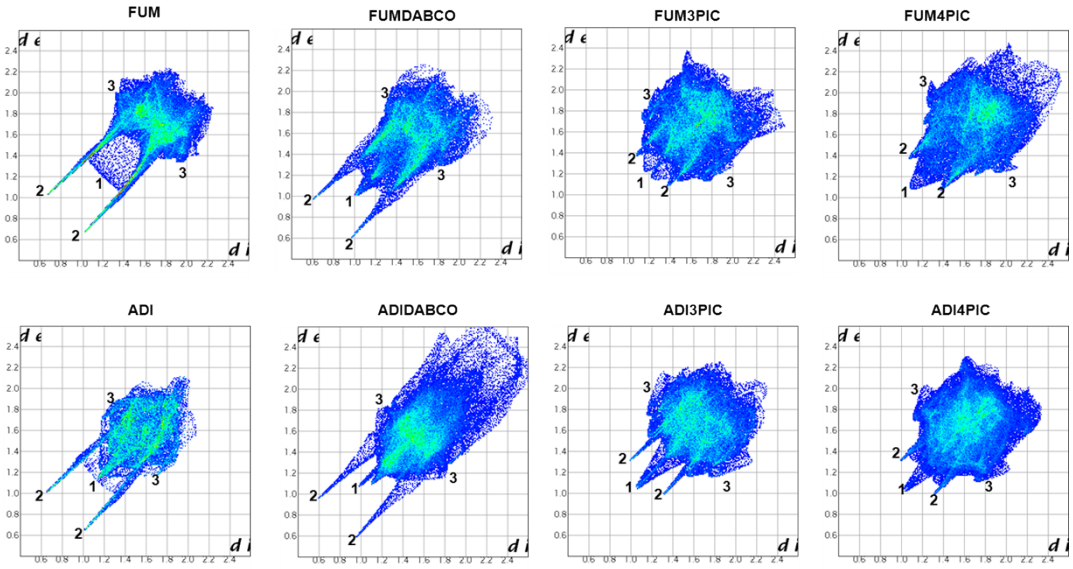

Fig. S9 The 2D plots derived from Hirshfeld surface analysis for **FUM**, **FUMDABCO**, **FUM3PIC**, **FUM4PIC**, **ADI**, **ADIDABCO**, **ADI3PIC** and **ADI4PIC**. Spikes labelled **1-3** represent the H•••H, O•••H and C•••H interactions