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Multicomponent supramolecular assembly of p-hydroxybenzoic acid and malonic acid: a deep insight into the formation of selective cocrystal

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Supporting Information

Table S1. Calculated geometrical parameters for PHBA-MA cocrystal using M062X-D3/6-311G (d,p) method.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.402076	-0.542629	0.321044
2	8	0	2.239931	1.668738	0.094248
3	8	0	6.382312	-0.087936	-0.648414
4	8	0	4.824326	-1.582088	-0.151545
5	6	0	2.914876	0.570858	0.237096
6	6	0	4.403606	0.772554	0.338266
7	1	0	4.691791	1.713385	-0.123210
8	1	0	4.632379	0.846791	1.407713
9	6	0	5.296175	-0.338303	-0.223679
10	1	0	1.250928	1.473800	0.071472
11	1	0	3.893692	-1.565844	0.131792
12	8	0	-0.292579	1.160813	0.034892
13	8	0	-6.463747	-0.259645	-0.171649
14	1	0	-6.866801	0.607652	-0.268892
15	8	0	-0.255690	-1.066013	0.221468
16	1	0	0.717321	-0.915074	0.259930
17	6	0	-2.347964	-0.013867	0.024229
18	6	0	-5.119412	-0.137261	-0.111272
19	6	0	-0.878100	0.086681	0.092945
20	6	0	-4.474308	1.099264	-0.182556
21	1	0	-5.056146	2.008615	-0.290804
22	6	0	-3.093208	1.155940	-0.114586
23	1	0	-2.573203	2.104260	-0.168323
24	6	0	-2.999974	-1.248537	0.094772
25	1	0	-2.415290	-2.153031	0.201966
26	6	0	-4.378417	-1.313104	0.027785
27	1	0	-4.907350	-2.255817	0.080023

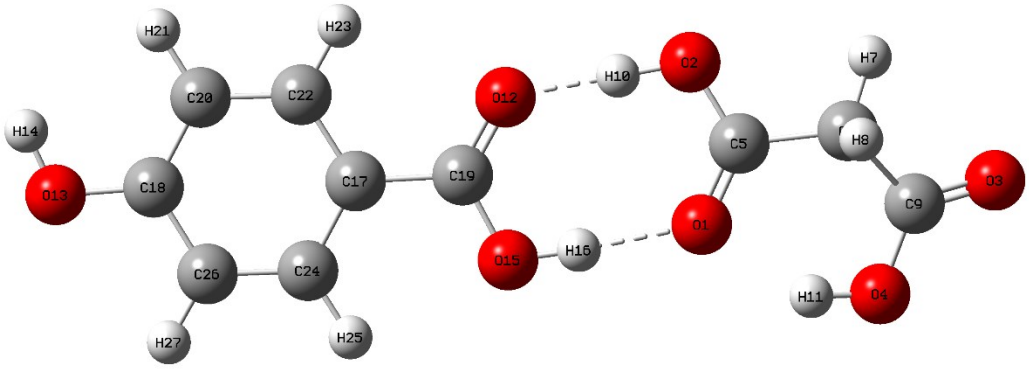

Fig.S1 Optimized structure for PHBA-MA cocrystal using M062X-D3/6-311G (d,p) method.

Table S2. Estimated physical components of the BEs for hydrogen bonds in PHBA-MA cocrystal[a].

Interactions	E_{elst}	E_{exch}	E_{ind}	E_{dis}
O7-H7···O5	-15.37	17.22	-7.30	-3.97
O6-H6···O16	-23.76	26.44	-11.56	-5.58
O15-H15···O5	-12.34	13.89	-5.76	-3.39
O17-H17···O7	-11.84	13.34	-5.51	-3.30

[b] E_{elst} term reflects the classical electrostatic interactions between the monomers; E_{exch} term represents the exchange-repulsion contribution; E_{ind} term signifies the induction contribution; E_{dis} term demonstrates the dispersion contribution.

[a] E_{elst}=1.718*BE+0.411; E_{exch}= -1.887*BE-0.115; E_{ind}=0.873*BE+0.719; E_{dis}=0.329*BE-0.949. Taken from reference [1].

References

[1] S. Emamian, T. Lu, H. Kruse and H. Emamian, J.Comput.Chem., 2019, 40, 2868-2881.