Supporting Information

Innovative Aminoglutethimide Co-crystals: Synthesis, Characterization, and Insights into Molecular Interactions

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Table S1. Geometric parameters of hydrogen bonds for co-crystals (Å, °).

compound	D-H…A	d(D-H)/ Å	d(H…A)/ Å	d(D…A)/ Å	∠(D-H…A)/ Å
AG-DNBA	N3-H3A…O7	0.860	2.348	2.950	127.450
	N3-H3B…O4	0.860	2.653	3.375	142.430
	N3-H3B…O8	0.859	2.654	3.306	133.670
	N3-H3B…O3	0.860	2.271	2.699	110.770
	N4-H4A…O3	0.860	2.158	2.990	162.800
AG-m-TA	O4-H4…N3	0.820	2.409	2.758	106.640
	O1-H1…O4	0.820	3.516	3.910	113.040

	N1-H1A…O1	0.860	2.200	2.994	153.610
	N2-H2A…O2	0.859	2.415	3.918	104.320
	N2-H2B…N2	0.860	3.201	3.743	123.360
	N2-H2B…O2	0.860	2.003	2.850	168.020
	N2-H2B…O3	0.860	2.590	2.982	108.880
	N2-H10…O10	0.820	1.980	2.736	152.100
	C31-H31…O2	0.930	2.640	3.213	120.500
	C31-H31…O2	0.930	2.130	3.028	162.900
	N3-H3…O3	0.860	2.080	2.936	179.100
AG-m-NBA	N1-H1A…O15	0.860	1.930	2.762	163.000
	N1-H1B…O9	0.860	2.230	2.765	119.900
	N2-H2B…O5	0.860	2.000	2.834	161.900
	C1-H1…O5	0.930	2.600	3.529	173.400
	C32-H32B…O2	0.970	2.480	3.294	141.000
	C38-H38…O9	0.930	2.490	3.387	162.700

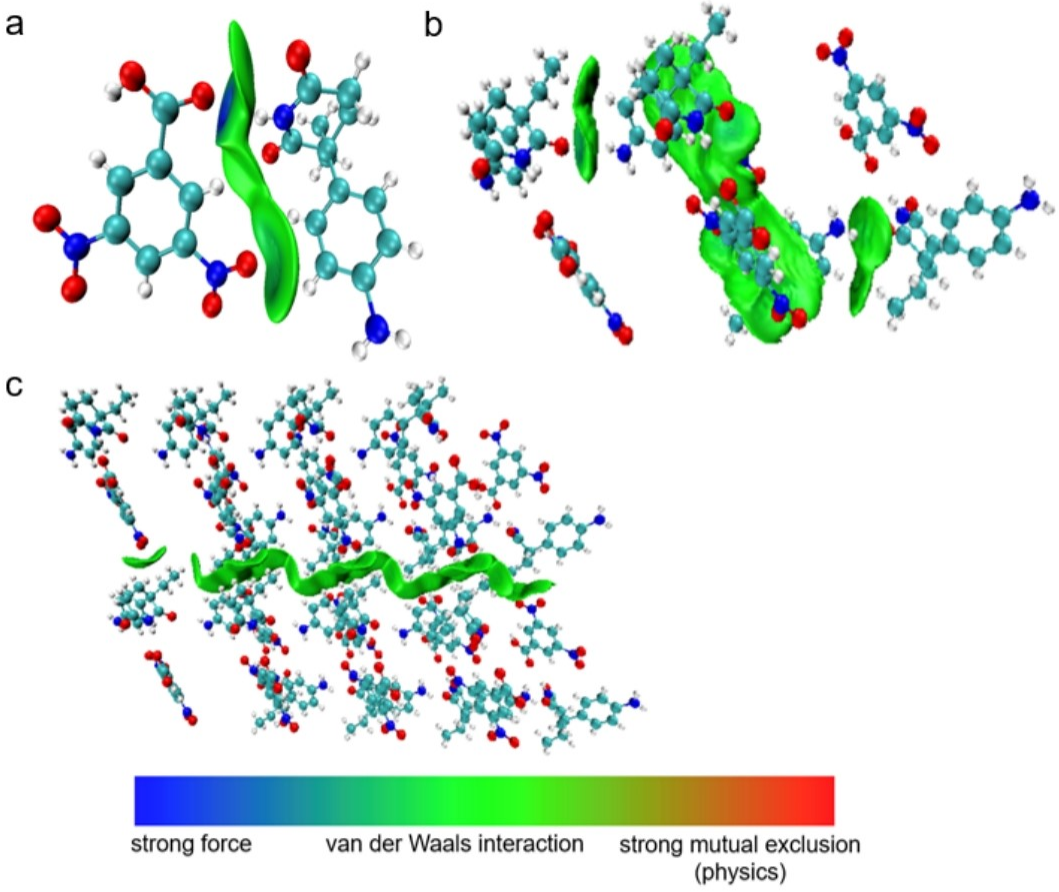

Figure S1. The sign(λ2)ρ colored isosurfaces of δg inter = 0.0004 a.u. corresponding to IGMH analysis of (a)asymmetric structural unit (b)one-dimensional chain structure and (c)two-dimensional plane structure of AG-DNBA co-crystal.

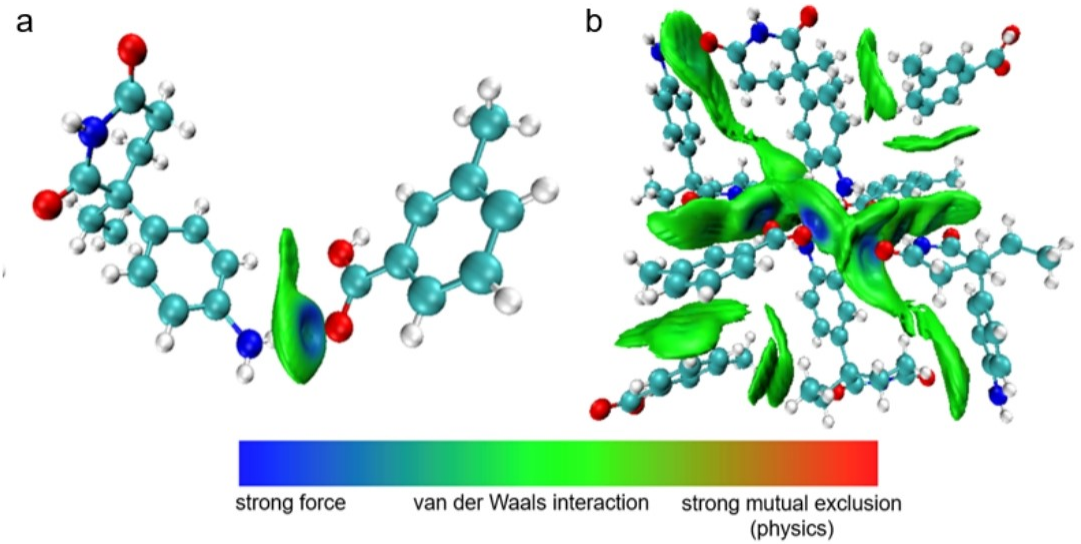

Figure S2. The sign(λ2)ρ colored isosurfaces of δg inter = 0.0004 a.u. corresponding to IGMH analysis of (a)asymmetric structural unit (b)octamer structure of AG-m-TA co-crystal.

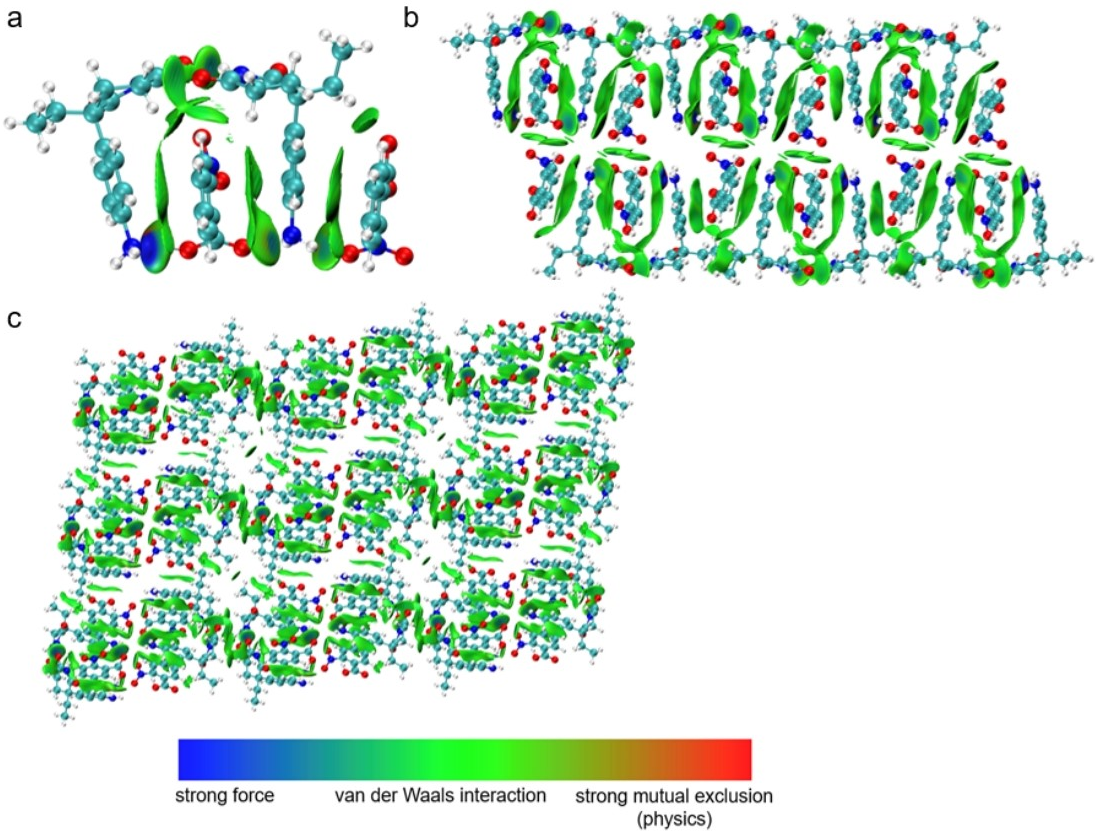

Figure S3. The sign(λ2)ρ colored isosurfaces of δg inter = 0.003 a.u. corresponding to IGMH analysis of (a)asymmetric structural unit (b)one-dimensional chain structure and (c)two-dimensional plane structure of AG-m-NBA co-crystal.