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SUPPLEMENTARY MATERIAL TO

Tuning crystal packing and reactivity through electrostatic and dispersion interactions: The case of phenytoin and its derivatives

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Table S-I. Comparation of total interaction energies (in kJ mol^{-1}) for the dimeric motif in compound **1-4**, calculated by using the DFT (CE‑B3LYP) method and the UNI force field.

Method	CrystalExplorer (CE-B3LYP)					UNI
	E_{ele}	E_{pol}	E_{dis}	E_{rep}	E_{tot}	E_{tot}
Comp. **1**						
D1	−39.80	−8.50	−20.50	40.00	−41.50	−38.49
D2	−37.30	−8.30	−6.80	39.30	−27.20	−26.06
D3	−9.00	−2.00	−26.20	14.90	−24.60	−5.63
D4	−1.70	−1.40	−26.60	13.70	−17.60	−21.60
D5	−9.00	−1.00	−26.00	26.70	−16.40	−15.10
D6	−2.30	−0.80	−4.40	1.80	−5.70	−25.32
Comp. **2**						
D1	−50.70	−12.10	−32.40	61.20	−53.00	−42.77
D2	−11.60	−1.80	−47.30	29.90	−36.40	−39.09
D3	−3.40	−2.80	−18.10	9.90	−15.40	−17.31
D4	−9.00	−2.20	−8.20	5.60	−14.80	−10.19
D5	−4.30	−0.70	−18.20	9.90	−14.70	−15.93
D6	−1.70	−0.80	−22.30	13.00	−13.80	−19.11
Comp. **3**						
D1	−91.30	−23.70	−24.10	98.70	−74.00	−53.44
D2	−21.70	−5.20	−42.30	29.40	−45.40	−36.79
D3	−9.90	−4.70	−41.90	24.70	−35.30	−38.34
D4	−9.00	−4.00	−32.50	15.80	−30.90	−35.34
Comp. **4**						
D1	−53.90	−12.60	−80.80	82.80	−85.50	−82.32
D2	−11.70	−1.80	−53.80	31.10	−41.30	−45.14
D3	−6.00	−0.40	−48.40	23.00	−34.60	−27.86
D4	−3.30	−2.90	−25.00	10.30	−20.90	−24.93

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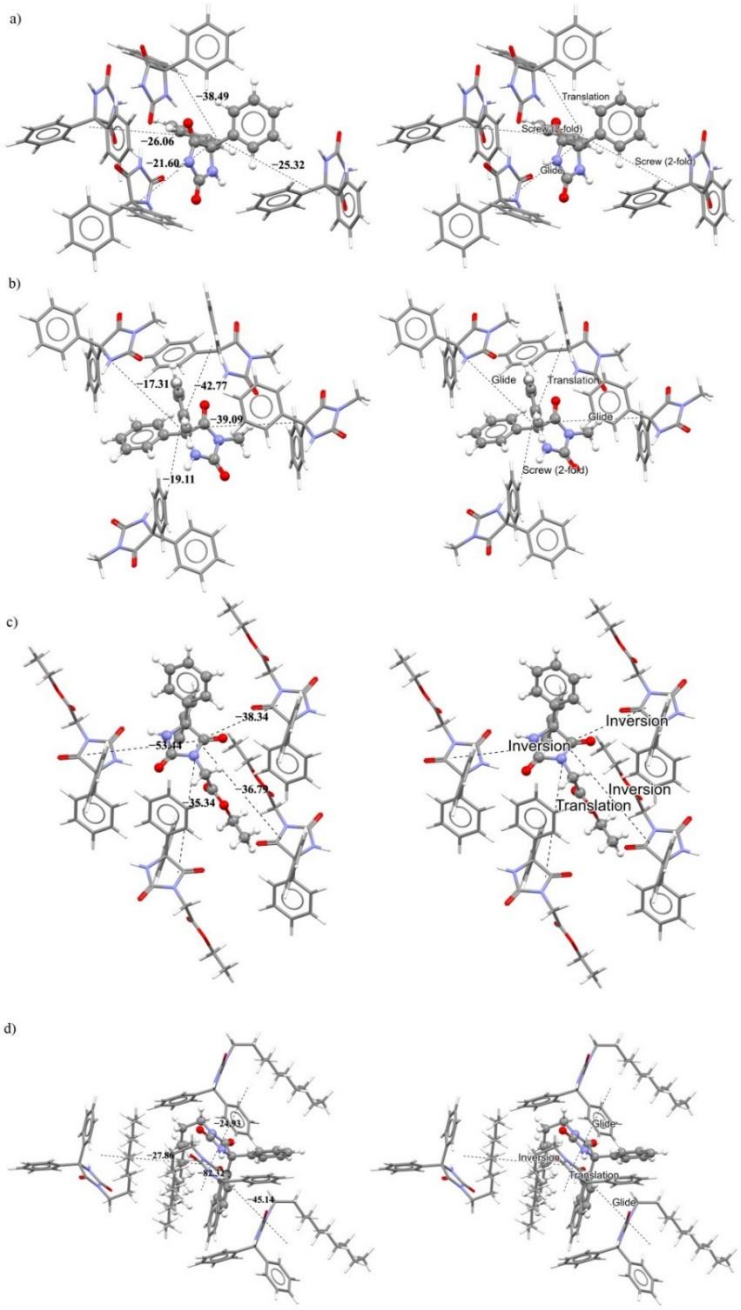

Figure S-1. The UNI force field calculated potentials (in kJ mol^{-1}) and a symmetry transformation for selected dimeric motifs in studied compounds **1-4**. The ball-and-stick style illustrates the asymmetric unit within the dimeric motif. Symmetry operations generating relevant molecular dimeric motifs: a) Identity (Translation): x, y, z; Screw axis (2-fold):

−x,1/2+y, −z (2-fold screw axis with direction [0, 1, 0] at 0, y, 0 with screw component [0, 1/2, 0]), Glide plane: 1/2+x, y, 1/2−z (Glide plane perpendicular to [0, 0, 1] with glide component [1/2, 0, 0]); b) Identity (Translation): x, y, z; Glide plane: 1/2+x, 1/2−y, 1/2+z (Glide plane perpendicular to [0, 1, 0] with glide component [1/2, 0, 1/2]); Screw axis (2-fold): 1/2−x, 1/2+y, 1/2−z (2-fold screw axis with direction [0, 1, 0] at 1/4, y, 1/4 with screw component [0, 1/2, 0]), c) Inversion centre: −x, −y, −z (Inversion at [0, 0, 0]), Identity (Translation): x, y, z, and, d) Identity (Translation): x, y, z; Glide plane: 1/2+x, 1/2−y, 1/2+z (Glide plane perpendicular to [0, 1, 0] with glide component [1/2, 0, 1/2]); Inversion centre: −x, −y, −z (Inversion at [0, 0, 0]); Glide plane: 1/2+x, 1/2−y, 1/2+z (Glide plane perpendicular to [0, 1, 0] with glide component [1/2, 0, 1/2]).

The equations for calculation of the global reactivity parameters

Ionization potential (IP) $= -E_{HOMO}$

Electron affinity (EA) $= -E_{LUMO}$

Chemical Hardness $(\eta) = 1/2\ (IP - EA)$

Chemical potential $(\mu) = -1/2(IP + EA)$

Electronegativity $(\chi) = -\mu$

Electrophilicity index $(\omega) = \mu^2/2\eta$