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Supplementary material

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

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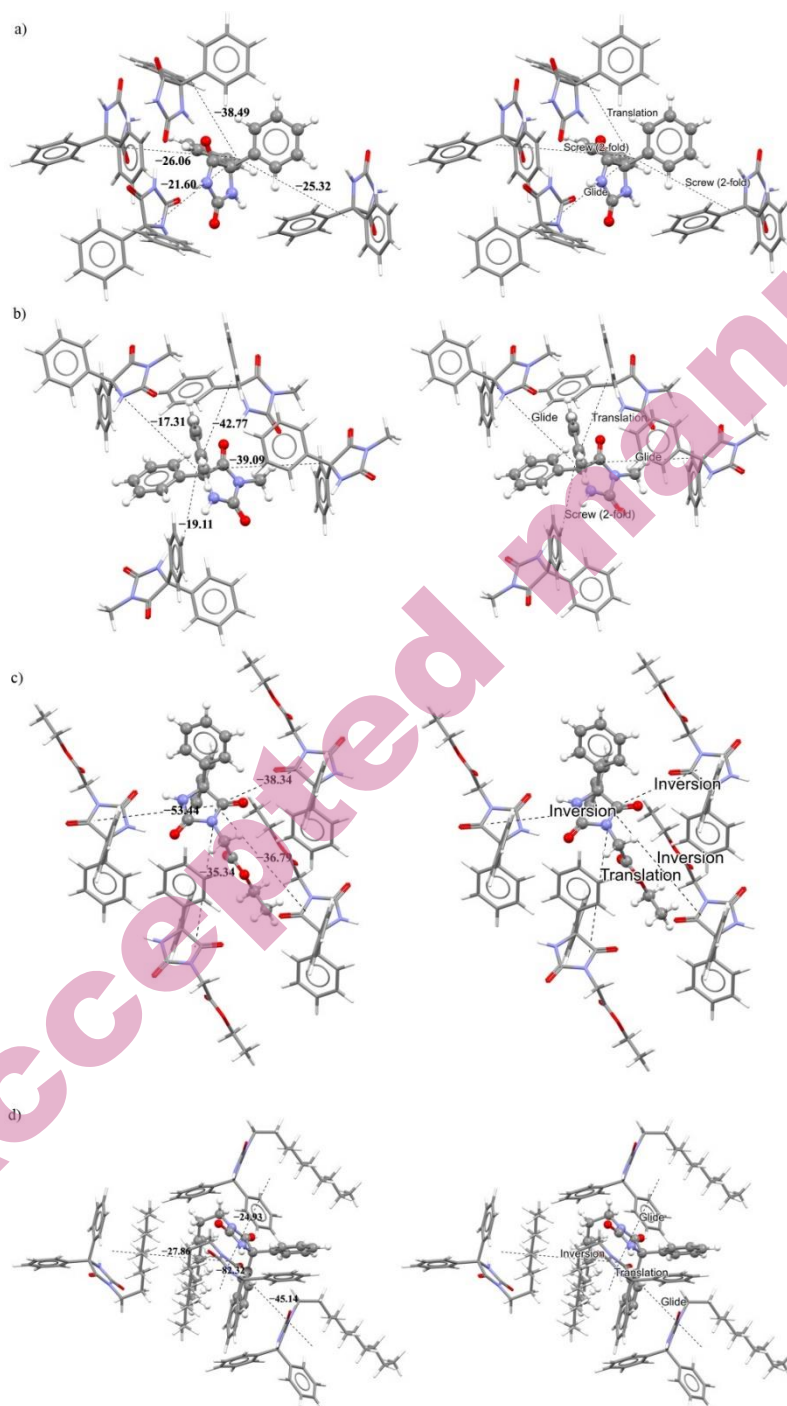


Figure S-I. The UNI force field calculated potentials (in kJ mol^{-1}) and a symmetry transformation for selected dimeric motifs in studied compounds 1-4. The ball-and-stick style illustrates the asymmetric unit within the dimeric motif. Symmetry operations generating relevant molecular dimeric motifs: 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 $[1/2, 0, 1/2]$).

Table S-I. Comparison 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

The equations for calculation of the global reactivity parameters

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

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

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

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

Electronegativity (χ) = $-\mu$

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