STRUCTURAL SCIENCE
CRYSTAL ENGINEERING
MATERIALS

Volume 76 (2020)

Supporting information for article:

Polymorphism of Monotropic Forms: Relationships of Thermochemical and Structural Characteristics

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Table S1 Average values of the descriptors selected for groups I and II

Group	α	ΣC_a	ΣC_d	N_{conf}	$N_{torsion}$	N_{rot}	N_d	N_a	N_{HB}
I	27.39	5.28	-2.50	60.31	9.69	5.15	1.03	3.42	0.95
II	29.91	5.50	-2.70	62.42	10.83	5.81	1.27	3.62	1.15
DELTA[a]	2.53	0.23	-0.2	2.12	1.13	0.66	0.24	0.20	0.20
ε [%][b]	9.2	4.3	7.9	3.5	11.7	12.9	23.0	5.7	21.3

[a] $DELTA = Y(II) - Y(I)$, where Y(I) and Y(II) are descriptors of groups I and II, respectively

[b] $\varepsilon = 100 \cdot |(Y(DO) - Y(I)) / Y(I)|$

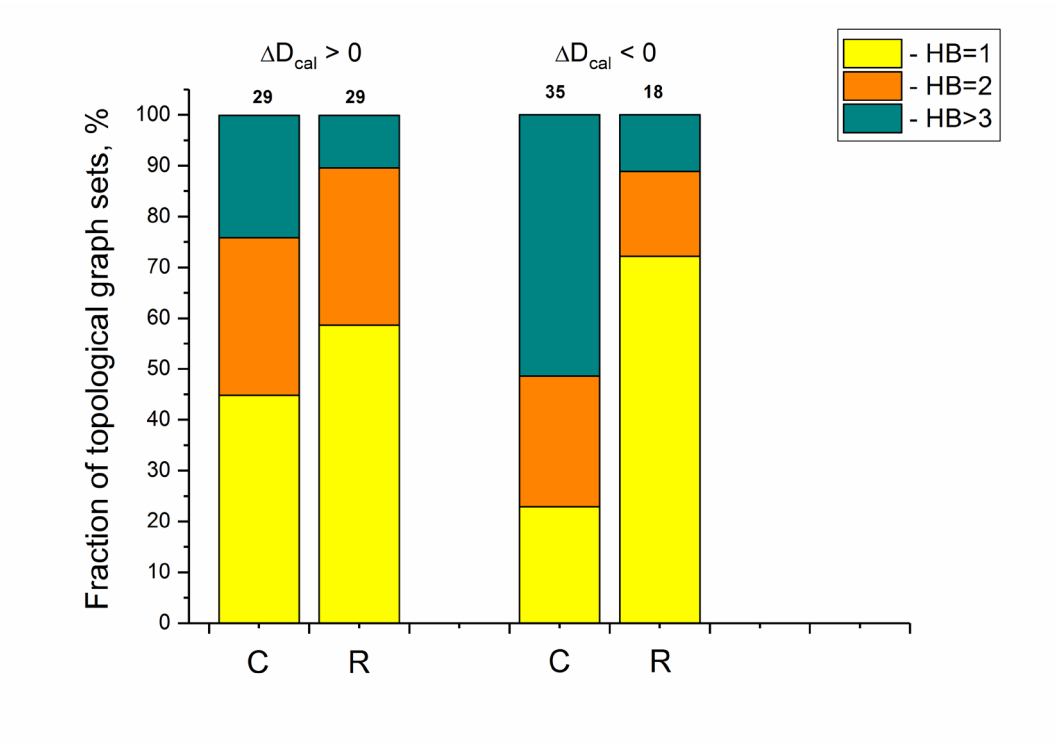
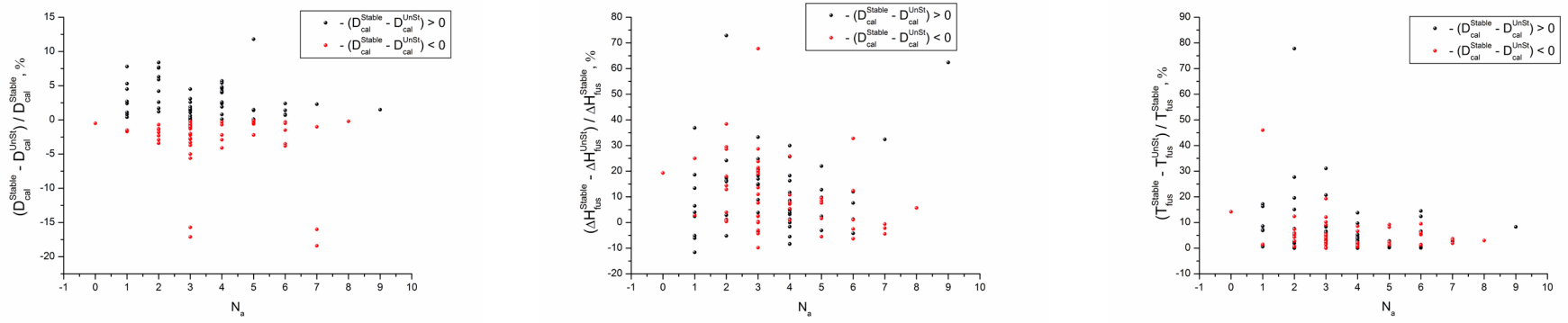
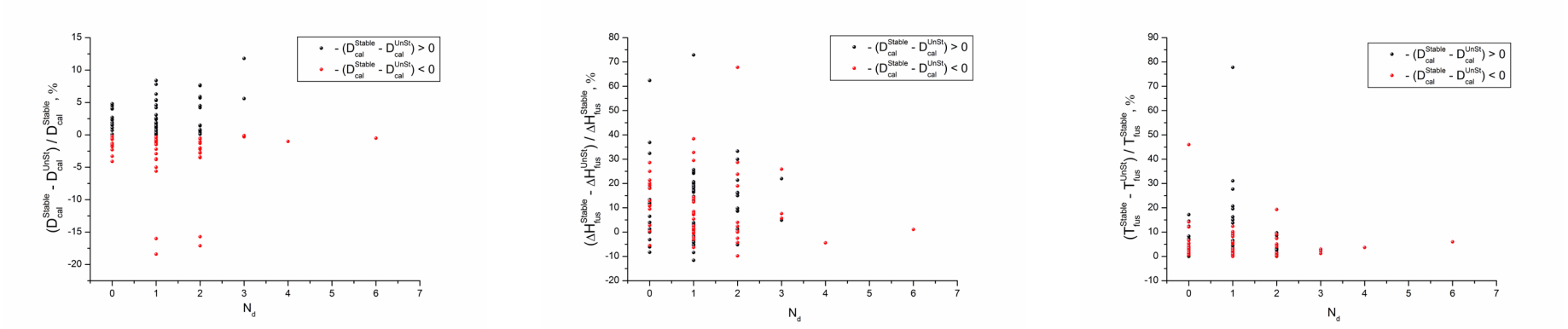


Figure S1 Relative distribution of the hydrogen bond number in group I ($\Delta D_{cal} > 0$) and group II ($\Delta D_{cal} < 0$) against topological graph sets



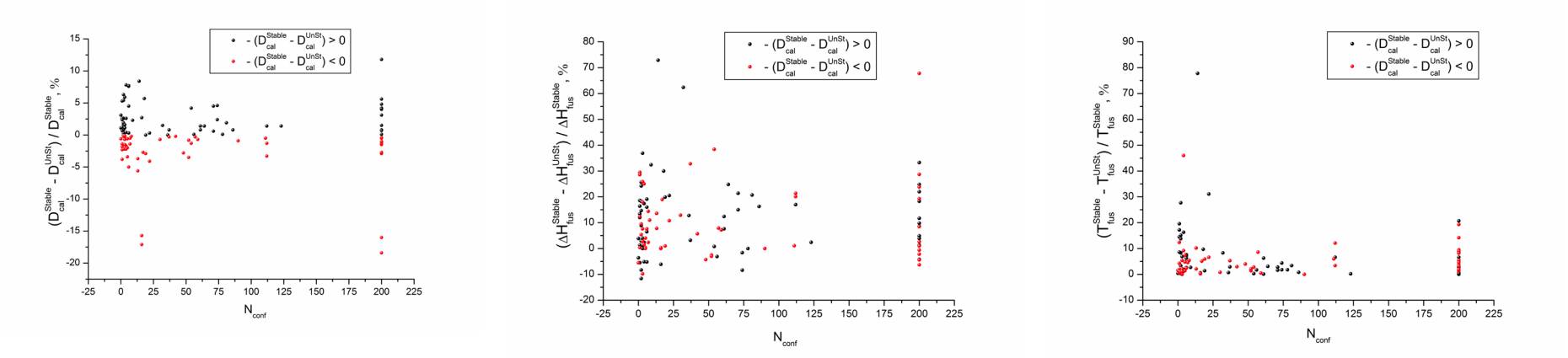
(a) (b) (c)

Figure S2 Distribution of the ΔD_{cal}, transition enthalpy and difference in melting points as a function the number of hydrogen bond acceptors (N_a)



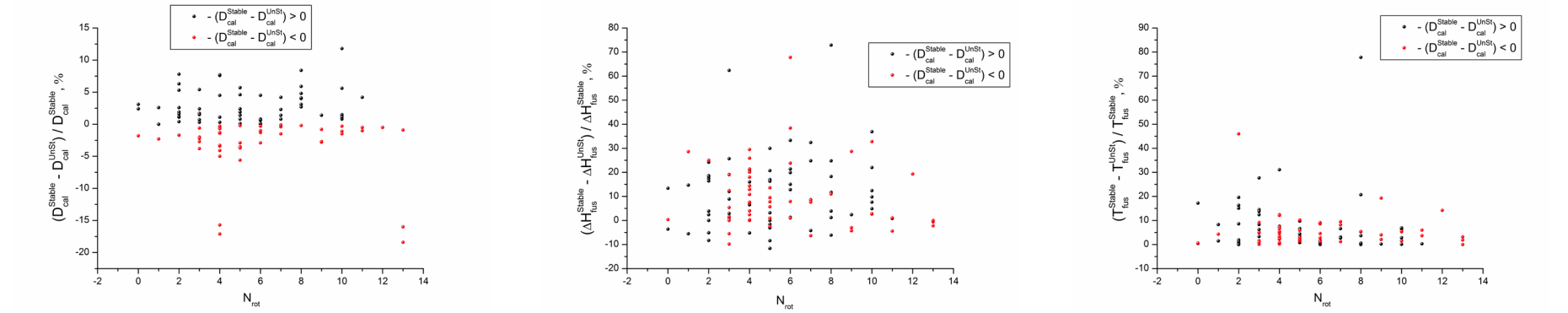
(a) (b) (c)

Figure S3 Distribution of the ΔD_{cal}, transition enthalpy and difference in melting points as a function the number of hydrogen bond donors (N_d)



(a) (b) (c)

Figure S4 Distribution of the ΔD_{cal} , transition enthalpy and difference in melting points as a function the number of conformers for a molecule (N_{conf})



(a) (b) (c)

Figure S5 Distribution of the ΔD_{cal}, transition enthalpy and difference in melting points as a function the number of rotatable bonds in a molecule (N_{rot})

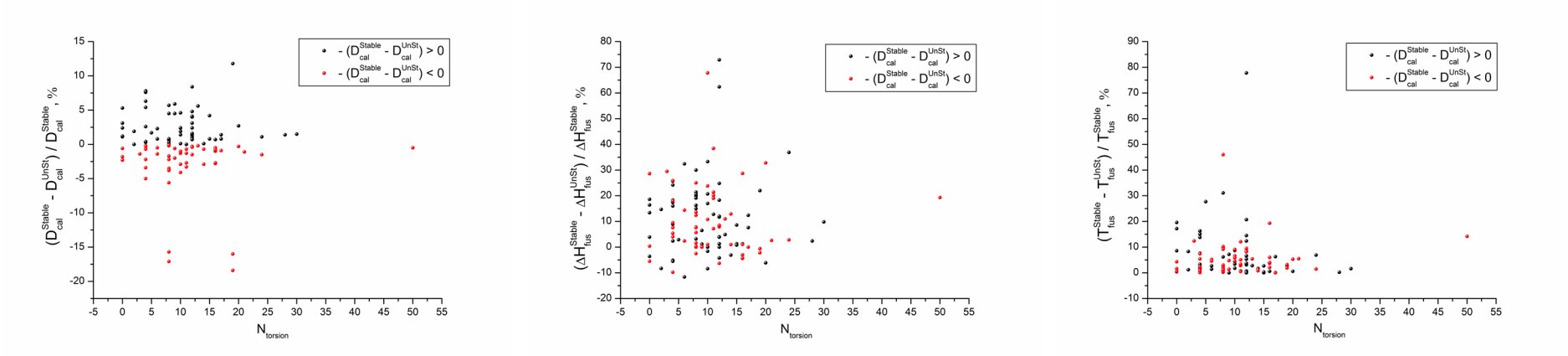
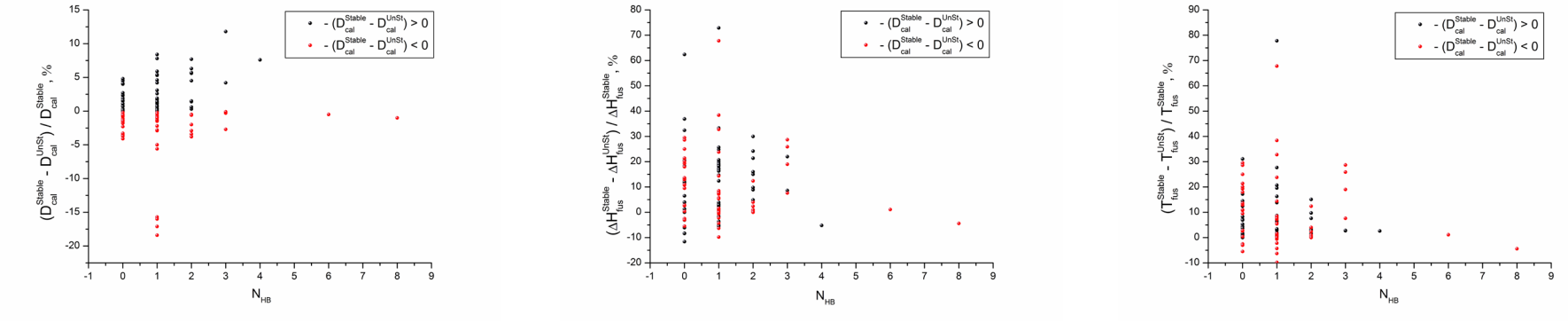
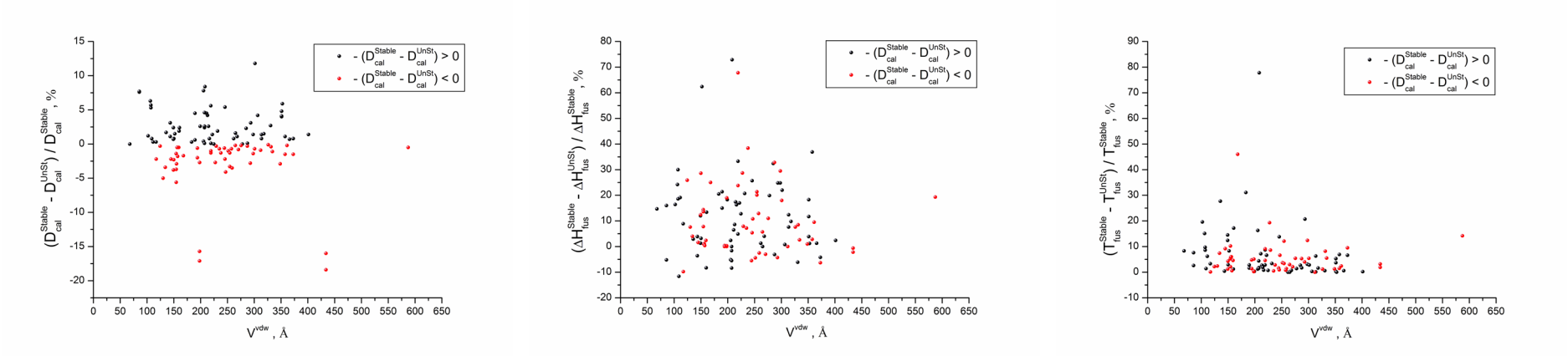


Figure S6 Distribution of the ΔD_{cal} , transition enthalpy and difference in melting points as a function the number of torsion angles in a molecule ($N_{torsion}$)



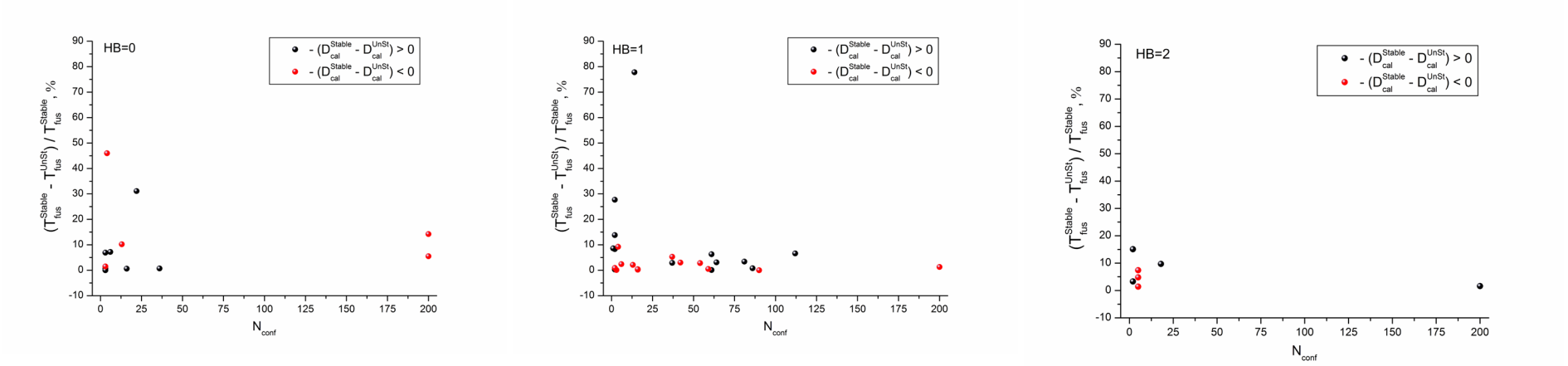
(a) (b) (c)

Figure S7 Distribution of the ΔD_{cal} , transition enthalpy and difference in melting points as a function the number of hydrogen bonds per molecule (N_{HB})



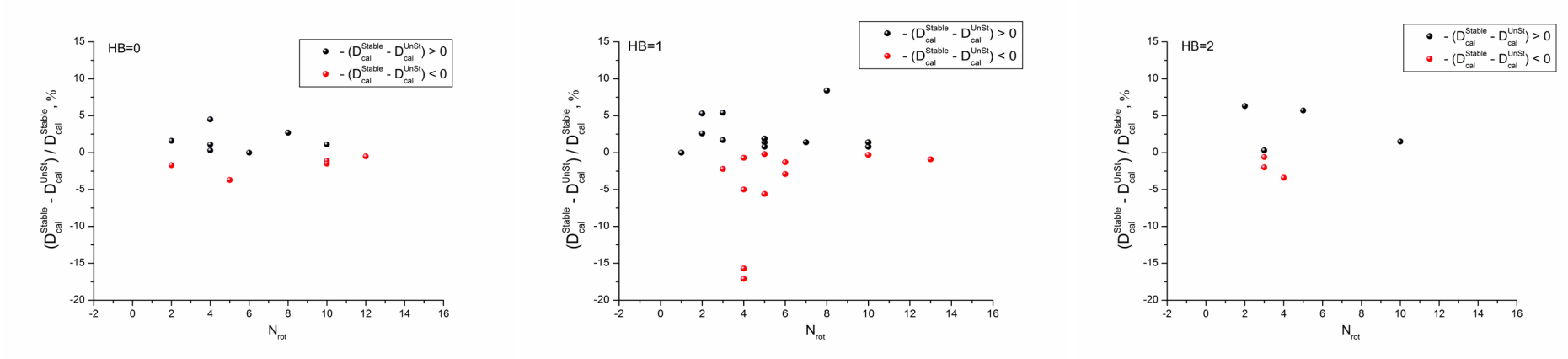
(a) (b) (c)

Figure S8 Distribution of the ΔD_{cal} , transition enthalpy and difference in melting points as a function of van der Waals volume of a molecule (V^{vdw})



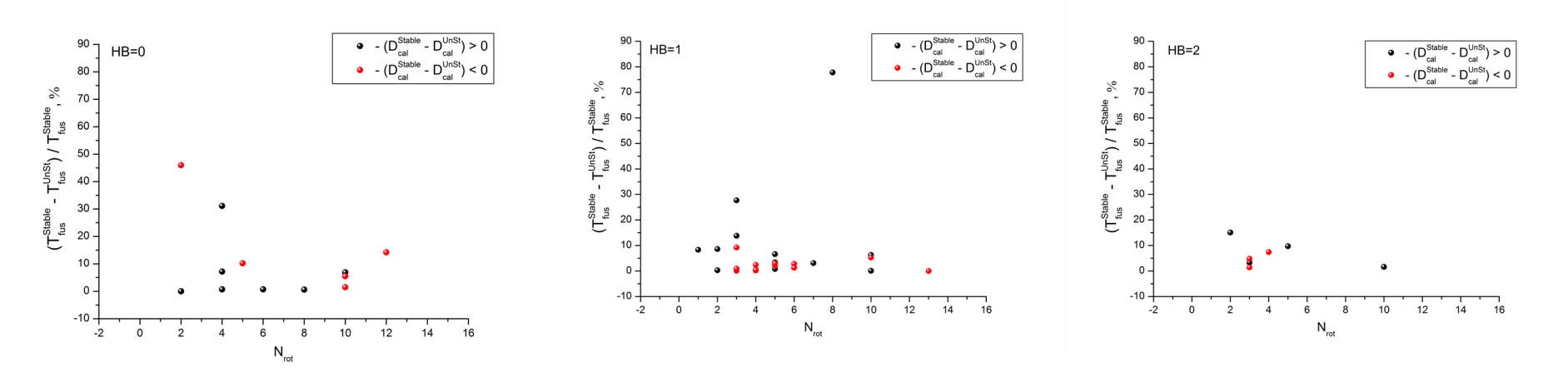
(a) (b) (c)

Figure S9 Distribution of the ΔT_{fus} parameter as a function of conformation numbers (N_{conf}) for different numbers of hydrogen bonds per molecule: (a) HB0, (b) HB1 and (c) HB2



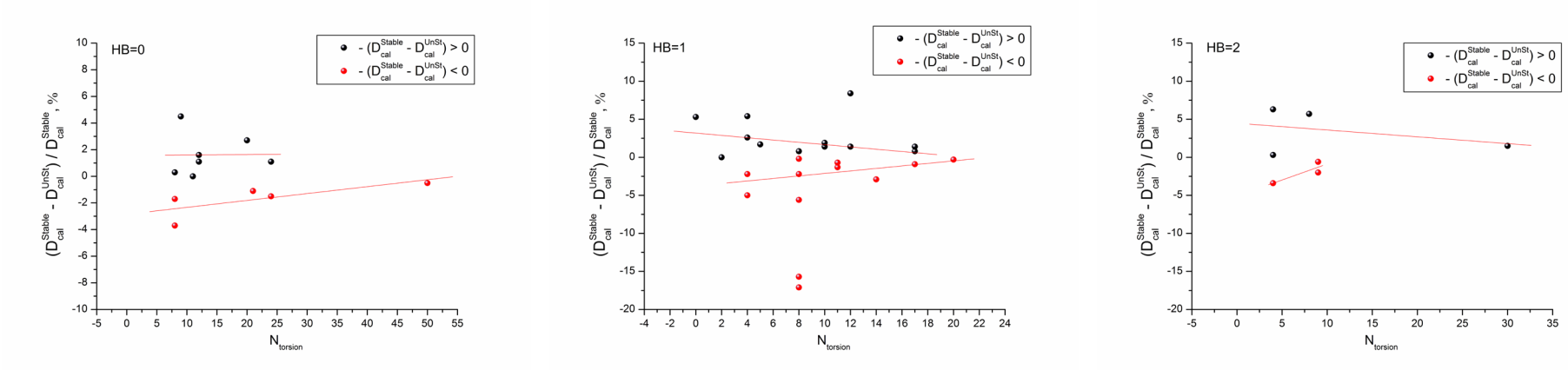
(a) (b) (c)

Figure S10 Distribution of the ΔD_{cal} parameter as a function of the number of rotatable bonds (N_{rot}) for different numbers of hydrogen bonds per molecule: (a) HB0, (b) HB1 and (c) HB2



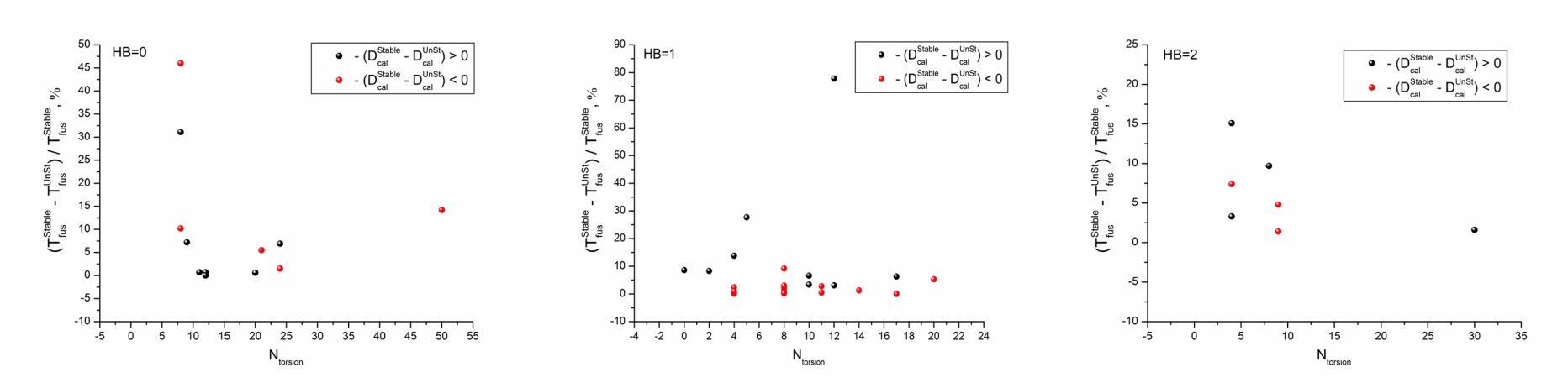
(a) (b) (c)

Figure S11 Distribution of the ΔT_{fus} parameter as a function of the number of rotatable bonds in a molecule (N_{rot}) for different numbers of hydrogen bonds per molecule: (a) HB0, (b) HB1 and (c) HB2



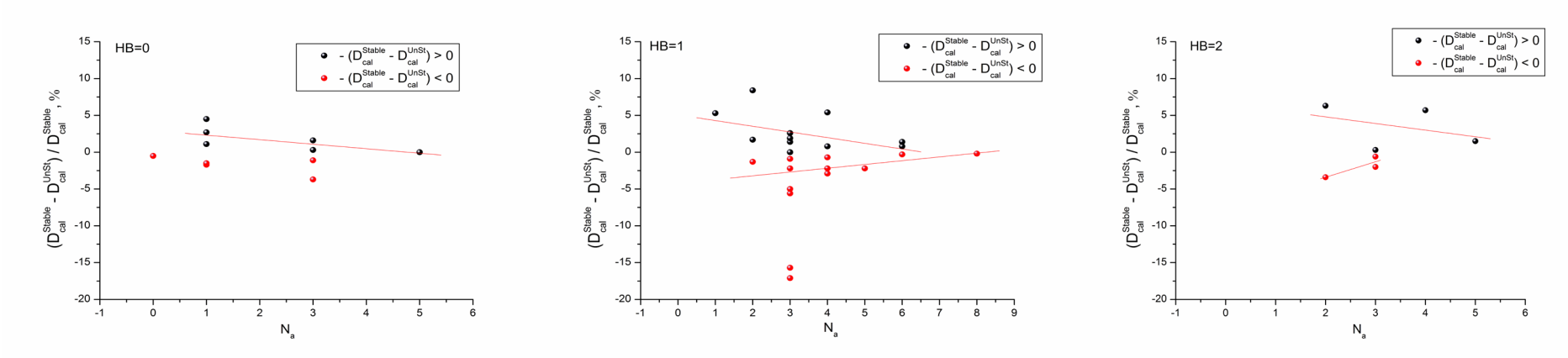
(a) (b) (c)

Figure S12 Distribution of the ΔD_{cal} parameter as a function of the number of torsion angles ($N_{torsion}$) for different numbers of hydrogen bonds per molecule: (a) HB0, (b) HB1 and (c) HB2



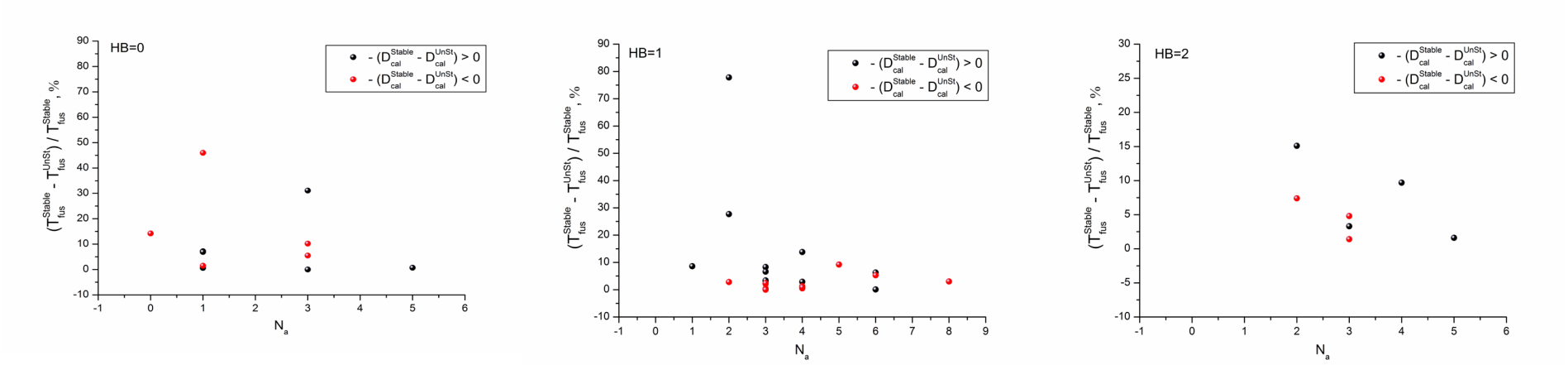
(a) (b) (c)

Figure S13 Distribution of the ΔT_{fus} parameter as a function of the number of torsion angles in a molecule ($N_{torsion}$) for different numbers of hydrogen bonds per molecule: (a) HB0, (b) HB1 and (c) HB2



(a) (b) (c)

Figure S14 Distribution of the ΔD_{cal} parameter as a function of the number of hydrogen bond acceptors (N_a) for different numbers of hydrogen bonds per molecule: (a) HB0, (b) HB1 and (c) HB2



(a) (b) (c)

Figure S15 Distribution of the ΔT_{fus} parameter as a function of the number of hydrogen bond acceptors (N_a) for different numbers of hydrogen bonds per molecule: (a) HB0, (b) HB1 and (c) HB2