

Supplementary Material

Table 1. Experimental folding free energies (in kJ mol^{-1}) for torsion balance molecules at 298 K.

Solvent	X	Y	ΔG
CDCl_3	NH_2	H	-1.00
CDCl_3	CH_3	H	-1.30
CDCl_3	H	H	-1.00
CDCl_3	OH	H	-1.09
CDCl_3	I	H	-1.21
CDCl_3	Br	H	-1.00
CDCl_3	CN	H	-1.00
CDCl_3	NO_2	H	-0.42
C_6D_6	H	CF_3	-3.31
C_6D_6	NH_2	CF_3	-3.88
C_6D_6	OH	CF_3	-2.75
C_6D_6	I	CF_3	-1.31
C_6D_6	Cl	CF_3	-1.71
C_6D_6	CN	CF_3	-0.65
C_6D_6	NO_2	CF_3	-0.24

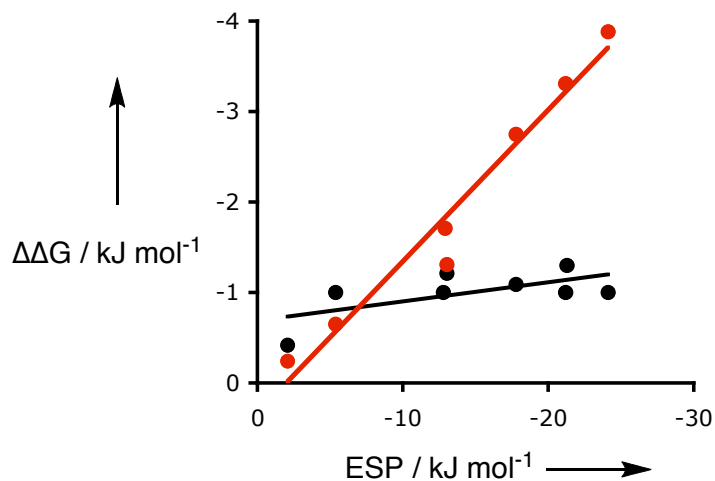


Figure 1. The experimental edge-to-face aromatic interaction free energies plotted as a function of the electrostatic potential (ESP) at the centre of the ‘face’ ring calculated at the DFT/B3LYP/6-31G* level (red: Y = CF_3 in benzene, black: Y = H in chloroform). The best fit straight lines are shown.