

Supporting Information for:

The Effect of Mechanical Interlocking on Crystal Packing: Prediction and testing

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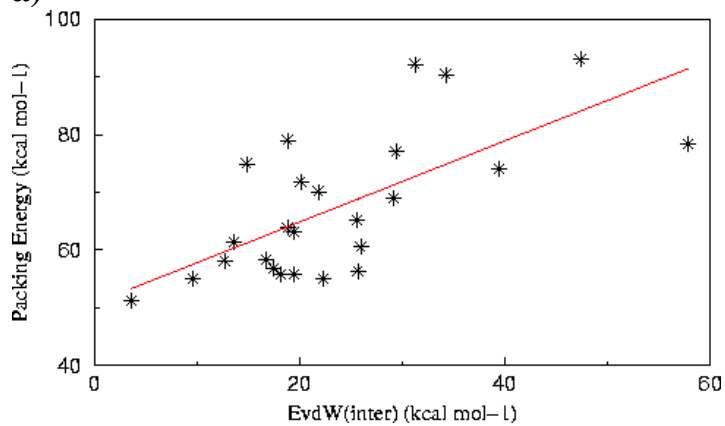
Table 1. PCA correlations matrix. The strongest correlations are shown in bold.

	PE	$E_{\text{mac-th}}$	$E_{\text{mac-xt}}$	E_{hb}	$E_{\text{hb(intra)}}$	$E_{\text{hb(inter)}}$	$E_{\text{hb(mac)}}$	$r_{\text{hb}(1)}$	$r_{\text{hb}(2)}$
PE	1	-0.28	0.87	0.64	-0.15	0.61	0.45	0.51	0.43
$E_{\text{mac-th}}$	-0.28	1	-0.48	-0.19	0.84	-0.71	-0.76	-0.78	-0.78
$E_{\text{mac-xt}}$	0.87	-0.48	1	0.45	-0.34	0.59	0.48	0.57	0.53
E_{hb}	0.64	-0.19	0.45	1	0.06	0.75	0.61	0.56	0.45
$E_{\text{hb(intra)}}$	-0.15	0.84	-0.34	0.06	1	-0.62	-0.72	-0.73	-0.80
$E_{\text{hb(inter)}}$	0.61	-0.71	0.59	0.75	-0.62	1	0.95	0.93	0.89
$E_{\text{hb(mac)}}$	0.45	-0.76	0.48	0.61	-0.72	0.95	1	0.92	0.91
$r_{\text{hb}(1)}$	0.51	-0.78	0.57	0.56	-0.73	0.93	0.92	1	0.98
$r_{\text{hb}(2)}$	0.43	-0.78	0.53	0.45	-0.80	0.89	0.91	0.98	1
W_m	0.45	-0.06	0.32	-0.03	0.15	-0.13	-0.19	-0.16	-0.21
Z_v	0.33	-0.07	0.32	-0.24	0.08	-0.24	-0.30	-0.21	-0.24
S_m	0.35	-0.14	0.40	-0.27	-0.03	-0.19	-0.23	-0.14	-0.15
V_m	0.35	-0.14	0.40	-0.27	-0.04	-0.18	-0.22	-0.13	-0.13
N_{nonH}	0.38	-0.01	0.27	-0.12	0.15	-0.20	-0.28	-0.20	-0.25
N_{nonH}/N_H	-0.05	0.22	-0.36	0.41	0.29	0.13	0.11	0.01	-0.05
S_{nonH}/S_H	0.11	0.26	-0.20	0.47	0.37	0.13	0.07	-0.01	-0.10
V_m/S_m	0.15	-0.08	0.19	-0.13	-0.13	-0.01	0.05	0.06	0.10
D_c	-0.19	-0.16	-0.33	-0.17	-0.10	-0.07	0.01	-0.13	-0.11
D_{el}	-0.32	-0.15	-0.37	-0.34	-0.16	-0.16	-0.07	-0.18	-0.13
C_k	-0.24	-0.24	-0.24	-0.42	-0.26	-0.16	-0.05	-0.15	-0.08

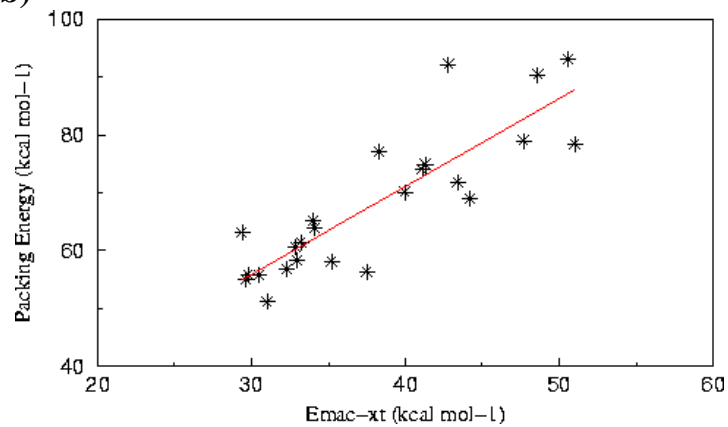
	W_m	Z_v	S_m	V_m	N_{nonH}	N_{nonH}/N_H	S_{nonH}/S_H	V_m/S_m	D_c	D_{el}	C_k
PE	0.45	0.33	0.35	0.35	0.38	-0.05	0.11	0.15	-0.19	-0.32	-0.24
$E_{\text{mac-th}}$	-0.06	-0.07	-0.14	-0.14	-0.01	0.22	0.26	-0.08	-0.16	-0.15	-0.24
$E_{\text{mac-xt}}$	0.32	0.32	0.40	0.40	0.27	-0.36	-0.20	0.19	-0.33	-0.37	-0.24
E_{hb}	-0.03	-0.24	-0.27	-0.27	-0.12	0.41	0.47	-0.13	-0.17	-0.34	-0.42
$E_{\text{hb(intra)}}$	0.15	0.08	-0.03	-0.04	0.15	0.29	0.37	-0.13	-0.10	-0.16	-0.26
$E_{\text{hb(inter)}}$	-0.13	-0.24	-0.19	-0.18	-0.20	0.13	0.13	-0.01	-0.07	-0.16	-0.16
$E_{\text{hb(mac)}}$	-0.19	-0.30	-0.23	-0.22	-0.28	0.11	0.07	0.05	0.01	-0.07	-0.05
$R_{\text{hb}(1)}$	-0.16	-0.21	-0.14	-0.13	-0.20	0.01	-0.01	0.06	-0.13	-0.18	-0.15
$R_{\text{hb}(2)}$	-0.21	-0.24	-0.15	-0.13	-0.25	-0.05	-0.10	0.10	-0.11	-0.13	-0.08
W_m	1.00	0.92	0.87	0.86	0.97	-0.17	-0.09	0.40	0.08	-0.02	0.11
Z_v	0.92	1.00	0.97	0.97	0.95	-0.47	-0.42	0.48	-0.03	-0.02	0.14
S_m	0.87	0.97	1.00	1.00	0.89	-0.62	-0.54	0.49	-0.10	-0.08	0.13
V_m	0.86	0.97	1.00	1.00	0.88	-0.62	-0.55	0.54	-0.12	-0.09	0.13
N_{nonH}	0.97	0.95	0.89	0.88	1.00	-0.21	-0.16	0.42	0.05	0.00	0.12
N_{nonH}/N_H	-0.17	-0.47	-0.62	-0.62	-0.21	1.00	0.92	-0.34	0.37	0.18	-0.04
S_{nonH}/S_H	-0.09	-0.42	-0.54	-0.55	-0.16	0.92	1.00	-0.44	0.27	0.05	-0.16
V_m/S_m	0.40	0.48	0.49	0.54	0.42	-0.34	-0.44	1.00	-0.21	-0.17	-0.02
D_c	0.08	-0.03	-0.10	-0.12	0.05	0.37	0.27	-0.21	1.00	0.95	0.90
D_{el}	-0.02	-0.02	-0.08	-0.09	0.00	0.18	0.05	-0.17	0.95	1.00	0.96
C_k	0.11	0.14	0.13	0.13	0.12	-0.04	-0.16	-0.02	0.90	0.96	1.00

Figure 1

a)



b)



c)

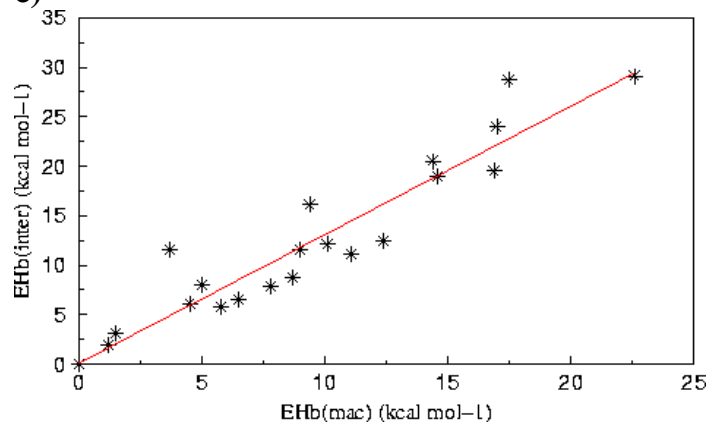


Figure 1 continued

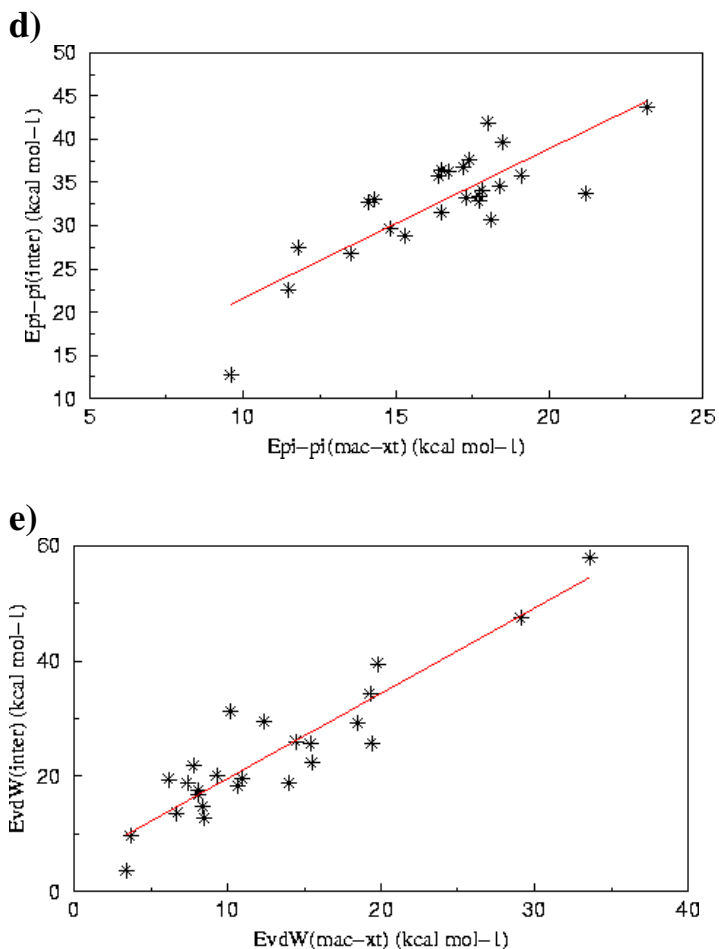


Figure 1. Correlation between some non-covalent interactions: a) PE versus other van der Waals energy; b) PE versus the interaction energies of the macrocycle with the crystal environment; c) rotaxane-crystal hydrogen bond energy versus macrocycle-crystal hydrogen bond energy; d) rotaxane-crystal π - π stacking energy versus macrocycle-crystal π - π stacking energy; e) rotaxane-crystal other van der Waals energy versus macrocycle-crystal other van der Waals energy.

