A Computational Characterization of the Hydrogen-Bonding and Stacking Interactions of Hypoxanthine

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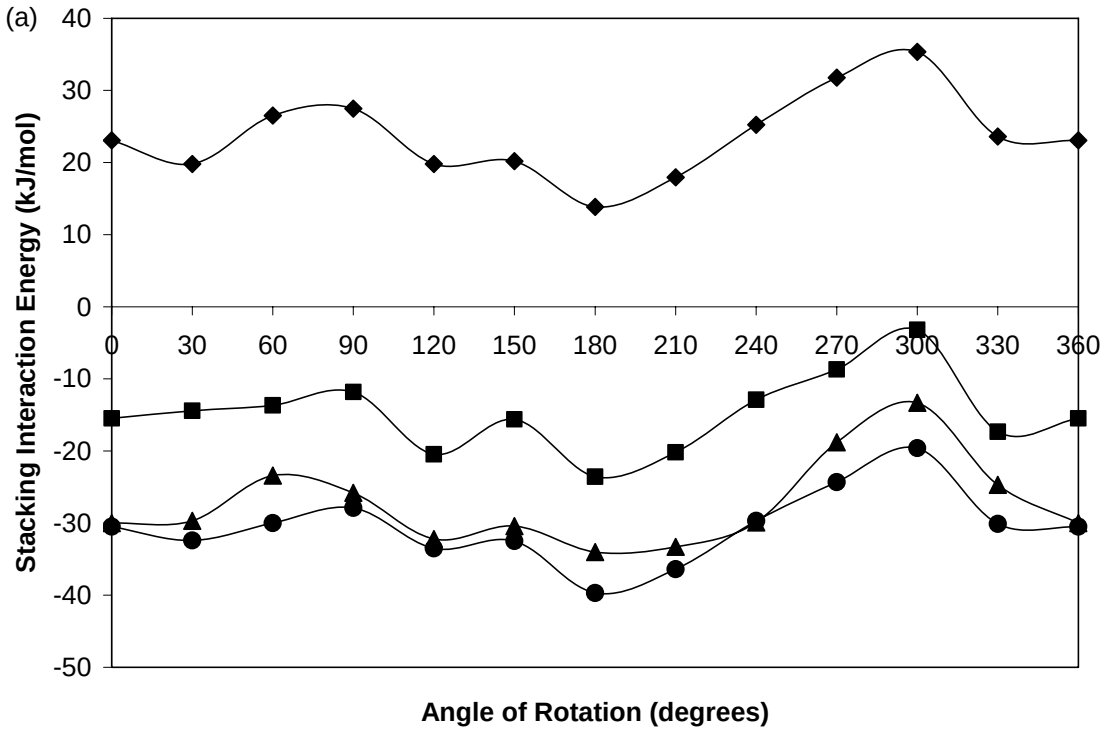
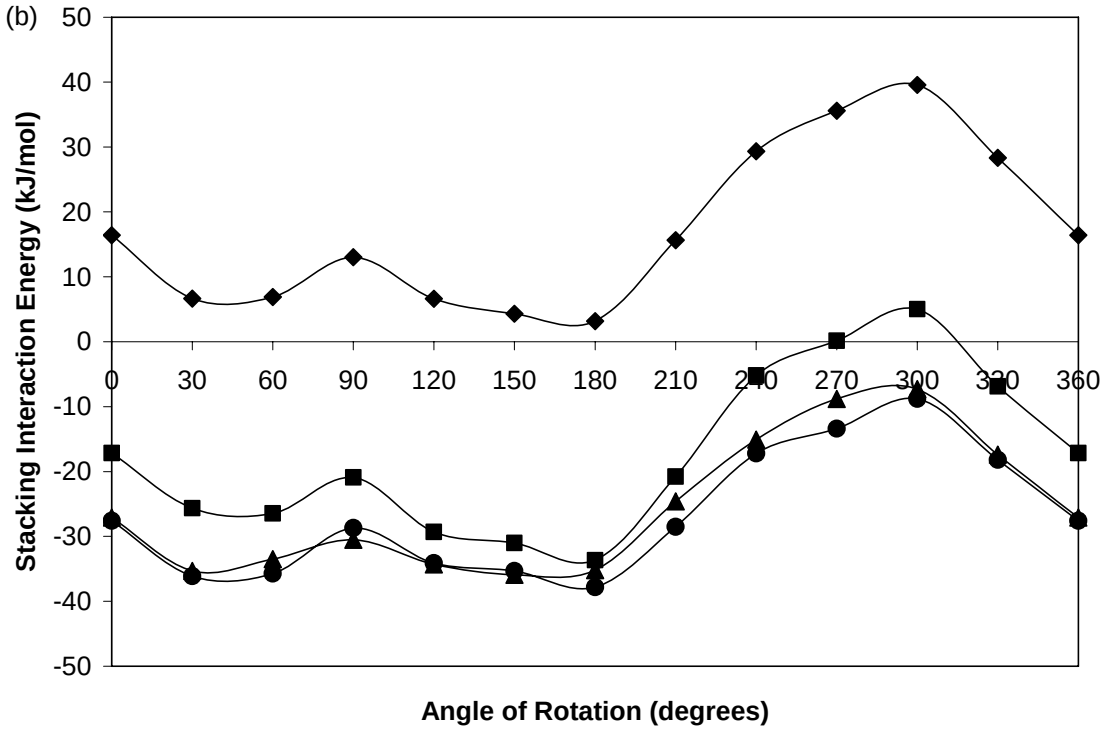
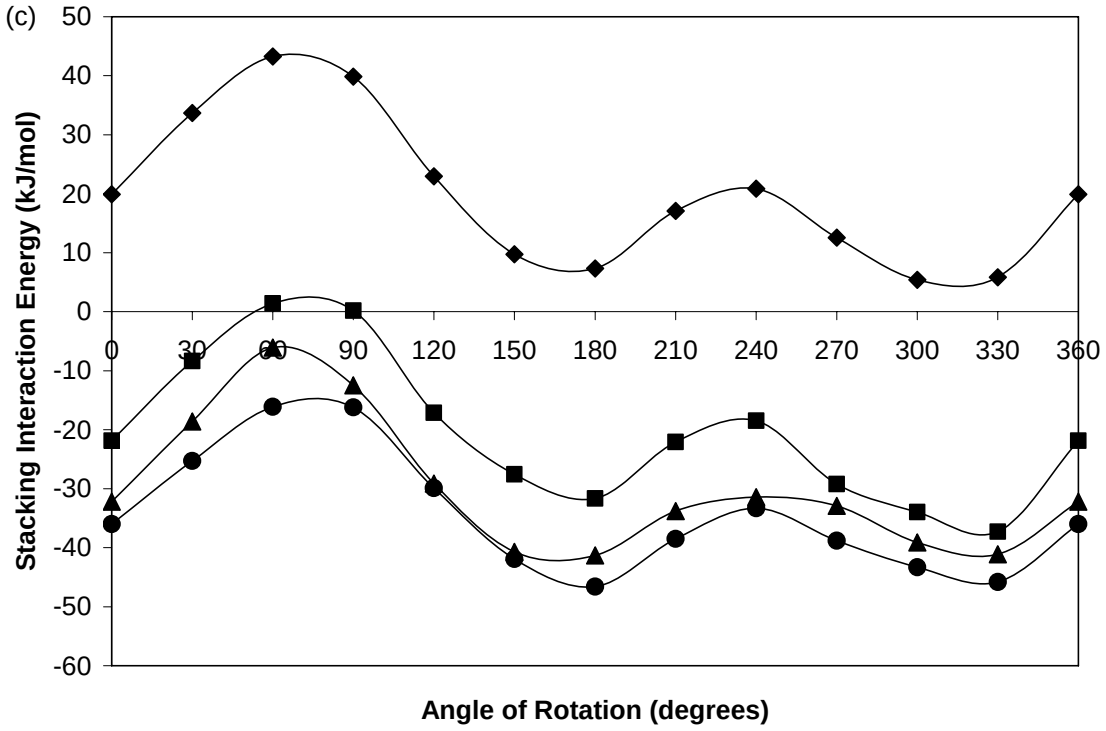
Supporting Information

(Figures S1 and S2, Table S1)

Figure S1: Stacking interaction energy (kJ mol^{-1}) as a function of the angle of rotation (α) for interstrand hypoxanthine pairs with (a) adenine, (b) cytosine, (c) guanine and (d) thymine calculated with MP2/6-31G*(0.25) (circles), AMBER (triangles), PWB6K (squares) and B3LYP (diamonds).






(c)
Stacking Interaction Energy (kJ/mol)
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
0
30
60
90
120
150
180
210
240
270
300
330
360
Angle of Rotation (degrees)

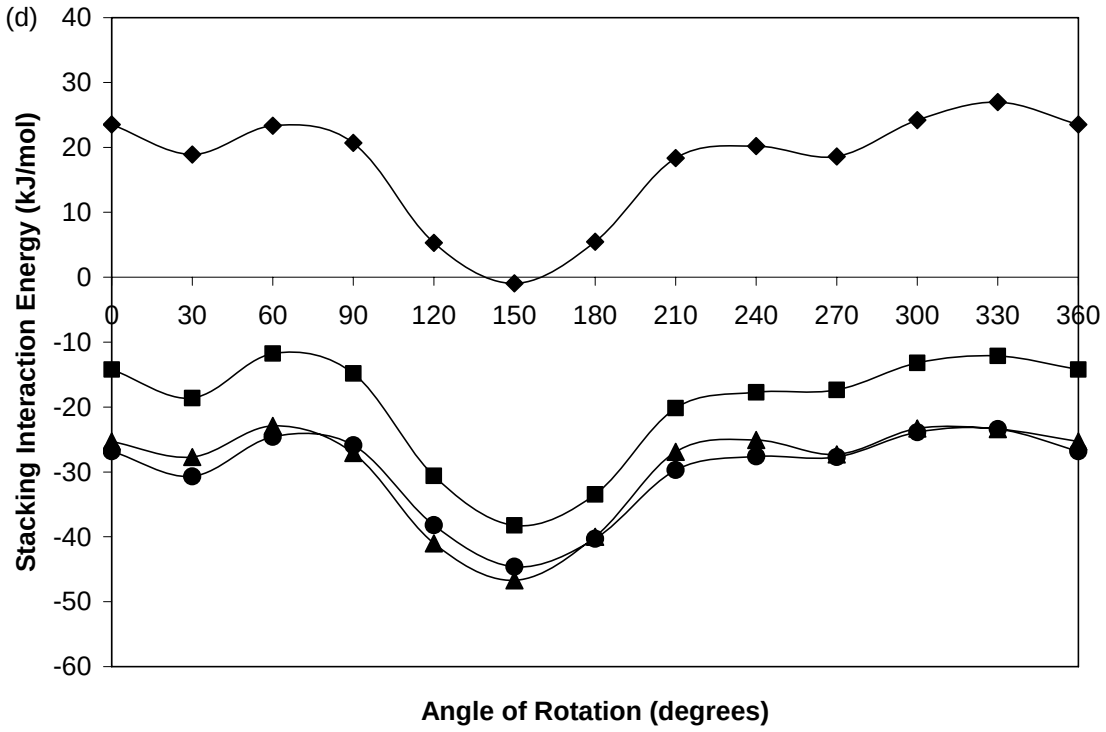

(d)
Stacking Interaction Energy (kJ/mol)
40
30
20
10
0
-10
-20
-30
-40
-50
-60
0
30
60
90
120
150
180
210
240
270
300
330
360
Angle of Rotation (degrees)

Figure S2: Interstrand hypoxanthine and natural nucleobase stacked dimers (a) with the angle of rotation (α) that leads to the strongest MP2/6-31G*(0.25) binding and (b) with dipole moments of the monomers aligned in opposing directions.

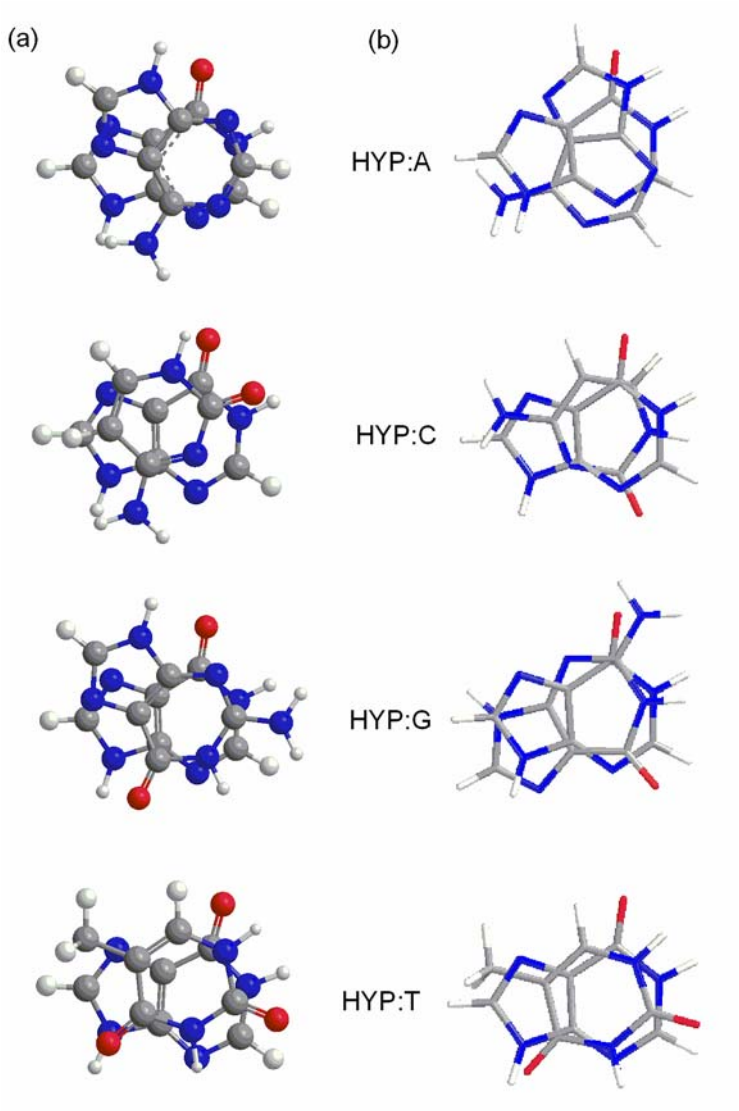
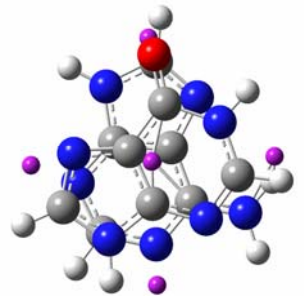
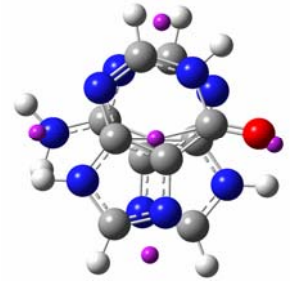
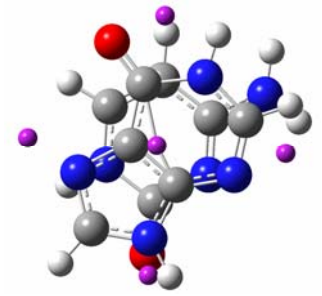
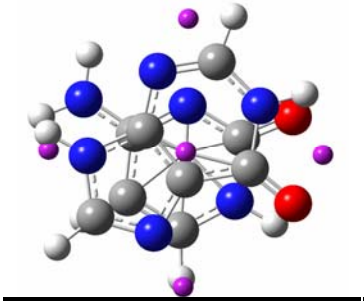
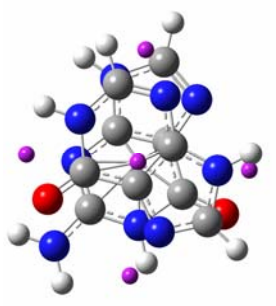
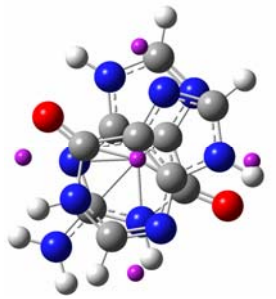
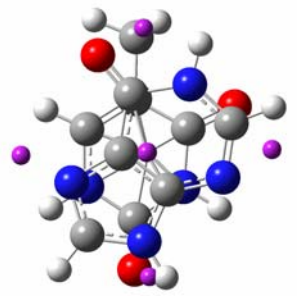
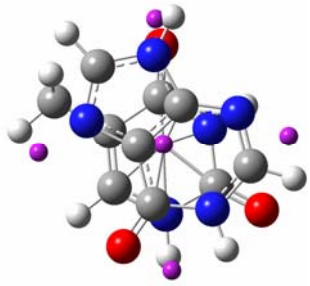


Table S1: Binding Strengths (kJ mol^{-1}) and Definition of Axes for R_2 Displacement Scans for Hypoxanthine Stacked with the Natural Nucleobases.[a]

Dimer	Direction (deg.)	R_2 = 0.5 Å	R_2 = 1.0 Å
HYP:A (intra) 	0	36.2	36.1
	45	40.7	44.2
	90	43.7	46.9
	135	44.2	44.2
	180	43.2	42.5
	225	41.0	39.0
	270	37.7	35.4
	315	35.0	32.7
	360	36.2	36.1
HYP:A (inter) 	0	40.1	39.1
	45	39.9	41.3
	90	38.7	37.9
	135	36.9	32.3
	180	37.8	34.5
	225	40.5	39.6
	270	42.7	44.6
	315	42.3	45.1
	360	40.1	39.1
HYP:C (intra) 	0	36.0	34.1
	45	38.2	38.8
	90	39.3	36.7
	135	39.9	39.1
	180	39.0	35.5
	225	38.8	37.7
	270	37.9	37.0
	315	35.7	32.2
	360	36.0	34.1
HYP:C (inter) 	0	34.7	31.3
	45	33.0	30.1
	90	32.4	26.6
	135	34.3	30.3
	180	37.6	35.0
	225	39.9	38.1
	270	39.9	37.6
	315	37.6	34.4
	360	34.7	31.3

HYP:G (intra) 	0	43.2	39.9
	45	40.9	35.1
	90	43.9	42.4
	135	47.7	48.4
	180	49.6	48.2
	225	50.1	50.7
	270	48.2	44.7
	315	46.5	44.9
	360	43.2	39.9
HYP:G (inter) 	0	43.0	37.5
	45	44.9	44.3
	90	45.9	47.3
	135	46.6	44.2
	180	49.1	49.2
	225	48.0	45.3
	270	44.5	38.1
	315	42.7	36.2
	360	43.0	37.5
HYP:T (intra) 	0	42.7	41.3
	45	41.2	36.9
	90	40.8	34.2
	135	43.5	39.2
	180	45.9	43.5
	225	46.3	44.2
	270	45.5	44.6
	315	43.7	40.7
	360	42.7	41.3
HYP:T (inter) 	0	45.4	42.5
	45	46.0	44.3
	90	45.0	43.3
	135	41.6	38.7
	180	39.1	33.5
	225	41.3	38.5
	270	44.3	42.7
	315	45.1	43.3
	360	45.4	42.5

[a]Note that the axes for the R_2 directional shifts are indicated with (purple) dummy atoms, where the 0º shift is to the right, 90º to the top, 180º to the left and 270º to the bottom.