Supplementary Material

Solution structures of purine base analogues 6-chloroguanine, 8-azaguanine and allopurinol

Spriha Gogia¹ and Mrinalini Puranik^{2*}

¹National Centre for Biological Sciences, Bangalore, India - 560065

²Indian Institute of Science Education and Research, Pune, India – 411 008

Submitted to: Journal of Biomolecular Structure and Dynamics

22 August 2012

*Correspondence to: Mrinalini Puranik, Indian Institute of Science Education and Research, Pune, India. E-mail: mrinalini@iiserpune.ac.in

Table SI

Interatomic bond distances and partial Mulliken charges of 6-chloroguanine and 8-azaguanine obtained from DFT (B3LYP/6-31G(d,p)) calculations.

Bond distances			Charge distribution		
Bond	6-ClG	8-azaG	Atom	6-ClG	8-azaG
C6—O/ C6—Cl	1.749	1.221	N1	-0.485	-0.609
N1—C2	1.36	1.387	C2	0.616	0.687
C2—N3	1.345	1.304	N3	-0.556	-0.549
N3—C4	1.329	1.366	C4	0.542	0.42
C4—C5	1.413	1.392	C5	0.224	0.29
C5—C6	1.397	1.438	C6	0.08	0.596
C6—N1	1.316	1.416	N7	-0.484	-0.447
C4—N9	1.373	1.37	C8/N8	0.282	-0.033
N9—C8/ N9—N8	1.387	1.307	N9	-0.586	-0.352
C8—N7/ N8—N7	1.306	1.349	N1H		0.281
N7—C5	1.384	1.357	N2	-0.631	-0.641
C2—N2	1.364	1.377	N2H2a	0.284	0.271
N2—H2a	1.007	1.011	N2H2b	0.278	0.295
N2—H2b	1.007	1.011	C6O/C6Cl	0.031	-0.508
N1—H		1.013	C8H	0.128	
N9—H	1.009		N9H	0.275	
N7—H		1.01	N7H		0.298

Table SII

Interatomic bond distances and partial Mulliken charges of Allopurinol (N8H and N9H tautomers) obtained from DFT (B3LYP/6-31G(d,p)) calculations.

Bond distances			Charge distribution		
Bond	Alp N8H	Alp N9H	Atom	Alp N8H	Alp N9H
C6—O	1.221	1.219	N1	-0.553	-0.55
N1—C2	1.38	1.367	C2	0.29	0.305
C2—N3	1.292	1.301	N3	-0.477	-0.502
N3—C4	1.38	1.366	C4	0.457	0.536
C4—C5	1.429	1.402	C5	-0.43	0.052
C5—C6	1.448	1.442	C6	0.552	0.551
C6—N1	1.414	1.431	N7	0.111	0.274
C5—C7	1.385	1.417	C8	-0.315	0.087
C7—N8	1.352	1.327	N9	-0.364	-0.422
N8—N9	1.356	1.363	N1H	0.28	0.284
C4—N9	1.336	1.353	C6O	-0.503	-0.501
N8—H/ N9—H	1.009	1.009	C2H	0.125	0.284
C7—H	1.079	1.081	C8H	0.291	
N1—H	1.012	1.013	N9H		0.286
C2—H	1.088	1.087	N7H/ C7H	0.148	0.128