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Deformations of Promoter DNA Bound to Carcinogens Help Interpret Effects on TATA-element Structure and Activity

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Supplementary Material

Table 1: Partial charges, atom types and topologies of $10S(+)$ - and $10R(-)$ -*trans-anti*-[BP]- N^6 -dA adducts at the position A_1 of the TATA box in the following systems.

Atom Name	Atom Type	Topology	Partial Charge				
			$10S(+)$ - <i>trans</i> -[A_1]		$10R(-)$ - <i>trans</i> -[A_1]		
			II	III	II	III	IV
P	P	M	1.2209	1.2212	1.2212	1.2212	1.2216
O1P	O2	E	-0.7932	-0.7936	-0.7931	-0.7939	-0.7930
O2P	O2	E	-0.7932	-0.7936	-0.7931	-0.7939	-0.7930
O5'	OS	M	-0.4914	-0.4890	-0.4964	-0.4873	-0.5033
C5'	CT	M	-0.0337	-0.0152	-0.0367	-0.0023	0.0236
H5'1	H1	E	0.0795	0.0847	0.0842	0.0810	0.0655
H5'2	H1	E	0.0795	0.0847	0.0842	0.0810	0.0655
C4'	CT	M	0.2233	0.1069	0.1927	0.0831	0.0893
H4'	H1	E	0.0944	0.1329	0.1067	0.1381	0.1246
O4'	OS	S	-0.4220	-0.3721	-0.3971	-0.3492	-0.3134
C1'	CT	B	0.2145	0.1059	0.0940	0.0381	0.0161
H1'	H2	E	0.1301	0.1620	0.1610	0.1777	0.1485
N9	N*	B	-0.0899	-0.0100	-0.0344	-0.0358	-0.0697
C8	CK	S	0.1461	0.0584	0.1268	0.1150	0.1104
H8	H5	E	0.1854	0.1991	0.1938	0.2022	0.1579
C4	CB	B	0.4535	0.4741	0.4964	0.4896	0.3803
N3	NC	E	-0.7712	-0.8080	-0.7845	-0.8019	-0.4965
C5	CB	B	0.0804	-0.0081	0.0260	0.0453	0.0811
N7	NB	E	-0.5937	-0.4918	-0.5855	-0.5690	-0.5258
C6	CA	B	0.4756	0.5417	0.4930	0.4451	0.4134
N1	NC	S	-0.7193	-0.7978	-0.7339	-0.7816	-0.6829
C2	CQ	S	0.6061	0.6830	0.6118	0.6803	0.4448
H2	H5	E	0.0439	0.0373	0.0467	0.0297	0.0562
N6	N2	B	-0.4766	-0.4544	-0.4421	-0.3934	-0.3821
H6	H	E	0.3166	0.3108	0.2948	0.2860	0.2674
CC1	CT	B	0.0259	0.0116	0.0245	0.0356	0.0265
HC1	H1	E	0.1196	0.1104	0.1708	0.1665	0.1646
CC2	CT	3	-0.0224	0.0019	0.0070	0.0541	0.0192
HC2	H1	E	0.1529	0.1372	0.1807	0.1580	0.1743
O9	OH	S	-0.6752	-0.6496	-0.6666	-0.6818	-0.6812
HO9	HO	E	0.4583	0.4305	0.4641	0.4684	0.4749
CC3	CT	3	0.1060	0.0836	0.0450	0.0526	0.0371
HC3	H1	E	0.1324	0.1292	0.0878	0.0850	0.0954

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Atom Name	Atom Type	Topology	Partial Charge					
			10 <i>S</i> (+)- <i>trans</i> -[A ₁]		10 <i>R</i> (-)- <i>trans</i> -[A ₁]			
			II	III	II	III	IV	
O8	OH	S	-0.6475	-0.6451	-0.6541	-0.6621	-0.6592	
HO8	HO	E	0.4443	0.4419	0.4407	0.4430	0.4473	
CC4	CT	3	0.2329	0.2682	0.2844	0.2459	0.2314	
HC4	H1	E	0.1549	0.1424	0.1203	0.1310	0.1349	
O7	OH	S	-0.6733	-0.6804	-0.6847	-0.6782	-0.6780	
HO7	HO	E	0.4313	0.4328	0.4214	0.4226	0.4230	
CC5	CA	S	-0.1012	-0.1021	-0.0748	-0.0821	-0.0494	
CC6	CA	B	-0.2048	-0.2065	-0.2274	-0.2257	-0.2443	
HC6	HA	E	0.1698	0.1707	0.1631	0.1626	0.1655	
CC7	CA	B	0.0282	0.0348	0.0291	0.0414	0.0491	
C20	CA	E	0.0337	0.0338	0.0272	0.0181	0.0213	
CC8	CA	B	-0.1631	-0.1687	-0.1540	-0.1550	-0.1626	
HC8	HA	E	0.1424	0.1431	0.1413	0.1375	0.1406	
CC9	CA	B	-0.2057	-0.2051	-0.2172	-0.2115	-0.2028	
HC9	HA	E	0.1463	0.1476	0.1491	0.1497	0.1450	
C10	CA	B	0.0532	0.0487	0.0592	0.0468	0.0534	
C19	CA	E	0.0929	0.1211	0.1010	0.1225	0.0995	
C11	CA	B	-0.1396	-0.1609	-0.1454	-0.1701	-0.1532	
HC11	HA	E	0.1399	0.1436	0.1419	0.1476	0.1439	
C12	CA	B	-0.2301	-0.2048	-0.2292	-0.1959	-0.2151	
HC12	HA	E	0.1656	0.1580	0.1650	0.1578	0.1623	
C13	CA	B	-0.1489	-0.1521	-0.1406	-0.1639	-0.1515	
HC13	HA	E	0.1442	0.1423	0.1413	0.1443	0.1421	
C14	CA	S	0.0487	0.0399	0.0411	0.0539	0.0446	
C15	CA	B	-0.2041	-0.2352	-0.2104	-0.2218	-0.2029	
HC15	HA	E	0.1523	0.1570	0.1556	0.1563	0.1509	
C16	CA	B	-0.2045	-0.1347	-0.1823	-0.1565	-0.1454	
HC16	HA	E	0.1758	0.1374	0.1561	0.1550	0.1327	
C17	CA	S	0.0289	-0.0011	0.0251	0.0005	-0.0153	
C18	CA	E	0.0225	0.0149	0.0301	0.0325	0.0545	
C3'	CT	M	0.0337	0.0396	0.0502	0.0291	0.0375	
H3'	H1	E	0.1112	0.1178	0.1126	0.1218	0.1296	
C2'	CT	B	-0.0695	-0.0563	-0.0814	-0.0418	-0.0308	
H2'1	HC	E	0.0502	0.0544	0.0598	0.0562	0.0526	
H2'2	HC	E	0.0502	0.0544	0.0598	0.0562	0.0526	
O3'	OS	M	-0.5241	-0.5151	-0.5238	-0.5111	-0.5209	

Table 2: Partial charges, atom types and topologies of $10S(+)$ - and $10R(-)$ -*trans-anti*-[BP]- N^6 -dA adducts at the position A_2 of the TATA box in the following systems.

Atom Name	Atom Type	Topology	Partial Charge					
			$10S(+)$ - <i>trans</i> -[A_2]			$10R(-)$ - <i>trans</i> -[A_2]		
			III	III-2	IV	I	III	IV
P	P	M	1.2212	1.2212	1.2212	1.2211	1.2208	1.2208
O1P	O2	E	-0.7930	-0.7930	-0.7930	-0.7928	-0.7928	-0.7928
O2P	O2	E	-0.7930	-0.7930	-0.7930	-0.7928	-0.7928	-0.7928
O5'	OS	M	-0.4972	-0.4972	-0.4972	-0.4987	-0.4947	-0.4947
C5'	CT	M	-0.0085	-0.0085	-0.0085	0.0304	0.0615	0.0615
H5'1	H1	E	0.0919	0.0919	0.0919	0.0783	0.0657	0.0657
H5'2	H1	E	0.0919	0.0919	0.0919	0.0783	0.0657	0.0657
C4'	CT	M	0.0634	0.0634	0.0634	0.0704	0.0844	0.0844
H4'	H1	E	0.1397	0.1397	0.1397	0.1336	0.1239	0.1239
O4'	OS	S	-0.3451	-0.3451	-0.3451	-0.3532	-0.3647	-0.3648
C1'	CT	B	0.0575	0.0575	0.0575	0.0346	0.0506	0.0506
H1'	H2	E	0.1426	0.1426	0.1426	0.1588	0.1484	0.1484
N9	N*	B	-0.0006	-0.0006	-0.0006	-0.0455	-0.0214	-0.0214
C8	CK	S	0.0522	0.0523	0.0523	0.1695	0.1229	0.1229
H8	H5	E	0.1969	0.1969	0.1969	0.1716	0.1754	0.1754
C4	CB	B	0.4703	0.4703	0.4704	0.4591	0.4633	0.4633
N3	NC	E	-0.8104	-0.8104	-0.8104	-0.7908	-0.8108	-0.8109
C5	CB	B	-0.0120	-0.0118	-0.0119	0.0742	0.0442	0.0442
N7	NB	E	-0.4877	-0.4877	-0.4877	-0.6090	-0.5572	-0.5572
C6	CA	B	0.6011	0.6007	0.6007	0.4802	0.4633	0.4633
N1	NC	S	-0.8096	-0.8096	-0.8095	-0.7455	-0.7870	-0.7870
C2	CQ	S	0.6799	0.6798	0.6798	0.6419	0.6887	0.6887
H2	H5	E	0.0386	0.0386	0.0387	0.0399	0.0293	0.0293
N6	N2	B	-0.5362	-0.5357	-0.5357	-0.4859	-0.4078	-0.4079
H6	H	E	0.3363	0.3361	0.3361	0.3100	0.2869	0.2869
CC1	CT	B	0.0014	0.0015	0.0015	0.0258	0.0243	0.0243
HC1	H1	E	0.1119	0.1118	0.1118	0.1701	0.1692	0.1692
CC2	CT	3	0.0044	0.0044	0.0044	0.0351	0.0377	0.0377
HC2	H1	E	0.1305	0.1304	0.1304	0.1700	0.1599	0.1599
O9	OH	S	-0.6594	-0.6594	-0.6594	-0.6755	-0.6778	-0.6778
HO9	HO	E	0.4389	0.4390	0.4390	0.4631	0.4659	0.4659
CC3	CT	3	0.1252	0.1253	0.1255	0.0913	0.0628	0.0628
HC3	H1	E	0.1227	0.1226	0.1226	0.0739	0.0816	0.0816

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Atom Name	Atom Type	Topology	Partial Charge					
			10 <i>S</i> (+)- <i>trans</i> -[A ₂]			10 <i>R</i> (-)- <i>trans</i> -[A ₂]		
			III	III-2	IV	I	III	IV
O8	OH	S	-0.6544	-0.6544	-0.6544	-0.6629	-0.6620	-0.6620
HO8	HO	E	0.4415	0.4415	0.4416	0.4358	0.4388	0.4388
CC4	CT	3	0.2593	0.2595	0.2595	0.2940	0.3009	0.3009
HC4	H1	E	0.1434	0.1433	0.1433	0.1129	0.1138	0.1138
O7	OH	S	-0.6825	-0.6825	-0.6823	-0.6854	-0.6857	-0.6857
HO7	HO	E	0.4320	0.4319	0.4318	0.4181	0.4174	0.4174
CC5	CA	S	-0.0993	-0.0994	-0.0995	-0.0995	-0.0897	-0.0897
CC6	CA	B	-0.2022	-0.2022	-0.2023	-0.2004	-0.2305	-0.2305
HC6	HA	E	0.1702	0.1702	0.1701	0.1559	0.1597	0.1597
CC7	CA	B	0.0297	0.0297	0.0298	0.0254	0.0508	0.0509
C20	CA	E	0.0237	0.0237	0.0237	0.0180	0.0154	0.0154
CC8	CA	B	-0.1585	-0.1585	-0.1585	-0.1694	-0.1580	-0.1580
HC8	HA	E	0.1424	0.1424	0.1424	0.1457	0.1394	0.1394
CC9	CA	B	-0.2212	-0.2212	-0.2212	-0.1994	-0.2244	-0.2244
HC9	HA	E	0.1516	0.1516	0.1516	0.1440	0.1520	0.1520
C10	CA	B	0.0674	0.0674	0.0674	0.0589	0.0637	0.0637
C19	CA	E	0.1164	0.1164	0.1164	0.1024	0.1204	0.1204
C11	CA	B	-0.1758	-0.1758	-0.1758	-0.1529	-0.1691	-0.1691
HC11	HA	E	0.1482	0.1482	0.1482	0.1429	0.1480	0.1480
C12	CA	B	-0.2044	-0.2044	-0.2044	-0.2146	-0.2087	-0.2087
HC12	HA	E	0.1588	0.1588	0.1588	0.1622	0.1611	0.1611
C13	CA	B	-0.1440	-0.1440	-0.1440	-0.1549	-0.1610	-0.1610
HC13	HA	E	0.1407	0.1407	0.1407	0.1442	0.1438	0.1438
C14	CA	S	0.0364	0.0364	0.0364	0.0484	0.0598	0.0598
C15	CA	B	-0.2458	-0.2458	-0.2458	-0.2254	-0.2383	-0.2383
HC15	HA	E	0.1602	0.1602	0.1602	0.1600	0.1609	0.1609
C16	CA	B	-0.1246	-0.1246	-0.1246	-0.1701	-0.1401	-0.1401
HC16	HA	E	0.1364	0.1364	0.1364	0.1605	0.1455	0.1454
C17	CA	S	0.0101	0.0101	0.0101	0.0267	0.0017	0.0017
C18	CA	E	0.0180	0.0181	0.0182	0.0344	0.0316	0.0316
C3'	CT	M	0.1127	0.1128	0.1127	0.1311	0.1338	0.1337
H3'	H1	E	0.1131	0.1130	0.1131	0.1082	0.0988	0.0989
C2'	CT	B	-0.0954	-0.0955	-0.0955	-0.1337	-0.1032	-0.1031
H2'1	HC	E	0.0773	0.0774	0.0774	0.0880	0.0774	0.0773
H2'2	HC	E	0.0773	0.0774	0.0774	0.0880	0.0774	0.0773
O3'	OS	M	-0.5247	-0.5248	-0.5247	-0.5284	-0.5310	-0.5310

Table 3: Added force field parameters.

Angle	K_θ (kcal mol ⁻¹ rad ⁻²)	θ_{eq} (deg)
OH-CT-CA	65.8	112.61
N2-CT-CA	50.0	108.75
H1-CT-CA	63.0	108.93