Supplementary Information

to

Effect of Size and Shape of Nitrogen-Containing Aromatics on Conformational Preferences of DNA Containing Damaged Guanine

Ryan W. Kung, Purshotam Sharma[§] and Stacey D. Wetmore[*]

Department of Chemistry and Biochemistry, University of Lethbridge, 4401 University Drive West, Lethbridge, Alberta, Canada T1K 3M4

[§]Currently at the Computational Biochemistry Laboratory, Department of Chemistry and Centre for Advanced Studies in Chemistry, Panjab University, Chandigarh, India 160014

*To whom correspondence should be addressed. Email: stacey.wetmore@uleth.ca

Table of Contents

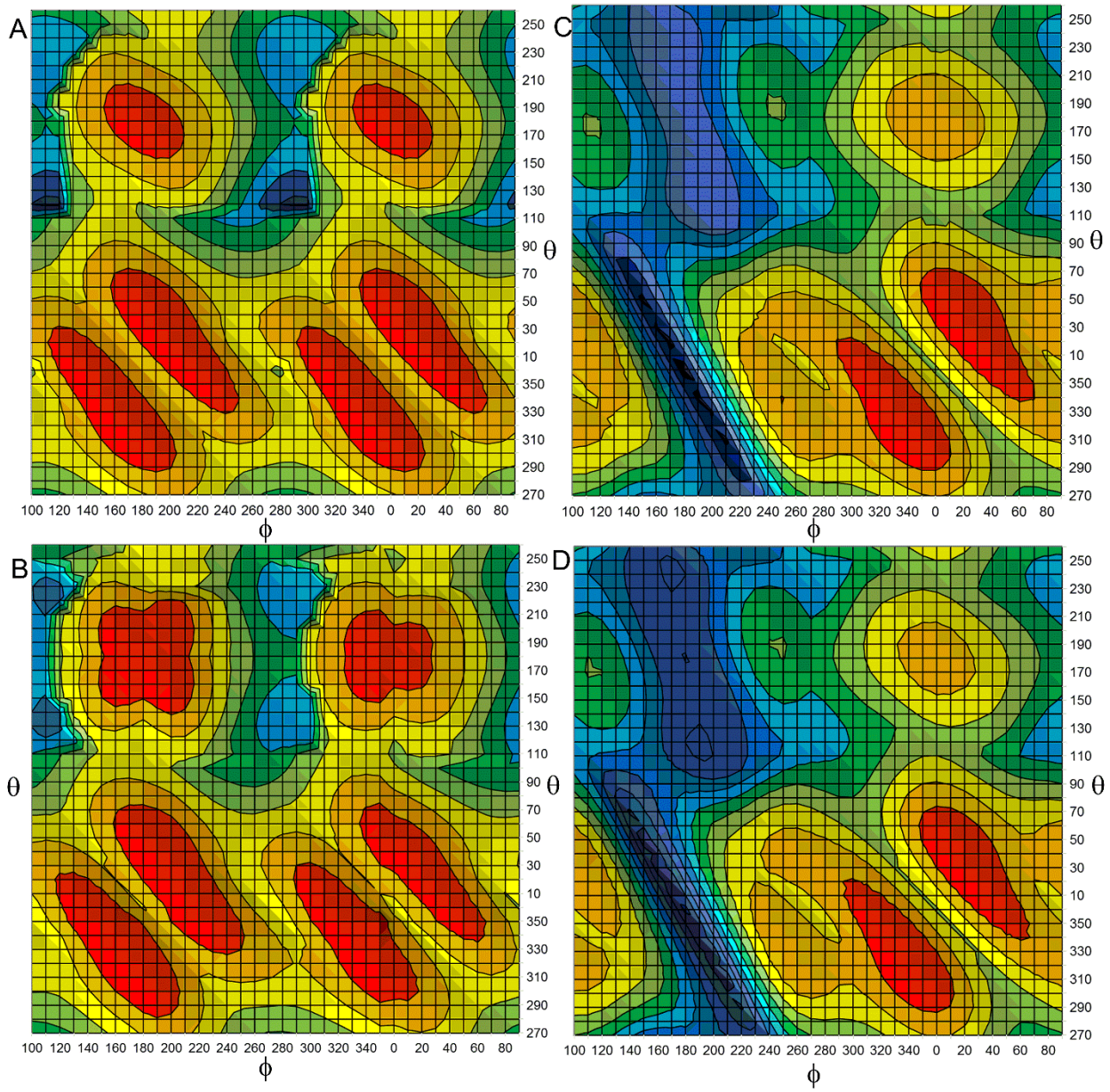


Figure S1. Contour plots of the B3LYP/6-31G(d) potential energy for the (A) ^{AN}G, (B) ^{3APHN}G, (C) ^{1ANP}G and (D) ^{1AP}G nucleobase adducts with respect to θ and ϕ (deg). The relative energy is represented by color; red represents the lowest energy regions, and each change in color in the surrounding regions represents an increase in the energy by 5 kJ mol^{-1}.

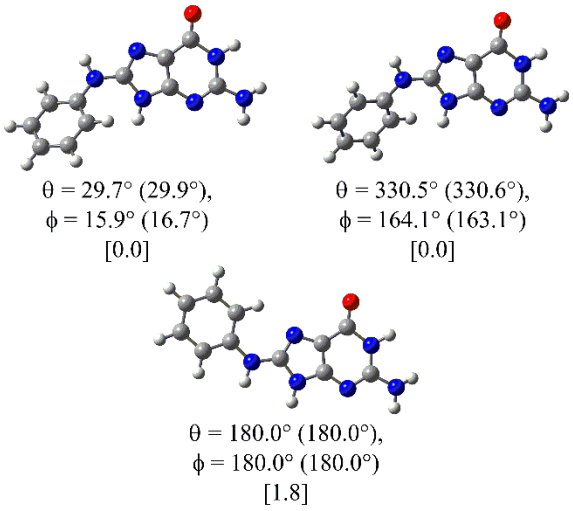


Figure S2. Select B3LYP/6-31G(d) and B3LYP-D3(BJ)/6-31G(d) (in parenthesis) dihedral angles (θ and ϕ, deg) for the fully optimized minima identified from the contour plots for the ^{AN}G nucleobase adduct. Zero-point vibrational energy corrected B3LYP-D3(BJ)/6-311+G(2df,p) relative energies are provided in parentheses (kJ mol^{-1}).

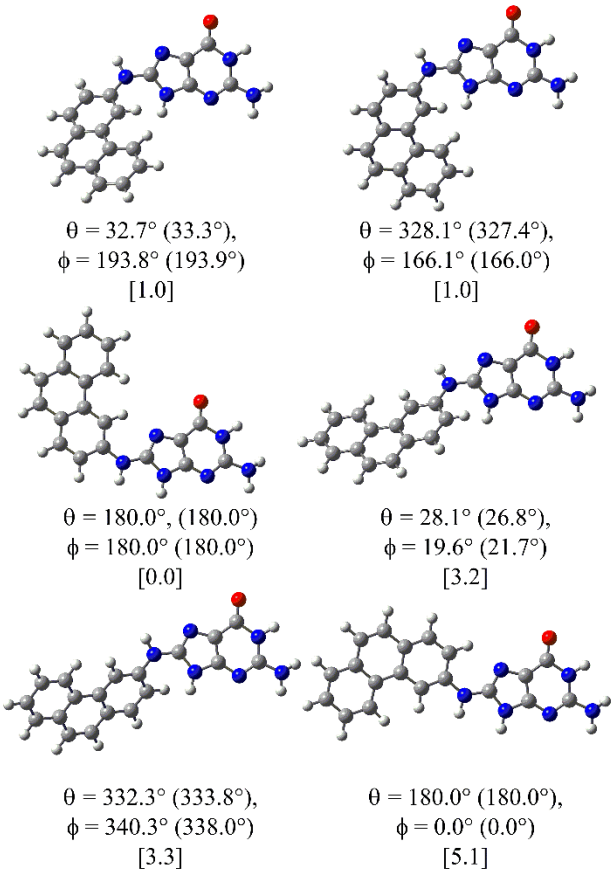


Figure S3. Select B3LYP/6-31G(d) and B3LYP-D3(BJ)/6-31G(d) (in parenthesis) dihedral angles (θ and ϕ, deg) for the fully optimized minima identified from the contour plots for the ^{3APHN}G nucleobase adduct. Zero-point vibrational energy corrected B3LYP-D3(BJ)/6-311+G(2df,p) relative energies are provided in parentheses (kJ mol^{-1}).

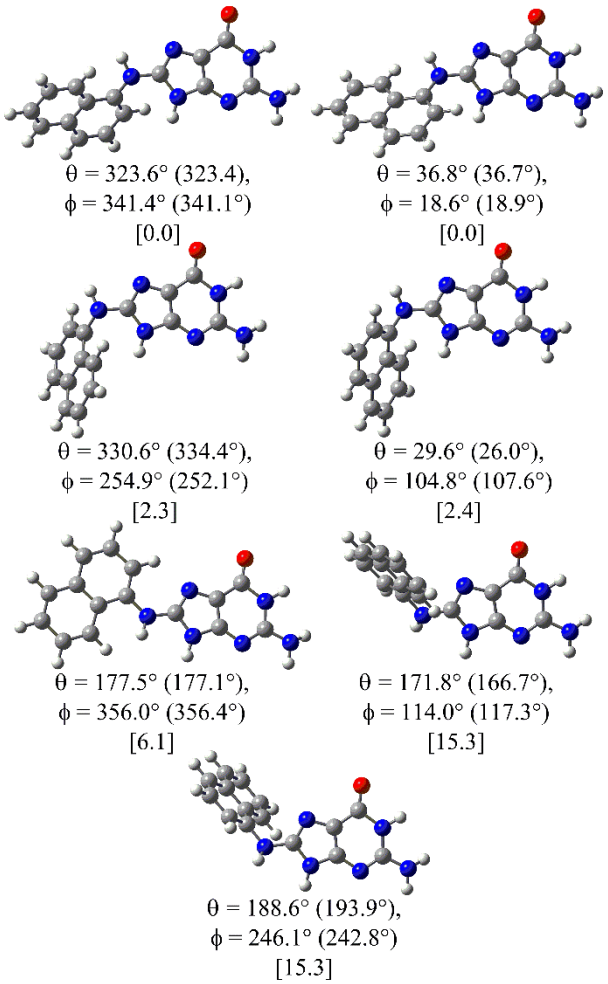


Figure S4. Select B3LYP/6-31G(d) and B3LYP-D3(BJ)/6-31G(d) (in parenthesis) dihedral angles (θ and ϕ, deg) for the fully optimized minima identified from the contour plots for the ^{1ANP}G nucleobase adduct. Zero-point vibrational energy corrected B3LYP-D3(BJ)/6-311+G(2df,p) relative energies are provided in parentheses (kJ mol^{-1}).

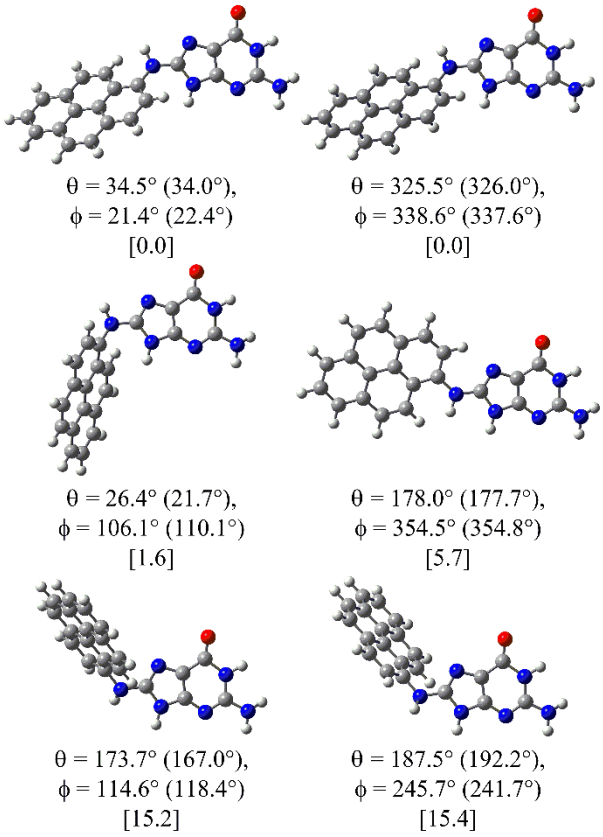


Figure S5. Select B3LYP/6-31G(d) and B3LYP-D3(BJ)/6-31G(d) (in parenthesis) dihedral angles (θ and ϕ, deg) for the fully optimized minima identified from the contour plots for the ^{1AP}G nucleobase adduct. Zero-point vibrational energy corrected B3LYP-D3(BJ)/6-311+G(2df,p) relative energies are provided in parentheses (kJ mol^{-1}).

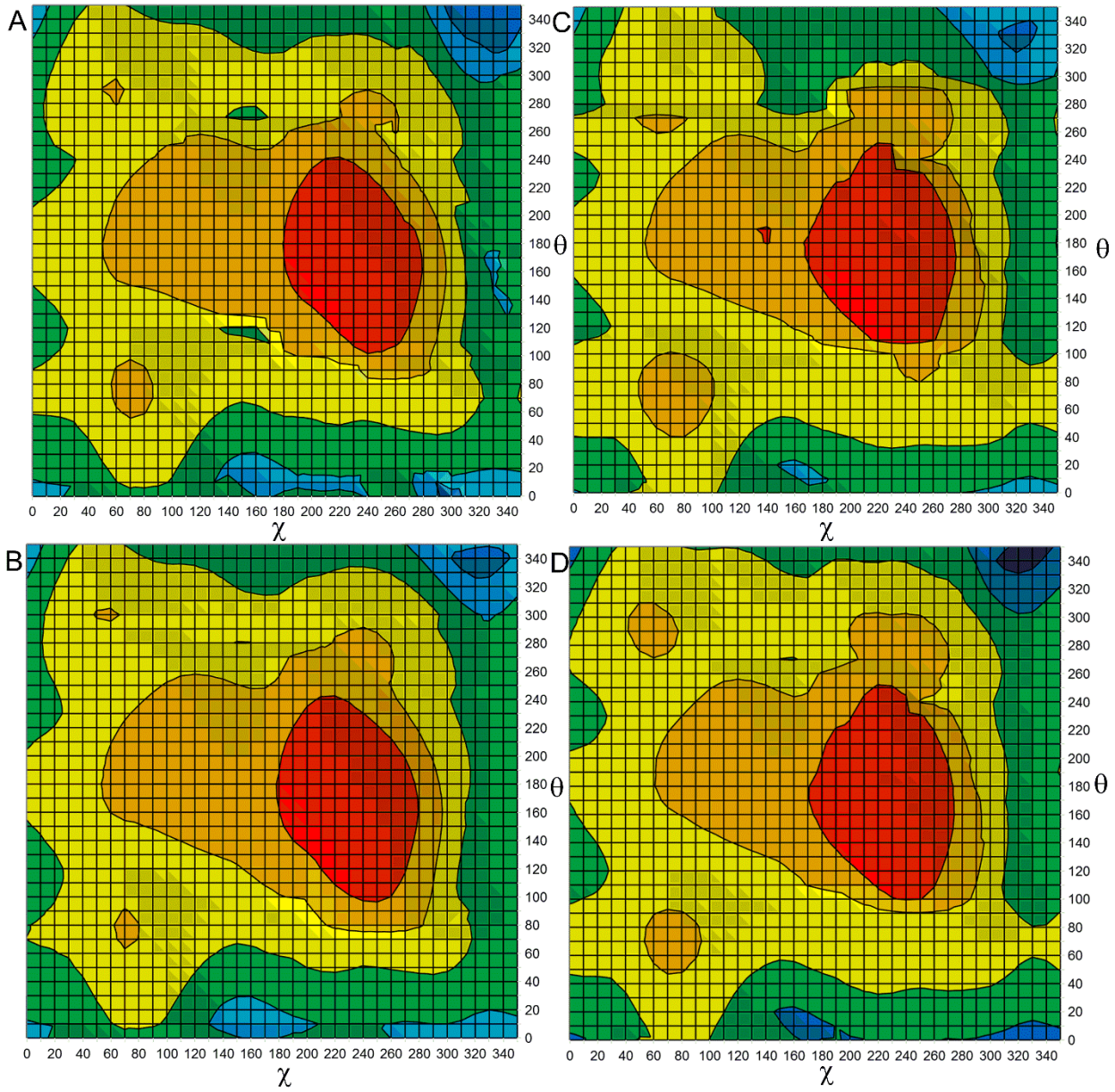


Figure S6. Contour plots of the B3LYP/6-31G(d) potential energy for the (A) ^{AN}dG, (B) ^{3APHN}dG, (C) ^{1ANP}dG and (D) ^{1AP}dG nucleoside adducts with respect to θ and χ (deg). The relative energy is represented by color; red represents the lowest energy regions, and each change in color in the surrounding regions represents an increase in the energy by 20 kJ mol^{-1}.

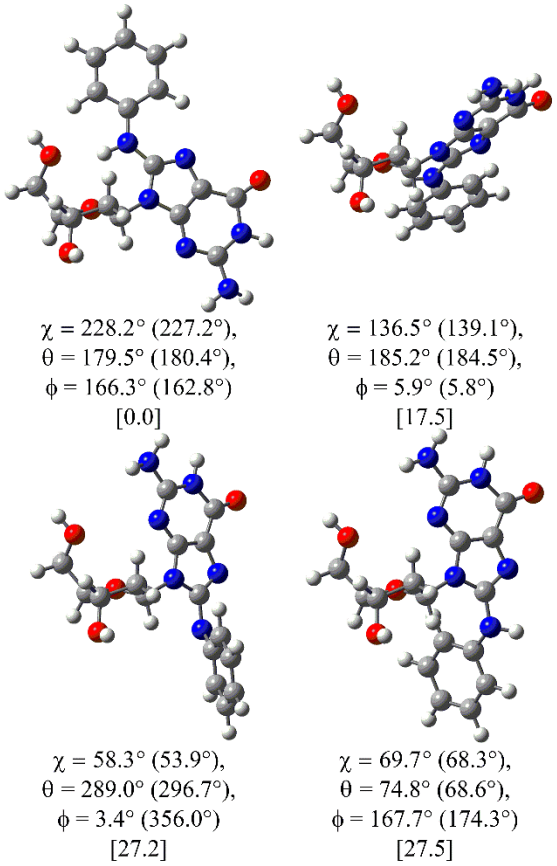


Figure S7. Select B3LYP/6-31G(d) and B3LYP-D3(BJ)/6-31G(d) (in parenthesis) dihedral angles (χ, θ and ϕ, deg) for the fully optimized minima identified from the contour plots for the ^{AN}dG nucleoside adduct. Zero-point vibrational energy corrected B3LYP-D3(BJ)/6-311+G(2df,p) relative energies are provided in parentheses (kJ mol^{-1}).

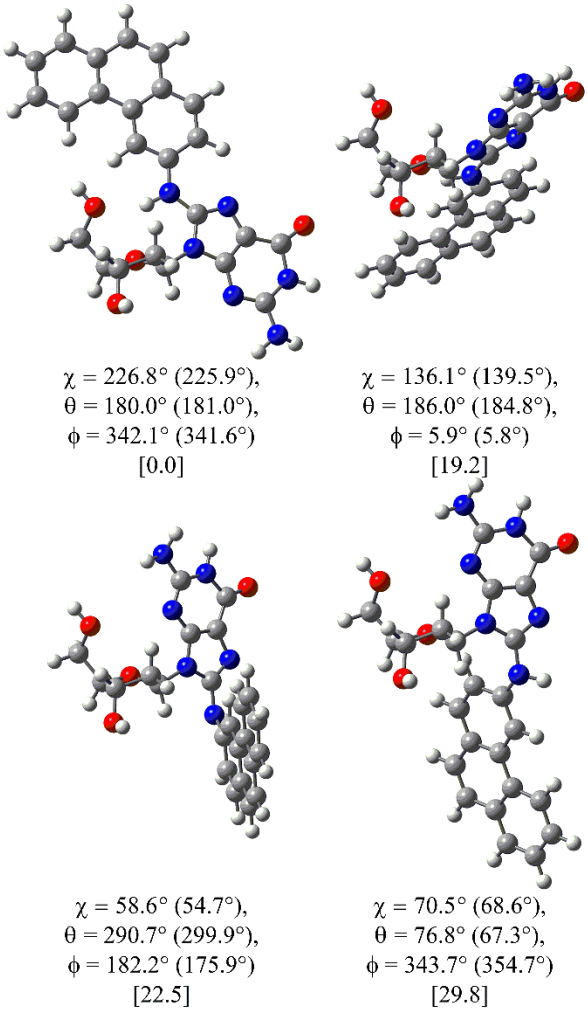


Figure S8. Select B3LYP/6-31G(d) and B3LYP-D3(BJ)/6-31G(d) (in parenthesis) dihedral angles (χ, θ and ϕ, deg) for the fully optimized minima identified from the contour plots for the ^{3APHN}dG nucleoside adduct. Zero-point vibrational energy corrected B3LYP-D3(BJ)/6-311+G(2df,p) relative energies are provided in parentheses (kJ mol^{-1}).

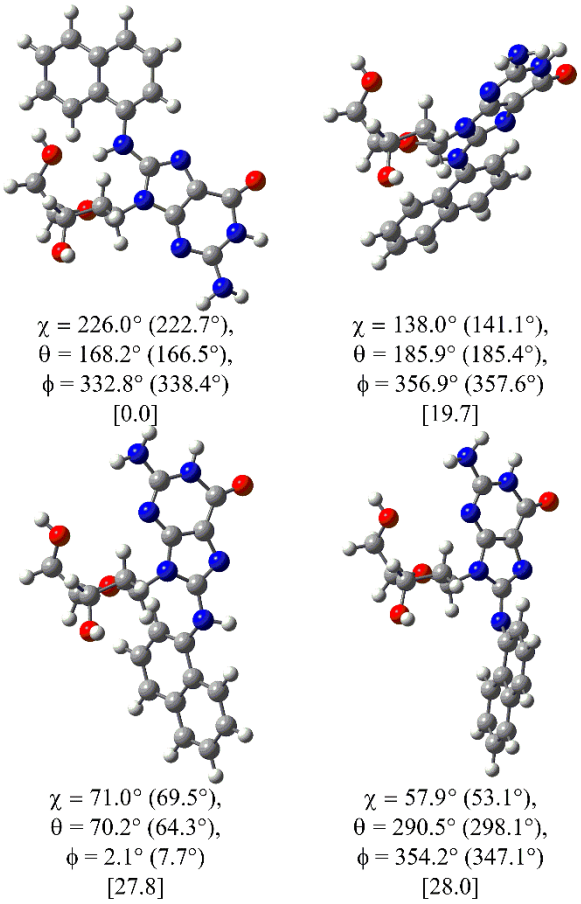


Figure S9. Select B3LYP/6-31G(d) and B3LYP-D3(BJ)/6-31G(d) (in parenthesis) dihedral angles (χ, θ and ϕ, deg) for the fully optimized minima identified from the contour plots for the ^{1ANP}dG nucleoside adduct. Zero-point vibrational energy corrected B3LYP-D3(BJ)/6-311+G(2df,p) relative energies are provided in parentheses (kJ mol^{-1}).

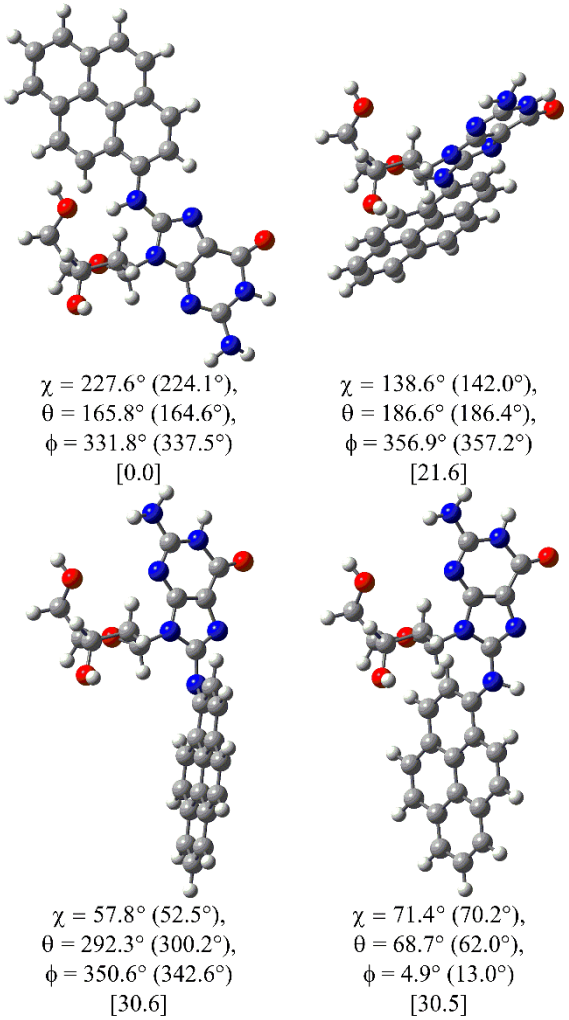


Figure S10. Select B3LYP/6-31G(d) and B3LYP-D3(BJ)/6-31G(d) (in parenthesis) dihedral angles (χ, θ and ϕ, deg) for the fully optimized minima identified from the contour plots for the ^{1AP}dG nucleoside adduct. Zero-point vibrational energy corrected B3LYP-D3(BJ)/6-311+G(2df,p) relative energies are provided in parentheses (kJ mol^{-1}).

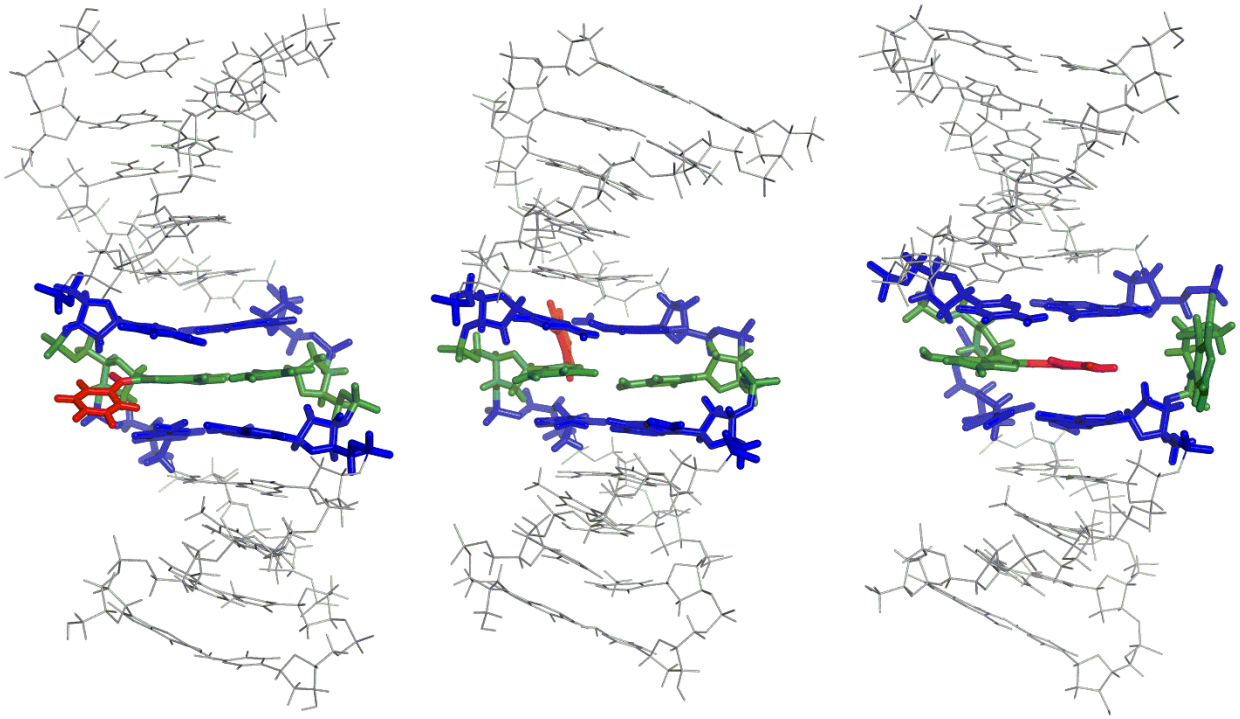


Figure S11. Representative structures obtained from MD simulations of the B (left), W (middle) and S (right) conformations of ^{AN}dG adducted DNA. The C^8-moiety is shown in red, the damaged dG and the opposing nucleotide in green, the base pairs flanking the lesion in blue, and rest of the DNA helix in grey.

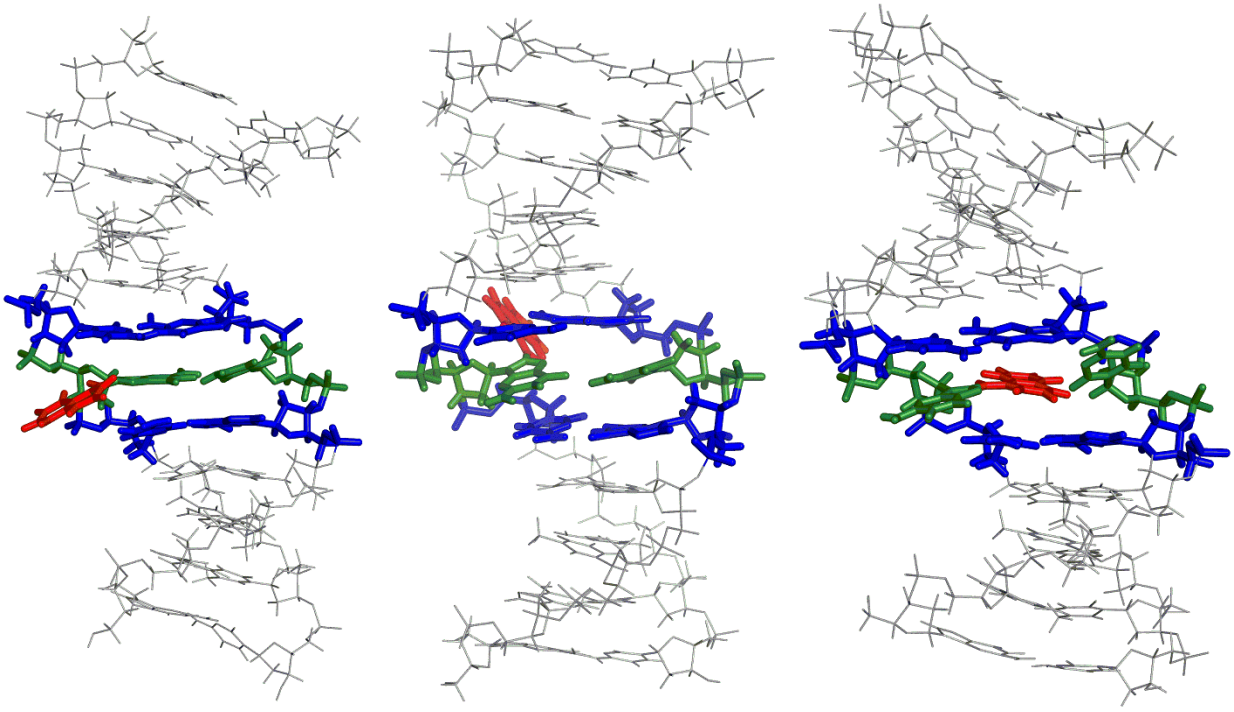


Figure S12. Representative structures obtained from MD simulations of the B (left), W (middle) and S (right) conformations of ^{1ANP}dG adducted DNA. The C^8-moiety is shown in red, the damaged dG and the opposing nucleotide in green, the base pairs flanking the lesion in blue, and rest of the DNA helix in grey.

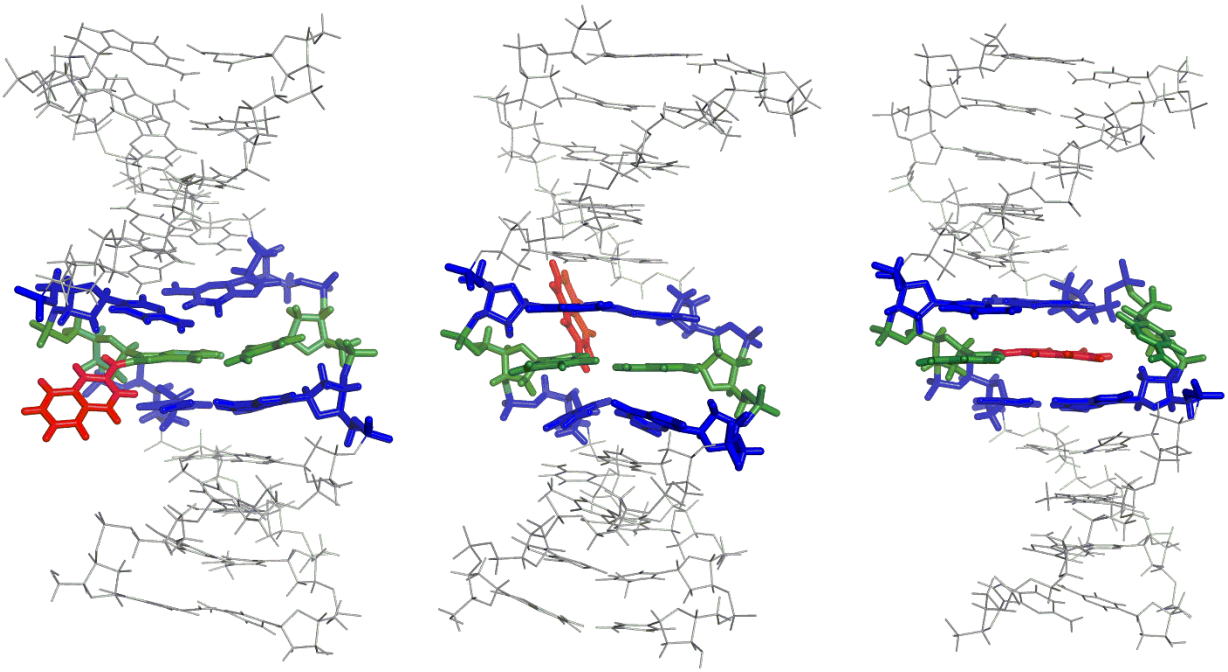


Figure S13. Representative structures obtained from MD simulations of the B (left), W (middle) and S (right) conformations of ^{2ANP}dG adducted DNA. The C^8-moiety is shown in red, the damaged dG and the opposing nucleotide in green, the base pairs flanking the lesion in blue, and rest of the DNA helix in grey.

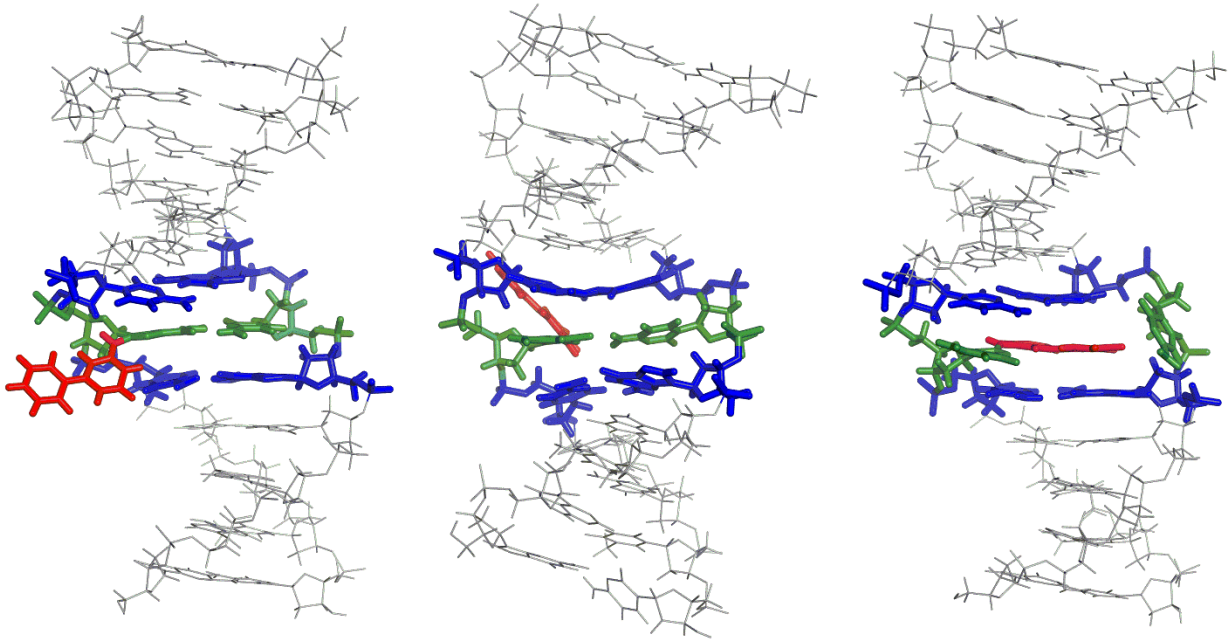


Figure S14. Representative structures obtained from MD simulations of the B (left), W (middle) and S (right) conformations of ^{3ABP}dG adducted DNA. The C^8-moiety is shown in red, the damaged dG and the opposing nucleotide in green, the base pairs flanking the lesion in blue, and rest of the DNA helix in grey.

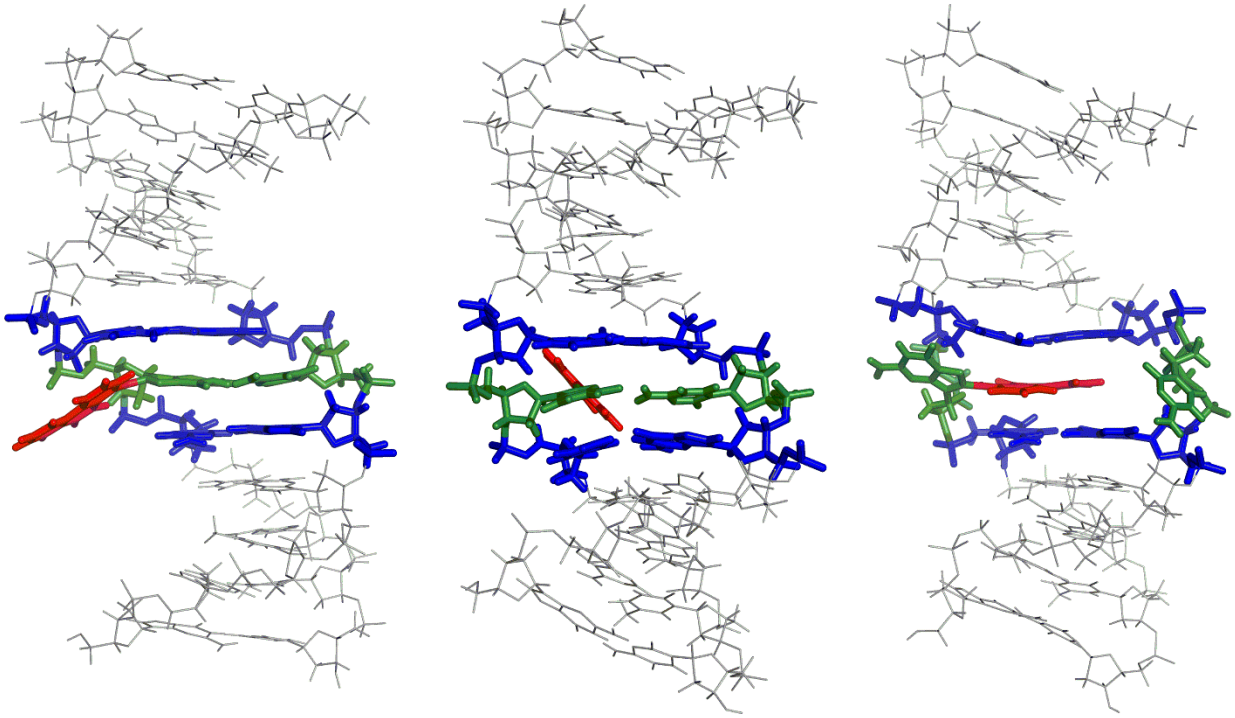


Figure S15. Representative structures obtained from MD simulations of the B (left), W (middle) and S (right) conformations of ^{1APHN}dG adducted DNA. The C^8-moiety is shown in red, the damaged dG and the opposing nucleotide in green, the base pairs flanking the lesion in blue, and rest of the DNA helix in grey.

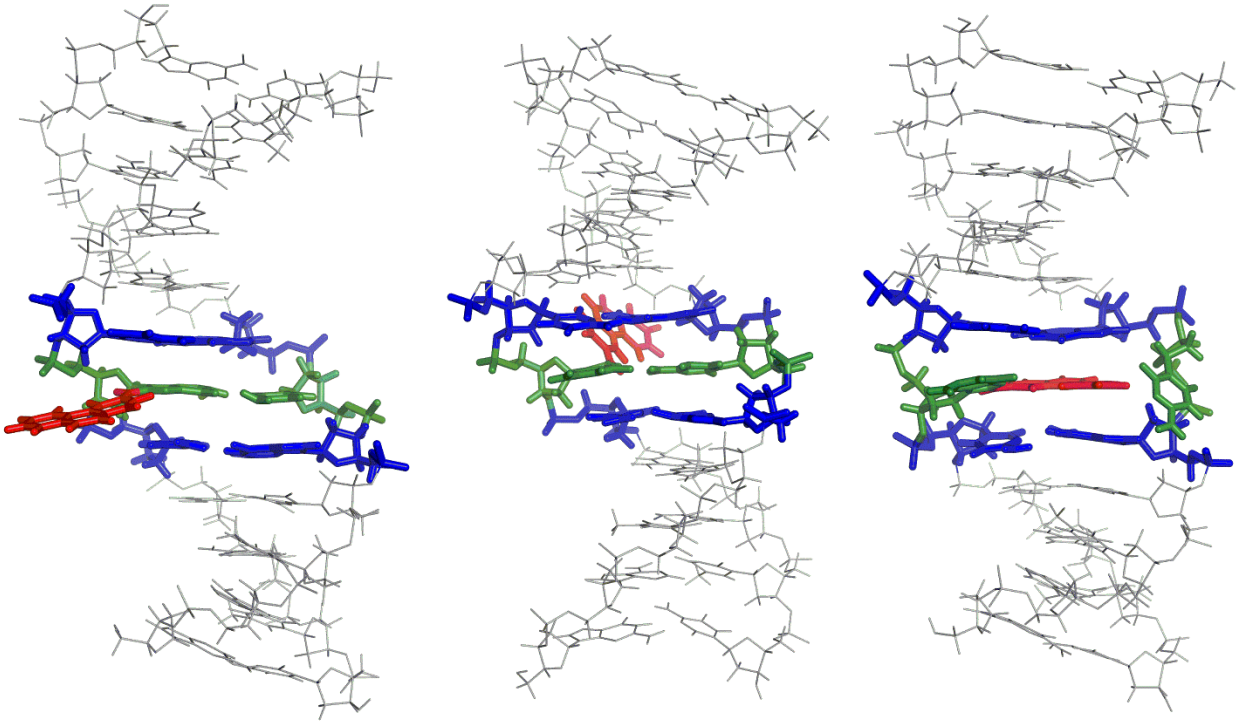


Figure S16. Representative structures obtained from MD simulations of the B (left), W (middle) and S (right) conformations of ^{3APHN}dG adducted DNA. The C^8-moiety is shown in red, the damaged dG and the opposing nucleotide in green, the base pairs flanking the lesion in blue, and rest of the DNA helix in grey.

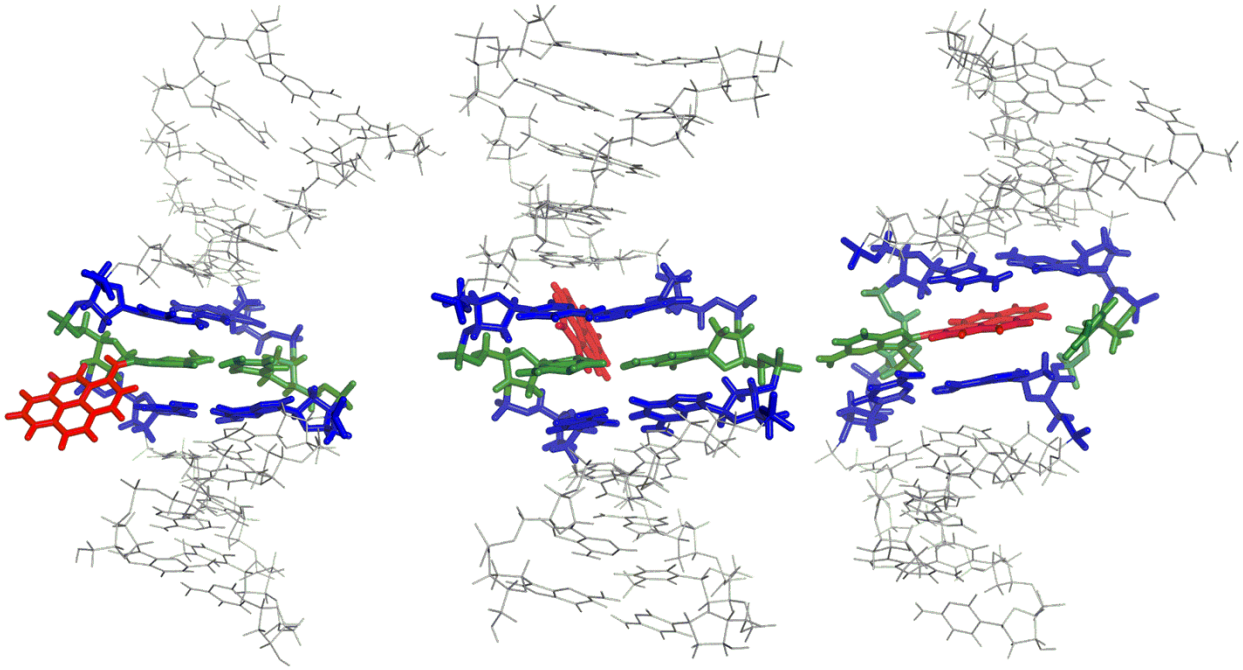


Figure S17. Representative structures obtained from MD simulations of the B (left), W (middle) and S (right) conformations of ^{1AP}dG adducted DNA. The C^8-moiety is shown in red, the damaged dG and the opposing nucleotide in green, the base pairs flanking the lesion in blue, and rest of the DNA helix in grey.

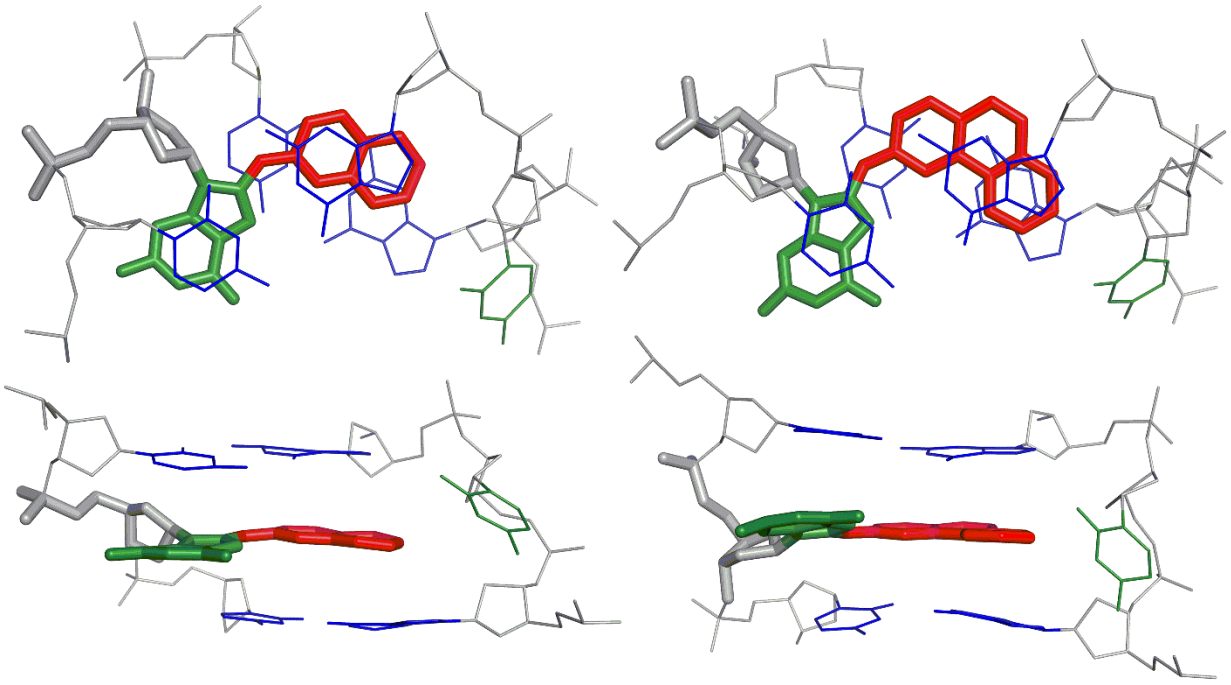


Figure S18. Lesion-site trimer of base pairs from ^{2ANP}dG (left, χ = 45.2°) and ^{3APHN}dG (right, χ = 132.3°) adducted DNA in the S conformer, highlighting how the changing χ allows different NCA moieties to optimize stacking interactions with the flanking base pairs. The C^8-moiety is shown in red, the damaged G and the opposing base in green, the base pairs flanking the lesion in blue, and the DNA backbone in grey.

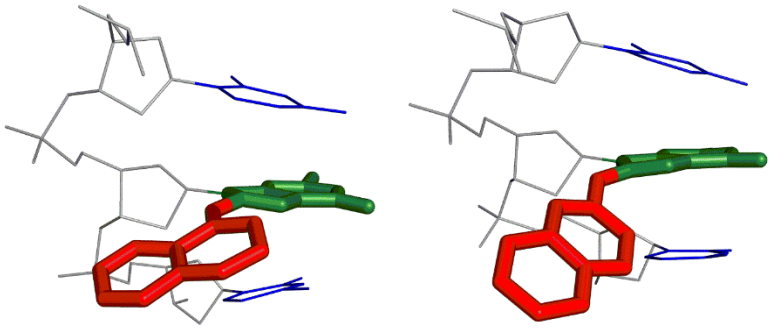


Figure S19. Structures of the ^{1ANP}dG (left, θ= 165.3°) and ^{2ANP}dG (right, θ = 139.9°) adducts in the B conformer of damaged DNA, highlighting the change in θ with the presence (left) or absence (right) of an α-fused ring due to the presence of a weak hydrogen bond between the bulky moiety and phosphate. The C^8-moiety is shown in red, the damaged G in green, the bases flanking the lesion in blue, and the DNA backbone in grey.

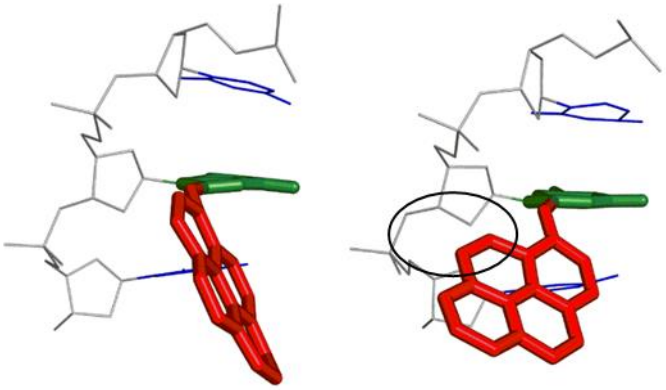


Figure S20. Structures of the ^{1AP}dG adduct in the B conformer of damaged DNA with ϕ ~ 0° (left) or 180° (right), highlighting minimal steric repulsion between the bulky group and the backbone for ϕ ~ 0°. The C^8-moiety is shown in red, the damaged G moiety in green, the bases flanking the lesion in blue, and the DNA backbone in grey.

Table S1. Comparison of the average structural and energetic parameters (standard deviations in parentheses) for damaged DNA containing select adducts deduced from 20 ns and 120 ns MD simulations.

Conformation	Parameter	^{AN}dG		^{1AP}dG	
		20 ns	**120 ns**	**20 ns**	**120 ns**
B	RMSD (Å)	4.0 (0.7)	4.2 (0.7)	2.6 (0.5)	4.2 (0.7)
	χ^{av} (deg)	227.8 (12.7)	226.6 (13.2)	218.5 (12.2)	215.2 (17.4)
	θ^{av} (deg)	139.9 (20.6)	140.8 (22.1)	166.4 (20.6)	167.2 (25.5)
	ϕ^{av} (deg)	2.9 (12.2)	3.2 (12.1)	17.6 (11.3)	15.0 (25.9)
	LSIE (kJ mol^{-1})[a]	–475.5 (19.2)	–474.8 (17.1)	–473.9 (17.9)	–473.3 (18.3)
W	RMSD (Å)	3.8 (0.8)	3.9 (0.7)	4.1 (0.7)	4.0 (0.7)
	χ^{av} (deg)	67.7 (13.2)	69.3 (13.4)	64.0 (12.5)	65.8 (12.9)
	θ^{av} (deg)	76.1 (18.1)	74.0 (17.8)	68.2 (12.9)	70.0 (13.3)
	ϕ^{av} (deg)	1.2 (9.9)	1.7 (10.0)	1.1 (10.2)	359.9 (10.2)
	LSIE (kJ mol^{-1})[a]	–361.9 (24.9)	–349.2 (39.8)	–367.5 (19.1)	–356.7 (34.5)
S	RMSD (Å)	2.5 (0.4)	3.3 (1.0)	5.0 (0.7)	4.7 (0.7)
	χ^{av} (deg)	42.1 (13.2)	54.7 (23.4)	48.4 (33.6)	45.3 (19.0)
	θ^{av} (deg)	167.0 (15.9)	147.9 (37.3)	205.6 (11.0)	175.9 (18.0)
	ϕ^{av} (deg)	357.6 (10.9)	358.7 (10.8)	353.2 (11.5)	352.8 (10.9)
	LSIE (kJ mol^{-1})[a]	–300.6 (17.1)	–300.3 (17.6)	–358.2 (21.5)	–355.6 (25.0)

[a]Lesion-site interaction energies (LSIE) were calculated as the sum of the van der Waals and electrostatic interactions between the bases constituting the 5′ and 3′ base pairs flanking the lesion, the lesions and the opposing base, and the lesion and the 5′ and 3′ flanking base pairs.

Table S2. Comparison of the average structural and energetic parameters (standard deviations in parentheses) for damaged DNA containing select adducts deduced from replicate 20 ns and 120 ns MD simulations.[a]

System	Parameter	^{AN}dG				^{1AP}dG			
		Replicate 1	Replicate 2	Replicate 3	Replicate Average[b]	Replicate 1	Replicate 2	Replicate 3	Replicate Average[b]
B 20 ns	RMSD (Å)	4.0 (0.7)	4.0 (0.7)	4.2 (0.8)	4.1 (0.1)	2.6 (0.5)	4.3 (0.7)	4.2 (0.7)	3.7 (1.0)
	χ^{av} (deg)	227.8 (12.7)	226.7 (12.9)	226.6 (12.9)	227.0 (0.5)	218.5 (12.2)	218.9 (13.3)	222.4 (13.8)	219.9 (1.8)
	θ^{av} (deg)	139.9 (20.6)	139.8 (21.6)	140.5 (22.2)	140.1 (0.3)	166.4 (20.6)	167.0 (20.9)	161.3 (25.0)	164.9 (2.6)
	ϕ^{av} (deg)	2.9 (12.2)	3.1 (12.1)	3.3 (12.1)	3.1 (0.2)	17.6 (11.3)	16.8 (11.6)	15.5 (11.5)	16.6 (0.9)
	LSIE (kJ mol^{-1})[c]	–475.5 (19.2)	–474.6 (17.0)	–473.8 (17.2)	–474.6 (0.7)	–473.9 (17.9)	–475.3 (16.6)	–477.3 (16.7)	–475.5 (1.4)
	G (kJ mol^{-1})[d]	–24010.0 (81.5)	–24009.8 (85.5)	–24013.8 (85.4)	–24011.2 (1.8)	–23774.0 (79.8)	–23757.3 (90.4)	–23771.7 (91.3)	–23767.7 (7.4)
B 120 ns	RMSD (Å)	4.2 (0.7)	4.0 (0.7)	4.0 (0.7)	4.1 (0.1)	4.2 (0.7)	4.3 (0.7)	4.2 (0.7)	4.2 (0.1)
	χ^{av} (deg)	226.6 (13.2)	227.2 (12.7)	227.2 (12.7)	227.0 (0.3)	215.2 (17.4)	220.1 (13.0)	216.1 (16.5)	217.1 (2.1)
	θ^{av} (deg)	140.8 (22.1)	139.5 (21.5)	139.3 (21.5)	139.9 (0.7)	167.2 (25.5)	163.8 (22.2)	168.3 (24.3)	166.6 (2.1)
	ϕ^{av} (deg)	3.2 (12.1)	3.0 (12.0)	3.0 (12.0)	3.1 (0.1)	15.0 (25.9)	16.2 (12.0)	14.9 (12.4)	15.4 (0.6)
	LSIE (kJ mol^{-1})[c]	–474.8 (17.1)	–474.4 (17.4)	–474.9 (16.9)	–474.7 (0.2)	–473.3 (18.3)	–475.2 (17.2)	–474.8 (17.4)	–474.4 (0.8)
	G (kJ mol^{-1})[d]	–24012.6 (86.7)	–24004.0 (79.5)	–24013.1 (89.8)	–24009.9 (4.2)	–23762.5 (84.1)	–23764.5 (87.2)	–23762.6 (86.7)	–23763.2 (0.9)
S 20 ns	RMSD (Å)	2.5 (0.4)	2.6 (0.7)	2.7 (0.5)	2.6 (0.1)	5.0 (0.7)	4.4 (0.8)	4.5 (0.7)	4.6 (0.3)
	χ^{av} (deg)	42.1 (13.2)	43.7 (12.6)	47.6 (13.1)	44.5 (2.3)	48.4 (33.6)	51.7 (30.6)	42.8 (13.0)	47.6 (3.7)
	θ^{av} (deg)	167.0 (15.9)	164.9 (15.5)	161.0 (15.0)	164.3 (2.5)	205.6 (11.0)	179.4 (18.1)	172.3 (14.5)	185.8 (14.3)
	ϕ^{av} (deg)	357.6 (10.9)	357.9 (10.7)	358.8 (10.8)	358.1 (0.5)	353.2 (11.5)	353.7 (11.1)	352.2 (10.8)	353.0 (0.6)
	LSIE (kJ mol^{-1})[c]	–300.6 (17.1)	–300.9 (16.2)	–306.2 (15.6)	–302.6 (2.6)	–358.2 (21.5)	–356.8 (17.7)	–344.4 (35.9)	–353.1 (6.2)
	G (kJ mol^{-1})[d]	–23925.1 (85.0)	–23921.1 (85.6)	–23915.7 (91.6)	–23920.6 (3.8)	–23738.9 (88.2)	–23724.9 (83.9)	–23723.5 (84.2)	–23729.1 (6.9)
S 120 ns	RMSD (Å)	3.3 (1.0)	2.6 (0.6)	3.0 (1.0)	3.0 (0.3)	4.7 (0.7)	4.7 (0.7)	4.6 (0.7)	4.7 (0.1)
	χ^{av} (deg)	54.7 (23.4)	43.7 (13.1)	50.5 (17.9)	49.6 (4.5)	45.3 (19.0)	52.8 (33.3)	42.7 (18.4)	46.9 (4.3)
	θ^{av} (deg)	147.9 (37.3)	163.9 (15.7)	160.5 (15.6)	157.4 (6.9)	175.9 (18.0)	181.7 (20.0)	181.7 (20.4)	179.8 (2.7)
	ϕ^{av} (deg)	358.7 (10.8)	358.2 (10.8)	359.4 (10.8)	358.8 (0.5)	352.8 (10.9)	354.5 (11.7)	352.8 (10.9)	353.4 (0.8)
	LSIE (kJ mol^{-1})[c]	–300.3 (17.6)	–300.8 (16.1)	–306.8 (15.8)	–302.6 (3.0)	–355.6 (25.0)	–351.6 (27.3)	–358.9 (22.4)	–355.4 (3.0)
	G (kJ mol^{-1})[d]	–23923.3 (100.8)	–23922.7 (90.2)	–23925.5 (82.0)	–23923.8 (1.2)	–23718.0 (84.4)	–23719.4 (90.2)	–23725.6 (88.5)	–23721.0 (3.3)

[a]Replicas were obtained from the same starting structure with different initial velocities. [b]Replicate averages calculated as the sum and standard deviation between the three replicate values reported. [c]Lesion-site interaction energies (LSIE) were calculated as the sum of the van der Waals and electrostatic interactions between the bases constituting the 5′ and 3′ base pairs flanking the lesion, the lesions and the opposing base, and the lesion and the 5′ and 3′ flanking base pairs. [d]G energies calculated using MM/PBSA enthalpies and normal mode entropies.

Table S3. MM/PBSA free energy rankings (G^{rel}, kJ mol^{-1}), and average θ and ϕ dihedral angles (deg) deduced from MD simulations on various damaged DNA conformations containing the ^{AN}G, ^{1ANP}dG or ^{2ANP}dG adducts.

Adduct	Conformation	Occupancy[a] (%)	θ^{av} (deg)	ϕ^{av} (deg)	G^{rel} (kJ mol^{-1})
^{AN}dG	B	100	139.9	2.9	0.0
		100	134.3	184.0	6.7
	W	100	76.1	1.2	47.0
		100	75.4	1.4	62.8
	S	100	167.0	357.6	85.0
		100	167.7	178.6	96.8
^{1ANP}dG	B	100	165.3	17.1	0.0
		100	131.1	165.5	34.2
		100	157.9	219.9	28.7
	W	100	70.7	359.6	39.0
		100	88.5	181.0	66.1
		58	225.4	356.8	69.1
		47	263.9	156.5	104.1
		53	218.8	190.4	88.1
	S	100	189.2	355.6	52.0
		100	303.5	4.2	100.8
		100	166.6	357.6	77.4
		100	294.5	7.9	127.5
		100	151.8	166.8	80.4
^{2ANP}dG	B	100	139.9	5.4	0.0
		47	130.7	183.8	11.2
		53	170.1	188.0	17.2
		29	121.5	185.3	6.9
		35	148.1	183.9	2.3
	W	100	76.2	180.5	40.5
		100	70.7	0.9	42.9
		44	166.1	358.1	83.0
		100	228.5	177.5	66.4
	S	100	177.1	175.2	62.3
		100	168.1	354.1	92.6
		30	294.6	4.0	101.0
		70	298.8	7.4	79.7
		100	232.8	179.9	81.9

[a]Occupancies of hydrogen-bonding interactions were determined using a cutoff of 3.4 Å for the donor–acceptor distance and 120° for the donor–hydrogen–acceptor angle.

Table S4. MM/PBSA free energy rankings (G^{rel}, kJ mol^{-1}), and average θ and ϕ dihedral angles (deg) deduced from MD simulations on various damaged DNA conformations containing the ^{3ABP}dG, ^{1APHN}dG and ^{3APHN}dG adducts.

Adduct	Conformation	Occupancy[a] (%)	θ^{av} (deg)	ϕ^{av} (deg)	G^{rel} (kJ mol^{-1})
^{3ABP}dG	B	100	124.6	5.3	0.0
		100	163.7	189.8	18.7
		41	171.3	12.2	7.3
	W	100	62.4	183.8	54.7
		100	72.1	0.8	78.2
		100	225.6	177.5	84.4
	S	100	196.5	175.9	37.6
		100	69.3	348.0	54.8
		100	166.0	356.0	79.1
		100	73.7	169.7	73.4
^{1APHN}dG	B	100	174.8	17.8	0.0
		27	126.8	10.8	17.3
		100	154.3	224.1	25.5
		37	141.3	160.5	38.4
	W	100	71.7	359.0	53.7
		100	73.2	188.9	82.4
		100	232.4	178.1	110.4
		100	232.1	356.9	74.3
	S	100	206.6	5.9	35.9
		100	300.4	1.2	108.7
		84	166.7	354.1	84.2
		100	152.1	164.9	113.8
^{3APHN}dG	B	100	135.4	8.6	0.0
		30	163.4	10.2	14.8
		70	118.9	8.3	17.0
		55	174.0	189.8	6.4
		45	131.5	186.9	11.0
		100	148.2	188.0	10.4
	W	100	72.5	0.1	49.3
		100	58.7	186.1	51.7
		100	229.4	171.8	63.4
		30	230.0	355.9	55.9
	S	100	191.9	177.5	50.9
		100	166.6	354.0	67.6
		100	298.2	11.8	89.0
		65	77.0	175.1	172.6

[a]Occupancies of hydrogen-bonding interactions were determined using a cutoff of 3.4 Å for the donor–acceptor distance and 120° for the donor–hydrogen–acceptor angle.

Table S5. MM/PBSA free energy rankings (G^{rel}, kJ mol^{-1}), and average θ and ϕ dihedral angles (deg) deduced from MD simulations on various damaged DNA conformations containing the ^{1AP}G adduct.

Adduct	Conformation	Occupancy[a] (%)	θ^{av} (deg)	ϕ^{av} (deg)	G^{rel} (kJ mol^{-1})
^{1AP}dG	B	100	166.4	17.6	0.0
		100	135.1	167.1	35.2
		65	179.3	12.7	14.5
		35	127.1	4.8	33.2
	W	100	68.2	1.1	37.5
		100	82.0	182.6	53.9
		46	259.1	150.0	92.0
		54	215.3	193.4	112.6
	S	100	205.6	353.2	35.1
		100	225.0	198.4	63.2
		100	177.7	354.3	43.8
		100	156.2	165.8	89.6

[a]Occupancies of hydrogen-bonding interactions were determined using a cutoff of 3.4 Å for the donor–acceptor distance and 120° for the donor–hydrogen–acceptor angle.

Table S6. Occupancies (%) of the hydrogen bonds within the trimer (5′–CXC–3′) containing the lesion pair (X:C) and the flanking base pairs in the B conformation of adducted DNA.[a]

Base pair	Hydrogen bond	^{AN}dG	^{1ANP}dG	^{2ANP}dG	^{3ABP}dG	^{1APHN}dG	^{3APHN}dG	^{1AP}dG
5′–C:G[b]	N1(G)–H•••N3(C)	99.9	99.9	100.0	100.0	99.9	99.9	100.0
	N2(G)–H•••O2(C)	99.8	99.8	99.8	99.9	99.9	99.8	99.9
	N4(C)–H•••O6(G)	98.0	98.6	98.8	98.5	98.7	98.6	98.7
X:C	N2(X)–H•••O2(C)	99.9	99.9	100.0	99.9	99.9	100.0	99.9
	N1(X)–H•••N3(C)	99.9	99.9	99.9	99.9	100.0	99.9	99.4
	N4(C)–H•••O6(X)	98.7	98.4	97.7	98.3	98.7	98.3	97.6
	N10(X)–H•••O4'(X)	81.0	57.1	74.4	66.0	64.8	65.5	63.1
3′–C:G[b]	N1(G)–H•••N3(C)	100.0	100.0	99.9	99.7	100.0	100.0	100.0
	N2(G)–H•••O2(C)	99.8	99.9	99.7	99.6	99.9	99.8	99.8
	N4(C)–H•••O6(G)	99.2	98.9	99.1	98.8	98.8	99.2	98.5

[a]Hydrogen-bonding interactions were determined using a cutoff of 3.4 Å for the donor–acceptor distance and 120° for the donor–hydrogen–acceptor angle. [b]5′–C:G and 3′–C:G represent the flanking base pairs present 5′ and 3′ with respect to the lesion, respectively.

Table S7. Average and standard deviations (in parentheses) of pseudostep parameters at the lesion site within different conformations of N-linked adducted DNA.[a]

Nucleoside	Conformation	Shift (Å)	Slide (Å)	Rise (Å)	Tilt (deg)	Roll (deg)	Twist (deg)
dG	B	0.4 (0.8)	–1.0 (0.9)	6.5 (0.4)	2.2 (5.0)	9.9 (7.5)	63.1 (6.3)
^{AN}dG		0.1 (0.8)	–1.8 (0.9)	6.4 (0.4)	4.2 (4.8)	9.5 (7.4)	59.5 (5.5)
^{1ANP}dG		–0.1 (0.8	–2.4 (0.8)	6.7 (0.4)	2.8 (4.9)	8.4 (6.9)	59.4 (4.8)
^{2ANP}dG		0.2 (0.8)	–1.9 (0.9)	6.5 (0.4)	3.9 (4.8)	8.9 (7.3)	60.7 (5.0)
^{3ABP}dG		0.3 (0.8)	–1.6 (1.0)	6.4 (0.4)	4.8 (5.0)	8.0 (7.5)	60.0 (6.5)
^{1APHN}dG		–0.1 (0.8)	–2.7 (0.8)	6.8 (0.5)	2.8 (5.0)	7.2 (7.3)	59.1 (4.9)
^{3APHN}dG		0.0 (0.9)	–2.3 (0.8)	6.6 (0.4)	3.4 (4.9)	9.6 (7.3)	59.9 (4.9)
^{1AP}dG		–0.1 (0.8)	–2.6 (0.9)	6.8 (0.5)	3.1 (4.9)	8.0 (7.1)	60.0 (4.9)
^{AN}dG	W	–0.1 (0.8	–1.1 (0.8)	6.2 (0.4)	2.5 (5.2)	14.1 (7.2)	59.7 (5.1)
^{1ANP}dG		–0.2 (0.7)	–1.1 (0.8)	6.2 (0.4)	1.9 (5.0)	13.7 (6.4)	58.9 (4.7)
^{2ANP}dG		–0.3 (0.7)	–1.4 (0.7)	6.2 (0.4)	3.1 (5.0)	14.0 (6.4)	59.7 (5.0)
^{3ABP}dG		0.1 (0.8)	–1.3 (0.8)	6.2 (0.4)	3.0 (5.1)	14.7 (6.5)	58.0 (4.7)
^{1APHN}dG		0.0 (0.7)	–0.9 (0.9)	6.3 (0.4)	3.0 (5.5)	12.0 (6.8)	60.5 (5.5)
^{3APHN}dG		0.0 (0.7)	–1.2 (0.8)	6.3 (0.4)	3.0 (5.4)	11.7 (6.5)	60.0 (5.4)
^{1AP}dG		–0.2 (0.7)	–1.3 (0.8)	6.2 (0.4)	2.3 (5.1)	14.5 (6.9)	59.1 (5.4)
^{AN}dG	S	–0.4 (0.9)	0.9 (1.0)	6.9 (0.5)	3.1 (5.8)	15.8 (6.7)	42.3 (6.9)
^{1ANP}dG		0.1 (1.0)	–3.4 (1.6)	6.8 (0.6)	0.9 (6.0)	16.7 (8.0)	56.6 (8.0)
^{2ANP}dG		–1.0 (0.9)	–2.4 (1.2)	6.9 (0.5)	2.2 (5.0)	10.4 (9.1)	49.5 (6.0)
^{3ABP}dG		–0.8 (0.9)	–1.4 (1.5)	6.9 (0.5)	1.6 (4.7)	–1.0 (8.0)	43.8 (5.9)
^{1APHN}dG		–0.3 0.8)	–1.5 (1.2)	6.6 (0.4)	2.2 (5.2)	–2.9 (9.5)	41.1 (5.0)
^{3APHN}dG		–0.7 (0.7)	0.3 (3.2)	6.9 (0.5)	1.9 (4.8)	–0.8 (7.1)	44.5 (5.7)
^{1AP}dG		–0.2 (0.7)	–2.9 (3.7)	7.1 (0.7)	–1.3 (5.9)	20.5 (7.9)	50.7 (11.2)

[a]Pseudostep parameters at the lesion site were calculated using a pseudostep consisting of the base pairs 5′ and 3′ with respect to the lesion.

Table S8. Average and standard deviations (in parentheses) of lesion-site van der Waals and electrostatic interactions (kJ mol^{-1}) within different conformations of N-linked adducted DNA.[a]

Nucleoside	Conformation	Lesion Stacking energy with 5′ bases	Lesion Stacking energy with 3′ bases	Base pair energy at the 5′ base pair	Base pair energy at the 3′ base pair	Base pair energy at the lesion site	Lesion-site Interaction energy[b]
dG	B	–61.0 (9.7)	–56.6 (10.5)	–118.2 (7.4)	–118.0 (7.4)	–118.4 (7.3)	–472.2 (17.7)
^{AN}dG		–65.5 (10.3)	–63.5 (9.8)	–117.7 (7.9)	–118.5 (7.2)	–110.3 (7.1)	–475.5 (19.2)
^{1ANP}dG		–65.6 (10.0)	–63.4 (10.1)	–118.2 (7.4)	–118.5 (7.3)	–110.5 (7.1)	–476.2 (19.0)
^{2ANP}dG		–66.7 (10.2)	–62.6 (10.0)	–118.6 (7.3)	–118.1 (7.5)	–109.4 (7.6)	–475.4 (19.2)
^{3ABP}dG		–64.7 (10.3)	–64.5 (9.7)	–118.1 (7.6)	–118.3 (8.0)	–110.0 (7.2)	–475.6 (19.3)
^{1APHN}dG		–63.8 (10.5)	–64.4 (10.0)	–118.7 (7.2)	–118.4 (7.3)	–110.0 (6.9)	–475.3 (19.0)
^{3APHN}dG		–66.5 (10.0)	–63.8 (9.9)	–118.1 (7.5)	–118.4 (7.3)	–109.7 (7.3)	–476.5 (18.9)
^{1AP}dG		–65.5 (10.4)	–62.5 (10.2)	–118.6 (7.2)	–117.8 (7.7)	–109.5 (7.9)	–473.9 (17.9)
^{AN}dG	W	–47.4 (8.3)	–44.9 (10.7)	–117.9 (7.3)	–116.0 (8.2)	–35.8 (17.8)	–361.9 (24.9)
^{1ANP}dG		–51.3 (8.2)	–45.0 (10.2)	–118.0 (7.1)	–114.8 (8.8)	–33.6 (15.8)	–362.8 (23.4)
^{2ANP}dG		–48.6 (7.8)	–40.9 (9.7)	–118.2 (7.2)	–115.5 (8.4)	–36.6 (15.4)	–359.8 (22.7)
^{3ABP}dG		–52.7 (7.8)	–44.3 (9.9)	–117.3 (7.6)	–115.8 (8.1)	–41.8 (9.4)	–372.0 (19.2)
^{1APHN}dG		–49.2 (9.3)	–43.0 (12.2)	–117.9 (7.4)	–113.9 (9.6)	–24.3 (24.9)	–348.3 (31.6)
^{3APHN}dG		–48.2 (8.4)	–45.0 (13.1)	–118.0 (7.5)	–114.9 (8.7)	–33.7 (19.0)	–359.8 (27.0)
^{1AP}dG		–53.4 (7.6)	–43.3 (9.3)	–118.1 (7.2)	–115.1 (9.0)	–37.6 (9.4)	–367.5 (19.1)
^{AN}dG	S	–44.2 (11.6)	–20.3 (11.3)	–117.7 (13.4)	–118.5 (14.9)	N/A	–300.6 (17.1)
^{1ANP}dG		–51.9 (11.0)	–45.9 (16.2)	–119.1 (13.4)	–111.2 (19.0)	N/A	–328.1 (19.9)
^{2ANP}dG		–52.5 (9.0)	–46.2 (11.3)	–117.8 (13.3)	–117.2 (13.7)	N/A	–333.7 (16.6)
^{3ABP}dG		–44.2 (12.2)	–49.0 (10.8)	–118.1 (13.2)	–118.0 (13.1)	N/A	–329.3 (17.7)
^{1APHN}dG		–64.6 (13.0)	–51.3 (17.5)	–116.9 (13.5)	–115.0 (17.3)	N/A	–347.8 (19.4)
^{3APHN}dG		–53.3 (21.8)	–41.0 (8.9)	–114.9 (14.4)	–117.4 (13.7)	N/A	–326.6 (20.5)
^{1AP}dG		–63.8 (14.3)	–61.6 (12.5)	–118.5 (13.3)	–114.3 (15.3)	N/A	–358.2 (21.5)

[a]Energies calculated with LIE of cpptraj. [b]Calculated as the sum of all other columns.

Table S9. Occupancies (%) of the hydrogen bonds within the trimer (5′–CXC–3′) containing the lesion pair (X:C) and the flanking base pairs in the W conformation of adducted DNA.[a]

Base pair	Hydrogen Bond	^{AN}dG	^{1ANP}dG	^{2ANP}dG	^{3ABP}dG	^{1APHN}dG	^{3APHN}dG	^{1AP}dG
5′–C:G[b]	N1(G)–H•••N3(C)	99.9	99.9	99.9	99.9	99.9	99.9	99.9
	N2(G)–H•••O2(C)	99.7	99.7	99.8	99.5	99.8	99.6	99.7
	N4(C)–H•••O6(G)	98.7	98.8	98.7	98.7	98.7	98.8	98.9
X:C	N4(C)–H•••O6(X)	78.9	79.7	76.3	80.1	93.0	73.0	75.0
	N4(C)–H•••N7(X)	42.7	45.4	56.1	59.8	38.5	38.5	61.0
X:3′–C[c]	N10(X)–H•••O4'(3′–C)	67.4	48.4	68.0	30.6	49.7	41.0	37.3
3′–C:G[b]	N1(G)–H•••N3(C)	99.9	99.9	99.9	99.9	99.8	99.9	99.8
	N2(G)–H•••O2(8)	99.3	99.2	99.3	99.4	99.4	99.4	99.0
	N4(C)–H•••O6(G)	98.1	97.2	98.1	98.0	95.6	97.7	97.8

[a]Hydrogen-bonding interactions were determined using a cutoff of 3.4 Å for the donor–acceptor distance and 120° for the donor–hydrogen–acceptor angle. [b]5′–C:G and 3′–C:G represent the flanking base pairs present 5′ and 3′ with respect to the lesion, respectively. [c]X:3′–C represents the interaction between the lesion (X) and the intrastrand C present 3' with respect to the lesion.

Table S10. Occupancies (%) of the hydrogen bonds within the trimer (5′–CXC–3′) containing the lesion (X), the opposing extrahelical base C (ex-C), and the flanking base pairs in the S conformation of the adducted DNA.[a]

Interaction	Hydrogen Bond	^{AN}dG	^{1ANP}dG	^{2ANP}dG	^{3ABP}dG	^{1APHN}dG	^{3APHN}dG	^{1AP}dG
5′–C:G[b]	N1(G)–H•••N3(C)	99.9	100.0	100.0	100.0	100.0	99.9	100.0
	N2(G)–H•••O2(C)	99.8	99.9	99.7	99.6	99.7	99.4	99.9
	N4(C)–H•••O6(G)	97.9	99.0	98.3	99.0	97.7	97.7	98.7
exC: 5′–G[c]	N4(exC)–H•••OP(3′–G)[b]	68.2	10.8	65.5	79.7	51.9	67.2	19.8
3′–C:G[b]	N2(G)–H•••O2(C)	99.7	99.9	99.9	100.0	99.9	96.3	99.9
	N1(G)–H•••N3(C)	99.2	93.5	99.8	99.9	96.4	67.3	99.7
	N4(C)–H•••O6(17)	96.5	87.0	97.3	98.6	92.9	66.3	91.5

[a]Hydrogen-bonding interactions were determined using a cutoff of 3.4 Å for the donor–acceptor distance and 120° for the donor–hydrogen–acceptor angle. [b]5′–C:G and 3′–C:G represent the flanking base pairs present 5′– and 3′– with respect to the lesion, respectively. [c]exC:5′–G represents the interaction between the extrahelical cytosine (exC) opposing the lesion, and a phosphate oxygen (OP) on the 5′-G.

Table S11. Average values and standard deviation (in parentheses) for the backbone RMSD[a] (Å) and key dihedral angles (deg) for different conformations of adducted DNA.

Adduct	Conformation	RMSD	χ	θ	ϕ
^{AN}dG	B	4.0 (0.7)	227.8 (12.7)	139.9 (20.6)	2.9 (12.2)
	W	3.8 (0.8)	67.7 (13.2)	76.1 (18.1)	1.2 (9.9)
	S	2.5 (0.4)	42.1 (13.2)	167.0 (15.9)	357.6 (10.9)
^{1ANP}dG	B	4.0 (0.7)	221.7 (13.1)	165.3 (21.2)	17.1 (11.0)
	W	2.1 (0.3)	66.2 (12.6)	70.7 (13.5)	359.6 (9.1)
	S	2.3 (0.4)	38.2 (15.8)	189.2 (18.3)	355.6 (9.8)
^{2ANP}dG	B	4.0 (0.7)	226.8 (12.7)	139.9 (22.3)	5.4 (11.4)
	W	1.9 (0.4)	64.7 (12.8)	76.2 (14.2)	180.5 (9.8)
	S	2.4 (0.5)	45.2 (21.7)	177.1 (14.1)	175.2 (10.5)
^{3ABP}dG	B	2.2 (0.5)	230.8 (12.2)	124.6 (13.9)	5.3 (12.8)
	W	2.2 (0.5)	69.1 (12.6)	62.4 (14.7)	183.8 (9.7)
	S	2.9 (0.5)	119.4 (18.9)	196.5 (13.8)	175.9 (10.2)
^{1APHN}dG	B	3.5 (0.6)	216.5 (11.0)	174.8 (12.2)	17.8 (10.8)
	W	2.3 (0.4)	67.9 (12.9)	71.7 (13.9)	359.0 (10.4)
	S	3.3 (0.5)	120.4 (23.1)	206.6 (15.0)	5.9 (11.9)
^{3APHN}dG	B	2.1 (0.4)	226.9 (13.1)	135.4 (25.9)	8.6 (12.9)
	W	2.4 (0.4)	71.2 (13.4)	72.5 (15.0)	0.1 (10.4)
	S	2.7 (0.5)	132.3 (24.4)	191.9 (18.1)	177.5 (11.1)
^{1AP}dG	B	2.6 (0.5)	218.5 (12.2)	166.4 (20.6)	17.6 (11.3)
	W	4.1 (0.7)	64.0 (12.5)	68.2 (12.9)	1.1 (10.2)
	S	5.0 (0.7)	48.4 (33.6)	205.6 (11.0)	353.2 (11.5)

[a]RMSD is calculated with respect to the first frame of the production run.

Table S12. Average and standard deviations (in parentheses) of the solvent accessible surface area (SASA, Å^2) of the NCA moiety within different conformations of N-linked adducted DNA.

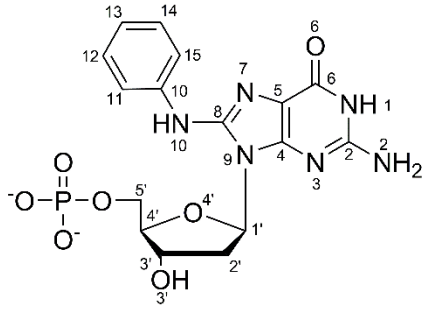
Nucleoside	Conformation	SASA
^{AN}dG	B	116.1 (6.3)
^{1ANP}dG		137.3 (6.5)
^{2ANP}dG		147.8 (5.8)
^{3ABP}dG		191.1 (7.1)
^{1APHN}dG		176.0 (6.1)
^{3APHN}dG		179.5 (7.3)
^{1AP}dG		175.6 (5.3)
^{AN}dG	W	92.2 (20.0)
^{1ANP}dG		115.5 (15.5)
^{2ANP}dG		109.5 (17.6)
^{3ABP}dG		159.7 (24.0)
^{1APHN}dG		153.1 (19.7)
^{3APHN}dG		159.7 (20.3)
^{1AP}dG		155.5 (18.2)
^{AN}dG	S	30.7 (12.3)
^{1ANP}dG		71.2 (11.9)
^{2ANP}dG		39.8 (7.0)
^{3ABP}dG		56.9 (6.8)
^{1APHN}dG		85.3 (12.3)
^{3APHN}dG		76.2 (8.8)
^{1AP}dG		107.8 (11.7)

Table S13. Occupancies (%) for the Watson-Crick hydrogen bonds within the base pairs present at the 5′– and 3′– terminals with respect to the lesion respectively, in three conformations of the adducted DNA.[a]

Conformation	Base pair[b]	Hydrogen bond	^{AN}dG	^{1ANP}dG	^{2ANP}dG	^{3ABP}dG	^{1APHN}dG	^{3APHN}dG	^{1AP}dG
B	5′–G:C	N1(G)–H•••N3(C)	100.0	100.0	100.0	100.0	100.0	100.0	100.0
		N2(G)–H•••O2(C)	99.9	99.9	99.9	99.9	99.9	99.9	99.9
		N4(C)–H•••O6(G)	98.9	98.8	99.0	99.2	99.1	98.9	99.1
	3′–G:C	N1(G)–H•••N3(C)	100.0	100.0	100.0	100.0	100.0	100.0	100.0
		N2(G)–H•••O2(C)	99.6	99.8	99.6	99.8	99.7	99.7	99.6
		N4(C)–H•••O6(G)	98.8	98.8	98.8	98.8	98.8	98.6	98.8
W	5′–G:C	N1(G)–H•••N3(C)	100.0	100.0	100.0	100.0	100.0	100.0	100.0
		N2(G)–H•••O2(C)	100.0	99.9	99.9	100.0	99.9	99.8	99.9
		N4(C)–H•••O6(G)	98.8	98.6	98.9	99.1	98.5	98.4	98.9
	3′–G:C	N1(G)–H•••N3(C)	100.0	100.0	100.0	100.0	100.0	100.0	100.0
		N2(G)–H•••O2(C)	99.7	99.8	99.6	99.8	99.7	99.7	99.7
		N4(C)–H•••O6(G)	98.8	98.8	98.6	98.9	98.5	98.5	98.8
S	5′–G:C	N1(G)–H•••N3(C)	100.0	100.0	100.0	100.0	100.0	100.0	100.0
		N2(G)–H•••O2(C)	99.9	99.8	99.9	99.9	99.9	99.9	99.9
		N4(C)–H•••O6(G)	99.1	98.8	98.8	98.7	98.8	98.8	99.0
	3′–G:C	N1(G)–H•••N3(C)	100.0	100.0	100.0	100.0	100.0	100.0	100.0
		N2(G)–H•••O2(C)	99.7	99.7	99.7	99.8	99.6	99.7	99.7
		N4(C)–H•••O6(G)	98.6	98.7	98.8	98.9	97.9	98.5	98.8

[a]Hydrogen-bonding interactions were determined using a cutoff of 3.4 Å for the donor–acceptor distance and 120° for the donor–hydrogen–acceptor angle. [b]5′–C:G and 3′–C:G present the terminal base pairs on the 5′ and 3′ terminal of the lesion containing strand, respectively.

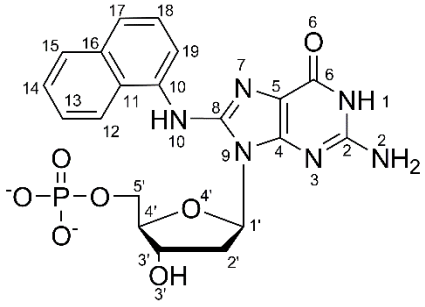
Table S14. MOL2 file containing partial charges and atom types of the ^{AN}dG adduct used for MD simulations (atom numbers are provided in the associated figure).



1	P	4.7050	0.0520	-1.1680	P	1	LIG	1.2090
2	O5'	4.1730	1.0760	0.0000	OS	1	LIG	-0.4900
3	OP1	4.6090	0.7320	-2.4680	O2	1	LIG	-0.7864
4	OP2	5.9220	-0.5810	-0.6380	O2	1	LIG	-0.7953
5	O3	0.0000	0.0000	0.0000	OS	1	LIG	-0.5474
6	C5'	3.1010	1.9490	-0.3030	CI	1	LIG	-0.0102
7	H5'	2.8330	2.4680	0.6250	H1	1	LIG	0.0752
8	H5''	3.3910	2.7140	-1.0420	H1	1	LIG	0.0752
9	C4'	1.8690	1.2180	-0.8380	CT	1	LIG	0.1830
10	H4'	1.0270	1.9170	-0.9140	H1	1	LIG	0.0978
11	O4'	2.1700	0.7140	-2.1590	OS	1	LIG	-0.4082
12	C1'	1.9220	-0.6850	-2.2280	CT	1	LIG	0.1596
13	H1'	0.9300	-0.8780	-2.6450	H2	1	LIG	0.0902
14	C3'	1.4280	0.0000	0.0000	CT	1	LIG	0.1484
15	H3'	1.8240	0.0530	1.0220	H1	1	LIG	0.0720
16	C2'	2.0070	-1.1870	-0.7800	CT	1	LIG	-0.0617
17	H2'	3.0480	-1.3520	-0.4920	HC	1	LIG	0.0466
18	H2''	1.4440	-2.1140	-0.6290	HC	1	LIG	0.0466
19	N9	2.8790	-1.2770	-3.1530	N*	1	LIG	-0.0563
20	C8	2.6100	-2.0090	-4.3140	CR	1	LIG	0.4678
21	C4	4.2540	-1.2720	-3.0400	CB	1	LIG	0.1484
22	N7	3.6880	-2.4790	-4.8900	NB	1	LIG	-0.5254
23	C5	4.7300	-2.0310	-4.1010	CB	1	LIG	0.0762
24	N4	4.9730	-0.6260	-2.0850	NC	1	LIG	-0.5421
25	C6	6.1500	-2.2180	-4.2500	C	1	LIG	0.5106
26	C2	6.2750	-0.7780	-2.1980	CA	1	LIG	0.6729
27	O6	6.7970	-2.8430	-5.0700	O	1	LIG	-0.5407
28	N1	6.8450	-1.5130	-3.1980	NA	1	LIG	-0.4810
29	H1	7.8500	-1.6540	-3.2180	H	1	LIG	0.3501
30	N2	7.0960	-0.2220	-1.2480	N2	1	LIG	-0.8752
31	H21	8.0220	0.0670	-1.5350	H	1	LIG	0.3884

32	H22	6.6240	0.4340	-0.6340	H	1	LIG	0.3884
33	N10	1.3100	-2.3020	-4.7270	N2	1	LIG	-0.5894
34	H10	1.3080	-3.1770	-5.2390	H	1	LIG	0.3511
35	C10	0.4170	-1.3450	-5.2830	CA	1	LIG	0.2156
36	C11	0.6440	0.0360	-5.2250	CA	1	LIG	-0.0547
37	H11	1.5430	0.4310	-4.7640	HA	1	LIG	0.1212
38	C15	-0.7540	-1.8230	-5.8900	CA	1	LIG	-0.2053
39	H15	-0.9360	-2.8950	-5.9310	HA	1	LIG	0.1458
40	C12	-0.2970	0.9160	-5.7630	CA	1	LIG	-0.2343
41	H12	-0.1060	1.9850	-5.7080	HA	1	LIG	0.1637
42	C14	-1.6780	-0.9360	-6.4340	CA	1	LIG	-0.1747
43	H14	-2.5760	-1.3250	-6.9060	HA	1	LIG	0.1548
44	C13	-1.4580	0.4430	-6.3720	CA	1	LIG	-0.1124
45	H13	-2.1820	1.1350	-6.7910	HA	1	LIG	0.1321

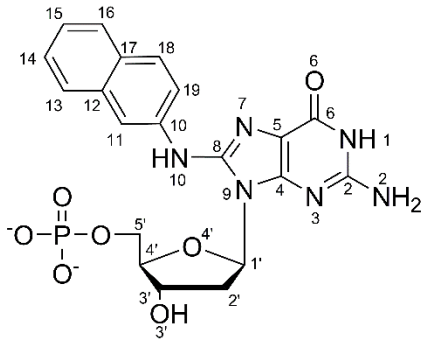
Table S15. MOL2 file containing partial charges and atom types of the ^{1ANP}dG adduct used for MD simulations (atom numbers are provided in the associated figure).



1	P	4.9460	0.3260	-1.3040	P	1	LIG	1.1661
2	O5'	4.1310	1.0120	0.0000	OS	1	LIG	-0.4975
3	OP1	5.0700	1.3460	-2.3940	O2	1	LIG	-0.7680
4	OP2	6.0760	-0.4560	-0.7070	O2	1	LIG	-0.7680
5	O3'	0.0000	0.0000	0.0000	OS	1	LIG	-0.5419
6	C5'	3.0960	1.8960	-0.3140	CI	1	LIG	-0.0178
7	H5'	3.4180	2.6460	-1.0320	H1	1	LIG	0.0805
8	H5''	2.8360	2.4120	0.6020	H1	1	LIG	0.0805
9	C4'	1.8580	1.1950	-0.8480	CT	1	LIG	0.1759
10	H4'	1.0450	1.9050	-0.9320	H1	1	LIG	0.1016
11	O4'	2.1310	0.6740	-2.1470	OS	1	LIG	-0.4096
12	C1'	1.8680	-0.6970	-2.2080	CT	1	LIG	0.1529
13	H1'	0.8770	-0.8680	-2.5990	H2	1	LIG	0.0818
14	C3'	1.4070	0.0000	0.0000	CT	1	LIG	0.1305
15	H3'	1.7900	0.0630	1.0110	H1	1	LIG	0.0783
16	C2'	1.9740	-1.1870	-0.7680	CT	1	LIG	-0.0617

17	H2'	3.0120	-1.3450	-0.5030	HC	1	LIG	0.0463
18	H2''	1.4240	-2.1060	-0.6070	HC	1	LIG	0.0463
19	N	2.7840	-1.3310	-3.1400	N*	1	LIG	-0.0146
20	C	4.1010	-1.0480	-3.4690	CR	1	LIG	0.2646
21	C6	2.4920	-2.4870	-3.8070	CB	1	LIG	0.1347
22	N1	4.6200	-1.9060	-4.2590	NB	1	LIG	-0.4291
23	C7	3.6230	-2.8360	-4.4770	CB	1	LIG	0.0774
24	N2	1.2990	-3.1310	-3.7570	NC	1	LIG	-0.5059
25	C8	3.6080	-4.0190	-5.2880	C	1	LIG	0.4773
26	C9	1.2730	-4.1920	-4.4890	CA	1	LIG	0.6026
27	O5	4.4510	-4.5170	-5.9710	O	1	LIG	-0.5400
28	N3	2.3330	-4.6330	-5.2100	NA	1	LIG	-0.4049
29	H	2.2290	-5.4250	-5.8090	H	1	LIG	0.3318
30	N4	0.1230	-4.9160	-4.5980	N2	1	LIG	-0.8791
31	H6	0.2020	-5.8970	-4.7470	H	1	LIG	0.3940
32	H7	-0.5810	-4.6540	-3.9430	H	1	LIG	0.3940
33	N5	4.7320	0.0820	-2.9520	N2	1	LIG	-0.1783
34	H8	4.1240	0.8710	-3.0190	H	1	LIG	0.2217
35	C10	6.0550	0.3790	-3.4120	CM	1	LIG	-0.0616
36	C11	7.1720	-0.2710	-2.8070	CM	1	LIG	0.0743
37	C12	6.2440	1.3280	-4.3640	CM	1	LIG	-0.0968
38	H9	5.3930	1.8050	-4.8190	HA	1	LIG	0.1341
39	C13	8.4670	0.0840	-3.2370	CA	1	LIG	0.1635
40	C14	7.0360	-1.2460	-1.7850	CA	1	LIG	-0.2174
41	H10	6.0550	-1.5200	-1.4480	HA	1	LIG	0.1272
42	C15	7.5470	1.6890	-4.7810	CA	1	LIG	-0.1760
43	H11	7.6660	2.4430	-5.5370	HA	1	LIG	0.1573
44	C16	9.5900	-0.5530	-2.6450	CA	1	LIG	-0.2093
45	H12	10.5740	-0.2810	-2.9810	HA	1	LIG	0.1434
46	C17	8.6280	1.0790	-4.2380	CA	1	LIG	-0.2327
47	H13	9.6220	1.3420	-4.5540	HA	1	LIG	0.1526
48	C18	8.1300	-1.8340	-1.2340	CA	1	LIG	-0.1129
49	H14	8.0110	-2.5710	-0.4600	HA	1	LIG	0.1354
50	C19	9.4290	-1.4860	-1.6720	CA	1	LIG	-0.1435
51	H15	10.2850	-1.9630	-1.2300	HA	1	LIG	0.1397

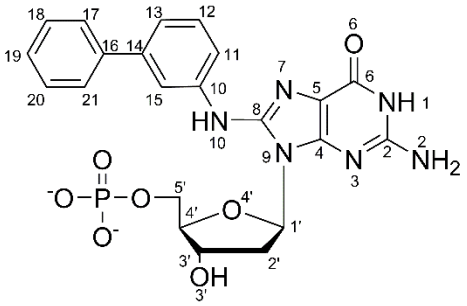
Table S16. MOL2 file containing partial charges and atom types of the ^{2ANP}dG adduct used for MD simulations (atom numbers are provided in the associated figure).



1	P	4.9500	0.3390	-1.3140	P	1	LIG	1.1662
2	O5'	4.1340	1.0060	0.0000	OS	1	LIG	-0.4947
3	OP1	5.0740	1.3760	-2.3880	O2	1	LIG	-0.7681
4	OP2	6.0790	-0.4520	-0.7290	O2	1	LIG	-0.7681
5	O3	0.0000	0.0000	0.0000	OS	1	LIG	-0.5427
6	C5'	3.1000	1.8950	-0.3000	CI	1	LIG	-0.0213
7	H5'	3.4210	2.6520	-1.0120	H1	1	LIG	0.0819
8	H5''	2.8450	2.4020	0.6220	H1	1	LIG	0.0819
9	C4'	1.8570	1.2030	-0.8360	CT	1	LIG	0.1693
10	H4'	1.0460	1.9160	-0.9090	H1	1	LIG	0.1034
11	O4'	2.1200	0.6960	-2.1430	OS	1	LIG	-0.4066
12	C1'	1.8670	-0.6760	-2.2160	CT	1	LIG	0.1659
13	H1'	0.8770	-0.8500	-2.6110	H2	1	LIG	0.0788
14	C3'	1.4070	0.0000	0.0000	CT	1	LIG	0.1359
15	H3'	1.7900	0.0530	1.0120	H1	1	LIG	0.0773
16	C2'	1.9750	-1.1790	-0.7800	CT	1	LIG	-0.0594
17	H2'	3.0120	-1.3380	-0.5180	HC	1	LIG	0.0441
18	H2''	1.4250	-2.1000	-0.6270	HC	1	LIG	0.0441
19	N9	2.7890	-1.3010	-3.1500	N*	1	LIG	-0.0377
20	C8	4.1030	-1.0080	-3.4810	CR	1	LIG	0.4496
21	C4	2.5170	-2.4780	-3.7870	CB	1	LIG	0.1103
22	N7	4.6370	-1.8800	-4.2460	NB	1	LIG	-0.5057
23	C5	3.6540	-2.8290	-4.4440	CB	1	LIG	0.0865
24	N3	1.3330	-3.1380	-3.7240	NC	1	LIG	-0.5039
25	C6	3.6620	-4.0360	-5.2180	C	1	LIG	0.5121
26	C2	1.3250	-4.2180	-4.4270	CA	1	LIG	0.6173
27	O6	4.5190	-4.5440	-5.8760	O	1	LIG	-0.5469
28	N1	2.3950	-4.6650	-5.1310	NA	1	LIG	-0.4417
29	H1	2.3050	-5.4750	-5.7070	H	1	LIG	0.3416
30	N2	0.1860	-4.9610	-4.5210	N2	1	LIG	-0.8699
31	H21	0.2770	-5.9440	-4.6480	H	1	LIG	0.3898

32	H22	-0.5260	-4.6910	-3.8780	H	1	LIG	0.3898
33	N10	4.7040	0.1470	-2.9940	N2	1	LIG	-0.4461
34	H10	4.0660	0.9130	-3.0200	H	1	LIG	0.2949
35	C10	6.0190	0.5050	-3.3890	CA	1	LIG	0.0740
36	C11	6.2680	1.7590	-3.8480	CA	1	LIG	-0.1637
37	H11	5.4580	2.4550	-3.9930	HA	1	LIG	0.1344
38	C19	7.0920	-0.4100	-3.2090	CA	1	LIG	-0.1758
39	H19	6.8840	-1.4000	-2.8560	HA	1	LIG	0.1831
40	C12	7.5910	2.1810	-4.1490	CA	1	LIG	0.0512
41	C18	8.3590	-0.0320	-3.5020	CA	1	LIG	-0.2300
42	H18	9.1660	-0.7300	-3.3690	HA	1	LIG	0.1580
43	C17	8.6530	1.2740	-3.9790	CA	1	LIG	0.1844
44	C13	7.8740	3.4880	-4.6240	CA	1	LIG	-0.2158
45	H13	7.0630	4.1820	-4.7560	HA	1	LIG	0.1417
46	C16	9.9740	1.6910	-4.2850	CA	1	LIG	-0.2256
47	H16	10.7820	0.9920	-4.1540	HA	1	LIG	0.1487
48	C14	9.1500	3.8610	-4.9100	CA	1	LIG	-0.1211
49	H14	9.3540	4.8530	-5.2700	HA	1	LIG	0.1365
50	C15	10.2180	2.9490	-4.7380	CA	1	LIG	-0.1481
51	H15	11.2220	3.2570	-4.9690	HA	1	LIG	0.1401

Table S17. MOL2 file containing partial charges and atom types of the ^{3ABP}dG adduct used for MD simulations (atom numbers are provided in the associated figure).

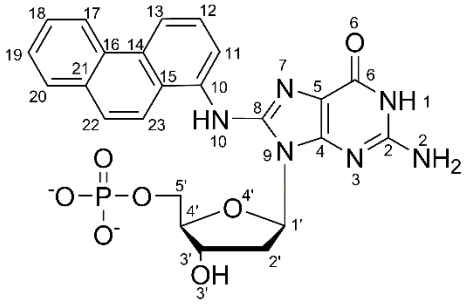


1	P	4.9540	0.3210	-1.2910	P	1	LIG	1.1662
2	O5'	4.1290	1.0200	0.0000	OS	1	LIG	-0.4955
3	OP1	5.0810	1.3290	-2.3930	O2	1	LIG	-0.7681
4	OP2	6.0840	-0.4490	-0.6780	O2	1	LIG	-0.7681
5	O3'	0.0000	0.0000	0.0000	OS	1	LIG	-0.5421
6	C5'	3.0930	1.8970	-0.3300	CI	1	LIG	-0.0196
7	H5'1	3.4150	2.6390	-1.0570	H1	1	LIG	0.0822
8	H5'2	2.8290	2.4240	0.5790	H1	1	LIG	0.0822
9	C4'	1.8570	1.1880	-0.8590	CT	1	LIG	0.1652
10	H4'	1.0430	1.8960	-0.9510	H1	1	LIG	0.1045

11	O4'	2.1310	0.6550	-2.1530	OS	1	LIG	-0.4045
12	C1'	1.8680	-0.7170	-2.2030	CT	1	LIG	0.1618
13	H1'	0.8770	-0.8900	-2.5920	H2	1	LIG	0.0837
14	C3'	1.4070	0.0000	0.0000	CT	1	LIG	0.1348
15	H3'	1.7900	0.0720	1.0110	H1	1	LIG	0.0780
16	C2'	1.9750	-1.1940	-0.7580	CT	1	LIG	-0.0575
17	H2'1	3.0130	-1.3480	-0.4930	HC	1	LIG	0.0444
18	H2'2	1.4250	-2.1110	-0.5880	HC	1	LIG	0.0444
19	N9	2.7840	-1.3660	-3.1260	N*	1	LIG	-0.0535
20	C8	4.1050	-1.0990	-3.4580	CR	1	LIG	0.4020
21	C4	2.5000	-2.5600	-3.7280	CB	1	LIG	0.1306
22	N7	4.6320	-2.0050	-4.1890	NB	1	LIG	-0.4841
23	C5	3.6370	-2.9460	-4.3650	CB	1	LIG	0.0745
24	N3	1.3090	-3.2040	-3.6490	NC	1	LIG	-0.4981
25	C6	3.6350	-4.1770	-5.0980	C	1	LIG	0.5012
26	C2	1.2920	-4.3060	-4.3170	CA	1	LIG	0.6022
27	O6	4.4910	-4.7170	-5.7330	O	1	LIG	-0.5467
28	N1	2.3600	-4.7880	-5.0000	NA	1	LIG	-0.4250
29	H1	2.2640	-5.6160	-5.5490	H	1	LIG	0.3383
30	N2	0.1440	-5.0380	-4.3930	N2	1	LIG	-0.8680
31	H21	0.2250	-6.0270	-4.4870	H	1	LIG	0.3898
32	H22	-0.5680	-4.7390	-3.7640	H	1	LIG	0.3898
33	N10	4.7040	0.0670	-3.0080	N2	1	LIG	-0.3808
34	H10	4.0510	0.8200	-3.0030	H	1	LIG	0.2905
35	C10	6.0120	0.4610	-3.3830	CA	1	LIG	0.0469
36	C15	6.2360	1.8120	-3.6080	CA	1	LIG	-0.1137
37	H15	5.4080	2.4990	-3.5780	HA	1	LIG	0.1068
38	C11	7.0730	-0.4330	-3.4560	CA	1	LIG	-0.0925
39	H11	6.9110	-1.4790	-3.2990	HA	1	LIG	0.1433
40	C14	7.5060	2.2950	-3.9050	cp	1	LIG	-0.0167
41	C12	8.3330	0.0450	-3.7620	CA	1	LIG	-0.2240
42	H12	9.1540	-0.6480	-3.8190	HA	1	LIG	0.1649
43	C16	7.7230	3.7520	-4.1390	cp	1	LIG	0.0101
44	C13	8.5600	1.3930	-3.9840	CA	1	LIG	-0.0936
45	H13	9.5530	1.7430	-4.1980	HA	1	LIG	0.1157
46	C17	7.1880	4.7030	-3.2750	CA	1	LIG	-0.0792
47	H17	6.6280	4.3820	-2.4150	HA	1	LIG	0.1073
48	C21	8.4700	4.1930	-5.2290	CA	1	LIG	-0.0822
49	H21	8.8760	3.4750	-5.9180	HA	1	LIG	0.1165
50	C18	7.3910	6.0550	-3.4940	CA	1	LIG	-0.1877
51	H18	6.9760	6.7740	-2.8100	HA	1	LIG	0.1447
52	C20	8.6730	5.5450	-5.4490	CA	1	LIG	-0.1870
53	H20	9.2470	5.8650	-6.3000	HA	1	LIG	0.1448

54	C19	8.1350	6.4820	-4.5820	CA	1	LIG	-0.1130
55	H19	8.2930	7.5320	-4.7520	HA	1	LIG	0.1337

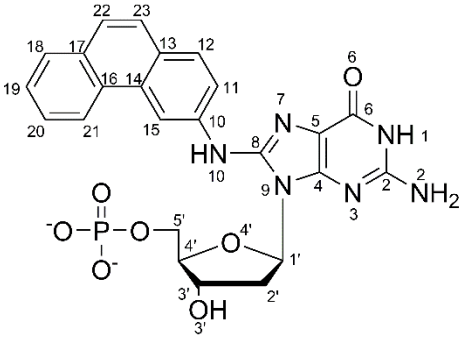
Table S18. MOL2 file containing partial charges and atom types of the ^{1APHN}dG adduct used for MD simulations (atom numbers are provided in the associated figure).



1	P	4.9390	0.3380	-1.3210	P	1	LIG	1.1662
2	O5'	4.1360	1.0060	0.0000	OS	1	LIG	-0.4960
3	OP1	5.0550	1.3730	-2.3970	O2	1	LIG	-0.7680
4	OP2	6.0730	-0.4550	-0.7460	O2	1	LIG	-0.7680
5	O3	0.0000	0.0000	0.0000	OS	1	LIG	-0.5443
6	C5'	3.1000	1.8960	-0.2910	CI	1	LIG	-0.0174
7	H5'	3.4190	2.6590	-0.9980	H1	1	LIG	0.0811
8	H5''	2.8460	2.3970	0.6360	H1	1	LIG	0.0811
9	C4'	1.8580	1.2080	-0.8300	CT	1	LIG	0.1705
10	H4'	1.0470	1.9210	-0.8980	H1	1	LIG	0.1016
11	O4'	2.1200	0.7070	-2.1400	OS	1	LIG	-0.4090
12	C1'	1.8680	-0.6660	-2.2190	CT	1	LIG	0.1650
13	H1'	0.8790	-0.8380	-2.6160	H2	1	LIG	0.0790
14	C3'	1.4070	0.0000	0.0000	CT	1	LIG	0.1414
15	H3'	1.7900	0.0480	1.0120	H1	1	LIG	0.0750
16	C2'	1.9750	-1.1760	-0.7860	CT	1	LIG	-0.0599
17	H2'	3.0120	-1.3360	-0.5240	HC	1	LIG	0.0433
18	H2''	1.4250	-2.0970	-0.6370	HC	1	LIG	0.0433
19	N9	2.7920	-1.2820	-3.1550	N*	1	LIG	-0.0483
20	C8	4.1100	-0.9870	-3.4700	CR	1	LIG	0.3864
21	C4	2.5270	-2.4550	-3.8040	CB	1	LIG	0.1609
22	N7	4.6520	-1.8510	-4.2380	NB	1	LIG	-0.4514
23	C5	3.6710	-2.7980	-4.4530	CB	1	LIG	0.0424
24	N3	1.3430	-3.1170	-3.7540	NC	1	LIG	-0.5186
25	C6	3.6850	-3.9970	-5.2400	C	1	LIG	0.5168
26	C2	1.3430	-4.1910	-4.4660	CA	1	LIG	0.6210
27	O6	4.5450	-4.4980	-5.8990	O	1	LIG	-0.5494
28	N1	2.4180	-4.6300	-5.1660	NA	1	LIG	-0.4362
29	H1	2.3330	-5.4340	-5.7500	H	1	LIG	0.3377
30	N2	0.2050	-4.9360	-4.5750	N2	1	LIG	-0.8693

31	H21	0.3020	-5.9190	-4.7020	H	1	LIG	0.3884
32	H22	-0.5100	-4.6730	-3.9330	H	1	LIG	0.3884
33	N10	4.7180	0.1580	-2.9650	N2	1	LIG	-0.4445
34	H10	4.0870	0.9300	-2.9790	H	1	LIG	0.3021
35	C10	6.0390	0.4770	-3.4140	CA	1	LIG	0.0699
36	C15	6.2480	1.3350	-4.5210	CA	1	LIG	0.0883
37	C11	7.0970	-0.0340	-2.7190	CA	1	LIG	-0.1367
38	H11	6.9150	-0.6850	-1.8850	HA	1	LIG	0.1436
39	C14	7.5620	1.6900	-4.8780	CA	1	LIG	0.0228
40	C23	5.1440	1.8530	-5.2910	CA	1	LIG	-0.1798
41	H23	4.1430	1.5500	-5.0490	HA	1	LIG	0.1390
42	C12	8.4040	0.2890	-3.0970	CA	1	LIG	-0.1725
43	H12	9.2330	-0.1240	-2.5510	HA	1	LIG	0.1602
44	C16	7.7770	2.6060	-5.9960	CA	1	LIG	0.0658
45	C13	8.6300	1.1380	-4.1430	CA	1	LIG	-0.2018
46	H13	9.6430	1.3750	-4.4010	HA	1	LIG	0.1547
47	C22	5.3460	2.6840	-6.3220	CA	1	LIG	-0.2403
48	H22	4.5110	3.0530	-6.8920	HA	1	LIG	0.1586
49	C21	6.6690	3.0960	-6.7040	CA	1	LIG	0.1173
50	C17	9.0590	3.0330	-6.4040	CA	1	LIG	-0.1932
51	H17	9.9330	2.6860	-5.8890	HA	1	LIG	0.1406
52	C20	6.8570	3.9810	-7.7840	CA	1	LIG	-0.1752
53	H20	5.9930	4.3420	-8.3140	HA	1	LIG	0.1388
54	C18	9.2230	3.8930	-7.4540	CA	1	LIG	-0.1292
55	H18	10.2120	4.2010	-7.7420	HA	1	LIG	0.1390
56	C29	8.1100	4.3760	-8.1570	CA	1	LIG	-0.1704
57	H19	8.2450	5.0520	-8.9830	HA	1	LIG	0.1492

Table S19. MOL2 file containing partial charges and atom types of the ^{3APHN}dG adduct used for MD simulations (atom numbers are provided in the associated figure).

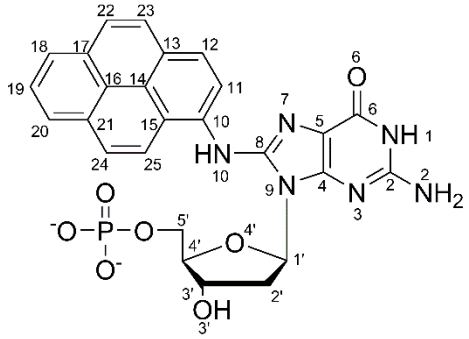


1	P	4.7030	0.0550	-1.1760	P	1	LIG	1.2091
2	O5'	4.1740	1.0720	0.0000	OS	1	LIG	-0.4894
3	OP1	4.6050	0.7450	-2.4710	O2	1	LIG	-0.7862

4	OP2	5.9200	-0.5830	-0.6540	O2	1	LIG	-0.7955
5	O3	0.0000	0.0000	0.0000	OS	1	LIG	-0.5485
6	C5'	3.1030	1.9480	-0.2950	CI	1	LIG	-0.0049
7	H5'	2.8380	2.4620	0.6370	H1	1	LIG	0.0737
8	H5''	3.3920	2.7170	-1.0290	H1	1	LIG	0.0737
9	C4'	1.8690	1.2220	-0.8310	CT	1	LIG	0.1806
10	H4'	1.0280	1.9230	-0.9010	H1	1	LIG	0.0973
11	O4'	2.1640	0.7260	-2.1570	OS	1	LIG	-0.4092
12	C1'	1.9180	-0.6730	-2.2330	CT	1	LIG	0.1631
13	H1'	0.9240	-0.8650	-2.6470	H2	1	LIG	0.0901
14	C3'	1.4280	0.0000	0.0000	CT	1	LIG	0.1539
15	H3'	1.8240	0.0460	1.0220	H1	1	LIG	0.0696
16	C2'	2.0060	-1.1830	-0.7870	CT	1	LIG	-0.0625
17	H2'	3.0470	-1.3500	-0.5020	HC	1	LIG	0.0462
18	H2''	1.4430	-2.1100	-0.6400	HC	1	LIG	0.0462
19	N9	2.8730	-1.2580	-3.1640	N*	1	LIG	-0.0458
20	C8	2.6000	-1.9810	-4.3310	CR	1	LIG	0.4616
21	C4	4.2480	-1.2530	-3.0550	CB	1	LIG	0.1258
22	N7	3.6770	-2.4460	-4.9130	NB	1	LIG	-0.5189
23	C5	4.7210	-2.0040	-4.1240	CB	1	LIG	0.0919
24	N3	4.9690	-0.6150	-2.0960	NC	1	LIG	-0.5254
25	C6	6.1410	-2.1900	-4.2770	C	1	LIG	0.5023
26	C2	6.2710	-0.7660	-2.2140	CA	1	LIG	0.6442
27	O6	6.7850	-2.8100	-5.1030	O	1	LIG	-0.5410
28	N1	6.8390	-1.4930	-3.2220	NA	1	LIG	-0.4656
29	H1	7.8430	-1.6340	-3.2440	H	1	LIG	0.3496
30	N2	7.0940	-0.2180	-1.2620	N2	1	LIG	-0.8684
31	H21	8.0210	0.0700	-1.5460	H	1	LIG	0.3883
32	H22	6.6230	0.4330	-0.6410	H	1	LIG	0.3883
33	N10	1.3000	-2.2720	-4.7430	N2	1	LIG	-0.5844
34	H10	1.2910	-3.1520	-5.2460	H	1	LIG	0.3515
35	C10	0.4040	-1.3200	-5.2950	CA	1	LIG	0.2030
36	C11	0.6360	0.0710	-5.2180	CA	1	LIG	-0.0909
37	H11	1.5320	0.4600	-4.7470	HA	1	LIG	0.1418
38	C15	-0.7530	-1.7900	-5.9070	CA	1	LIG	-0.2595
39	H15	-0.9090	-2.8640	-5.9430	HA	1	LIG	0.1563
40	C12	-0.2930	0.9410	-5.7500	CA	1	LIG	-0.2651
41	H12	-0.1140	2.0120	-5.6900	HA	1	LIG	0.1669
42	C14	-1.7080	-0.9190	-6.4670	CA	1	LIG	0.0047
43	C13	-1.4710	0.4860	-6.3810	CA	1	LIG	0.1187
44	C16	-2.9230	-1.3900	-7.1230	CA	1	LIG	0.0738
45	C22	-2.4200	1.4080	-6.9330	CA	1	LIG	-0.1827
46	H22'	-2.2110	2.4720	-6.8510	HA	1	LIG	0.1524

47	C17	-3.8380	-0.4320	-7.6570	CA	1	LIG	0.1448
48	C21	-3.2440	-2.7600	-7.2590	CA	1	LIG	-0.2055
49	H21'	-2.5720	-3.5150	-6.8670	HA	1	LIG	0.1475
50	C23	-3.5530	0.9700	-7.5430	CA	1	LIG	-0.2670
51	H23	-4.2670	1.6770	-7.9590	HA	1	LIG	0.1612
52	C18	-5.0190	-0.8780	-8.2950	CA	1	LIG	-0.2005
53	H18	-5.7040	-0.1350	-8.6960	HA	1	LIG	0.1440
54	C20	-4.4060	-3.1720	-7.8880	CA	1	LIG	-0.1450
55	H20	-4.6230	-4.2330	-7.9770	HA	1	LIG	0.1421
56	C19	-5.3040	-2.2240	-8.4120	CA	1	LIG	-0.1486
57	H19	-6.2150	-2.5510	-8.9050	HA	1	LIG	0.1462

Table S20. MOL2 file containing partial charges and atom types of the ^{1AP}dG adduct used for MD simulations (atom numbers are provided in the associated figure).



1	P	4.9760	0.3860	-1.3260	P	1	LIG	1.1662
2	O5'	4.1390	0.9990	0.0000	OS	1	LIG	-0.4956
3	OP1	5.1120	1.4640	-2.3580	O2	1	LIG	-0.7681
4	OP2	6.1010	-0.4220	-0.7550	O2	1	LIG	-0.7681
5	O3	0.0000	0.0000	0.0000	OS	1	LIG	-0.5424
6	C5'	3.1040	1.8950	-0.2820	CI	1	LIG	-0.0196
7	H5'	3.4230	2.6620	-0.9830	H1	1	LIG	0.0821
8	H5''	2.8550	2.3890	0.6500	H1	1	LIG	0.0821
9	C4'	1.8570	1.2140	-0.8200	CT	1	LIG	0.1633
10	H4'	1.0480	1.9310	-0.8780	H1	1	LIG	0.1054
11	O4'	2.1080	0.7240	-2.1370	OS	1	LIG	-0.4032
12	C1'	1.8650	-0.6500	-2.2260	CT	1	LIG	0.1513
13	H1'	0.8780	-0.8250	-2.6240	H2	1	LIG	0.0873
14	C3'	1.4070	0.0000	0.0000	CT	1	LIG	0.1347
15	H3'	1.7910	0.0400	1.0120	H1	1	LIG	0.0784
16	C2'	1.9750	-1.1690	-0.7950	CT	1	LIG	-0.0572
17	H2'	3.0130	-1.3300	-0.5360	HC	1	LIG	0.0443
18	H2''	1.4270	-2.0920	-0.6530	HC	1	LIG	0.0443
19	N9	2.7970	-1.2560	-3.1630	N*	1	LIG	-0.0519

20	C8	4.0990	-0.9300	-3.5110	CR	1	LIG	0.3777
21	C4	2.5500	-2.4460	-3.7900	CB	1	LIG	0.1445
22	N7	4.6490	-1.7930	-4.2750	NB	1	LIG	-0.4566
23	C5	3.6890	-2.7690	-4.4570	CB	1	LIG	0.0570
24	N3	1.3850	-3.1370	-3.7080	NC	1	LIG	-0.4990
25	C6	3.7200	-3.9790	-5.2240	C	1	LIG	0.4977
26	C2	1.3980	-4.2210	-4.4050	CA	1	LIG	0.5921
27	O6	4.5820	-4.4690	-5.8910	O	1	LIG	-0.5456
28	N1	2.4720	-4.6420	-5.1190	NA	1	LIG	-0.4138
29	H1	2.3970	-5.4580	-5.6890	H	1	LIG	0.3351
30	N2	0.2780	-4.9950	-4.4810	N2	1	LIG	-0.8656
31	H21	0.3970	-5.9770	-4.5990	H	1	LIG	0.3895
32	H22	-0.4320	-4.7410	-3.8300	H	1	LIG	0.3895
33	N10	4.6780	0.2390	-3.0360	N2	1	LIG	-0.3628
34	H10	4.0050	0.9680	-2.9720	H	1	LIG	0.2783
35	C10	5.9550	0.6490	-3.5100	CA	1	LIG	0.0814
36	C15	6.1060	1.8360	-4.2310	CA	1	LIG	0.0633
37	C11	7.0640	-0.1160	-3.1790	CA	1	LIG	-0.2616
38	H11	6.9210	-1.0300	-2.6350	HA	1	LIG	0.1751
39	C14	7.4130	2.2570	-4.5810	CA	1	LIG	0.0181
40	C23	4.9910	2.6640	-4.6450	CA	1	LIG	-0.1706
41	H23	3.9870	2.3450	-4.4390	HA	1	LIG	0.1296
42	C12	8.3300	0.2810	-3.5480	CA	1	LIG	-0.1240
43	H12	9.1750	-0.3300	-3.2860	HA	1	LIG	0.1527
44	C16	7.6070	3.4880	-5.2930	CA	1	LIG	0.0859
45	C13	8.5310	1.4720	-4.2390	CA	1	LIG	0.0232
46	C22	5.1770	3.8110	-5.3090	CA	1	LIG	-0.2254
47	H22'	4.3310	4.4020	-5.6120	HA	1	LIG	0.1573
48	C21	6.4980	4.2810	-5.6550	CA	1	LIG	0.0462
49	C17	8.9100	3.9110	-5.6360	CA	1	LIG	0.0488
50	C24	9.8500	1.9270	-4.6100	CA	1	LIG	-0.1744
51	H24	10.6920	1.3130	-4.3430	HA	1	LIG	0.1419
52	C20	6.7030	5.4740	-6.3400	CA	1	LIG	-0.1411
53	H20	5.8560	6.0770	-6.6170	HA	1	LIG	0.1383
54	C18	9.0760	5.1110	-6.3220	CA	1	LIG	-0.1473
55	H18	10.0680	5.4350	-6.5840	HA	1	LIG	0.1409
56	C25	10.0320	3.0790	-5.2670	CA	1	LIG	-0.1962
57	H25	11.0200	3.4070	-5.5350	HA	1	LIG	0.1453
58	C19	7.9830	5.8840	-6.6680	CA	1	LIG	-0.2217
59	H19	8.1290	6.8080	-7.1990	HA	1	LIG	0.1629

Table S21. Cartesian coordinates of the nucleobase minimum for the ^{AN}G adduct with θ = 29.9° and ϕ = 16.7°.

Calculated energy (in Hartrees) = –829.3022069			
Atom	X	Y	Z
N	-0.06926100	0.46196200	-0.34668600
C	0.36255100	-0.83952200	-0.13182800
N	-0.62197900	-1.66773600	0.12555900
C	-1.76302700	-0.88013200	0.06605300
C	-3.14133000	-1.22591300	0.27780200
O	-3.67376800	-2.28962300	0.54653900
N	-3.95774100	-0.04763900	0.13461900
H	-4.93548300	-0.21028200	0.34652800
C	-3.52219600	1.21669300	-0.15888600
N	-4.47557500	2.21503400	-0.19219900
H	-5.37876500	1.96528100	-0.57618400
H	-4.10773300	3.07863000	-0.57202800
N	-2.25953000	1.51823900	-0.35395900
C	-1.44222000	0.44483200	-0.21787800
H	0.49182900	1.25207700	-0.62913500
N	1.67717600	-1.22237200	-0.27218300
H	1.79065200	-2.22480500	-0.33485400
C	2.82627500	-0.44676400	-0.06812300
C	4.04225100	-0.90686200	-0.59942700
C	2.80909700	0.75946800	0.65048000
C	5.21007000	-0.17334200	-0.42118000
C	3.98409000	1.49507500	0.80382400
H	1.89486700	1.09888900	1.12470500
C	5.18943700	1.03977400	0.27166900
H	3.95361800	2.42493600	1.36501200
H	4.05801900	-1.83803800	-1.15985900
H	6.14109900	-0.54780600	-0.83727900
H	6.10043800	1.61583900	0.39968000

Table S22. Cartesian coordinates of the nucleobase minimum for the ^{AN}G adduct with θ = 180.0° and ϕ = 0.0°.

Calculated energy (in Hartrees) = –829.3011175			
Atom	X	Y	Z
N	-0.71971200	-1.62217300	-0.00300100
C	0.34768300	-0.72606200	0.00014100
N	-0.04848800	0.52486400	0.00689100
C	-1.43564900	0.45607300	0.00749200
C	-2.41328200	1.50716100	0.00050600
O	-2.29293000	2.72075700	-0.00934100
N	-3.73435600	0.93089300	-0.00467900
H	-4.47160500	1.62174600	-0.08528700
C	-4.04281500	-0.40239300	-0.00206000
N	-5.38073900	-0.73663600	-0.06938500
H	-6.02269400	-0.13814300	0.43574200
H	-5.53578000	-1.72206600	0.10426700
N	-3.13657200	-1.35285600	0.00977600
C	-1.87219800	-0.86355200	-0.00026400
H	-0.69216600	-2.63138300	-0.01400800
N	1.63298000	-1.20806800	-0.00257200
H	1.73139600	-2.21225600	-0.00625100
C	2.83877100	-0.48739000	-0.00063700
C	4.03030100	-1.23011600	-0.00360500
C	2.89475400	0.91416400	0.00401800
C	5.26172700	-0.58395500	-0.00187500
C	4.13920600	1.54342300	0.00566500
H	1.97546400	1.48378600	0.00615900
C	5.32598100	0.81060800	0.00282400
H	4.17293700	2.62943100	0.00916300
H	3.98743900	-2.31795600	-0.00735900
H	6.17304700	-1.17551000	-0.00427200
H	6.28673000	1.31636700	0.00412800

Table S23. Cartesian coordinates of the nucleobase minimum for the ^{AN}G adduct with θ = 330.6° and ϕ = 163.1°.

Calculated energy (in Hartrees) = –829.3021875			
Atom	X	Y	Z
N	0.06882000	0.46199600	-0.33584200
C	-0.36201300	-0.83862600	-0.11443300
N	0.62295600	-1.66482700	0.14819700
C	1.76340000	-0.87670400	0.08514400
C	3.14441300	-1.22562400	0.27292300
O	3.68027600	-2.29385500	0.51566900
N	3.96079700	-0.04898500	0.11733800
H	4.95462100	-0.24310600	0.16175500
C	3.52277300	1.21696400	-0.16560000
N	4.48804200	2.18985700	-0.33512400
H	5.29755000	2.13326300	0.27071300
H	4.08715700	3.11884300	-0.37642400
N	2.25680800	1.52327800	-0.32862700
C	1.44219500	0.44576300	-0.20945800
H	-0.49169300	1.24843600	-0.62957200
N	-1.67618500	-1.22376900	-0.25156700
H	-1.78837700	-2.22640000	-0.31278200
C	-2.82675200	-0.44772000	-0.06130200
C	-2.81422500	0.76651800	0.64383100
C	-4.04019700	-0.91551400	-0.59196100
C	-3.99091900	1.50197900	0.78451700
C	-5.20964600	-0.18176200	-0.42647700
H	-4.05253700	-1.85298700	-1.14188600
C	-5.19352500	1.03908600	0.25288500
H	-6.13849200	-0.56221400	-0.84199900
H	-1.90239000	1.11259800	1.11779500
H	-3.96388300	2.43819400	1.33524100
H	-6.10584600	1.61520300	0.37076300

Table S24. Cartesian coordinates of the nucleobase minimum for the ^{1ANP}G adduct with θ = 36.7° and ϕ = 18.9°.

Calculated energy (in Hartrees) = –983.0063609			
Atom	X	Y	Z
N	1.09192600	0.52696100	0.40380500
C	0.55296900	-0.60271600	-0.19375000
N	1.46763100	-1.43568300	-0.62933700
C	2.67290500	-0.83352500	-0.29511100
C	4.02267800	-1.26433400	-0.53165400
O	4.46766600	-2.26564300	-1.06692300
N	4.93726100	-0.27501800	-0.02096200
H	5.90790200	-0.48530300	-0.22340800
C	4.60605800	0.90045900	0.59772200
N	5.64682500	1.73327200	0.95776200
H	6.48952200	1.28431200	1.29512600
H	5.33695300	2.49337500	1.55071900
N	3.36769200	1.28069400	0.81074300
C	2.46186400	0.38912300	0.33829600
H	0.58681700	1.28238200	0.84345900
N	-0.80283900	-0.85214200	-0.21753800
H	-1.00778800	-1.78862200	-0.54221800
C	-1.81593300	0.11472400	-0.36474900
C	-3.14501200	-0.24382800	0.03753400
C	-1.56522100	1.37561300	-0.87817700
C	-4.19727300	0.71088200	-0.14311000
C	-3.45607600	-1.50305900	0.61215200
C	-2.60748400	2.32015200	-1.00852400
H	-0.56929100	1.62966200	-1.22437900
C	-5.51987600	0.34535900	0.21948700
C	-3.89764700	1.99786200	-0.66282000
C	-4.75083900	-1.82347700	0.95671400
H	-2.65823900	-2.21079500	0.81064200
H	-2.37836200	3.30080900	-1.41542500
C	-5.79565800	-0.89443600	0.74901900
H	-4.96888800	-2.79046600	1.40042800
H	-4.70275700	2.71741800	-0.78137500
H	-6.31558300	1.07101300	0.07193000
H	-6.81381400	-1.15802500	1.02039700

Table S25. Cartesian coordinates of the nucleobase minimum for the ^{1ANP}G adduct with θ = 323.4° and ϕ = 341.1°.

Calculated energy (in Hartrees) = –983.006339			
Atom	X	Y	Z
N	-1.09272700	0.53158000	0.39535500
C	-0.55347200	-0.59686200	-0.20423200
N	-1.46786400	-1.42835700	-0.64328100
C	-2.67332200	-0.82666100	-0.30897500
C	-4.02294800	-1.26876600	-0.52475700
O	-4.46741300	-2.28358400	-1.03441200
N	-4.93791300	-0.28334700	-0.00734800
H	-5.90818600	-0.57162600	-0.06030200
C	-4.60707300	0.89876200	0.59885400
N	-5.64776300	1.66938500	1.07777200
H	-6.49300600	1.68554900	0.52032400
H	-5.33926200	2.59176300	1.35954200
N	-3.36894400	1.29391600	0.78387600
C	-2.46269100	0.39272400	0.33071800
H	-0.58798500	1.28227100	0.84349100
N	0.80218300	-0.84642700	-0.22848800
H	1.00748600	-1.78261000	-0.55354500
C	1.81700500	0.11943300	-0.36653000
C	3.14485600	-0.24424700	0.03551700
C	1.56944100	1.38457900	-0.87111500
C	4.19900700	0.71000500	-0.13628400
C	3.45283000	-1.50805000	0.60169200
C	2.61353100	2.32821300	-0.99273000
H	0.57450200	1.64281400	-1.21700200
C	5.52033600	0.33971800	0.22608500
C	3.90253600	2.00126000	-0.64714100
C	4.74643300	-1.83306900	0.94631300
H	2.65361700	-2.21591800	0.79409800
H	2.38683000	3.31228600	-1.39273100
C	5.79313200	-0.90430200	0.74718900
H	4.96201800	-2.80350800	1.38362900
H	4.70906100	2.72031300	-0.75890800
H	6.31747400	1.06514500	0.08528100
H	6.81034200	-1.17147200	1.01860500

Table S26. Cartesian coordinates of the nucleobase minimum for the ^{1ANP}G adduct with θ = 334.4° and ϕ = 252.1°.

Calculated energy (in Hartrees) = –983.0056003			
Atom	X	Y	Z
N	0.56164000	0.10570700	0.08398800
C	0.40044400	-1.13466500	-0.50854600
N	1.53787900	-1.73256800	-0.76899100
C	2.50632800	-0.83615000	-0.33490400
C	3.93904100	-0.92844100	-0.36786900
O	4.68257700	-1.80249600	-0.78203800
N	4.50869200	0.26763700	0.19834600
H	5.51965100	0.29881600	0.13323900
C	3.82179500	1.34062700	0.69991300
N	4.57301900	2.41471700	1.13885700
H	5.43763500	2.19205800	1.61724700
H	4.00766200	3.08898200	1.64031000
N	2.51184600	1.40825900	0.73132000
C	1.92195400	0.31088700	0.19481700
H	-0.16282800	0.76045000	0.34149100
N	-0.84376200	-1.67130300	-0.81357300
H	-0.75040100	-2.66313800	-1.00069200
C	-2.02305100	-1.29957200	-0.11303400
C	-2.60850600	-0.01649200	-0.35246600
C	-2.62022500	-2.18177100	0.76529700
C	-3.77053900	0.35582500	0.39998200
C	-2.09930500	0.89075500	-1.32092200
C	-3.79459000	-1.82417900	1.46364000
H	-2.16324300	-3.15271000	0.93593100
C	-4.33180600	1.64420500	0.19672700
C	-4.34551400	-0.57420800	1.30447400
C	-2.67550400	2.12916100	-1.49652200
H	-1.26184400	0.58317100	-1.93717600
H	-4.24219600	-2.53759200	2.14911200
C	-3.79359600	2.51650400	-0.72083800
H	-2.27775600	2.80825400	-2.24492000
H	-5.23360600	-0.28489000	1.85952000
H	-5.20516300	1.92632300	0.77903200
H	-4.23528700	3.49818100	-0.86492200

Table S27. Cartesian coordinates of the nucleobase minimum for the ^{1ANP}G adduct with θ = 26.0° and ϕ = 107.6°.

Calculated energy (in Hartrees) = –983.0055845			
Atom	X	Y	Z
N	-0.56203000	0.11250900	0.07006900
C	-0.40148700	-1.12705100	-0.52430900
N	-1.53918400	-1.72345700	-0.78664300
C	-2.50723600	-0.82682700	-0.35204600
C	-3.93959300	-0.93013500	-0.36022300
O	-4.68295900	-1.81720100	-0.74604700
N	-4.50854500	0.26216700	0.21455200
H	-5.51683000	0.21945100	0.30831700
C	-3.82133200	1.34175900	0.70132500
N	-4.57040900	2.35754900	1.26496600
H	-5.44822000	2.57438000	0.80841900
H	-4.00926100	3.17985300	1.45100500
N	-2.51185500	1.42399800	0.70050300
C	-1.92217700	0.31735500	0.18305100
H	0.16300100	0.76478000	0.33223700
N	0.84277800	-1.66366700	-0.83007800
H	0.74772100	-2.65469500	-1.02086800
C	2.01956900	-1.29892000	-0.12104300
C	2.61064400	-0.01704800	-0.35218700
C	2.60806800	-2.18619500	0.75792500
C	3.76930200	0.34869000	0.40866200
C	2.11021800	0.89551000	-1.32019700
C	3.77924400	-1.83502300	1.46490300
H	2.14654700	-3.15599700	0.92263200
C	4.33607600	1.63590500	0.21355200
C	4.33545400	-0.58645100	1.31344500
C	2.69170700	2.13255200	-1.48785800
H	1.27542300	0.59284700	-1.94256200
H	4.21990200	-2.55220900	2.15091700
C	3.80641500	2.51334700	-0.70409600
H	2.30094700	2.81568100	-2.23631300
H	5.22089900	-0.30204900	1.87521000
H	5.20669400	1.91303100	0.80230900
H	4.25232200	3.49401900	-0.84193600

Table S28. Cartesian coordinates of the nucleobase minimum for the ^{1ANP}G adduct with θ = 177.1° and ϕ = 356.4°.

Calculated energy (in Hartrees) = –983.0036838			
Atom	X	Y	Z
N	-1.47743200	-1.43280100	-0.13440700
C	-0.56851000	-0.37866200	-0.05444600
N	-1.16273900	0.78611900	0.04854900
C	-2.52029300	0.49329600	0.04768500
C	-3.65489100	1.36946000	0.12239800
O	-3.73235700	2.58355000	0.20660000
N	-4.86521200	0.58833500	0.07437400
H	-5.70581300	1.15415700	0.04964200
C	-4.95336100	-0.77365100	-0.02640600
N	-6.21988600	-1.31487400	-0.11482900
H	-6.94344400	-0.86850200	0.43519400
H	-6.21141400	-2.32286700	-0.01967500
N	-3.90515400	-1.56245800	-0.09243900
C	-2.73687900	-0.87528800	-0.06583800
H	-1.28432400	-2.42358300	-0.15939300
N	0.77835500	-0.65737300	-0.06535800
H	1.01457600	-1.58629600	-0.37796500
C	1.84932400	0.25444300	-0.04994400
C	3.17578600	-0.29525800	0.01637000
C	1.66166200	1.62482100	-0.09290200
C	4.28913600	0.60637500	-0.03551900
C	3.44481200	-1.68433400	0.14029700
C	2.77605700	2.49143400	-0.10792800
H	0.65574900	2.02029300	-0.12136700
C	5.60495000	0.07465400	-0.00972900
C	4.06072100	2.00520700	-0.09772400
C	4.73493600	-2.16707400	0.16959400
H	2.63067000	-2.39373800	0.25986200
H	2.59773800	3.56224400	-0.14536400
C	5.82997200	-1.27925500	0.08203500
H	4.91006700	-3.23408600	0.27260800
H	4.91463300	2.67618400	-0.12807000
H	6.43996100	0.76897500	-0.05866800
H	6.84439500	-1.66683400	0.10151400

Table S29. Cartesian coordinates of the nucleobase minimum for the ^{1ANP}G adduct with θ = 166.7° and ϕ = 117.3°.

Calculated energy (in Hartrees) = –983.0002316			
Atom	X	Y	Z
N	-1.48124800	-1.39739000	-1.15125000
C	-0.34412700	-1.17495100	-0.38209200
N	-0.57007500	-0.38824000	0.63835900
C	-1.91387900	-0.05776200	0.53554100
C	-2.72672400	0.78878300	1.36497400
O	-2.45934300	1.44643200	2.35542400
N	-4.07400500	0.80849300	0.85215400
H	-4.68138000	1.44953100	1.34969100
C	-4.53846000	0.13990000	-0.24829300
N	-5.85575500	0.35352500	-0.60041100
H	-6.51624900	0.46510800	0.15886900
H	-6.17052900	-0.29492500	-1.31148000
N	-3.78682000	-0.63707700	-0.99331400
C	-2.50050800	-0.68112800	-0.56450300
H	-1.53229600	-1.88097600	-2.03615500
N	0.86973000	-1.73728000	-0.77492200
H	0.82901100	-2.74824900	-0.85793100
C	2.07944300	-1.29232200	-0.17092800
C	2.53105800	0.04600900	-0.39091700
C	2.84407900	-2.17535900	0.56122300
C	3.76485000	0.45148100	0.21222000
C	1.82421700	0.97793000	-1.19328300
C	4.07694500	-1.77449100	1.12264600
H	2.48144600	-3.18727100	0.72522300
C	4.21660600	1.78350100	0.01871400
C	4.52149800	-0.48408000	0.96649400
C	2.29626000	2.25856800	-1.36810000
H	0.90650800	0.66941100	-1.67898000
H	4.65759600	-2.49142100	1.69561600
C	3.49889700	2.67093600	-0.74833400
H	1.74202100	2.95887600	-1.98636000
H	5.45963400	-0.16225300	1.41037900
H	5.14894000	2.08704600	0.48806900
H	3.85630700	3.68735900	-0.88683300

Table S30. Cartesian coordinates of the nucleobase minimum for the ^{1ANP}G adduct with θ = 193.9° and ϕ = 242.8°.

Calculated energy (in Hartrees) = –983.0002151			
Atom	X	Y	Z
N	1.47685000	-1.37099600	-1.17772700
C	0.34258600	-1.16798900	-0.39910500
N	0.57049200	-0.39991700	0.63500000
C	1.91243500	-0.06244000	0.53231000
C	2.73225800	0.74965700	1.38889100
O	2.47485800	1.36081200	2.41124800
N	4.07820700	0.77972400	0.87334400
H	4.72528700	1.27705100	1.47444500
C	4.53598700	0.14825300	-0.25155500
N	5.88190500	0.26823000	-0.53199000
H	6.31157100	1.16076100	-0.32230100
H	6.11208400	-0.07917600	-1.45473200
N	3.77573900	-0.58958600	-1.02714700
C	2.49692400	-0.66489700	-0.58061500
H	1.52713400	-1.84371600	-2.06850600
N	-0.87153900	-1.72676200	-0.79736700
H	-0.83054000	-2.73708000	-0.88872000
C	-2.07984700	-1.28805500	-0.18600900
C	-2.53159900	0.05248900	-0.39190700
C	-2.84289500	-2.17771100	0.53967400
C	-3.76358700	0.45273700	0.21827400
C	-1.82643100	0.99165100	-1.18726700
C	-4.07407600	-1.78165900	1.10822000
H	-2.48014500	-3.19118500	0.69327700
C	-4.21522300	1.78672300	0.03849900
C	-4.51859400	-0.48966100	0.96566000
C	-2.29840500	2.27407300	-1.34889800
H	-0.91031700	0.68692500	-1.67843800
H	-4.65337500	-2.50375800	1.67603000
C	-3.49922500	2.68108000	-0.72211100
H	-1.74576100	2.97990700	-1.96234700
H	-5.45533200	-0.17170200	1.41523500
H	-5.14618600	2.08627600	0.51311000
H	-3.85670400	3.69885300	-0.85018500

Table S31. Cartesian coordinates of the nucleobase minimum for the ^{3APHN}G adduct with θ = 33.3° and ϕ = 193.9°.

Calculated energy (in Hartrees) = –1136.7154178			
Atom	X	Y	Z
N	-1.66986700	-0.33928200	-0.61953400
C	-1.67468000	-1.54206300	0.07343000
N	-2.82014300	-1.78546800	0.66455300
C	-3.61796500	-0.69813600	0.33755400
C	-4.97142400	-0.39414200	0.71207700
O	-5.77663400	-1.00687700	1.39244700
N	-5.35096800	0.87508700	0.14576900
H	-6.27248300	1.18275400	0.43482100
C	-4.57095400	1.68769900	-0.63253500
N	-5.11835300	2.89293100	-1.02398100
H	-6.10623100	2.89103600	-1.24652000
H	-4.55356900	3.35763600	-1.72428600
N	-3.33610900	1.39611200	-0.96998600
C	-2.92161000	0.21372700	-0.45193100
N	-0.61273500	-2.41935300	0.04929200
H	-0.85809500	-3.33846300	0.39220400
C	0.74954100	-2.10436900	-0.04124800
C	1.24040100	-0.81877700	0.15591300
C	1.64810400	-3.15317100	-0.35044100
C	2.61437900	-0.52610700	0.02061300
C	2.99384500	-2.89263000	-0.45897000
H	1.26214800	-4.15652400	-0.50836400
C	3.14737200	0.81583000	0.20249000
C	3.51185700	-1.58735100	-0.29042500
H	3.68283700	-3.70061300	-0.69087600
C	2.33283700	1.93184500	0.50076200
C	4.55217100	1.02707200	0.07119900
C	4.91317600	-1.32680700	-0.41873700
C	2.87194200	3.19342400	0.66911900
C	5.07986100	2.32642700	0.24892500
C	5.41377800	-0.07437900	-0.24302500
H	5.57179300	-2.15799600	-0.65742900
C	4.25892400	3.39565700	0.54417000
H	2.21997300	4.03129100	0.89854700
H	6.15281400	2.46849100	0.14689900
H	6.47941900	0.11552200	-0.33924100
H	4.67874800	4.38841400	0.67792700
H	1.25984800	1.80922400	0.60000300

H	0.55618600	-0.04102200	0.46687600
H	-0.93241500	0.02258700	-1.20656800

Table S32. Cartesian coordinates of the nucleobase minimum for the ^{3APHN}G adduct with θ = 327.4° and ϕ = 166.0°.

Calculated energy (in Hartrees) = –1136.7153814			
Atom	X	Y	Z
N	1.66917700	-0.32454400	-0.60170400
C	1.67705200	-1.53262100	0.08194200
N	2.82486500	-1.78045600	0.66669600
C	3.62141000	-0.69089300	0.34438200
C	4.98518200	-0.40253200	0.69303500
O	5.80323600	-1.03553700	1.33864200
N	5.36504800	0.86744900	0.12884900
H	6.34222200	1.09360200	0.27496000
C	4.57619100	1.69434400	-0.62525000
N	5.16481100	2.84020100	-1.12102600
H	5.83495000	3.30284400	-0.51920800
H	4.48537400	3.47426300	-1.52302000
N	3.32874000	1.42176100	-0.93048900
C	2.92307500	0.22535000	-0.43809900
N	0.61526400	-2.40989000	0.05779000
H	0.86315900	-3.33212400	0.39014100
C	-0.74713300	-2.09928200	-0.03634000
C	-1.24303000	-0.81523600	0.15908900
C	-1.64163900	-3.15140200	-0.34654300
C	-2.61779400	-0.52762700	0.02102600
C	-2.98800000	-2.89572100	-0.45777200
H	-1.25201500	-4.15355900	-0.50308000
C	-3.15606600	0.81251700	0.20071100
C	-3.51098800	-1.59220000	-0.29090000
H	-3.67363400	-3.70630800	-0.69050200
C	-2.34614300	1.93187600	0.49899700
C	-4.56141900	1.01856800	0.06694900
C	-4.91298100	-1.33686100	-0.42174900
C	-2.89008400	3.19166800	0.66515300
C	-5.09408700	2.31620200	0.24251500
C	-5.41856100	-0.08618800	-0.24774800
H	-5.56810700	-2.17062800	-0.66104300
C	-4.27758900	3.38876500	0.53790100
H	-2.24159600	4.03229800	0.89449800

H	-6.16736900	2.45426400	0.13853500
H	-6.48471000	0.09975500	-0.34593700
H	-4.70127200	4.38012900	0.66982300
H	-1.27282900	1.81308600	0.59963400
H	-0.56224500	-0.03490600	0.47103200
H	0.93246300	0.03757300	-1.18956400

Table S33. Cartesian coordinates of the nucleobase minimum for the ^{3APHN}G adduct with θ = 180.0° and ϕ = 180.0°.

Calculated energy (in Hartrees) = –1136.7153462			
Atom	X	Y	Z
N	-2.99392500	-1.87130400	0.00181000
C	-1.67760900	-1.41392200	0.00052800
N	-1.60401600	-0.10303500	0.00260600
C	-2.92415600	0.32590900	0.00468300
C	-3.46167900	1.65644400	-0.00613000
O	-2.91354800	2.74606600	-0.02101100
N	-4.90089800	1.58993900	-0.00821100
H	-5.34394200	2.49772700	-0.09197600
C	-5.66432600	0.45377300	0.00051600
N	-7.03311300	0.61818600	-0.06407700
H	-7.41921200	1.40989800	0.43535500
H	-7.53006200	-0.24595900	0.11331600
N	-5.15667600	-0.75769200	0.01570500
C	-3.80129600	-0.75206300	0.00261700
N	-0.64391300	-2.31707700	-0.00112900
H	-0.90135500	-3.29251100	-0.00433000
C	0.73596400	-2.05502200	-0.00178500
C	1.26115000	-0.77002800	-0.00013300
C	1.60255200	-3.17307500	-0.00383500
C	2.65541800	-0.56138100	-0.00005900
C	2.96528100	-2.98386400	-0.00382400
H	1.18903200	-4.17967900	-0.00534700
C	3.22991400	0.77609000	0.00187000
C	3.52789700	-1.68738400	-0.00176800
H	3.63019900	-3.84374500	-0.00535800
C	2.43830500	1.94736400	0.00306400
C	4.64875500	0.92041100	0.00257000
C	4.94644200	-1.49429600	-0.00127700
C	3.01752700	3.20279900	0.00508700
C	5.21581500	2.21511400	0.00473200

C	5.48441100	-0.24496500	0.00094400
H	5.58680200	-2.37305900	-0.00264700
C	4.41791700	3.34147600	0.00602200
H	2.38443100	4.08534600	0.00580900
H	6.29924600	2.30751100	0.00525900
H	6.56247300	-0.10599200	0.00139500
H	4.86722900	4.33060600	0.00760400
H	1.35659000	1.87233800	0.00215700
H	0.57220000	0.05996600	0.00108400
H	-3.32714000	-2.82439000	-0.00409300

Table S34. Cartesian coordinates of the nucleobase minimum for the ^{3APHN}G adduct with θ = 26.8° and ϕ = 21.7°.

Calculated energy (in Hartrees) = –1136.7143743			
Atom	X	Y	Z
N	2.30200400	0.39726100	0.32317500
C	1.85732000	-0.77311900	-0.27630300
N	2.83834500	-1.56359600	-0.64273500
C	3.98893600	-0.89098000	-0.25622500
C	5.37088500	-1.25407300	-0.40679000
O	5.89681900	-2.24083200	-0.89338700
N	6.20207500	-0.20812700	0.13224500
H	7.19233800	-0.37036400	-0.01058100
C	5.77569300	0.95914600	0.70663900
N	6.74975700	1.85208100	1.10702700
H	7.59333400	1.45451400	1.50182800
H	6.36766100	2.60640900	1.66415000
N	4.50906800	1.27687500	0.84147300
C	3.67959800	0.33012500	0.33735500
N	0.52403500	-1.09424300	-0.38838500
H	0.36353300	-2.07292300	-0.58216200
C	-0.56947400	-0.22166200	-0.44369400
C	-1.83247400	-0.70866900	-0.12323400
C	-0.42384000	1.13043200	-0.83537500
C	-2.97805300	0.10803200	-0.17162100
C	-1.53026900	1.95191700	-0.86344400
H	0.54241800	1.50552200	-1.15327900
C	-4.31022400	-0.38328200	0.15251300
C	-2.81877300	1.47816300	-0.53568400
H	-1.41936400	2.98939700	-1.16823600
C	-4.56680700	-1.72471100	0.51386100

C	-5.41228400	0.52086900	0.10499200
C	-3.95629900	2.34677000	-0.57312400
C	-5.84398600	-2.15825100	0.81788300
C	-6.70846400	0.05481000	0.42102300
C	-5.19907700	1.89008900	-0.26451500
H	-3.80188600	3.38491100	-0.85594200
C	-6.92719200	-1.26183700	0.77304900
H	-6.00973400	-3.19621900	1.09150000
H	-7.53652100	0.75798700	0.38036000
H	-6.05776800	2.55542100	-0.29449800
H	-7.92912600	-1.60572500	1.01296900
H	-3.75230800	-2.43941100	0.55419300
H	-1.91331500	-1.74545700	0.18470600
H	1.73790400	1.11820700	0.74864600

Table S35. Cartesian coordinates of the nucleobase minimum for the ^{3APHN}G adduct with θ = 333.8° and ϕ = 338.0°.

Calculated energy (in Hartrees) = –1136.7143537			
Atom	X	Y	Z
N	-2.30268200	0.40375800	0.30971900
C	-1.85784200	-0.76630700	-0.29017000
N	-2.83864300	-1.55712100	-0.65661100
C	-3.98932600	-0.88525200	-0.26920600
C	-5.37039500	-1.26087500	-0.39540000
O	-5.89483700	-2.26212300	-0.85313700
N	-6.20185000	-0.21849200	0.15003300
H	-7.18691600	-0.45701200	0.16030900
C	-5.77623100	0.95677000	0.70868600
N	-6.74631600	1.78964700	1.22994600
H	-7.62107000	1.83870500	0.72213300
H	-6.37530400	2.70027500	1.47175600
N	-4.51081700	1.29037800	0.81203200
C	-3.68028400	0.33423600	0.32763700
N	-0.52462200	-1.08638300	-0.40553500
H	-0.36355000	-2.06556500	-0.59614300
C	0.56989200	-0.21506800	-0.45187000
C	1.83161400	-0.70568600	-0.13164600
C	0.42706400	1.13969400	-0.83542700
C	2.97834200	0.10977800	-0.17230400
C	1.53464300	1.95982600	-0.85589300
H	-0.53799800	1.51803200	-1.15304100

C	4.30913600	-0.38534500	0.15175200
C	2.82177700	1.48236200	-0.52823200
H	1.42583500	2.99938400	-1.15433500
C	4.56305900	-1.72924700	0.50565900
C	5.41255800	0.51752100	0.11200700
C	3.96055600	2.34960500	-0.55786900
C	5.83898900	-2.16640400	0.80976000
C	6.70741200	0.04774400	0.42791200
C	5.20205200	1.88928400	-0.24953000
H	3.80817400	3.38971600	-0.83450400
C	6.92354900	-1.27129800	0.77249600
H	6.00266000	-3.20618700	1.07765700
H	7.53652900	0.74998900	0.39327300
H	6.06172700	2.55358500	-0.27354500
H	7.92448200	-1.61802200	1.01249600
H	3.74748700	-2.44301500	0.54020500
H	1.91050000	-1.74448700	0.16994200
H	-1.73875000	1.12104500	0.74162500

Table S36. Cartesian coordinates of the nucleobase minimum for the ^{3APHN}G adduct with θ = 180.0° and ϕ = 0.0°.

Calculated energy (in Hartrees) = –1136.7133475			
Atom	X	Y	Z
N	-2.81301400	-1.57816200	0.00049300
C	-1.85929600	-0.56250000	0.00204700
N	-2.40021300	0.63267000	0.00603100
C	-3.76948800	0.40101900	0.00652000
C	-4.86427900	1.32962100	-0.00314900
O	-4.88703400	2.54880100	-0.01570900
N	-6.10794100	0.60162100	-0.00747100
H	-6.92164200	1.20034500	-0.09001600
C	-6.25686600	-0.75891600	-0.00209000
N	-7.54543300	-1.24866900	-0.06917000
H	-8.25533600	-0.72818700	0.43125500
H	-7.58461300	-2.24530100	0.10512700
N	-5.24468200	-1.59588300	0.01207100
C	-4.04713700	-0.96088500	0.00145100
N	-0.52545500	-0.89115000	0.00080300
H	-0.31185300	-1.87750400	-0.00300300
C	0.58965100	-0.03995500	0.00175600
C	1.84883500	-0.63236800	0.00003200

C	0.47097900	1.36893900	0.00445500
C	3.02908800	0.13316900	0.00098800
C	1.62025100	2.12976900	0.00550600
H	-0.51128100	1.82111800	0.00551200
C	4.35831500	-0.46231300	-0.00083700
C	2.90912600	1.55366200	0.00391200
H	1.53678300	3.21357900	0.00748900
C	4.57653300	-1.85812400	-0.00393700
C	5.50008900	0.39286300	0.00048000
C	4.08517500	2.36998900	0.00510300
C	5.85232700	-2.39126400	-0.00564400
C	6.79435700	-0.17512400	-0.00128200
C	5.32712400	1.81633900	0.00349900
H	3.96028700	3.44982600	0.00728300
C	6.97488700	-1.54358600	-0.00429500
H	5.98627100	-3.46930500	-0.00808100
H	7.65261900	0.49227900	-0.00026800
H	6.21478200	2.44335400	0.00439100
H	7.97621800	-1.96454700	-0.00566400
H	3.73071900	-2.53709500	-0.00512300
H	1.90932500	-1.71679100	-0.00208700
H	-2.66686600	-2.57718300	-0.00755300

Table S37. Cartesian coordinates of the nucleobase minimum for the ^{1AP}G adduct with θ = 34.0° and ϕ = 22.4°.

Calculated energy (in Hartrees) = –1212.9766572			
Atom	X	Y	Z
N	2.43931300	0.38308200	0.43537700
C	1.99297000	-0.68480100	-0.32959900
N	2.97255300	-1.39845800	-0.83146100
C	4.12532800	-0.77989900	-0.36778000
C	5.50689000	-1.09866800	-0.59915400
O	6.03151600	-1.99217800	-1.24217200
N	6.33975500	-0.13759800	0.07787700
H	7.32818500	-0.26351000	-0.10789200
C	5.91477300	0.92326600	0.83166500
N	6.88858600	1.75690900	1.34436900
H	7.74458000	1.31481200	1.65633600
H	6.51151400	2.41247500	2.01773400
N	4.64840600	1.20127300	1.03816600
C	3.81690500	0.33245500	0.41196900

H	1.87521700	1.04113900	0.95304500
N	0.65764800	-1.00066900	-0.45202900
H	0.51515800	-1.90023100	-0.89240300
C	-0.41153800	-0.08682100	-0.46960800
C	-1.70804200	-0.54995200	-0.13605500
C	-0.21735600	1.25638100	-0.82093900
C	-2.80325900	0.36291100	-0.19867300
C	-1.96440400	-1.90304100	0.26740000
C	-1.28216000	2.14816600	-0.84277000
H	0.76996200	1.59234500	-1.11861100
C	-4.12376000	-0.08781100	0.09911300
C	-2.58708200	1.73046600	-0.54770200
C	-3.22652800	-2.33160600	0.54807400
H	-1.12957500	-2.58699900	0.37811700
H	-1.10767100	3.18268600	-1.12628100
C	-4.35270200	-1.44843600	0.46390600
C	-5.22301700	0.82248800	0.03605800
C	-3.70868600	2.62298100	-0.59591800
H	-3.39820800	-3.35887500	0.85853100
C	-5.66106100	-1.87209000	0.74615000
C	-6.51290500	0.35314600	0.32675700
C	-4.96924400	2.19003400	-0.32101100
H	-3.52800600	3.66066400	-0.86449700
C	-6.72694000	-0.97900200	0.67560300
H	-5.83258400	-2.90881800	1.02334800
H	-7.34923900	1.04551000	0.27816000
H	-5.81096400	2.87596800	-0.36607700
H	-7.73341500	-1.32250800	0.89685000

Table S38. Cartesian coordinates of the nucleobase minimum for the ^{1AP}G adduct with θ = 326.0° and ϕ = 337.6°.

Calculated energy (in Hartrees) = –1212.9766571			
Atom	X	Y	Z
N	-2.43931800	0.38308600	0.43537700
C	-1.99297100	-0.68479800	-0.32959600
N	-2.97255000	-1.39846100	-0.83145500
C	-4.12532900	-0.77989900	-0.36778400
C	-5.50688500	-1.09868200	-0.59915100
O	-6.03151700	-1.99220000	-1.24215100
N	-6.33975700	-0.13759800	0.07787300
H	-7.32818800	-0.26353400	-0.10787900

C	-5.91478100	0.92326700	0.83165100
N	-6.88859000	1.75692100	1.34435000
H	-7.74458500	1.31482300	1.65631900
H	-6.51151200	2.41246800	2.01773000
N	-4.64841200	1.20128000	1.03815200
C	-3.81691000	0.33245900	0.41196300
N	-0.65764800	-1.00066400	-0.45202200
H	-0.51515800	-1.90022100	-0.89240700
C	0.41154000	-0.08681700	-0.46959900
C	1.70804000	-0.54995000	-0.13605000
C	0.21735700	1.25638700	-0.82092800
C	2.80326000	0.36291200	-0.19866800
C	1.96440400	-1.90304000	0.26740500
C	1.28216200	2.14817100	-0.84275900
H	-0.76996000	1.59235100	-1.11860200
C	4.12376200	-0.08781100	0.09911300
C	2.58708500	1.73046700	-0.54769400
C	3.22652700	-2.33160600	0.54807500
H	1.12957500	-2.58699800	0.37812700
H	1.10767600	3.18269200	-1.12626700
C	4.35270500	-1.44844100	0.46390500
C	5.22301600	0.82248400	0.03605500
C	3.70868800	2.62298200	-0.59591200
H	3.39820200	-3.35887600	0.85853300
C	5.66106100	-1.87209200	0.74614000
C	6.51291100	0.35314200	0.32674700
C	4.96924700	2.19003100	-0.32100900
H	3.52800800	3.66066500	-0.86448700
C	6.72694500	-0.97900200	0.67558900
H	5.83259500	-2.90881900	1.02333900
H	7.34923800	1.04551300	0.27814500
H	5.81096900	2.87596300	-0.36607700
H	7.73341700	-1.32251900	0.89683200
H	-1.87522400	1.04116400	0.95301900

Table S39. Cartesian coordinates of the nucleobase minimum for the ^{1AP}G adduct with θ = 21.7° and ϕ = 110.1°.

Calculated energy (in Hartrees) = –1212.9762440			
Atom	X	Y	Z
N	-1.71781700	-0.08005700	0.05700800
C	-1.84349900	-1.26341700	-0.64941300

N	-3.09028200	-1.58768800	-0.89392200
C	-3.83181200	-0.56033500	-0.32446400
C	-5.25344600	-0.36878000	-0.25490800
O	-6.18039800	-1.04469700	-0.66992500
N	-5.53756100	0.85312200	0.45347900
H	-6.52789900	1.00719900	0.60430500
C	-4.62131500	1.71797100	0.98944500
N	-5.11844000	2.80432300	1.68441300
H	-5.95046000	3.23885200	1.30374600
H	-4.39135600	3.47293300	1.90800400
N	-3.32450800	1.53236200	0.91548400
C	-2.99996000	0.38450100	0.26992700
H	-0.86368200	0.37994400	0.33709400
N	-0.75359000	-2.01379400	-1.06812100
H	-1.05084600	-2.95154300	-1.31148700
C	0.52612000	-1.91585300	-0.46554500
C	1.31670100	-0.76041000	-0.65891100
C	1.01443700	-2.97963700	0.30063100
C	2.57527900	-0.66916300	0.01146500
C	0.91553900	0.31941100	-1.51931200
C	2.25799600	-2.90814200	0.91483900
H	0.39244800	-3.86086500	0.43206300
C	3.37161700	0.50606900	-0.12700000
C	3.04909100	-1.75453100	0.80792100
C	1.67971100	1.43919000	-1.64813500
H	-0.00301400	0.21534900	-2.08544200
H	2.61427800	-3.74308300	1.51193400
C	2.92290200	1.58484500	-0.94660600
C	4.62430500	0.60613500	0.55139600
C	4.31545600	-1.62905900	1.47082800
H	1.36343400	2.24178500	-2.30921800
C	3.71794100	2.73548100	-1.06005400
C	5.38440100	1.77709100	0.40879100
C	5.06562800	-0.49961100	1.35385000
H	4.66294900	-2.46188200	2.07655800
C	4.93352500	2.82858600	-0.38620100
H	3.37475500	3.55522100	-1.68557400
H	6.33671500	1.85367800	0.92678500
H	6.02065900	-0.41630100	1.86574300
H	5.53687600	3.72635200	-0.48475700

Table S40. Cartesian coordinates of the nucleobase minimum for the ^{1AP}G adduct with θ = 177.7° and ϕ = 354.8°.

Calculated energy (in Hartrees) = –1212.9740911			
Atom	X	Y	Z
N	-2.94633700	-1.48193600	-0.16389400
C	-2.00722500	-0.45673100	-0.06327100
N	-2.56703700	0.72232000	0.06665700
C	-3.93231100	0.46963200	0.05977400
C	-5.04079000	1.37683300	0.15574600
O	-5.08197500	2.59046700	0.26641900
N	-6.27335000	0.63273400	0.09284000
H	-7.09707300	1.22331900	0.08219400
C	-6.40151200	-0.72357300	-0.03818500
N	-7.68289000	-1.22549200	-0.13712700
H	-8.39441700	-0.76887400	0.42002500
H	-7.70491800	-2.23508400	-0.06404000
N	-5.37669000	-1.54109100	-0.12294000
C	-4.18904700	-0.88921600	-0.08286300
N	-0.66910500	-0.77302400	-0.09056600
H	-0.46231500	-1.72474600	-0.34853000
C	0.43516200	0.09168000	-0.04901300
C	1.73222700	-0.48476800	0.01623100
C	0.28018100	1.48466800	-0.07734200
C	2.86895100	0.37988100	-0.01316400
C	1.96660800	-1.89815700	0.11722000
C	1.39524100	2.31082600	-0.07823600
H	-0.71810400	1.89958300	-0.10145400
C	4.18796000	-0.16652900	0.01174500
C	2.69799600	1.79565000	-0.06321300
C	3.22491400	-2.41928500	0.14309300
H	1.13070300	-2.58482600	0.21952500
H	1.25350000	3.38801400	-0.10605000
C	4.38258100	-1.57859100	0.07811400
C	5.32486300	0.69925000	-0.02682900
C	3.85661600	2.63911400	-0.09475000
H	3.36938200	-3.49311000	0.22891600
C	5.68735600	-2.09630300	0.09626400
C	6.61032600	0.13626100	-0.00812200
C	5.11366400	2.11808300	-0.08122600
H	3.70543600	3.71494800	-0.13257800
C	6.78754700	-1.24449300	0.05150400
H	5.82841000	-3.17277900	0.14768200

H	7.47359500	0.79595200	-0.03889300
H	5.98362900	2.76884800	-0.10887100
H	7.79176900	-1.65863300	0.06550000
H	-2.78378900	-2.47631700	-0.23043200

Table S41. Cartesian coordinates of the nucleobase minimum for the ^{1AP}G adduct with θ = 167.0° and ϕ = 118.4°.

Calculated energy (in Hartrees) = –1212.9706277			
Atom	X	Y	Z
N	2.97329200	1.29324600	-1.22716200
C	1.77482200	1.34356800	-0.52333100
N	1.78976600	0.60258300	0.55459500
C	3.04864700	0.01856300	0.56102900
C	3.63742900	-0.90567400	1.49089000
O	3.19571900	-1.42920500	2.49864600
N	4.98109400	-1.21584800	1.06990000
H	5.42562000	-1.92385000	1.64307400
C	5.62381300	-0.72662400	-0.03518700
N	6.89152200	-1.21024500	-0.28717600
H	7.47665500	-1.39301400	0.51866900
H	7.36343700	-0.68494700	-1.01278600
N	5.07698400	0.12414400	-0.87254000
C	3.80248000	0.44042500	-0.53261300
N	0.71440300	2.09286900	-1.02917900
H	0.95671600	3.06392000	-1.19733800
C	-0.59084500	1.94122000	-0.48638700
C	-1.27952700	0.71457700	-0.60906200
C	-1.20924900	3.03991800	0.11315400
C	-2.59464800	0.61479100	-0.06339100
C	-0.72206700	-0.42946600	-1.27244700
C	-2.50120700	2.95049800	0.61660200
H	-0.65753400	3.97273900	0.20229200
C	-3.31014300	-0.61686800	-0.15017700
C	-3.21125700	1.74446700	0.55613600
C	-1.40799200	-1.60131800	-1.35581100
H	0.26008400	-0.34657000	-1.72064700
H	-2.96147400	3.81721600	1.08309500
C	-2.71752000	-1.74606800	-0.78933500
C	-4.62451500	-0.72422400	0.39815600
C	-4.53481800	1.60831400	1.09384400
H	-0.96859500	-2.45649000	-1.86269700

C	-3.43581200	-2.94980800	-0.85823900
C	-5.30415800	-1.94820900	0.30642600
C	-5.20917000	0.42891300	1.02317000
H	-4.98842500	2.47596200	1.56625900
C	-4.71368500	-3.04760200	-0.31342100
H	-2.98063500	-3.80886000	-1.34414100
H	-6.30349500	-2.02907200	0.72621000
H	-6.20950400	0.33869300	1.43856200
H	-5.25525600	-3.98741000	-0.37364600
H	3.16376200	1.69172500	-2.13516600

Table S42. Cartesian coordinates of the nucleobase minimum for the ^{1AP}G adduct with θ = 192.2° and ϕ = 241.7°.

Calculated energy (in Hartrees) = –1212.9705809			
Atom	X	Y	Z
N	-2.96132200	1.26047100	-1.25586500
C	-1.77189400	1.33877500	-0.53951000
N	-1.79339500	0.62361300	0.55560700
C	-3.04713900	0.02915900	0.56166200
C	-3.64890800	-0.85577300	1.52105300
O	-3.22653800	-1.32503800	2.56320700
N	-4.98720800	-1.18217500	1.09566500
H	-5.49385500	-1.74628900	1.76835700
C	-5.61468700	-0.73944700	-0.03745100
N	-6.92319400	-1.13594500	-0.22319900
H	-7.16080900	-2.07395000	0.07479400
H	-7.26255300	-0.91261100	-1.15057400
N	-5.05257700	0.06769400	-0.90736900
C	-3.79270200	0.42037400	-0.54918800
N	-0.71167600	2.08562200	-1.05115500
H	-0.95446800	3.05624700	-1.22196600
C	0.59198600	1.93748700	-0.50360100
C	1.28004500	0.70963100	-0.61753700
C	1.20960200	3.03877100	0.09183600
C	2.59343900	0.61137400	-0.06773100
C	0.72322700	-0.43736800	-1.27629000
C	2.50000900	2.95066200	0.59962500
H	0.65848300	3.97248900	0.17467800
C	3.30804800	-0.62134700	-0.14618800
C	3.20921600	1.74374100	0.54769000
C	1.40832300	-1.61028000	-1.35191600

H	-0.25747600	-0.35541000	-1.72803600
H	2.95958300	3.81936000	1.06310100
C	2.71626200	-1.75330300	-0.78131000
C	4.62079900	-0.72700700	0.40637000
C	4.53103200	1.60909800	1.09005300
H	0.96981100	-2.46759600	-1.85602200
C	3.43386300	-2.95789300	-0.84239800
C	5.29971700	-1.95195800	0.32252900
C	5.20457700	0.42877900	1.02735100
H	4.98399400	2.47869700	1.55947500
C	4.71017200	-3.05392500	-0.29364200
H	2.97946500	-3.81897700	-1.32547100
H	6.29781200	-2.03152500	0.74548800
H	6.20357100	0.33978900	1.44620300
H	5.25128300	-3.99436700	-0.34788300
H	-3.14686700	1.64218800	-2.17203200

Table S43. Cartesian coordinates of nucleoside minimum for the ^{AN}dG adduct with χ = 227.2°, θ = 180.4° and ϕ = 162.8°.

Calculated energy (in Hartrees) = –1250.4854482			
Atom	X	Y	Z
N	-0.84202700	0.32347400	-0.11559100
C	0.06232400	-0.74988600	-0.04674900
N	-0.54490100	-1.91429500	-0.00085800
C	-1.89847600	-1.61754400	-0.04169500
C	-3.03925300	-2.48762500	0.00076800
O	-3.12725200	-3.70111500	0.09206600
N	-4.24544200	-1.70028900	-0.07107500
H	-5.08997600	-2.25185500	0.02762600
C	-4.32431200	-0.33736800	-0.15689400
N	-5.58941000	0.22118700	-0.15202200
H	-6.30295800	-0.28725100	-0.66060300
H	-5.56504000	1.20516500	-0.39106700
N	-3.26988700	0.44311500	-0.18902300
C	-2.10414600	-0.24778300	-0.12015000
N	1.41072300	-0.50879400	-0.04820600
H	1.69743000	0.43503300	-0.28702200
C	2.43617000	-1.46536900	0.00756800
C	3.72625700	-1.05714600	-0.37224100
C	2.23712600	-2.78599900	0.44057700
C	4.79797000	-1.94097400	-0.30363800

C	3.32178700	-3.65948100	0.49934100
H	1.24123600	-3.11556000	0.70159400
C	4.60560100	-3.25156000	0.13632400
H	3.15201200	-4.67921100	0.83439900
H	3.87288300	-0.04604200	-0.73864300
H	5.78655100	-1.60425700	-0.60507600
H	5.44044700	-3.94415100	0.18651600
C	-0.60317000	1.74155700	-0.06187500
O	0.36525400	2.09741000	-1.05335800
C	-0.01632200	2.27075200	1.24976500
C	1.01657100	3.31326500	-0.65402300
C	0.57389700	3.60745100	0.79822700
H	0.77293100	1.60245700	1.60367400
H	-0.77514100	2.37650100	2.03049600
C	2.51381900	3.13646400	-0.81880100
H	0.67677500	4.13767200	-1.29256500
O	-0.41405900	4.63366600	0.71372600
H	1.41845800	3.92337700	1.42275600
O	2.93424900	2.14680000	0.11905800
H	3.01048600	4.09952500	-0.63122500
H	2.73077400	2.82502500	-1.84961300
H	-0.72588900	4.81727800	1.61356000
H	3.88960000	2.01090400	0.03808000
H	-1.56456400	2.21798500	-0.27641000

Table S44. Cartesian coordinates of nucleoside minimum for the ^{AN}dG adduct with χ = 139.1°, θ = 184.5° and ϕ = 5.8°.

Calculated energy (in Hartrees) = –1250.4780571			
Atom	X	Y	Z
N	0.49152500	0.08143800	-0.27512200
C	-0.81650300	0.56225300	-0.08625600
N	-0.85858000	1.85218400	0.15099000
C	0.46315300	2.26195400	0.09826700
C	1.01543400	3.57396400	0.28455500
O	0.48209900	4.64270700	0.53443300
N	2.44614400	3.51979000	0.14042300
H	2.90594600	4.40143200	0.33644600
C	3.18686500	2.40755900	-0.14680700
N	4.56051200	2.56653200	-0.19904200

H	4.89430300	3.42481300	-0.62149100
H	5.01891100	1.74349600	-0.57042300
N	2.66530900	1.21712800	-0.32044600
C	1.31507600	1.19473400	-0.16436700
N	-1.86321400	-0.31725600	-0.18094400
H	-1.60097700	-1.29111200	-0.07799300
C	-3.23528600	-0.03458200	-0.11519000
C	-4.11219500	-1.13240800	-0.13400600
C	-3.75914800	1.26565600	-0.05196100
C	-5.48800900	-0.93619500	-0.09175700
C	-5.14187300	1.44260700	-0.01359100
H	-3.08368800	2.10953000	-0.01893000
C	-6.01554100	0.35545200	-0.03234500
H	-5.53642700	2.45393900	0.03700200
H	-3.70615400	-2.14049000	-0.18761100
H	-6.14944600	-1.79832700	-0.10679700
H	-7.08992900	0.50981500	0.00084200
C	0.80996500	-1.25631100	-0.73809400
O	0.14133600	-2.19234900	0.11743400
C	2.28020200	-1.65767400	-0.67476800
C	0.91877600	-3.39693900	0.25065200
C	2.17173200	-3.18299300	-0.61092700
H	2.72784700	-1.27902000	0.24309200
H	2.85838300	-1.29651200	-1.52780800
C	1.20032300	-3.65677900	1.72095400
H	0.34073800	-4.23438200	-0.15603200
O	1.89190700	-3.76299000	-1.88540600
H	3.06120100	-3.63545900	-0.15580600
O	2.14535300	-2.70379800	2.18584000
H	1.58264700	-4.68553000	1.82182900
H	0.25152100	-3.58926500	2.27285400
H	2.66224800	-3.60771000	-2.45362900
H	2.31781000	-2.87765900	3.12247300
H	0.40982000	-1.37660800	-1.75359600

Table S45. Cartesian coordinates of nucleoside minimum for the ^{AN}dG adduct with χ = 68.3°, θ = 68.6° and ϕ = 174.3°.

Calculated energy (in Hartrees) = –1250.4741386			
Atom	X	Y	Z
N	0.22199600	-0.47054500	0.47999300
C	-0.37944500	-1.72717200	0.60990700

N	0.46435300	-2.71758600	0.46032000
C	1.68165800	-2.10922100	0.20356300
C	2.96661800	-2.69288000	-0.07459100
O	3.32578000	-3.85684400	-0.12862900
N	3.92368200	-1.64862600	-0.33135000
H	4.83179100	-1.99420600	-0.61997200
C	3.67761700	-0.30193500	-0.30465900
N	4.72306300	0.54034800	-0.63187100
H	5.63743300	0.28373200	-0.27931500
H	4.48051700	1.50709500	-0.44867400
N	2.50354200	0.21264500	-0.03790300
C	1.54951300	-0.72348600	0.18795500
N	-1.70966800	-1.87660800	0.98581200
H	-1.84018200	-2.77323600	1.44007700
C	-2.80773000	-1.49787100	0.17135300
C	-4.09676600	-1.81548400	0.62258300
C	-2.65216500	-0.80813500	-1.03674600
C	-5.21173900	-1.45173800	-0.12600300
C	-3.77880800	-0.43287900	-1.76788900
H	-1.66529900	-0.55327700	-1.40271600
C	-5.06181500	-0.75227400	-1.32544700
H	-3.64252700	0.10686900	-2.70087500
H	-4.21619900	-2.34385000	1.56534600
H	-6.20309200	-1.71117000	0.23518600
H	-5.93282600	-0.46125100	-1.90460500
C	-0.40954600	0.81811700	0.64295900
O	-0.44024700	1.48126200	-0.61737200
C	0.30198800	1.80344200	1.57215600
C	-0.51542800	2.89718200	-0.39970100
C	-0.31514300	3.12670100	1.11410200
H	1.37262700	1.79521200	1.36235700
H	0.12288000	1.58944500	2.63044000
C	0.49537300	3.60704200	-1.28447900
H	-1.52042200	3.24613100	-0.66922800
O	-1.61579100	3.33812500	1.66647000
H	0.34197500	3.98139700	1.31141300
O	1.80086600	3.48191800	-0.73008800
H	0.20000900	4.66633100	-1.35700500
H	0.44056900	3.16614700	-2.29004300
H	-1.51133900	3.45468100	2.62355500
H	2.41158000	3.94556200	-1.32127400
H	-1.42621700	0.62484800	0.99689500

Table S46. Cartesian coordinates of nucleoside minimum for the ^{AN}dG adduct with χ = 53.9°, θ = 296.7° and ϕ = 356.0°.

Calculated energy (in Hartrees) = –1250.4739861			
Atom	X	Y	Z
N	0.08879300	-0.45457900	-0.27720100
C	-0.53535800	-1.61779200	-0.73620900
N	0.25338500	-2.66256300	-0.74211600
C	1.47225900	-2.18188700	-0.28730500
C	2.72764400	-2.85999700	-0.10595700
O	3.05586400	-4.01481200	-0.31991300
N	3.70563600	-1.93353300	0.40348800
H	4.63780900	-2.32586500	0.47031700
C	3.49534900	-0.61015200	0.68633800
N	4.58275700	0.13077400	1.11119600
H	5.21095800	-0.32446200	1.76290200
H	4.28895600	1.05151200	1.41677300
N	2.34232100	-0.01230900	0.52591000
C	1.38658000	-0.82659900	0.01857200
N	-1.85092400	-1.60022200	-1.18039900
H	-2.03038100	-2.35391800	-1.83288800
C	-2.94241900	-1.27533500	-0.34053800
C	-2.78184300	-1.00278300	1.02486400
C	-4.22229500	-1.20439700	-0.90829500
C	-3.88657500	-0.64739200	1.79807700
C	-5.32029600	-0.86776200	-0.12245000
H	-4.34417400	-1.40414600	-1.96958000
C	-5.16054100	-0.57811900	1.23464500
H	-6.30574900	-0.82127900	-0.57741400
H	-1.80159700	-1.08715900	1.48076800
H	-3.74727100	-0.44317700	2.85635900
H	-6.01763200	-0.30693600	1.84333000
C	-0.41469000	0.89866900	-0.38555700
O	0.39334300	1.61328700	-1.31316500
C	-0.36269100	1.73104900	0.89639700
C	0.36051600	3.01184000	-0.99161700
C	-0.43418800	3.14747900	0.32312200
H	0.59666700	1.57316800	1.39331800
H	-1.18666600	1.50172700	1.57825400
C	1.77255700	3.57640400	-0.94258200
H	-0.19045300	3.53764000	-1.78155100
O	-1.76669200	3.50860900	-0.04630100
H	0.00734800	3.89164900	0.99545400

O	2.38143700	3.29525600	0.31506300
H	1.70900900	4.66432200	-1.10534100
H	2.34256700	3.13643800	-1.77268100
H	-2.29155600	3.56290400	0.76734400
H	3.27213800	3.67430600	0.29194800
H	-1.43941800	0.82222600	-0.75797500

Table S47. Cartesian coordinates of nucleoside minimum for the ^{1ANP}dG adduct with χ = 222.7°, θ = 166.5° and ϕ = 338.4°.

Calculated energy (in Hartrees) = –1404.1903584			
Atom	X	Y	Z
N	-1.52525200	0.29828500	-0.18423500
C	-0.56545200	-0.72509700	-0.11377400
N	-1.10394200	-1.92326100	-0.11804500
C	-2.47027700	-1.70194200	-0.19094100
C	-3.56098700	-2.63554500	-0.19937900
O	-3.58240900	-3.85377000	-0.13779900
N	-4.80774000	-1.91579900	-0.28435000
H	-5.62157500	-2.51658000	-0.22118700
C	-4.96217700	-0.55751300	-0.33471000
N	-6.25686300	-0.07182900	-0.34633400
H	-6.92851700	-0.60558700	-0.88510000
H	-6.28383000	0.91829000	-0.55816200
N	-3.95370000	0.28190300	-0.31836300
C	-2.75198600	-0.34343900	-0.23889000
N	0.76929000	-0.41806100	-0.10139800
H	1.00934100	0.56472000	-0.17877900
C	1.82108600	-1.28624300	0.22622700
C	3.13519300	-0.92924400	-0.22774000
C	1.64253900	-2.42951500	0.98756200
C	4.25646300	-1.69003900	0.23871200
C	3.37243400	0.12998000	-1.14531900
C	2.75494300	-3.19756500	1.38819000
H	0.64193400	-2.72675000	1.27098800
C	5.56335200	-1.29162300	-0.15264200
C	4.03815800	-2.82765400	1.05570800
C	4.65295400	0.48135600	-1.51559500
H	2.52681800	0.63463700	-1.59913100
H	2.58364400	-4.08398400	1.99245400
C	5.76438400	-0.22256500	-0.99429300
H	4.80881700	1.28082100	-2.23503000

C	-1.37757800	1.72463300	-0.02382800
O	-0.35859800	2.20242100	-0.90430600
C	-0.93529400	2.18827400	1.36767100
C	0.23114500	3.39380700	-0.35048700
C	-0.36595700	3.57456700	1.06136400
H	-0.15071500	1.53046500	1.75017900
H	-1.76562700	2.21091200	2.07943400
C	1.73860700	3.22636500	-0.37299700
H	-0.05225800	4.25674700	-0.96420700
O	-1.38845000	4.56246000	0.93865900
H	0.39656300	3.88218600	1.78735600
O	2.06283400	2.18621100	0.54219400
H	2.21195900	4.17595300	-0.08289200
H	2.06156300	2.97542700	-1.39304100
H	-1.79705700	4.67343600	1.81121600
H	3.02369200	2.05324600	0.55187600
H	-2.34694100	2.15800300	-0.28740400
H	6.77113900	0.06404800	-1.28478700
H	6.40908200	-1.86242500	0.22271900
H	4.89309000	-3.40678300	1.39355000

Table S48. Cartesian coordinates of nucleoside minimum for the ^{1ANP}dG adduct with χ = 141.1°, θ = 185.4° and ϕ = 357.6°.

Calculated energy (in Hartrees) = –1404.1821590			
Atom	X	Y	Z
N	-1.20610400	-0.03236400	-0.23142700
C	-0.15090400	-0.94087100	-0.02580500
N	-0.56431600	-2.17113600	0.16406900
C	-1.94322200	-2.09877800	0.05692700
C	-2.91965500	-3.14397600	0.18061800
O	-2.79628400	-4.33646100	0.40742200
N	-4.23765100	-2.59616900	-0.00193500
H	-4.98005000	-3.26958600	0.14827300
C	-4.53879300	-1.28998800	-0.26934100
N	-5.87957100	-0.96432700	-0.36730200
H	-6.47279200	-1.64549600	-0.82601700
H	-6.01343800	-0.02519800	-0.72145600
N	-3.63353300	-0.34812900	-0.38365600
C	-2.36500400	-0.79638300	-0.18877700
N	1.13306500	-0.46205200	-0.06107900
H	1.19246000	0.53086000	0.12446700

C	2.32985100	-1.18613400	0.01223300
C	3.54965400	-0.43398200	-0.11512400
C	2.37156600	-2.55918000	0.18651700
C	4.79607700	-1.13357800	-0.00987500
C	3.58158200	0.96721300	-0.34890100
C	3.61348400	-3.22619600	0.25989500
H	1.44419600	-3.10741300	0.28043600
C	6.00612500	-0.39751400	-0.10616400
C	4.80117900	-2.54015000	0.17800000
C	4.77520600	1.64924900	-0.44239100
H	2.65923100	1.52324300	-0.48674800
H	3.61475000	-4.30362700	0.39960500
C	6.00287900	0.96270000	-0.31147200
H	4.77142200	2.71981200	-0.62723200
C	-1.02971800	1.33876500	-0.67789100
O	-0.08032600	1.97186400	0.19043600
C	-2.26872100	2.22604800	-0.60624900
C	-0.39712200	3.36685700	0.36034400
C	-1.64033200	3.61781400	-0.50473900
H	-2.82948400	2.00460600	0.30106300
H	-2.92752300	2.10758800	-1.46878400
C	-0.57971900	3.66825800	1.83792800
H	0.43719800	3.96292800	-0.02530000
O	-1.16680600	4.09348300	-1.76489100
H	-2.32234100	4.33913700	-0.03829600
O	-1.79591000	3.08457600	2.28183600
H	-0.58676600	4.76273500	1.96705700
H	0.28625600	3.26561300	2.38319800
H	-1.93822700	4.22710200	-2.33711500
H	-1.90281500	3.28215900	3.22353900
H	-0.60551000	1.32348300	-1.69007600
H	6.93940500	1.50852400	-0.38356700
H	6.94495500	-0.93865900	-0.01737800
H	5.75399200	-3.05730400	0.25083000

Table S49. Cartesian coordinates of nucleoside minimum for the ^{1ANP}dG adduct with χ = 69.5°, θ = 64.3° and ϕ = 7.7°.

Calculated energy (in Hartrees) = –1404.1788452			
Atom	X	Y	Z
N	-0.85583900	-0.45924900	-0.37159800
C	-0.08465500	-1.62208200	-0.27248800

N	-0.80225400	-2.70299600	-0.09521500
C	-2.11217500	-2.25320400	-0.05523600
C	-3.33272500	-2.98439000	0.15274400
O	-3.53848100	-4.17551300	0.31441900
N	-4.44407700	-2.06981900	0.17084700
H	-5.32714800	-2.51081100	0.40114900
C	-4.37670900	-0.71250000	0.00534700
N	-5.55774000	-0.00272300	0.11255800
H	-6.37888400	-0.42792700	-0.30117800
H	-5.42811800	0.96418200	-0.16136200
N	-3.25680500	-0.06403100	-0.19457600
C	-2.16606300	-0.86947800	-0.19773100
N	1.29011400	-1.61710200	-0.47117500
H	1.60148600	-2.55551900	-0.69992900
C	2.18584800	-0.91348100	0.38069300
C	3.55472600	-0.82977600	-0.02915900
C	1.77143400	-0.31324200	1.55227200
C	4.48339400	-0.14768400	0.82175300
C	4.02482300	-1.38905300	-1.24560800
C	2.69087500	0.39422500	2.35779700
H	0.73349900	-0.37449300	1.85576600
C	5.84798000	-0.09240600	0.43560100
C	4.01968500	0.46572500	2.01517500
C	5.35620800	-1.31323000	-1.59117200
H	3.31775500	-1.85635300	-1.92291400
H	2.33345300	0.86438200	3.26920800
C	6.27982300	-0.66703500	-0.73790600
H	5.69760400	-1.74346100	-2.52835300
C	-0.37106300	0.88696400	-0.56829200
O	-0.53494900	1.61857500	0.64280600
C	-1.10166400	1.72356800	-1.61979700
C	-0.60552500	3.01821100	0.33752100
C	-0.68601400	3.13528900	-1.19979900
H	-2.17897500	1.59784200	-1.50371700
H	-0.79963300	1.47349700	-2.64163800
C	-1.77480000	3.64407100	1.07823100
H	0.32056300	3.50359400	0.67097500
O	0.62870600	3.46999900	-1.64853700
H	-1.41465900	3.89219500	-1.51219500
O	-2.99475300	3.30736200	0.42684200
H	-1.62476800	4.73587000	1.09378900
H	-1.75840900	3.28099100	2.11587900
H	0.60379000	3.51827500	-2.61680500

H	-3.71429800	3.72175100	0.92474900
H	0.68983100	0.80348700	-0.81955800
H	7.32825800	-0.61583500	-1.01755300
H	6.54980400	0.41966600	1.08906900
H	4.73044100	0.99378200	2.64481700

Table S50. Cartesian coordinates of nucleoside minimum for the ^{1ANP}dG adduct with χ = 53.1°, θ = 298.1° and ϕ = 347.1°.

Calculated energy (in Hartrees) = –1404.1786742			
Atom	X	Y	Z
N	0.78307900	-0.43781700	-0.17868600
C	0.06177800	-1.59867100	-0.46249700
N	0.80274300	-2.67749300	-0.49315500
C	2.08837200	-2.22345400	-0.23572500
C	3.33007400	-2.94464800	-0.16086500
O	3.58595000	-4.12545000	-0.32755500
N	4.39814600	-2.03190100	0.15726000
H	5.31554500	-2.46253400	0.14188900
C	4.27437500	-0.68481100	0.36998900
N	5.43178900	0.03189500	0.61263700
H	6.11817200	-0.41092600	1.21212600
H	5.20935000	0.98021300	0.89332300
N	3.13409600	-0.04580100	0.30543200
C	2.09299400	-0.84751300	-0.02119500
N	-1.30121700	-1.54766200	-0.72523300
H	-1.60186900	-2.37574300	-1.22808100
C	-2.22545400	-1.08191500	0.24716900
C	-3.55180700	-0.76828800	-0.18843200
C	-1.86897100	-0.90604900	1.57063600
C	-4.50132100	-0.30850000	0.78036600
C	-3.95549400	-0.88590300	-1.54333600
C	-2.80502100	-0.41399200	2.50757100
H	-0.86766000	-1.16734800	1.89551200
C	-5.82614400	-0.02742100	0.35557500
C	-4.09632200	-0.13128100	2.12961100
C	-5.24880200	-0.60028500	-1.92120900
H	-3.22409700	-1.17789100	-2.28929700
H	-2.49736700	-0.28863900	3.54193700
C	-6.19667500	-0.17658300	-0.96127100
H	-5.54069500	-0.68996400	-2.96350300
C	0.30522700	0.92609700	-0.26410600
O	1.03122600	1.60633100	-1.28050600

C	0.50625500	1.77518500	0.99147100
C	1.06238400	3.00989700	-0.98003400
C	0.40291400	3.18299400	0.40350400
H	1.50979900	1.60432100	1.38707500
H	-0.24538000	1.57155500	1.75952700
C	2.48465200	3.54226700	-1.07629300
H	0.44931300	3.53754200	-1.72143600
O	-0.95370600	3.56055300	0.15967100
H	0.91989300	3.92996700	1.01641300
O	3.20635100	3.26668300	0.12176100
H	2.42880400	4.62882300	-1.25038700
H	2.96259700	3.07709400	-1.94960700
H	-1.39552700	3.63661900	1.01958700
H	4.09850500	3.62483200	0.00606700
H	-0.75333900	0.87077000	-0.53059400
H	-7.21489700	0.04266300	-1.26961300
H	-6.54611900	0.31304400	1.09545600
H	-4.82211300	0.22934000	2.85326400

Table S51. Cartesian coordinates of nucleoside minimum for the ^{3APHN}dG adduct with χ = 225.9°, θ = 181.0° and ϕ = 341.6°.

Calculated energy (in Hartrees) = –1557.8987699			
Atom	X	Y	Z
N	-2.51965200	0.23390500	-0.10745900
C	-1.44284600	-0.66040000	0.00516500
N	-1.82743600	-1.91620500	-0.01403300
C	-3.20715500	-1.86747400	-0.14304300
C	-4.17059400	-2.93011400	-0.19730300
O	-4.04122400	-4.14162000	-0.13589400
N	-5.49262100	-2.37150300	-0.33798600
H	-6.22700600	-3.06943700	-0.30975400
C	-5.81294900	-1.04317600	-0.40262000
N	-7.15554000	-0.72256200	-0.47452600
H	-7.73300600	-1.33738000	-1.03543600
H	-7.29752400	0.25630500	-0.69236100
N	-4.91842400	-0.08429500	-0.34643600
C	-3.65352200	-0.55519700	-0.21007300
N	-0.16555500	-0.17486000	0.10153700
H	-0.05066000	0.81530000	-0.08981900
C	1.01827700	-0.91462800	0.20051900
C	2.21247200	-0.25269100	-0.07231700

C	1.04803200	-2.27521000	0.58951500
C	3.46141900	-0.88327000	0.05627100
C	2.26603400	-2.90799400	0.71431500
H	0.11846500	-2.79890900	0.76405800
C	4.71907200	-0.20036800	-0.21217200
C	3.49004700	-2.24736500	0.46745400
H	2.29240700	-3.95248800	1.01477000
C	4.78837500	1.14333800	-0.64331300
C	5.94445500	-0.90892000	-0.03513000
C	4.74425100	-2.91922800	0.62170900
C	5.99867500	1.76796600	-0.88154000
C	7.17007000	-0.24930900	-0.28270200
C	5.92165800	-2.27930200	0.38660200
H	4.73396900	-3.95974200	0.93660800
C	7.20450700	1.06697800	-0.69714800
H	6.01761400	2.80172600	-1.21544000
H	8.09427100	-0.80434500	-0.14154500
H	6.86955800	-2.79622500	0.51052800
H	8.15494300	1.55858100	-0.88392300
C	-2.54309300	1.67100700	-0.01576700
O	-1.56742100	2.21816900	-0.90834500
C	-2.17885100	2.25872200	1.35045500
C	-1.18194300	3.51981900	-0.43781400
C	-1.79646000	3.69065400	0.97091000
H	-1.31828400	1.72932300	1.76830200
H	-3.01058600	2.20899600	2.05909900
C	0.33133500	3.62128500	-0.46794100
H	-1.60819900	4.28665300	-1.09575200
O	-2.93844500	4.53029500	0.80806100
H	-1.07934300	4.13104500	1.67438400
O	0.84263300	2.69857800	0.49234500
H	0.62417000	4.65297900	-0.22505200
H	0.69095500	3.38413700	-1.47851400
H	-3.35672200	4.63148100	1.67726800
H	1.81055900	2.73863100	0.49826600
H	-3.55068100	1.97647400	-0.31393400
H	2.15482500	0.77845400	-0.39512500
H	3.87292000	1.70298000	-0.80785800

Table S52. Cartesian coordinates of nucleoside minimum for the ^{3APHN}dG adduct with χ = 139.5°, θ = 184.8° and ϕ = 5.8°.

Calculated energy (in Hartrees) = –1557.8907377			
Atom	X	Y	Z
N	-2.21786700	-0.00674600	-0.28093600
C	-1.09251800	-0.82604200	-0.08420000
N	-1.40518000	-2.07881000	0.14797100
C	-2.78774200	-2.11349000	0.08266300
C	-3.67752700	-3.22641500	0.25843200
O	-3.45639200	-4.40029300	0.50706000
N	-5.03799700	-2.78450600	0.10386800
H	-5.72210500	-3.50842500	0.29137600
C	-5.44561500	-1.51183400	-0.18376500
N	-6.80956800	-1.29084400	-0.24699800
H	-7.36274900	-2.02626700	-0.67063500
H	-7.02524800	-0.37384300	-0.61834500
N	-4.61830600	-0.50759400	-0.34786600
C	-3.31447900	-0.85393700	-0.18145500
N	0.15574600	-0.26369700	-0.16491100
H	0.16575300	0.74534000	-0.06464500
C	1.39900700	-0.90301900	-0.09515500
C	2.53159800	-0.09234300	-0.09903400
C	1.54121000	-2.30936700	-0.04030100
C	3.83024100	-0.62955400	-0.04972200
C	2.80871800	-2.84850200	0.00710500
H	0.65816600	-2.93306300	-0.01920800
C	5.02930800	0.19760900	-0.05310300
C	3.97122700	-2.04741000	0.00532000
H	2.92376200	-3.92862300	0.05294900
C	4.98956900	1.60869100	-0.11027300
C	6.30758000	-0.43357400	0.00242800
C	5.27575700	-2.63405600	0.05985200
C	6.14656400	2.36601600	-0.11180700
C	7.47623000	0.36147200	0.00016600
C	6.39655200	-1.86370700	0.05928400
H	5.34938000	-3.71793700	0.10216700
C	7.40451200	1.73888500	-0.05580600
H	6.08177600	3.44958100	-0.15708500
H	8.44152700	-0.13711300	0.04331200
H	7.38314800	-2.31774100	0.10109300
H	8.31221200	2.33572700	-0.05713500
C	-2.15792200	1.37166700	-0.73314100

O	-1.25649900	2.08044100	0.12651700
C	-3.46304600	2.15830600	-0.66035600
C	-1.68156400	3.44655900	0.28950300
C	-2.94318100	3.59541000	-0.57231600
H	-4.00082300	1.90083400	0.25119800
H	-4.11449500	1.98228900	-1.51881300
C	-1.88406900	3.74192200	1.76606000
H	-0.89823700	4.10529800	-0.10179900
O	-2.51136000	4.09563900	-1.83802900
H	-3.67654700	4.26649000	-0.10892700
O	-3.05098300	3.06939700	2.21654300
H	-1.97491000	4.83335200	1.88937000
H	-0.98884000	3.41001300	2.31177600
H	-3.29240900	4.16570700	-2.40858800
H	-3.17077900	3.26395300	3.15732800
H	-1.74176700	1.38582900	-1.74908500
H	2.39079800	0.98301700	-0.14756600
H	4.03399600	2.11975700	-0.15564500

Table S53. Cartesian coordinates of nucleoside minimum for the ^{3APHN}dG adduct with χ = 54.7°, θ = 299.9° and ϕ = 175.9°.

Calculated energy (in Hartrees) = –1557.8895159			
Atom	X	Y	Z
N	1.40590300	-0.63621600	-0.56097700
C	1.09476300	-1.96163500	-0.87874500
N	1.92416100	-2.82953000	-0.35680700
C	2.85112700	-2.05847700	0.32815100
C	4.01383500	-2.45288800	1.07745000
O	4.49885200	-3.55143000	1.28938400
N	4.65712600	-1.28327000	1.61819300
H	5.53465600	-1.48368300	2.08417700
C	4.24144200	0.01237500	1.46353300
N	5.03249900	1.00524000	2.01054900
H	5.42643600	0.81667300	2.92473400
H	4.56792300	1.90422800	1.95218600
N	3.17330400	0.35156800	0.78747400
C	2.54009500	-0.70554900	0.22644200
N	0.03297500	-2.27990400	-1.71577700
H	0.16445900	-3.18226500	-2.15663500
C	-1.30634800	-1.93530600	-1.43945900
C	-1.67414200	-1.27332900	-0.27667800

C	-2.28714900	-2.23830600	-2.41104100
C	-2.99824000	-0.83963400	-0.06405600
C	-3.59325300	-1.85696100	-2.20544800
H	-1.99521000	-2.75453400	-3.32136800
C	-3.39253100	-0.09224200	1.12056700
C	-3.98129800	-1.13893900	-1.05042600
H	-4.34767700	-2.09010800	-2.95231900
C	-2.48412100	0.25129200	2.14833200
C	-4.74936300	0.32710300	1.25593400
C	-5.33339500	-0.70707800	-0.86607300
C	-2.88727500	0.97756500	3.25372300
C	-5.13709600	1.06710500	2.39638700
C	-5.70286500	-0.00224700	0.23731000
H	-6.06171700	-0.95305200	-1.63467800
C	-4.22599800	1.39150300	3.38132900
H	-2.16633100	1.22495800	4.02756600
H	-6.17520300	1.37787700	2.48429000
H	-6.73066100	0.32588100	0.36745900
H	-4.53974300	1.96052900	4.25170700
C	0.84841800	0.56038500	-1.15950700
O	1.85813200	1.19896900	-1.93180900
C	0.37319900	1.63403500	-0.17884600
C	1.57699100	2.60556100	-2.00402700
C	0.36319600	2.86302200	-1.08849000
H	1.11528500	1.75634800	0.61262000
H	-0.60814600	1.41722600	0.25136200
C	2.81952600	3.41083100	-1.65493100
H	1.28909800	2.85031700	-3.03417300
O	-0.78684600	2.88535800	-1.93637000
H	0.46101200	3.79786500	-0.52524100
O	2.97960900	3.49958600	-0.24131500
H	2.70719300	4.41526400	-2.09381400
H	3.68366600	2.92325000	-2.12741000
H	-1.56514900	3.00610900	-1.37014000
H	3.78010900	4.01904400	-0.07717700
H	0.02901800	0.23696600	-1.80528800
H	-0.91761200	-1.09117700	0.47421600
H	-1.44826400	-0.06191700	2.08163800

Table S54. Cartesian coordinates of nucleoside minimum for the ^{3APHN}dG adduct with χ = 68.6°, θ = 67.3° and ϕ = 354.7°.

Calculated energy (in Hartrees) = –1557.8864595			
Atom	X	Y	Z
N	1.84983800	-0.50148900	0.44164300
C	1.03585000	-1.64004000	0.41641100
N	1.70072600	-2.74037800	0.16691600
C	3.01271200	-2.33077500	-0.00035700
C	4.18549700	-3.09759000	-0.32583400
O	4.33824300	-4.29335100	-0.50825400
N	5.31723600	-2.21662400	-0.44757700
H	6.16086900	-2.68280700	-0.76117700
C	5.30776100	-0.85886300	-0.27056000
N	6.49415000	-0.18414900	-0.48441300
H	7.33824700	-0.63719900	-0.15528100
H	6.42016900	0.78410000	-0.19496800
N	4.23231200	-0.17777200	0.03680300
C	3.12311900	-0.95025400	0.14085500
N	-0.31075800	-1.60025300	0.75782200
H	-0.60716900	-2.50218100	1.11190500
C	-1.30887200	-0.93079400	0.00927900
C	-2.62918700	-1.05324300	0.42377900
C	-0.99781400	-0.13883300	-1.11656300
C	-3.68107700	-0.40580900	-0.25185600
C	-2.01172800	0.52086400	-1.77704600
H	0.02583500	-0.03451100	-1.45273200
C	-5.07381100	-0.52594700	0.15633600
C	-3.36039000	0.40981700	-1.37676400
H	-1.77322900	1.13693200	-2.64018400
C	-5.48793600	-1.31808300	1.25046300
C	-6.07375200	0.18214500	-0.57404700
C	-4.39978400	1.09941100	-2.08001500
C	-6.81900100	-1.40959800	1.61324600
C	-7.42777600	0.07392500	-0.18376700
C	-5.69964400	0.99297300	-1.69623800
H	-4.12265400	1.71354800	-2.93316100
C	-7.80104800	-0.70692500	0.89156700
H	-7.10576300	-2.02814000	2.45894000
H	-8.17610000	0.62087700	-0.75203600
H	-6.48271000	1.51976400	-2.23518900
H	-8.84595900	-0.78067500	1.17905900
C	1.44307000	0.85431400	0.72750200

O	1.55530800	1.62961100	-0.46236700
C	2.28677100	1.61282800	1.75330900
C	1.70607100	3.01149400	-0.10707600
C	1.90687300	3.05819200	1.42332800
H	3.34541900	1.44666600	1.54920300
H	2.05142600	1.33123700	2.78438200
C	2.83952200	3.62555800	-0.91071800
H	0.77741100	3.54455200	-0.34743200
O	0.64661900	3.42981800	1.98440100
H	2.69142700	3.76850100	1.70813000
O	4.09239000	3.22475800	-0.36635800
H	2.72803700	4.72139600	-0.87530700
H	2.73296500	3.30362000	-1.95650900
H	0.74574100	3.43563600	2.94913200
H	4.78604100	3.63457600	-0.90332400
H	0.40011700	0.80609800	1.05382600
H	-2.83405400	-1.65943700	1.29993300
H	-4.75362300	-1.87322000	1.82365900

Table S55. Cartesian coordinates of nucleoside minimum for the ^{1AP}dG adduct with χ = 224.1°, θ = 164.6° and ϕ = 337.5°.

Calculated energy (in Hartrees) = –1634.1616705			
Atom	X	Y	Z
N	-2.65120200	0.23691900	-0.17530600
C	-1.56371900	-0.65010800	-0.20737200
N	-1.93707300	-1.90458100	-0.31620600
C	-3.32193800	-1.86353300	-0.35220100
C	-4.27900900	-2.93094600	-0.43326000
O	-4.13664900	-4.14145100	-0.48002600
N	-5.61163800	-2.38025200	-0.44154700
H	-6.33695500	-3.08799800	-0.42507900
C	-5.94609100	-1.05560800	-0.37019000
N	-7.29290200	-0.74830500	-0.32653100
H	-7.90180200	-1.32180200	-0.89783700
H	-7.45669000	0.24338200	-0.45107400
N	-5.05778100	-0.09285100	-0.28946100
C	-3.78261300	-0.55572500	-0.27632000
N	-0.28084700	-0.16876100	-0.17164700
H	-0.17388200	0.83987800	-0.20711000
C	0.87815400	-0.90327900	0.10360600
C	2.12388900	-0.36664300	-0.31085900

C	0.84151500	-2.11094700	0.81806900
C	3.32877700	-0.99029900	0.13297800
C	2.23157500	0.77427300	-1.17697300
C	2.01806100	-2.73774600	1.19812800
H	-0.11815100	-2.54452100	1.06518000
C	4.59477500	-0.41762300	-0.19557100
C	3.27620100	-2.18924800	0.90281400
C	3.44072000	1.31990100	-1.49363300
H	1.33002000	1.17552700	-1.62653900
H	1.96664300	-3.66535000	1.76242300
C	4.66582100	0.76481500	-0.99288300
C	5.79960600	-1.02800000	0.27175800
C	4.50107700	-2.78761900	1.34353000
H	3.49738900	2.16825700	-2.17161300
C	5.92010100	1.31885400	-1.29101000
C	7.03147300	-0.43523700	-0.04939400
C	5.70865200	-2.23038400	1.05028400
H	4.44383400	-3.70247500	1.92802500
C	7.08826800	0.72435400	-0.81873100
H	5.97055400	2.21632800	-1.90231800
H	7.94746200	-0.89801700	0.30866600
H	6.62967200	-2.69095900	1.39777700
H	8.05198100	1.16522000	-1.05802700
C	-2.68480800	1.65391100	0.09578900
O	-1.76938200	2.32572000	-0.77150100
C	-2.25401200	2.06537100	1.50701200
C	-1.32022300	3.54123800	-0.14200200
C	-1.88130500	3.53402700	1.29622400
H	-1.37672700	1.49073600	1.81423100
H	-3.05307400	1.92418000	2.24055400
C	0.19411400	3.57895700	-0.22023800
H	-1.73814100	4.40145800	-0.67757300
O	-3.02734300	4.38411300	1.28161100
H	-1.13777200	3.88414500	2.02254000
O	0.68726000	2.53027400	0.60528100
H	0.54945800	4.56063000	0.12589500
H	0.50773100	3.44527800	-1.26512600
H	-3.41302500	4.37386500	2.17140600
H	1.65727000	2.52716700	0.57702700
H	-3.71114800	1.97411100	-0.10679800

Table S56. Cartesian coordinates of nucleoside minimum for the ^{1AP}dG adduct with χ = 142.0°, θ = 186.4° and ϕ = 357.2°.

Calculated energy (in Hartrees) = –1634.1528866			
Atom	X	Y	Z
N	2.18671300	0.09706400	-0.54759700
C	1.09459700	-0.76538100	-0.40654200
N	1.43798900	-2.01922500	-0.23856500
C	2.82038100	-2.00259400	-0.26984200
C	3.73181800	-3.10129300	-0.12775400
O	3.53061700	-4.28090800	0.07337400
N	5.08038500	-2.62854400	-0.24673700
H	5.77876800	-3.34765000	-0.09714300
C	5.45647400	-1.33236000	-0.47117800
N	6.81886000	-1.07535000	-0.51089200
H	7.38666100	-1.78928000	-0.95314400
H	7.00474500	-0.15353000	-0.88871600
N	4.61357300	-0.33947700	-0.59374200
C	3.31289100	-0.71199800	-0.46440000
N	-0.17856700	-0.24268500	-0.45949200
H	-0.23483000	0.73094400	-0.69998900
C	-1.39772300	-0.85790800	-0.16089300
C	-2.58858800	-0.09617000	-0.31805000
C	-1.45994500	-2.18076600	0.30131900
C	-3.83583200	-0.69074600	0.04601900
C	-2.61077900	1.24774300	-0.82513200
C	-2.68114000	-2.74568100	0.63752700
H	-0.54262000	-2.74763400	0.38343600
C	-5.04943100	0.05310100	-0.07244500
C	-3.88229400	-2.03130400	0.53276900
C	-3.76855100	1.95621500	-0.94123300
H	-1.69602600	1.72680300	-1.16540700
H	-2.70663900	-3.77116200	0.99682600
C	-5.02957500	1.39301400	-0.56279200
C	-6.29585200	-0.54091300	0.29912100
C	-5.14647400	-2.60140000	0.89374400
H	-3.75168800	2.96813600	-1.33767900
C	-6.23266900	2.10847400	-0.67002000
C	-7.47323900	0.21337700	0.17615700
C	-6.30238800	-1.89119100	0.78534900
H	-5.15993600	-3.62463700	1.26068800
C	-7.44026600	1.52136900	-0.30243100
H	-6.21000800	3.12816300	-1.04570300

H	-8.41958600	-0.23980900	0.45977800
H	-7.25428200	-2.33514300	1.06435000
H	-8.36398700	2.08641600	-0.39029000
C	2.05548300	1.56508100	-0.63919200
O	3.28729600	2.17567300	-0.88107500
C	1.48076800	2.17645700	0.66536500
C	3.67603300	3.01152200	0.22316200
C	2.36085800	3.41050700	0.89845700
H	1.59621400	1.46452500	1.48274300
H	0.42471100	2.45028600	0.57636000
C	4.66798600	2.31555200	1.14313100
H	4.15629600	3.89170200	-0.21378400
O	1.87763000	4.56035600	0.20875900
H	2.49809000	3.61534200	1.96757600
O	3.97652900	1.35254000	1.93013500
H	5.13940900	3.08075900	1.78115800
H	5.43428100	1.84033100	0.52100400
H	1.02611100	4.80311700	0.60405200
H	4.61678900	0.91678300	2.51065700
H	1.41302700	1.76552600	-1.50842300

Table S57. Cartesian coordinates of nucleoside minimum for the ^{1AP}dG adduct with χ = 70.2°, θ = 62.0° and ϕ = 13.0°.

Calculated energy (in Hartrees) = –1634.1492840			
Atom	X	Y	Z
N	-1.98114000	-0.51606200	-0.37525800
C	-1.30317100	-1.72742200	-0.20092400
N	-2.09799700	-2.72673700	0.08996800
C	-3.36504000	-2.16712700	0.13072700
C	-4.63190900	-2.77448800	0.43717900
O	-4.92655100	-3.92715000	0.70508800
N	-5.66458100	-1.77212400	0.41188400
H	-6.57102200	-2.11795000	0.70537000
C	-5.49425800	-0.44296700	0.13186800
N	-6.60879100	0.36962000	0.21678800
H	-7.47739300	-0.01708300	-0.13276700
H	-6.41209200	1.29721500	-0.14044500
N	-4.33398800	0.09128100	-0.15671100
C	-3.31273700	-0.79993400	-0.12671700
N	0.05879800	-1.84917300	-0.43762800
H	0.29765300	-2.82294900	-0.59252600

C	1.03426200	-1.11809400	0.29425300
C	2.35744500	-1.08652700	-0.20238200
C	0.70563300	-0.43545200	1.46907200
C	3.35222500	-0.37873900	0.53598300
C	2.73836000	-1.73151500	-1.42653100
C	1.67069100	0.28091100	2.16516300
H	-0.31390800	-0.46056200	1.83483900
C	4.70032300	-0.35368100	0.07105100
C	3.00345000	0.31636100	1.73291600
C	4.02694600	-1.70805100	-1.86733300
H	1.97233900	-2.22093600	-2.01844200
H	1.39296200	0.80603800	3.07501700
C	5.05661200	-1.03052600	-1.13409200
C	5.69892300	0.35416500	0.80766100
C	4.02656900	1.02255000	2.44876200
H	4.29518400	-2.19704800	-2.80032800
C	6.39038300	-0.99573600	-1.57066700
C	7.01890500	0.36052100	0.33192000
C	5.31489800	1.03870300	2.01037400
H	3.74711300	1.54653200	3.35929800
C	7.35823700	-0.30839800	-0.84263500
H	6.65963900	-1.51203200	-2.48843200
H	7.77891600	0.89850300	0.89261800
H	6.08052200	1.57503600	2.56486000
H	8.38603900	-0.29153400	-1.19409300
C	-1.39611500	0.76206600	-0.70679900
O	-1.44078000	1.60384100	0.44089300
C	-2.09982700	1.56932600	-1.79850300
C	-1.39988800	2.97314000	0.01537800
C	-1.53691200	2.96556800	-1.52254400
H	-3.17699600	1.55610800	-1.62761500
H	-1.87191500	1.20510100	-2.80521400
C	-2.47663300	3.76440300	0.73791000
H	-0.42088600	3.39764100	0.27175500
O	-0.21777100	3.13080500	-2.04571700
H	-2.20479200	3.75972400	-1.87544200
O	-3.74832300	3.48382200	0.16332100
H	-2.23166500	4.83531500	0.64927900
H	-2.44676800	3.49277700	1.80288300
H	-0.27986600	3.09773600	-3.01292100
H	-4.40716900	4.00308400	0.64667700
H	-0.35884300	0.56677300	-0.99288400

Table S58. Cartesian coordinates of nucleoside minimum for the ^{1AP}dG adduct with χ = 52.5°, θ = 300.2° and ϕ = 342.6°.

Calculated energy (in Hartrees) = –1634.1490684			
Atom	X	Y	Z
N	1.88711900	-0.46267400	-0.25264100
C	1.27820000	-1.68404400	-0.54615100
N	2.10342500	-2.69996600	-0.50793400
C	3.33199200	-2.13741700	-0.19186400
C	4.62080000	-2.75349500	-0.02692800
O	4.97965300	-3.91287200	-0.14809200
N	5.59161900	-1.75067400	0.32971900
H	6.53970700	-2.10572300	0.37895700
C	5.34799500	-0.41400900	0.50090500
N	6.42747100	0.39956800	0.79281900
H	7.10962100	0.02653300	1.44254600
H	6.11243600	1.33166000	1.03694000
N	4.16632000	0.12870400	0.35374300
C	3.21421100	-0.76162300	-0.01170500
N	-0.06955200	-1.74826300	-0.87296200
H	-0.28666700	-2.61399500	-1.35482300
C	-1.06598700	-1.29976200	0.03587600
C	-2.35764600	-1.01180400	-0.45929300
C	-0.77753700	-1.12128500	1.39362900
C	-3.36082700	-0.56624200	0.45285800
C	-2.69455200	-1.13769000	-1.84848700
C	-1.74788200	-0.65615200	2.27274200
H	0.21355700	-1.36655100	1.76016000
C	-4.67889100	-0.29326100	-0.01844400
C	-3.05077100	-0.37968100	1.83398700
C	-3.95505700	-0.87950300	-2.29479100
H	-1.91502000	-1.41869600	-2.54826200
H	-1.50464500	-0.53319900	3.32496500
C	-4.99514700	-0.46049500	-1.40018700
C	-5.68650800	0.15293800	0.89032800
C	-4.08142200	0.07523400	2.72216800
H	-4.19101500	-0.97308600	-3.35158900
C	-6.30062000	-0.19171200	-1.84063100
C	-6.97723200	0.40908400	0.40345700
C	-5.34160200	0.32668100	2.27356700
H	-3.83256100	0.20970100	3.77184500
C	-7.27847100	0.23614200	-0.94609000
H	-6.53976500	-0.31940100	-2.89306400

H	-7.74435700	0.74772700	1.09490800
H	-6.11405400	0.66608600	2.95867100
H	-8.28386500	0.43941900	-1.30365700
C	1.31002300	0.85762700	-0.39732300
O	2.04765500	1.57721800	-1.37708200
C	1.35609400	1.73910100	0.85138800
C	1.95593300	2.98326400	-1.10047100
C	1.18552300	3.12496900	0.22780200
H	2.33940200	1.65445400	1.31916500
H	0.57020300	1.48857400	1.56952900
C	3.33952100	3.61776100	-1.10294300
H	1.36292400	3.45403900	-1.89444700
O	-0.17491200	3.38859000	-0.12109900
H	1.59626100	3.92031800	0.85984100
O	3.98477000	3.42359700	0.15355700
H	3.21905500	4.69308800	-1.31050300
H	3.91600000	3.17002100	-1.92423000
H	-0.68444500	3.44301600	0.70228300
H	4.85473000	3.84473100	0.09507600
H	0.27951700	0.71439500	-0.73218400