

The activation of N-glycosidic bond cleavage operated by base-excision repair enzyme hOGG1; theoretical study of the role of Lys 249 residue in activation of G, OxoG and FapyG

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The supplementary information includes Tables S1-S15, Figures S1-S6 and xyz coordinates of optimized structures.

Table S1. The interatomic distances (Å) and angles (degrees) of G calculated employing small model and B3LYP-D2/6-31G**/PCM method. The interactions of Lys 249 with G are indicated in parenthesis as follows: C1'-pathway (C1'), N3-pathway (N3), N3-pathway with proton transferred from Nε-ammonium to N3 nitrogen (N3H). The numbering of atoms can be found in Figure 1.

Geometry Parameter	G	G (C1')	G (N3)	G (N3H)
Interatomic distance				
C1'-N9	1.468	1.460	1.461	1.471
Nε-N9	-	4.262	3.912	3.902
Nε-C1'	-	3.291	3.481	3.448
Nε-N3	-	3.954	2.734	2.681
N9-C8	1.382	1.382	1.387	1.389
C8-O8	-	-	-	-
N9-C4	1.368	1.369	1.368	1.358
C4-N3	1.358	1.358	1.366	1.375
C8-N7	1.313	1.312	1.309	1.309
N7-C5	1.382	1.382	1.380	1.378
C4-C5	1.397	1.397	1.392	1.387
N7-H7	-	-	-	-
C1'-H1'	1.095	1.093	1.097	1.097
N9-Hε1	-	-	3.114	2.822
Nε-Hε1	-	-	1.088	1.574
Nε-Hε2	-	1.018	1.024	1.021
Nε-Hε3	-	1.018	1.023	1.020
Angle				
C8-N9-C4	106.4	106.3	106.0	105.4
C8-N9-C1'	128.5	127.3	126.1	126.3
C4-N9-Nε	-	90.7	68.6	68.3
C1'-N9-Nε	-	35.8	62.3	61.4
N9-Hε1-Nε	-	-	130.7	122.6
Dihedral angle				
χ	193.5	217.7	229.5	223.0
κ'	-3.1	-3.8	1.5	2.3

Table S2. The interatomic distances (Å) and angles (degrees) of OxoG calculated employing small model and B3LYP-D2/6-31G**/PCM method. The interactions of Lys 249 with OxoG are indicated in parenthesis as follows: C1'-pathway (C1'), N3-pathway (N3), N3-pathway with proton transferred from Nε-ammonium to N3 nitrogen (N3H), N9-pathway (N9). The numbering of atoms can be found in Figure 1.

Geometry Parameter	OxoG	OxoG (C1')	OxoG (N3)	OxoG (N3H)	OxoG (N9)
Interatomic distance					
C1'-N9	1.456	1.454	1.458	1.464	1.479
Nε-N9	-	3.505	3.802	3.772	2.929
Nε-C1'	-	3.208	3.516	3.435	3.358
Nε-N3	-	3.104	2.769	2.644	3.518
N9-C8	1.415	1.413	1.423	1.429	1.442
C8-O8	1.226	1.225	1.221	1.217	1.220
N9-C4	1.384	1.381	1.380	1.368	1.407
C4-N3	1.350	1.352	1.362	1.372	1.348
C8-N7	1.378	1.380	1.378	1.380	1.372
N7-C5	1.392	1.392	1.390	1.389	1.394
C4-C5	1.380	1.382	1.376	1.371	1.371
N7-H7	1.008	1.008	1.009	1.009	1.009
C1'-H1'	1.095	1.091	1.097	1.096	1.092
N9-Hε1	-	-	3.050	2.790	1.958
Nε-Hε1	-	-	1.075	1.508	1.039
Nε-Hε2	-	1.017	1.024	1.021	1.024
Nε-Hε3	-	1.018	1.024	1.021	1.024
Angle					
C8-N9-C4	109.3	109.5	109.0	108.5	107.6
C8-N9-C1'	126.1	125.6	124.1	123.7	123.4
C4-N9-Nε	-	77.1	70.2	69.5	92.7
C1'-N9-Nε	-	66.2	67.6	65.5	93.3
N9-Hε1-Nε	-	-	127.5	119.7	154.4
Dihedral angle					
χ	262.0	251.1	261.6	256.3	285.3
κ'	10.5	2.6	17.1	18.4	37.8

Table S3. The interatomic distances (Å) and angles (degrees) of FapyG calculated employing small model and B3LYP-D2/6-31G**/PCM method. The interactions of Lys 249 with FapyG are indicated in parenthesis as follows: C1'-pathway (C1'), N3-pathway (N3), N3-pathway with proton transferred from Nε-ammonium to N3 nitrogen (N3H), N9-pathway (N9), N9-pathway with proton transferred from Nε-ammonium to N9 nitrogen (N9H). The numbering of atoms can be found in Figure 1.

Geometry Parameter	FapyG	FapyG (C1')	FapyG (N3)	FapyG (N3H)	FapyG (N9)	FapyG (N9H)
Interatomic distance						
C1'-N9	1.446	1.446	1.463	1.464	1.480	1.514
Nε-N9	-	4.494	3.115	3.480	2.753	2.656
Nε-C1'	-	3.402	3.297	3.388	3.301	3.205
Nε-N3	-	4.771	2.733	2.680	3.289	3.270
N9-C8	3.173	3.172	3.213	3.201	3.211	3.170
C8-O8	1.237	1.237	1.234	1.232	1.234	1.237
N9-C4	1.361	1.359	1.379	1.361	1.409	1.445
C4-N3	1.369	1.369	1.381	1.395	1.366	1.354
C8-N7	1.348	1.348	1.352	1.355	1.353	1.350
N7-C5	1.422	1.422	1.417	1.414	1.415	1.408
C4-C5	1.404	1.404	1.386	1.382	1.381	1.374
N7-H7	1.017	1.016	1.017	1.016	1.017	1.018
N9-H9	1.024	1.023	1.025	1.026	1.026	1.051
C1'-H1'	1.091	1.089	1.093	1.091	1.090	1.091
N9-He1	-	-	2.587	2.521	1.699	1.130
N3-He1			1.666	1.106	2.695	2.467
Nε-He1	-	-	1.077	1.576	1.078	1.543
Nε-He2	-	1.019	1.022	1.020	1.022	1.019
Nε-He3	-	1.018	1.024	1.020	1.023	1.019
Angle						
C8-N9-C4	81.0	81.0	78.8	78.0	78.3	78.7
H9-N9-C4	114.2	114.0	112.2	112.2	111.0	108.6
C8-N9-C1'	151.0	150.8	133.1	134.8	128.0	111.6
H9-N9-C1'	116.1	115.9	115.0	115.8	113.5	110.2
C4-N9-Nε	-	111.4	86.9	82.1	112.8	110.6
C1'-N9-Nε	-	34.5	83.9	74.2	98.0	96.6
N9-He1-Nε	-	-	109.4	114.3	164.4	166.6
Dihedral angle						
χ	288.8	288.4	305.7	297.8	300.9	306.0
κ ¹	37.8	39.5	76.9	75.0	84.4	93.3
κ ²	30.3	31.6	41.9	38.3	49.6	58.0

¹κ' for torsional angle C4-N9-C1'-C8 - 180°

²κ' for torsional angle C4-N9-C1'-H9 - 180°

Table S4. The calculated and experimental interatomic distances (Å) and angles (degrees) of G, OxoG and FapyG.

Parameter	Calc. Medium Model ^{a)}			Calc. Large Model ^{b)}		Experiment ^{c)}			
	G	OxoG	FapyG	OxoG	OxoG	G	G	OxoG	OxoG
C1'-N9	1.464	1.461	1.440	1.455	1.485	1.461	1.461	1.455	1.458
N ϵ -N9	3.629	3.021	2.777	3.075	2.911	4.178	5.175	3.366	3.027
N ϵ -N3	2.704	3.425	3.260	3.363	3.261	3.510	5.527	3.470	3.341
N ϵ -C1'	3.289	3.175	3.121	3.375	3.354	4.293	4.199	3.370	3.172
N7-O _{Gly42}	3.565	2.936	2.595	3.003	2.790	3.199	7.783	2.729	2.785
χ	248.7	272.9	287.6	288.3	269.5	266.3	286.9	275.1	258.0
κ'	29.9	38.8	48.2	42.2	41.8	0.5	-0.3	1.9	2.8

^{a)} Calculations employing medium structural model and ONIOM method (see Computational details).

^{b)} Calculations employing large structural model and AM1/OPLS_2005 QM/MM method (left column) and B3LYP/OPLS_2005 QM/MM method (right column) (see Computational details).

^{c)} X-ray structures with PDB ID 3IH7, 1YQK, 1N3C, 2NOZ (from left to right).

Table S5. The Wiberg bond orders calculated for pairs of atoms of G, OxoG, and FapyG employing B3LYP-D2/6-31G**/PCM. The interactions of Lys 249 with nucleosides are indicated in parenthesis as follows: C1'-pathway (C1'), N3-pathway (N3), N3-pathway with proton transferred from N ϵ -ammonium to N3 nitrogen (N3H), N9-pathway (N9), N9-pathway with proton transferred from N ϵ -ammonium to N9 nitrogen (N9H).

Pair of atoms	G	G (C1')	G (N3)	G (N3H)	G (N9)	G (N9H)
C1'-N9	0.8981	0.9083	0.9125	0.8965	-	-
N9-C8	1.1360	1.1325	1.1158	1.1158	-	-
N9-C4	1.1513	1.1516	1.1589	1.1902	-	-
N9-H ⁺ (N ϵ)	-	-	-	-	-	-
N3-H ⁺ (N ϵ)	-	-	0.1639	0.5452	-	-
N ϵ -H ⁺ (N ϵ)	-	-	0.5938	0.2085	-	-
	OxoG	OxoG (C1')	OxoG (N3)	OxoG (N3H)	OxoG (N9)	OxoG (N9H)
C1'-N9	0.9241	0.9224	0.9231	0.9119	0.9052	-
N9-C8	1.0265	1.0285	1.0031	0.9867	0.9734	-
N9-C4	1.1050	1.1154	1.1180	1.1522	1.0507	-
N9-H ⁺ (N ϵ)	-	-	-	-	0.0431	-
N3-H ⁺ (N ϵ)	-	-	0.1394	0.5098	-	-
N ϵ -H ⁺ (N ϵ)	-	-	0.6172	0.2456	0.7074	-
	FapyG	FapyG (C1')	FapyG (N3)	FapyG (N3H)	FapyG (N9)	FapyG (N9H)
C1'-N9	0.9713	0.9687	0.9566	0.9466	0.9285	0.8674
N9-H9	0.7039	0.7073	0.6998	0.6902	0.6986	0.6310
N9-C4	1.2023	1.2071	1.1346	1.1909	1.0421	0.9530
N9-H ⁺ (N ϵ)	-	-	-	-	0.1307	0.5111
N3-H ⁺ (N ϵ)	-	-	0.1452	0.5467	-	-
N ϵ -H ⁺ (N ϵ)	-	-	0.6086	0.2070	0.6174	0.2281

Table S6. The NBO atomic charges in e calculated for G employing B3LYP-D2/6-31G**/PCM method. The interactions of Lys 249 with G are indicated in parenthesis as follows: C1'-pathway (C1'), N3-pathway (N3), N3-pathway with proton transferred from Nε-ammonium to N3 nitrogen (N3H).

Atom	G	G (C1')	G (N3)	G (N3H)
C1'	0.279	0.269	0.280	0.278
N9	-0.420	-0.415	-0.419	-0.410
C8	0.198	0.201	0.211	0.220
C4	0.359	0.366	0.375	0.378
N3	-0.598	-0.595	-0.655	-0.612
N7	-0.486	-0.484	-0.461	-0.453
C5	-0.056	-0.058	-0.046	-0.036
O4'	-0.597	-0.603	-0.591	-0.590
C2'	-0.504	-0.495	-0.496	-0.498
Nε	-	-0.924	-0.822	-0.922

Table S7. The NBO atomic charges in e calculated for OxoG employing B3LYP-D2/6-31G**/PCM method. The interactions of Lys 249 with OxoG are indicated in parenthesis as follows: C1'-pathway (C1'), N3-pathway (N3), N3-pathway with proton transferred from Nε-ammonium to N3 nitrogen (N3H), N9-pathway (N9).

Atom	OxoG	OxoG (C1')	OxoG (N3)	OxoG (N3H)	OxoG (N9)
C1'	0.264	0.273	0.279	0.276	0.261
N9	-0.469	-0.460	-0.474	-0.465	-0.544
C8	0.821	0.821	0.826	0.830	0.828
C4	0.399	0.404	0.402	0.412	0.380
N3	-0.590	-0.596	-0.651	-0.616	-0.610
N7	-0.619	-0.621	-0.614	-0.613	-0.615
C5	-0.040	-0.040	-0.026	-0.015	-0.029
O4'	-0.605	-0.608	-0.598	-0.596	-0.595
C2'	-0.504	-0.502	-0.500	-0.500	-0.512
Nε	-	-0.922	-0.818	-0.912	-0.799

Table S8. The NBO atomic charges in e calculated for FapyG employing B3LYP-D2/6-31G**/PCM method. The interactions of Lys 249 with FapyG are indicated in parenthesis as follows: C1'-pathway (C1'), N3-pathway (N3), N3-pathway with proton transferred from Nε-ammonium to N3 nitrogen (N3H), N9-pathway (N9), N9-pathway with proton transferred from Nε-ammonium to N9 nitrogen (N9H).

Atoms	FapyG	FapyG (C1')	FapyG (N3)	FapyG (N3H)	FapyG (N9)	FapyG (N9H)
C1'	0.244	0.239	0.251	0.253	0.250	0.275
N9	-0.647	-0.645	-0.705	-0.672	-0.745	-0.707
C8	0.508	0.507	0.520	0.525	0.521	0.527
C4	0.431	0.433	0.424	0.438	0.405	0.383
N3	-0.603	-0.599	-0.657	-0.614	-0.620	-0.598
N7	-0.622	-0.622	-0.626	-0.627	-0.626	-0.617
C5	-0.084	-0.086	-0.048	-0.041	-0.037	-0.011
O4'	-0.607	-0.610	-0.602	-0.604	-0.595	-0.595
C2'	-0.500	-0.495	-0.505	-0.502	-0.511	-0.512
Nε	-	-0.917	-0.817	-0.923	-0.814	-0.910

Table S9. The f, f^+, f^2 Fukui indices calculated for G employing B3LYP-D2/6-31G**/PCM method. The interactions of Lys 249 with G are indicated in parenthesis as follows: C1'-pathway (C1'), N3-pathway (N3), N3-pathway with proton transferred from N ϵ -ammonium to N3 nitrogen (N3H).

Atoms	G	G (C1')	G (N3)	G (N3H)
f				
C1'	-0.009	-0.008	-0.007	-0.004
N9	0.011	0.011	0.006	0.004
N3	0.130	0.123	0.091	0.039
N ϵ	-	-0.001	0.002	-0.001
f^+				
C1'	-0.009	-0.001	-0.001	-0.003
N9	0.031	0.008	0.017	0.015
N3	0.026	0.006	0.023	0.054
N ϵ	-	0.004	0.001	-0.005
f^2				
C1'	0.000	0.007	0.006	0.001
N9	0.020	-0.003	0.011	0.011
N3	-0.104	-0.117	-0.068	0.015
N ϵ	-	0.005	-0.001	-0.004

Table S10. The Fukui indices f, f^+, f^2 calculated for OxoG employing B3LYP-D2/6-31G**/PCM method. The interactions of Lys 249 with OxoG are indicated in parenthesis as follows: C1'-pathway (C1'), N3-pathway (N3), N3-pathway with proton transferred from N ϵ -ammonium to N3 nitrogen (N3H), N9-pathway (N9).

Atoms	OxoG	OxoG (C1')	OxoG (N3)	OxoG (N3H)	OxoG (N9)
f					
C1'	-0.007	-0.008	-0.009	-0.008	-0.007
N9	0.035	0.038	0.043	0.047	0.026
N3	0.075	0.066	0.053	0.025	0.093
N ϵ	-	-0.006	0.002	-0.001	0.001
f^+					
C1'	-0.004	-0.001	-0.001	-0.003	-0.003
N9	0.022	0.010	0.014	0.025	0.009
N3	0.027	0.007	0.007	0.004	0.013
N ϵ	-	0.003	0.001	-0.003	0.001
f^2					
C1'	0.003	0.007	0.008	0.005	0.004
N9	-0.013	-0.028	-0.029	-0.022	-0.017
N3	-0.048	-0.059	-0.046	-0.021	-0.080
N ϵ	-	0.009	-0.001	-0.002	0.000

Table S11. The Fukui indices f^+ , f , f^2 calculated for FapyG employing B3LYP-D2/6-31G**/PCM method. The interactions of Lys 249 with FapyG are indicated in parenthesis as follows: C1'-pathway (C1'), N3-pathway (N3), N3-pathway with proton transferred from N ϵ -ammonium to N3 nitrogen (N3H), N9-pathway (N9), N9-pathway with proton transferred from N ϵ -ammonium to N9 nitrogen (N9H).

Atoms	FapyG	FapyG (C1')	FapyG (N3)	FapyG (N3H)	FapyG (N9)	FapyG (N9H)
f						
C1'	-0.011	-0.011	-0.011	-0.011	-0.007	-0.002
N9	0.113	0.116	0.112	0.124	0.046	0.000
N3	0.044	0.042	0.042	0.013	0.085	0.100
N ϵ	-	-0.007	0.002	-0.001	0.005	0.008
f^+						
C1'	-0.002	-0.001	-0.003	-0.003	-0.003	0.003
N9	0.050	0.024	0.026	0.044	0.010	-0.006
N3	0.010	0.004	0.001	-0.005	0.008	0.022
N ϵ	-	0.001	0.000	-0.006	0.001	-0.005
f^2						
C1'	0.009	0.010	0.008	0.008	0.004	0.005
N9	-0.063	-0.092	-0.086	-0.080	-0.036	-0.006
N3	-0.034	-0.038	-0.041	-0.018	-0.077	-0.078
N ϵ	-	0.008	-0.002	-0.005	-0.004	-0.013

Table S12. The Hardness η ^{a)} in (eV) calculated for G, OxoG and FapyG. The numbering of atoms is according to IUPAC.

Substrates	η (eV)
G	2.74
OxoG	2.46
FapyG	2.39

^{a)} The global reactivity descriptor of a molecule called chemical hardness $\eta = \frac{1}{2}(\epsilon_{LUMO} - \epsilon_{HOMO})$ was calculated employing the B3LYP-D2/6-31G**/PCM method. ϵ_{LUMO} and ϵ_{HOMO} are electronic energies of lowest unoccupied and highest occupied molecular orbital.

Table S13. The interaction energies in kcal/mol of G, OxoG and FapyG interacting with Lys 249 calculated employing small model and B3LYP-D2/PCM method including the BSSE correction that was calculated in gas phase.^{a)}

Complexes	$\Delta E_{\text{int}}^{\text{b)}$	$\Delta E_{\text{int}} \text{ (BSSE)}^{\text{b)}$	$\Delta E_{\text{int}}^{\text{c)}$	$\Delta E_{\text{int}} \text{ (BSSE)}^{\text{c)}$
G (N3)	-9.1	-8.3	-10.4	-8.7
OxoG (N3)	-8.5	-7.6	-9.4	-7.9
OxoG (N9)	-3.6	-2.5	-4.4	-2.4
FapyG (N3)	-12.0	-11.0	-12.8	-11.1
FapyG (N9)	-10.9	-9.8	-11.8	-9.8

^{a)} The interaction energy for Lys249 and nucleoside employing small model was computed using the following protocol: (i) the geometry optimization of complexes and monomers using the B3LYP-D2/6-31G(d,p)/PCM=diethylether method keeping the constraint defined for small model, (ii) the energy calculation for the complex (E_{complex}) and the monomers (E_1, E_2) employing the B3LYP-D2/6-311++G(d,p)/PCM=diethylether method, (iii) the BSSE calculation employing the B3LYP-D2/6-311++G(d,p) method, (iv) the interaction energy calculation: $\Delta E_{\text{int}} = E_{\text{complex}} - (E_1 + E_2)$, $\Delta E_{\text{int}} \text{ (BSSE)} = \Delta E_{\text{int}} + E_{\text{BSSE}}$. ^{b)} Calculated with 6-311++G(d,p) basis set. ^{c)} Calculated with aug-cc-pVDZ basis set.

Table S14. The reaction energies ΔE_r , the activation energies ΔE^\ddagger , the Gibbs free reaction energies ΔG_r , and the Gibbs free activation energies ΔG^\ddagger in kcal/mol calculated employing small model and B3LYP-D2/6-31G**/PCM method for proton transfer from Lys 249 to nucleobase owing to N3-pathway and N9-pathway.

Nucleoside (pathway) ^{a)}	ΔE_r ^{b)}	ΔE^\ddagger ^{c)}	ΔG_r ^{b)}	ΔG^\ddagger ^{c)}
G (N3)	1.7	2.4	-0.4	0.1
OxoG (N3)	3.8	3.9	3.7	1.3
FapyG (N3)	2.4	2.9	2.0	1.5
FapyG (N9)	2.8	3.1	2.0	1.3

^{b)} The N3-pathway and N9-pathway depicted in Figure S4 and Figure S5 are indicated in parenthesis. ^{b)} The energy of complex with proton at nucleobase minus energy of complex with proton at Lys 249. ^{c)} The energy of transition state of proton transfer minus energy of complex with proton at Lys 249.

Table S15. The electronic and Gibbs free activation and reaction energies in kcal/mol calculated for cleavage of N-glycosidic bond with S_N2 reaction mechanism initiated by C1'-pathway as depicted in Figure S3. The calculations employing B3LYP-D2/6-31G**/PCM method.

Complexes	ΔE^\ddagger	ΔG^\ddagger	ΔE_r	ΔG_r
G	29.1	30.7	9.3	14.7
OxoG	33.8	32.0	11.5	12.9
FapyG	36.6	35.2	26.0	25.5

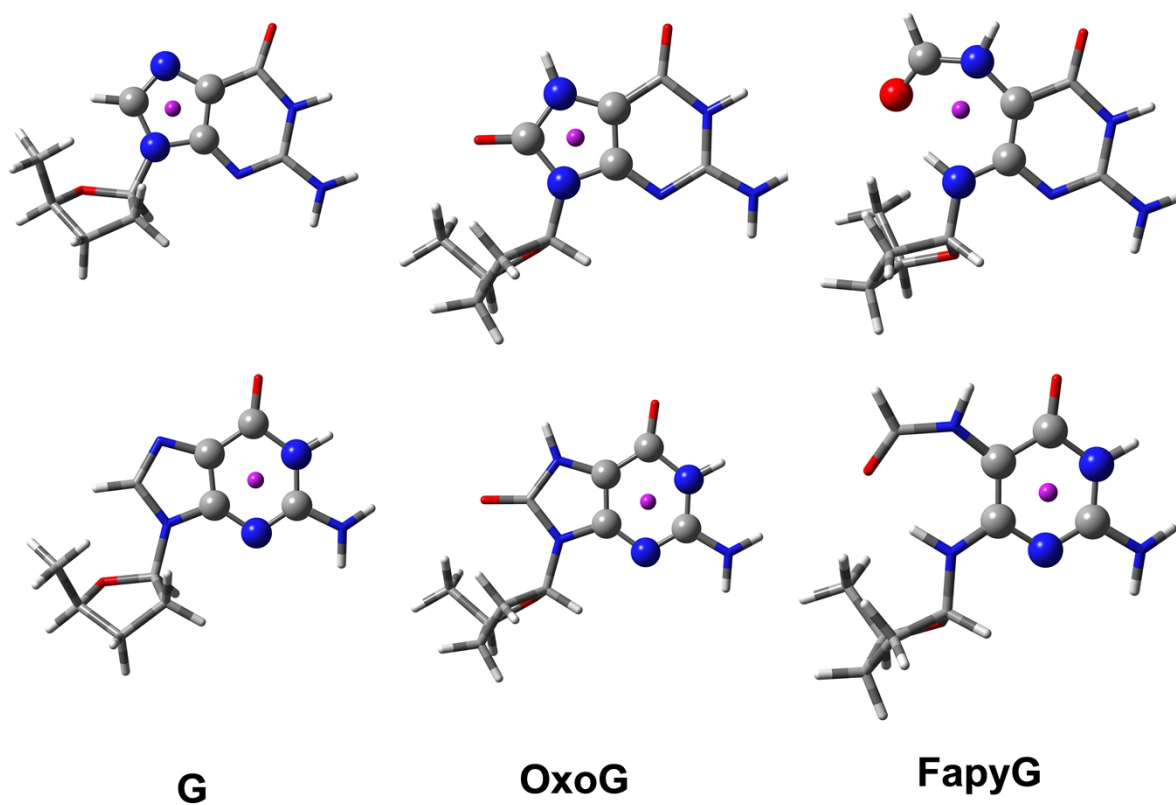


Figure S1. The NICSs were calculated at the centre of mass of 5 and 6-membered ring of G, OxoG and FapyG indicated by purple ball.

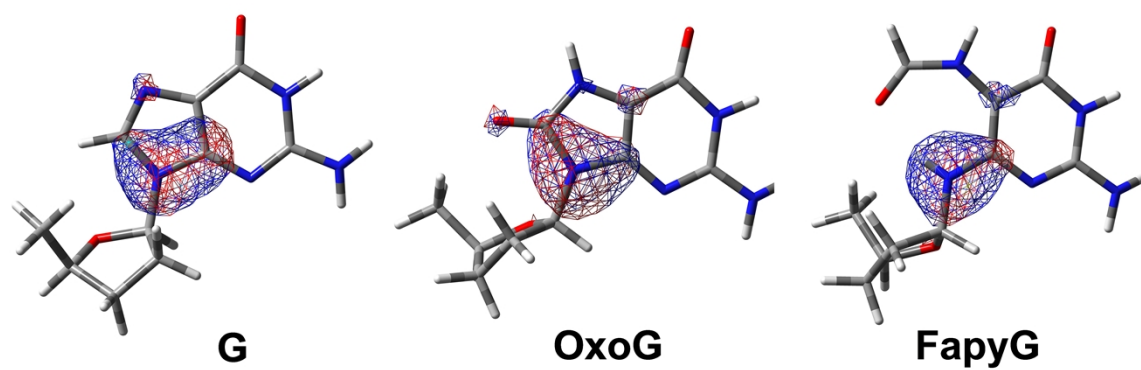


Figure S2. The NLMO of lone-pair electrons at N9 nitrogen calculated for G, OxoG and FapyG.

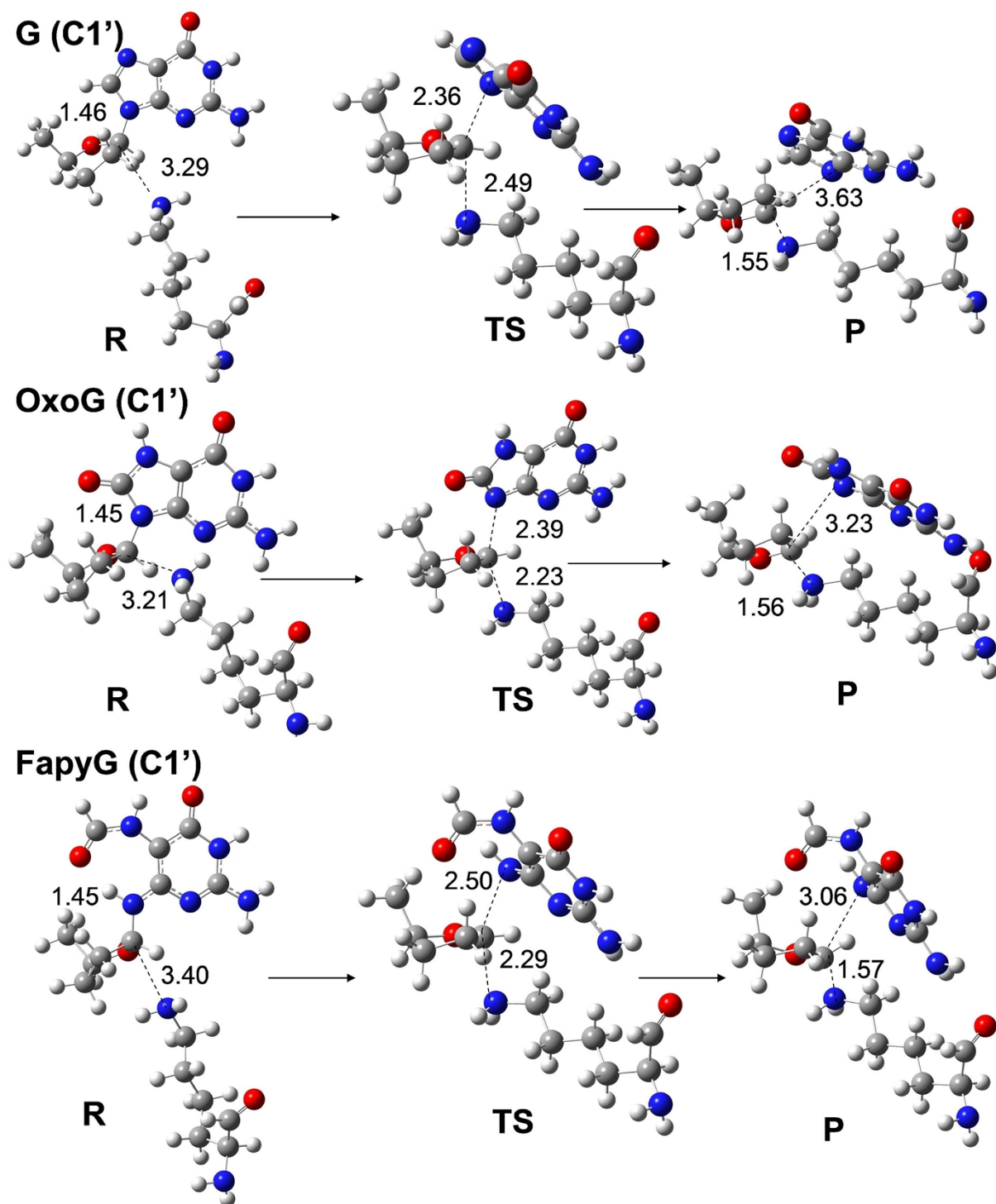


Figure S3. The reactant (R), transition state (TS) and product (P) of N-glycosidic bond cleavage of G, OxoG and FapyG employing C1'-pathway. The C1'-N9 and C1'-Nε distances between atoms indicated by dashed lines are in Å.

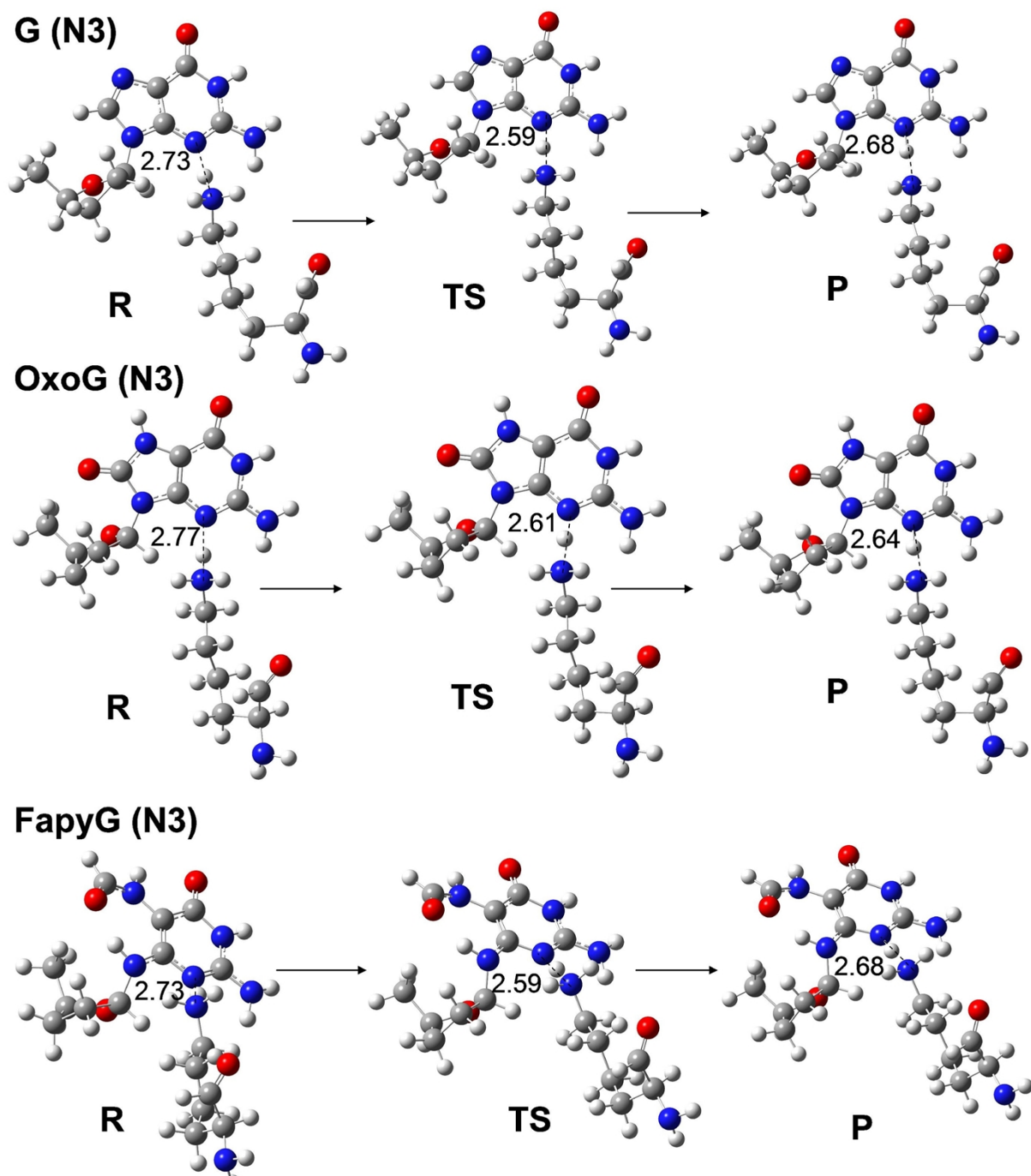


Figure S4. The reactant (R), transition state (TS), and product (P) calculated for proton addition to nitrogen N3 of G, OxoG and FapyG employing Lys 249. The N3-N ϵ distances between atoms indicated by dashed line are in Å.

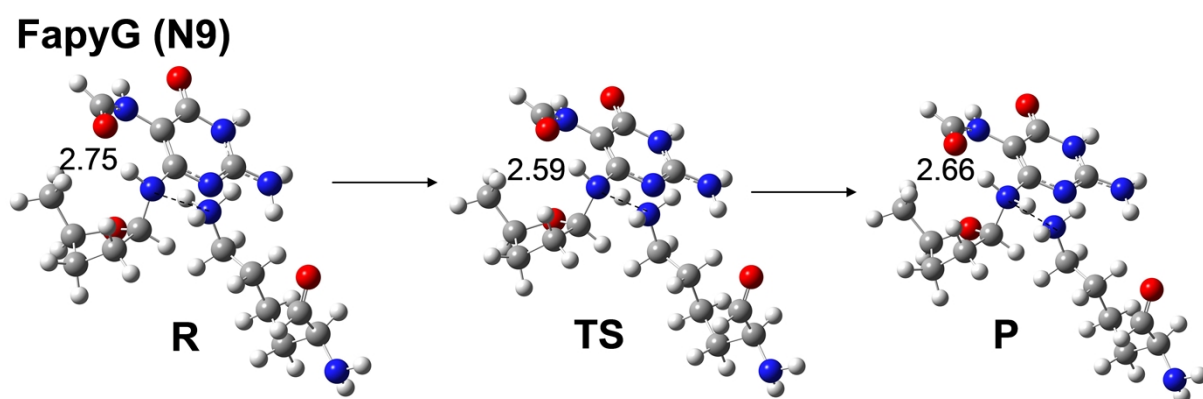


Figure S5. The reactant (R), transition state (TS), and product (P) calculated for proton addition to glycosidic nitrogen N9 of FapyG owing to deprotonation of Lys 249. The N9-N ϵ distances between atoms indicated by dashed lines are in Å.

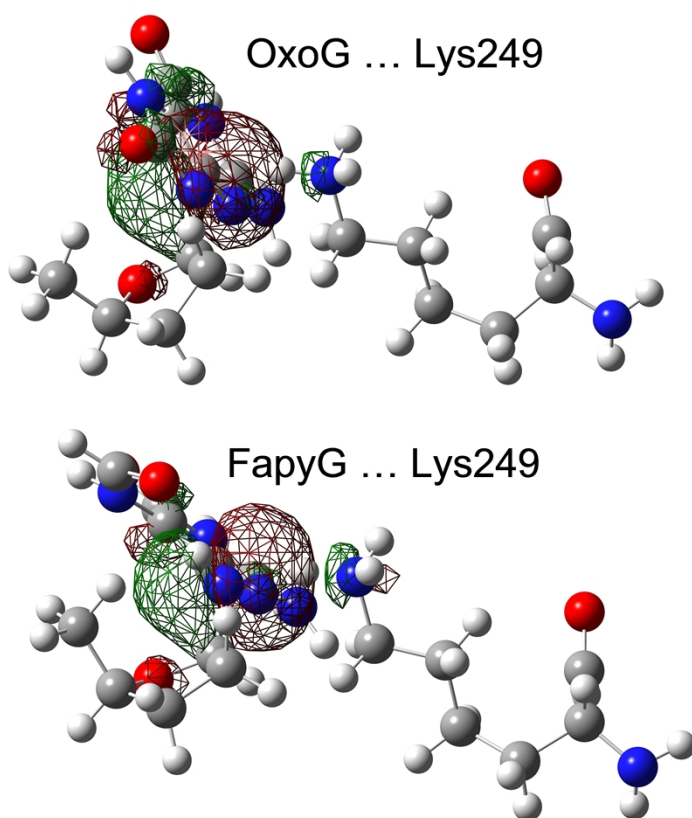


Figure S6. The NLMO of lone-pair electrons at N9 nitrogen calculated for N9-pathway of OxoG and FapyG.

Optimized Geometries (Small model)

G

C	22.85767200	23.29809500	37.87293800
C	22.97834600	24.74550200	37.40633800
O	23.40560800	24.80226300	36.01987900
C	21.64657100	25.50707000	37.41416700
C	21.03820400	25.09308900	36.06724700
C	22.28581100	24.94200000	35.17240800
N	22.19763000	23.77317200	34.28817900
C	22.82006300	22.54583100	34.42005200
N	22.48838700	21.69487800	33.47631900
C	21.59899300	22.39438400	32.68316900
C	20.88385300	21.99622500	31.50349400
O	20.87792000	20.93077600	30.89718600
N	20.07181800	23.07695200	31.03726400
C	19.96411300	24.32329900	31.60729700
N	19.08128400	25.19201800	31.02805500
N	20.62203100	24.68268900	32.68948400
C	21.40748800	23.68750600	33.17508400
H	23.51268800	22.36819800	35.22811900
H	22.62111600	23.26583900	38.94228700
H	22.06476700	22.77669500	37.32586800
H	23.75479700	25.26064700	37.97960200
H	21.01563500	25.24136400	38.26673300
H	20.53072100	24.12753900	36.14670600
H	20.33440000	25.81750200	35.65346000
H	22.42586300	25.81113600	34.52081000
H	19.16864200	26.14788500	31.34382200
H	23.80039500	22.76601500	37.70931000
H	21.83360700	26.58544600	37.43738500
H	19.51047800	22.85150300	30.22438800
H	18.88061000	25.08484700	30.04383300

G (C1')

C*	22.98299200	25.18401500	36.84898400
O	22.69765800	24.30372100	35.73430600
C*	21.67600300	25.24698500	37.63902000
C	21.13101900	23.82669900	37.45601700
C	21.53571200	23.52875700	36.00634200
N	21.84232900	22.12123200	35.77030900
C	22.99734100	21.44578300	36.11670900
N	22.95880000	20.16665800	35.82577700
C	21.70917500	19.98456700	35.26352400
C	21.08290100	18.79842900	34.75318600
O	21.49451700	17.64499700	34.69050400
N	19.77473800	19.10754700	34.26757000
C	19.17495800	20.34439800	34.27334300
N	17.88934600	20.40790100	33.80724600
N	19.75390900	21.42771300	34.74450900
C	21.00272200	21.18950500	35.22074000
N*	13.56100000	29.92299800	34.24600500
C*	14.57800000	28.98100300	33.82998300
C*	14.09301200	27.55499700	34.08701000
O*	14.09599300	26.72300200	33.16999800
C	15.94598400	29.25100500	34.50632300
C	17.10791900	28.31165100	34.14481300
C	17.15438800	27.01602800	34.96805300
C	18.51531200	26.31464400	34.86429300
N	18.66705100	25.11026800	35.68719800
H	15.79734400	29.24435400	35.59626300
H	16.20541500	30.28256700	34.23571300
H	18.04756400	28.85373100	34.31381500
H	17.07633200	28.07242100	33.07349300
H	16.97089100	27.25667800	36.02599600

H	16.36261500	26.32412700	34.65598000
H	19.29887700	27.02660400	35.15705800
H	18.71565200	26.04085900	33.82112500
H	18.38386800	25.32078500	36.64234000
H	18.03199900	24.38628800	35.35843100
H	14.70037400	29.05002400	32.74412800
H	13.80723800	30.84866700	33.90346900
H	13.55617500	29.99490800	35.26264100
C	24.15791700	24.63943600	37.65687400
H	23.25013400	26.15478600	36.41770800
H	21.82984500	25.52397300	38.68600200
H	20.98888100	25.96157000	37.17389600
H	21.62232600	23.12101100	38.13384400
H	20.04957900	23.75245900	37.57876500
H	20.72305700	23.79822300	35.32730500
H	17.55983100	21.34722500	33.63255200
H	17.60024100	19.72615700	33.11970600
H	19.26050600	18.30589900	33.92164800
H	23.83084500	21.97521800	36.55453800
H	13.74359600	27.30438200	35.10919400
H	24.45707300	25.35943000	38.42715300
H	23.88503800	23.69985100	38.15049500
H	25.01430500	24.45268700	37.00107700

G (C1') TS

C*	22.98300000	25.18400000	36.84900000
O	22.55700600	25.32766800	35.42794600
C*	21.67600000	25.24700000	37.63900000
C	20.61287900	24.81219500	36.61216000
C	21.28342100	25.15649000	35.31616500
N	20.93707200	23.07848700	34.25186500
C	21.21217100	22.00084700	35.05426000
N	20.17526700	21.36641600	35.59748400
C	19.10035800	22.08459900	35.10359000
C	17.69981900	21.95445800	35.36152800
O	17.07603200	21.14580300	36.05016300
N	16.97832600	22.98582800	34.68202500
C	17.52875000	23.99277400	33.92312700
N	16.66525400	24.96057500	33.46768600
N	18.81409100	24.10142800	33.68496600
C	19.57259200	23.12324200	34.28241200
H	22.23605200	21.68549100	35.22757400
N*	13.56100000	29.92300000	34.24600000
C*	14.57800000	28.98100000	33.83000000
C*	14.09300000	27.55500000	34.08700000
O*	14.09600000	26.72300000	33.17000000
C	15.92133000	29.22226400	34.55183500
C	17.05822000	28.29014500	34.14833500
C	18.32563000	28.54094700	34.96708300
C	19.36795600	27.45505100	34.71745700
N	20.55763800	27.51890500	35.57594000
H	15.74231500	29.12833100	35.63389000
H	16.20134100	30.26918600	34.37315100
H	17.27376300	28.40380300	33.07681400
H	16.75079900	27.24872100	34.29423200
H	18.74271600	29.53255100	34.74521200
H	18.06704900	28.53627700	36.03652100
H	19.70589200	27.48050500	33.67498900
H	18.89839200	26.47319000	34.85619400
H	21.17480100	28.27232600	35.28466800
H	20.28416100	27.71326600	36.53671000
H	14.71651600	29.05715600	32.74694100
H	13.79649500	30.84563000	33.88919600
H	13.56557900	30.00605800	35.26146300
C	23.73683200	23.87277600	36.97818700
H	23.63579100	26.04162100	37.02010500

H	21.70733400	24.58672200	38.50788200
H	21.48443700	26.26808700	37.97740700
H	20.42971100	23.73424500	36.66028500
H	19.65432100	25.32219000	36.71121300
H	20.82411900	25.36477700	34.36656600
H	17.03947400	25.54072800	32.73112900
H	15.67742800	24.76367800	33.38304500
H	15.97736700	22.96432400	34.83482400
H	24.15051000	23.79463300	37.98877000
H	23.05842000	23.03145100	36.80872100
H	24.55710800	23.82327200	36.25623700
H	13.74901900	27.30402300	35.11046600

G (C1') P

C*	22.98300000	25.18400000	36.84900000
O	22.57855600	25.75516100	35.54401300
C*	21.67600000	25.24700000	37.63900000
C	20.64669500	24.86158800	36.57311600
C	21.20992800	25.56824500	35.34507900
N	19.47492500	24.31132400	32.41587700
C	20.54757700	23.53210200	32.74699500
N	20.45623000	22.77967800	33.85388000
C	19.18417500	23.08034200	34.28771700
C	18.49861400	22.67825000	35.47076200
O	18.87048900	21.97072100	36.41551900
N	17.20566600	23.27293500	35.52134100
C	16.67992100	24.14351100	34.58604400
N	15.42062500	24.64574400	34.88488800
N	17.32758700	24.54907600	33.52851900
C	18.59228400	24.00871700	33.39910500
H	21.44592400	23.53213100	32.13541800
N*	13.56100000	29.92300000	34.24600000
C*	14.57800000	28.98100000	33.83000000
C*	14.09300000	27.55500000	34.08700000
O*	14.09600000	26.72300000	33.17000000
C	15.97205600	29.13509400	34.51338600
C	16.95142100	27.99181000	34.18566900
C	18.35986800	28.19206700	34.77712500
C	19.15287100	26.89440300	34.63585100
N	20.54867200	26.96955000	35.21597000
H	15.81732500	29.18289100	35.60112000
H	16.38998700	30.10306200	34.20752700
H	17.02707700	27.86357700	33.09973600
H	16.55353100	27.04445500	34.56633100
H	18.87266200	29.01978200	34.27127100
H	18.27790000	28.45638800	35.84084900
H	19.27078300	26.57187200	33.59971100
H	18.64865100	26.08524400	35.16213300
H	21.15196200	27.54462800	34.62108500
H	20.53955200	27.41591600	36.13834000
H	14.70485000	29.05409600	32.74561400
H	13.79358700	30.84830500	33.89345900
H	13.55701200	30.00186700	35.26196300
C	23.53135200	23.78309200	36.62768300
H	23.75230200	25.85368300	37.24162500
H	21.66767800	24.56769700	38.49522700
H	21.51068400	26.26626100	38.00918500
H	20.64379800	23.78718900	36.39130700
H	19.62239300	25.15734800	36.80934400
H	21.00352800	25.08763900	34.39035500
H	14.97484000	25.09512800	34.08899900
H	14.80141400	23.99069000	35.34753100
H	16.66934600	23.04613900	36.34980800
H	23.83656000	23.34492800	37.58433200
H	22.77504200	23.14085700	36.16498200
H	24.40148800	23.82226600	35.96556400

H 13.78295400 27.29011200 35.11677800

G (N3)

C 24.01577000 24.23864000 37.45217000
C* 22.98298700 25.18398600 36.84898400
O 22.59087300 24.72212700 35.52615200
C* 21.67601300 25.24701700 37.63901700
C 20.90221900 24.06139300 37.04994500
C 21.32356800 24.10596800 35.56974400
N 21.40593700 22.78458400 34.95228600
C 22.36899000 21.82016600 35.21061900
N 22.21214900 20.73276700 34.49965000
C 21.09437700 20.98314500 33.73020700
C 20.44861800 20.16102900 32.74466400
O 20.70877100 19.03554300 32.35491100
N 19.33589800 20.86793400 32.16962100
C 18.90218300 22.11627000 32.50157100
N 17.79059500 22.59164100 31.87906000
N 19.49331400 22.85184700 33.43650100
C 20.58584200 22.25135600 33.99539000
H 23.16256600 22.01171100 35.91739000
N* 13.56100100 29.92300500 34.24599200
C* 14.57800100 28.98099700 33.83004000
C* 14.09299300 27.55500400 34.08695900
O* 14.09600500 26.72299100 33.17000800
C 15.87511300 29.23389100 34.63437700
C 17.05438500 28.33897100 34.21280600
C 17.07387200 26.97090000 34.91265100
C 18.07567100 26.02929600 34.25882400
N 17.96527800 24.64128700 34.82760800
H 15.66265400 29.12452300 35.70551000
H 16.14374600 30.28459600 34.47206000
H 17.99751200 28.85409200 34.42475100
H 17.01492300 28.18862300 33.12595300
H 17.31108800 27.09681300 35.97630700
H 16.08883800 26.49820700 34.85467300
H 19.11020700 26.35154100 34.40088800
H 17.88453200 25.94114900 33.18684900
H 18.22603500 24.62887100 35.81625500
H 18.59270700 23.93921900 34.28257200
H 16.99839600 24.30827000 34.77328800
H 14.83073900 29.01913700 32.75811300
H 13.94101600 30.86610700 34.24822100
H 12.78321200 29.91789500 33.59193800
H 24.43039500 24.67306600 38.36818500
H 23.56443500 23.27329000 37.70865600
H 23.42486600 26.17407400 36.70429200
H 21.83252000 25.15885000 38.71700500
H 21.23499800 23.11670800 37.48917100
H 19.81882000 24.12306900 37.18726900
H 20.61771200 24.67668300 34.95320200
H 17.69048800 23.59506900 31.83003600
H 24.83249200 24.06822500 36.74438400
H 21.15298000 26.18750400 37.43703600
H 18.85766000 20.35514200 31.43706900
H 17.43586900 22.09486200 31.07429600
H 13.73370000 27.32179200 35.10838300

G (N3) TS

C 24.00068700 24.20551700 37.42302400
C* 22.98300000 25.18400000 36.84900000
O 22.57756100 24.76475400 35.51303600
C* 21.67600000 25.24700000 37.63900000
C 20.88864700 24.08258500 37.02707300

C	21.30537800	24.16362900	35.54787500
N	21.38372800	22.85196000	34.89497000
C	22.39922900	21.91933300	35.05480900
N	22.22556400	20.84111400	34.33364300
C	21.04253400	21.06207100	33.66208400
C	20.35706800	20.23499200	32.70662400
O	20.62725400	19.13189500	32.27361000
N	19.17442100	20.91057300	32.22272500
C	18.70723900	22.12222900	32.60838900
N	17.54763700	22.57486400	32.09208200
N	19.35355000	22.85670000	33.52182300
C	20.51621300	22.30209900	33.99969500
H	23.23811000	22.12941800	35.70088000
N*	13.56100000	29.92300000	34.24600000
C*	14.57800000	28.98100000	33.83000000
C*	14.09300000	27.55500000	34.08700000
O*	14.09600000	26.72300000	33.17000000
C	15.87895900	29.23289900	34.62774500
C	17.05139700	28.33114500	34.20062900
C	17.08165700	26.96949700	34.91124400
C	18.05685900	26.00316200	34.24602300
N	17.98582400	24.63092800	34.82549200
H	15.67152500	29.12527100	35.70012000
H	16.14771900	30.28335300	34.46225900
H	17.99828700	28.84764500	34.39307200
H	16.99717900	28.17109500	33.11543800
H	17.34827900	27.10433500	35.96728900
H	16.09188000	26.50220500	34.89037500
H	19.09211700	26.34687000	34.33659700
H	17.82795300	25.91830600	33.17854800
H	18.26373200	24.65668200	35.80735000
H	18.72267200	23.73845600	34.14563000
H	17.01386000	24.31312000	34.82782600
H	14.82737500	29.01857600	32.75723000
H	13.94242800	30.86553800	34.25122100
H	12.78510500	29.92062600	33.58967700
H	24.41914000	24.60559000	38.35273500
H	23.53591300	23.23873500	37.64816000
H	23.44025100	26.16983800	36.72722600
H	21.83009100	25.13559300	38.71516400
H	21.21628500	23.12473800	37.44097400
H	19.80766500	24.15326200	37.16973200
H	20.59859600	24.75208600	34.94994800
H	17.35467300	23.56458500	32.12430800
H	24.81767800	24.04745600	36.71242600
H	21.16385300	26.19690800	37.45390900
H	18.66657100	20.39284000	31.51352700
H	17.10201000	22.06415500	31.34360100
H	13.73366700	27.32165900	35.10827900

G (N3H)

C	24.00983300	24.22168100	37.43402500
C*	22.98299900	25.18400300	36.84899900
O	22.57688700	24.74613600	35.51898800
C*	21.67600000	25.24699600	37.63900100
C	20.90014500	24.06291500	37.04857100
C	21.31759100	24.12231000	35.56903400
N	21.42816200	22.79462500	34.94435100
C	22.48210500	21.90201900	35.09082400
N	22.33083900	20.80774500	34.38867900
C	21.12490400	20.97401000	33.74351800
C	20.44947100	20.11201300	32.81075200
O	20.74929500	19.01686800	32.38267400
N	19.22661500	20.73656500	32.34416000
C	18.71664100	21.92983300	32.71994800
N	17.54508400	22.34738500	32.22490200

N	19.37239700	22.69230700	33.61036000
C	20.56573900	22.19686100	34.08186400
H	23.32740900	22.15353400	35.71281700
N*	13.56099700	29.92299600	34.24600000
C*	14.57800900	28.98099900	33.82997400
C*	14.09298600	27.55498800	34.08704200
O*	14.09600900	26.72301800	33.16998300
C	15.88164500	29.23453700	34.62250800
C	17.05204500	28.32991700	34.19483300
C	17.08402800	26.97195400	34.91079600
C	18.05931300	25.99241100	34.26009700
N	17.98555900	24.62826400	34.84129700
H	15.67771700	29.12981300	35.69591400
H	16.14894700	30.28492300	34.45304800
H	17.99979600	28.84754400	34.38121200
H	16.99432000	28.16522100	33.11035700
H	17.34687700	27.11339600	35.96740400
H	16.09379600	26.50463800	34.89292600
H	19.09363400	26.34144500	34.35500700
H	17.84236100	25.91016000	33.18880900
H	18.25155300	24.66703200	35.82472300
H	18.83832100	23.53249300	34.10030000
H	17.01138200	24.32127000	34.84605800
H	14.82475200	29.01785300	32.75653700
H	13.94317700	30.86523400	34.25260500
H	12.78615900	29.92205200	33.58841100
H	24.42706400	24.63833800	38.35693500
H	23.55447500	23.25413200	37.67426500
H	23.43223700	26.17151100	36.71271300
H	21.83168800	25.15622300	38.71687700
H	21.23770300	23.11691700	37.48130600
H	19.81821200	24.12592600	37.18446700
H	20.59732700	24.68048200	34.95848800
H	17.24971200	23.30182700	32.36464400
H	24.82694600	24.06094800	36.72407600
H	21.15401000	26.18790300	37.43717500
H	18.71865900	20.18498700	31.66120400
H	17.07211300	21.81658100	31.50814400
H	13.73355300	27.32151800	35.10823100

OxoG

C	23.79928700	23.83854700	37.55214100
C	23.07932100	25.06960900	37.01295200
O	22.77213900	24.88818800	35.60915200
C	21.72031400	25.33688500	37.68102400
C	20.76406600	24.49057600	36.83212900
C	21.38348500	24.62608300	35.43315700
N	21.19651200	23.46573900	34.57292500
C	21.46252600	22.11977500	34.91967100
N	21.29984800	21.40926100	33.74996200
C	20.97499600	22.26555700	32.70111100
C	20.72246900	22.02249500	31.32677100
O	20.72110600	20.96179000	30.70273400
N	20.43794500	23.25538000	30.66664300
C	20.41352700	24.49208300	31.25830200
N	20.07049000	25.55439100	30.47434100
N	20.65606500	24.68249800	32.54209400
C	20.92561500	23.54475400	33.21768000
O	21.75876300	21.67489100	36.02295900
H	24.07887300	23.99392000	38.60107700
H	23.15544700	22.95869200	37.46821600
H	23.73526000	25.94534100	37.07788900
H	21.71528000	25.05611000	38.73791600
H	20.78454300	23.44692900	37.14624900
H	19.73226200	24.85061700	36.84320200
H	20.93537400	25.45641600	34.87811700

H	21.41975300	20.41030500	33.69296100
H	20.24646900	26.45898300	30.88843900
H	24.71054600	23.65449200	36.97298200
H	21.46612500	26.39962900	37.60121200
H	20.21706900	23.16169500	29.68217200
H	20.22925700	25.49588400	29.47870400

OxoG (C1')

C	23.96818600	24.14526900	37.37500600
C*	22.98299000	25.18399800	36.84898700
O	22.58829400	24.84136800	35.49693100
C*	21.67600800	25.24700300	37.63901500
C	20.83480500	24.16574400	36.95585600
C	21.24042000	24.36973000	35.49518800
N	21.12506800	23.18637500	34.65838500
C	21.68595700	21.92093100	34.94089300
N	21.35757900	21.13374200	33.85581700
C	20.62123600	21.86720300	32.92941000
C	20.04414400	21.50683700	31.68538500
O	20.05686800	20.42677200	31.09513200
N	19.36943200	22.63316900	31.12331000
C	19.28678100	23.87729400	31.69118800
N	18.53906700	24.81665500	31.04187000
N	19.84464700	24.18107300	32.84769900
C	20.48723400	23.14613100	33.43470200
O	22.31676000	21.58933800	35.93759200
N*	13.56099900	29.92299700	34.24600400
C*	14.57800400	28.98100300	33.83000000
C*	14.09299700	27.55500000	34.08699300
O*	14.09600200	26.72299900	33.17000100
C	15.84450200	29.25248200	34.67960500
C	17.08369400	28.39433200	34.38367800
C	16.91460900	26.89908000	34.70364100
C	18.22006200	26.18451600	35.06240600
N	18.05983300	24.75068300	35.32275800
H	15.56741900	29.13930400	35.73618900
H	16.09769800	30.31133700	34.53289600
H	17.90548700	28.79594600	34.99176700
H	17.38501900	28.51978100	33.33540600
H	16.22523000	26.78302000	35.55406600
H	16.45479400	26.37643100	33.86012000
H	18.66318800	26.66018300	35.94949500
H	18.94432200	26.28662100	34.24617200
H	17.23824700	24.60373000	35.90645600
H	17.88300700	24.27980900	34.43926400
H	14.84541300	29.02201400	32.76179500
H	13.94577400	30.86411500	34.25854900
H	12.78792900	29.92910900	33.58573900
H	24.31237700	24.42304000	38.37862500
H	23.49381900	23.16065800	37.40400000
H	23.46969600	26.16548500	36.79621400
H	21.82742200	25.06906100	38.70794100
H	21.13380500	23.17014700	37.28848500
H	19.75641400	24.28828400	37.05708100
H	20.59428700	25.10982100	35.02132500
H	21.61710800	20.16295700	33.78124200
H	18.66039700	25.76079500	31.38025800
H	24.83814100	24.08510900	36.71237200
H	21.20530600	26.22954000	37.51468500
H	18.89467100	22.44434400	30.24823600
H	18.40598800	24.72844200	30.04467500
H	13.73202800	27.32306400	35.10754700

OxoG (C1') TS

C*	22.98300000	25.18400000	36.84900000
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O	22.56115800	25.34265900	35.43567800
C*	21.67600000	25.24700000	37.63900000
C	20.64788500	24.70677900	36.62414500
C	21.29244600	25.09683200	35.32278400
N	21.42072400	22.86022100	34.48518600
C	21.20002200	21.67583300	35.15329200
N	20.73994700	20.72817900	34.23518200
C	20.60808300	21.34905600	32.99563400
C	20.14470300	20.89620200	31.74580400
O	19.72675800	19.78574100	31.38957600
N	20.19493400	21.97149700	30.79852300
C	20.61024000	23.24959000	31.06697300
N	20.50048200	24.16098700	30.03457600
N	21.04433700	23.64442000	32.24159300
C	21.03356800	22.66705500	33.20380500
O	21.35846700	21.46389400	36.37285500
N*	13.56100000	29.92300000	34.24600000
C*	14.57800000	28.98100000	33.83000000
C*	14.09300000	27.55500000	34.08700000
O*	14.09600000	26.72300000	33.17000000
C	15.94356800	29.17990800	34.52248400
C	17.00821000	28.17046000	34.09080600
C	18.32869600	28.34902800	34.84110900
C	19.24193700	27.14349200	34.63208600
N	20.50376400	27.18676400	35.37556200
H	15.79212300	29.10831200	35.61008000
H	16.28083700	30.20457800	34.31773900
H	17.17717300	28.24629900	33.00893300
H	16.63831700	27.15240500	34.26930600
H	18.83461300	29.26909900	34.52081500
H	18.12671600	28.45120100	35.91725800
H	19.48364800	27.01873100	33.57093600
H	18.70605200	26.23649200	34.94298300
H	21.17384600	27.82220500	34.95136100
H	20.35537600	27.48391300	36.33700700
H	14.70597900	29.05500900	32.74534000
H	13.80233000	30.84900100	33.90115000
H	13.55580900	29.99638200	35.26241900
C	23.72065600	23.86063100	36.96883900
H	23.64290600	26.03345500	37.03877100
H	21.72755200	24.63531100	38.54167200
H	21.44462600	26.27773500	37.92407200
H	20.60038700	23.61600500	36.67935400
H	19.64309200	25.12060000	36.72760900
H	20.87514600	25.08570300	34.32959800
H	20.44805600	19.79450800	34.47562200
H	21.03212900	25.00448700	30.20537200
H	20.62828200	23.79555200	29.09963100
H	19.82830700	21.74156500	29.88315800
H	24.13585500	23.77851400	37.97960700
H	23.03629100	23.02388500	36.78938600
H	24.54397100	23.81862900	36.24913000
H	13.74836200	27.30516200	35.11137100

OxoG (C1') P

C*	22.98278600	25.18392500	36.84878400
O	22.57961400	25.74021600	35.53979300
C*	21.67614500	25.24705300	37.63925800
C	20.64937400	24.84195900	36.57483500
C	21.21758500	25.52868300	35.33261800
N	20.00609100	23.45165400	33.17901100
C	20.04839700	22.65757500	34.30929000
N	18.78757300	22.66911600	34.92318800
C	17.94386000	23.47701800	34.17043400
C	16.61653300	23.89660300	34.36303800
O	15.80811800	23.63598000	35.27070200

N	16.22703900	24.76914300	33.30115400
C	17.04827100	25.18795300	32.28643900
N	16.52324600	26.12048800	31.42117500
N	18.29881300	24.80866900	32.14507600
C	18.74232400	23.92991500	33.10430800
O	21.03416200	22.06680600	34.79405300
N*	13.56106700	29.92297000	34.24623300
C*	14.57779500	28.98102100	33.82952000
C*	14.09287500	27.55491100	34.08730100
O*	14.09633100	26.72312100	33.16990400
C	15.96900600	29.13412700	34.52823700
C	16.95527900	27.99945300	34.19189100
C	18.35000700	28.14897600	34.82555100
C	19.15809000	26.87143900	34.58269700
N	20.54334200	26.92698700	35.18878200
H	15.80153500	29.16948700	35.61435200
H	16.38347700	30.10743600	34.23600600
H	17.05478800	27.90657500	33.10509900
H	16.53734800	27.04485000	34.53189900
H	18.87104500	29.01741700	34.40295800
H	18.24999000	28.31652400	35.90704000
H	19.28966700	26.65668600	33.52056300
H	18.65891000	26.00534800	35.02445500
H	21.15838600	27.50851900	34.61287800
H	20.51520200	27.36649600	36.11428600
H	14.71167000	29.05636000	32.74630000
H	13.78472000	30.84512400	33.88073500
H	13.56376700	30.01112700	35.26112900
C	23.54094200	23.78356000	36.64321100
H	23.74593700	25.86338300	37.23739300
H	21.67249600	24.57654400	38.50227200
H	21.50351600	26.26912300	37.99862700
H	20.66906600	23.76574100	36.40942600
H	19.62091700	25.13770800	36.79553300
H	21.01764900	25.02839100	34.38092300
H	18.53980700	22.12449400	35.73320600
H	16.97853400	26.16574300	30.52146100
H	15.52392500	26.26938800	31.43307100
H	15.27907200	25.13114800	33.36018500
H	23.83525000	23.35619800	37.60874900
H	22.79799500	23.13377200	36.16737900
H	24.42409000	23.82769200	35.99829100
H	13.75892200	27.29038000	35.10795900

OxoG (N3)

C	24.05553300	24.31705400	37.49517700
C*	22.98292000	25.18401200	36.84888200
O	22.61803100	24.62988100	35.55449500
C*	21.67606300	25.24699800	37.63913100
C	20.88936100	24.05514100	37.08006000
C	21.32418300	24.06495300	35.60828300
N	21.31928100	22.75462600	34.96964500
C	22.04759800	21.62970700	35.44941600
N	22.01041500	20.71686600	34.41823500
C	21.32069300	21.23880700	33.33043600
C	21.02511700	20.69059900	32.05294000
O	21.30930300	19.59625100	31.58391600
N	20.30213400	21.65172700	31.27156800
C	19.90445600	22.88582300	31.68481100
N	19.16479500	23.64419900	30.83308100
N	20.16871800	23.34862500	32.90419400
C	20.90635000	22.50408100	33.67646700
O	22.57299900	21.50482200	36.54460400
N*	13.56101400	29.92302100	34.24598800
C*	14.57800400	28.98098400	33.83008200
C*	14.09298600	27.55500400	34.08690000

O*	14.09601300	26.72298100	33.17001700
C	15.87353300	29.23333900	34.63998600
C	17.10037900	28.44216700	34.15391300
C	17.14051700	26.97923600	34.62222700
C	18.30238500	26.22623700	33.98756600
N	18.16890200	24.74447900	34.21466500
H	15.68146300	29.04190200	35.70346300
H	16.09347400	30.30402700	34.54931900
H	18.00770400	28.94664700	34.50546600
H	17.12902500	28.46935600	33.05658600
H	17.21763700	26.93646200	35.71528200
H	16.21997700	26.46411100	34.33803100
H	19.27367100	26.52578400	34.38819200
H	18.31437700	26.36410700	32.90400000
H	18.19174300	24.51666800	35.21249900
H	18.95439300	24.21172100	33.70939900
H	17.27080800	24.41101100	33.85334300
H	14.83144900	29.02140700	32.75813500
H	13.93802500	30.86716200	34.24187300
H	12.77855800	29.91123300	33.59768600
H	24.38548000	24.77269200	38.43581300
H	23.66751400	23.31367900	37.68783300
H	23.38002100	26.18601900	36.65317200
H	21.83985400	25.17782800	38.71756400
H	21.20496600	23.12141000	37.54553900
H	19.80465400	24.15643500	37.18362900
H	20.65008400	24.68141300	35.00169800
H	22.45240600	19.81161500	34.46663500
H	19.20937900	24.64391200	30.97153500
H	24.91937900	24.23067300	36.82822100
H	21.15017000	26.18534600	37.42997000
H	20.09500300	21.34781600	30.32653400
H	19.09248500	23.35525600	29.86764100
H	13.74060900	27.31992400	35.11009900

OxoG (N3) TS

C	24.07280500	24.35477500	37.51329700
C*	22.98286000	25.18403700	36.84884400
O	22.61618200	24.58660900	35.56944200
C*	21.67609800	25.24697100	37.63918700
C	20.92006100	24.01717300	37.12470400
C	21.32209100	24.03014300	35.64723300
N	21.30933700	22.71413800	35.01015600
C	22.13543200	21.62378400	35.41887300
N	22.04664500	20.71005400	34.38872400
C	21.21100000	21.18487500	33.38611500
C	20.80084900	20.61191000	32.14971700
O	21.09155800	19.53897400	31.64835900
N	19.92891700	21.52364100	31.44830700
C	19.48497100	22.71933300	31.89474100
N	18.60044200	23.42389200	31.17214800
N	19.89014800	23.20041200	33.08182000
C	20.77188000	22.42154300	33.78548900
O	22.76138000	21.53307000	36.45917300
N*	13.56098200	29.92295500	34.24605900
C*	14.57805500	28.98104100	33.82992000
C*	14.09301500	27.55498800	34.08699900
O*	14.09598900	26.72300900	33.16999200
C	15.87724300	29.24036700	34.63030500
C	17.09629900	28.43754100	34.14388200
C	17.16268800	26.99832400	34.67320600
C	18.28618900	26.19731800	34.01856100
N	18.22058800	24.74860400	34.35010100
H	15.69005600	29.05944000	35.69663600
H	16.09491200	30.31070500	34.52742000
H	18.01054800	28.96277800	34.44416400

H	17.09334300	28.41792900	33.04559800
H	17.29898100	27.00623600	35.76229600
H	16.22661100	26.47050000	34.46994400
H	19.27334100	26.56545700	34.31618200
H	18.21744900	26.28705300	32.92860300
H	18.31663300	24.62464600	35.35940400
H	19.17029500	23.95728300	33.65668300
H	17.28952100	24.39524600	34.12053200
H	14.82694200	29.02012300	32.75676500
H	13.93781100	30.86718300	34.23849100
H	12.77761100	29.90989900	33.59878500
H	24.40919100	24.85324000	38.42948400
H	23.70187400	23.35546600	37.75237700
H	23.36156900	26.18589200	36.62026100
H	21.84228000	25.22410500	38.71922200
H	21.28776900	23.10171700	37.59080100
H	19.83554300	24.07480000	37.25405100
H	20.63077400	24.64495300	35.05950200
H	22.52953900	19.82423300	34.39290900
H	18.46215500	24.40153000	31.38039800
H	24.92854100	24.25113300	36.83864000
H	21.12521500	26.16165800	37.39305100
H	19.62625700	21.19035600	30.53905900
H	18.32369600	23.10962700	30.25354100
H	13.73993400	27.31981700	35.10989900

OxoG (N3H)

C	24.07624900	24.36251000	37.51714900
C*	22.98283700	25.18392100	36.84883600
O	22.61525200	24.58077500	35.57238600
C*	21.67612900	25.24712500	37.63914800
C	20.92953500	24.00600600	37.13647900
C	21.32566600	24.01495600	35.65784800
N	21.32548900	22.69557500	35.02421600
C	22.18219500	21.62366200	35.42292900
N	22.12938900	20.72349700	34.37809600
C	21.28709700	21.18773600	33.37625400
C	20.91677800	20.62986400	32.12001500
O	21.25595500	19.58216200	31.59802500
N	20.02232800	21.52593100	31.42391400
C	19.52249600	22.69136700	31.88820400
N	18.62283800	23.37741200	31.17373400
N	19.90693800	23.16099900	33.08862200
C	20.80878000	22.40314000	33.79215300
O	22.80209800	21.53675300	36.46644500
N*	13.56102700	29.92307600	34.24589400
C*	14.57805600	28.98091600	33.83042400
C*	14.09287300	27.55504600	34.08662300
O*	14.09607800	26.72291600	33.17007600
C	15.87722900	29.23865900	34.63102200
C	17.09299700	28.42938500	34.14682800
C	17.16048600	26.99460100	34.68782800
C	18.27585600	26.18355500	34.03009800
N	18.22265500	24.74070300	34.37641900
H	15.68861900	29.06083000	35.69763600
H	16.09786600	30.30819500	34.52552200
H	18.00957900	28.95569600	34.43816200
H	17.08544200	28.40039700	33.04870200
H	17.30747300	27.01188200	35.77557000
H	16.22093900	26.46691900	34.49968400
H	19.26508200	26.56097400	34.31054600
H	18.19449800	26.26432400	32.93970500
H	18.33575400	24.62946700	35.38463400
H	19.22296500	23.89062200	33.63394400

H	17.28907100	24.38282100	34.16929800
H	14.82760700	29.02033300	32.75743100
H	13.93884100	30.86693500	34.24022000
H	12.77899000	29.91167600	33.59697300
H	24.41475700	24.87099700	38.42701900
H	23.70891000	23.36489000	37.76795200
H	23.35845900	26.18562100	36.61463200
H	21.84229400	25.23639200	38.71935600
H	21.30906400	23.09728500	37.60653800
H	19.84517200	24.05312900	37.27019700
H	20.62617700	24.62013300	35.07019800
H	22.63839500	19.85235000	34.37284400
H	18.39916200	24.32915600	31.42283700
H	24.92984800	24.25401900	36.84057800
H	21.11862100	26.15491800	37.38295900
H	19.75940400	21.21006700	30.49635600
H	18.29529300	23.03646700	30.28216800
H	13.73950900	27.32001200	35.10949500

OxoG (N9)

C	23.70573200	23.84637300	36.97473800
C*	22.98300700	25.18399700	36.84900700
O	22.62556000	25.42299400	35.47056800
C*	21.67599400	25.24700300	37.63899100
C	20.65376200	24.72290000	36.61320900
C	21.24783400	25.21398500	35.27872000
N	21.03368000	24.29976900	34.13594100
C	21.41026000	22.90758000	34.15087200
N	21.66722700	22.58640800	32.84194400
C	21.57035500	23.71536900	32.02982400
C	21.76337300	23.88899400	30.62834300
O	22.07213600	23.06308500	29.77730800
N	21.54261100	25.25511900	30.28064500
C	21.18378700	26.25538200	31.14472700
N	20.95886300	27.49045300	30.62986000
N	21.00041300	26.04969200	32.44131900
C	21.21412100	24.77496400	32.82430900
O	21.44598600	22.17141800	35.12320300
N*	13.56100100	29.92300700	34.24598700
C*	14.57798900	28.98099700	33.83002200
C*	14.09302000	27.55499500	34.08699300
O*	14.09598900	26.72300100	33.16999900
C	15.84025400	29.23787700	34.68772300
C	17.11035400	28.49335900	34.25706700
C	16.95108300	26.96446800	34.21536400
C	18.29354000	26.27517000	34.30250500
N	18.14619300	24.78819700	34.06520800
H	15.60194900	28.99626000	35.73166900
H	16.04344200	30.31534100	34.65538000
H	17.90722200	28.75944100	34.96331300
H	17.43443400	28.84291600	33.26935500
H	16.32510800	26.62719100	35.05138000
H	16.44470900	26.66993200	33.29300400
H	18.73040600	26.38539100	35.29483300
H	19.00662600	26.62617200	33.55425900
H	17.51408400	24.35756000	34.74649400
H	19.07582700	24.32913800	34.12774800
H	17.76312200	24.60831700	33.13270500
H	14.84836900	29.02467600	32.76236800
H	13.93701100	30.86733400	34.24005800
H	12.77465000	29.91070600	33.60206500
H	24.05941700	23.70795000	38.00272700
H	23.03640400	23.02266500	36.70945100
H	23.66048900	25.99648700	37.13273900
H	21.70835000	24.63945100	38.54621600
H	20.61597900	23.63465200	36.62263600

H	19.64749300	25.11637800	36.78373400
H	20.80714200	26.15795100	34.95010400
H	21.97067000	21.66833500	32.55289700
H	20.90305900	28.24048500	31.30405700
H	24.57017800	23.82250700	36.30323900
H	21.44536800	26.28079000	37.91618100
H	21.65813300	25.45713900	29.29358600
H	21.34444800	27.73412300	29.72912500
H	13.73023200	27.32394400	35.10732100

FapyG

C	23.63199500	23.61655400	36.75532400
C	22.96857500	24.99322300	36.80188900
O	22.34025100	25.31430700	35.54820300
C	21.82158700	25.08757400	37.81818700
C	20.64409700	24.49812200	37.02667400
C	20.98499100	24.83492300	35.55574200
H	24.16791400	23.42283000	37.69215100
H	22.89519000	22.82186000	36.60304200
H	23.72957600	25.76313900	36.97098500
H	22.02747400	24.54343500	38.74465700
H	20.59564200	23.41246600	37.15991900
H	19.67653000	24.91327800	37.31832800
H	20.37148100	25.63779900	35.14559600
H	24.34715000	23.57452200	35.92734700
H	21.63235500	26.13805500	38.06263400
N	20.81943500	24.94461900	32.79780200
C	20.83444800	23.70076800	33.36964500
C	20.85344300	22.53303700	32.59126600
C	20.77583600	22.63164000	31.16524600
N	20.75716700	23.94766900	30.67368500
C	20.77753800	25.03854800	31.49276400
N	20.80487800	21.18339000	33.03631100
C	21.24095200	20.57334700	34.15638800
N	20.80146600	23.66272600	34.72921300
O	21.72326100	21.10358500	35.16420700
O	20.70380400	21.67695200	30.37683800
N	20.70292600	26.26746100	30.90451700
H	20.91328100	27.03971800	31.52127500
H	21.03033100	26.36959800	29.95454700
H	20.67588900	24.04092400	29.66860200
H	20.53040200	20.56217500	32.27986700
H	21.10197400	19.48166500	34.09440600
H	21.11312800	22.77418400	35.13146100

FapyG (C1')

C*	22.98302500	25.18399400	36.84903100
O	22.61674800	24.50024200	35.63949500
C*	21.67597600	25.24700900	37.63895900
C	21.07546900	23.86252400	37.35303900
C	21.57415400	23.54603700	35.92789400
N	22.05068100	22.18203000	35.86267700
C	23.81259600	19.80708700	37.00991600
N	23.41122300	19.51251900	35.75710900
C	23.02189300	20.32468500	34.65643900
C	23.23038300	19.66938400	33.40161500
O	23.71869500	18.53946700	33.24651800
N	22.80102900	20.40511600	32.28401100
C	22.20464900	21.62763900	32.39438000
N	21.77896400	22.22473800	31.24315100
N	21.99141500	22.21218000	33.54552600
C	22.36776700	21.56681600	34.69274600
N*	13.56100400	29.92300800	34.24599000
C*	14.57799800	28.98098800	33.83001600

C*	14.09299400	27.55500200	34.08700300
O*	14.09600400	26.72299900	33.17000100
C	15.95564900	29.23023800	34.49624600
C	17.08719700	28.26931200	34.08935900
C	17.15540600	26.98912200	34.93197800
C	18.37259700	26.12116200	34.58986200
N	18.49710800	24.89099000	35.38171900
H	15.82412800	29.20823500	35.58809700
H	16.22729100	30.26148500	34.23714400
H	18.04693600	28.79263800	34.18575000
H	16.98143600	28.00523400	33.02819700
H	17.20196500	27.26086700	35.99687200
H	16.24859300	26.38678600	34.79670600
H	19.28926000	26.70900600	34.72927500
H	18.33530400	25.84191200	33.52935000
H	18.50734100	25.13999900	36.36919200
H	17.65766900	24.32867300	35.25083500
H	14.69774300	29.05029500	32.74383900
H	13.81579500	30.85125100	33.91640000
H	13.54683700	29.98435500	35.26337400
C	24.10873600	24.45256400	37.58237000
H	23.32967300	26.18001000	36.54974400
H	21.82544600	25.43981000	38.70581200
H	21.03415100	26.03198200	37.22337800
H	21.46120900	23.12396700	38.06394200
H	19.98541200	23.84069100	37.39413700
H	20.79216100	23.69060700	35.18395100
H	21.51795900	23.19518200	31.34888800
H	22.24438100	21.99245600	30.37741200
H	22.91097800	19.94847200	31.38695200
O	23.83166200	20.91804300	37.55264000
H	13.74490900	27.30428400	35.10961700
H	24.42615000	25.02648400	38.46138800
H	23.79248600	23.45713000	37.90888600
H	24.96813600	24.32906200	36.91553400
H	23.56638400	18.55163000	35.46437200
H	22.60100900	21.86226800	36.66390300
H	24.12678700	18.89887400	37.55020600

FapyG (C1') TS

C*	22.98300000	25.18400000	36.84900000
O	22.55680400	25.33487700	35.42953700
C*	21.67600000	25.24700000	37.63900000
C	20.61829200	24.80414800	36.61206200
C	21.27132700	25.18976700	35.32405700
N	20.95987600	22.96932500	34.21442600
C	20.54332400	20.70529600	36.57747000
N	19.57863500	20.70360500	35.63706100
C	18.93699100	21.83127300	35.04895900
C	17.52480600	21.74969100	35.03343800
O	16.81454600	20.83611000	35.49596000
N	16.89522400	22.84874700	34.39728200
C	17.60803600	23.87936100	33.85161200
N	16.87897000	24.95318500	33.39255000
N	18.90931500	23.91714300	33.79953200
C	19.65297800	22.85964800	34.35385500
O	21.13830400	21.69440000	37.01804300
N*	13.56100000	29.92300000	34.24600000
C*	14.57800000	28.98100000	33.83000000
C*	14.09300000	27.55500000	34.08700000
O*	14.09600000	26.72300000	33.17000000
C	15.93071200	29.20892200	34.54141900

C	17.03653200	28.24165500	34.12970500
C	18.33410500	28.45534700	34.91182600
C	19.31757500	27.31705600	34.64988200
N	20.54978500	27.36027900	35.44645500
H	15.76106300	29.12793200	35.62581800
H	16.23214800	30.24720200	34.34844000
H	17.22996500	28.33522200	33.05189500
H	16.70182700	27.21185800	34.29412100
H	18.78782000	29.42258200	34.65727600
H	18.10629800	28.48170600	35.98760700
H	19.60795600	27.29444100	33.59355900
H	18.82481400	26.35785200	34.84734100
H	21.20475700	28.05175600	35.09222600
H	20.34717000	27.59237600	36.41587500
H	14.71305100	29.05622100	32.74635800
H	13.79864300	30.84658900	33.89280700
H	13.56318300	30.00317400	35.26177900
C	23.73066000	23.86720700	36.96366500
H	23.64013100	26.03713400	37.03108300
H	21.70712900	24.58354700	38.50570700
H	21.48569600	26.26787100	37.98402700
H	20.50177600	23.71501700	36.62896400
H	19.63866300	25.26803200	36.73537400
H	20.82886400	25.22015000	34.34478300
H	19.09041100	19.82380900	35.51009300
H	17.38452300	25.55807400	32.76223800
H	15.89757800	24.84195700	33.17571700
H	15.88389000	22.83914800	34.39199400
H	24.14984400	23.78103300	37.97210100
H	23.04677100	23.03045500	36.79454700
H	24.55063300	23.82814500	36.23993200
H	13.74855300	27.30379200	35.11038800
H	21.42154000	22.22483400	34.73284100
H	20.79097900	19.68147500	36.91281900

FapyG (C1') P

C*	22.98294400	25.18408300	36.84887600
O	22.55913700	25.65499800	35.50699100
C*	21.67604400	25.24690800	37.63915600
C	20.63693500	24.82109200	36.59299900
C	21.18566300	25.48263500	35.33879900
N	20.62497500	22.82145300	33.94704400
C	20.49975600	20.57698300	36.38432400
N	19.43446100	20.58474300	35.55952400
C	18.72408400	21.72350200	35.07874800
C	17.32861500	21.64860000	35.24607600
O	16.66858100	20.73949200	35.79311200
N	16.62526500	22.75132500	34.68829100
C	17.26996600	23.76791000	34.04318500
N	16.48326700	24.83787500	33.65165700
N	18.55389000	23.81577700	33.84128300
C	19.36304900	22.74619300	34.28652500
O	21.12728900	21.56089000	36.78589400
N*	13.56099700	29.92298900	34.24601800
C*	14.57800200	28.98102200	33.82993100
C*	14.09304300	27.55499500	34.08702800
O*	14.09597000	26.72300500	33.16999100
C	15.97045100	29.15916800	34.52178700
C	16.98720800	28.06179600	34.15730100
C	18.36963000	28.18853800	34.83040700
C	19.15894800	26.89416200	34.60422900
N	20.54512300	26.91112500	35.20742300
H	15.81049000	29.16053600	35.60987200
H	16.35159400	30.15319400	34.25417200
H	17.11880700	28.03574600	33.06704400

H	16.57478900	27.08738300	34.43505100
H	18.91692500	29.05239200	34.43227200
H	18.23934100	28.34919600	35.90939600
H	19.29722900	26.67263200	33.54500600
H	18.64438300	26.03499600	35.03470800
H	21.17668900	27.48148700	34.63890700
H	20.52821100	27.34054900	36.13793900
H	14.70702600	29.05518100	32.74573800
H	13.79363700	30.84850700	33.89444900
H	13.55485000	30.00011500	35.26194700
C	23.59387700	23.79949700	36.72400500
H	23.72221000	25.91163600	37.19607700
H	21.68373300	24.58712200	38.51061400
H	21.49799400	26.27206700	37.98921100
H	20.64515400	23.73911600	36.44170700
H	19.61439800	25.13032600	36.82574100
H	20.94386100	24.95126800	34.41315400
H	18.94650700	19.70101500	35.46416300
H	16.89441200	25.38154200	32.90614500
H	15.48911100	24.69448400	33.52828200
H	15.61948500	22.73427000	34.78852500
H	23.99203700	23.48701600	37.69646900
H	22.84609100	23.06960700	36.40328200
H	24.41631100	23.82076800	36.00179400
H	13.75332300	27.30179100	35.11123100
H	21.12559500	22.03735800	34.36309800
H	20.79817700	19.54618900	36.65599000

FapyG (N3)

C	23.59954300	23.78547500	36.82036400
C*	22.98302500	25.18399200	36.84902800
O	22.61330500	25.62308900	35.52593000
C*	21.67598400	25.24700600	37.63896800
C	20.62508300	24.82874500	36.58984300
C	21.29260700	25.18077100	35.23711000
N	21.25898600	24.01411400	34.35550700
C	22.79923700	21.19408400	34.38401700
N	23.30502600	21.96008200	33.39133100
C	22.80148800	23.08832800	32.69792100
C	23.43595700	23.24898300	31.40925100
O	24.28560600	22.49355200	30.93640600
N	23.06106000	24.41074100	30.71232300
C	22.15926600	25.30766700	31.18827500
N	21.82858400	26.36317500	30.40648100
N	21.57127500	25.13835800	32.35689000
C	21.91612600	24.05682000	33.14384500
O	21.76659100	21.39403300	35.02916300
N*	13.56100200	29.92300400	34.24599700
C*	14.57799300	28.98099600	33.83000200
C*	14.09298800	27.55500500	34.08700300
O*	14.09600700	26.72299800	33.17000200
C	15.86218700	29.24785000	34.65810600
C	17.16368800	28.81423600	33.97728200
C	17.32651400	27.30031700	33.79073300
C	18.67666600	27.01687000	33.15109500
N	18.93777400	25.55310000	32.95928600
H	15.77030800	28.78429200	35.64937300
H	15.92143300	30.32908800	34.83186300
H	18.00633900	29.18737600	34.57293300
H	17.22844600	29.30303500	32.99611500
H	17.26392200	26.79582200	34.76451800
H	16.52659900	26.90320900	33.15881700
H	19.49640100	27.40036800	33.76352600
H	18.74562500	27.47349200	32.16069600
H	18.86051000	25.02888100	33.83557900
H	19.94993200	25.41530100	32.61882500

H	18.28122800	25.14076600	32.29273500
H	14.83141200	29.02369000	32.75736800
H	13.92049800	30.87143900	34.18327200
H	12.75134700	29.87119500	33.63309000
H	24.01534800	23.54086400	37.80422400
H	22.85302800	23.02600800	36.56764500
H	23.72096800	25.90708500	37.20980000
H	21.67957500	24.59002400	38.51268200
H	20.42332200	23.75475800	36.64169600
H	19.67385900	25.35198500	36.71830400
H	20.81509300	26.01656000	34.72009000
H	24.12344000	21.57924700	32.92342500
H	21.40427900	27.15718500	30.86367800
H	24.40310700	23.74188700	36.07833700
H	21.49096000	26.27217000	37.97417600
H	23.53273700	24.56102800	29.82791800
H	22.38787800	26.57057800	29.59170200
H	13.73105300	27.32255500	35.10710100
H	21.37464700	23.11164800	34.82650200
H	23.44521400	20.32561100	34.58462000

FapyG (N3) TS

C	23.68395800	23.82932200	36.93414600
C*	22.98284400	25.18403600	36.84880900
O	22.57418800	25.47885700	35.49402100
C*	21.67609300	25.24697500	37.63922900
C	20.66293500	24.63483800	36.65563000
C	21.27002900	24.95396800	35.27027400
N	21.29506600	23.74621300	34.44593600
C	23.15744500	21.13894900	34.42136100
N	23.47163800	21.90766100	33.35136000
C	22.75486100	22.91621900	32.66530600
C	23.22246500	23.08785600	31.30770000
O	24.10724700	22.42735800	30.77128900
N	22.63658100	24.16706500	30.60681700
C	21.68346400	24.96801900	31.12758500
N	21.13269200	25.93567600	30.37748100
N	21.25698900	24.77246500	32.37107200
C	21.80958300	23.78458800	33.18009800
O	22.16178500	21.23818500	35.14074300
N*	13.56095400	29.92290800	34.24609500
C*	14.57809300	28.98108400	33.82985700
C*	14.09307300	27.55497800	34.08702600
O*	14.09594400	26.72301800	33.16998400
C	15.86664900	29.24679400	34.65044700
C	17.16403700	28.78842200	33.97521800
C	17.27756800	27.27598000	33.75456600
C	18.66065500	26.90748300	33.22931200
N	18.84275700	25.44836400	33.00912100
H	15.77152400	28.79375000	35.64640100
H	15.93500500	30.32958400	34.81283600
H	18.00786000	29.12137700	34.59336500
H	17.26137200	29.29845800	33.00750800
H	17.09982900	26.74625100	34.70118700
H	16.51594700	26.93595000	33.04628700
H	19.43608100	27.23407100	33.92993200
H	18.84823000	27.40892000	32.27287700
H	18.62209900	24.93372900	33.86342400
H	20.11423200	25.13650600	32.67159300
H	18.18637500	25.11566600	32.30115500
H	14.82772900	29.02311800	32.75626600
H	13.92241000	30.87095600	34.18888500
H	12.75403000	29.87492700	33.62935900
H	24.09428900	23.68369400	37.93968600
H	22.99448600	23.00574700	36.72284900
H	23.67784900	25.98010400	37.13283900

H	21.72627900	24.70092400	38.58511100
H	20.58996200	23.55173500	36.79161400
H	19.65882200	25.05241800	36.76418800
H	20.72164400	25.72835500	34.73091300
H	24.29372800	21.61346200	32.83152200
H	20.60814100	26.66894200	30.83030200
H	24.50499500	23.78438700	36.21130800
H	21.42024600	26.28997300	37.85041200
H	23.00918200	24.33406600	29.67844500
H	21.45749500	26.11235300	29.43873200
H	13.73193700	27.32223900	35.10740400
H	21.54181000	22.88170200	34.93854000
H	23.93077900	20.37798300	34.60510900

FapyG (N3H)

C	23.73769400	23.86602900	37.01248500
C*	22.98291700	25.18402500	36.84891400
O	22.55699800	25.37782500	35.47989000
C*	21.67605200	25.24698200	37.63910000
C	20.69417600	24.51743400	36.70554600
C	21.27540500	24.78690300	35.29951100
N	21.35390700	23.53648200	34.54232300
C	23.30703800	21.00030500	34.57519300
N	23.54464000	21.71247300	33.44686000
C	22.76120000	22.65561800	32.74217600
C	23.15264800	22.76301600	31.35370100
O	24.02973000	22.10177700	30.80931900
N	22.49473000	23.78098500	30.61795100
C	21.54356300	24.58180500	31.13220100
N	20.92646300	25.49321100	30.37533200
N	21.19854000	24.43813900	32.41264200
C	21.81120000	23.51561300	33.26101100
O	22.34372400	21.11274900	35.33485900
N*	13.56099600	29.92297900	34.24603800
C*	14.57803600	28.98100400	33.82989700
C*	14.09297900	27.55495800	34.08709800
O*	14.09602000	26.72305200	33.16995300
C	15.86275400	29.24522500	34.65727000
C	17.16292100	28.75517900	34.00962300
C	17.25167900	27.23928100	33.80510400
C	18.64092900	26.82102200	33.33160200
N	18.77681000	25.36636700	33.08609500
H	15.74795700	28.81194900	35.65999400
H	15.94262600	30.33020000	34.80014200
H	18.00128000	29.07940900	34.64007300
H	17.28878600	29.25359700	33.03901300
H	17.02251700	26.72015800	34.74682800
H	16.50911200	26.91174600	33.07116000
H	19.39671800	27.11020700	34.07065600
H	18.88800200	27.34289800	32.39856500
H	18.50949600	24.85310100	33.92637700
H	20.22712400	24.86730700	32.72232900
H	18.11184900	25.07771600	32.36851600
H	14.83140400	29.02363800	32.75734900
H	13.92453900	30.87055700	34.19431800
H	12.75639200	29.87931800	33.62593800
H	24.14847800	23.79365700	38.02569100
H	23.08384700	23.00410800	36.84506400
H	23.64692700	26.02302900	37.07791100
H	21.75137300	24.77446300	38.62214000
H	20.68862900	23.44224800	36.90846300
H	19.66725200	24.87937200	36.79592900
H	20.68418400	25.50228100	34.72655300
H	24.35245400	21.41514200	32.90681000
H	20.31094500	26.16919500	30.80209200
H	24.56376100	23.81404300	36.29584100

H	21.37338400	26.29013600	37.77313600
H	22.80116400	23.88899500	29.65699000
H	21.16130800	25.61457500	29.40204700
H	13.73274300	27.32217200	35.10779300
H	21.65027200	22.71038700	35.07356400
H	24.11230100	20.27530700	34.76518800

FapyG (N9)

C	23.46584600	23.75420800	36.60609800
C*	22.98299200	25.18400500	36.84899000
O	22.69603800	25.85520800	35.61007000
C*	21.67600500	25.24699500	37.63901300
C	20.61805900	25.11332700	36.52418300
C	21.34543300	25.63732300	35.26043200
N*	13.56099900	29.92299700	34.24600400
C*	14.57800300	28.98100300	33.82998800
C*	14.09300100	27.55499700	34.08700900
O*	14.09600000	26.72300400	33.16999600
C	15.83905100	29.24225500	34.68509100
C	17.12966200	28.62349300	34.14523500
C	17.06835700	27.10002000	33.95012800
C	18.47254900	26.53766500	33.95813700
N	18.51637100	25.06781800	33.65705300
H	15.65112100	28.89228300	35.70886300
H	15.97792400	30.32848700	34.75025600
H	17.93675300	28.86742000	34.84844000
H	17.39388600	29.09208600	33.18941800
H	16.49768900	26.63485700	34.76417000
H	16.55191300	26.85474700	33.01786700
H	18.91064200	26.65907100	34.94822400
H	19.13501000	27.00471000	33.22778000
H	17.89961800	24.54024900	34.27907200
H	19.53364200	24.74022900	33.79818000
H	18.22306000	24.88087400	32.69565600
H	14.84509100	29.02607600	32.76125500
H	13.92749100	30.87005100	34.20490600
H	12.75968800	29.88744000	33.62115200
H	23.82949600	23.31875500	37.54330500
H	22.66054400	23.11844300	36.22524400
H	23.78007100	25.76288900	37.32573000
H	21.59938200	24.45574700	38.38872400
H	20.32829400	24.06692500	36.38155200
H	19.71053300	25.68342400	36.74077000
H	20.96949800	26.58893300	34.88511800
H	24.28140600	23.75107800	35.87597400
H	21.58192000	26.21585300	38.13829300
H	13.73319800	27.32359400	35.10812900
N	21.35458700	26.13184000	32.38106900
C	21.83025200	24.98295700	32.94712400
C	22.80920100	24.20109700	32.36514100
C	23.40746700	24.64460800	31.12078800
N	22.87806000	25.84093100	30.62268000
C	21.88984900	26.54219600	31.25166000
N	23.41797000	23.02288700	32.85843100
C	22.92470600	22.01278800	33.61060400
N	21.19152000	24.65915600	34.16072000
O	21.82690700	21.98293500	34.17310700
O	24.32807400	24.07327200	30.53600000
N	21.42708900	27.66518700	30.64986400
H	20.84447200	28.26394300	31.21641300
H	21.97830700	28.12178800	29.93796900
H	23.28348000	26.16572400	29.75206700
H	24.29533100	22.82776400	32.38326500
H	23.64176800	21.18210400	33.69160700
H	21.40065400	23.69395500	34.44028200

FapyG (N9) TS

C	23.63206300	23.80324900	36.88347500
C*	22.98300000	25.18400000	36.84900000
O	22.64727000	25.53548800	35.48764200
C*	21.67600000	25.24700000	37.63900000
C	20.63502800	24.87262900	36.56910600
C	21.26939400	25.41418000	35.27690400
N*	13.56100000	29.92300000	34.24600000
C*	14.57800000	28.98100000	33.83000000
C*	14.09300000	27.55500000	34.08700000
O*	14.09600000	26.72300000	33.17000000
C	15.83763000	29.24130600	34.68650800
C	17.11620000	28.55600800	34.19945700
C	17.02218100	27.02570800	34.09592400
C	18.40664100	26.41047600	34.15055800
N	18.44363500	24.94657200	33.89902200
H	15.62211500	28.94447200	35.72151800
H	16.00583200	30.32563100	34.70324600
H	17.92191600	28.82177900	34.89679600
H	17.40401000	28.96182300	33.22125600
H	16.42338400	26.62389600	34.92432800
H	16.51635500	26.73587100	33.17106900
H	18.82941800	26.58052400	35.14357200
H	19.08064200	26.86038000	33.41686900
H	17.85297500	24.44959500	34.56656500
H	19.74934400	24.58038300	33.98149800
H	18.07497400	24.74574600	32.96905500
H	14.84700200	29.02537700	32.76191800
H	13.93237800	30.86876300	34.21831100
H	12.76600100	29.89761600	33.61275000
H	24.02210200	23.59850200	37.88640500
H	22.90593900	23.02623500	36.62413600
H	23.70010100	25.93760200	37.18920800
H	21.67119000	24.56096800	38.48883000
H	20.53194100	23.78458500	36.49640000
H	19.64545700	25.29592100	36.75558500
H	20.87801300	26.38260100	34.95927500
H	24.46019200	23.75765300	36.16899700
H	21.49473300	26.26202800	38.00552700
H	13.73372800	27.32345600	35.10832900
N	21.05906000	25.81757200	32.24734600
C	21.66454200	24.80959300	32.92483600
C	22.81529000	24.17553500	32.51683400
C	23.46627800	24.65597500	31.30595000
N	22.79128300	25.70008300	30.66898400
C	21.62505100	26.24149400	31.13395100
N	23.54055300	23.13368000	33.12928800
C	23.15188900	22.15019600	33.96917400
N	20.98141500	24.47015200	34.14348700
O	22.03338000	22.01753200	34.47818900
O	24.52867600	24.22272100	30.86542900
N	21.04191700	27.21334300	30.40613700
H	20.24180200	27.68116100	30.80330500
H	21.51388500	27.65076800	29.63004100
H	23.22695400	26.04464900	29.82044200
H	24.46989000	23.03599300	32.72748300
H	23.96695700	21.44421400	34.17808900
H	21.24502900	23.49709500	34.41411900

FapyG (N9H)

C	23.65143500	23.81410700	36.90677700
C*	22.98302100	25.18399200	36.84902200
O	22.63857000	25.50633000	35.47975400

C*	21.67598400	25.24700800	37.63897300
C	20.63824500	24.83860800	36.57760300
C	21.26524700	25.37375800	35.28085600
N*	13.56100100	29.92300400	34.24599300
C*	14.57799800	28.98099500	33.83000900
C*	14.09299200	27.55500200	34.08700300
O*	14.09600400	26.72300000	33.17000000
C	15.83890800	29.24103000	34.68571000
C	17.11575600	28.54449700	34.20736500
C	17.01060600	27.01516200	34.10982900
C	18.38348100	26.37030600	34.17112000
N	18.39515800	24.90957800	33.93281500
H	15.61941100	28.95242800	35.72226000
H	16.01127300	30.32494300	34.69509700
H	17.92001400	28.80729600	34.90778900
H	17.41137000	28.94550300	33.22928000
H	16.40228800	26.62271400	34.93632600
H	16.50567000	26.72641900	33.18414700
H	18.80699900	26.54940100	35.16393800
H	19.06392100	26.81175400	33.43646100
H	17.79351900	24.43484200	34.60410400
H	19.87649200	24.48085500	33.99629200
H	18.01376600	24.71267300	33.00874600
H	14.84654300	29.02510200	32.76182100
H	13.93343900	30.86845700	34.22104300
H	12.76755100	29.89977000	33.61071600
H	24.04974400	23.63624100	37.91144300
H	22.93581600	23.02115100	36.66797100
H	23.69026300	25.95451300	37.17043200
H	21.68017300	24.57724000	38.50160700
H	20.55414700	23.74807600	36.52120500
H	19.64202800	25.24822700	36.75638700
H	20.85531100	26.32640100	34.94156600
H	24.47696100	23.76677700	36.18939200
H	21.48263600	26.26648200	37.98587300
H	13.73415500	27.32334800	35.10847500
N	21.06828900	25.74603600	32.24526300
C	21.68189400	24.74940900	32.92543900
C	22.84648300	24.13035000	32.53949400
C	23.50264100	24.61759400	31.33212400
N	22.81817300	25.64823100	30.68463400
C	21.63927300	26.17540400	31.13562300
N	23.57498200	23.09507700	33.15658100
C	23.19093800	22.12508500	34.01275500
N	20.99393300	24.40607200	34.14898700
O	22.07359200	22.00377000	34.52986200
O	24.57342300	24.19457500	30.90421800
N	21.05217200	27.13970700	30.40408100
H	20.23156500	27.58568800	30.78450500
H	21.52051300	27.57951000	29.62723900
H	23.25480700	25.99248300	29.83620900
H	24.50388800	22.99657900	32.75324900
H	24.00306800	21.41889900	34.22830900
H	21.27252900	23.43234400	34.42872600

* The atoms indicated by star were fixed during geometry optimizations. The initial geometries were derived from the 1N3C PDB x-ray structure.