Essential Reactive Intermediates In Nucleoside Chemistry: Cyclonucleoside Cations

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SUPPLEMENTARY INFORMATION

Content

Computations (general methodology)

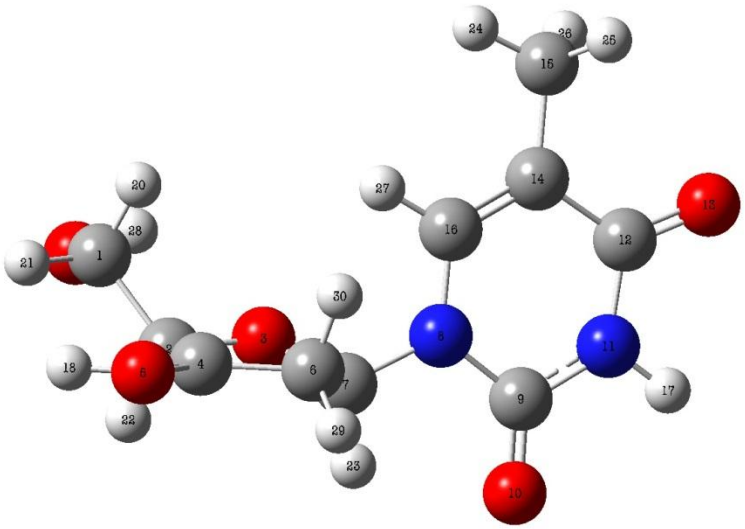
Methods. Theoretical calculations performed are based on DFT (density functional theory) – they have used hybrid functional B3LYP that has shown trustworthy results also in modeling carbocations (see, *e.g.*, M. R. Siebert and D. J. Tantillo *J. Phys. Org. Chem.*, 2007; **20**, 384–394; Y. J. Hong and D. J. Tantillo *Chem. Commun*., 2012, **48**, 1571–1573). Among basis function sets, the 6-31+G(d,p) set (for common basis sets, see D. Feller and E. R. Davidson In: *Reviews In Computational. Chemistry*, 1990, VCH Publishers, New York, pp. 1-43) has been chosen as a set that, in combination with B3LYP, provides accurate parameters of molecular geometry as well as sufficiently accurate values of molecular energy for single organic molecules, which are composed of atoms of the elements of the first three rows. A low computational cost, but successful model of solvation, PCM (polarized continuum model), which is an implicit model (a model that represents the solution as a non-structured bulk), has been employed in order quantitatively to take into account solvation effects of water. Bond orders have been calculated within the limits of the NBO (natural bond orbital) approach that, by relating purposefully designed orbitals (natural orbitals) to individual atoms as well as atom pairs, permits to characterize chemical functionality in terms of Lewis structures (see Ref. 8 for the basics of this description of molecular structures). Technically, our calculations that combine all these methods, have been performed using the Gaussian09 calculation package.

Procedural details.

a) *Location of energy minima*. In order to locate cyclonucleoside as well as "open cycle" nucleoside cations of rotational orientation *syn*, initial molecular structures of *syn*-shaped 2'- and 3'-dehydro nucleosides of arbitrary twist or envelope geometry of the sugar ring, which have interatomic distances C2′⋯2-O (for $\mathbf{5}_{iso}$ and $\mathbf{6}_{iso}$) or C3′⋯2-O (for $\mathbf{3}_{syn}$, $\mathbf{3}_{iso}$, $\mathbf{4}_{iso}$, $\mathbf{12}_{syn}$ and $\mathbf{12}_{iso}$) of 0.15, 0.20, 0.25 and 0.30 nm, were used in geometry optimization that has been performed at the B3LYP/6-31+G(d,p) level, for water solution in the PCM approximation [Gaussian option SCRF=(PCM, Solvent=water)]. In locating cations $\mathbf{3}_{anti}$ and $\mathbf{12}_{anti}$, initial structures of *anti* orientation of the nucleobase were subjected to energy minimization at the same theory level. Combination of linear minimization and the Newton-Raphson algorithm (Gaussian option SCF=XQC) was employed in order to overcome convergence problems in energy minimization.

b) *Structure analysis*. For optimized cationic structures, highly delocalized structure option (Gaussian keyword Resonance) was used in NBO calculations [Gaussian command Pop=(NBOread, saveNBOs) of molecular orbitals. Calculated LUMOs (lowest unoccupied molecular orbitals; here, among NBOs) were visualized by means of the GaussVIew5 program. Wiberg coefficients (bond order equivalents) were calculated in the natural atom orbital basis (Gaussian keyword BNDIDX). According to these coefficient values, the obtained structures have been assigned to isouronium (Figs. 1 and 2 in the main text), guanidinium (Fig. 1) or ammidinium (Fig. 2) cations.

2. Cation 3_{anti} (oxacarbenium ion)



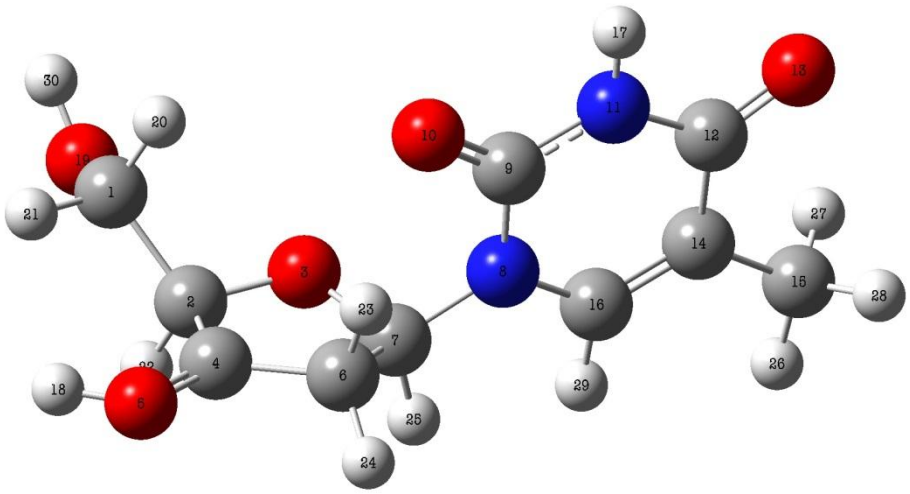
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-3.371297	1.425532	-0.453945
2	6	0	-2.776421	-0.009097	-0.414696
3	8	0	-1.411841	0.037107	-0.820186
4	6	0	-2.736185	-0.685252	0.918631
5	8	0	-3.706723	-0.904339	1.704745
6	6	0	-1.369311	-1.125864	1.234808
7	6	0	-0.659760	-0.979290	-0.131739
8	7	0	0.725534	-0.569035	-0.080566
9	6	0	1.687047	-1.449930	-0.585153
10	8	0	1.417477	-2.553455	-1.049063
11	7	0	2.975804	-0.970787	-0.506138
12	6	0	3.411104	0.260638	-0.003690
13	8	0	4.611703	0.532901	-0.003861
14	6	0	2.346832	1.134561	0.484550
15	6	0	2.711078	2.488922	1.021305
16	6	0	1.074197	0.681344	0.418605
17	1	0	3.693187	-1.596680	-0.858298
18	1	0	-4.580491	-0.573719	1.407664
19	8	0	-3.357044	1.914118	-1.775201
20	1	0	-2.803163	2.067557	0.227463
21	1	0	-4.416043	1.396068	-0.136303
22	1	0	-3.369510	-0.652181	-1.089319
23	1	0	-0.686828	-1.920138	-0.682979
24	1	0	1.819649	3.033219	1.341082
25	1	0	3.389316	2.399083	1.876337
26	1	0	3.227730	3.083674	0.260744
27	1	0	0.239495	1.294988	0.734331
28	1	0	-2.448664	2.146225	-2.017930
29	1	0	-1.338961	-2.128081	1.670588
30	1	0	-0.967357	-0.431310	1.990030

ENERGY (a.u):

HF=-=-874.396164

3. Cation 3_{syn} (oxacarbenium ion)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.395547	1.328347	0.206562
2	6	0	2.716473	0.019660	0.639803
3	8	0	1.335230	0.220558	0.908613
4	6	0	2.742008	-1.086164	-0.369547
5	8	0	3.762320	-1.584688	-0.935343
6	6	0	1.393128	-1.580656	-0.641014
7	6	0	0.559514	-0.909697	0.472328
8	7	0	-0.764065	-0.453088	0.094510
9	6	0	-0.923459	0.373255	-1.019481
10	8	0	0.002566	0.683859	-1.766071
11	7	0	-2.213837	0.805389	-1.222910
12	6	0	-3.350120	0.527096	-0.453650
13	8	0	-4.439775	1.000262	-0.776665
14	6	0	-3.107883	-0.334108	0.699566
15	6	0	-4.262520	-0.697631	1.588866
16	6	0	-1.845125	-0.767992	0.914578
17	1	0	-2.347316	1.402687	-2.033000
18	1	0	4.619956	-1.172472	-0.699297
19	8	0	3.464719	2.143573	1.362863
20	1	0	2.798168	1.789237	-0.586919
21	1	0	4.399573	1.107236	-0.181140
22	1	0	3.241391	-0.360211	1.536975
23	1	0	1.116846	-1.180299	-1.631027
24	1	0	1.335435	-2.671284	-0.679380
25	1	0	0.423538	-1.603855	1.304532
26	1	0	-3.935909	-1.347285	2.404062
27	1	0	-4.720231	0.198754	2.020231

28	1	0	-5.041725	-1.217153	1.021259
29	1	0	-1.602376	-1.405367	1.756426
30	1	0	3.652110	3.052740	1.090839

ENERGY (a.u):

HF=-874.3942935

Wiberg bond index matrix in the NAO basis:

Atom	1	2	3	4	5	6	7	8	9
1. C	0.0000	0.9693	0.0216	0.0198	0.0097	0.0050	0.0060	0.0004	0.0003
2. C	0.9693	0.0000	0.9160	1.0342	0.0364	0.0085	0.0079	0.0079	0.0005
3. O	0.0216	0.9160	0.0000	0.0272	0.0089	0.0211	0.8919	0.0338	0.0047
4. C	0.0198	1.0342	0.0272	0.0000	1.4382	1.0945	0.0139	0.0055	0.0006
5. O	0.0097	0.0364	0.0089	1.4382	0.0000	0.0342	0.0084	0.0008	0.0002
6. C	0.0050	0.0085	0.0211	1.0945	0.0342	0.0000	0.9766	0.0106	0.0029
7. C	0.0060	0.0079	0.8919	0.0139	0.0084	0.9766	0.0000	0.9578	0.0093
8. N	0.0004	0.0079	0.0338	0.0055	0.0008	0.0106	0.9578	0.0000	1.0442
9. C	0.0003	0.0005	0.0047	0.0006	0.0002	0.0029	0.0093	1.0442	0.0000
10. O	0.0008	0.0010	0.0038	0.0056	0.0017	0.0080	0.0061	0.1140	1.5957
11. N	0.0001	0.0003	0.0013	0.0006	0.0001	0.0010	0.0090	0.0154	1.1306
12. C	0.0000	0.0002	0.0011	0.0001	0.0000	0.0005	0.0006	0.0216	0.0082
13. O	0.0000	0.0003	0.0016	0.0002	0.0001	0.0008	0.0012	0.0259	0.0142
14. C	0.0000	0.0007	0.0029	0.0006	0.0002	0.0013	0.0082	0.0499	0.0250
15. C	0.0000	0.0000	0.0002	0.0000	0.0000	0.0002	0.0004	0.0094	0.0011
16. C	0.0001	0.0005	0.0055	0.0004	0.0002	0.0058	0.0111	1.0855	0.0128
17. H	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0006	0.0100	0.0022
18. H	0.0014	0.0019	0.0006	0.0045	0.6304	0.0179	0.0010	0.0005	0.0001
19. O	0.9518	0.0184	0.0038	0.0113	0.0023	0.0007	0.0006	0.0001	0.0001
20. H	0.8985	0.0025	0.0031	0.0013	0.0006	0.0002	0.0001	0.0002	0.0001
21. H	0.9003	0.0042	0.0092	0.0010	0.0007	0.0007	0.0006	0.0002	0.0001
22. H	0.0042	0.8176	0.0234	0.0191	0.0111	0.0046	0.0013	0.0005	0.0000
23. H	0.0017	0.0032	0.0003	0.0251	0.0149	0.7913	0.0033	0.0025	0.0008

24.	H	0.0004	0.0071	0.0062	0.0117	0.0070	0.8438	0.0025
0.0008	0.0001							
25.	H	0.0007	0.0011	0.0214	0.0009	0.0004	0.0025	0.8778
0.0013	0.0068							
26.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0004	0.0000							
27.	H	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0002
0.0018	0.0010							
28.	H	0.0000	0.0000	0.0001	0.0000	0.0000	0.0001	0.0002
0.0018	0.0010							
29.	H	0.0000	0.0001	0.0004	0.0000	0.0000	0.0002	0.0008
0.0015	0.0066							
30.	H	0.0011	0.0087	0.0002	0.0010	0.0002	0.0003	0.0001
0.0000	0.0000							

Atom	10	11	12	13	14	15	16	17	18
1.	C	0.0008	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0014
2.	C	0.0010	0.0003	0.0002	0.0003	0.0007	0.0000	0.0005	0.0000	0.0019
3.	O	0.0038	0.0013	0.0011	0.0016	0.0029	0.0002	0.0055	0.0001	0.0006
4.	C	0.0056	0.0006	0.0001	0.0002	0.0006	0.0000	0.0004	0.0000	0.0045
5.	O	0.0017	0.0001	0.0000	0.0001	0.0002	0.0000	0.0002	0.0000	0.6304
6.	C	0.0080	0.0010	0.0005	0.0008	0.0013	0.0002	0.0058	0.0000	0.0179
7.	C	0.0061	0.0090	0.0006	0.0012	0.0082	0.0004	0.0111	0.0006	0.0010
8.	N	0.1140	0.0154	0.0216	0.0259	0.0499	0.0094	1.0855	0.0100	0.0005
9.	C	1.5957	1.1306	0.0082	0.0142	0.0250	0.0011	0.0128	0.0022	0.0001
10.	O	0.0000	0.1258	0.0132	0.0079	0.0239	0.0006	0.0098	0.0033	0.0001
11.	N	0.1258	0.0000	1.0652	0.1279	0.0057	0.0079	0.0214	0.7381	0.0000
12.	C	0.0132	1.0652	0.0000	1.6306	1.0820	0.0098	0.0319	0.0038	0.0000
13.	O	0.0079	0.1279	1.6306	0.0000	0.0666	0.0052	0.0587	0.0045	0.0000
14.	C	0.0239	0.0057	1.0820	0.0666	0.0000	1.0298	1.6756	0.0112	0.0001
15.	C	0.0006	0.0079	0.0098	0.0052	1.0298	0.0000	0.0187	0.0005	0.0000
16.	C	0.0098	0.0214	0.0319	0.0587	1.6756	0.0187	0.0000	0.0003	0.0000
17.	H	0.0033	0.7381	0.0038	0.0045	0.0112	0.0005	0.0003	0.0000	0.0000
18.	H	0.0001	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
19.	O	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0014
20.	H	0.0012	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0001
21.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0018

22.	H	0.0003	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000	0.0003
23.	H	0.0152	0.0011	0.0000	0.0001	0.0003	0.0000	0.0002	0.0001	0.0000
24.	H	0.0009	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
25.	H	0.0003	0.0002	0.0001	0.0000	0.0005	0.0000	0.0009	0.0004	0.0001
26.	H	0.0000	0.0001	0.0082	0.0009	0.0017	0.9192	0.0011	0.0004	0.0000
27.	H	0.0010	0.0002	0.0017	0.0013	0.0021	0.9030	0.0172	0.0000	0.0000
28.	H	0.0010	0.0002	0.0017	0.0013	0.0020	0.9030	0.0171	0.0000	0.0000
29.	H	0.0016	0.0002	0.0100	0.0016	0.0071	0.0017	0.8931	0.0006	0.0000
30.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom		19	20	21	22	23	24	25	26	27
1.	C	0.9518	0.8985	0.9003	0.0042	0.0017	0.0004	0.0007	0.0000	0.0000
2.	C	0.0184	0.0025	0.0042	0.8176	0.0032	0.0071	0.0011	0.0000	0.0000
3.	O	0.0038	0.0031	0.0092	0.0234	0.0003	0.0062	0.0214	0.0000	0.0001
4.	C	0.0113	0.0013	0.0010	0.0191	0.0251	0.0117	0.0009	0.0000	0.0000
5.	O	0.0023	0.0006	0.0007	0.0111	0.0149	0.0070	0.0004	0.0000	0.0000
6.	C	0.0007	0.0002	0.0007	0.0046	0.7913	0.8438	0.0025	0.0000	0.0000
7.	C	0.0006	0.0001	0.0006	0.0013	0.0033	0.0025	0.8778	0.0000	0.0002
8.	N	0.0001	0.0002	0.0002	0.0005	0.0025	0.0008	0.0013	0.0004	0.0018
9.	C	0.0001	0.0001	0.0001	0.0000	0.0008	0.0001	0.0068	0.0000	0.0010
10.	O	0.0003	0.0012	0.0000	0.0003	0.0152	0.0009	0.0003	0.0000	0.0010
11.	N	0.0000	0.0001	0.0000	0.0000	0.0011	0.0001	0.0002	0.0001	0.0002
12.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0082	0.0017
13.	O	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0009	0.0013
14.	C	0.0000	0.0001	0.0000	0.0001	0.0003	0.0000	0.0005	0.0017	0.0021
15.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9192	0.9030
16.	C	0.0000	0.0000	0.0000	0.0001	0.0002	0.0001	0.0009	0.0011	0.0172
17.	H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0004	0.0004	0.0000
18.	H	0.0014	0.0001	0.0018	0.0003	0.0000	0.0000	0.0001	0.0000	0.0000
19.	O	0.0000	0.0208	0.0285	0.0052	0.0004	0.0001	0.0000	0.0000	0.0000

20.	H	0.0208	0.0000	0.0003	0.0091	0.0002	0.0000	0.0000	0.0000
0.0000									
21.	H	0.0285	0.0003	0.0000	0.0001	0.0000	0.0001	0.0001	0.0000
0.0000									
22.	H	0.0052	0.0091	0.0001	0.0000	0.0013	0.0007	0.0017	0.0000
0.0000									
23.	H	0.0004	0.0002	0.0000	0.0013	0.0000	0.0042	0.0051	0.0000
0.0000									
24.	H	0.0001	0.0000	0.0001	0.0007	0.0042	0.0000	0.0006	0.0000
0.0000									
25.	H	0.0000	0.0000	0.0001	0.0017	0.0051	0.0006	0.0000	0.0000
0.0000									
26.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000									
27.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0007									
28.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0007									
29.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0019	0.0000
0.0005									
30.	H	0.7036	0.0005	0.0000	0.0003	0.0001	0.0000	0.0000	0.0000
0.0000									

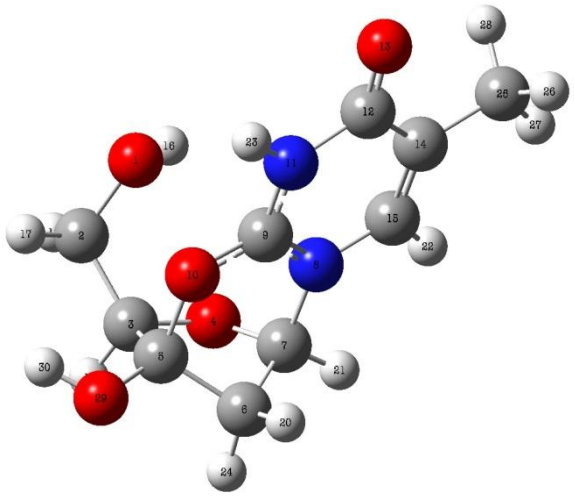
Atom		28	29	30
1.	C	0.0000	0.0000	0.0011
2.	C	0.0000	0.0001	0.0087
3.	O	0.0001	0.0004	0.0002
4.	C	0.0000	0.0000	0.0010
5.	O	0.0000	0.0000	0.0002
6.	C	0.0001	0.0002	0.0003
7.	C	0.0002	0.0008	0.0001
8.	N	0.0018	0.0015	0.0000
9.	C	0.0010	0.0066	0.0000
10.	O	0.0010	0.0016	0.0000
11.	N	0.0002	0.0002	0.0000
12.	C	0.0017	0.0100	0.0000
13.	O	0.0013	0.0016	0.0000
14.	C	0.0020	0.0071	0.0000
15.	C	0.9030	0.0017	0.0000
16.	C	0.0171	0.8931	0.0000
17.	H	0.0000	0.0006	0.0000
18.	H	0.0000	0.0000	0.0000
19.	O	0.0000	0.0000	0.7036
20.	H	0.0000	0.0000	0.0005
21.	H	0.0000	0.0000	0.0000
22.	H	0.0000	0.0000	0.0003
23.	H	0.0000	0.0000	0.0001
24.	H	0.0000	0.0000	0.0000
25.	H	0.0000	0.0019	0.0000
26.	H	0.0007	0.0005	0.0000
27.	H	0.0006	0.0001	0.0000
28.	H	0.0000	0.0001	0.0000
29.	H	0.0001	0.0000	0.0000
30.	H	0.0000	0.0000	0.0000

Wiberg bond index, Totals by atom:

Atom		1
1.	C	3.7934

2.	C	3.8481
3.	O	2.0104
4.	C	3.7176
5.	O	2.2067
6.	C	3.8333
7.	C	3.7974
8.	N	3.4042
9.	C	3.8690
10.	O	1.9432
11.	N	3.2526
12.	C	3.8908
13.	O	1.9508
14.	C	3.9976
15.	C	3.8107
16.	C	3.8681
17.	H	0.7762
18.	H	0.6624
19.	O	1.7494
20.	H	0.9392
21.	H	0.9480
22.	H	0.9012
23.	H	0.8714
24.	H	0.8866
25.	H	0.9250
26.	H	0.9341
27.	H	0.9310
28.	H	0.9310
29.	H	0.9283
30.	H	0.7162

4. Cation 3_{iso} (isouronium ion)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.817891	-1.204087	1.946877

2	6	0	-2.192817	-0.878102	1.778122
3	6	0	-2.431720	0.217261	0.734038
4	8	0	-1.567472	1.355574	1.010751
5	6	0	-2.169558	-0.084269	-0.761349
6	6	0	-1.753236	1.267262	-1.311933
7	6	0	-0.848439	1.676510	-0.157050
8	7	0	0.391114	0.828807	-0.228200
9	6	0	0.238284	-0.460457	-0.566808
10	8	0	-0.921013	-0.974811	-0.869968
11	7	0	1.312344	-1.252171	-0.629281
12	6	0	2.638661	-0.850149	-0.316976
13	8	0	3.544449	-1.665945	-0.401418
14	6	0	2.764534	0.548299	0.088403
15	6	0	1.648970	1.315473	0.117245
16	1	0	-0.423675	-0.565267	2.556532
17	1	0	-2.712484	-1.792026	1.474683
18	1	0	-2.634161	-0.546526	2.723369
19	1	0	-3.474443	0.547777	0.805350
20	1	0	-1.266059	1.216276	-2.286408
21	1	0	-0.531156	2.715882	-0.126903
22	1	0	1.663146	2.359807	0.404098
23	1	0	1.171989	-2.224475	-0.893983
24	1	0	-2.616980	1.932759	-1.360415
25	6	0	4.125565	1.062652	0.452495
26	1	0	4.814929	0.952369	-0.390684
27	1	0	4.081899	2.116043	0.735059
28	1	0	4.540801	0.490502	1.288319
29	8	0	-3.133856	-0.716246	-1.469971
30	1	0	-3.493208	-1.482333	-0.993934

ENERGY (a.u):

HF=-874.4138392

Wiberg bond index matrix in the NAO basis:

```
     Atom    1        2        3        4        5        6        7
8        9
     ---- ------   ------   ------   ------   ------   ------   ------   -
-----   ------
   1.  O  0.0000   0.9443   0.0321   0.0052   0.0022   0.0006   0.0008
0.0048   0.0109
   2.  C  0.9443   0.0000   0.9917   0.0197   0.0080   0.0063   0.0047
0.0008   0.0008
   3.  C  0.0321   0.9917   0.0000   0.8782   0.9682   0.0081   0.0087
0.0016   0.0047
```

4.	O	0.0052	0.0197	0.8782	0.0000	0.0188	0.0222	0.9519	0.0472	0.0060		
5.	C	0.0022	0.0080	0.9682	0.0188	0.0000	0.9893	0.0121	0.0028	0.0062		
6.	C	0.0006	0.0063	0.0081	0.0222	0.9893	0.0000	0.9954	0.0098	0.0036		
7.	C	0.0008	0.0047	0.0087	0.9519	0.0121	0.9954	0.0000	0.8622	0.0087		
8.	N	0.0048	0.0008	0.0016	0.0472	0.0028	0.0098	0.8622	0.0000	1.2242		
9.	C	0.0109	0.0008	0.0047	0.0060	0.0062	0.0036	0.0087	1.2242	0.0000		
10.	O	0.0046	0.0038	0.0129	0.0021	0.7178	0.0142	0.0035	0.0754	1.1779		
11.	N	0.0029	0.0003	0.0020	0.0021	0.0090	0.0010	0.0090	0.0403	1.2747		
12.	C	0.0003	0.0000	0.0002	0.0013	0.0007	0.0003	0.0005	0.0224	0.0089		
13.	O	0.0001	0.0000	0.0002	0.0016	0.0014	0.0004	0.0008	0.0300	0.0136		
14.	C	0.0007	0.0001	0.0004	0.0021	0.0002	0.0010	0.0067	0.0291	0.0456		
15.	C	0.0006	0.0001	0.0002	0.0053	0.0005	0.0056	0.0104	1.0698	0.0176		
16.	H	0.7058	0.0029	0.0005	0.0022	0.0001	0.0001	0.0001	0.0002	0.0001		
17.	H	0.0116	0.8987	0.0045	0.0098	0.0010	0.0004	0.0007	0.0001	0.0001		
18.	H	0.0182	0.9055	0.0025	0.0012	0.0081	0.0003	0.0001	0.0002	0.0002		
19.	H	0.0095	0.0033	0.8673	0.0159	0.0057	0.0008	0.0025	0.0008	0.0005		
20.	H	0.0003	0.0003	0.0087	0.0099	0.0025	0.8810	0.0028	0.0006	0.0003		
21.	H	0.0001	0.0002	0.0078	0.0081	0.0072	0.0035	0.8731	0.0015	0.0048		
22.	H	0.0000	0.0000	0.0000	0.0007	0.0000	0.0003	0.0010	0.0016	0.0066		
23.	H	0.0001	0.0000	0.0000	0.0002	0.0002	0.0001	0.0006	0.0099	0.0026		
24.	H	0.0000	0.0002	0.0001	0.0009	0.0054	0.8676	0.0034	0.0083	0.0010		
25.	C	0.0000	0.0000	0.0000	0.0003	0.0000	0.0002	0.0004	0.0092	0.0020		
26.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0001	0.0010	0.0020		
27.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000		
28.	H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0001	0.0010	0.0019		
29.	O	0.0006	0.0021	0.0316	0.0101	1.0681	0.0176	0.0086	0.0010	0.0087		
30.	H	0.0001	0.0008	0.0011	0.0001	0.0035	0.0149	0.0010	0.0001	0.0001		

Atom	10	11	12	13	14	15	16	17	18
1. O	0.0046	0.0029	0.0003	0.0001	0.0007	0.0006	0.7058	0.0116	0.0182

2.	C	0.0038	0.0003	0.0000	0.0000	0.0001	0.0001	0.0029
0.8987	0.9055							
3.	C	0.0129	0.0020	0.0002	0.0002	0.0004	0.0002	0.0005
0.0045	0.0025							
4.	O	0.0021	0.0021	0.0013	0.0016	0.0021	0.0053	0.0022
0.0098	0.0012							
5.	C	0.7178	0.0090	0.0007	0.0014	0.0002	0.0005	0.0001
0.0010	0.0081							
6.	C	0.0142	0.0010	0.0003	0.0004	0.0010	0.0056	0.0001
0.0004	0.0003							
7.	C	0.0035	0.0090	0.0005	0.0008	0.0067	0.0104	0.0001
0.0007	0.0001							
8.	N	0.0754	0.0403	0.0224	0.0300	0.0291	1.0698	0.0002
0.0001	0.0002							
9.	C	1.1779	1.2747	0.0089	0.0136	0.0456	0.0176	0.0001
0.0001	0.0002							
10.	O	0.0000	0.0701	0.0071	0.0038	0.0182	0.0097	0.0003
0.0003	0.0003							
11.	N	0.0701	0.0000	1.0079	0.1217	0.0107	0.0177	0.0000
0.0000	0.0001							
12.	C	0.0071	1.0079	0.0000	1.6795	1.0861	0.0343	0.0000
0.0000	0.0000							
13.	O	0.0038	0.1217	1.6795	0.0000	0.0701	0.0648	0.0000
0.0000	0.0000							
14.	C	0.0182	0.0107	1.0861	0.0701	0.0000	1.6737	0.0001
0.0000	0.0000							
15.	C	0.0097	0.0177	0.0343	0.0648	1.6737	0.0000	0.0001
0.0000	0.0000							
16.	H	0.0003	0.0000	0.0000	0.0000	0.0001	0.0001	0.0000
0.0088	0.0007							
17.	H	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0088
0.0000	0.0009							
18.	H	0.0003	0.0001	0.0000	0.0000	0.0000	0.0000	0.0007
0.0009	0.0000							
19.	H	0.0102	0.0004	0.0001	0.0000	0.0001	0.0001	0.0000
0.0000	0.0007							
20.	H	0.0021	0.0001	0.0000	0.0000	0.0001	0.0001	0.0000
0.0001	0.0004							
21.	H	0.0003	0.0003	0.0001	0.0001	0.0003	0.0005	0.0000
0.0003	0.0000							
22.	H	0.0009	0.0002	0.0096	0.0017	0.0071	0.8863	0.0000
0.0000	0.0000							
23.	H	0.0031	0.7184	0.0037	0.0040	0.0097	0.0003	0.0000
0.0000	0.0000							
24.	H	0.0119	0.0010	0.0001	0.0002	0.0002	0.0002	0.0000
0.0000	0.0000							
25.	C	0.0007	0.0085	0.0106	0.0048	1.0326	0.0202	0.0000
0.0000	0.0000							
26.	H	0.0008	0.0005	0.0018	0.0014	0.0022	0.0174	0.0000
0.0000	0.0000							
27.	H	0.0000	0.0002	0.0084	0.0008	0.0017	0.0011	0.0000
0.0000	0.0000							
28.	H	0.0008	0.0005	0.0018	0.0013	0.0022	0.0174	0.0000
0.0000	0.0000							
29.	O	0.0592	0.0017	0.0007	0.0004	0.0001	0.0002	0.0001
0.0006	0.0004							
30.	H	0.0008	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0007	0.0002							

Atom	19	20	21	22	23	24	25
26	27						

1.	O	0.0095	0.0003	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
2.	C	0.0033	0.0003	0.0002	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000
3.	C	0.8673	0.0087	0.0078	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000
4.	O	0.0159	0.0099	0.0081	0.0007	0.0002	0.0009	0.0003	0.0000	0.0000
5.	C	0.0057	0.0025	0.0072	0.0000	0.0002	0.0054	0.0000	0.0000	0.0000
6.	C	0.0008	0.8810	0.0035	0.0003	0.0001	0.8676	0.0002	0.0001	0.0000
7.	C	0.0025	0.0028	0.8731	0.0010	0.0006	0.0034	0.0004	0.0001	0.0000
8.	N	0.0008	0.0006	0.0015	0.0016	0.0099	0.0083	0.0092	0.0010	0.0003
9.	C	0.0005	0.0003	0.0048	0.0066	0.0026	0.0010	0.0020	0.0020	0.0000
10.	O	0.0102	0.0021	0.0003	0.0009	0.0031	0.0119	0.0007	0.0008	0.0000
11.	N	0.0004	0.0001	0.0003	0.0002	0.7184	0.0010	0.0085	0.0005	0.0002
12.	C	0.0001	0.0000	0.0001	0.0096	0.0037	0.0001	0.0106	0.0018	0.0084
13.	O	0.0000	0.0000	0.0001	0.0017	0.0040	0.0002	0.0048	0.0014	0.0008
14.	C	0.0001	0.0001	0.0003	0.0071	0.0097	0.0002	1.0326	0.0022	0.0017
15.	C	0.0001	0.0001	0.0005	0.8863	0.0003	0.0002	0.0202	0.0174	0.0011
16.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
17.	H	0.0000	0.0001	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
18.	H	0.0007	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
19.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
20.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0018	0.0000	0.0000	0.0000
21.	H	0.0000	0.0000	0.0000	0.0013	0.0003	0.0010	0.0000	0.0000	0.0000
22.	H	0.0000	0.0000	0.0013	0.0000	0.0005	0.0000	0.0017	0.0001	0.0005
23.	H	0.0000	0.0000	0.0003	0.0005	0.0000	0.0000	0.0005	0.0000	0.0004
24.	H	0.0000	0.0018	0.0010	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
25.	C	0.0000	0.0000	0.0000	0.0017	0.0005	0.0001	0.0000	0.8975	0.9155
26.	H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.8975	0.0000	0.0008
27.	H	0.0000	0.0000	0.0000	0.0005	0.0004	0.0000	0.9155	0.0008	0.0000
28.	H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.8977	0.0007	0.0008
29.	O	0.0016	0.0005	0.0002	0.0000	0.0001	0.0012	0.0000	0.0000	0.0000
30.	H	0.0001	0.0000	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

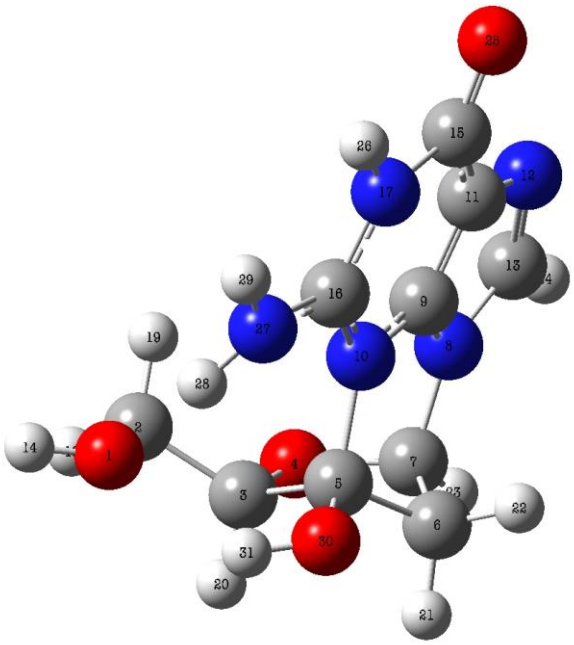
	Atom	28	29	30
1.	O	0.0000	0.0006	0.0001
2.	C	0.0000	0.0021	0.0008
3.	C	0.0000	0.0316	0.0011
4.	O	0.0001	0.0101	0.0001
5.	C	0.0000	1.0681	0.0035
6.	C	0.0000	0.0176	0.0149
7.	C	0.0001	0.0086	0.0010
8.	N	0.0010	0.0010	0.0001
9.	C	0.0019	0.0087	0.0001
10.	O	0.0008	0.0592	0.0008
11.	N	0.0005	0.0017	0.0000
12.	C	0.0018	0.0007	0.0000
13.	O	0.0013	0.0004	0.0000
14.	C	0.0022	0.0001	0.0000
15.	C	0.0174	0.0002	0.0000
16.	H	0.0000	0.0001	0.0000
17.	H	0.0000	0.0006	0.0007
18.	H	0.0000	0.0004	0.0002
19.	H	0.0000	0.0016	0.0001
20.	H	0.0000	0.0005	0.0000
21.	H	0.0000	0.0002	0.0004
22.	H	0.0001	0.0000	0.0000
23.	H	0.0000	0.0001	0.0000
24.	H	0.0000	0.0012	0.0000
25.	C	0.8977	0.0000	0.0000
26.	H	0.0007	0.0000	0.0000
27.	H	0.0008	0.0000	0.0000
28.	H	0.0000	0.0000	0.0000
29.	O	0.0000	0.0000	0.6833
30.	H	0.0000	0.6833	0.0000

Wiberg bond index, Totals by atom:

	Atom	1
1.	O	1.7565
2.	C	3.7948
3.	C	3.8331
4.	O	2.0233
5.	C	3.8389
6.	C	3.8444
7.	C	3.7701
8.	N	3.4560
9.	C	3.8343
10.	O	2.2130
11.	N	3.3012
12.	C	3.8863
13.	O	2.0029
14.	C	4.0010
15.	C	3.8543
16.	H	0.7221
17.	H	0.9389
18.	H	0.9400
19.	H	0.9196
20.	H	0.9117
21.	H	0.9114
22.	H	0.9201
23.	H	0.7549

24.	H	0.9049
25.	C	3.8025
26.	H	0.9264
27.	H	0.9305
28.	H	0.9264
29.	O	1.8986
30.	H	0.7075

5. Cation 4_{iso} (guanidinium ion)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.804282	-1.552624	-0.997868
2	6	0	2.332912	-0.325738	-1.591001
3	6	0	2.234062	0.643045	-0.422713
4	8	0	1.576003	1.871679	-0.798954
5	6	0	1.438173	0.139763	0.805645
6	6	0	1.139915	1.489042	1.480531
7	6	0	0.707130	2.297080	0.255379
8	7	0	-0.659880	1.839726	-0.044328
9	6	0	-0.914570	0.515865	0.058472
10	7	0	0.055963	-0.425284	0.331927
11	6	0	-2.259567	0.329133	-0.158045
12	7	0	-2.856036	1.554853	-0.399392
13	6	0	-1.881453	2.434037	-0.322506
14	1	0	3.300658	-2.073549	-1.643948
15	6	0	-2.772374	-1.011237	-0.101418

16	6	0	-0.367894	-1.716550	0.255703
17	7	0	-1.702264	-1.948609	0.113823
18	1	0	3.043040	0.048106	-2.332105
19	1	0	1.362425	-0.479106	-2.074497
20	1	0	3.244961	0.870884	-0.062443
21	1	0	2.079947	1.864884	1.887505
22	1	0	0.390480	1.447214	2.271265
23	1	0	0.725969	3.380965	0.341680
24	1	0	-1.974451	3.502699	-0.450198
25	8	0	-3.912978	-1.428400	-0.225548
26	1	0	-1.998218	-2.917996	0.040767
27	7	0	0.480719	-2.738164	0.310491
28	1	0	1.442067	-2.589750	0.008854
29	1	0	0.125979	-3.683085	0.249867
30	8	0	2.075402	-0.749807	1.632823
31	1	0	2.747945	-1.242346	1.131699

ENERGY (a.u):

HF=-962.855431097

Wiberg bond index matrix in the NAO basis

Atom	1	2	3	4	5	6	7	8	9
1. O	0.0000	0.9087	0.0205	0.0123	0.0054	0.0010	0.0013	0.0002	0.0004
2. C	0.9087	0.0000	0.9944	0.0171	0.0071	0.0066	0.0059	0.0005	0.0005
3. C	0.0205	0.9944	0.0000	0.8963	0.9646	0.0086	0.0078	0.0018	0.0023
4. O	0.0123	0.0171	0.8963	0.0000	0.0216	0.0190	0.9203	0.0418	0.0053
5. C	0.0054	0.0071	0.9646	0.0216	0.0000	0.9776	0.0103	0.0034	0.0070
6. C	0.0010	0.0066	0.0086	0.0190	0.9776	0.0000	0.9943	0.0094	0.0040
7. C	0.0013	0.0059	0.0078	0.9203	0.0103	0.9943	0.0000	0.8929	0.0100
8. N	0.0002	0.0005	0.0018	0.0418	0.0034	0.0094	0.8929	0.0000	1.1868
9. C	0.0004	0.0005	0.0023	0.0053	0.0070	0.0040	0.0100	1.1868	0.0000
10. N	0.0010	0.0025	0.0114	0.0018	0.8036	0.0093	0.0013	0.0280	1.0726
11. C	0.0001	0.0002	0.0010	0.0021	0.0074	0.0013	0.0103	0.0487	1.3859
12. N	0.0001	0.0001	0.0003	0.0048	0.0017	0.0022	0.0121	0.0861	0.0591

13.	C	0.0000	0.0001	0.0004	0.0082	0.0008	0.0074	0.0091	1.1256	0.0668	
14.	H	0.6800	0.0016	0.0063	0.0013	0.0003	0.0001	0.0002	0.0000	0.0000	
15.	C	0.0001	0.0000	0.0004	0.0002	0.0003	0.0003	0.0003	0.0100	0.0311	
16.	C	0.0011	0.0004	0.0036	0.0004	0.0076	0.0068	0.0003	0.0109	0.0122	
17.	N	0.0004	0.0003	0.0009	0.0003	0.0083	0.0012	0.0001	0.0059	0.0116	
18.	H	0.0134	0.9057	0.0020	0.0007	0.0084	0.0003	0.0001	0.0000	0.0001	
19.	H	0.0221	0.9065	0.0020	0.0016	0.0008	0.0002	0.0001	0.0001	0.0004	
20.	H	0.0006	0.0023	0.8724	0.0195	0.0040	0.0007	0.0014	0.0009	0.0003	
21.	H	0.0000	0.0003	0.0002	0.0007	0.0045	0.8739	0.0027	0.0072	0.0013	
22.	H	0.0001	0.0006	0.0083	0.0089	0.0022	0.8840	0.0027	0.0007	0.0004	
23.	H	0.0003	0.0003	0.0055	0.0097	0.0071	0.0031	0.8754	0.0012	0.0056	
24.	H	0.0000	0.0000	0.0000	0.0001	0.0001	0.0000	0.0001	0.0012	0.0072	
25.	O	0.0001	0.0001	0.0008	0.0003	0.0005	0.0005	0.0008	0.0065	0.0495	
26.	H	0.0000	0.0000	0.0001	0.0000	0.0006	0.0002	0.0000	0.0003	0.0004	
27.	N	0.0139	0.0008	0.0017	0.0002	0.0029	0.0019	0.0001	0.0039	0.0081	
28.	H	0.0375	0.0005	0.0001	0.0000	0.0005	0.0002	0.0000	0.0000	0.0002	
29.	H	0.0005	0.0000	0.0000	0.0000	0.0002	0.0001	0.0000	0.0003	0.0004	
30.	O	0.0064	0.0010	0.0263	0.0111	1.0368	0.0223	0.0086	0.0010	0.0050	
31.	H	0.0170	0.0003	0.0018	0.0004	0.0028	0.0090	0.0007	0.0001	0.0001	

Atom		10	11	12	13	14	15	16	17	18
1.	O	0.0010	0.0001	0.0001	0.0000	0.6800	0.0001	0.0011	0.0004	0.0134
2.	C	0.0025	0.0002	0.0001	0.0001	0.0016	0.0000	0.0004	0.0003	0.9057
3.	C	0.0114	0.0010	0.0003	0.0004	0.0063	0.0004	0.0036	0.0009	0.0020
4.	O	0.0018	0.0021	0.0048	0.0082	0.0013	0.0002	0.0004	0.0003	0.0007
5.	C	0.8036	0.0074	0.0017	0.0008	0.0003	0.0003	0.0076	0.0083	0.0084
6.	C	0.0093	0.0013	0.0022	0.0074	0.0001	0.0003	0.0068	0.0012	0.0003
7.	C	0.0013	0.0103	0.0121	0.0091	0.0002	0.0003	0.0003	0.0001	0.0001
8.	N	0.0280	0.0487	0.0861	1.1256	0.0000	0.0100	0.0109	0.0059	0.0000
9.	C	1.0726	1.3859	0.0591	0.0668	0.0000	0.0311	0.0122	0.0116	0.0001

10.	N	0.0000	0.0241	0.0101	0.0096	0.0001	0.0176	1.1939
0.0372	0.0003							
11.	C	0.0241	0.0000	1.2082	0.0349	0.0000	1.1049	0.0259
0.0077	0.0000							
12.	N	0.0101	1.2082	0.0000	1.6158	0.0000	0.0153	0.0042
0.0131	0.0000							
13.	C	0.0096	0.0349	1.6158	0.0000	0.0000	0.0276	0.0107
0.0013	0.0000							
14.	H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0008							
15.	C	0.0176	1.1049	0.0153	0.0276	0.0000	0.0000	0.0079
0.9900	0.0000							
16.	C	1.1939	0.0259	0.0042	0.0107	0.0000	0.0079	0.0000
1.2309	0.0001							
17.	N	0.0372	0.0077	0.0131	0.0013	0.0000	0.9900	1.2309
0.0000	0.0000							
18.	H	0.0003	0.0000	0.0000	0.0000	0.0008	0.0000	0.0001
0.0000	0.0000							
19.	H	0.0009	0.0001	0.0000	0.0000	0.0002	0.0000	0.0002
0.0001	0.0003							
20.	H	0.0104	0.0002	0.0002	0.0001	0.0000	0.0000	0.0004
0.0004	0.0012							
21.	H	0.0094	0.0004	0.0008	0.0004	0.0000	0.0000	0.0004
0.0003	0.0000							
22.	H	0.0011	0.0001	0.0003	0.0001	0.0000	0.0000	0.0001
0.0000	0.0002							
23.	H	0.0002	0.0003	0.0001	0.0005	0.0001	0.0002	0.0002
0.0000	0.0000							
24.	H	0.0001	0.0117	0.0099	0.8971	0.0000	0.0001	0.0003
0.0003	0.0000							
25.	O	0.0237	0.0749	0.0071	0.0163	0.0000	1.6743	0.0138
0.1230	0.0000							
26.	H	0.0088	0.0088	0.0004	0.0003	0.0000	0.0031	0.0023
0.7336	0.0000							
27.	N	0.0786	0.0164	0.0012	0.0070	0.0003	0.0077	1.3514
0.0808	0.0004							
28.	H	0.0009	0.0004	0.0000	0.0001	0.0000	0.0005	0.0035
0.0088	0.0009							
29.	H	0.0098	0.0001	0.0000	0.0001	0.0000	0.0002	0.0027
0.0011	0.0000							
30.	O	0.0507	0.0016	0.0008	0.0004	0.0009	0.0004	0.0037
0.0010	0.0004							
31.	H	0.0018	0.0001	0.0000	0.0001	0.0000	0.0000	0.0001
0.0001	0.0000							

Atom	19	20	21	22	23	24	25	26	27
1.	O	0.0221	0.0006	0.0000	0.0001	0.0003	0.0000	0.0001	0.0000	0.0139
2.	C	0.9065	0.0023	0.0003	0.0006	0.0003	0.0000	0.0001	0.0000	0.0008
3.	C	0.0020	0.8724	0.0002	0.0083	0.0055	0.0000	0.0008	0.0001	0.0017
4.	O	0.0016	0.0195	0.0007	0.0089	0.0097	0.0001	0.0003	0.0000	0.0002
5.	C	0.0008	0.0040	0.0045	0.0022	0.0071	0.0001	0.0005	0.0006	0.0029
6.	C	0.0002	0.0007	0.8739	0.8840	0.0031	0.0000	0.0005	0.0002	0.0019

7.	C	0.0001	0.0014	0.0027	0.0027	0.8754	0.0001	0.0008	0.0000	0.0001
8.	N	0.0001	0.0009	0.0072	0.0007	0.0012	0.0012	0.0065	0.0003	0.0039
9.	C	0.0004	0.0003	0.0013	0.0004	0.0056	0.0072	0.0495	0.0004	0.0081
10.	N	0.0009	0.0104	0.0094	0.0011	0.0002	0.0001	0.0237	0.0088	0.0786
11.	C	0.0001	0.0002	0.0004	0.0001	0.0003	0.0117	0.0749	0.0088	0.0164
12.	N	0.0000	0.0002	0.0008	0.0003	0.0001	0.0099	0.0071	0.0004	0.0012
13.	C	0.0000	0.0001	0.0004	0.0001	0.0005	0.8971	0.0163	0.0003	0.0070
14.	H	0.0002	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0003
15.	C	0.0000	0.0000	0.0000	0.0000	0.0002	0.0001	1.6743	0.0031	0.0077
16.	C	0.0002	0.0004	0.0004	0.0001	0.0002	0.0003	0.0138	0.0023	1.3514
17.	N	0.0001	0.0004	0.0003	0.0000	0.0000	0.0003	0.1230	0.7336	0.0808
18.	H	0.0003	0.0012	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0004
19.	H	0.0000	0.0101	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
20.	H	0.0101	0.0000	0.0001	0.0000	0.0000	0.0000	0.0001	0.0001	0.0002
21.	H	0.0000	0.0001	0.0000	0.0017	0.0011	0.0000	0.0001	0.0001	0.0001
22.	H	0.0000	0.0000	0.0017	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
23.	H	0.0000	0.0000	0.0011	0.0000	0.0000	0.0008	0.0001	0.0000	0.0000
24.	H	0.0000	0.0000	0.0000	0.0000	0.0008	0.0000	0.0001	0.0000	0.0000
25.	O	0.0000	0.0001	0.0001	0.0000	0.0001	0.0001	0.0000	0.0047	0.0051
26.	H	0.0000	0.0001	0.0001	0.0000	0.0000	0.0000	0.0047	0.0000	0.0011
27.	N	0.0001	0.0002	0.0001	0.0000	0.0000	0.0000	0.0051	0.0011	0.0000
28.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0010	0.0002	0.7208
29.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0007	0.7597
30.	O	0.0002	0.0013	0.0013	0.0004	0.0004	0.0000	0.0005	0.0003	0.0039
31.	H	0.0004	0.0003	0.0000	0.0000	0.0003	0.0000	0.0000	0.0000	0.0004

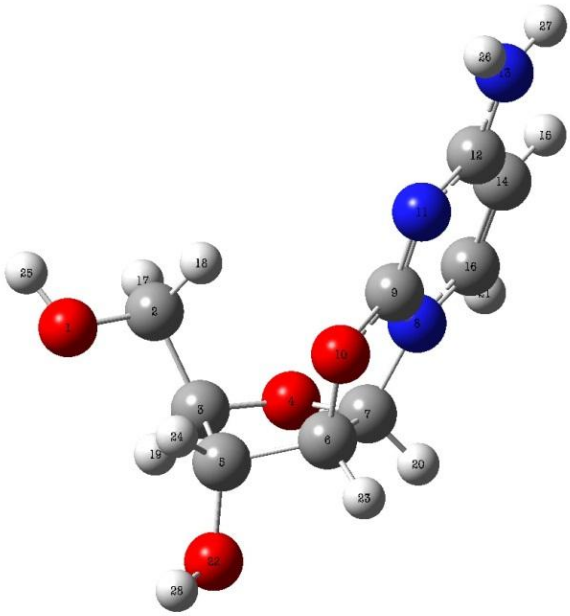
Atom	28	29	30	31
1.	O	0.0375	0.0005	0.0064	0.0170
2.	C	0.0005	0.0000	0.0010	0.0003
3.	C	0.0001	0.0000	0.0263	0.0018
4.	O	0.0000	0.0000	0.0111	0.0004
5.	C	0.0005	0.0002	1.0368	0.0028
6.	C	0.0002	0.0001	0.0223	0.0090
7.	C	0.0000	0.0000	0.0086	0.0007
8.	N	0.0000	0.0003	0.0010	0.0001
9.	C	0.0002	0.0004	0.0050	0.0001

10.	N	0.0009	0.0098	0.0507	0.0018
11.	C	0.0004	0.0001	0.0016	0.0001
12.	N	0.0000	0.0000	0.0008	0.0000
13.	C	0.0001	0.0001	0.0004	0.0001
14.	H	0.0000	0.0000	0.0009	0.0000
15.	C	0.0005	0.0002	0.0004	0.0000
16.	C	0.0035	0.0027	0.0037	0.0001
17.	N	0.0088	0.0011	0.0010	0.0001
18.	H	0.0009	0.0000	0.0004	0.0000
19.	H	0.0000	0.0000	0.0002	0.0004
20.	H	0.0000	0.0000	0.0013	0.0003
21.	H	0.0000	0.0000	0.0013	0.0000
22.	H	0.0000	0.0000	0.0004	0.0000
23.	H	0.0000	0.0000	0.0004	0.0003
24.	H	0.0000	0.0000	0.0000	0.0000
25.	O	0.0010	0.0001	0.0005	0.0000
26.	H	0.0002	0.0007	0.0003	0.0000
27.	N	0.7208	0.7597	0.0039	0.0004
28.	H	0.0000	0.0008	0.0017	0.0006
29.	H	0.0008	0.0000	0.0008	0.0000
30.	O	0.0017	0.0008	0.0000	0.6698
31.	H	0.0006	0.0000	0.6698	0.0000

Wiberg bond index, Totals by atom:

Atom		1
1.	O	1.7446
2.	C	3.7644
3.	C	3.8420
4.	O	2.0063
5.	C	3.8983
6.	C	3.8454
7.	C	3.7693
8.	N	3.4753
9.	C	3.9347
10.	N	3.4208
11.	C	3.9776
12.	N	3.0541
13.	C	3.8408
14.	H	0.6924
15.	C	3.8926
16.	C	3.8960
17.	N	3.2589
18.	H	0.9355
19.	H	0.9466
20.	H	0.9272
21.	H	0.9070
22.	H	0.9121
23.	H	0.9124
24.	H	0.9291
25.	O	2.0039
26.	H	0.7663
27.	N	3.0687
28.	H	0.7792
29.	H	0.7778
30.	O	1.8590
31.	H	0.7062

6. Cation 5_{iso}



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.689620	2.491978	0.096469
2	6	0	1.722452	1.732331	0.805462
3	6	0	2.204733	0.281242	0.742699
4	8	0	1.260021	-0.595525	1.424122
5	6	0	2.351639	-0.289282	-0.681093
6	6	0	1.033804	-1.054924	-0.905969
7	6	0	0.519144	-1.353731	0.523230
8	7	0	-0.884659	-0.879744	0.410325
9	6	0	-1.075230	-0.195944	-0.753740
10	8	0	0.001875	-0.216657	-1.521895
11	7	0	-2.173211	0.419791	-1.093736
12	6	0	-3.194570	0.370509	-0.205043
13	7	0	-4.321330	0.992499	-0.556249
14	6	0	-3.073669	-0.313817	1.053709
15	1	0	-3.892689	-0.343255	1.762780
16	6	0	-1.889667	-0.925784	1.335046
17	1	0	1.650786	2.032677	1.858702
18	1	0	0.725440	1.839244	0.349079
19	1	0	3.155723	0.186827	1.270062
20	1	0	0.523673	-2.403515	0.824342
21	1	0	-1.682944	-1.456309	2.257924
22	8	0	3.405289	-1.239051	-0.698355
23	1	0	1.164555	-1.929051	-1.543297
24	1	0	2.486503	0.504872	-1.420046
25	1	0	2.600080	3.434447	0.304207
26	1	0	-4.371828	1.459447	-1.454797
27	1	0	-5.140288	1.003591	0.036995
28	1	0	3.989127	-1.086356	-1.456871

ENERGY (a.u):

HF=-815.1177223

Wiberg bond index matrix in the NAO basis:

Atom	1	2	3	4	5	6	7	8	9
1. O	0.0000	0.9456	0.0215	0.0129	0.0040	0.0008	0.0010	0.0008	0.0007
2. C	0.9456	0.0000	0.9893	0.0236	0.0081	0.0009	0.0030	0.0013	0.0003
3. C	0.0215	0.9893	0.0000	0.8647	0.9797	0.0086	0.0120	0.0033	0.0009
4. O	0.0129	0.0236	0.8647	0.0000	0.0169	0.0239	0.9772	0.0492	0.0066
5. C	0.0040	0.0081	0.9797	0.0169	0.0000	0.9691	0.0074	0.0025	0.0056
6. C	0.0008	0.0009	0.0086	0.0239	0.9691	0.0000	0.9752	0.0059	0.0094
7. C	0.0010	0.0030	0.0120	0.9772	0.0074	0.9752	0.0000	0.8715	0.0096
8. N	0.0008	0.0013	0.0033	0.0492	0.0025	0.0059	0.8715	0.0000	1.1316
9. C	0.0007	0.0003	0.0009	0.0066	0.0056	0.0094	0.0096	1.1316	0.0000
10. O	0.0006	0.0014	0.0016	0.0029	0.0138	0.8498	0.0137	0.0645	1.1110
11. N	0.0002	0.0005	0.0003	0.0020	0.0015	0.0120	0.0101	0.0459	1.4622
12. C	0.0000	0.0001	0.0003	0.0024	0.0006	0.0013	0.0008	0.0425	0.0157
13. N	0.0000	0.0000	0.0002	0.0022	0.0005	0.0005	0.0012	0.0367	0.0245
14. C	0.0000	0.0001	0.0002	0.0030	0.0002	0.0005	0.0092	0.0385	0.0441
15. H	0.0000	0.0000	0.0000	0.0002	0.0000	0.0004	0.0003	0.0078	0.0005
16. C	0.0001	0.0001	0.0004	0.0063	0.0004	0.0073	0.0107	1.1467	0.0169
17. H	0.0213	0.9106	0.0016	0.0013	0.0088	0.0004	0.0001	0.0001	0.0001
18. H	0.0295	0.9186	0.0020	0.0009	0.0008	0.0002	0.0002	0.0003	0.0007
19. H	0.0012	0.0022	0.8778	0.0095	0.0020	0.0047	0.0047	0.0009	0.0003
20. H	0.0005	0.0009	0.0059	0.0189	0.0014	0.0035	0.8766	0.0034	0.0053
21. H	0.0000	0.0000	0.0000	0.0012	0.0000	0.0002	0.0011	0.0017	0.0072
22. O	0.0007	0.0073	0.0234	0.0020	0.9518	0.0368	0.0014	0.0006	0.0016
23. H	0.0001	0.0001	0.0060	0.0057	0.0020	0.8807	0.0026	0.0011	0.0043
24. H	0.0036	0.0012	0.0038	0.0061	0.8822	0.0020	0.0064	0.0002	0.0001
25. H	0.7205	0.0015	0.0086	0.0016	0.0004	0.0001	0.0001	0.0000	0.0000
26. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0002
27. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001	0.0005

28.	H	0.0001	0.0005	0.0048	0.0003	0.0015	0.0020	0.0001	0.0000
0.0000									

Atom		10	11	12	13	14	15	16	17	18
1.	O	0.0006	0.0002	0.0000	0.0000	0.0000	0.0000	0.0001	0.0213	0.0295
2.	C	0.0014	0.0005	0.0001	0.0000	0.0001	0.0000	0.0001	0.9106	0.9186
3.	C	0.0016	0.0003	0.0003	0.0002	0.0002	0.0000	0.0004	0.0016	0.0020
4.	O	0.0029	0.0020	0.0024	0.0022	0.0030	0.0002	0.0063	0.0013	0.0009
5.	C	0.0138	0.0015	0.0006	0.0005	0.0002	0.0000	0.0004	0.0088	0.0008
6.	C	0.8498	0.0120	0.0013	0.0005	0.0005	0.0004	0.0073	0.0004	0.0002
7.	C	0.0137	0.0101	0.0008	0.0012	0.0092	0.0003	0.0107	0.0001	0.0002
8.	N	0.0645	0.0459	0.0425	0.0367	0.0385	0.0078	1.1467	0.0001	0.0003
9.	C	1.1110	1.4622	0.0157	0.0245	0.0441	0.0005	0.0169	0.0001	0.0007
10.	O	0.0000	0.0853	0.0157	0.0064	0.0205	0.0005	0.0080	0.0003	0.0008
11.	N	0.0853	0.0000	1.2806	0.0840	0.0260	0.0089	0.0499	0.0000	0.0002
12.	C	0.0157	1.2806	0.0000	1.3467	1.1949	0.0035	0.0297	0.0000	0.0001
13.	N	0.0064	0.0840	1.3467	0.0000	0.0390	0.0005	0.0441	0.0000	0.0000
14.	C	0.0205	0.0260	1.1949	0.0390	0.0000	0.8896	1.6345	0.0000	0.0001
15.	H	0.0005	0.0089	0.0035	0.0005	0.8896	0.0000	0.0058	0.0000	0.0000
16.	C	0.0080	0.0499	0.0297	0.0441	1.6345	0.0058	0.0000	0.0000	0.0001
17.	H	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002
18.	H	0.0008	0.0002	0.0001	0.0000	0.0001	0.0000	0.0001	0.0002	0.0000
19.	H	0.0002	0.0000	0.0001	0.0001	0.0000	0.0000	0.0002	0.0012	0.0104
20.	H	0.0034	0.0011	0.0006	0.0007	0.0009	0.0000	0.0007	0.0000	0.0000
21.	H	0.0009	0.0005	0.0083	0.0002	0.0051	0.0014	0.8921	0.0000	0.0000
22.	O	0.0113	0.0007	0.0003	0.0001	0.0001	0.0000	0.0001	0.0010	0.0001
23.	H	0.0085	0.0018	0.0005	0.0004	0.0002	0.0000	0.0001	0.0001	0.0000
24.	H	0.0029	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0006	0.0002
25.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006	0.0000
26.	H	0.0001	0.0053	0.0033	0.7667	0.0127	0.0001	0.0005	0.0000	0.0000
27.	H	0.0002	0.0111	0.0026	0.7813	0.0005	0.0003	0.0002	0.0000	0.0000
28.	H	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000

Atom	19	20	21	22	23	24	25	26	27
1. O	0.0012	0.0005	0.0000	0.0007	0.0001	0.0036	0.7205	0.0000	0.0000
2. C	0.0022	0.0009	0.0000	0.0073	0.0001	0.0012	0.0015	0.0000	0.0000
3. C	0.8778	0.0059	0.0000	0.0234	0.0060	0.0038	0.0086	0.0000	0.0000
4. O	0.0095	0.0189	0.0012	0.0020	0.0057	0.0061	0.0016	0.0000	0.0000
5. C	0.0020	0.0014	0.0000	0.9518	0.0020	0.8822	0.0004	0.0000	0.0000
6. C	0.0047	0.0035	0.0002	0.0368	0.8807	0.0020	0.0001	0.0000	0.0001
7. C	0.0047	0.8766	0.0011	0.0014	0.0026	0.0064	0.0001	0.0000	0.0000
8. N	0.0009	0.0034	0.0017	0.0006	0.0011	0.0002	0.0000	0.0002	0.0001
9. C	0.0003	0.0053	0.0072	0.0016	0.0043	0.0001	0.0000	0.0002	0.0005
10. O	0.0002	0.0034	0.0009	0.0113	0.0085	0.0029	0.0000	0.0001	0.0002
11. N	0.0000	0.0011	0.0005	0.0007	0.0018	0.0000	0.0000	0.0053	0.0111
12. C	0.0001	0.0006	0.0083	0.0003	0.0005	0.0000	0.0000	0.0033	0.0026
13. N	0.0001	0.0007	0.0002	0.0001	0.0004	0.0000	0.0000	0.7667	0.7813
14. C	0.0000	0.0009	0.0051	0.0001	0.0002	0.0000	0.0000	0.0127	0.0005
15. H	0.0000	0.0000	0.0014	0.0000	0.0000	0.0000	0.0000	0.0001	0.0003
16. C	0.0002	0.0007	0.8921	0.0001	0.0001	0.0001	0.0000	0.0005	0.0002
17. H	0.0012	0.0000	0.0000	0.0010	0.0001	0.0006	0.0006	0.0000	0.0000
18. H	0.0104	0.0000	0.0000	0.0001	0.0000	0.0002	0.0000	0.0000	0.0000
19. H	0.0000	0.0001	0.0000	0.0039	0.0001	0.0007	0.0000	0.0000	0.0000
20. H	0.0001	0.0000	0.0005	0.0002	0.0005	0.0000	0.0001	0.0000	0.0000
21. H	0.0000	0.0005	0.0000	0.0000	0.0000	0.0000	0.0000	0.0005	0.0000
22. O	0.0039	0.0002	0.0000	0.0000	0.0030	0.0144	0.0001	0.0000	0.0000
23. H	0.0001	0.0005	0.0000	0.0030	0.0000	0.0002	0.0000	0.0000	0.0000
24. H	0.0007	0.0000	0.0000	0.0144	0.0002	0.0000	0.0000	0.0000	0.0000
25. H	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
26. H	0.0000	0.0000	0.0005	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
27. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
28. H	0.0003	0.0000	0.0000	0.7163	0.0003	0.0012	0.0000	0.0000	0.0000

Atom	28
1. O	0.0001
2. C	0.0005

3.	C	0.0048
4.	O	0.0003
5.	C	0.0015
6.	C	0.0020
7.	C	0.0001
8.	N	0.0000
9.	C	0.0000
10.	O	0.0004
11.	N	0.0000
12.	C	0.0000
13.	N	0.0000
14.	C	0.0000
15.	H	0.0000
16.	C	0.0000
17.	H	0.0002
18.	H	0.0000
19.	H	0.0003
20.	H	0.0000
21.	H	0.0000
22.	O	0.7163
23.	H	0.0003
24.	H	0.0012
25.	H	0.0000
26.	H	0.0000
27.	H	0.0000
28.	H	0.0000

Wiberg bond index, Totals by atom:

Atom		1
1.	O	1.7658
2.	C	3.8174
3.	C	3.8170
4.	O	2.0417
5.	C	3.8611
6.	C	3.7964
7.	C	3.7964
8.	N	3.4572
9.	C	3.8602
10.	O	2.2247
11.	N	3.0902
12.	C	3.9508
13.	N	3.1362
14.	C	3.9199
15.	H	0.9202
16.	C	3.8550
17.	H	0.9485
18.	H	0.9655
19.	H	0.9208
20.	H	0.9254
21.	H	0.9211
22.	O	1.7773
23.	H	0.9180
24.	H	0.9261
25.	H	0.7338
26.	H	0.7897
27.	H	0.7971
28.	H	0.7281

CHELPG charges:

```
Charge= 1.00000 Dipole=    -7.4736     0.3730     1.0307 Tot= 7.5535

     1  O   -0.759860
     2  C    0.173073
     3  C    0.354385
     4  O   -0.535016
     5  C    0.380108
     6  C    0.079743
     7  C    0.537374
     8  N   -0.515333
     9  C    0.912233
    10  O   -0.398075
    11  N   -0.726933
    12  C    0.967121
    13  N   -0.992768
    14  C   -0.521923
    15  H    0.216107
    16  C    0.244789
    17  H    0.036422
    18  H   -0.010232
    19  H    0.061553
    20  H    0.042185
    21  H    0.166984
    22  O   -0.736430
    23  H    0.077072
    24  H    0.047190
    25  H    0.493341
    26  H    0.482470
    27  H    0.468405
    28  H    0.456015
 ----------------------------------------------------------------
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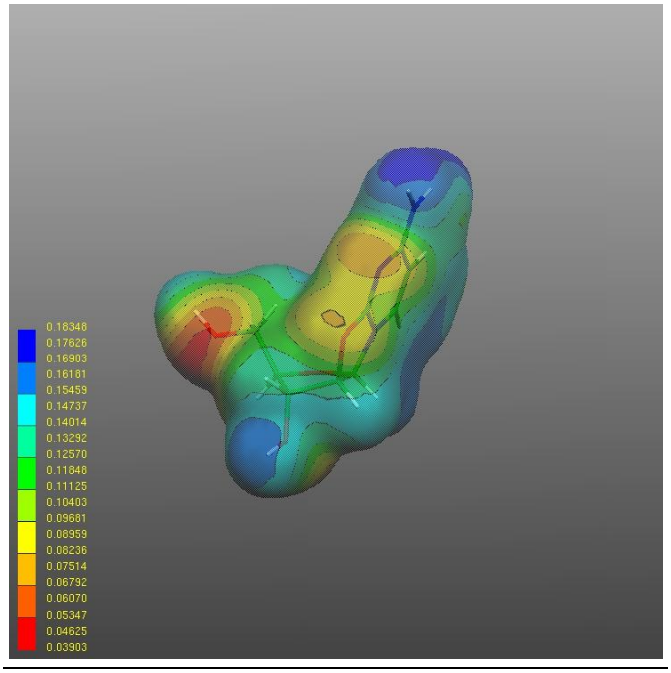
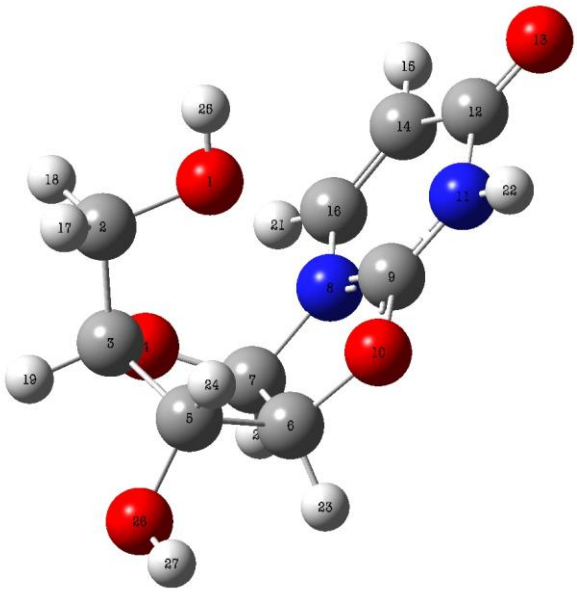
Electrostatic potential at the van der Waals surface:



7. Cation 6_{iso}



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.332421	1.428404	-1.304158
2	6	0	1.555836	1.979475	-0.811883
3	6	0	2.238705	0.961225	0.083654
4	8	0	1.503428	0.756335	1.327795
5	6	0	2.421734	-0.445520	-0.521125
6	6	0	1.310151	-1.295202	0.133208
7	6	0	0.793417	-0.437238	1.316894
8	7	0	-0.638646	-0.271266	0.934426
9	6	0	-0.863144	-0.831646	-0.255035
10	8	0	0.155944	-1.464269	-0.768927
11	7	0	-2.052159	-0.767117	-0.838744
12	6	0	-3.159937	-0.064834	-0.259960
13	8	0	-4.222790	-0.041348	-0.856535
14	6	0	-2.856672	0.555313	1.021239
15	1	0	-3.646323	1.106842	1.512994
16	6	0	-1.629841	0.446435	1.579669
17	1	0	2.236752	2.221887	-1.638176
18	1	0	1.370791	2.891250	-0.232185
19	1	0	3.213822	1.358010	0.375015
20	1	0	0.840585	-0.899004	2.302722
21	1	0	-1.352279	0.892448	2.526153
22	1	0	-2.192690	-1.217061	-1.740500
23	1	0	1.639567	-2.296463	0.401898
24	1	0	2.308856	-0.446320	-1.608924

25	1	0	-0.116135	2.085506	-1.852835
26	8	0	3.699902	-0.919265	-0.123956
27	1	0	3.919963	-1.715309	-0.629649

ENERGY (a.u):

HF =-835.0862024

Wiberg bond index matrix in the NAO basis:

Atom	1	2	3	4	5	6	7	8	9
1. O	0.0000	0.9228	0.0161	0.0024	0.0048	0.0009	0.0011	0.0047	0.0100
2. C	0.9228	0.0000	1.0088	0.0241	0.0082	0.0010	0.0032	0.0013	0.0004
3. C	0.0161	1.0088	0.0000	0.8622	0.9798	0.0077	0.0126	0.0025	0.0011
4. O	0.0024	0.0241	0.8622	0.0000	0.0175	0.0252	0.9811	0.0512	0.0081
5. C	0.0048	0.0082	0.9798	0.0175	0.0000	0.9717	0.0064	0.0016	0.0054
6. C	0.0009	0.0010	0.0077	0.0252	0.9717	0.0000	0.9754	0.0065	0.0101
7. C	0.0011	0.0032	0.0126	0.9811	0.0064	0.9754	0.0000	0.8647	0.0096
8. N	0.0047	0.0013	0.0025	0.0512	0.0016	0.0065	0.8647	0.0000	1.2210
9. C	0.0100	0.0004	0.0011	0.0081	0.0054	0.0101	0.0096	1.2210	0.0000
10. O	0.0035	0.0005	0.0017	0.0047	0.0135	0.8311	0.0128	0.0741	1.1619
11. N	0.0032	0.0003	0.0003	0.0026	0.0019	0.0117	0.0086	0.0422	1.2969
12. C	0.0005	0.0000	0.0001	0.0011	0.0002	0.0009	0.0005	0.0227	0.0087
13. O	0.0002	0.0000	0.0001	0.0015	0.0003	0.0013	0.0009	0.0303	0.0136
14. C	0.0009	0.0001	0.0002	0.0024	0.0002	0.0006	0.0087	0.0327	0.0445
15. H	0.0000	0.0000	0.0000	0.0002	0.0000	0.0004	0.0004	0.0086	0.0004
16. C	0.0010	0.0001	0.0002	0.0039	0.0003	0.0070	0.0107	1.0739	0.0149
17. H	0.0237	0.8994	0.0061	0.0123	0.0005	0.0002	0.0006	0.0002	0.0002
18. H	0.0224	0.9040	0.0028	0.0031	0.0096	0.0006	0.0001	0.0001	0.0001
19. H	0.0087	0.0037	0.8761	0.0098	0.0024	0.0040	0.0050	0.0008	0.0004
20. H	0.0002	0.0006	0.0076	0.0136	0.0025	0.0036	0.8688	0.0038	0.0052
21. H	0.0000	0.0000	0.0000	0.0014	0.0000	0.0002	0.0011	0.0015	0.0063
22. H	0.0001	0.0000	0.0000	0.0004	0.0000	0.0001	0.0006	0.0101	0.0028

23.	H	0.0002	0.0001	0.0049	0.0039	0.0019	0.8756	0.0027	0.0017	0.0047
24.	H	0.0010	0.0010	0.0035	0.0060	0.8810	0.0021	0.0053	0.0002	0.0001
25.	H	0.6999	0.0014	0.0093	0.0001	0.0001	0.0000	0.0000	0.0002	0.0001
26.	O	0.0012	0.0054	0.0162	0.0028	0.9463	0.0383	0.0017	0.0005	0.0016
27.	H	0.0000	0.0007	0.0090	0.0004	0.0015	0.0002	0.0001	0.0000	0.0000

Atom		10	11	12	13	14	15	16	17	18
1.	O	0.0035	0.0032	0.0005	0.0002	0.0009	0.0000	0.0010	0.0237	0.0224
2.	C	0.0005	0.0003	0.0000	0.0000	0.0001	0.0000	0.0001	0.8994	0.9040
3.	C	0.0017	0.0003	0.0001	0.0001	0.0002	0.0000	0.0002	0.0061	0.0028
4.	O	0.0047	0.0026	0.0011	0.0015	0.0024	0.0002	0.0039	0.0123	0.0031
5.	C	0.0135	0.0019	0.0002	0.0003	0.0002	0.0000	0.0003	0.0005	0.0096
6.	C	0.8311	0.0117	0.0009	0.0013	0.0006	0.0004	0.0070	0.0002	0.0006
7.	C	0.0128	0.0086	0.0005	0.0009	0.0087	0.0004	0.0107	0.0006	0.0001
8.	N	0.0741	0.0422	0.0227	0.0303	0.0327	0.0086	1.0739	0.0002	0.0001
9.	C	1.1619	1.2969	0.0087	0.0136	0.0445	0.0004	0.0149	0.0002	0.0001
10.	O	0.0000	0.0688	0.0070	0.0036	0.0191	0.0004	0.0090	0.0001	0.0001
11.	N	0.0688	0.0000	0.9819	0.1213	0.0114	0.0071	0.0194	0.0001	0.0000
12.	C	0.0070	0.9819	0.0000	1.6961	1.1177	0.0033	0.0328	0.0000	0.0000
13.	O	0.0036	0.1213	1.6961	0.0000	0.0736	0.0018	0.0663	0.0000	0.0000
14.	C	0.0191	0.0114	1.1177	0.0736	0.0000	0.8798	1.7127	0.0000	0.0000
15.	H	0.0004	0.0071	0.0033	0.0018	0.8798	0.0000	0.0067	0.0000	0.0000
16.	C	0.0090	0.0194	0.0328	0.0663	1.7127	0.0067	0.0000	0.0000	0.0001
17.	H	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003
18.	H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0003	0.0000
19.	H	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001	0.0001	0.0002
20.	H	0.0024	0.0007	0.0004	0.0008	0.0010	0.0000	0.0006	0.0004	0.0001
21.	H	0.0007	0.0002	0.0085	0.0015	0.0064	0.0016	0.8834	0.0000	0.0000
22.	H	0.0028	0.7143	0.0036	0.0038	0.0096	0.0003	0.0003	0.0000	0.0000
23.	H	0.0062	0.0015	0.0002	0.0002	0.0001	0.0000	0.0001	0.0000	0.0001

24.	H	0.0031	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
0.0001	0.0005							
25.	H	0.0003	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
0.0002	0.0002							
26.	O	0.0103	0.0008	0.0002	0.0001	0.0001	0.0000	0.0001
0.0002	0.0005							
27.	H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0003							

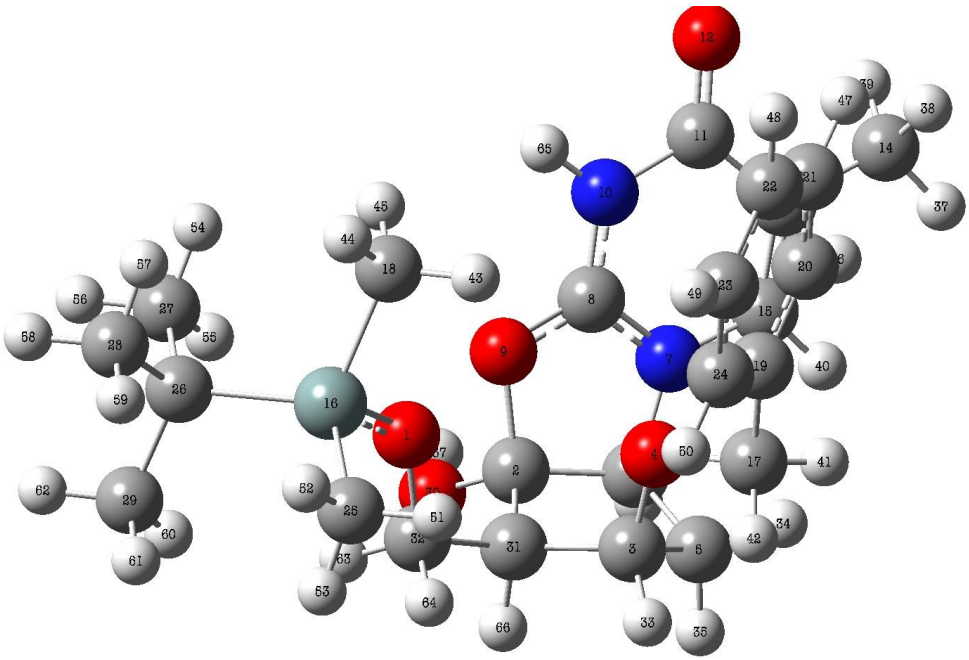
Atom	19	20	21	22	23	24	25	26	27
1.	O	0.0087	0.0002	0.0000	0.0001	0.0002	0.0010	0.6999	0.0012	0.0000
2.	C	0.0037	0.0006	0.0000	0.0000	0.0001	0.0010	0.0014	0.0054	0.0007
3.	C	0.8761	0.0076	0.0000	0.0000	0.0049	0.0035	0.0093	0.0162	0.0090
4.	O	0.0098	0.0136	0.0014	0.0004	0.0039	0.0060	0.0001	0.0028	0.0004
5.	C	0.0024	0.0025	0.0000	0.0000	0.0019	0.8810	0.0001	0.9463	0.0015
6.	C	0.0040	0.0036	0.0002	0.0001	0.8756	0.0021	0.0000	0.0383	0.0002
7.	C	0.0050	0.8688	0.0011	0.0006	0.0027	0.0053	0.0000	0.0017	0.0001
8.	N	0.0008	0.0038	0.0015	0.0101	0.0017	0.0002	0.0002	0.0005	0.0000
9.	C	0.0004	0.0052	0.0063	0.0028	0.0047	0.0001	0.0001	0.0016	0.0000
10.	O	0.0001	0.0024	0.0007	0.0028	0.0062	0.0031	0.0003	0.0103	0.0001
11.	N	0.0001	0.0007	0.0002	0.7143	0.0015	0.0000	0.0002	0.0008	0.0000
12.	C	0.0000	0.0004	0.0085	0.0036	0.0002	0.0000	0.0000	0.0002	0.0000
13.	O	0.0000	0.0008	0.0015	0.0038	0.0002	0.0000	0.0000	0.0001	0.0000
14.	C	0.0000	0.0010	0.0064	0.0096	0.0001	0.0000	0.0000	0.0001	0.0000
15.	H	0.0000	0.0000	0.0016	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000
16.	C	0.0001	0.0006	0.8834	0.0003	0.0001	0.0001	0.0000	0.0001	0.0000
17.	H	0.0001	0.0004	0.0000	0.0000	0.0000	0.0001	0.0002	0.0002	0.0000
18.	H	0.0002	0.0001	0.0000	0.0000	0.0001	0.0005	0.0002	0.0005	0.0003
19.	H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0010	0.0006	0.0047	0.0006
20.	H	0.0001	0.0000	0.0004	0.0002	0.0007	0.0001	0.0000	0.0004	0.0000
21.	H	0.0000	0.0004	0.0000	0.0005	0.0000	0.0000	0.0000	0.0000	0.0000
22.	H	0.0000	0.0002	0.0005	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
23.	H	0.0000	0.0007	0.0000	0.0000	0.0000	0.0005	0.0000	0.0030	0.0005
24.	H	0.0010	0.0001	0.0000	0.0000	0.0005	0.0000	0.0000	0.0223	0.0004

```
  25.  H  0.0006  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000
0.0001  0.0000
  26.  O  0.0047  0.0004  0.0000  0.0000  0.0030  0.0223  0.0001
0.0000  0.7049
  27.  H  0.0006  0.0000  0.0000  0.0000  0.0005  0.0004  0.0000
0.7049  0.0000
```

Wiberg bond index, Totals by atom:

Atom		1
1.	O	1.7295
2.	C	3.7872
3.	C	3.8293
4.	O	2.0417
5.	C	3.8579
6.	C	3.7766
7.	C	3.7828
8.	N	3.4572
9.	C	3.8281
10.	O	2.2377
11.	N	3.2953
12.	C	3.8864
13.	O	2.0174
14.	C	3.9218
15.	H	0.9110
16.	C	3.8436
17.	H	0.9448
18.	H	0.9451
19.	H	0.9187
20.	H	0.9140
21.	H	0.9140
22.	H	0.7496
23.	H	0.9088
24.	H	0.9286
25.	H	0.7129
26.	O	1.7615
27.	H	0.7187

8. Cation 12_{iso}



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.035718	-0.326405	-0.289910
2	6	0	-0.141659	-2.538603	-0.729295
3	6	0	-0.397643	-0.805893	-2.423282
4	8	0	-0.651141	0.327690	-1.595520
5	6	0	-1.637576	-1.724024	-2.526782
6	6	0	-1.631423	-2.559087	-1.232186
7	7	0	-2.349520	-1.922051	-0.108690
8	6	0	-1.487347	-1.511218	0.819943
9	8	0	-0.237478	-1.773839	0.586363
10	7	0	-1.913939	-0.888918	1.917399
11	6	0	-3.291191	-0.636121	2.181774
12	8	0	-3.601385	-0.061636	3.214208
13	6	0	-4.214756	-1.116913	1.150040
14	6	0	-5.682829	-0.897843	1.368182
15	6	0	-3.714417	-1.737469	0.052326
16	14	0	3.300997	0.683280	0.202352
17	6	0	-1.316396	1.402198	-2.287899
18	6	0	2.451608	1.929497	1.331043
19	6	0	-1.527397	2.548847	-1.332735
20	6	0	-2.701267	2.633483	-0.569882
21	6	0	-2.893860	3.688520	0.326591
22	6	0	-1.913319	4.676639	0.465030
23	6	0	-0.741391	4.604050	-0.295302

24	6	0	-0.551549	3.545765	-1.188669
25	6	0	4.039385	1.555813	-1.302372
26	6	0	4.642494	-0.311496	1.157898
27	6	0	3.983318	-1.107201	2.306142
28	6	0	5.676908	0.670798	1.754913
29	6	0	5.380835	-1.297435	0.224759
30	8	0	0.465855	-3.731809	-0.464590
31	6	0	0.644652	-1.735967	-1.773121
32	6	0	2.034841	-1.211056	-1.392982
33	1	0	-0.054793	-0.475847	-3.411919
34	1	0	-2.572627	-1.176270	-2.661248
35	1	0	-1.531728	-2.402708	-3.377973
36	1	0	-2.008969	-3.574162	-1.366475
37	1	0	-6.264234	-1.295634	0.534395
38	1	0	-5.900420	0.170017	1.471463
39	1	0	-6.011056	-1.386530	2.291178
40	1	0	-4.334502	-2.120470	-0.748467
41	1	0	-2.280676	1.056725	-2.682420
42	1	0	-0.692689	1.714000	-3.136701
43	1	0	1.674803	2.466542	0.776014
44	1	0	3.162146	2.668804	1.717035
45	1	0	1.975993	1.439713	2.187637
46	1	0	-3.469105	1.872028	-0.680867
47	1	0	-3.808416	3.742827	0.909995
48	1	0	-2.063546	5.500169	1.157100
49	1	0	0.020685	5.371653	-0.196256
50	1	0	0.358094	3.494697	-1.781528
51	1	0	3.266961	2.131077	-1.825626
52	1	0	4.822030	2.257148	-0.990912
53	1	0	4.486782	0.859942	-2.019869
54	1	0	3.477086	-0.449952	3.022573
55	1	0	3.245769	-1.826120	1.932208
56	1	0	4.745101	-1.672110	2.862426
57	1	0	5.216409	1.379901	2.451717
58	1	0	6.445117	0.115998	2.312041
59	1	0	6.191876	1.247897	0.977923
60	1	0	4.706051	-2.050182	-0.197106
61	1	0	5.877152	-0.786759	-0.608229
62	1	0	6.157134	-1.837485	0.785881
63	1	0	2.664303	-2.084790	-1.178833
64	1	0	2.446906	-0.726445	-2.288772
65	1	0	-1.236383	-0.587660	2.613728
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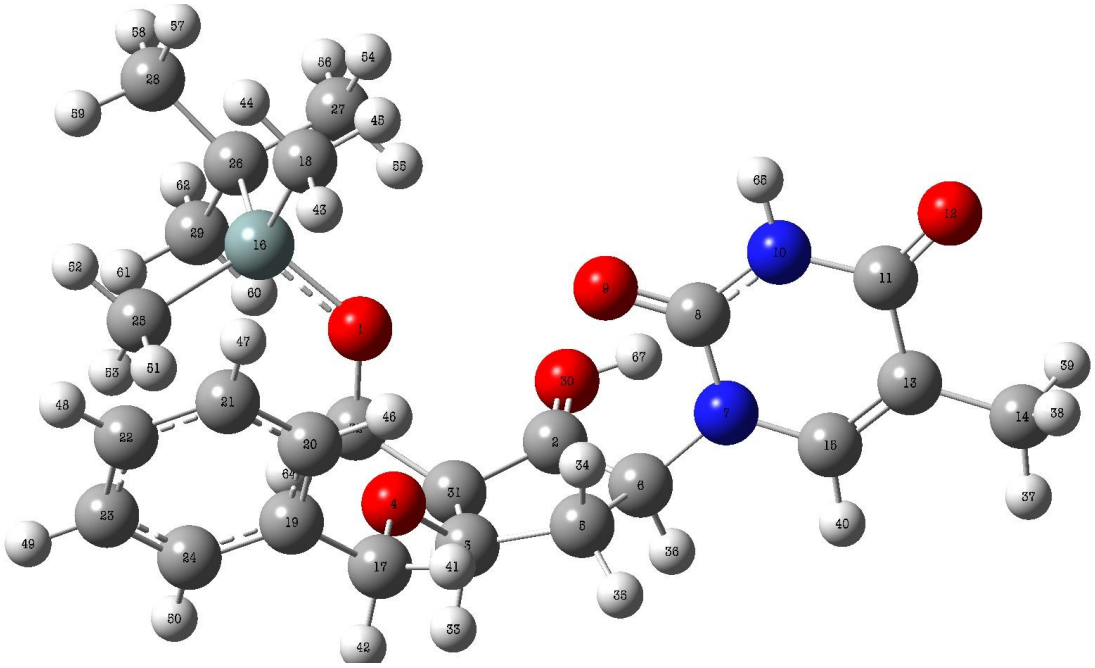
67	1	0	-0.084007	-4.302258	0.096031

ENERGY (a.u):

HF = -1710.78095427

9. Cation 12$_{syn}$



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26	6	0	-2.598309	3.730345	0.247101
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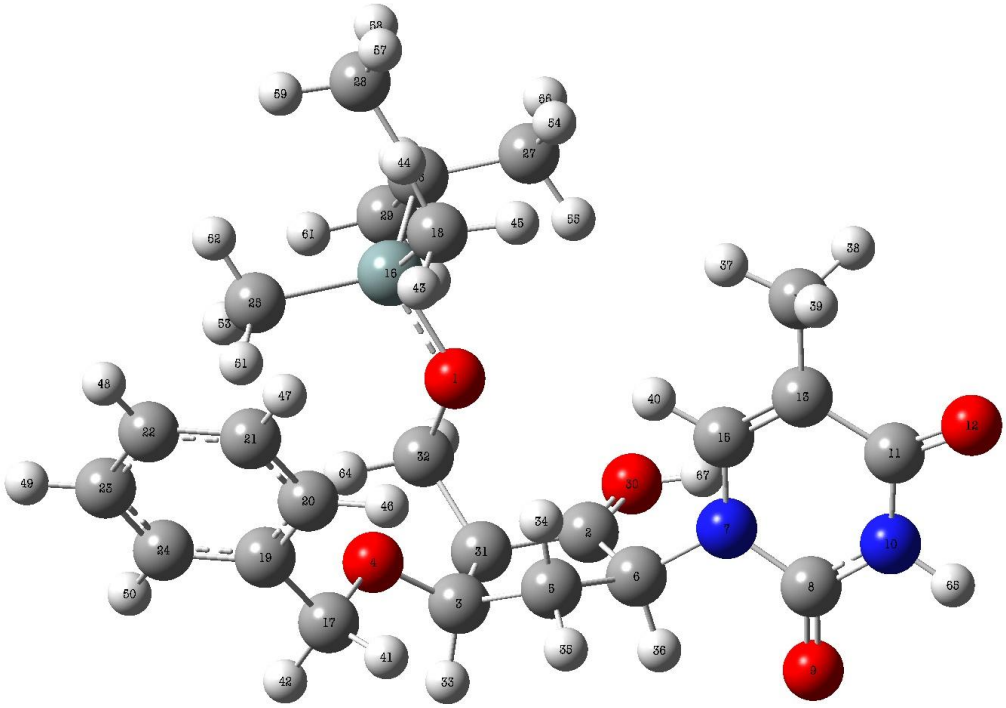
ENERGY (a.u):

HF = -1710.76256618

10. Cation 12*anti*



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55	1	0	-1.855361	3.200815	0.564773
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ENERGY (a.u):

HF = -1710.7654645

Characterization of new compounds 9a,b, 7a,b, 10a,b and 11a-c

Starting oxirane **8** {(2R,3S)-2-benzyloxymethyl-6-oxabicyclo[3.1.0]-3-hexanol} was prepared according to the known procedure (Biggadike, K.; Borthwick, A. D.; Evans, D.; Exall, A. M.; Kirk, B. E.; Roberts, S. M.; Stephenson, L.; Youds, P. *J. Chem. Soc., Perkin Trans. I*, **1988**, 549-554).

For compounds **7a,b-11a,b**, NMR spectra have been registered for solutions in $CDCl_3$, at room temperature, while ^1H and ^{13}C NMR spectra of compound **11c** have been taken for $CD_3C(O)CD_3$ and CD_3OD solutions, respectively (Bruker DPX-300 NMR spectrometer).

Methane has been used as the reagent gas, recording HRMS/CI mass-spectra (VG-Fison AutoSpec mass-spectrometer).

(2R,3S)-2-Benzyloxymethyl-3-(*tert*-butyldimethyl)silyloxy-6-oxabicylo[3.1.0]hexane (9a).

^{13}C NMR (ppm): 130.11, 128.39, 127,66, 127.48 (Ph), 75.42 (C-3), 73.19 (Ph$\underline{C}H_2O$), 69.20 (O$\underline{C}H_2CH$), 60.13, 58.20 (C-5 and C-1), 50.78 (C-2), 38.29 (C-4), 25.94 (3 $\underline{C}H_3C$), 18.81 ($Me_2Si\underline{C}$), -4.62 (2 $\underline{C}H_3Si$).

^1H NMR (ppm): 7.35 (5H, m, Ph), 4.51 (2H, q, BnOC$\underline{H_2}$), 4.21 (1H, d, H-3), 3.42-3.53 (4H, overlapping multiplets, H-1, H-5 and PhC$\underline{H_2}$O), 2.34 (1H, td, H-2), 2.12 (1H, ddd, H-4'), 1.91 (1H, dd, H-4"), 0.85 (9H, s, 3 C$\underline{H_3}$C), 0.01 (6H, 2 C$\underline{H_3}$Si).

HRMS: found 335.2040 $[M+H]^+$, calc. 335.2043 for $C_{19}H_{31}O_3Si$.

(2R,3S)-2-(*Tert*-butyldimethylsilyl)oxymethyl-3-benzyloxy-6-oxabicylo[3.1.0]hexane (9b).

^{13}C NMR (ppm): 138.49, 128.29, 127, 69, 127.40 (Ph), 80.98 (C-3), 70.86 (Ph$\underline{C}H_2O$), 62.38 (BnO$\underline{C}H_2$), 59.88, 57.95 (C-5 and C-1), 49.39 (C-2), 35.00 (C-4), 25.79 (3 $CH_3\underline{C}$), 18.16 ($Me_2Si\underline{C}$), -5.58 (2 $\underline{C}H_3Si$).

^1H NMR (ppm): 7.30 (5H, m, Ph), 4.51 (2H, q, PhC$\underline{H_2}$), 3.88 (1H, d, H-3), 3.58 (2H, d, SiOC$\underline{H_2}$), 3.55, 3.45 (2H, H-1 and H-5), 2.51 (1H, t, H-2), 2.17 (1H, d, H-4'), 2.08 (1H, ddd, H-4"), 0.88 (9H, s, 3 C$\underline{H_3}$C), 0.03 (6H, 2 C$\underline{H_3}$Si).

HRMS: found 335.2087 $[M+H]^+$, calc. 335.2043 for $C_{19}H_{31}O_3Si$.

(1S,2R,3S,5S)-5-Thymino-2-benzyloxymethyl-3-(*tert*-butyldimethyl)silyloxycyclopentanol (10a).

^{13}C NMR (ppm): 163.99 (C-4), 151.35 (C-2), 138.76 (C-6), 137.95, 128.43, 127.75, 127.68 (Ph), 110.68 (C-5), 75.76 (C-1'), 73.49 (Ph$\underline{C}H_2O$), 69.96 (C-3'), 69.45 (BnO$\underline{C}H_2$), 63.91 (C-5'), 54.22 (C-2'), 37.11 (C-4'), 25.73 (3 $\underline{C}H_3C$), 17.90 ($Me_3Si\underline{C}$), 12.32 (5-$\underline{C}H_3$), -4.67, -4.92 (2 $\underline{C}H_3Si$).

^1H NMR (ppm): 9.49 (1H, N*H*), 7.25-7.35 (5H, m, Ph), 6.96 (1H, d, H-6), 4.60 (1H, q, H-5'), 4.49 (2H, q, PhC$\underline{H_2}$), 4.17 (1H, t, H-1'), 4.15 (1H, td, H-3'), 3.69 (1H, dd, BnOC$\underline{H_a}$), 3.56 (1H, dd, BnOC$\underline{H_b}$), 3.36 (1H, broadened, OH), 2.11 (1H, dtd, H-4'$_a$), 2.05 (1H, m, H-2'), 1.99 (1H, ddd, H-4'$_b$), 1.80 (3H, 5-C$\underline{H_3}$), 0.82 (9H, s, 3 C$\underline{H_3}$C), 0.02 (6H, s, 2 C$\underline{H_3}$Si).

HRMS: found 461.2410 $[M+H]^+$, calc. 461.2372 for $C_{24}H_{37}N_2O_5Si$.

(1S,2R,3S,5S)-5-Thymino-2-(*tert*-butyldimethyl)silyloxymethyl-3-benzyloxycyclopentanol (10b).

^{13}C NMR (ppm): 163.60 (C-4), 151.18 (C-2), 138.48 (C-6), 137.97, 128.46, 127.78, 127.68 (Ph), 110.81 (C-5), 76.14, 76.03 (C-1' and C-3'), 71.30 (Ph$\underline{C}$H$_2$O), 63.96 (C-5'), 63.30 (BnO$\underline{C}$H$_2$), 53.21 (C-2'), 33.44 (C-4'), 25.84 (3 $\underline{C}$H$_3$C), 18.14 (Me$_2$Si$\underline{C}$), 12.43 (5-$\underline{C}$H$_3$), -5.54, -5.59 (2 $\underline{C}$H$_3$Si).

^{1}H NMR (ppm): 8.79 (1H, N*H*), 7.25-7.37 (5H, m, Ph), 6.99 (1H, d, H-6), 4.63 (1H, q, H-5'), 4.52, 4.44 (2H, q, PhC$\underline{H_2}$), 4.21 (1H, t, H-1'), 3.89 (1H, dd, BnOC$\underline{H}_a$), 3.86 (1H, m, H-3'), 3.72 (1H, dd, BnOC$\underline{H}_b$), 3.45 (1H, broadened, OH), 2.12-2.22 (3H, overlapping multiplets, H-2', 2 H-4'), 1.90 (3H, d, 5-C$\underline{H_3}$), 0.88 (9H, s, 3 C$\underline{H_3}$C), 0.06, 0.07 (6H, s, 2 C$\underline{H_3}$Si).

HRMS: found 461.2432 [M+H]$^+$, calc. 461.2372 for $C_{24}H_{37}N_2O_5Si$.

(1S,2R,3S,5S)-5-Thymino-2-benzyloxymethyl-3-(*tert*-butyldimethyl)silyloxycyclopentanone (7a, crude).

^{1}H NMR (ppm): 9.49 (1H, N*H*), 7.25-7.35 (5H, m, Ph), 6.67 (1H, d, H-6), 5.33 (1H, dd, H-5'), 4.60 (1H, m, H-3'), 4.48 (2H, s, PhC$\underline{H_2}$), 3.95 (1H, dd, BnOC$\underline{H}_a$C), 3.78 (1H, dd, BnOC$\underline{H}_b$C), 2.3-2.5 (3H, overlapping multiplets, H-2', 2 H-4'), 1.56 (3H, d, 5-C$\underline{H_3}$), 0.87 (9H, s, 3 C$\underline{H_3}$C), 0.07 (6H, s, 2 C$\underline{H_3}$Si).

HRMS: found 459.2291 [M+H]$^+$, calc. 459.2315 for $C_{24}H_{35}N_2O_5Si$.

(1S,2R,3S,5S)-5-Thymino-2-(*tert*-butyldimethyl)silyloxymethyl-3-benzyloxy cyclopentanone (7b, crude).

^{13}C NMR (ppm): 211.49 (C-1'), 163.56 (C-4), 150.54 (C-2), 138.31 (C-6), 137.44, 128.55, 127.95, 127.71 (Ph), 111.32 (C-5), 76.16 (C-3'), 70.89 (Ph$\underline{C}$H$_2$O), 62.79 (SiO$\underline{C}$H$_2$), 61.34 (C-5'), 54.64 (C-3'), 51.58 (C-2'), 33.20 (C-4'), 25.62 (3 $\underline{C}$H$_3$C), 18.29 (Me$_2$Si$\underline{C}$), 12.28 (5-$\underline{C}$H$_3$), -5.51, -5.60 (2 $\underline{C}$H$_3$Si).

^{1}H NMR (ppm): 8.3 (1H, N*H*), 7.3-7.4 (5H, m, Ph), 6.74 (1H, d, H-6), 5.26 (1H, q, H-5'), 4.57 (2H, q, PhC$\underline{H_2}$), 4.30 (1H, d, H-3'), 4.01 (1H, dd, BnOC$\underline{H}_a$), 3.86 (1H, dd, BnOC$\underline{H}_b$), 2.4-2.7 (3H, overlapping multiplets, H-2', 2 H-4'), 1.87 (3H, d, 5-C$\underline{H_3}$), 0.89 (9H, s, 3 C$\underline{H_3}$C), 0.08 (6H, s, 2 C$\underline{H_3}$Si).

HRMS: found 459.2273 [M+H]$^+$, calc. 459.2315 for $C_{24}H_{35}N_2O_5Si$.

5-Thymino-2-benzyloxymethyl-2-cyclopentenone (11a)

^{13}C NMR (ppm): 200.65 (C-1'), 163.59 (C-4), 155.93 (C-3'), 150.29 (C-2), 142.39 (C-2'), 139.01 (C-6), 137.59, 128.48, 127.91, 127.84 (Ph), 110.54 (C-5), 73.36 (Ph$\underline{C}$H$_2$O), 63.93 (BnO$\underline{C}$H$_2$), 61.20 (C-5'), 32.93 (C-4'), 12.34 (5-$\underline{C}$H$_3$).

^{1}H NMR (ppm): 8.59 (1H, N*H*), 7.58 (1H, m, H-3'), 7.25-7.35 (5H, m, Ph), 6.72 (1H, d, 1.0 Hz, H-6), 4.58 (1H, dd, 7.5, 3.8 Hz, H-5'), 4.55 (2H, s, PhC$\underline{H_2}$), 4.22 (2H, m, BnOC$\underline{H_2}$), 3.09 (1H, dddt, 18.5, 7.5, 3.0, 1.5 Hz, H-4'$_a$), 2.74 (1H, dddt, 18.5, 3.8, 2.5, 2.0 Hz, H-4'$_b$), 1.86 (3H, d, 1.0 Hz, H-4'$_b$),

HRMS: found 327.1304 [M+H]$^+$, calc. 327.1345 for $C_{18}H_{19}N_2O_4$.

5-Thymino-2-(*tert*-butyldimethyl)silyloxymethyl-2-cyclopentenone (11b)

^{13}C NMR (ppm): 200.66 (C-1'), 163.40 (C-4), 154.95 (C-2), 154.38 (C-3'), 145.29 (C-2'), 138.85 (C-6), 111.56 (C-5), 61.38 (C-5'), 57.44 (BnO<u>*C*</u>H$_2$), 32.87 (C-4'), 25.83 (3 <u>*C*</u>H$_3$C), 18.29 (Me$_2$Si<u>*C*</u>), 12.37 (5-<u>*C*</u>H$_3$), -5.47 (2 <u>*C*</u>H$_3$Si).

^{1}H NMR (ppm): 8.30 (1H, N*H*), 7.50 (1H, m, H-3'), 6.82 (1H, dd, (H-6), 4.70 (1H, dd, H-5'), 4.43 (2H, m, SiOC<u>*H*$_2$</u>), 3.15 (1H, ddd, H-4'$_a$), 2.77 (1H, dddt, H-4'$_b$), 1.95 (3H, s, 5-C<u>*H*$_3$</u>), 0.95 (9H, s, 3 C<u>*H*$_3$</u>C), 0.12 (6H, s, 2 C<u>*H*$_3$</u>Si).

HRMS: found 351.1712 $[M+H]^+$, calc. 351.1740 for $C_{17}H_{27}N_2O_4Si$.

5-Thymino-2-hydroxymethyl-2-cyclopentenone (11c)

^{13}C NMR (ppm): 203.56 (C-1'), 166.75 (C-4), 156.61 (C-3'), 152.25 (C-2), 145.42 (C-2'), 143.08 (C-6), 111.48 (C-5), 62.87 (C-5'), 57.27 (O<u>*C*</u>H$_2$), 33.27 (C-4'), 12.22 (5-<u>*C*</u>H$_3$).

^{1}H NMR (ppm): 10.05 (1H, N*H*), 7.55 (1H, m, H-6), 7.31 (1H, d, 1.0 Hz, H-6), 4.70 (1H, dd, H-5'), 4.25 (2H, m, C<u>*H*$_2$</u>), 3.41 (1H, ddt, H-4'$_a$), 2.86 (1H, dq, H-4'$_b$), 1.82 (3H, d, 1.0 Hz, (5-<u>*C*</u>H$_3$).

HRMS: found 237.0844 $[M+H]^+$, calc. 237.0875 for $C_{11}H_{13}N_2O_4$.