Supporting Information

Ground State Destabilization in Uracil DNA Glycosylase (UDG): Let's Not Forget "Tautomeric Strain" in Substrates

Ranjita Das,[†] Erik A. Vázquez-Montelongo,[‡] G. Andrés Cisneros[‡] and Judy I. Wu[†,*]

[†] *Department of Chemistry, University of Houston, Houston, Texas 77204, United States*
[‡]*Department of Chemistry, University of North Texas, Denton, Texas 76201, United States*

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Full citation for Gaussian09:

Gaussian 09, Revision E.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.

Supplementary Note 1: Harmonic Oscillator Model of Electron Delocalization (HOMED)

HOMED is a geometric criterion for quantifying the aromaticity of heterocycles:

$$\mathrm{HOMED} = 1 - \frac{1}{n}\left\{\alpha_{CC}\sum[R_o(\mathrm{CC}) - R_i(\mathrm{CC})]^2 + \alpha_{CX}\sum[R_o(\mathrm{CX}) - R_i(\mathrm{CX})]^2\right\}$$

where α_{CC} and α_{CX} are based on:

$\alpha_{2i} = 2\{(R_o - R_s)^2 + (R_o - R_d)^2\}^{-1}$ for heterocycles with an even number of bonds.

$\alpha_{2i+1} = (2i+1)\{(i+1)(R_o - R_s)^2 + i(R_o - R_d)^2\}^{-1}$ for heterocycles with an odd number of bonds.

Based on the computed geometries of selected reference compounds (see right): R_s (single bond length), R_d (double bond length), and R_o (optimal bond length) are the reference bond lengths for CC and CN bonds. All reference bond lengths and HOMED parameters were computed at ωB97X-D/6-31+G(d).

Bond	R_s	R_d	R_0
C-C	$H_3C—CH_3$	$H_2C=CH_2$	
C-N	$H_3C—NH_2$	$H_2C=NH$	

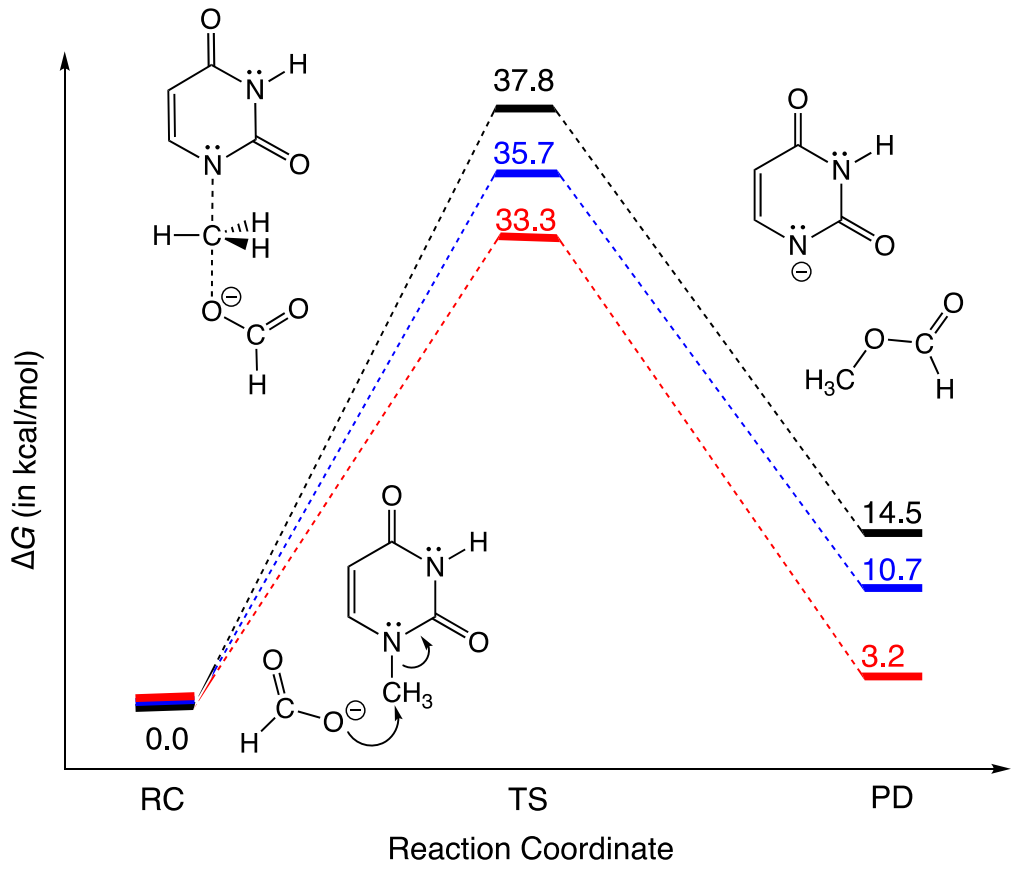


Figure S1: Computed gas-phase S_N2 activation free energy barrier for N–CH_3 bond cleavage in naked (in black), three water bound (in blue), and two zwitterionic glycine bound 1-methyl-uracil with formate as the nucleophile. Free energies (ΔG, in kcal/mol) were computed at 298 K at ωB97X-D/6-31+G(d).

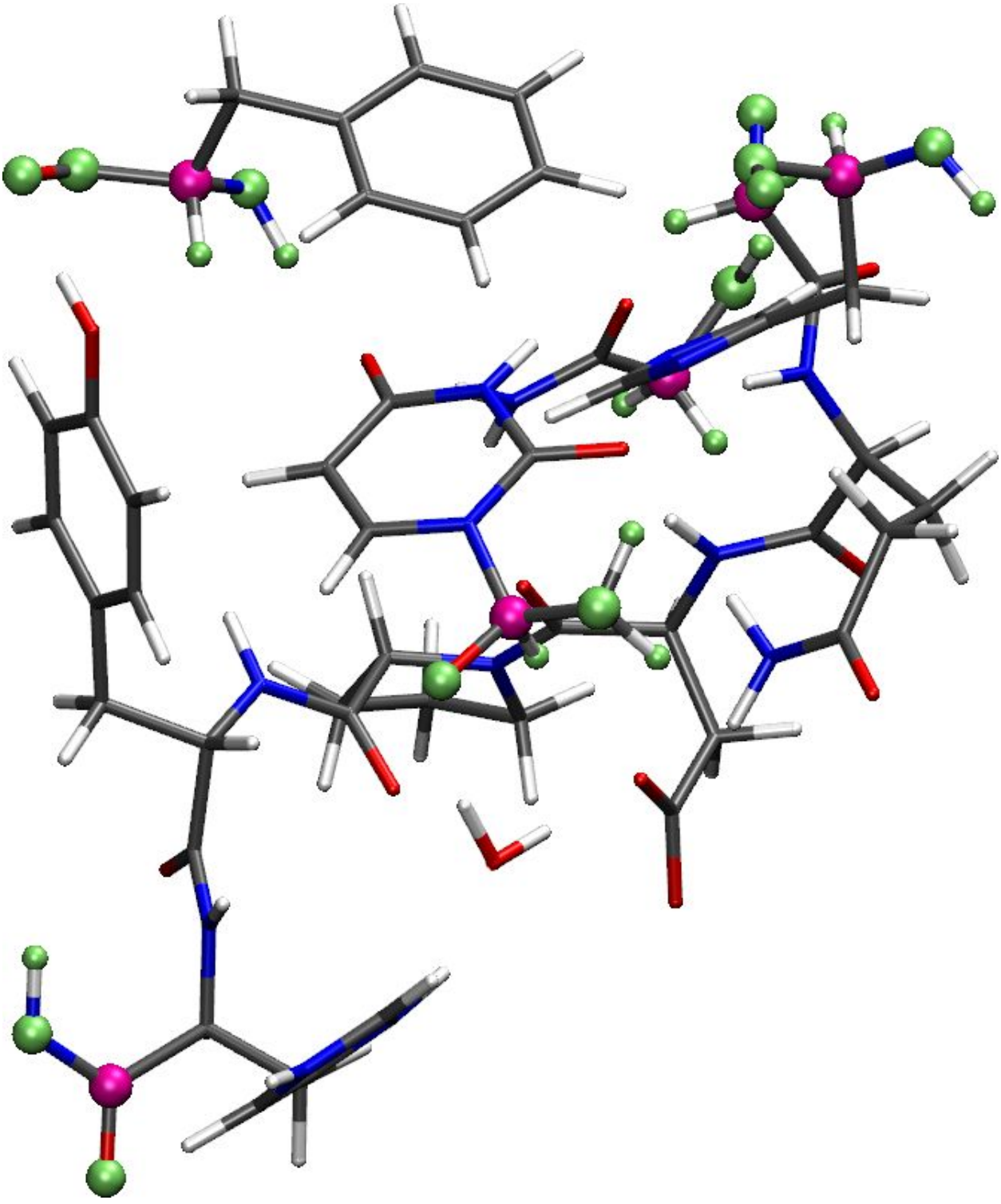


Figure S2. QM/MM model of the UDG active site used for geometry optimization: Green and pink dots represents boundary atoms and pseudo-bonds, respectively.

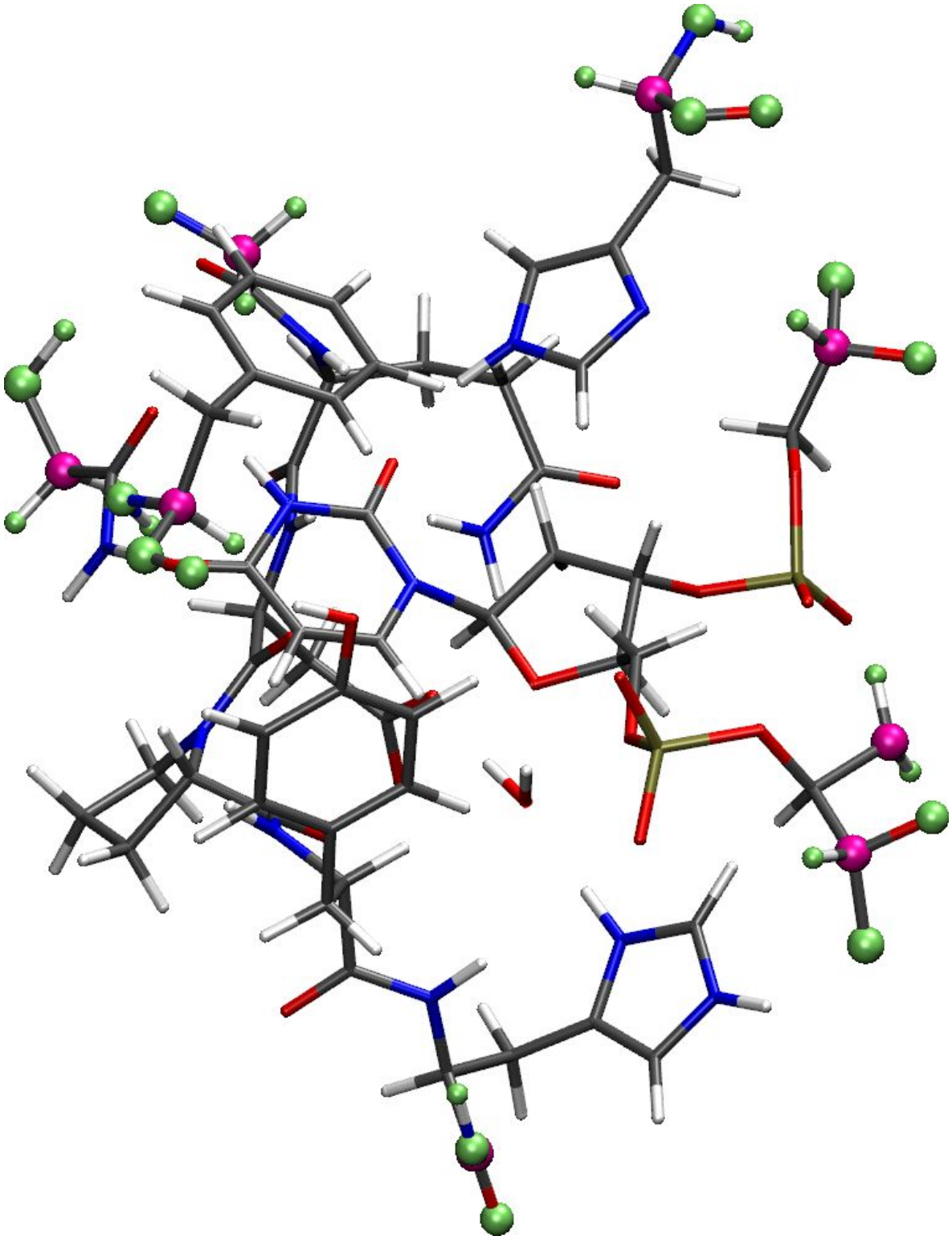
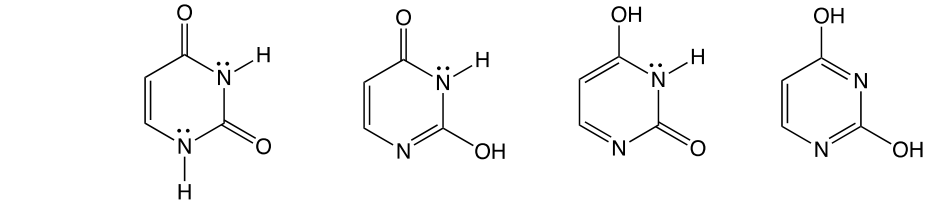


Figure S3. QM/MM model of the UDG active site used for single-point calculation: Green and pink dots represents boundary atoms and pseudo-bonds, respectively.

Table S1. Computed relative energies (ΔE, in the gas-phase, and at ε = 4) for substrate (**1-4**)-residue complexes.



Complex	ΔE (kcal/mol)	
	Gas phase	ε = 4.0
1-residue	0.00	0.00
2-residue	15.57	18.42
3-residue	24.12	22.18
4-residue	17.53	19.75

Optimized Cartesian coordinates at ωB97X-D/6-31+G(d).

Uracil

N	-1.19417	0.94912	0.00000
C	-0.05599	1.71901	0.00000
H	-0.22201	2.79047	0.00000
C	1.17287	1.17070	0.00000
H	2.07135	1.77228	0.00000
C	1.31599	-0.28180	0.00000
O	2.36601	-0.89601	0.00000
N	0.09204	-0.97104	0.00000
C	-1.18124	-0.43788	0.00000
O	-2.19667	-1.10466	0.00000
H	0.14442	-1.98317	0.00000
H	-2.11196	1.37027	0.00000

Charge: 0 Point Group: C_s
Total electronic energy = –414.70095 a.u.
Zero-point corrected total electronic energy (E_{ZPE}) = –414.61247 a.u.
No. of imaginary frequency = 0

Uracil (in implicit solvation at ε = 4.0, with IEF-PCM model)

N	-1.13713	-1.02353	0.00000
C	0.05335	-1.70429	0.00000
H	-0.03184	-2.78450	0.00000
C	1.23904	-1.06308	0.00000
H	2.17782	-1.59951	0.00000
C	1.26761	0.38945	0.00000
O	2.27138	1.08859	0.00000
N	0.00000	0.98540	0.00000
C	-1.22579	0.35408	0.00000
O	-2.28999	0.95108	0.00000
H	-0.02616	1.99910	0.00000
H	-2.01631	-1.52258	0.00000

Charge: 0 Point Group: C_s
Total electronic energy = –414.71309 a.u.
Zero-point corrected total electronic energy (E_{ZPE}) = –414.62466 a.u.
No. of imaginary frequency = 0

Uracil (in implicit water solvation, with IEF-PCM model)

C	-0.40973	1.20636	0.00000
N	-0.98372	-0.04709	0.00000
C	-0.32718	-1.28110	0.00000
C	1.11918	-1.18530	0.00000
C	1.70386	0.03057	0.00000
N	0.96694	1.18580	0.00000
O	-1.06275	2.24035	0.00000
O	-0.98063	-2.31986	0.00000
H	2.77817	0.16818	0.00000
H	1.70322	-2.09533	0.00000
H	-1.99771	-0.06845	0.00000
H	1.42775	2.08649	0.00000

Charge: 0 Point Group: C_s
Total electronic energy = –414.71928 a.u.
Zero-point corrected total electronic energy (E_{ZPE}) = –414.63091 a.u.
No. of imaginary frequency = 0

Uracil : $3H_2O$

C	1.15187	0.73967	-0.04793
N	-0.00115	0.00216	-0.03728
C	-0.08759	-1.38619	-0.04130
C	1.18686	-2.08745	0.01888
C	2.32979	-1.37679	0.03629
N	2.31647	-0.00525	0.00143
O	1.18820	1.96383	-0.09734
O	-1.17765	-1.94775	-0.09368
H	-0.90041	0.54579	-0.01557
H	1.17869	-3.16847	0.03693
H	3.31215	-1.83372	0.07211
H	3.17326	0.52962	-0.00963
O	-0.93392	3.51766	-1.14572
O	-2.33687	1.43392	0.00050
O	-3.55884	-0.79108	-1.05974
H	-0.13274	3.08856	-0.78643
H	-0.99477	4.37342	-0.70718
H	-2.96211	0.86602	-0.49332
H	-2.13320	2.22695	-0.53351
H	-2.78869	-1.29595	-0.72876
H	-4.32650	-1.14770	-0.59960

Charge: 0 Point Group: C_1
Total electronic energy = –643.95359 a.u.
Zero-point corrected total electronic energy (E_{ZPE}) = –643.78786 a.u.
No. of imaginary frequency = 0

2 (keto-enol tautomer of uracil)

N	1.19364	-1.05638	0.00000
C	-0.01732	-1.70386	0.00000
H	0.05124	-2.78783	0.00000
C	-1.22777	-1.08685	0.00000
H	-2.15835	-1.63997	0.00000
C	-1.30077	0.35909	0.00000
O	-2.29448	1.06410	0.00000
N	-0.01806	0.95459	0.00000
C	1.12805	0.23824	0.00000
O	2.23378	0.98538	0.00000
H	0.01990	1.96778	0.00000
H	2.98796	0.37521	0.00000

Charge: 0 Point Group: C_s
Total electronic energy = –414.68015 a.u.
Zero-point corrected total electronic energy (E_{ZPE}) = –414.59201 a.u.
No. of imaginary frequency = 0

2 (keto-enol tautomer of uracil in implicit solvation at ε = 4.0, with IEF-PCM model)

N	1.16583	-1.09364	0.00000
C	-0.05787	-1.71125	0.00000
H	-0.01870	-2.79647	0.00000
C	-1.25463	-1.06393	0.00000
H	-2.19638	-1.59783	0.00000
C	-1.28719	0.37834	0.00000
O	-2.27256	1.10776	0.00000
N	0.00000	0.94507	0.00000
C	1.13187	0.20514	0.00000
O	2.24681	0.93062	0.00000
H	0.06587	1.95773	0.00000
H	3.00132	0.31969	0.00000

Charge: 0 Point Group: C_s
Total electronic energy = –414.68943 a.u.
Zero-point corrected total electronic energy (E_{ZPE}) = – 414.60144 a.u.

No. of imaginary frequency = 0

3 (keto-enol tautomer of uracil)

N	-1.27575	-1.10077	0.00000
C	-0.11626	-1.70564	0.00000
H	-0.15472	-2.79461	0.00000
C	1.15717	-1.08454	0.00000
H	2.07637	-1.65682	0.00000
C	1.14302	0.28642	0.00000
O	2.20213	1.10447	0.00000
N	-0.03861	0.93091	0.00000
C	-1.30368	0.27853	0.00000
O	-2.30358	0.96611	0.00000
H	-0.05751	1.94421	0.00000
H	3.02092	0.59140	0.00000

Charge: 0 Point Group: C_s
Total electronic energy = –414.66307 a.u.
Zero-point corrected total electronic energy (E_{ZPE}) = –414.57575 a.u.
No. of imaginary frequency = 0

3 (keto-enol tautomer of uracil in implicit solvation at ε = 4.0, with IEF-PCM model)

N	-1.27566	-1.09325	0.00000
C	-0.11096	-1.70631	0.00000
H	-0.15228	-2.79419	0.00000
C	1.15400	-1.08866	0.00000
H	2.07373	-1.65906	0.00000
C	1.14200	0.28616	0.00000
O	2.19410	1.10064	0.00000
N	-0.04208	0.93029	0.00000
C	-1.29328	0.27926	0.00000
O	-2.30701	0.96464	0.00000
H	-0.05319	1.94468	0.00000
H	3.02013	0.59548	0.00000

Charge: 0 Point Group: C_s
Total electronic energy = –414.67851 a.u.
Zero-point corrected total electronic energy (E_{ZPE}) = –414.59101a.u.
No. of imaginary frequency = 0

4 (dienol tautomer of uracil)

N	-1.24331	-1.05382	0.00000
C	-0.08441	-1.72838	0.00000
H	-0.16735	-2.81214	0.00000
C	1.15172	-1.11290	0.00000
H	2.08524	-1.66014	0.00000
C	1.11842	0.28705	0.00000
O	2.26749	0.97080	0.00000
N	-0.00714	0.98684	0.00000
C	-1.13012	0.27128	0.00000
O	-2.26013	0.98441	0.00000
H	2.04122	1.91475	0.00000
H	-2.99369	0.35078	0.00000

Charge: 0 Point Group: C_s
Total electronic energy = –414.67518 a.u.
Zero-point corrected total electronic energy (E_{ZPE}) = –414.58702 a.u.
No. of imaginary frequency = 0

4 (dienol tautomer of uracil in implicit solvation at ε = 4.0, with IEF-PCM model)

N	-1.24438	-1.05862	0.00000
C	-0.08174	-1.73090	0.00000
H	-0.15923	-2.81454	0.00000
C	1.15179	-1.11126	0.00000
H	2.08544	-1.65833	0.00000
C	1.11700	0.28839	0.00000
O	2.26694	0.96940	0.00000
N	-0.01264	0.98477	0.00000
C	-1.13343	0.26574	0.00000
O	-2.26203	0.98419	0.00000
H	2.05642	1.91751	0.00000
H	-3.00620	0.36217	0.00000

Charge: 0 Point Group: C_s
Total electronic energy = –414.68207 a.u.
Zero-point corrected total electronic energy (E_{ZPE}) = –414.59423 a.u.
No. of imaginary frequency = 0

1uracil (hydrogen-bonded to His, Asn, and a fragment of protein backbone)

C	-2.36335	1.06679	0.65946

N	-2.47624	0.31487	-0.47599
C	-3.61585	0.18946	-1.27207
C	-4.74793	1.00195	-0.85500
C	-4.64213	1.76582	0.24835
N	-3.48576	1.79388	0.99001
O	-1.34862	1.10342	1.35221
O	-3.61502	-0.56410	-2.23780
H	-1.63335	-0.22289	-0.77068
N	2.16390	-1.05714	0.43280
C	1.86314	-1.55440	1.76692
C	0.59739	-2.41082	1.64421
O	0.65764	-3.60640	1.36732
C	1.79655	-0.43266	2.80682
N	-0.58511	-1.77376	1.80862
C	-1.82923	-2.44924	1.51155
C	0.78650	-3.19103	-1.89647
C	-0.34503	-2.20257	-1.89984
O	-0.24605	-1.11612	-1.29582
N	-1.47322	-2.53406	-2.54311
C	4.27805	3.65595	-0.69346
C	2.93181	3.00815	-0.66809
N	2.15685	2.89600	-1.80251
C	2.27772	2.44699	0.39895
C	1.06020	2.27993	-1.41937
N	1.08116	1.98587	-0.09541
H	1.06106	0.33566	2.54265
H	2.77868	0.04443	2.86617
H	2.66568	-2.24295	2.04401
H	-0.60248	-0.76262	1.86065
H	0.89322	-3.59348	-0.88252
H	0.63271	-4.01437	-2.59865
H	-2.26235	-1.88418	-2.55433
H	-1.55642	-3.41279	-3.02931
H	4.20327	4.70118	-1.01310
H	4.74298	3.62854	0.29662
H	2.56037	2.31932	1.43308
H	0.34181	1.53850	0.43515
H	0.22924	2.01267	-2.05837
H	-5.44720	2.39136	0.61611
H	4.94354	3.14467	-1.39807

H	1.71538	-2.67141	-2.14450
H	1.39325	-0.89493	-0.21036
C	3.43929	-0.81264	0.02929
H	1.54152	-0.83096	3.79467
O	4.40227	-0.95523	0.77558
C	3.59718	-0.38905	-1.41758
H	2.65184	-0.11018	-1.89203
H	4.27685	0.46394	-1.46418
H	4.05434	-1.21488	-1.97346
H	-5.65425	0.96462	-1.44345
H	-1.89480	-3.38217	2.07653
H	-2.65901	-1.79937	1.80047
H	-1.91608	-2.69103	0.44478
H	-3.40700	2.36451	1.82047

Charge: 0 Point Group: C_1
Total electronic energy = –1385.10132 a.u.
Zero-point corrected total electronic energy (E_{ZPE}) = –1384.64141a.u.
No. of imaginary frequency = 1 (18.5i cm^{-1}, corresponding to His methyl rotation)

1uracil (hydrogen-bonded to His, Asn, and a fragment of protein backbone in implicit solvation at ε = 4.0, with IEF-PCM model)

C	2.26678	1.28540	-1.10062
N	2.52367	0.77688	0.14105
C	3.71568	0.90764	0.85257
C	4.73670	1.69874	0.19549
C	4.48764	2.21792	-1.02333
N	3.28670	2.01314	-1.65589
O	1.19806	1.10189	-1.69092
O	3.83663	0.36620	1.94976
H	1.75941	0.23357	0.58979
N	-1.94188	-1.24283	-0.22925
C	-1.65183	-1.90906	-1.49311
C	-0.29131	-2.60304	-1.34334
O	-0.21358	-3.77298	-0.96185
C	-1.75869	-0.96271	-2.69067
N	0.79795	-1.85926	-1.61739
C	2.13484	-2.34455	-1.34109
C	-0.20870	-2.79880	2.30692

C	0.77226	-1.68112	2.08514
O	0.48833	-0.72466	1.33216
N	1.95956	-1.75355	2.69428
C	-4.52415	3.35092	0.28779
C	-3.11094	2.86556	0.28638
N	-2.28189	3.02781	1.37756
C	-2.43492	2.21546	-0.71454
C	-1.13257	2.48281	1.03132
N	-1.17383	1.97785	-0.22348
H	-1.09279	-0.09816	-2.59635
H	-2.78518	-0.59232	-2.75900
H	-2.38263	-2.71247	-1.61272
H	0.69311	-0.86477	-1.78625
H	-0.34910	-3.33256	1.36148
H	0.12000	-3.50528	3.07233
H	2.65389	-1.01691	2.54911
H	2.18972	-2.52622	3.30032
H	-4.56962	4.43299	0.45430
H	-5.01216	3.12943	-0.66596
H	-2.73760	1.89648	-1.70068
H	-0.40151	1.54400	-0.72281
H	-0.24789	2.42245	1.65038
H	5.20522	2.81568	-1.57170
H	-5.10324	2.87145	1.08547
H	-1.17353	-2.37496	2.59748
H	-1.16025	-0.90441	0.33189
C	-3.20655	-1.07781	0.22443
H	-1.51559	-1.48705	-3.62058
O	-4.19227	-1.45478	-0.41402
C	-3.34495	-0.42734	1.58560
H	-2.41247	0.01731	1.94414
H	-4.10837	0.35155	1.52923
H	-3.68337	-1.18352	2.30174
H	5.68218	1.85084	0.69741
H	2.27849	-3.32909	-1.79175
H	2.85636	-1.64873	-1.77399
H	2.31703	-2.42707	-0.26253
H	3.11053	2.40590	-2.57144

Charge: 0 Point Group: C_1
Total electronic energy = –1385.12824a.u.
Zero-point corrected total electronic energy (E_{ZPE}) = – 1384.66917a.u.
No. of imaginary frequency = 1 (19.0i cm^{-1}, corresponding to methyl rotation)

2 (keto-enol tautomer of uracil) hydrogen-bonded to His, Asn, and a fragment of protein backbone

C	-2.52027	1.09279	0.61932
N	-2.55745	0.22501	-0.40913
C	-3.74097	-0.02361	-1.11669
C	-4.85996	0.75934	-0.65652
C	-4.69443	1.61836	0.38507
N	-3.51344	1.79914	1.05695
O	-1.31512	1.18698	1.21174
O	-3.74715	-0.84650	-2.03110
H	-1.69880	-0.28139	-0.71282
N	2.16048	-1.05270	0.43283
C	1.86565	-1.55443	1.76701
C	0.60399	-2.41603	1.64167
O	0.66946	-3.60362	1.34029
C	1.79655	-0.43271	2.80685
N	-0.58153	-1.78733	1.82789
C	-1.82927	-2.44924	1.51154
C	0.78650	-3.19105	-1.89646
C	-0.37353	-2.23654	-1.85151
O	-0.27842	-1.14343	-1.25093
N	-1.51518	-2.60600	-2.44015
C	4.27809	3.65602	-0.69350
C	2.94764	3.00013	-0.86194
N	2.30079	2.96638	-2.07884
C	2.20192	2.34074	0.08012
C	1.19030	2.29605	-1.87107
N	1.07905	1.89620	-0.57861
H	1.08581	0.35127	2.51644
H	2.78492	0.02753	2.88838
H	2.67086	-2.23949	2.04625
H	-0.58907	-0.78174	1.91736
H	0.92440	-3.61610	-0.89572
H	0.63901	-4.00134	-2.61497
H	-2.34090	-1.99866	-2.39681

H	-1.59013	-3.49582	-2.90789
H	4.21773	4.72903	-0.90605
H	4.65269	3.52455	0.32610
H	2.38739	2.11757	1.12002
H	0.33416	1.34671	-0.17713
H	0.43882	2.06833	-2.61469
H	-5.52171	2.21986	0.74927
H	5.01150	3.22636	-1.38461
H	1.69576	-2.64229	-2.15418
H	1.39589	-0.96726	-0.23271
C	3.43440	-0.77783	0.03760
H	1.50871	-0.82160	3.78916
O	4.38732	-0.86298	0.80399
C	3.59717	-0.38904	-1.41757
H	2.64970	-0.14613	-1.90719
H	4.25899	0.47633	-1.48344
H	4.07502	-1.22021	-1.94760
H	-5.80989	0.63688	-1.16071
H	-1.84890	-3.43742	1.97561
H	-2.65658	-1.85393	1.90495
H	-1.95902	-2.57723	0.43015
H	-1.38327	1.89051	1.87822

Charge: 0 Point Group: C_1
Total electronic energy = –1385.07518 a.u.
Zero-point corrected total electronic energy (E_{ZPE}) = –1384.61660a.u.
No. of imaginary frequency = 1 ($5.1i$ cm^{-1}, corresponding to methyl rotation)

2 (keto-enol tautomer of uracil) hydrogen-bonded to His, Asn, and a fragment of protein backbone in implicit solvation at ε = 4.0, with IEF-PCM model

C	2.40948	1.39215	-1.12586
N	2.58207	0.83071	0.08661
C	3.78810	0.94857	0.78400
C	4.78108	1.72616	0.09200
C	4.48904	2.25135	-1.12916
N	3.28916	2.09078	-1.77158
O	1.19696	1.16343	-1.65916
O	3.91408	0.40663	1.88558
H	1.81069	0.29438	0.53612
N	-1.91375	-1.29887	-0.23470

C	-1.59067	-2.02583	-1.45635
C	-0.21141	-2.66565	-1.25234
O	-0.09794	-3.79920	-0.78498
C	-1.71592	-1.15165	-2.70583
N	0.85748	-1.90872	-1.57281
C	2.20686	-2.32362	-1.24666
C	-0.16069	-2.65989	2.39871
C	0.81391	-1.55185	2.10857
O	0.52905	-0.64959	1.28708
N	1.99527	-1.57845	2.72764
C	-4.65884	3.21954	0.00712
C	-3.23788	2.80517	0.20460
N	-2.54528	3.09798	1.36217
C	-2.43368	2.09484	-0.64823
C	-1.34941	2.56923	1.20388
N	-1.23210	1.95152	0.00447
H	-1.10121	-0.24627	-2.63954
H	-2.75726	-0.83778	-2.81611
H	-2.29526	-2.85703	-1.53935
H	0.71344	-0.94324	-1.83265
H	-0.25806	-3.28136	1.50240
H	0.15005	-3.28694	3.23719
H	2.70110	-0.86255	2.52801
H	2.22239	-2.31306	3.38079
H	-4.76554	4.30776	0.07492
H	-5.02589	2.89737	-0.97181
H	-2.61510	1.66735	-1.62285
H	-0.41218	1.48374	-0.35670
H	-0.54124	2.60089	1.92152
H	5.22222	2.84127	-1.67018
H	-5.30555	2.77828	0.77408
H	-1.14174	-2.22929	2.61508
H	-1.14641	-0.94012	0.33324
C	-3.19135	-1.13564	0.18698
H	-1.42257	-1.70761	-3.60203
O	-4.15539	-1.54946	-0.45997
C	-3.36707	-0.44012	1.51996
H	-2.44983	0.03332	1.88045
H	-4.14539	0.31970	1.42629
H	-3.70156	-1.17896	2.25594

H	5.74328	1.87252	0.56573
H	2.39825	-3.32210	-1.64600
H	2.91037	-1.62199	-1.69798
H	2.36802	-2.34830	-0.16265
H	1.14868	1.64602	-2.50194

Charge: 0 Point Group: C_1
Total electronic energy = –1385.09886a.u.
Zero-point corrected total electronic energy (E_{ZPE}) = –1384.63980a.u.
No. of imaginary frequency = 0

3 (keto-enol tautomer of uracil) hydrogen-bonded to His, Asn, and a fragment of protein backbone

C	-2.32101	1.12124	0.73330
N	-2.40493	0.47730	-0.51232
C	-3.49839	0.55299	-1.28900
C	-4.58901	1.27674	-0.87721
C	-4.46245	1.88908	0.38683
N	-3.40882	1.82635	1.16626
O	-1.27461	1.01744	1.37462
O	-3.39881	-0.13316	-2.44065
H	-1.58658	-0.07997	-0.83274
N	2.16493	-1.05348	0.43277
C	1.86059	-1.55316	1.76513
C	0.59647	-2.41022	1.63076
O	0.65964	-3.59964	1.32055
C	1.79655	-0.43266	2.80682
N	-0.58365	-1.78024	1.80910
C	-1.82923	-2.44924	1.51155
C	0.78650	-3.19103	-1.89647
C	-0.34316	-2.20287	-1.92041
O	-0.25385	-1.09058	-1.37675
N	-1.48337	-2.57890	-2.53493
C	4.27805	3.65595	-0.69346
C	2.93074	3.01252	-0.62691
N	2.13921	2.86243	-1.74555
C	2.28551	2.50142	0.47071
C	1.04183	2.27506	-1.31952
N	1.07811	2.03333	0.01372

H	1.05388	0.33107	2.55263
H	2.77684	0.04922	2.85778
H	2.66392	-2.24279	2.03633
H	-0.60998	-0.77036	1.89715
H	0.88533	-3.57858	-0.87472
H	0.63613	-4.02330	-2.58862
H	-2.25406	-1.92516	-2.59287
H	-1.57148	-3.47831	-2.98046
H	4.19865	4.69215	-1.04040
H	4.75806	3.65610	0.28982
H	2.57739	2.42397	1.50723
H	0.33366	1.62005	0.57041
H	0.19692	1.99527	-1.93452
H	-5.30144	2.46618	0.77252
H	4.93208	3.12439	-1.39387
H	1.71700	-2.67378	-2.14238
H	1.39586	-0.82385	-0.18902
C	3.44346	-0.85093	0.01681
H	1.55304	-0.83374	3.79639
O	4.41117	-1.05740	0.74112
C	3.59718	-0.38905	-1.41758
H	2.65139	-0.10193	-1.88589
H	4.27081	0.47003	-1.44153
H	4.06216	-1.19627	-1.99377
H	-5.48984	1.36231	-1.47211
H	-1.91337	-3.37426	2.08784
H	-2.65362	-1.78474	1.78144
H	-1.90448	-2.70742	0.44686
H	-4.18607	0.01330	-2.98246

Charge: 0 Point Group: C_1
Total electronic energy = –1385.06104 a.u.
Zero-point corrected total electronic energy (E_{ZPE}) = –1384.60298a.u.
No. of imaginary frequency = 0

3 (keto-enol tautomer of uracil) hydrogen-bonded to His, Asn, and a fragment of protein backbone in implicit solvation at ε = 4.0, with IEF-PCM model

C	2.26092	1.22420	-1.22684
N	2.50740	0.81169	0.08439
C	3.66527	1.07203	0.71889

C	4.65932	1.76718	0.07093
C	4.36620	2.14899	-1.24724
N	3.23806	1.90240	-1.88667
O	1.16008	0.94929	-1.72998
O	3.71573	0.59470	1.96509
H	1.76657	0.27203	0.57625
N	-1.95693	-1.21401	-0.19715
C	-1.70420	-1.90847	-1.45406
C	-0.36123	-2.63660	-1.31126
O	-0.31067	-3.80601	-0.91872
C	-1.80764	-0.97944	-2.66584
N	0.74101	-1.92182	-1.59710
C	2.06924	-2.44362	-1.35579
C	-0.22660	-2.77958	2.33512
C	0.79736	-1.70622	2.09323
O	0.54102	-0.71657	1.38043
N	2.00724	-1.86602	2.65006
C	-4.41019	3.45125	0.28744
C	-3.01142	2.92708	0.25975
N	-2.15585	3.06982	1.33291
C	-2.37264	2.25957	-0.75426
C	-1.02794	2.49695	0.96070
N	-1.10776	1.99131	-0.29154
H	-1.11023	-0.13768	-2.60360
H	-2.82315	-0.57707	-2.71677
H	-2.45864	-2.69325	-1.54471
H	0.66636	-0.92548	-1.78345
H	-0.39014	-3.32204	1.39772
H	0.07519	-3.48658	3.11071
H	2.71479	-1.15021	2.53111
H	2.22032	-2.65980	3.23467
H	-4.42182	4.53445	0.45278
H	-4.92141	3.24301	-0.65713
H	-2.70290	1.95223	-1.73523
H	-0.35424	1.53960	-0.81003
H	-0.13163	2.41900	1.56079
H	5.11926	2.69509	-1.81131
H	-4.98831	2.98930	1.09621
H	-1.17263	-2.31176	2.61843
H	-1.16319	-0.85168	0.32767

C	-3.20909	-1.02663	0.28213
H	-1.60374	-1.52809	-3.59109
O	-4.21230	-1.41590	-0.32008
C	-3.31038	-0.33676	1.62581
H	-2.36298	0.09603	1.95872
H	-4.05589	0.45864	1.55943
H	-3.65621	-1.06523	2.36669
H	5.60633	1.99571	0.54221
H	2.19263	-3.41342	-1.84421
H	2.79814	-1.74417	-1.76970
H	2.26078	-2.57284	-0.28318
H	4.55085	0.83350	2.39394

Charge: 0 Point Group: C_1
Total electronic energy = –1385.09257a.u.
Zero-point corrected total electronic energy (E_{ZPE}) = –1384.63382a.u.
No. of imaginary frequency = 1 ($16.3i$ cm^{-1}, corresponding to methyl rotation)

4 (dienol tautomer of uracil) hydrogen-bonded to His, Asn, and a fragment of protein backbone

C	2.49963	2.00861	-0.98590
N	2.04605	1.09106	-0.12741
C	2.88186	0.74781	0.85677
C	4.16507	1.30618	0.96698
C	4.50459	2.23613	0.00740
N	3.67987	2.60656	-0.98637
O	1.62907	2.33363	-1.94757
O	2.48479	-0.14377	1.74716
N	-1.74484	-1.07243	-0.71890
C	-1.11877	-1.40417	-1.98918
C	0.09601	-2.28170	-1.66663
O	0.00079	-3.50405	-1.57796
C	-0.82368	-0.16388	-2.83710
N	1.26524	-1.64014	-1.43876
C	2.42592	-2.36776	-0.97321
C	-0.91163	-3.49455	1.59551
C	0.19323	-2.53505	1.92503
O	0.15458	-1.34935	1.55366
N	1.25016	-3.01217	2.61016

C	-4.14023	3.48933	0.44622
C	-2.82494	2.82582	0.70574
N	-2.38133	2.57703	1.98742
C	-1.89650	2.38072	-0.20141
C	-1.21003	1.99638	1.84773
N	-0.86868	1.85148	0.54286
H	-0.19885	0.56460	-2.30948
H	-1.77313	0.32032	-3.08224
H	-1.81528	-2.04754	-2.53266
H	1.26506	-0.63480	-1.31967
H	-0.82213	-3.76519	0.53589
H	-0.87962	-4.40245	2.20310
H	2.03616	-2.40903	2.81503
H	1.30366	-3.97833	2.89233
H	-4.17621	4.47742	0.91744
H	-4.31238	3.60980	-0.62758
H	-1.88168	2.38015	-1.28087
H	-0.00092	1.45719	0.19346
H	-0.57171	1.65754	2.65259
H	5.47722	2.72026	0.01947
H	-4.96476	2.89815	0.86024
H	-1.87285	-2.99476	1.73269
H	-1.15554	-0.94805	0.09812
C	-3.08695	-0.88385	-0.60023
H	-0.32015	-0.43922	-3.76996
O	-3.84839	-0.95800	-1.55787
C	-3.57797	-0.62191	0.80884
H	-2.77846	-0.34300	1.50104
H	-4.31561	0.18237	0.78378
H	-4.07836	-1.52486	1.17618
H	4.83249	1.01793	1.76860
H	2.67821	-3.16373	-1.67820
H	3.26613	-1.67323	-0.90092
H	2.25285	-2.82562	0.00799
H	2.04641	3.00920	-2.50373
H	1.55559	-0.47196	1.57196

Charge: 0 Point Group: C_1
Total electronic energy = –1385.07115a.u.
Zero-point corrected total electronic energy (E_{ZPE}) = –1384.61348a.u.
No. of imaginary frequency = 1 ($9.8i$ cm^{-1}, corresponding to methyl rotation)

4 (dienol tautomer of uracil) hydrogen-bonded to His, Asn, and a fragment of protein backbone in implicit solvation at ε = 4.0, with IEF-PCM model

C	-2.48511	1.98050	1.04705
N	-2.00655	1.10000	0.16165
C	-2.81265	0.80183	-0.86234
C	-4.09088	1.36695	-0.98743
C	-4.46037	2.25271	0.00140
N	-3.66517	2.57807	1.03680
O	-1.63889	2.26178	2.04296
O	-2.39013	-0.04967	-1.77973
N	1.74912	-1.08635	0.72602
C	1.12265	-1.40998	2.00153
C	-0.10066	-2.28871	1.70751
O	-0.02286	-3.51912	1.73307
C	0.82215	-0.16413	2.83737
N	-1.24311	-1.64678	1.39507
C	-2.42926	-2.36455	0.97258
C	0.90794	-3.49553	-1.59473
C	-0.16152	-2.50166	-1.94641
O	-0.09515	-1.32004	-1.54895
N	-1.20187	-2.93476	-2.67070
C	4.14411	3.48480	-0.44524
C	2.82089	2.83603	-0.70119
N	2.35916	2.60467	-1.98149
C	1.89973	2.38455	0.20994
C	1.18401	2.02616	-1.83395
N	0.86153	1.86937	-0.52884
H	0.18308	0.54949	2.30812
H	1.76462	0.33757	3.07431
H	1.81751	-2.04795	2.55236
H	-1.22877	-0.64557	1.23779
H	0.82215	-3.72864	-0.52755
H	0.83136	-4.42097	-2.16922
H	-1.95649	-2.30567	-2.91332
H	-1.26272	-3.88911	-2.99216
H	4.19341	4.47330	-0.91490
H	4.31745	3.60445	0.62827
H	1.89644	2.37387	1.28956

H	-0.00809	1.47822	-0.17435
H	0.53232	1.70081	-2.63349
H	-5.43253	2.73649	-0.02040
H	4.96323	2.88417	-0.85726
H	1.88729	-3.04127	-1.76153
H	1.15866	-0.99530	-0.09825
C	3.08396	-0.89876	0.59818
H	0.32837	-0.43823	3.77543
O	3.85801	-0.97319	1.55467
C	3.57728	-0.62585	-0.80747
H	2.77167	-0.37884	-1.50411
H	4.28833	0.20244	-0.78011
H	4.10617	-1.51388	-1.17017
H	-4.73545	1.11545	-1.81949
H	-2.71378	-3.10312	1.72577
H	-3.24264	-1.64622	0.85272
H	-2.26753	-2.88499	0.02142
H	-2.06396	2.90830	2.62811
H	-1.47510	-0.40778	-1.58888

Charge: 0 Point Group: C_1
Total electronic energy = –1385.09523a.u.
Zero-point corrected total electronic energy (E_{ZPE}) = –1384.63769a.u.
No. of imaginary frequency = 1 ($4.8i$ cm^{-1}, corresponding to methyl rotation)

1-methyl-uracil

C	-0.63627	-0.86343	0.00000
N	-1.08576	0.45218	0.00000
C	-0.20356	1.50605	0.00000
C	1.13516	1.35109	0.00000
C	1.70701	0.01329	0.00000
N	0.73715	-0.99895	0.00000
H	-0.66493	2.48799	0.00000
H	1.80609	2.19918	0.00000
O	-1.39871	-1.81245	0.00000
O	2.89225	-0.26584	0.00000
C	-2.53158	0.64885	0.00000
H	-2.97416	0.19001	0.88682
H	-2.73641	1.72021	0.00000
H	-2.97416	0.19001	-0.88682
H	1.07856	-1.95310	0.00000

Charge: 0 Point Group: C_s
Total electronic energy = –454.00026 a.u.
Zero-point corrected total electronic energy (E_{ZPE}) = –453.883767 a.u.
No. of imaginary frequency = 1 (72.4i cm^{-1}, corresponding to methyl rotation)

1-methyl-uracil (hydrogen-bonded to His, Asn, and a fragment of protein backbone)

C	-1.92437	-2.13969	-0.81726
N	-1.12372	-0.99800	-0.86980
C	-1.48640	0.26840	-0.49665
C	-3.66418	-0.62459	-0.07937
O	-1.43323	-3.23853	-1.09962
O	-0.66551	1.19689	-0.49008
C	-6.95853	0.79423	0.81660
O	-6.51414	-0.38148	0.78496
O	-6.33543	1.86641	0.63472
C	3.55449	-2.12516	-0.91251
C	2.08681	-2.24805	-1.24153
O	1.50468	-1.34668	-1.86099
N	1.44724	-3.36604	-0.85155
C	4.69592	-0.58079	2.89755
C	3.34152	-0.46794	2.27447
N	2.42855	-1.49827	2.34166
C	2.81064	0.58272	1.56673
C	1.36816	-1.06491	1.69032
N	1.54658	0.18534	1.20258
H	4.10505	-1.93918	-1.83917
H	3.68989	-1.25761	-0.25923
H	0.43119	-3.43245	-0.98921
H	1.88452	-3.99643	-0.19746
H	5.25547	-1.41989	2.46729
H	5.27401	0.33511	2.73908
H	3.21496	1.54758	1.29546
H	0.88040	0.69952	0.62695
H	0.45183	-1.61838	1.53510
H	-4.69611	-0.40553	0.24626
H	4.61618	-0.75769	3.97605
H	3.96142	-3.00824	-0.41369
N	-2.79125	0.43803	-0.11568
C	-3.27715	-1.88224	-0.41014
H	-0.17216	-1.09961	-1.25883

H	-3.98124	-2.70174	-0.35841
H	-8.05335	0.89337	1.03467
C	-3.22185	1.77792	0.29875
N	1.75129	2.71353	-0.92246
C	1.24435	3.76228	-0.06240
H	1.74274	3.73996	0.91327
H	1.08972	2.02129	-1.25311
C	3.07329	2.58763	-1.18292
O	3.90447	3.37026	-0.72077
C	3.46551	1.43382	-2.08120
H	2.71776	0.63557	-2.11436
H	3.62483	1.81568	-3.09611
H	4.41536	1.02789	-1.72366
H	1.41598	4.74945	-0.50471
H	0.17428	3.59841	0.07365
H	-2.95558	2.49668	-0.47897
H	-4.31054	1.77332	0.44888
H	-2.70854	2.05536	1.22395

Charge: 0 Point Group: C_1
Total electronic energy = -1366.33949 a.u.
Zero-point corrected total electronic energy (E_{ZPE}) = -1365.91482 a.u.
No. of imaginary frequency = 1 ($13.67i$ cm^{-1})

1-methyl-uracil : formate (reaction complex)

C	1.32283	-1.45363	0.00000
N	0.09827	-0.81676	0.00000
C	0.00000	0.55455	0.00000
C	1.09075	1.36106	0.00000
C	2.41774	0.79756	0.00000
N	2.41338	-0.60438	0.00000
H	-1.02029	0.96890	0.00000
H	0.97499	2.43658	0.00000
O	1.45261	-2.67159	0.00000
O	3.48905	1.39766	0.00000
C	-1.10148	-1.65707	0.00000
H	-1.09703	-2.29704	0.88645
H	-1.99395	-1.01744	0.00000
H	-1.09703	-2.29704	-0.88645
O	-2.66818	1.99670	0.00000
C	-3.70300	1.28374	0.00000
H	-4.67597	1.84420	0.00000

O	-3.79225	0.03385	0.00000
H	3.31678	-1.06033	0.00000

Charge: –1 Point Group: C_s
Total electronic energy = –643.19696 a.u.
Zero-point corrected total electronic energy (E_{ZPE}) = –643.05831 a.u.
Sum of electronic and thermal Enthalpies (H) = -643.04512 a.u.
Sum of electronic and thermal Free Energies (G) = -643.10006 a.u.
No. of imaginary frequency = 0

1-methyl-uracil : formate (TS)

C	-0.65214	1.47755	0.00000
N	0.00000	0.27985	0.00000
C	1.34702	0.26473	0.00000
C	2.16030	1.36566	0.00000
C	1.55358	2.67097	0.00000
N	0.15930	2.61650	0.00000
H	1.78352	-0.73473	0.00000
H	3.24005	1.28702	0.00000
O	-1.87804	1.60370	0.00000
O	2.12887	3.76293	0.00000
C	-0.99825	-1.45828	0.00000
H	-0.51733	-1.71697	0.92861
H	-1.93580	-0.92572	0.00000
H	-0.51733	-1.71697	-0.92861
O	-1.97653	-3.10634	0.00000
C	-1.25006	-4.16026	0.00000
H	-1.84957	-5.09994	0.00000
O	-0.01842	-4.23939	0.00000
H	-0.32847	3.50334	0.00000

Charge: –1 Point Group: C_s
Total electronic energy = –643.13646 a.u.
Zero-point corrected total electronic energy (E_{ZPE}) = –642.99928 a.u.
Sum of electronic and thermal Enthalpies (H) = –642.98659 a.u.
Sum of electronic and thermal Free Energies (G) = – 643.03978 a.u.
No. of imaginary frequency = 1 (616.56i cm^{-1})

1-methyl-uracil : formate (product)

C	-1.29438	0.36534	0.00000
N	0.00000	0.78355	0.00000

C	0.20681	2.10965	0.00000
C	-0.74532	3.10700	0.00000
C	-2.12722	2.72954	0.00000
N	-2.29652	1.34623	0.00000
H	1.26046	2.39866	0.00000
H	-0.48579	4.15908	0.00000
O	-1.64747	-0.82507	0.00000
O	-3.11886	3.47448	0.00000
C	1.41963	-1.96471	0.00000
H	1.82050	-1.47923	0.89051
H	0.33131	-1.92508	0.00000
H	1.82050	-1.47923	-0.89051
O	1.78759	-3.37165	0.00000
C	3.07223	-3.66644	0.00000
H	3.19816	-4.76076	0.00000
O	4.00243	-2.89152	0.00000
H	-3.24955	1.00599	0.00000

Charge: –1 Point Group: C_s
Total electronic energy = –643.17198 a.u.
Zero-point corrected total electronic energy (E_{ZPE}) = –643.03348 a.u.
Sum of electronic and thermal Enthalpies (H) = –643.02018 a.u.
Sum of electronic and thermal Free Energies (G) = –643.07691 a.u.
No. of imaginary frequency = 0

Three water bound 1-methyl-uracil : formate (reaction complex)

C	-2.12744	0.63116	-0.12685
N	-2.88351	-0.49299	0.09329
C	-2.43751	-1.80847	0.03685
C	-1.02912	-1.94520	-0.20337
C	-0.25756	-0.84338	-0.38180
N	-0.78606	0.42321	-0.34613
O	-2.62145	1.76395	-0.12791
O	-3.24048	-2.74064	0.18804
H	0.82536	-0.91853	-0.57611
H	-0.59332	-2.93401	-0.25050
H	-3.87564	-0.33064	0.34709
H	-4.31781	2.20560	-0.45103
O	-5.27999	2.39172	-0.54185
H	-5.45723	3.07859	0.11018
O	-5.60637	-0.04770	0.75107
H	-5.99228	-0.84077	0.32903

H	-5.78277	0.73198	0.18979
H	-4.98722	-2.72426	-0.05762
O	-5.96872	-2.64992	-0.12627
H	-6.30494	-3.16865	0.61269
C	0.06245	1.59508	-0.58487
H	-0.20896	2.05302	-1.54036
H	-0.10417	2.32499	0.20977
H	1.11474	1.28050	-0.59409
O	2.65598	-1.35879	-0.92999
C	3.42173	-0.37098	-0.79487
H	4.51615	-0.58715	-0.91437
O	3.12218	0.81994	-0.54553

Charge: –1 Point Group: C_1
Total electronic energy = –872.45409 a.u.
Zero-point corrected total electronic energy (E_{ZPE}) = –872.23733 a.u.
Sum of electronic and thermal Enthalpies (H) = –872.21650 a.u.
Sum of electronic and thermal Free Energies (G) = –872.28930 a.u.
No. of imaginary frequency = 0

Three water bound 1-methyl-uracil : formate (TS)

C	-2.06139	0.57173	-0.09243
N	-2.88425	-0.52691	0.11480
C	-2.49751	-1.85421	0.03819
C	-1.09848	-2.04693	-0.20774
C	-0.30863	-0.94172	-0.36353
N	-0.74456	0.33153	-0.31776
O	-2.53919	1.71973	-0.06648
O	-3.33512	-2.76498	0.17961
H	0.76018	-1.04528	-0.55033
H	-0.70999	-3.05500	-0.27190
H	-3.86434	-0.32965	0.37572
H	-4.18378	2.18505	-0.41767
O	-5.13872	2.41738	-0.52479
H	-5.28483	3.12568	0.11169
O	-5.63628	0.01227	0.77508
H	-6.01746	-0.75356	0.30365
H	-5.73158	0.80844	0.21585
H	-5.06100	-2.67150	-0.08763
O	-6.04239	-2.57905	-0.16317
H	-6.38634	-3.04308	0.60801

O	3.46117	1.68470	-1.07718
C	3.03367	2.84291	-1.04956
H	3.74785	3.68382	-1.20678
O	1.83154	3.23721	-0.85808
C	0.56388	1.79764	-0.59290
H	0.80381	1.39854	-1.56428
H	-0.21062	2.53948	-0.48339
H	1.11938	1.45774	0.26531

Charge: –1 Point Group: C_1
Total electronic energy = –872.39637 a.u.
Zero-point corrected total electronic energy (E_{ZPE}) = –872.18141 a.u.
Sum of electronic and thermal Enthalpies (H) = –872.16091 a.u.
Sum of electronic and thermal Free Energies (G) = –872.23249 a.u.
No. of imaginary frequency = 1 (609.82i cm^{-1})

Three water bound 1-methyl-uracil : formate (product)

C	-0.04516	-0.08018	-0.19186
N	1.28675	-0.48643	-0.23103
C	1.73026	-1.79347	-0.13326
C	0.68029	-2.75469	-0.0602
C	-0.61912	-2.29779	-0.07208
N	-1.01758	-1.01834	-0.12851
O	-0.29196	1.14862	-0.21823
O	2.95646	-2.04587	-0.11725
H	-1.43338	-3.02311	-0.02389
H	0.93125	-3.80604	0.0094
H	1.99589	0.24635	-0.37046
H	0.70294	2.41102	0.36576
O	1.30744	3.15961	0.61266
H	1.13784	3.82769	-0.06059
O	3.33373	1.60543	-0.50527
H	3.97736	1.13692	0.06081
H	2.8373	2.2417	0.0463
H	4.21913	-0.99963	0.40248
O	4.95832	-0.37286	0.61578
H	5.59589	-0.51388	-0.09269
O	-6.24836	0.26576	0.21406
C	-5.82973	1.39515	0.09746
H	-6.47968	2.28375	0.07959
O	-4.57039	1.76899	-0.02589

C	-3.55982	0.72647	-0.02234
H	-2.59814	1.22435	-0.12852
H	-3.59983	0.17437	0.91746
H	-3.72999	0.04137	-0.85364

Charge: –1 Point Group: C_1
Total electronic energy = –872.43533 a.u.
Zero-point corrected total electronic energy (E_{ZPE}) = –872.21855 a.u.
Sum of electronic and thermal Enthalpies (H) = –872.19765 a.u.
Sum of electronic and thermal Free Energies (G) = –872.27217 a.u.
No. of imaginary frequency = 0

Two glycine bound 1-methyl-uracil : formate (reactant)

C	-1.40324	-1.91849	0.00241
N	-1.75402	-0.59180	0.16630
C	-3.03376	-0.07513	0.10581
C	-4.06126	-1.02797	-0.13184
C	-3.74183	-2.34304	-0.28515
N	-2.45127	-2.78484	-0.22177
O	-0.23573	-2.29271	0.05784
O	-3.21956	1.15683	0.25798
H	-4.53396	-3.09183	-0.46561
H	-5.09196	-0.70641	-0.18915
H	-0.97121	0.05736	0.32801
N	2.20518	-0.72704	0.31440
H	1.66680	0.15359	0.39695
H	2.78414	-0.88786	1.18290
C	3.28113	-0.67499	-0.71294
H	3.16137	-1.50003	-1.41674
H	3.21986	0.26884	-1.25584
C	4.64431	-0.80805	0.04716
O	5.65877	-0.76434	-0.65780
O	4.51175	-0.94909	1.29661
H	1.50929	-1.47009	0.18295
N	-1.53480	3.08318	0.81446
H	-2.03516	3.91184	1.13220
H	-0.92250	2.70731	1.54933
C	-0.67426	3.31230	-0.37874
H	-1.29975	3.31490	-1.27251
H	-0.16442	4.27386	-0.28771
C	0.36933	2.16923	-0.44759

O	1.10918	2.14635	-1.42381
O	0.32651	1.38016	0.55725
H	-2.23130	2.28781	0.60758
C	-2.13185	-4.20795	-0.39603
H	-1.47272	-4.32468	-1.25935
H	-1.61047	-4.56882	0.49329
H	-3.06943	-4.75980	-0.54629
O	-6.21480	-3.91126	-0.72615
C	-5.96489	-5.13714	-0.85749
H	-6.85034	-5.79649	-1.04433
O	-4.85109	-5.70931	-0.80660

Charge: –1 Point Group: C_1
Total electronic energy = -1211.93926 a.u.
Zero-point corrected total electronic energy (E_{ZPE}) = -1211.63152 a.u.
Sum of electronic and thermal Enthalpies (H) = -1211.60669 a.u.
Sum of electronic and thermal Free Energies (G) = -1211.69016 a.u.
No. of imaginary frequency = 1 ($5.22i$ cm^{-1})

Two glycine bound 1-methyl-uracil : formate (TS)

C	-1.44424	-1.87628	-0.08023
N	-1.75944	-0.52709	0.10953
C	-3.02232	0.01759	0.05681
C	-4.06882	-0.90508	-0.20801
C	-3.73474	-2.22517	-0.37863
N	-2.48847	-2.71499	-0.32207
O	-0.27014	-2.24852	-0.02089
O	-3.19459	1.25363	0.23831
H	-4.50526	-2.96965	-0.57695
H	-5.08924	-0.55126	-0.26545
H	-0.96367	0.09870	0.28540
N	2.17662	-0.75588	0.24769
H	1.67873	0.14429	0.36576
H	2.75210	-0.96331	1.10502
C	3.24233	-0.70396	-0.78927
H	3.11210	-1.52704	-1.49382
H	3.18097	0.24181	-1.32901
C	4.61469	-0.84669	-0.04815
O	5.62077	-0.77884	-0.76487
O	4.50061	-1.02020	1.19834
H	1.44314	-1.46239	0.09888

N	-1.46594	3.08029	0.92783
H	-1.92642	3.89123	1.33687
H	-0.83907	2.61458	1.59969
C	-0.62494	3.38499	-0.26114
H	-1.26097	3.44113	-1.14532
H	-0.11021	4.33761	-0.11810
C	0.41580	2.24443	-0.40909
O	1.12790	2.26281	-1.40598
O	0.39660	1.41624	0.56370
H	-2.19349	2.32329	0.66754
O	-4.41857	-6.58015	-0.95477
C	-3.31094	-7.13102	-0.92852
H	-3.25963	-8.23586	-1.05948
O	-2.16666	-6.58580	-0.76523
C	-2.29586	-4.63324	-0.54119
H	-2.79425	-4.58912	-1.49507
H	-2.87903	-4.80722	0.34747
H	-1.21908	-4.60648	-0.48650

Charge: –1 Point Group: C_1
Total electronic energy = –1211.88319 a.u.
Zero-point corrected total electronic energy (E_{ZPE}) = –1211.57680 a.u.
Sum of electronic and thermal Enthalpies (H) = –1211.55149 a.u.
Sum of electronic and thermal Free Energies (G) = –1211.63710 a.u.
No. of imaginary frequency = 1 (602.47i cm^{-1})

Two glycine bound 1-methyl-uracil : formate (product)

C	-1.38221	-0.65117	-0.02125
N	-0.43469	-1.67903	-0.14482
C	-0.69526	-3.01913	0.02250
C	-2.03506	-3.33159	0.33130
C	-2.93394	-2.28286	0.42967
N	-2.66392	-0.98799	0.26733
O	-1.00342	0.52022	-0.18662
O	0.23425	-3.87617	-0.10373
H	-3.97609	-2.50525	0.66296
H	-2.32075	-4.36511	0.47833
H	0.52309	-1.38616	-0.36034
N	1.57681	1.67922	-0.37785
H	2.09825	0.79484	-0.50966

H	1.73205	2.31942	-1.19494
C	2.09986	2.51088	0.73851
H	1.29120	2.74506	1.43293
H	2.87665	1.95844	1.26904
C	2.67185	3.82868	0.11863
O	3.16728	4.62813	0.92470
O	2.54295	3.90076	-1.13579
H	0.58444	1.40259	-0.29107
N	2.66780	-3.50907	-0.84444
H	3.05759	-4.38089	-1.19667
H	2.63635	-2.78159	-1.57275
C	3.42667	-2.91149	0.28468
H	3.09871	-3.36818	1.21955
H	4.49717	-3.08297	0.15046
C	3.13946	-1.38737	0.29882
O	3.60220	-0.74174	1.23462
O	2.44695	-0.99199	-0.69666
H	1.61843	-3.65340	-0.54855
O	-6.82901	2.31711	0.05098
C	-6.00231	3.18487	-0.11412
H	-6.25200	4.24770	-0.25018
O	-4.69110	3.03164	-0.16204
C	-4.17447	1.68999	0.00113
H	-3.09294	1.76619	-0.08180
H	-4.45667	1.29688	0.97873
H	-4.57136	1.03878	-0.77903

Charge: –1 Point Group: C_1
Total electronic energy = –1211.92929 a.u.
Zero-point corrected total electronic energy (E_{ZPE}) = –1211.622169 a.u.
Sum of electronic and thermal Enthalpies (H) = –1211.596191 a.u.
Sum of electronic and thermal Free Energies (G) = –1211.685003 a.u.
No. of imaginary frequency = 0

Optimized Cartesian coordinates for stationary points on the stepwise reaction pathway of glycosidic N1–C1' bond cleavage, using a constrained and truncated QM model. All geometries were optimized in the gas-phase at ωB97X-D/6-31+G(d).

Reaction complex (RC)

C	-1.29532	0.16691	-0.34553
N	-1.92897	0.24983	-1.56309
C	-1.34587	0.09081	-2.81086
C	0.04417	-0.28940	-2.76972
C	0.70034	-0.28251	-1.58773
N	0.07867	-0.00738	-0.39837
O	-1.91135	0.23439	0.71030
O	-2.00505	0.27709	-3.83897
C	0.86404	0.40308	0.80775
C	0.60611	-0.44386	2.05581
C	1.99584	-0.70397	2.65020
C	2.94033	-0.49184	1.47654
O	2.39970	0.08833	3.72907
O	2.22530	0.25105	0.48463
C	3.38578	-1.83638	1.02733
O	4.26269	-1.81354	-0.09708
P	5.28532	-3.17311	-0.51525
N	-3.81211	2.73365	1.15767
C	-4.05504	2.60687	2.59005
C	-3.17459	1.60674	3.34399
C	-1.61099	5.35547	1.07633
C	-0.48415	4.33376	0.93885
O	0.69504	4.81250	0.89923
O	-0.77777	3.11853	0.90645
C	5.83462	5.01493	-0.78953
C	5.69612	3.51548	-0.86549
N	4.58637	2.84140	-0.38112
C	6.51645	2.55322	-1.38985
C	4.72194	1.53867	-0.60299
N	5.88590	1.33318	-1.21262
C	-2.43556	-4.29389	-4.74974
C	-3.11388	-3.83590	-3.48013
C	-3.64610	-2.54705	-3.37885
C	-3.24215	-4.69483	-2.38372

C	-4.29086	-2.12473	-2.21713
C	-3.88740	-4.28029	-1.22002
C	-4.41357	-2.99189	-1.13298
C	-5.51366	3.54863	-2.08775
C	-4.66695	2.33353	-2.40539
O	-4.62487	1.36576	-1.63694
N	-3.97385	2.34857	-3.56120
C	-2.72359	-4.28906	5.33427
C	-2.58189	-3.54895	4.03965
N	-2.48808	-4.22022	2.84017
C	-2.52576	-2.19390	3.81878
C	-2.37617	-3.28356	1.92146
N	-2.40201	-2.03964	2.45780
O	2.74964	3.45427	1.41186
H	-2.93058	0.48384	-1.52954
H	0.62507	1.46238	0.95564
H	0.14717	-1.39713	1.78105
H	-0.05974	0.05914	2.75898
H	2.05728	-1.72679	3.02666
H	3.79539	0.11760	1.78752
H	2.29923	1.02067	3.48939
H	2.50144	-2.45100	0.78746
H	3.90284	-2.31219	1.87302
H	-4.17511	1.92563	0.65901
H	-2.79963	2.73712	0.99054
H	-2.11927	1.82681	3.15369
H	-3.38428	0.59600	2.98438
H	-1.74944	5.57495	2.14218
H	-1.34238	6.29189	0.57886
H	5.80717	5.35564	0.24997
H	6.78441	5.32284	-1.23255
H	3.80373	3.21851	0.23689
H	7.47923	2.63427	-1.86884
H	3.99717	0.77566	-0.35666
H	-1.95727	-3.45516	-5.26606
H	-3.16007	-4.74036	-5.44259
H	-3.53197	-1.85142	-4.20639
H	-2.82013	-5.69654	-2.43589
H	-4.68397	-1.11293	-2.15528
H	-3.96579	-4.95774	-0.37327

H	-4.89960	-2.66159	-0.21877
H	-5.19303	3.92796	-1.11121
H	-5.43757	4.33891	-2.83974
H	-3.93243	3.17963	-4.12880
H	-3.32813	1.57856	-3.76848
H	-1.90203	-5.00194	5.46329
H	-2.71798	-3.59851	6.18408
H	-2.56189	-1.34758	4.48924
H	-2.27487	-3.45004	0.85758
H	1.85342	3.91885	1.14547
H	3.06181	3.97120	2.16355
H	-1.66807	-5.04701	-4.54301
H	-3.66085	-4.85676	5.35933
H	5.01867	5.50418	-1.32957
H	6.22565	0.39675	-1.43402
H	-6.55771	3.23537	-1.99618
H	-2.55216	4.96682	0.68037
H	-3.36033	1.65314	4.42216
H	1.75812	-0.49883	-1.50314
H	0.55025	-0.52388	-3.69605
H	-2.29802	-1.16855	1.93805
O	6.27533	-2.21215	-1.47203
O	5.99063	-3.58190	0.73084
O	4.55029	-4.08512	-1.44324
H	6.13836	-2.54032	-2.37071
H	-5.11255	2.31555	2.71457
C	-4.00607	3.99543	3.20533
O	-3.66140	4.25454	4.33742
H	-4.35112	4.79638	2.51817

Charge: –1 Point Group: C_1
Total electronic energy = –2968.22362 a.u.
Zero-point corrected total electronic energy (E_{ZPE}) = –2967.37893 a.u.
No. of imaginary frequency = 5 (58.6i cm^{-1}, 35.63i cm^{-1}, 24.63i cm^{-1}, 22.02i cm^{-1}, 1.22i cm^{-1})

Transition State 1 (TS1)

C	-1.44533	-0.14575	-0.39928
N	-2.14244	0.00051	-1.57288
C	-1.65287	-0.27459	-2.84201
C	-0.30907	-0.80497	-2.85239

C	0.38105	-0.87288	-1.68692
N	-0.14509	-0.55933	-0.46413
O	-2.00057	0.10945	0.68404
O	-2.34270	-0.03438	-3.83841
C	1.08548	0.73824	0.51657
C	0.76814	0.67566	1.96779
C	1.82903	-0.28216	2.53371
C	2.90964	-0.34133	1.42668
O	2.34336	0.10174	3.79046
O	2.30588	0.31648	0.26628
C	3.38982	-1.72862	1.05614
O	4.33901	-1.64714	0.01015
P	5.32786	-2.98828	-0.50340
N	-4.74284	0.42345	1.78956
C	-4.45522	1.69965	2.45141
C	-3.23251	1.56410	3.37960
C	-1.72367	5.39186	1.26675
C	-0.48301	4.72537	0.67446
O	-0.24000	4.94389	-0.54162
O	0.23893	4.01605	1.44922
C	5.73680	5.21248	-0.54148
C	5.69700	3.70686	-0.63968
N	4.50774	3.00224	-0.71324
C	6.69083	2.76524	-0.68323
C	4.76074	1.70103	-0.79912
N	6.08040	1.52609	-0.78168
C	-2.32947	-4.12120	-4.84868
C	-2.58929	-3.78770	-3.39690
C	-3.73367	-3.06955	-3.02924
C	-1.70321	-4.17680	-2.39036
C	-3.99333	-2.76599	-1.69620
C	-1.95823	-3.87487	-1.05152
C	-3.10780	-3.17456	-0.69834
C	-5.57066	3.58885	-1.99963
C	-4.78143	2.32223	-2.26924
O	-4.71681	1.41866	-1.42662
N	-4.16822	2.21493	-3.46551
C	-2.71855	-4.41678	5.22800
C	-2.21344	-3.60098	4.07642
N	-1.05851	-3.94805	3.40974

C	-2.74770	-2.46259	3.52070
C	-0.90609	-3.03387	2.47500
N	-1.89725	-2.10960	2.50000
O	2.01128	3.58914	-0.40771
H	-3.10489	0.35770	-1.49497
H	0.76189	1.55750	-0.11642
H	-0.26567	0.39031	2.15602
H	0.88860	1.70216	2.34888
H	1.40443	-1.27611	2.69487
H	3.76806	0.28594	1.69507
H	2.56473	1.04203	3.76637
H	2.52447	-2.33840	0.75087
H	3.82773	-2.18453	1.95608
H	-5.53484	0.53348	1.15975
H	-3.94554	0.17953	1.20000
H	-2.46334	2.31533	3.16190
H	-2.77059	0.58164	3.25499
H	-1.52006	6.46206	1.38915
H	-2.57320	5.29291	0.58589
H	5.16629	5.55585	0.32645
H	6.76974	5.55324	-0.44072
H	3.50352	3.37825	-0.63452
H	7.76347	2.87202	-0.64965
H	4.02718	0.90747	-0.84837
H	-2.33407	-3.21237	-5.46167
H	-3.10190	-4.79243	-5.24299
H	-4.41982	-2.72713	-3.80085
H	-0.79623	-4.71775	-2.65173
H	-4.88005	-2.19385	-1.43545
H	-1.25783	-4.19164	-0.28382
H	-3.30638	-2.94265	0.34444
H	-5.20089	4.04297	-1.07549
H	-5.51560	4.31264	-2.81778
H	-4.13617	2.99482	-4.10222
H	-3.58499	1.39519	-3.66825
H	-1.97206	-4.45823	6.02902
H	-3.63999	-3.98876	5.63653
H	-3.63863	-1.88947	3.73524
H	-0.10887	-3.00053	1.74377
H	1.33230	4.13254	-0.88440

H	1.56699	3.65945	0.49083
H	-1.35962	-4.61235	-4.97649
H	-2.92440	-5.44663	4.91541
H	5.30133	5.66833	-1.43557
H	6.50792	0.60002	-0.81038
H	-6.61661	3.31679	-1.82983
H	-1.97713	4.96913	2.24201
H	-3.51938	1.67137	4.42965
H	1.42140	-1.19200	-1.66426
H	0.12912	-1.09220	-3.79906
H	-1.99024	-1.31267	1.86673
O	6.43707	-1.96187	-1.23211
O	5.90066	-3.59749	0.72715
O	4.62810	-3.71622	-1.60454
H	6.38068	-2.16307	-2.17565
H	-5.34247	1.99812	3.02020
C	-4.20520	2.78221	1.41837
O	-4.91572	3.75476	1.25985
H	-3.31810	2.61523	0.77421

Charge: –1 Point Group: C_1
Total electronic energy = –2968.19049 a.u.
Zero-point corrected total electronic energy (E_{ZPE}) = –2967.35032 a.u.
No. of imaginary frequency = 6 (236.81i cm^{-1}, corresponding to N1–C1' bond cleavage, and 74.81i cm^{-1}, 48.25i cm^{-1}, 30.50i cm^{-1}, 13.64i cm^{-1}, 6.12i cm^{-1})

Intermediate (INT)

C	-1.74014	-0.45001	-0.45558
N	-2.41082	-0.03891	-1.59030
C	-2.01658	-0.30767	-2.89186
C	-0.80395	-1.06372	-2.98058
C	-0.16047	-1.41645	-1.82376
N	-0.58099	-1.12578	-0.56863
O	-2.22996	-0.14754	0.66324
O	-2.69469	0.12031	-3.84501
C	1.14073	0.75099	0.46848
C	0.78803	0.65853	1.88692
C	1.91125	-0.20717	2.48651
C	2.89446	-0.41358	1.31649
O	2.54624	0.33432	3.61963
O	2.22811	0.20531	0.14051

C	3.20646	-1.85213	1.01694
O	4.12208	-1.94756	-0.04775
P	4.88959	-3.45504	-0.51636
N	-4.49098	1.49439	1.71935
C	-3.46117	2.48860	2.01131
C	-2.88958	2.31639	3.41344
C	-1.14531	5.74478	0.79719
C	0.21909	5.10274	0.76929
O	0.54061	4.60285	-0.42057
O	0.97026	5.08061	1.72978
C	6.12136	4.61042	-1.42300
C	6.06049	3.10807	-1.39424
N	4.97279	2.43206	-0.87427
C	6.97709	2.19348	-1.84693
C	5.22898	1.14349	-1.01948
N	6.43004	0.95264	-1.59941
C	-3.13190	-4.17010	-4.25039
C	-3.53057	-3.60956	-2.90402
C	-4.58178	-2.69269	-2.79664
C	-2.86751	-3.99309	-1.73515
C	-4.96826	-2.18588	-1.55809
C	-3.25090	-3.49115	-0.49195
C	-4.30763	-2.58921	-0.39859
C	-5.36668	4.08126	-2.01758
C	-4.76835	2.70594	-2.25691
O	-4.78410	1.85772	-1.35743
N	-4.21240	2.46672	-3.45524
C	-2.83021	-3.44505	5.80727
C	-2.24369	-3.03494	4.49571
N	-1.18644	-3.71125	3.93111
C	-2.62785	-2.00334	3.67472
C	-0.94762	-3.09311	2.79017
N	-1.78880	-2.05186	2.59042
O	2.65368	3.16582	0.42521
H	-3.30322	0.44244	-1.45418
H	0.60029	1.29759	-0.29627
H	-0.22520	0.25077	1.97919
H	0.73858	1.67733	2.29488
H	1.51271	-1.16958	2.81547
H	3.80917	0.17191	1.44308

H	2.84890	1.23013	3.41699
H	2.26933	-2.38503	0.78833
H	3.62201	-2.27914	1.94390
H	-4.93193	1.71413	0.82647
H	-4.02245	0.60329	1.55634
H	-2.14042	3.08235	3.63460
H	-2.40520	1.33725	3.50558
H	-1.77864	5.35888	-0.00319
H	-1.60326	5.56134	1.77069
H	6.09343	5.02457	-0.40891
H	7.04198	4.95101	-1.90614
H	3.52904	2.99573	-0.02152
H	7.94282	2.31556	-2.31354
H	4.60041	0.30505	-0.74625
H	-3.10873	-3.38168	-5.01077
H	-3.84358	-4.93582	-4.58369
H	-5.08491	-2.34988	-3.69819
H	-2.02887	-4.68327	-1.79623
H	-5.76939	-1.45348	-1.50100
H	-2.71232	-3.79030	0.40297
H	-4.58901	-2.17932	0.56726
H	-4.73060	4.61445	-1.30307
H	-5.45627	4.68282	-2.92687
H	-4.15890	3.18937	-4.15531
H	-3.72162	1.57180	-3.62968
H	-2.06834	-3.44108	6.59507
H	-3.63566	-2.76484	6.10406
H	-3.40899	-1.26083	3.75939
H	-0.19007	-3.36787	2.06783
H	1.38554	4.09159	-0.31296
H	2.77119	3.80604	1.14199
H	-2.13966	-4.63027	-4.20912
H	-3.24079	-4.46000	5.75245
H	5.26927	5.02166	-1.97474
H	6.82683	0.03962	-1.78300
H	-6.35195	3.96181	-1.56057
H	-1.03008	6.82691	0.66834
H	-3.69738	2.37067	4.14833
H	0.77495	-1.97265	-1.87224
H	-0.42248	-1.32960	-3.95819

H	-1.84202	-1.42030	1.77992
O	5.82738	-2.72480	-1.67441
O	5.73447	-3.88223	0.63106
O	3.85719	-4.28510	-1.20951
H	5.37649	-2.88217	-2.51452
H	-3.94294	3.47961	1.94411
C	-2.36556	2.51919	0.95655
O	-1.18649	2.69917	1.18833
H	-2.72129	2.40692	-0.08502

Charge: –1 Point Group: C_1
Total electronic energy = –2968.19461 a.u.
Zero-point corrected total electronic energy (E_{ZPE}) = –2967.35378 a.u.
No. of imaginary frequency = 5 (54.77i cm^{-1}, 54.13i cm^{-1}, 18.67i cm^{-1}, 15.29i cm^{-1}, 5.01i cm^{-1})

Transition State 2 (TS2)

C	-1.02839	0.38773	1.17240
N	-1.35422	-0.37112	2.28292
C	-0.44267	-0.91358	3.17559
C	0.91731	-0.61005	2.85782
C	1.18143	0.13842	1.73724
N	0.26058	0.62523	0.87653
O	-1.97114	0.81392	0.45437
O	-0.84917	-1.60579	4.13066
C	0.75532	-1.07028	-1.49301
C	-0.15026	-0.19659	-2.29234
C	0.78052	0.91030	-2.83806
C	2.18832	0.46950	-2.38388
O	0.70066	1.13279	-4.23352
O	1.95395	-0.59558	-1.40229
C	3.07028	1.51629	-1.73787
O	4.31193	0.91257	-1.43332
P	5.68226	1.77993	-0.80981
N	-4.94112	0.53229	0.39902
C	-4.64824	-0.39336	-0.69210
C	-4.59431	0.31443	-2.03969
C	-3.53864	-4.21462	-2.15980
C	-2.10967	-3.88264	-2.53635
O	-1.22503	-4.20378	-1.58905
O	-1.77697	-3.41520	-3.61091

C	3.84224	-5.67551	-3.71184
C	4.29989	-4.36327	-3.12228
N	3.45927	-3.35139	-2.66378
C	5.58631	-3.94333	-2.91539
C	4.22607	-2.37235	-2.19465
N	5.51376	-2.69519	-2.33411
C	0.55963	1.86726	6.43930
C	-0.31225	2.22172	5.25570
C	-1.67877	1.91977	5.26389
C	0.21624	2.85650	4.12941
C	-2.49523	2.25939	4.18798
C	-0.59698	3.20087	3.04968
C	-1.95778	2.91041	3.07809
C	-5.41453	-3.52413	2.79141
C	-4.26057	-2.58866	3.11816
O	-4.30016	-1.40645	2.76191
N	-3.21362	-3.09996	3.78639
C	-3.12144	6.37268	-1.80232
C	-2.27234	5.23909	-1.32444
N	-0.90707	5.35905	-1.20224
C	-2.66433	3.97805	-0.94704
C	-0.49451	4.18759	-0.75658
N	-1.51630	3.31640	-0.59108
O	1.02357	-2.76974	-2.51789
H	-2.34595	-0.49001	2.49388
H	0.42737	-1.68368	-0.66547
H	-0.89873	0.19705	-1.59465
H	-0.70699	-0.73851	-3.06159
H	0.52164	1.87094	-2.38810
H	2.72724	0.00058	-3.21733
H	0.81941	0.29246	-4.69543
H	2.58048	1.89892	-0.83074
H	3.18649	2.34366	-2.45379
H	-5.09239	0.00256	1.25697
H	-4.09501	1.07443	0.57526
H	-4.39063	-0.39063	-2.85083
H	-3.79223	1.06153	-2.03879
H	-3.67023	-4.18774	-1.07729
H	-4.20525	-3.50177	-2.64616
H	3.22450	-5.51727	-4.60171

H	4.71268	-6.27204	-3.99564
H	2.21952	-3.14839	-2.64742
H	6.52749	-4.42632	-3.12770
H	3.90144	-1.44177	-1.74689
H	0.44460	0.81015	6.70532
H	0.29225	2.46483	7.31953
H	-2.10512	1.39697	6.11791
H	1.28096	3.07546	4.08613
H	-3.55063	1.99901	4.20705
H	-0.16425	3.68340	2.17830
H	-2.58415	3.16587	2.22820
H	-5.50811	-3.59176	1.70301
H	-5.29320	-4.53094	3.20184
H	-3.17688	-4.07860	4.02258
H	-2.37932	-2.51509	3.97509
H	-2.80394	6.70544	-2.79735
H	-4.17388	6.07454	-1.85911
H	-3.63490	3.50468	-0.89520
H	0.53033	3.92494	-0.52829
H	-0.34577	-3.84138	-1.85928
H	0.54229	-2.73647	-3.36067
H	1.61684	2.04656	6.21962
H	-3.04440	7.23363	-1.12806
H	3.25077	-6.24485	-2.98773
H	6.26871	-2.07606	-2.05758
H	-6.33929	-3.08631	3.17668
H	-3.77451	-5.22233	-2.52111
H	-5.54282	0.82603	-2.22611
H	2.21374	0.37379	1.47953
H	1.70255	-0.97264	3.50901
H	-1.48987	2.35622	-0.22119
O	6.56063	0.38086	-0.56970
O	6.27549	2.55051	-1.93551
O	5.30655	2.32313	0.53188
H	6.48905	0.19203	0.37539
H	-5.46637	-1.13465	-0.71353
C	-3.39252	-1.21603	-0.44899
O	-2.61837	-1.55842	-1.31992
H	-3.24752	-1.54842	0.59489

Charge: –1 Point Group: C_1
Total electronic energy = –2968.180515 a.u.
Zero-point corrected total electronic energy (E_{ZPE}) = –2967.34326 a.u.
No. of imaginary frequency = 6 (141.66i cm^{-1}, corresponding to C1'–O bond formation at the positively charged oxocarbenium center, and 52.95i cm^{-1}, 23.66i cm^{-1}, 14.10i cm^{-1}, 11.75i cm^{-1}, 5.21i cm^{-1})

Product (PD)

C	-1.29783	1.22234	0.53992
N	-2.22528	0.87763	1.50732
C	-1.92173	0.49889	2.80437
C	-0.52340	0.49157	3.08339
C	0.35189	0.85184	2.08306
N	0.01280	1.20893	0.82938
O	-1.73312	1.52403	-0.60396
O	-2.84612	0.19076	3.58982
C	0.69007	-1.73350	-0.74831
C	0.56939	-0.77994	-1.93202
C	2.00733	-0.33110	-2.24489
C	2.85112	-0.92769	-1.10066
O	2.48833	-0.72331	-3.52174
O	1.91800	-1.47749	-0.15335
C	3.76273	0.06088	-0.40131
O	4.51587	-0.63651	0.58387
P	5.76768	0.07474	1.53695
N	-4.28724	1.76352	-2.06723
C	-3.93582	0.45629	-2.61455
C	-3.14214	0.57176	-3.91142
C	-3.86203	-3.75969	-2.38358
C	-2.41056	-3.87940	-1.99765
O	-2.21782	-3.94898	-0.67546
O	-1.49138	-3.95406	-2.79471
C	2.48413	-7.31178	0.09477
C	3.13994	-6.00149	0.48128
N	2.61931	-4.73255	0.22581
C	4.31259	-5.77519	1.14643
C	3.43171	-3.79373	0.71562
N	4.46622	-4.40567	1.27618
C	-1.19870	4.09803	5.28938
C	-1.71549	4.10515	3.86835
C	-3.06989	3.88072	3.60102

C	-0.85982	4.34276	2.78904
C	-3.55828	3.91070	2.29683
C	-1.34253	4.37706	1.48151
C	-2.69639	4.16819	1.23211
C	-6.99582	-0.80911	0.77546
C	-5.76387	-0.15444	1.37851
O	-5.21690	0.78521	0.79096
N	-5.30166	-0.64271	2.54033
C	0.26941	5.75755	-4.55231
C	0.35989	4.77663	-3.42891
N	1.50307	4.64190	-2.67528
C	-0.60111	3.90574	-2.97671
C	1.22405	3.70509	-1.78727
N	-0.03200	3.22619	-1.93063
O	0.65102	-3.15013	-1.12444
H	-3.21043	0.99971	1.26605
H	-0.07971	-1.58795	0.01142
H	-0.04258	0.06922	-1.62146
H	0.07653	-1.22403	-2.80203
H	2.07668	0.75880	-2.25111
H	3.46626	-1.74747	-1.50643
H	2.36906	-1.67754	-3.61369
H	3.15602	0.85064	0.06326
H	4.42424	0.51196	-1.15471
H	-4.91208	1.63418	-1.27155
H	-3.43962	2.15659	-1.65667
H	-2.19185	1.08478	-3.72478
H	-3.71281	1.15260	-4.64149
H	-3.93253	-3.12645	-3.26867
H	-4.25006	-4.75426	-2.63137
H	2.33239	-7.37140	-0.98719
H	3.12736	-8.13838	0.40333
H	1.77526	-4.44826	-0.29509
H	5.03782	-6.47224	1.53515
H	3.26819	-2.71875	0.67443
H	-1.63938	3.27494	5.86274
H	-1.44794	5.03518	5.80320
H	-3.74615	3.65314	4.42265
H	0.20350	4.48537	2.96844
H	-4.60805	3.70288	2.10755

H	-0.65618	4.53772	0.65464
H	-3.06671	4.16456	0.21113
H	-6.71883	-1.24520	-0.18959
H	-7.43280	-1.58892	1.40644
H	-5.73778	-1.44128	2.97295
H	-4.42213	-0.27446	2.95546
H	1.04500	5.56596	-5.30317
H	-0.70746	5.69685	-5.04461
H	-1.61745	3.71840	-3.29420
H	1.89055	3.34423	-1.01528
H	-1.25757	-3.86291	-0.51117
H	0.12990	-3.27133	-1.94253
H	-0.11057	3.98166	5.31293
H	0.40830	6.78382	-4.19194
H	1.51304	-7.42174	0.58693
H	5.22973	-3.88265	1.70141
H	-7.74621	-0.03700	0.58555
H	-4.44876	-3.33965	-1.56586
H	-2.91148	-0.41448	-4.32461
H	1.42299	0.85327	2.28292
H	-0.18486	0.21584	4.07432
H	-0.51731	2.52300	-1.35497
O	5.91866	-1.30450	2.48772
O	6.97818	0.21336	0.68162
O	5.16999	1.14343	2.39577
H	5.48128	-1.07821	3.31936
H	-4.88480	-0.06759	-2.82920
C	-3.23034	-0.44236	-1.61049
O	-2.38275	-1.26096	-1.90886
H	-3.59254	-0.36072	-0.57090

Charge: –1 Point Group: C_1
Total electronic energy = –2968.20967 a.u.
Zero-point corrected total electronic energy (E_{ZPE}) = –2967.36479 a.u.
No. of imaginary frequency = 5 (45.54i cm^{-1}, 34.55i cm^{-1}, 31.19i cm^{-1}, 13.88i cm^{-1}, 13.24i cm^{-1}, 3.08i cm^{-1})

Optimized Cartesian coordinates for QM/MM active site for geometry optimization calculations.

N	15.752078	0.078982	2.223261
C	15.352022	0.627332	3.526157
C	14.644657	1.934920	3.326255
O	14.256236	2.271930	2.222163
H	14.675673	-0.119318	4.036244
H	16.253719	0.731993	4.165399
N	14.436877	2.662162	4.437750
C	13.680223	3.913344	4.379914
C	14.540414	5.188737	4.328315
O	14.135136	6.122699	3.624809
H	14.914592	2.412769	5.295590
H	13.224852	3.931767	3.388503
C	12.448027	4.006024	5.335221
C	12.466784	3.549037	6.806386
C	12.822241	4.626590	7.818169
O	12.079833	4.918270	8.747394
N	13.977144	5.270016	7.543426
H	11.703319	3.392871	4.830089
H	12.069712	5.032740	5.280659
H	13.083593	2.657629	6.970343
H	11.450366	3.260574	7.072843
H	14.688840	4.793643	7.012691
H	14.349437	6.005358	8.131999
N	15.684914	5.301496	5.023618
C	16.435915	6.553395	5.021215
C	17.750034	6.283047	5.754384
O	17.905731	5.292060	6.473388
H	16.069374	4.538015	5.566136
H	16.659143	6.765587	3.968277
C	15.655256	7.781538	5.589276
C	15.759459	8.109043	7.087270
O	15.677774	9.324720	7.388816
O	15.834379	7.179639	7.929012
H	14.592641	7.654015	5.356743
H	15.970152	8.668476	5.027386
N	18.785076	7.129016	5.510924
C	20.095436	6.856766	6.102253
C	20.077831	6.898629	7.636403
O	19.283844	7.599756	8.240597

H	20.456308	5.881739	5.748318
C	20.982666	8.010913	5.580772
C	20.252045	8.512588	4.334601
C	18.783350	8.374353	4.733791
H	22.001421	7.674568	5.382652
H	21.034349	8.806389	6.331767
H	20.467443	7.869385	3.473745
H	20.531044	9.535983	4.065864
H	18.126755	8.314421	3.864768
H	18.464373	9.213358	5.364721
N	21.082838	6.219333	8.262930
C	21.322899	6.373165	9.690621
C	21.495468	7.864827	10.052977
O	22.177322	8.610364	9.359995
H	21.658148	5.581976	7.725415
H	20.467724	5.961179	10.240077
C	22.620472	5.673297	10.155339
C	22.609983	4.167785	10.087546
C	21.737619	3.441041	10.911067
C	23.479818	3.452909	9.262919
C	21.672733	2.060058	10.854263
C	23.446516	2.055555	9.208814
C	22.528248	1.366073	10.000522
O	22.423021	0.008365	10.034642
H	22.789976	5.970278	11.196630
H	23.458712	6.076375	9.572258
H	21.103409	3.968572	11.616649
H	24.221052	3.984174	8.660973
H	20.990770	1.506775	11.491181
H	24.142971	1.535164	8.556179
H	23.038301	-0.365981	9.398880
N	20.886927	8.271312	11.203234
C	20.871489	9.630448	11.608357
C	21.844379	10.012078	12.774839
O	21.811766	11.145904	13.261987
H	20.437326	7.575240	11.793870
H	21.213842	10.209388	10.755707
C	19.444748	10.079127	11.934148
C	18.805054	9.263219	13.005756
N	17.728586	8.428773	12.767531
C	19.119408	9.103217	14.321095
C	17.411936	7.775981	13.884099
N	18.243158	8.186244	14.829288
H	18.846922	9.992870	11.025056
H	19.440689	11.140196	12.206861
H	17.323063	8.211041	11.839332

H	19.918043	9.492722	14.929389
H	16.625290	7.046117	14.006152
H	18.308775	7.841568	15.778944
N	22.736551	9.078996	13.223666
H	22.759466	8.110551	12.875205
N	21.868481	0.272998	5.413549
C	22.224897	-0.443233	6.611400
C	23.701492	-0.607805	6.926183
O	24.072870	-1.067651	8.009961
H	21.304222	1.099829	5.647434
H	21.831137	0.155781	7.463301
C	21.473915	-1.889570	6.637934
C	20.011524	-1.619597	6.512905
C	19.343903	-1.830317	5.311726
C	19.298033	-1.170930	7.627682
C	17.985119	-1.537079	5.203970
C	17.940393	-0.898233	7.531697
C	17.278700	-1.082531	6.314719
H	21.718403	-2.356897	7.592275
H	21.869608	-2.492802	5.819544
H	19.884970	-2.185176	4.436600
H	19.823839	-0.998037	8.565915
H	17.481073	-1.685168	4.253067
H	17.396366	-0.547861	8.403154
H	16.211023	-0.894919	6.242177
C	16.893831	3.753932	0.663465
H	16.323528	2.857632	1.011309
C	17.453266	4.553248	1.862038
C	17.960442	3.663676	2.999638
O	17.400364	2.631854	3.317163
N	19.021223	4.169069	3.609412
H	16.671930	5.196695	2.300503
H	18.250805	5.251284	1.518492
H	19.498816	5.001467	3.282586
H	19.449623	3.624696	4.352129
N	10.638093	-3.649339	8.715250
C	11.963569	-3.054270	8.756299
C	12.762704	-3.728999	9.876611
O	12.225430	-4.015554	10.936936
H	9.858944	-3.076314	9.067353
H	12.437235	-3.226084	7.773444
C	11.829623	-1.476700	9.057896
C	13.129450	-0.770593	8.937304
N	13.959358	-0.613388	10.020822
C	13.656327	-0.135985	7.841864
C	14.984964	0.074676	9.587685

N	14.857794	0.382936	8.264218
H	11.440448	-1.368919	10.066413
H	11.111961	-1.059667	8.355946
H	13.324331	-0.062693	6.814118
H	15.843544	0.370218	10.180643
H	15.446890	1.018719	7.742387
O	17.029850	7.234459	10.420996
H	17.342482	6.336794	10.569186
H	16.653114	7.233153	9.505423
C	20.080198	3.007446	7.818487
C	19.619120	2.652313	6.516631
N	18.286671	2.357966	6.403207
C	17.318993	2.740470	7.289341
N	17.823990	3.196675	8.503980
C	19.162142	3.344300	8.726004
O	20.304827	2.665358	5.486454
O	16.135563	2.654685	6.992979
C	16.927969	4.013493	9.426923
C	15.542454	3.522684	9.715269
O	17.495325	4.360402	10.687547
H	17.954605	2.148684	5.455725
H	15.240127	2.682515	9.104226
H	14.844276	4.320371	9.480477
H	16.844381	4.917233	8.834065
H	19.454878	3.747385	9.684919
H	21.119961	3.213169	8.024668

Cartesian coordinates for QM/MM active site for single-point calculations.

C	19.295973	4.731270	18.024103
C	18.944773	3.377273	17.448734
O	18.263023	2.589793	18.434092
C	18.114044	3.285540	16.168749
C	16.711210	2.994697	16.683485
O	18.543661	2.182240	15.350052
H	19.912823	2.891420	17.281736
H	18.094881	4.232559	15.614800
H	16.157433	3.928630	16.788385
H	16.126926	2.372768	15.998198
P	13.671378	3.538978	13.061518
O	12.874393	4.695830	13.563131
O	14.739105	2.889890	13.888484
O	12.815276	2.368018	12.391223

C	11.669369	2.676332	11.612541
C	10.790257	1.453644	11.713755
O	10.413697	1.229677	13.084391
C	9.482544	1.365052	10.939628
H	11.940639	2.847831	10.565754
H	11.117413	3.553992	11.951826
H	11.434203	0.620661	11.406176
N	15.752078	0.078982	2.223261
C	15.352022	0.627332	3.526157
C	14.644657	1.934920	3.326255
O	14.256236	2.271930	2.222163
H	14.675673	-0.119318	4.036244
H	16.253719	0.731993	4.165399
N	14.436877	2.662162	4.437750
C	13.680223	3.913344	4.379914
C	14.540414	5.188737	4.328315
O	14.135136	6.122699	3.624809
H	14.914592	2.412769	5.295590
H	13.224852	3.931767	3.388503
C	12.448027	4.006024	5.335221
C	12.466784	3.549037	6.806386
C	12.822241	4.626590	7.818169
O	12.079833	4.918270	8.747394
N	13.977144	5.270016	7.543426
H	11.703319	3.392871	4.830089
H	12.069712	5.032740	5.280659
H	13.083593	2.657629	6.970343
H	11.450366	3.260574	7.072843
H	14.688840	4.793643	7.012691
H	14.349437	6.005358	8.131999
N	15.684914	5.301496	5.023618
C	16.435915	6.553395	5.021215
C	17.750034	6.283047	5.754384
O	17.905731	5.292060	6.473388
H	16.069374	4.538015	5.566136
H	16.659143	6.765587	3.968277
C	15.655256	7.781538	5.589276
C	15.759459	8.109043	7.087270
O	15.677774	9.324720	7.388816
O	15.834379	7.179639	7.929012
H	14.592641	7.654015	5.356743
H	15.970152	8.668476	5.027386
N	18.785076	7.129016	5.510924
C	20.095436	6.856766	6.102253
C	20.077831	6.898629	7.636403
O	19.283844	7.599756	8.240597

H	20.456308	5.881739	5.748318
C	20.982666	8.010913	5.580772
C	20.252045	8.512588	4.334601
C	18.783350	8.374353	4.733791
H	22.001421	7.674568	5.382652
H	21.034349	8.806389	6.331767
H	20.467443	7.869385	3.473745
H	20.531044	9.535983	4.065864
H	18.126755	8.314421	3.864768
H	18.464373	9.213358	5.364721
N	21.082838	6.219333	8.262930
C	21.322899	6.373165	9.690621
C	21.495468	7.864827	10.052977
O	22.177322	8.610364	9.359995
H	21.658148	5.581976	7.725415
H	20.467724	5.961179	10.240077
C	22.620472	5.673297	10.155339
C	22.609983	4.167785	10.087546
C	21.737619	3.441041	10.911067
C	23.479818	3.452909	9.262919
C	21.672733	2.060058	10.854263
C	23.446516	2.055555	9.208814
C	22.528248	1.366073	10.000522
O	22.423021	0.008365	10.034642
H	22.789976	5.970278	11.196630
H	23.458712	6.076375	9.572258
H	21.103409	3.968572	11.616649
H	24.221052	3.984174	8.660973
H	20.990770	1.506775	11.491181
H	24.142971	1.535164	8.556179
H	23.038301	-0.365981	9.398880
N	20.886927	8.271312	11.203234
C	20.871489	9.630448	11.608357
C	21.844379	10.012078	12.774839
O	21.811766	11.145904	13.261987
H	20.437326	7.575240	11.793870
H	21.213842	10.209388	10.755707
C	19.444748	10.079127	11.934148
C	18.805054	9.263219	13.005756
N	17.728586	8.428773	12.767531
C	19.119408	9.103217	14.321095
C	17.411936	7.775981	13.884099
N	18.243158	8.186244	14.829288
H	18.846922	9.992870	11.025056
H	19.440689	11.140196	12.206861
H	17.323063	8.211041	11.839332

H	19.918043	9.492722	14.929389
H	16.625290	7.046117	14.006152
H	18.308775	7.841568	15.778944
N	22.736551	9.078996	13.223666
H	22.759466	8.110551	12.875205
N	21.868481	0.272998	5.413549
C	22.224897	-0.443233	6.611400
C	23.701492	-0.607805	6.926183
O	24.072870	-1.067651	8.009961
H	21.304222	1.099829	5.647434
H	21.831137	0.155781	7.463301
C	21.473915	-1.889570	6.637934
C	20.011524	-1.619597	6.512905
C	19.343903	-1.830317	5.311726
C	19.298033	-1.170930	7.627682
C	17.985119	-1.537079	5.203970
C	17.940393	-0.898233	7.531697
C	17.278700	-1.082531	6.314719
H	21.718403	-2.356897	7.592275
H	21.869608	-2.492802	5.819544
H	19.884970	-2.185176	4.436600
H	19.823839	-0.998037	8.565915
H	17.481073	-1.685168	4.253067
H	17.396366	-0.547861	8.403154
H	16.211023	-0.894919	6.242177
C	16.893831	3.753932	0.663465
H	16.323528	2.857632	1.011309
C	17.453266	4.553248	1.862038
C	17.960442	3.663676	2.999638
O	17.400364	2.631854	3.317163
N	19.021223	4.169069	3.609412
H	16.671930	5.196695	2.300503
H	18.250805	5.251284	1.518492
H	19.498816	5.001467	3.282586
H	19.449623	3.624696	4.352129
N	10.638093	-3.649339	8.715250
C	11.963569	-3.054270	8.756299
C	12.762704	-3.728999	9.876611
O	12.225430	-4.015554	10.936936
H	9.858944	-3.076314	9.067353
H	12.437235	-3.226084	7.773444
C	11.829623	-1.476700	9.057896
C	13.129450	-0.770593	8.937304
N	13.959358	-0.613388	10.020822
C	13.656327	-0.135985	7.841864
C	14.984964	0.074676	9.587685

N	14.857794	0.382936	8.264218
H	11.440448	-1.368919	10.066413
H	11.111961	-1.059667	8.355946
H	13.324331	-0.062693	6.814118
H	15.843544	0.370218	10.180643
H	15.446890	1.018719	7.742387
O	17.029850	7.234459	10.420996
H	17.342482	6.336794	10.569186
H	16.653114	7.233153	9.505423
C	20.080198	3.007446	7.818487
C	19.619120	2.652313	6.516631
N	18.286671	2.357966	6.403207
C	17.318993	2.740470	7.289341
N	17.823990	3.196675	8.503980
C	19.162142	3.344300	8.726004
O	20.304827	2.665358	5.486454
O	16.135563	2.654685	6.992979
C	16.927969	4.013493	9.426923
C	15.542454	3.522684	9.715269
C	15.468281	3.283112	11.197873
C	16.786394	3.782352	11.791101
O	14.385630	4.056007	11.712134
O	17.495325	4.360402	10.687547
C	17.616854	2.739578	12.512065
O	18.722490	3.374149	13.151029
P	19.595367	2.448941	14.160312
O	19.889328	1.122723	13.522293
O	20.716814	3.344510	14.600105
H	17.954605	2.148684	5.455725
H	15.240127	2.682515	9.104226
H	14.844276	4.320371	9.480477
H	16.844381	4.917233	8.834065
H	15.343510	2.207129	11.373619
H	17.929085	1.976827	11.793000
H	16.934200	2.278136	13.241313
H	16.590733	4.588815	12.508771
H	19.454878	3.747385	9.684919
H	21.119961	3.213169	8.024668