Supporting Information

Reaction Kinetics, Product Branching and Potential Energy Surfaces of $^1O_2$-induced 9-Methylguanine–Lysine Cross-linking: A Combined Mass Spectrometry, Spectroscopy and Computational Study

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Table of Contents

Fig. S1 Schematic of experimental setup S2

Cablibaryion of [$^1O_2$] in solution and Fig. S2 ..... S3

Fig. S3 Stable tautomers/rotamers of neutral N^{α}-acetyl-lysine methyl ester S6

Fig. S4 Stable tautomers/rotamers of protonated N^{α}-acetyl-lysine methyl ester S8

Cartesian coordinates for the structures in Fig. S3 ..... S10

Cartesian coordinates for the structures in Fig. S4 ..... S22

Cartesian coordinates for the structures in Fig. 3 ..... S33

Cartesian coordinates for the structures in Fig. 4 ..... S42

Cartesian coordinates for the structures in Fig. 5 ..... S49

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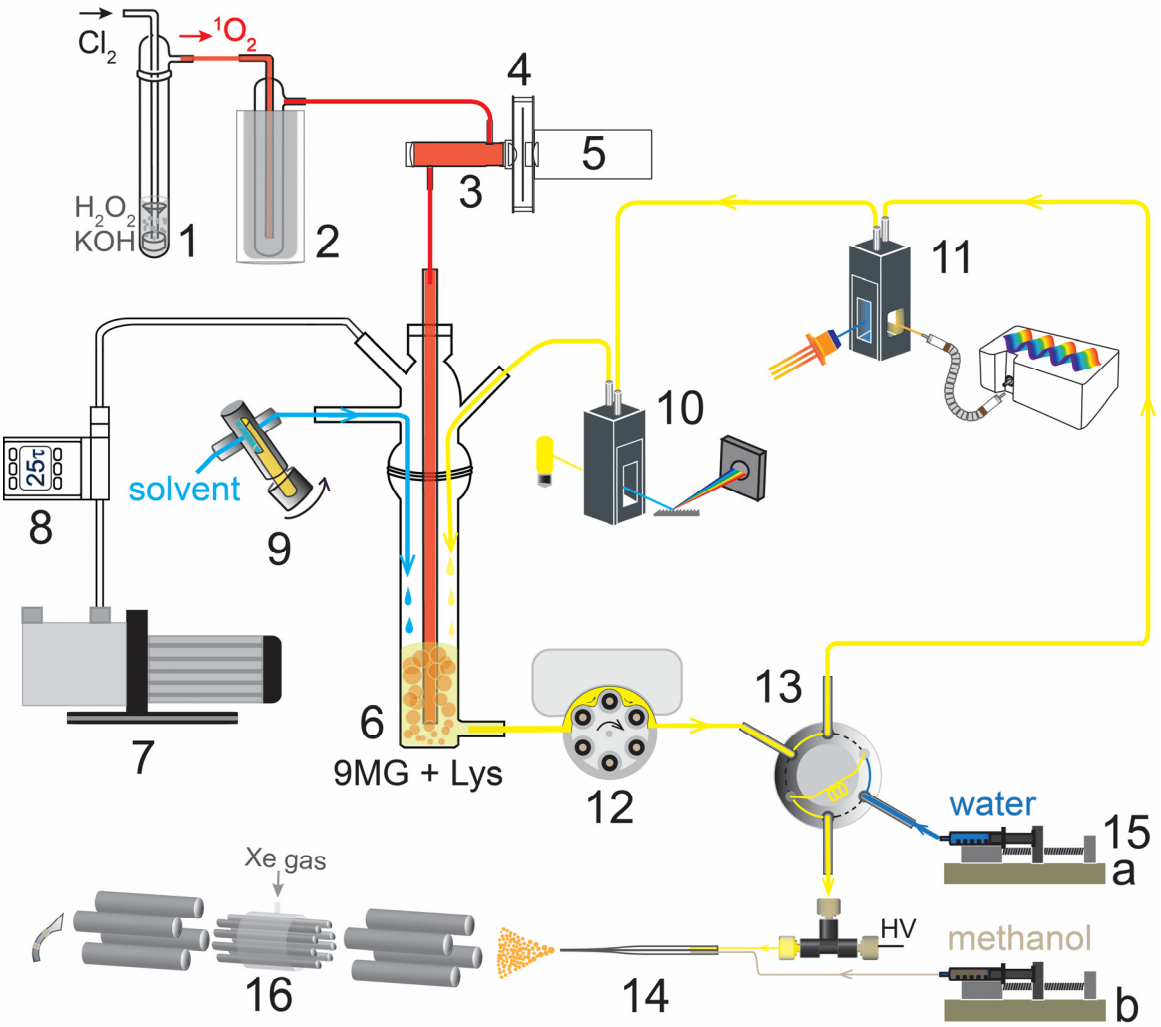


Fig. S1 Schematic of experimental setup: (**1**) sparger; (**2**) cold trap; (**3**) emission cell; (**4**) optical chopper; (**5**) InGaAs photodetector; (**6**) reaction vessel; (**7**) mechanical pump; (**8**) pressure relay; (**9**) piston pump; (**10**) UV-Vis spectrometer; (**11**) fluorometer; (**12**) peristaltic pump; (**13**) two-position switching valve; (**14**) θ-ESI emitter; (**15a – b**) syringe pumps; and (**16**) tandem MS.

Calibration of [$^1O_2$] in solution In the experiment, chemically generated $^1O_2$ was continuously bubbled into the reaction vessel. $^1O_2$ had a longer lifetime in the interior of bubbles (because of reduced encounters with water) than in bulk solution. After diffusing into the bulk water, $^1O_2$ could travel ~ 150 nm within a lifetime of ~ 2 μs.[1] Therefore, $^1O_2$ reactions occurred both at the gas/solution interface and in the bulk solution. On the basis of the steady concentration of airborne $^1O_2$ (determined on the basis of its emission intensity) and the continuously bubbling of $^1O_2$ into the solution, quasi-steady-state $[^1O_2]_{sol}$ was assumed for the solution reaction and its amount was determined as

$$[^1O_2]_{sol} = m \cdot (I_{EM} - I_B) \quad \text{(S1)}$$

where I_{EM} is the $^1O_2$ emission intensity (mV) measured by the lock-in amplifier in the gas phase, I_B (= 43 mV) represents a threshold $^1O_2$ emission intensity below which all of the airborne $^1O_2$ quenched in the bubbles and/or during diffusion before reaching aqueous substrates as we determined in the previous experiment,[2,3] and m is a scaling factor ($M \cdot mv^{-1}$).

To validate this assumption and calibrate the value of the scaling factor m, 3-(10-(2-carboxy-ethyl)-anthracen-9-yl)-propionic acid (ADPA, Aldrich) was used as a calibration compound. ADPA is known to react with $^1O_2$ chemically (*i.e.* without physical quenching) and produces an endoperoxide *via* a [4 + 2] cycloaddition accompanied by bleaching of the absorption band of ADPA.[4] To take into account the physical quenching of $^1O_2$ by $LysNH_2$ (N^{α}-acetyl-L-lysine-methyl ester, 15 mM) in the actual reaction solution, the calibration experiment was carried out in the presence of the same $LysNH_2$ concentration in the ADPA solution. pH of the ADPA solution (0.1 mM) was maintained at 10.0 using borax/NaOH buffer. The rate law for the decay of ADPA could be described as

$$In\frac{A_t}{A_0} = -k_r \int [^1O_2]_{sol,t} dt \quad \text{(S2)}$$

where A_t and A_0 are the ADPA peak absorption (at 378.7 nm) at different reaction times and time zero, respectively; and $[^1O_2]_{sol,t}$ represents the $[^1O_2]_{sol}$ at the time instant t. The combination of Eqs (S1) and (S2) gives

$$In\frac{A_t}{A_0} = -k_r m \int (I_{EM,t} - I_B) dt \quad \text{(S3)}$$

Figure S2a shows the absorption changes of ADPA throughout the reaction, and the plot of $In\frac{A_t}{A_0}$ $vs.$ $\int(I_{EM,t} - I_B)dt$ is depicted in Figure S2b. The observation of a linear relationship between $In\frac{A_t}{A_0}$ and $\int(I_{EM,t} - I_B)dt$ has verified the pseudo first-order consumption of ADPA and the linear dependence of $[^1O_2]_{sol}$ on I_{EM}. Accordingly, the value of m (8.39×10^{-15} $M \cdot mV^{-1}$) was extracted from the slope of the calibration plot using the reaction rate k_r of 8.2×10^7 $M^{-1} \cdot s^{-1}$ for ADPA + $^1O_2$.[4]

During the experiment, emission of airborne $^1O_2$ was continuously monitored, and the Eq. S1 was used to determine $[^1O_2]_{sol}$ in the reactions.

1. Skovsen, E.; Snyder, J. W.; Lambert, J. D. C.; Ogilby, P. R. Lifetime and Diffusion of Singlet Oxygen in a Cell. *J. Phys. Chem. B* **2005**, 109, 8570-8573.
2. Liu, F.; Lu, W.; Yin, X.; Liu, J. Mechnistic and Kinetic Study of Singlet O_2 Oxidation of Methionine by On-Line Electrospray Ionization Mass Spectrometry. *J. Am. Soc. Mass Spectrom.* **2016**, 27, 59-72.
3. Lu, W.; Sun, Y.; Zhou, W.; Liu, J. pH-Dependent Singlet O_2 Oxidation Kinetics of Guanine and 9-Methylguanine: An Online Mass Spectrometry and Spectroscopy Study Combined with Theoretical Exploration. *J. Phys. Chem. B* **2018,** *122*, 40-53.
4. Lindig, B. A.; Rodgers, M. A. J. Rate Parameters for the Quenching of Singlet Oxygen by Water-Soluble and Lipid-Soluble Substrates in Aqueous and Micellar Systems. *Photochem. Photobiol.* **1981**, 33, 627-34.

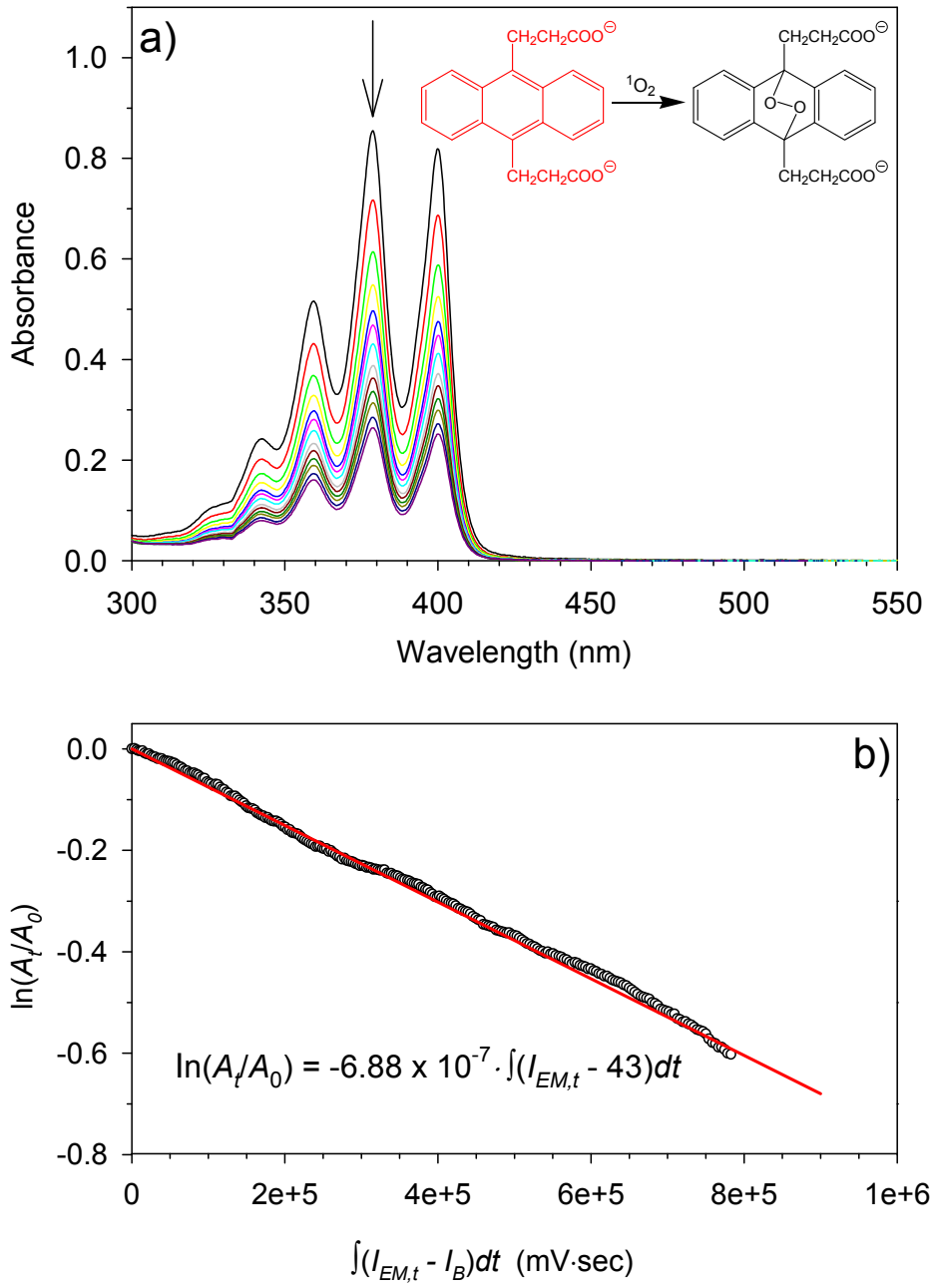


Fig. S2 (a) UV-Vis absorption spectra of ADPA over the course of the reaction with $^1O_2$; and (b) the linear relationship of $In\frac{A_t}{A_0}$ against $\int(I_{EM,t} - I_B)dt$.

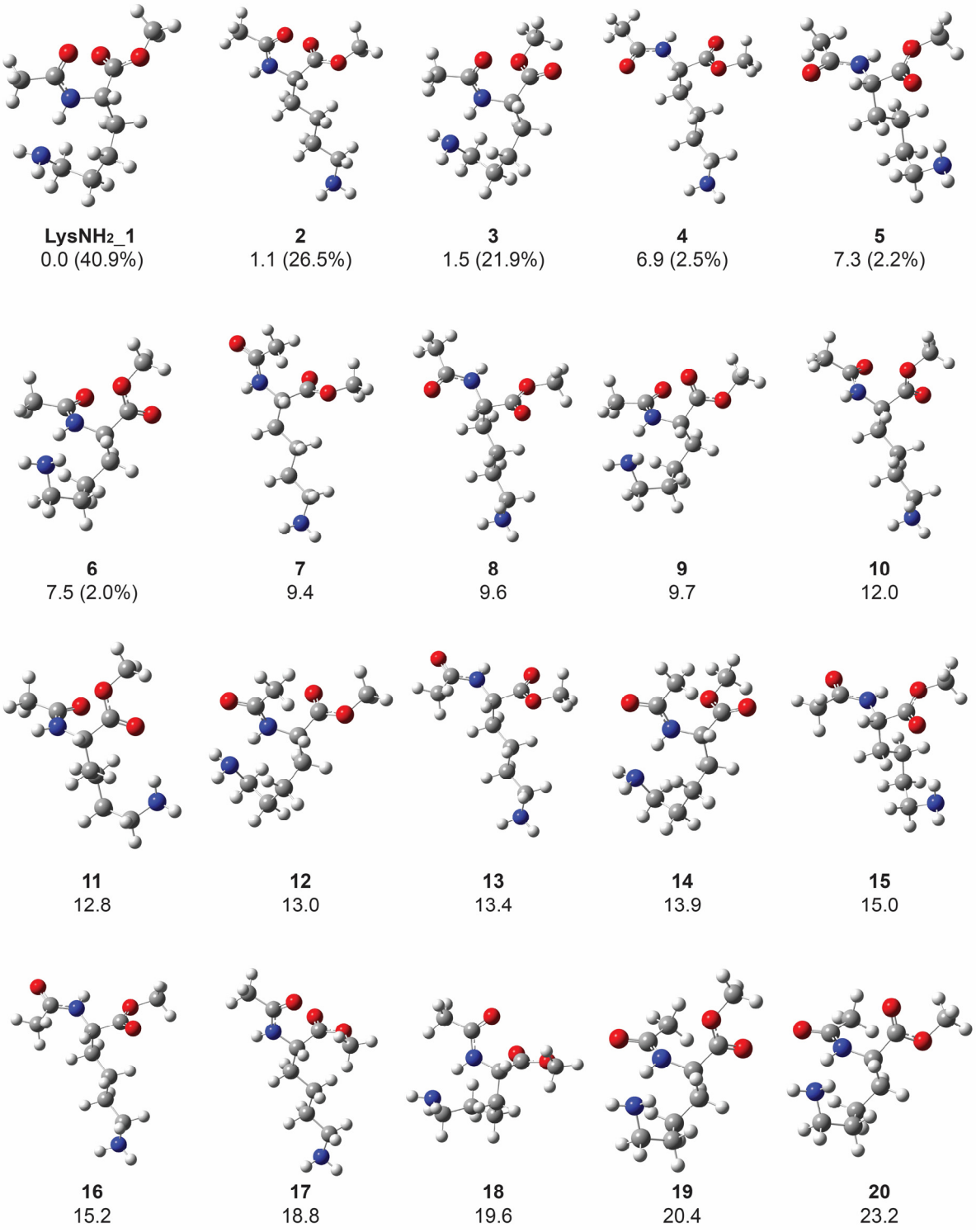


Fig. S3 Stable conformers of neutral $LysNH_2$ (N^{α}-acetyl-L-lysine-methyl ester). Relative energies (kJ/mol, including ZPE and thermal corrections at 298 K) were calculated at the SMD-ωB97XD/6-31+G(d,p) level of theory. Populations for major conformers are indicated in parenthesis.

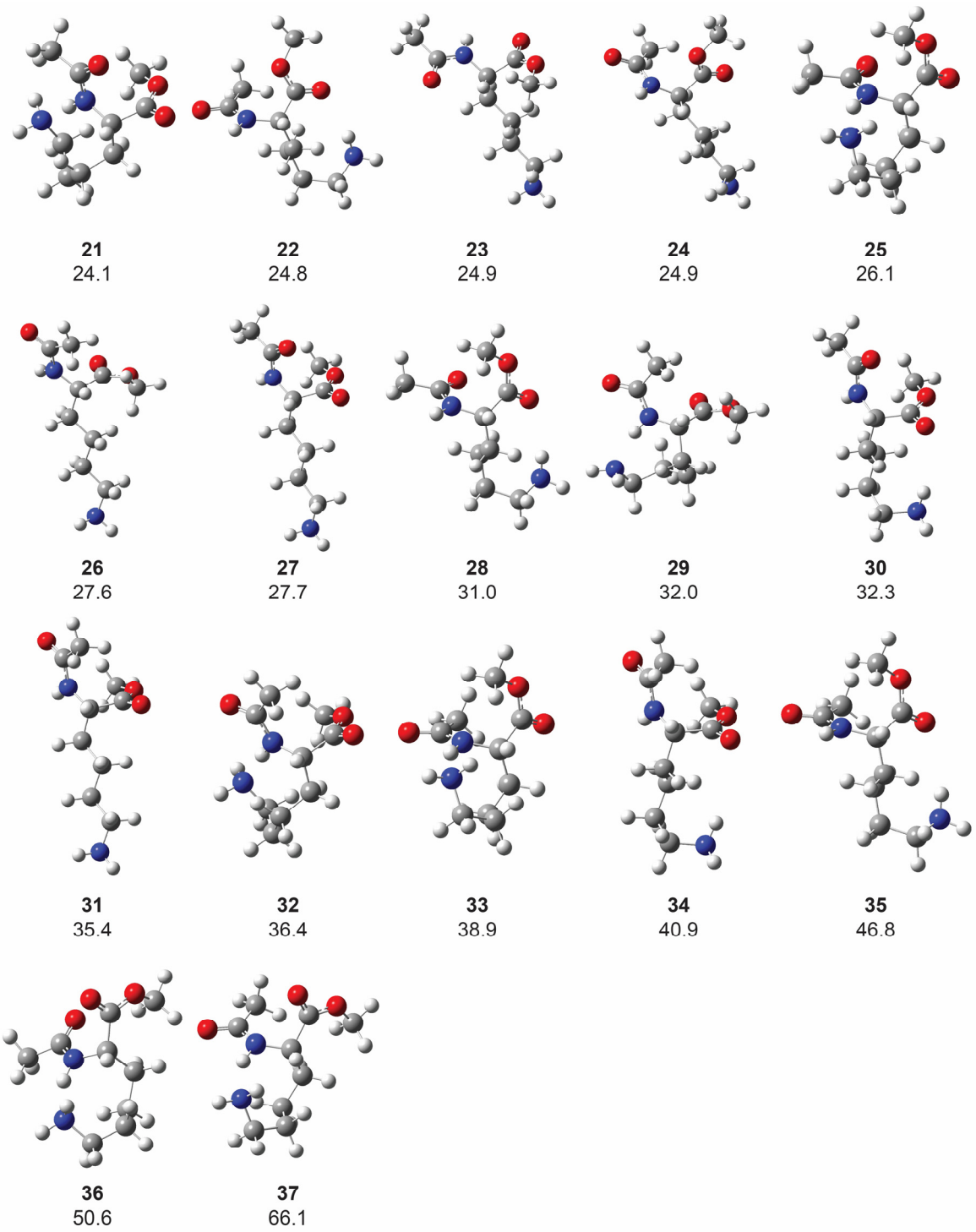


Fig. S3 (Continued.)

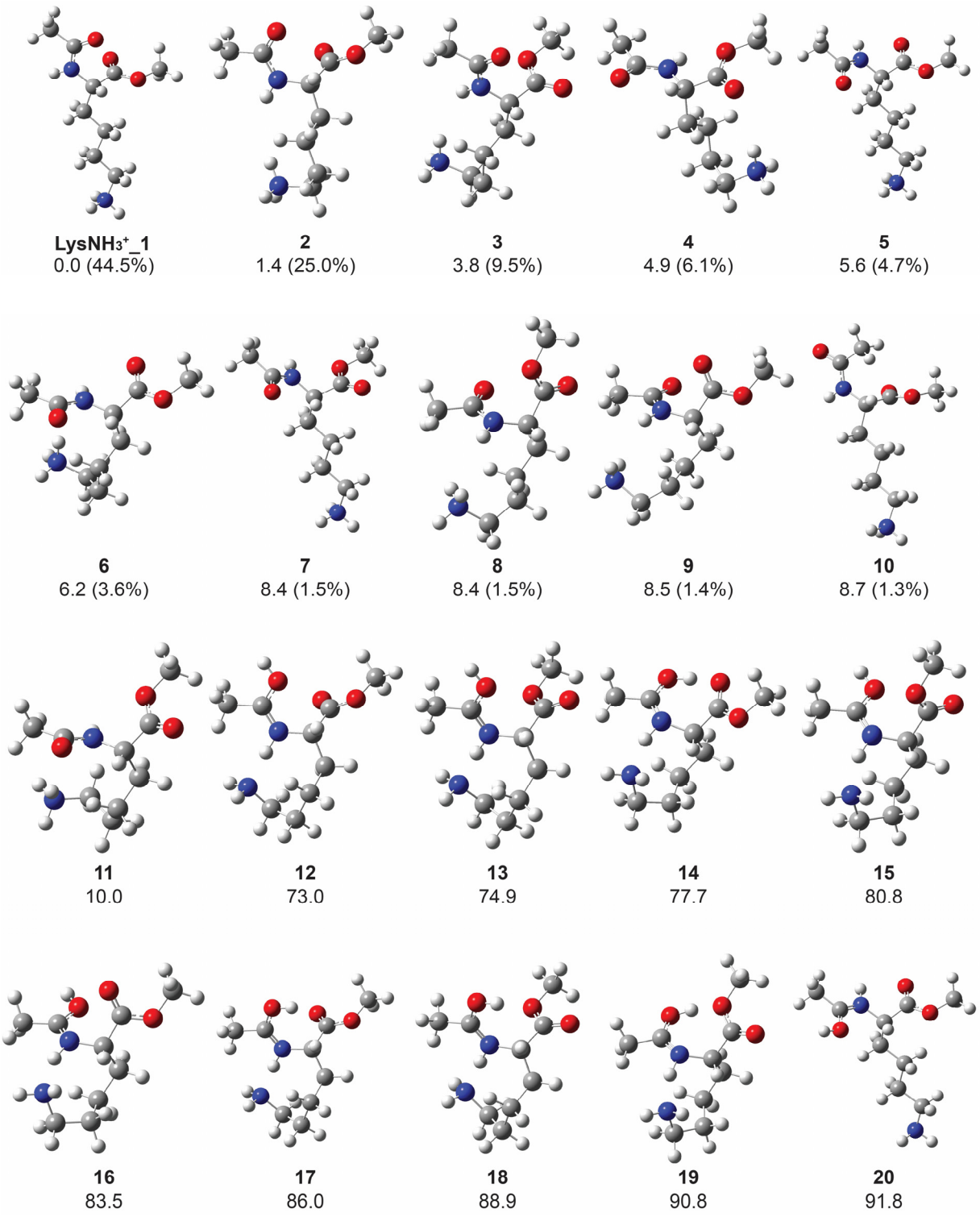


Fig. S4 Stable conformers of protonated $LysNH_3^+$ (protonated N^{α}-acetyl-L-lysine-methyl ester). Relative energies (kJ/mol, including ZPE and thermal corrections at 298 K) were calculated at the SMD-ωB97XD/6-31+G(d,p) level of theory. Populations for major conformers are indicated in parenthesis.

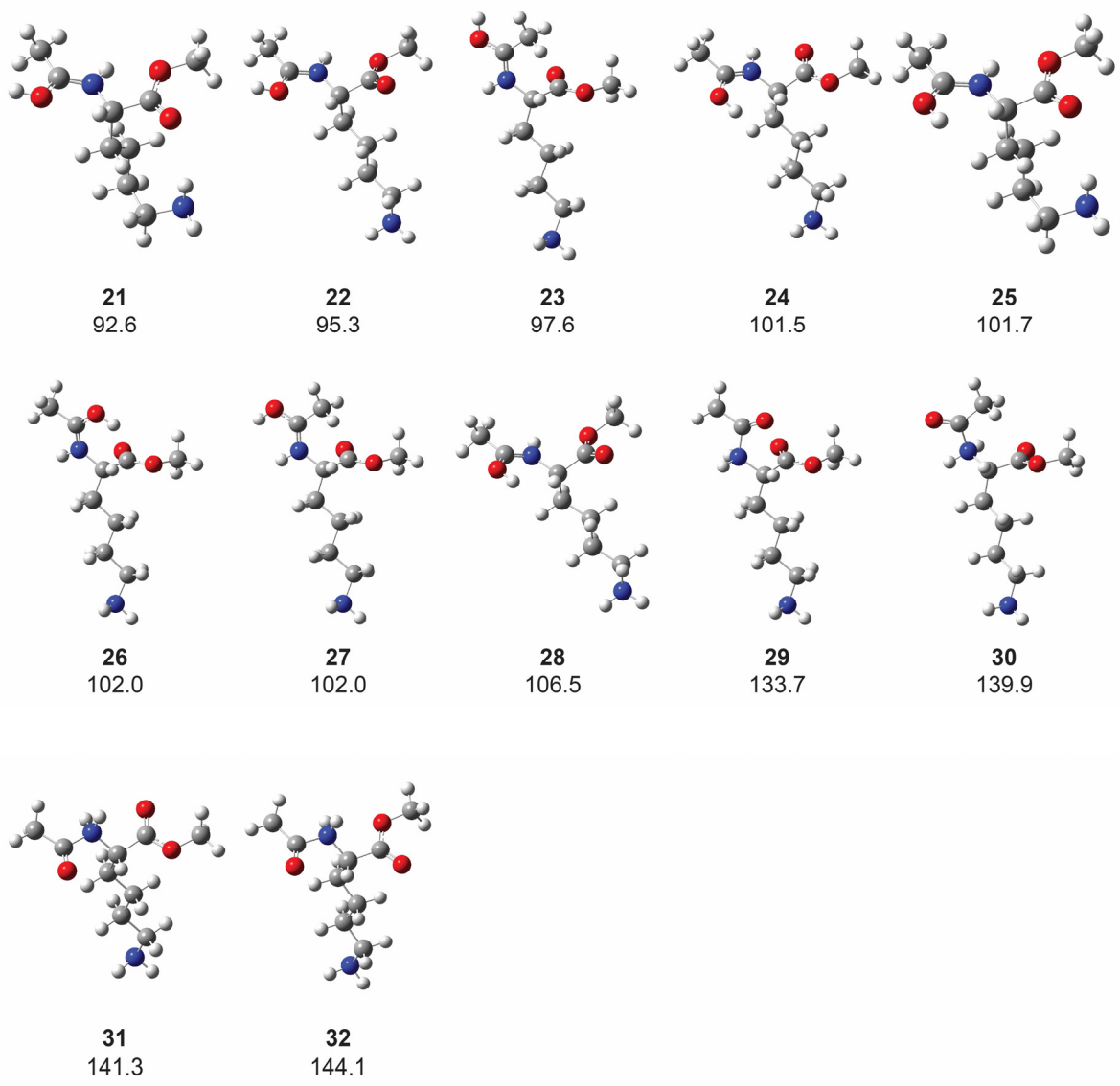


Fig. S4 (Continued.)

Cartesian coordinates for the structures in Fig. S3, optimized at SMD-ωB97XD/6-31+ G(d,p).

LysNH$_2$_1

C1	-0.472120	-0.351185	-0.516146
H2	-0.742063	-0.358051	-1.577699
C3	0.439716	-1.549790	-0.210453
H4	0.651786	-1.543678	0.864183
H5	-0.130400	-2.461366	-0.409742
C6	-1.752634	-0.515329	0.287912
O7	-2.710405	-1.096955	-0.430093
O8	-1.877836	-0.224631	1.465315
N9	0.193181	0.891772	-0.179982
H10	1.208859	0.874215	0.032278
C11	1.745224	-1.545450	-1.031900
H12	1.714083	-2.354747	-1.767425
H13	1.818141	-0.620220	-1.613173
C14	3.018879	-1.702933	-0.191200
H15	3.881991	-1.676747	-0.868515
H16	3.028493	-2.688097	0.290312
C17	3.215448	-0.648234	0.897105
H18	2.478974	-0.781648	1.696894
H19	4.203212	-0.800040	1.352922
N20	3.051696	0.713031	0.367346
H21	3.319095	1.392228	1.074006
H22	3.682728	0.848862	-0.419088
C23	-0.435997	2.068934	-0.300910
C24	0.351791	3.302139	0.045509
H25	1.393265	3.083577	0.288815
H26	0.313865	3.998414	-0.796028
H27	-0.122200	3.787330	0.903569
O28	-1.629298	2.143657	-0.661741
C29	-3.936502	-1.402060	0.257444
H30	-4.392542	-0.485992	0.636957
H31	-4.580088	-1.863762	-0.488753
H32	-3.743840	-2.097025	1.076917

2

N1	-5.583724	-0.770426	0.155295
C2	-4.353328	-0.055967	-0.205218
H3	-4.329662	0.885966	0.352731
H4	-4.319575	0.205407	-1.273733
C5	-3.120555	-0.879436	0.139134
H6	-3.170369	-1.839427	-0.392776
H7	-3.127868	-1.108209	1.212521
C8	-1.819878	-0.165134	-0.224306
H9	-1.808788	0.057290	-1.298868
H10	-1.782272	0.798068	0.300211
C11	-0.594482	-1.004324	0.131899
H12	-0.680325	-1.991215	-0.336198
H13	-0.548160	-1.159223	1.216856
C14	0.735534	-0.397215	-0.336151
H15	0.717903	-0.267315	-1.421731
C16	0.935246	0.976930	0.292464
N17	1.823247	-1.280552	0.032158
O18	1.328343	1.161323	1.431479
O19	0.576989	1.954548	-0.532620
H20	-6.386325	-0.198027	-0.091199
H21	-5.653384	-1.608698	-0.417126
H22	1.618586	-2.074995	0.623706
C23	0.640322	3.295138	-0.013521
H24	0.284249	3.934265	-0.818926
H25	-0.004500	3.389477	0.862068
H26	1.670951	3.545527	0.244124
C27	3.106024	-0.989508	-0.253465
C28	4.152403	-1.932425	0.267625
H29	4.840519	-2.186086	-0.541655
H30	4.721922	-1.415257	1.045659
H31	3.727387	-2.845574	0.687732
O32	3.402834	0.027443	-0.905901

3

C1	-0.376260	-0.461853	-0.779066
H2	-0.496871	-0.397759	-1.866301
C3	0.691357	-1.516200	-0.449510
H4	0.766626	-1.598988	0.640141
H5	0.324437	-2.480966	-0.810038
C6	-1.718190	-0.946086	-0.252641
O7	-1.944473	-0.624366	1.015346
O8	-2.477427	-1.631542	-0.919520
N9	0.000325	0.834095	-0.248768
H10	0.960777	0.965143	0.120575
C11	2.065657	-1.199936	-1.073839
H12	2.269780	-1.912297	-1.878878
H13	2.041484	-0.213169	-1.548589
C14	3.232152	-1.243475	-0.080169
H15	4.156007	-1.006291	-0.622695
H16	3.352315	-2.260838	0.311521
C17	3.105934	-0.297113	1.113356
H18	2.316363	-0.639594	1.791180
H19	4.044429	-0.333014	1.682937
N20	2.763734	1.068684	0.691483
H21	2.831503	1.699765	1.484986
H22	3.440970	1.392943	0.005061
C23	-0.800479	1.896082	-0.413363
C24	-0.304191	3.217080	0.105486
H25	0.666386	3.138070	0.597904
H26	-0.231527	3.918862	-0.729858
H27	-1.036224	3.613458	0.814194
O28	-1.917018	1.795151	-0.964013
C29	-3.171639	-1.099096	1.596325
H30	-3.190865	-2.190509	1.594463
H31	-3.172685	-0.720570	2.616557
H32	-4.026023	-0.704046	1.043851

4

N1	5.180838	-1.446069	-0.231507
C2	4.100076	-0.524371	0.137549
H3	4.295665	0.439780	-0.343370
H4	4.062907	-0.337363	1.221441
C5	2.746061	-1.050682	-0.316296
H6	2.587020	-2.048989	0.114311
H7	2.750157	-1.170892	-1.407251
C8	1.597174	-0.133605	0.099608
H9	1.574975	-0.048987	1.193807
H10	1.781792	0.875295	-0.291129
C11	0.245510	-0.642837	-0.397702
H12	0.119151	-1.695255	-0.121444
H13	0.195026	-0.583603	-1.491399
C14	-0.966337	0.110735	0.186942
H15	-0.957501	0.023440	1.274989
C16	-0.897001	1.578436	-0.182687
N17	-2.220383	-0.426742	-0.309117
O18	-1.312768	2.032631	-1.235778
O19	-0.293900	2.302545	0.750289
H20	6.066896	-1.062421	0.085683
H21	5.056005	-2.316395	0.280519
H22	-2.580582	-0.055378	-1.179483
C23	-0.065896	3.692103	0.448245
H24	0.460045	4.091040	1.312973
H25	0.548154	3.782685	-0.449338
H26	-1.019091	4.205299	0.311791
C27	-2.818016	-1.497940	0.244597
C28	-4.061554	-2.007569	-0.430293
H29	-3.876239	-3.030200	-0.770139
H30	-4.869624	-2.038320	0.304720
H31	-4.368697	-1.397761	-1.281880
O32	-2.372000	-2.043666	1.270463

5

C1	-0.690122	0.087239	0.694101
H2	-1.078123	0.007775	1.712692
C3	0.540572	-0.830669	0.570909
H4	1.231345	-0.561798	1.375861
H5	0.204320	-1.855551	0.761655
C6	-0.260146	1.533160	0.523079
O7	-0.798878	2.142824	-0.524052
O8	0.539385	2.063931	1.276481
N9	-1.763577	-0.279774	-0.208508
H10	-1.723354	0.051338	-1.162883
C11	1.237177	-0.746059	-0.787161
H12	0.521013	-0.978968	-1.583501
H13	1.568903	0.285228	-0.969127
C14	2.431310	-1.699195	-0.911611
H15	2.854294	-1.606570	-1.919192
H16	2.077026	-2.732322	-0.806631
C17	3.538455	-1.469657	0.112855
H18	3.159159	-1.691477	1.120765
H19	4.345315	-2.182977	-0.078792
N20	4.099141	-0.115531	0.017385
H21	3.388851	0.558878	0.293364
H22	4.845631	-0.020550	0.700206
C23	-0.392125	3.502987	-0.765066
H24	-0.671693	4.132805	0.081055
H25	0.685516	3.545415	-0.932068
H26	-0.928494	3.808569	-1.661057
C27	-2.729592	-1.153782	0.130957
C28	-3.737453	-1.489354	-0.933427
H29	-4.736158	-1.262366	-0.551753
H30	-3.573705	-0.946276	-1.865673
H31	-3.690955	-2.563825	-1.130050
O32	-2.797544	-1.660280	1.265718

6

C1	0.219298	-0.622016	0.033281
H2	-0.174987	-1.162686	0.902182
C3	-0.481777	-1.134180	-1.230247
H4	0.021471	-0.721514	-2.110672
H5	-0.362272	-2.222040	-1.269206
C6	1.707492	-0.934003	0.033620
O7	2.348377	-0.349900	1.043388
O8	2.248254	-1.697533	-0.748309
N9	-0.044422	0.783518	0.291180
H10	-0.947407	0.945321	0.764297
C11	-1.968857	-0.770661	-1.283951
H12	-2.068328	0.321703	-1.283975
H13	-2.349015	-1.103309	-2.254932
C14	-2.843066	-1.369019	-0.159217
H15	-2.245728	-2.025314	0.488299
H16	-3.615373	-2.009443	-0.597900
C17	-3.548811	-0.334136	0.714437
H18	-4.062541	0.390689	0.073884
H19	-4.321277	-0.838444	1.311394
N20	-2.606467	0.406845	1.569197
H21	-3.109693	1.127822	2.078456
H22	-2.239321	-0.229822	2.274162
C23	3.758682	-0.606181	1.148973
H24	3.938531	-1.671175	1.307373
H25	4.269688	-0.265020	0.246676
H26	4.092460	-0.034479	2.012873
C27	0.512671	1.757641	-0.445480
C28	-0.056142	3.139331	-0.277322
H29	-0.459484	3.466946	-1.239744
H30	-0.847004	3.178895	0.473815
H31	0.745663	3.827514	0.001884
O32	1.465106	1.538828	-1.220837

7

N1	-5.587299	-0.691965	0.042170
C2	-4.333979	-0.011018	-0.305025
H3	-4.328794	0.967218	0.186672

H4	-4.244227	0.174828	-1.385875
C5	-3.127466	-0.816188	0.155629
H6	-3.164619	-1.811291	-0.308450
H7	-3.186240	-0.967878	1.240889
C8	-1.803475	-0.141821	-0.199106
H9	-1.756432	0.031758	-1.281673
H10	-1.762146	0.843257	0.282629
C11	-0.605678	-0.987586	0.227685
H12	-0.693062	-1.989097	-0.207401
H13	-0.594610	-1.103080	1.318528
C14	0.749153	-0.421086	-0.222758
H15	0.746525	-0.324513	-1.311023
C16	0.950349	0.967790	0.375904
N17	1.802171	-1.329909	0.193780
O18	1.300906	1.177572	1.524095
O19	0.669541	1.926115	-0.499318
H20	-6.370799	-0.142737	-0.300040
H21	-5.626750	-1.574023	-0.463563
H22	1.570493	-2.009971	0.909062
C23	0.764207	3.283324	-0.028627
H24	0.509791	3.904226	-0.885245
H25	0.055718	3.447969	0.785150
H26	1.782411	3.490442	0.305008
C27	3.108165	-1.257343	-0.143325
C28	3.534972	-0.190263	-1.112089
H29	3.609888	0.767528	-0.585056
H30	4.518657	-0.443755	-1.506467
H31	2.829106	-0.068450	-1.936684
O32	3.927491	-2.052958	0.350494

8

N1	5.383594	-1.003616	-0.425600
C2	4.239567	-0.343970	0.214090
H3	4.346635	0.736030	0.068383
H4	4.209685	-0.517932	1.300288
C5	2.924797	-0.807701	-0.396475
H6	2.844130	-1.898456	-0.293144
H7	2.929108	-0.588699	-1.472017
C8	1.712565	-0.148262	0.258411
H9	1.696261	-0.386282	1.329981
H10	1.814012	0.942316	0.178841
C11	0.399725	-0.594582	-0.382015
H12	0.334625	-1.688360	-0.383745
H13	0.357513	-0.262095	-1.425959
C14	-0.851142	-0.081673	0.351230
H15	-0.876006	-0.489863	1.361748
C16	-0.809138	1.429846	0.494984
N17	-2.071226	-0.491997	-0.321815
O18	-0.527943	2.007078	1.531093
O19	-1.070315	2.052712	-0.648972
H20	6.242912	-0.659527	-0.006158
H21	5.348181	-1.997757	-0.212373
H22	-2.284592	-0.062329	-1.212771
C23	-1.012517	3.491095	-0.639427
H24	-1.261020	3.795325	-1.654052
H25	-1.739993	3.890714	0.069157
H26	-0.005473	3.820822	-0.377957
C27	-2.810791	-1.546815	0.075325
C28	-3.982798	-1.904877	-0.796445
H29	-3.808751	-2.896254	-1.224101
H30	-4.880566	-1.958958	-0.175961
H31	-4.143575	-1.189455	-1.604761
O32	-2.548151	-2.194578	1.103934

9

C1	0.314017	-0.413660	0.261573
H2	-0.097291	-1.007946	1.086748
C3	-0.067376	-1.092175	-1.062254
H4	0.470982	-0.611592	-1.884954
H5	0.262762	-2.134929	-1.021712
C6	1.806264	-0.366445	0.561604
O7	2.515149	-1.193391	-0.198790
O8	2.297747	0.302538	1.455720
N9	-0.271418	0.907246	0.403303
H10	-1.241630	0.884268	0.754725
C11	-1.571772	-1.039390	-1.348620
H12	-1.884921	0.009190	-1.421560
H13	-1.724878	-1.465425	-2.345113
C14	-2.469675	-1.779336	-0.332116
H15	-1.859683	-2.287944	0.426796
H16	-3.023160	-2.572550	-0.845609
C17	-3.492223	-0.895519	0.378795
H18	-4.033299	-0.297098	-0.362001
H19	-4.233629	-1.537296	0.874548
N20	-2.860173	0.030809	1.333576
H21	-3.569647	0.639723	1.731526
H22	-2.486655	-0.511197	2.110511
C23	3.925252	-1.273649	0.073035
H24	4.391785	-0.297446	-0.070685
H25	4.092120	-1.626585	1.092313
H26	4.316504	-1.990853	-0.645964
C27	0.144880	1.948449	-0.335863
C28	-0.717164	3.180672	-0.309948
H29	-1.145327	3.322754	-1.306802
H30	-1.526850	3.113633	0.418997
H31	-0.094746	4.049756	-0.083634
O32	1.196538	1.908537	-1.004871

10

N1	5.645365	-0.279143	-0.486980
C2	4.468752	0.222809	0.232934
H3	4.375384	1.294361	0.027390
H4	4.571163	0.116165	1.323345
C5	3.198635	-0.487220	-0.212614
H6	3.306098	-1.565487	-0.029051
H7	3.073319	-0.359667	-1.295384

C8	1.957456	0.034355	0.509199
H9	2.094087	-0.064390	1.594210
H10	1.843162	1.104571	0.301886
C11	0.689722	-0.717493	0.102734
H12	0.773969	-1.757994	0.432381
H13	0.583168	-0.731081	-0.987161
C14	-0.580823	-0.139550	0.736256
H15	-0.360514	0.146085	1.770858
C16	-1.044369	1.145217	0.049939
N17	-1.671789	-1.098577	0.814823
O18	-0.410878	1.741840	-0.801738
O19	-2.201778	1.584928	0.538958
H20	6.472556	0.204707	-0.148425
H21	5.780372	-1.258776	-0.247577
H22	-1.832189	-1.560042	1.698761
C23	-2.720939	2.795786	-0.037942
H24	-3.665323	2.978575	0.470814
H25	-2.028122	3.621627	0.133880
H26	-2.887520	2.657285	-1.107844
C27	-2.424048	-1.440238	-0.245449
C28	-3.487196	-2.478036	-0.021956
H29	-4.464925	-2.013001	-0.176765
H30	-3.368627	-3.268500	-0.766960
H31	-3.451315	-2.912897	0.978316
O32	-2.258958	-0.901927	-1.355493

11

C1	-0.496644	0.009399	1.171214
H2	-0.711885	0.315552	2.200925
C3	0.987200	-0.366154	1.111603
H4	1.550360	0.531124	1.389022
H5	1.162958	-1.101579	1.905518
C6	-0.843022	1.241383	0.340663
O7	-2.145017	1.517118	0.371690
O8	-0.021083	1.957139	-0.203751
N9	-1.399828	-1.097588	0.892712
H10	-1.672856	-1.673066	1.676850
C11	1.493387	-0.927943	-0.217209
H12	0.954675	-1.851915	-0.454620
H13	1.267814	-0.227059	-1.027691
C14	2.995232	-1.240160	-0.203380
H15	3.274746	-1.648198	-1.182297
H16	3.195712	-2.024830	0.537456
C17	3.896922	-0.050255	0.115428
H18	3.754177	0.246425	1.164738
H19	4.939975	-0.366989	0.022852
N20	3.681146	1.066969	-0.812151
H21	2.744198	1.440305	-0.676829
H22	4.315147	1.822922	-0.569827
C23	-1.822455	-1.445010	-0.337292
C24	-2.704373	-2.659054	-0.430919
H25	-2.901787	-3.119861	0.538487
H26	-3.650853	-2.367619	-0.893582
H27	-2.221814	-3.389138	-1.085999
C28	-2.577739	2.661686	-0.382238
H29	-2.090206	3.566036	-0.013967
H30	-2.355658	2.514770	-1.441172
H31	-3.653053	2.721240	-0.225832
O32	-1.514140	-0.788899	-1.347337

12

C1	-0.476710	-0.244663	-0.480623
H2	-0.772713	-0.158678	-1.531077
C3	0.507153	-1.419387	-0.338986
H4	0.754036	-1.518922	0.723362
H5	-0.016086	-2.335839	-0.623539
C6	-1.720882	-0.575549	0.332537
O7	-2.601869	-1.259597	-0.391866
O8	-1.885325	-0.294127	1.506674
N9	0.158194	0.978101	-0.026290
H10	1.140483	0.913849	0.296551
C11	1.778412	-1.238214	-1.189276
H12	1.717519	-1.877455	-2.075559
H13	1.831733	-0.211446	-1.565726
C14	3.080794	-1.553756	-0.444460
H15	3.918762	-1.347934	-1.122308
H16	3.127876	-2.622836	-0.204095
C17	3.290534	-0.772710	0.853266
H18	2.609606	-1.135700	1.630143
H19	4.308929	-0.971068	1.213965
N20	3.033047	0.663827	0.675995
H21	3.315009	1.161850	1.515527
H22	3.618040	1.018819	-0.077234
C23	-0.335386	2.220057	-0.181570
C24	-1.711825	2.382971	-0.768695
H25	-1.825838	1.811758	-1.693983
H26	-2.468120	2.032741	-0.058709
H27	-1.889249	3.438778	-0.971495
O28	0.335056	3.213183	0.171010
C29	-3.788068	-1.712425	0.285832
H30	-4.344324	-0.858895	0.676877
H31	-4.371786	-2.232736	-0.470796
H32	-3.519596	-2.393391	1.095470

13

N1	5.191340	-1.367291	-0.204867
C2	4.087218	-0.471408	0.158014
H3	4.262817	0.496280	-0.323717
H4	4.040146	-0.283467	1.241339
C5	2.749049	-1.031192	-0.302771
H6	2.610357	-2.031927	0.129144
H7	2.764177	-1.154157	-1.393311
C8	1.574843	-0.141080	0.100410
H9	1.536301	-0.056528	1.194086
H10	1.743248	0.871387	-0.288955
C11	0.242765	-0.680394	-0.417328

H12	0.125741	-1.730944	-0.128109
H13	0.218722	-0.639121	-1.512885
C14	-0.997141	0.060811	0.119613
H15	-1.045593	-0.041911	1.204127
C16	-0.900325	1.539603	-0.207655
N17	-2.220914	-0.456076	-0.469459
O18	-1.229231	2.019166	-1.279407
O19	-0.371981	2.239775	0.787479
H20	6.066926	-0.961776	0.114047
H21	5.086101	-2.239687	0.307940
H22	-2.406625	-0.185997	-1.429808
C23	-0.112022	3.633801	0.534283
H24	0.373460	4.004005	1.434709
H25	0.548393	3.739329	-0.328156
H26	-1.051159	4.162329	0.362889
C27	-2.968669	-1.471350	0.009816
C28	-2.655639	-2.003345	1.381668
H29	-3.346619	-2.813849	1.610625
H30	-1.629204	-2.378740	1.429496
H31	-2.762000	-1.216741	2.134722
O32	-3.904869	-1.932390	-0.669848

14

C1	-0.375763	-0.364359	-0.768498
H2	-0.532825	-0.221463	-1.843087
C3	0.776029	-1.364541	-0.565713
H4	0.894207	-1.522579	0.511543
H5	0.468699	-2.323038	-0.991321
C6	-1.652547	-1.007181	-0.244437
O7	-1.909217	-0.735520	1.027780
O8	-2.343333	-1.742357	-0.931812
N9	-0.044782	0.896591	-0.130179
H10	0.882512	0.970644	0.327325
C11	2.095281	-0.890883	-1.205066
H12	2.263752	-1.437460	-2.138083
H13	2.013408	0.163025	-1.488887
C14	3.325195	-1.057429	-0.304969
H15	4.195332	-0.654986	-0.838343
H16	3.526008	-2.121944	-0.134278
C17	3.220874	-0.374356	1.059380
H18	2.530674	-0.923810	1.707889
H19	4.205116	-0.420761	1.544664
N20	2.719523	1.003297	0.944936
H21	2.801863	1.465986	1.845795
H22	3.311440	1.524310	0.301499
C23	-0.761372	2.031130	-0.217426
C24	-2.067387	2.003977	-0.966410
H25	-1.969497	1.511530	-1.937761
H26	-2.821579	1.461914	-0.385606
H27	-2.414950	3.026347	-1.112979
O28	-0.352533	3.079112	0.326191
C29	-3.084509	-1.339501	1.596966
H30	-2.989087	-2.426621	1.586620
H31	-3.130652	-0.971337	2.619912
H32	-3.971745	-1.029988	1.041559

15

C1	-0.735490	0.084078	0.626541
H2	-1.134604	-0.030646	1.636653
C3	0.525641	-0.792741	0.496477
H4	1.186808	-0.543872	1.332569
H5	0.214452	-1.834752	0.629493
C6	-0.336260	1.547267	0.524960
O7	-0.834436	2.178113	-0.528566
O8	0.410327	2.069522	1.336376
N9	-1.775085	-0.265832	-0.325672
H10	-1.670270	0.072084	-1.275486
C11	1.254717	-0.625179	-0.836322
H12	0.556075	-0.801718	-1.662484
H13	1.596812	0.413049	-0.942077
C14	2.445366	-1.577157	-0.997295
H15	2.924319	-1.382199	-1.964355
H16	2.076056	-2.609893	-1.026578
C17	3.492852	-1.481938	0.107822
H18	3.056812	-1.833566	1.054375
H19	4.312791	-2.166575	-0.127840
N20	4.051164	-0.129091	0.223199
H21	3.320855	0.508514	0.532812
H22	4.750404	-0.125279	0.960530
C23	-0.457030	3.557216	-0.700295
H24	-0.776423	4.142420	0.163433
H25	0.623136	3.634228	-0.835044
H26	-0.976895	3.886786	-1.597423
C27	-2.712751	-1.221416	-0.156379
C28	-2.865716	-1.844317	1.203871
H29	-1.935189	-2.321652	1.523712
H30	-3.127443	-1.084691	1.946402
H31	-3.656674	-2.592152	1.161724
O32	-3.443585	-1.552697	-1.108984

16

N1	5.330571	-0.911799	-0.423207
C2	4.180547	-0.261802	0.215541
H3	4.285481	0.819914	0.081882
H4	4.143795	-0.447013	1.299711
C5	2.871513	-0.722935	-0.409082
H6	2.798571	-1.816117	-0.327352
H7	2.878300	-0.483792	-1.480300
C8	1.650879	-0.086783	0.253360
H9	1.626643	-0.355663	1.317546
H10	1.746508	1.006069	0.206186
C11	0.347041	-0.522877	-0.411465
H12	0.298585	-1.616846	-0.458496
H13	0.303229	-0.149757	-1.441353
C14	-0.916382	-0.058522	0.333538
H15	-0.922041	-0.476845	1.340267

C16	-0.903133	1.450184	0.512941
N17	-2.132905	-0.466390	-0.356333
O18	-0.627429	2.006703	1.561584
O19	-1.177430	2.093433	-0.615655
H20	6.186288	-0.568463	0.004119
H21	5.297379	-1.907872	-0.218746
H22	-2.374192	0.040638	-1.201198
C23	-1.137561	3.532098	-0.577067
H24	-1.392948	3.853900	-1.584513
H25	-1.867520	3.908451	0.141460
H26	-0.133596	3.868169	-0.311836
C27	-2.780687	-1.638347	-0.177636
C28	-2.368400	-2.515686	0.971907
H29	-2.966326	-3.426234	0.951884
H30	-1.308744	-2.777949	0.904286
H31	-2.528569	-2.001755	1.924508
O32	-3.709817	-1.959323	-0.941365

17

N1	-5.583743	-0.736776	0.026117
C2	-4.353585	0.040138	-0.166410
H3	-4.366959	0.877763	0.538774
H4	-4.286068	0.473691	-1.175480
C5	-3.119740	-0.815194	0.083575
H6	-3.158186	-1.697012	-0.571207
H7	-3.135362	-1.184748	1.116702
C8	-1.820482	-0.054921	-0.173987
H9	-1.826324	0.340000	-1.197715
H10	-1.770639	0.811145	0.499591
C11	-0.592285	-0.942717	0.013282
H12	-0.649743	-1.790477	-0.678351
H13	-0.569547	-1.350077	1.031199
C14	0.737052	-0.226417	-0.259656
H15	0.724532	0.185461	-1.269659
C16	0.942267	0.889909	0.770575
N17	1.828502	-1.176385	-0.158092
O18	1.209596	0.640528	1.934715
O19	0.772099	2.166420	0.430214
H20	-6.386011	-0.139160	-0.152691
H21	-5.619878	-1.467555	-0.680877
H22	1.625429	-2.117797	0.150773
C23	0.569078	2.587127	-0.933352
H24	0.506162	3.672570	-0.882402
H25	1.419866	2.294403	-1.551266
H26	-0.363891	2.185104	-1.330654
C27	3.108400	-0.795429	-0.321164
C28	4.167373	-1.842410	-0.133290
H29	4.812510	-1.855387	-1.015149
H30	4.780301	-1.563713	0.728672
H31	3.750815	-2.837939	0.028661
O32	3.389705	0.382468	-0.607746

18

C1	-0.617186	-0.174306	-0.606368
H2	-1.292950	0.041291	-1.437565
C3	0.268946	-1.367001	-1.026777
H4	-0.390473	-2.106715	-1.490955
H5	0.921583	-1.008674	-1.828015
C6	-1.458372	-0.531786	0.620240
O7	-2.624667	-1.161144	0.449893
O8	-1.094777	-0.317366	1.763540
N9	0.166341	1.015237	-0.349349
H10	1.196352	0.946316	-0.386073
C11	1.066787	-2.091721	0.067582
H12	0.353701	-2.567328	0.752102
H13	1.600786	-2.913491	-0.426111
C14	2.073777	-1.299838	0.911937
H15	2.442239	-1.982058	1.687707
H16	1.574219	-0.479527	1.439118
C17	3.299334	-0.751815	0.183623
H18	4.000506	-0.380797	0.936649
H19	3.806804	-1.570138	-0.346081
N20	2.990101	0.369660	-0.724574
H21	3.789530	0.992442	-0.781093
H22	2.843053	0.022096	-1.667944
C23	-3.230706	-1.333928	-0.845497
H24	-3.434733	-0.363609	-1.301648
H25	-2.605663	-1.950175	-1.493228
H26	-4.169075	-1.849801	-0.649740
C27	-0.435051	2.182170	-0.082299
C28	0.449970	3.371092	0.169473
H29	1.507415	3.154521	0.009205
H30	0.142416	4.186531	-0.489884
H31	0.304703	3.701275	1.201963
O32	-1.679369	2.280555	-0.033736

19

C1	0.183018	-0.578707	0.001254
H2	-0.253876	-1.138120	0.838378
C3	-0.519926	-1.023606	-1.287068
H4	-0.010216	-0.584859	-2.151649
H5	-0.418995	-2.110450	-1.373332
C6	1.650588	-0.981054	0.036169
O7	2.302003	-0.446023	1.063107
O8	2.164988	-1.751261	-0.755978
N9	-0.049870	0.819868	0.335347
H10	-0.953851	0.948669	0.817944
C11	-2.000450	-0.633104	-1.325476
H12	-2.081995	0.458174	-1.253273
H13	-2.380505	-0.895771	-2.317528
C14	-2.887279	-1.290509	-0.244573
H15	-2.297438	-1.979491	0.375411
H16	-3.654446	-1.906549	-0.725209
C17	-3.597862	-0.299419	0.674097
H18	-4.103451	0.458753	0.066507

H19	-4.377195	-0.828434	1.240081
N20	-2.656381	0.393315	1.568907
H21	-3.153404	1.106278	2.095261
H22	-2.309934	-0.273622	2.255859
C23	3.700585	-0.760007	1.176907
H24	3.837489	-1.832278	1.327555
H25	4.230320	-0.432555	0.280263
H26	4.049631	-0.208292	2.047459
C27	0.442949	1.909532	-0.285541
C28	1.648845	1.785132	-1.179156
H29	1.583831	0.944988	-1.873893
H30	1.756252	2.707460	-1.749699
H31	2.544631	1.651520	-0.563744
O32	-0.065229	3.028879	-0.065360

20

C1	0.257587	-0.383235	0.224058
H2	-0.204043	-0.974731	1.025533
C3	-0.151506	-1.016442	-1.113783
H4	0.396661	-0.538477	-1.932283
H5	0.142693	-2.070528	-1.099076
C6	1.740313	-0.458113	0.566960
O7	2.397580	-1.344124	-0.171343
O8	2.262410	0.187771	1.459550
N9	-0.267477	0.960658	0.410861
H10	-1.233628	0.946147	0.775001
C11	-1.655224	-0.905875	-1.387605
H12	-1.936569	0.153546	-1.413614
H13	-1.826014	-1.285778	-2.399589
C14	-2.567553	-1.661523	-0.396157
H15	-1.967898	-2.221636	0.334320
H16	-3.150135	-2.413649	-0.938412
C17	-3.555158	-0.776993	0.360898
H18	-4.089165	-0.138353	-0.350812
H19	-4.307575	-1.415826	0.843963
N20	-2.883198	0.096386	1.336961
H21	-3.567716	0.715850	1.761422
H22	-2.518843	-0.481156	2.092245
C23	3.795088	-1.520975	0.124245
H24	4.324066	-0.574170	0.003515
H25	3.918629	-1.898901	1.140698
H26	4.151852	-2.251497	-0.598936
C27	0.104434	2.083039	-0.233633
C28	1.405634	2.128561	-0.991025
H29	1.682166	1.182180	-1.458856
H30	1.331419	2.896097	-1.762034
H31	2.202665	2.414590	-0.297443
O32	-0.601932	3.109643	-0.148724

21

C1	-0.491037	-0.690841	-0.721673
H2	-0.724016	-0.778252	-1.788198
C3	0.742420	-1.561870	-0.425279
H4	0.911701	-1.599562	0.654807
H5	0.489359	-2.581063	-0.728631
C6	-1.710643	-1.301469	-0.030649
O7	-1.994298	-1.090698	1.255533
O8	-2.431593	-2.078992	-0.639025
N9	-0.263343	0.703841	-0.401389
H10	0.685822	1.011416	-0.111703
C11	2.017630	-1.086729	-1.151382
H12	2.310499	-1.833785	-1.894709
H13	1.812171	-0.170419	-1.715071
C14	3.209726	-0.846326	-0.215908
H15	4.061817	-0.512142	-0.821318
H16	3.508952	-1.793114	0.249561
C17	2.973361	0.168625	0.901199
H18	2.249676	-0.220592	1.626733
H19	3.917397	0.311199	1.443743
N20	2.437264	1.432238	0.376728
H21	2.431016	2.136898	1.108706
H22	3.048087	1.781720	-0.357895
C23	-1.237123	1.610909	-0.555272
C24	-0.901557	3.041554	-0.237876
H25	0.100209	3.158896	0.178683
H26	-0.981313	3.631427	-1.155453
H27	-1.637163	3.425363	0.473546
O28	-2.382261	1.283063	-0.931532
C29	-1.229118	-0.267242	2.157498
H30	-1.485478	0.782865	2.014768
H31	-1.536093	-0.590257	3.151344
H32	-0.156830	-0.419791	2.039959

22

C1	-0.505517	0.014019	-1.176892
H2	-0.695142	-0.267409	-2.219703
C3	0.988352	0.349619	-1.083643
H4	1.534053	-0.549840	-1.385178
H5	1.189362	1.107523	-1.849478
C6	-0.895028	-1.246552	-0.413419
O7	-2.209755	-1.387440	-0.294999
O8	-0.090854	-2.070678	-0.015724
N9	-1.391543	1.145664	-0.932356
H10	-1.606384	1.703877	-1.749888
C11	1.493780	0.853239	0.267589
H12	0.942999	1.756322	0.555712
H13	1.292036	0.107020	1.044704
C14	2.990683	1.187425	0.258176
H15	3.271972	1.559379	1.250804
H16	3.174673	2.003049	-0.452590
C17	3.903831	0.022313	-0.114134
H18	3.749732	-0.239466	-1.171044
H19	4.943250	0.351501	-0.024678
N20	3.718454	-1.129675	0.776805
H21	2.788684	-1.518246	0.636128
H22	4.366061	-1.863442	0.504067

C23	-1.865439	1.665395	0.219255
C24	-1.651007	0.971110	1.536233
H25	-0.874444	0.209075	1.541061
H26	-1.400811	1.728516	2.281187
H27	-2.597136	0.504343	1.826724
C28	-2.674219	-2.540965	0.427456
H29	-2.367501	-3.455691	-0.082574
H30	-2.280869	-2.523447	1.445751
H31	-3.758894	-2.455784	0.437741
O32	-2.533470	2.717765	0.182770

23

N1	5.282123	-1.221140	-0.134976
C2	4.157347	-0.346506	0.215807
H3	4.319024	0.623309	-0.266687
H4	4.096363	-0.157173	1.298125
C5	2.834809	-0.933441	-0.256084
H6	2.704251	-1.929219	0.189658
H7	2.868274	-1.072983	-1.344087
C8	1.641542	-0.054993	0.114641
H9	1.609399	0.078361	1.203311
H10	1.782673	0.942940	-0.322746
C11	0.318675	-0.651944	-0.359768
H12	0.172091	-1.639282	0.092086
H13	0.331680	-0.787630	-1.447790
C14	-0.919967	0.185590	0.006799
H15	-0.989900	0.281019	1.089039
C16	-0.837656	1.552249	-0.664858
N17	-2.140720	-0.453355	-0.452984
O18	-1.006488	1.670327	-1.868328
O19	-0.549361	2.643710	0.037398
H20	6.146574	-0.797923	0.191264
H21	5.189431	-2.094635	0.378399
H22	-2.351575	-0.396210	-1.441407
C23	-0.418303	2.629281	1.474027
H24	-0.224195	3.665449	1.743894
H25	-1.346952	2.293340	1.937895
H26	0.422739	2.004904	1.777994
C27	-2.859039	-1.293512	0.317232
C28	-4.023845	-1.978699	-0.342695
H29	-3.857479	-3.058575	-0.301189
H30	-4.930303	-1.756396	0.226078
H31	-4.165812	-1.677047	-1.381930
O32	-2.585086	-1.495155	1.513832

24

N1	5.617762	-0.210049	-0.457908
C2	4.438501	0.288115	0.260292
H3	4.356766	1.364222	0.074913
H4	4.528954	0.158711	1.349276
C5	3.167048	-0.401876	-0.212244
H6	3.268585	-1.485561	-0.060211
H7	3.047343	-0.241602	-1.291333
C8	1.924886	0.101695	0.520330
H9	2.045565	-0.054847	1.600230
H10	1.825536	1.182350	0.365715
C11	0.652722	-0.607279	0.054782
H12	0.726806	-1.672835	0.293959
H13	0.560219	-0.526627	-1.033084
C14	-0.618128	-0.071034	0.732587
H15	-0.353196	0.236732	1.750690
C16	-1.131878	1.210726	0.073814
N17	-1.670132	-1.062289	0.910160
O18	-0.458521	1.913148	-0.659008
O19	-2.383415	1.499147	0.414070
H20	6.445465	0.260819	-0.102628
H21	5.742895	-1.194919	-0.235126
H22	-1.928926	-1.287246	1.862269
C23	-2.951651	2.686478	-0.167600
H24	-3.963172	2.746108	0.229000
H25	-2.375431	3.565581	0.126503
H26	-2.973772	2.592283	-1.254847
C27	-2.377482	-1.705950	-0.040637
C28	-2.076067	-1.439241	-1.489975
H29	-1.198684	-2.022761	-1.785682
H30	-2.928514	-1.762814	-2.087038
H31	-1.868826	-0.388654	-1.704977
O32	-3.252905	-2.528842	0.288501

25

C1	0.237273	-0.704046	-0.003341
H2	-0.246337	-1.044402	0.920938
C3	-0.532899	-1.285617	-1.193069
H4	0.008046	-1.053078	-2.116089
H5	-0.550571	-2.375591	-1.089128
C6	1.662778	-1.241849	0.074867
O7	2.460223	-0.866531	1.079704
O8	2.097919	-2.075246	-0.702566
N9	0.181811	0.745788	0.030168
H10	-0.675657	1.106134	0.476262
C11	-1.964575	-0.748556	-1.295304
H12	-1.927635	0.336638	-1.448381
H13	-2.399583	-1.163421	-2.209805
C14	-2.884438	-1.071977	-0.096470
H15	-2.371665	-1.728710	0.619538
H16	-3.753849	-1.638174	-0.446514
C17	-3.411002	0.151301	0.651721
H18	-3.846904	0.854798	-0.065837
H19	-4.219924	-0.163657	1.325156
N20	-2.348305	0.858608	1.385875
H21	-2.737740	1.690239	1.820793
H22	-2.031378	0.264841	2.150408
C23	2.044069	0.001459	2.150319
H24	2.141936	1.043130	1.843720
H25	1.022768	-0.213876	2.467398
H26	2.731730	-0.211269	2.967616

C27	0.957146	1.533309	-0.725895
C28	0.645852	3.004530	-0.704292
H29	0.412260	3.327195	-1.722537
H30	-0.190406	3.248492	-0.046589
H31	1.535877	3.547685	-0.375647
O32	1.909265	1.080644	-1.393991

26

N1	5.538047	-0.737691	0.120986
C2	4.300499	0.037823	0.268462
H3	4.338037	0.874788	-0.436572
H4	4.196416	0.472533	1.274011
C5	3.077943	-0.818890	-0.027472
H6	3.089784	-1.699006	0.630578
H7	3.136640	-1.191486	-1.057953
C8	1.769092	-0.057810	0.172700
H9	1.716042	0.310028	1.204997
H10	1.764746	0.826106	-0.479924
C11	0.550656	-0.931898	-0.113909
H12	0.551645	-1.794959	0.560065
H13	0.597136	-1.316418	-1.140285
C14	-0.797050	-0.218448	0.077441
H15	-0.870495	0.127790	1.107309
C16	-0.892581	0.956482	-0.905071
N17	-1.873513	-1.158672	-0.178829
O18	-1.059532	0.769514	-2.098980
O19	-0.768449	2.213085	-0.480844
H20	6.333019	-0.136852	0.320476
H21	5.553009	-1.463136	0.834194
H22	-1.720732	-1.832591	-0.921032
C23	-0.615611	2.552765	0.912231
H24	-0.566401	3.639867	0.929819
H25	-1.479796	2.214401	1.485795
H26	0.309775	2.137592	1.312981
C27	-3.141240	-1.081347	0.284673
C28	-3.472911	-0.004885	1.280890
H29	-3.342120	0.983773	0.829163
H30	-4.510262	-0.120569	1.592630
H31	-2.822798	-0.064413	2.158456
O32	-3.996790	-1.894555	-0.107611

27

N1	-5.654839	-0.504163	0.375253
C2	-4.450388	0.009781	-0.289004
H3	-4.403582	1.090459	-0.118754
H4	-4.478008	-0.140832	-1.378625
C5	-3.193102	-0.642376	0.267511
H6	-3.247707	-1.727392	0.103972
H7	-3.154835	-0.484320	1.352854
C8	-1.917451	-0.092652	-0.368628
H9	-1.941798	-0.255823	-1.453403
H10	-1.881846	0.992314	-0.210580
C11	-0.669533	-0.749020	0.217139
H12	-0.727786	-1.833440	0.074332
H13	-0.630215	-0.568310	1.297251
C14	0.643277	-0.292893	-0.439139
H15	0.597399	-0.534215	-1.504439
C16	0.795618	1.233201	-0.428794
N17	1.764088	-1.000295	0.145802
O18	0.474146	1.882748	-1.411942
O19	1.230525	1.911334	0.632878
H20	-6.472960	-0.058819	-0.031168
H21	-5.745704	-1.495181	0.163478
H22	1.620233	-1.485498	1.021967
C23	1.616283	1.327737	1.892934
H24	1.629561	2.163366	2.591013
H25	0.893591	0.587373	2.233306
H26	2.613968	0.895213	1.816048
C27	3.018844	-0.874670	-0.328736
C28	4.101409	-1.617779	0.400424
H29	4.569551	-2.320623	-0.293891
H30	4.861975	-0.900710	0.719427
H31	3.729908	-2.162776	1.269833
O32	3.262049	-0.173777	-1.326218

28

C1	0.548172	-0.351254	0.964692
H2	0.844939	-0.827961	1.906582
C3	-0.929393	0.037003	1.104898
H4	-1.496625	-0.891201	1.224292
H5	-1.022384	0.585042	2.050128
C6	0.775458	-1.428590	-0.099642
O7	1.993441	-1.949733	-0.278097
O8	-0.140527	-1.931738	-0.727765
N9	1.420801	0.801552	0.801862
H10	1.700110	1.279256	1.647422
C11	-1.510219	0.889361	-0.023529
H12	-0.936164	1.818541	-0.111353
H13	-1.402490	0.371581	-0.982250
C14	-2.980324	1.259585	0.205776
H15	-3.310172	1.906461	-0.616309
H16	-3.064900	1.848391	1.128210
C17	-3.933548	0.073090	0.314072
H18	-3.713142	-0.494074	1.230251
H19	-4.952996	0.454629	0.424643
N20	-3.895500	-0.772739	-0.884889
H21	-2.988757	-1.230592	-0.943598
H22	-4.576446	-1.519793	-0.781682
C23	1.774266	1.331070	-0.383760
C24	2.598892	2.586948	-0.347538
H25	2.794331	2.941206	0.665889
H26	3.549192	2.396005	-0.853194
H27	2.070935	3.364524	-0.905660
C28	3.156735	-1.566515	0.475381
H29	3.581286	-0.645755	0.073781
H30	2.930560	-1.458829	1.537026

H31	3.862358	-2.384434	0.337369
O32	1.453715	0.794111	-1.458195

29

C1	-0.590440	-0.151403	-0.577251
H2	-1.316081	0.026315	-1.374438
C3	0.404349	-1.214870	-1.102130
H4	-0.177572	-1.965933	-1.642876
H5	1.020328	-0.717744	-1.856626
C6	-1.336278	-0.683993	0.648707
O7	-2.382712	-1.493916	0.467607
O8	-1.001071	-0.438422	1.793780
N9	0.092111	1.093361	-0.283529
H10	1.124669	1.081931	-0.277747
C11	1.264093	-1.964120	-0.072463
H12	0.596941	-2.572881	0.550657
H13	1.876700	-2.677947	-0.637450
C14	2.186665	-1.167425	0.859315
H15	2.593813	-1.879363	1.587700
H16	1.612013	-0.435846	1.437953
C17	3.375689	-0.466351	0.208035
H18	4.018662	-0.083214	1.005621
H19	3.970404	-1.199515	-0.354638
N20	2.986610	0.678324	-0.636033
H21	3.737644	1.361041	-0.652282
H22	2.866444	0.374022	-1.598023
C23	-2.994757	-1.696473	-0.821620
H24	-3.389432	-0.753059	-1.203798
H25	-2.294313	-2.143369	-1.527927
H26	-3.814212	-2.388348	-0.636281
C27	-0.503771	2.274737	-0.045787
C28	-2.007807	2.342549	-0.072270
H29	-2.419072	1.878391	-0.973108
H30	-2.424566	1.819751	0.794821
H31	-2.316833	3.386614	-0.030478
O32	0.183402	3.288772	0.198444

30

C1	0.507590	-0.041186	-0.839635
H2	0.795584	0.096010	-1.885140
C3	-0.896504	-0.670480	-0.838114
H4	-1.520634	-0.028444	-1.466841
H5	-0.818584	-1.635419	-1.350939
C6	0.447184	1.401866	-0.317456
O7	0.783360	1.780737	0.913347
O8	0.040642	2.273185	-1.072907
N9	1.495394	-0.899591	-0.225221
H10	1.190347	-1.637271	0.395153
C11	-1.551945	-0.857463	0.531185
H12	-0.933490	-1.507199	1.162185
H13	-1.607381	0.109176	1.049106
C14	-2.951372	-1.477376	0.443914
H15	-3.330991	-1.624949	1.461949
H16	-2.875332	-2.470431	-0.016505
C17	-3.969967	-0.660683	-0.346298
H18	-3.686528	-0.640285	-1.408663
H19	-4.936799	-1.169445	-0.294238
N20	-4.138654	0.687381	0.210586
H21	-3.282705	1.217534	0.065636
H22	-4.856588	1.174548	-0.317969
C23	1.190158	0.923872	1.998764
H24	0.584044	0.021288	2.054082
H25	2.249619	0.683550	1.903541
H26	1.030433	1.522474	2.894260
C27	2.815605	-0.664578	-0.353506
C28	3.748025	-1.610104	0.347657
H29	4.408759	-1.029555	0.996413
H30	3.222378	-2.359567	0.941646
H31	4.367296	-2.112156	-0.400617
O32	3.234844	0.297629	-1.020399

31

N1	5.651298	-0.492653	-0.321519
C2	4.428284	-0.033213	0.346851
H3	4.431373	1.061859	0.344356
H4	4.382547	-0.349445	1.399890
C5	3.187507	-0.539473	-0.375078
H6	3.216973	-1.637188	-0.411148
H7	3.205243	-0.186572	-1.414154
C8	1.892205	-0.089615	0.298256
H9	1.871495	-0.448805	1.334948
H10	1.871814	1.006281	0.341822
C11	0.662320	-0.610191	-0.442218
H12	0.729020	-1.699002	-0.540538
H13	0.635219	-0.196355	-1.456624
C14	-0.668321	-0.323355	0.274349
H15	-0.614154	-0.775748	1.267180
C16	-0.837362	1.174396	0.564321
N17	-1.761503	-0.931948	-0.459030
O18	-0.510754	1.617214	1.655198
O19	-1.306291	2.041355	-0.330792
H20	6.459796	-0.147883	0.188228
H21	5.696241	-1.507136	-0.259617
H22	-1.625776	-1.089922	-1.451329
C23	-1.694355	1.711302	-1.680009
H24	-1.791680	2.673942	-2.179126
H25	-0.928155	1.120375	-2.181649
H26	-2.654550	1.195955	-1.680858
C27	-3.023835	-1.116943	-0.010490
C28	-3.314652	-0.803552	1.430607
H29	-3.152577	0.259315	1.637052
H30	-4.353896	-1.049995	1.644288
H31	-2.659219	-1.377307	2.092470
O32	-3.900333	-1.545607	-0.780767

32

C1	-0.520169	-0.595141	-0.715416
H2	-0.829932	-0.592661	-1.764841
C3	0.779827	-1.416924	-0.611783
H4	1.024749	-1.566203	0.443802
H5	0.564975	-2.407946	-1.019038
C6	-1.636526	-1.354718	0.004964
O7	-1.852270	-1.251018	1.315054
O8	-2.350775	-2.123049	-0.622296
N9	-0.315425	0.769083	-0.267502
H10	0.609342	1.014693	0.135336
C11	1.965345	-0.769516	-1.353818
H12	2.192249	-1.349167	-2.253695
H13	1.689088	0.229490	-1.706009
C14	3.241232	-0.663421	-0.508272
H15	4.005140	-0.145434	-1.101657
H16	3.634571	-1.665726	-0.299991
C17	3.081511	0.059609	0.828855
H18	2.479412	-0.542059	1.518344
H19	4.074564	0.159811	1.287428
N20	2.409477	1.357804	0.673679
H21	2.446287	1.863105	1.554525
H22	2.919580	1.921739	-0.002688
C23	-1.194051	1.778064	-0.400122
C24	-2.545644	1.488526	-0.996241
H25	-2.472161	0.903963	-1.917288
H26	-3.153303	0.920492	-0.283026
H27	-3.050028	2.431744	-1.204423
O28	-0.896790	2.926275	-0.008485
C29	-1.061754	-0.463578	2.229696
H30	-1.334501	0.588525	2.153822
H31	-1.324058	-0.846715	3.214698
H32	0.005713	-0.600928	2.060106

33

C1	0.222499	-0.656833	-0.046573
H2	-0.310006	-1.034008	0.836777
C3	-0.520570	-1.166116	-1.285087
H4	0.039137	-0.895375	-2.186189
H5	-0.551818	-2.259759	-1.239198
C6	1.622474	-1.251151	0.083813
O7	2.368700	-0.961834	1.151122
O8	2.084879	-2.030308	-0.732364
N9	0.180315	0.791074	0.087817
H10	-0.678091	1.100849	0.570293
C11	-1.945038	-0.610823	-1.386195
H12	-1.897787	0.482068	-1.462352
H13	-2.358833	-0.958633	-2.337714
C14	-2.896329	-1.013529	-0.236749
H15	-2.410689	-1.736067	0.433591
H16	-3.764494	-1.535689	-0.652243
C17	-3.427765	0.150159	0.598203
H18	-3.825356	0.921489	-0.070232
H19	-4.267617	-0.207205	1.209957
N20	-2.383098	0.771194	1.429680
H21	-2.775151	1.573795	1.913978
H22	-2.106925	0.111380	2.154482
C23	1.921665	-0.133479	2.241704
H24	2.056371	0.918386	1.988905
H25	0.881925	-0.337786	2.500231
H26	2.565485	-0.402253	3.077898
C27	0.878960	1.724957	-0.580105
C28	2.058275	1.314570	-1.421882
H29	1.824708	0.481002	-2.087856
H30	2.375778	2.169792	-2.018127
H31	2.890467	1.017923	-0.774474
O32	0.577341	2.930601	-0.454131

34

C1	0.532553	-0.065484	-0.721301
H2	0.847055	-0.023192	-1.766224
C3	-0.895341	-0.643402	-0.722686
H4	-1.483042	-0.024848	-1.407273
H5	-0.835933	-1.642039	-1.168478
C6	0.501176	1.418095	-0.315777
O7	0.906153	1.894543	0.857911
O8	0.085734	2.227965	-1.132041
N9	1.453761	-0.923656	-0.008119
H10	1.102641	-1.439886	0.790050
C11	-1.585380	-0.714442	0.640204
H12	-0.972315	-1.283732	1.349110
H13	-1.676098	0.296999	1.058675
C14	-2.965302	-1.379884	0.577730
H15	-3.398081	-1.379692	1.585072
H16	-2.841017	-2.429889	0.285015
C17	-3.952103	-0.733331	-0.389354
H18	-3.597753	-0.871670	-1.421223
H19	-4.907001	-1.261715	-0.316657
N20	-4.192148	0.678948	-0.067773
H21	-3.337286	1.207578	-0.225554
H22	-4.872119	1.054412	-0.722678
C23	1.261554	1.114722	2.018070
H24	0.521826	0.339884	2.216754
H25	2.259571	0.692994	1.904007
H26	1.258347	1.834316	2.835343
C27	2.794174	-0.979302	-0.175009
C28	3.410679	-0.164365	-1.277292
H29	2.997742	-0.450642	-2.249095
H30	3.212208	0.902140	-1.129731
H31	4.487141	-0.330748	-1.279457
O32	3.481959	-1.696628	0.572389

35

C1	0.569615	0.331036	-0.935318
H2	0.859735	0.798603	-1.884512
C3	-0.924858	0.000766	-1.060308

H4	-1.455691	0.950720	-1.175717
H5	-1.042764	-0.539251	-2.007271
C6	0.856830	1.422142	0.099328
O7	2.095114	1.895542	0.248243
O8	-0.025332	1.944311	0.758207
N9	1.416244	-0.852416	-0.823240
H10	1.642296	-1.290912	-1.708309
C11	-1.540540	-0.831985	0.063065
H12	-0.973805	-1.762402	0.183421
H13	-1.463901	-0.297679	1.016382
C14	-3.003567	-1.202640	-0.207239
H15	-3.359557	-1.839864	0.611226
H16	-3.057977	-1.802605	-1.124720
C17	-3.951154	-0.016515	-0.359954
H18	-3.702274	0.538610	-1.276289
H19	-4.967368	-0.398365	-0.495499
N20	-3.946920	0.844914	0.828729
H21	-3.041814	1.303480	0.905418
H22	-4.623242	1.591396	0.695407
C23	1.810788	-1.564627	0.255741
C24	1.584041	-1.023477	1.640313
H25	0.609747	-0.553009	1.773004
H26	1.681083	-1.843005	2.351979
H27	2.359906	-0.281683	1.859672
C28	3.223555	1.486174	-0.547430
H29	3.619928	0.538416	-0.182547
H30	2.962584	1.418113	-1.604328
H31	3.962428	2.273511	-0.406914
O32	2.424864	-2.634452	0.086299

36

C1	0.254328	-0.440365	0.366794
H2	-0.368920	-0.813594	1.186426
C3	-0.108745	-1.254880	-0.878811
H4	0.495577	-0.940356	-1.731947
H5	0.106993	-2.310257	-0.679504
C6	1.651749	-0.532151	1.004012
O7	2.674668	-1.231472	0.514603
O8	1.816263	-0.023057	2.104149
N9	-0.105923	0.960686	0.223569
H10	-1.102114	1.153817	0.400794
C11	-1.586693	-1.096472	-1.263401
H12	-1.767780	-0.049054	-1.531814
H13	-1.739316	-1.668307	-2.183801
C14	-2.617882	-1.539932	-0.203427
H15	-2.119287	-1.935498	0.691617
H16	-3.216572	-2.367994	-0.596786
C17	-3.581451	-0.434434	0.223147
H18	-4.034340	0.012172	-0.668476
H19	-4.398576	-0.876350	0.809696
N20	-2.898450	0.637327	0.967763
H21	-3.553880	1.393242	1.144390
H22	-2.631548	0.277243	1.882189
C23	2.867179	-1.592527	-0.865423
H24	2.275905	-2.470365	-1.122981
H25	2.637282	-0.749516	-1.515842
H26	3.927138	-1.832221	-0.939467
C27	0.677237	1.841492	-0.411966
C28	0.103431	3.209599	-0.655094
H29	0.042601	3.374433	-1.734605
H30	-0.888550	3.334625	-0.216645
H31	0.782924	3.957863	-0.239082
O32	1.837590	1.549785	-0.767312

37

C1	0.284600	-0.358609	0.326974
H2	-0.317238	-0.793832	1.134789
C3	-0.078593	-1.129216	-0.950510
H4	0.527154	-0.785194	-1.792868
H5	0.127731	-2.191329	-0.797271
C6	1.686646	-0.420522	0.968864
O7	2.682843	-1.211958	0.580311
O8	1.896232	0.256874	1.964196
N9	-0.151042	1.030239	0.261665
H10	-1.138312	1.140693	0.538500
C11	-1.558910	-0.966959	-1.322999
H12	-1.771210	0.093616	-1.500095
H13	-1.694952	-1.462383	-2.289222
C14	-2.571592	-1.540868	-0.307964
H15	-2.052886	-2.042210	0.520805
H16	-3.171302	-2.318314	-0.792838
C17	-3.538539	-0.512059	0.273353
H18	-3.998426	0.053559	-0.544085
H19	-4.350120	-1.038366	0.795050
N20	-2.858482	0.446115	1.159926
H21	-3.522517	1.151208	1.466537
H22	-2.561823	-0.044867	2.001090
C23	2.753471	-2.013974	-0.612556
H24	2.087307	-2.872110	-0.535896
H25	2.539439	-1.419111	-1.499403
H26	3.786499	-2.356549	-0.645382
C27	0.407422	2.031444	-0.439725
C28	1.794465	1.864856	-1.003502
H29	1.982356	0.870645	-1.414574
H30	1.943073	2.605343	-1.789728
H31	2.526615	2.052685	-0.211130
O32	-0.197642	3.117267	-0.567885

Cartesian coordinates for the structures in Fig. S4, optimized at SMD-ωB97XD/6-31+ G(d,p).

$LysNH_3^+$_1

N1	-5.541400	-0.702935	0.108660
C2	-4.272147	-0.003797	-0.255529
H3	-4.264558	0.940959	0.289215
H4	-4.323904	0.203849	-1.325077
C5	-3.070358	-0.863022	0.093342
H6	-3.130755	-1.812362	-0.452142
H7	-3.089524	-1.096160	1.164942
C8	-1.765931	-0.147443	-0.253752
H9	-1.746221	0.081467	-1.326110
H10	-1.730488	0.809763	0.280285
C11	-0.551585	-0.999242	0.109454
H12	-0.639793	-1.982122	-0.365948
H13	-0.517709	-1.160076	1.193796
C14	0.784878	-0.395462	-0.343073
H15	0.777437	-0.259263	-1.427951
C16	0.986957	0.974213	0.295589
N17	1.864751	-1.286167	0.029386
O18	1.372587	1.148694	1.438556
O19	0.640396	1.958733	-0.525983
H20	-6.357708	-0.136636	-0.131122
H21	-5.620978	-1.595325	-0.385360
H22	1.653806	-2.079091	0.620822
C23	0.712371	3.296123	0.000711
H24	0.370254	3.942923	-0.804604
H25	0.060488	3.392383	0.870837
H26	1.743085	3.534657	0.268882
C27	3.150678	-0.998068	-0.246706
C28	4.190781	-1.944943	0.279325
H29	4.886300	-2.195255	-0.524579
H30	4.753351	-1.432407	1.065487
H31	3.760662	-2.859590	0.690868
O32	3.454128	0.019563	-0.894642
H33	-5.577956	-0.900073	1.111814

2

C1	-0.528551	-0.131881	-0.438390
H2	-0.769298	-0.207088	-1.503118
C3	0.866837	-0.720192	-0.189843
H4	1.117798	-0.570901	0.867572
H5	0.817004	-1.800345	-0.361152
C6	-1.560406	-0.954703	0.323262
O7	-1.980622	-1.986651	-0.401251
O8	-1.926134	-0.732515	1.463732
N9	-0.576943	1.254633	-0.028828
H10	0.204454	1.635981	0.487842
C11	1.932537	-0.113934	-1.103463
H12	1.621740	-0.240721	-2.145859
H13	2.006479	0.968142	-0.938036
C14	3.311435	-0.760277	-0.937569
H15	4.013774	-0.294070	-1.637388
H16	3.254842	-1.821593	-1.201804
C17	3.899473	-0.698520	0.463845
H18	3.295335	-1.235573	1.195303
H19	4.907419	-1.112260	0.477307
N20	4.009512	0.711172	0.952959
H21	4.493350	0.747809	1.852674
H22	4.531785	1.288069	0.288507
C23	-1.671383	2.015197	-0.218744
C24	-1.620727	3.426589	0.294422
H25	-0.645257	3.693749	0.704613
H26	-1.871559	4.108335	-0.521758
H27	-2.380341	3.540229	1.072927
O28	-2.678674	1.561338	-0.790465
C29	-2.904105	-2.892000	0.229768
H30	-3.813013	-2.360177	0.516428
H31	-3.127401	-3.646414	-0.521757
H32	-2.440941	-3.351559	1.104729
H33	3.088633	1.138705	1.078189

3

C1	-0.465014	-0.148443	-0.698030
H2	-0.598347	-0.003235	-1.774621
C3	0.958710	-0.653160	-0.429614
H4	1.100139	-0.740138	0.654438
H5	1.043572	-1.660734	-0.849792
C6	-1.461471	-1.232212	-0.309701
O7	-1.865695	-1.162240	0.951633
O8	-1.802200	-2.112838	-1.082540
N9	-0.701738	1.105514	-0.014570
H10	0.003693	1.456485	0.619531
C11	2.030556	0.240877	-1.054455
H12	1.808997	0.374874	-2.118654
H13	2.001288	1.243504	-0.610526
C14	3.442466	-0.340939	-0.934106
H15	4.151857	0.328155	-1.433812
H16	3.490296	-1.302831	-1.455516
C17	3.926647	-0.595320	0.485036
H18	3.301404	-1.309320	1.021568
H19	4.951731	-0.964916	0.482550
N20	3.926973	0.663072	1.294469
H21	4.353896	0.510566	2.210334
H22	4.452171	1.402737	0.820873
C23	-1.852157	1.787420	-0.162976
C24	-1.986005	3.077663	0.594398
H25	-1.065054	3.365658	1.104142
H26	-2.276706	3.865677	-0.104176
H27	-2.785536	2.970023	1.332836
O28	-2.762349	1.357631	-0.894515
C29	-2.772370	-2.187068	1.398229
H30	-2.309314	-3.169750	1.294005
H31	-2.964460	-1.966688	2.446287

H32	-3.699002	-2.141709	0.823321
H33	2.976519	1.008221	1.448609

4

C1	-0.721391	0.077438	0.687661
H2	-1.106454	0.007943	1.708246
C3	0.466757	-0.893408	0.554102
H4	1.164099	-0.662410	1.365385
H5	0.088329	-1.905461	0.731142
C6	-0.228261	1.504369	0.523048
O7	-0.766139	2.151403	-0.501191
O8	0.615301	1.987066	1.260545
N9	-1.813917	-0.235566	-0.211168
H10	-1.770777	0.109435	-1.160572
C11	1.166876	-0.819687	-0.803191
H12	0.462202	-1.081540	-1.599003
H13	1.478369	0.213869	-1.008409
C14	2.377702	-1.750428	-0.919810
H15	2.815418	-1.646076	-1.918774
H16	2.058020	-2.792900	-0.818131
C17	3.468641	-1.530176	0.117938
H18	3.136269	-1.750514	1.132478
H19	4.340126	-2.146411	-0.101677
N20	3.939832	-0.108560	0.125990
H21	3.213189	0.524512	0.470299
H22	4.756778	0.001564	0.730058
C23	-0.297273	3.491336	-0.743886
H24	-0.534007	4.130632	0.108039
H25	0.778725	3.481084	-0.926177
H26	-0.831216	3.825219	-1.631121
C27	-2.808483	-1.077806	0.127815
C28	-3.844988	-1.355429	-0.925130
H29	-4.819776	-1.042089	-0.541543
H30	-3.647006	-0.841360	-1.867166
H31	-3.884878	-2.433275	-1.101996
O32	-2.880972	-1.595765	1.256840
H33	4.198183	0.197767	-0.815669

5

N1	5.159214	-1.344776	-0.139848
C2	4.034244	-0.414699	0.177741
H3	4.257819	0.531650	-0.316309
H4	4.050082	-0.261967	1.257733
C5	2.710630	-0.993846	-0.288244
H6	2.566752	-1.982253	0.164986
H7	2.735694	-1.130753	-1.376156
C8	1.549600	-0.079390	0.098807
H9	1.520675	0.026166	1.190305
H10	1.723748	0.921732	-0.313962
C11	0.211441	-0.623217	-0.397883
H12	0.108203	-1.675756	-0.113584
H13	0.161143	-0.571967	-1.491697
C14	-1.015503	0.108359	0.183333
H15	-1.006413	0.022350	1.271440
C16	-0.974810	1.577211	-0.186993
N17	-2.255882	-0.456992	-0.314186
O18	-1.402883	2.024137	-1.238027
O19	-0.380675	2.310957	0.744183
H20	6.055829	-0.951853	0.154462
H21	5.037106	-2.241980	0.336018
H22	-2.621893	-0.096886	-1.186788
C23	-0.178335	3.704723	0.443247
H24	0.345241	4.111164	1.305935
H25	0.429427	3.807108	-0.457293
H26	-1.140645	4.202172	0.312641
C27	-2.831792	-1.538248	0.243725
C28	-4.064613	-2.076452	-0.428070
H29	-3.884541	-3.121423	-0.693644
H30	-4.890055	-2.049862	0.288165
H31	-4.344631	-1.519396	-1.323842
O32	-2.376710	-2.067892	1.273900
H33	5.210117	-1.530146	-1.144597

6

C1	-0.856301	0.131259	-0.332440
H2	-1.028639	0.417286	-1.372407
C3	-0.001934	-1.150287	-0.275623
H4	0.232417	-1.337668	0.779091
H5	-0.593860	-1.999786	-0.628794
C6	-2.204384	-0.113286	0.320612
O7	-2.992153	-0.852194	-0.453149
O8	-2.520549	0.281644	1.429183
N9	-0.178504	1.223941	0.331796
H10	2.590371	0.092973	1.021719
C11	1.270642	-1.020789	-1.114826
H12	1.012849	-1.128081	-2.173139
H13	1.688580	-0.011823	-1.014577
C14	2.354834	-2.045832	-0.771152
H15	3.184701	-1.933619	-1.477296
H16	1.967854	-3.063089	-0.893033
C17	2.901382	-1.953505	0.647075
H18	2.158070	-2.209134	1.401905
H19	3.760728	-2.611274	0.773663
N20	3.370633	-0.567960	0.969625
H21	3.850404	-0.548327	1.872038
H22	4.020572	-0.224305	0.258139
C23	0.433768	2.237912	-0.313102
C24	1.297934	3.130631	0.534834
H25	1.150881	2.970451	1.604677
H26	2.344479	2.925685	0.288413
H27	1.090549	4.174001	0.288686
O28	0.312087	2.424111	-1.535922
C29	-4.272576	-1.225406	0.089834
H30	-4.875235	-0.334129	0.272638
H31	-4.737118	-1.849168	-0.670999
H32	-4.137629	-1.787496	1.015420

H33	0.039856	1.092963	1.311745

7

N1	5.357928	-0.957797	-0.310356
C2	4.166530	-0.259796	0.260098
H3	4.312604	0.806519	0.083375
H4	4.180261	-0.445632	1.334903
C5	2.886040	-0.765462	-0.379508
H6	2.818287	-1.852234	-0.249556
H7	2.910712	-0.562159	-1.456962
C8	1.664917	-0.097664	0.250281
H9	1.643387	-0.316374	1.325188
H10	1.759228	0.990676	0.147586
C11	0.363538	-0.571042	-0.393752
H12	0.320178	-1.665685	-0.394335
H13	0.315366	-0.238677	-1.437146
C14	-0.894381	-0.082320	0.344157
H15	-0.906163	-0.493020	1.353920
C16	-0.880050	1.429743	0.491545
N17	-2.108972	-0.515098	-0.323837
O18	-0.599618	2.008501	1.526878
O19	-1.163034	2.050561	-0.648004
H20	6.222715	-0.609761	0.109378
H21	5.306902	-1.965457	-0.141990
H22	-2.344299	-0.077564	-1.205364
C23	-1.134756	3.489945	-0.633727
H24	-1.395968	3.792500	-1.645640
H25	-1.865682	3.872008	0.080891
H26	-0.133084	3.839159	-0.377003
C27	-2.827577	-1.583482	0.075757
C28	-4.005192	-1.952713	-0.783617
H29	-3.827097	-2.942775	-1.212532
H30	-4.895660	-2.014499	-0.153364
H31	-4.181301	-1.238922	-1.590169
O32	-2.541905	-2.233964	1.096336
H33	5.418970	-0.811871	-1.320910

8

C1	0.518239	-0.705268	0.273120
H2	0.298719	-1.216983	1.216090
C3	-0.214256	-1.425761	-0.875962
H4	0.261765	-1.173072	-1.827002
H5	-0.085928	-2.502522	-0.727834
C6	2.030016	-0.820856	0.127356
O7	2.690957	0.025870	0.910270
O8	2.578304	-1.651450	-0.576365
N9	0.098142	0.671305	0.466303
H10	-0.600707	0.848293	1.175172
C11	-1.699214	-1.074827	-0.960196
H12	-1.788928	-0.006081	-1.188149
H13	-2.130894	-1.597012	-1.820254
C14	-2.506619	-1.435962	0.292386
H15	-1.947763	-1.218588	1.210816
H16	-2.699518	-2.512976	0.304487
C17	-3.848563	-0.727885	0.380067
H18	-4.388360	-0.752071	-0.567736
H19	-4.477821	-1.159891	1.157728
N20	-3.671707	0.715402	0.743320
H21	-4.576226	1.183439	0.830099
H22	-3.181774	0.803478	1.637303
C23	4.126870	-0.044261	0.870055
H24	4.465581	-1.031487	1.190147
H25	4.484683	0.169826	-0.138691
H26	4.472320	0.718182	1.565387
C27	0.347188	1.635949	-0.439432
C28	-0.336831	2.957460	-0.232246
H29	-1.034422	3.116811	-1.059720
H30	-0.885478	3.008396	0.710015
H31	0.411012	3.753240	-0.262739
O32	1.111044	1.436418	-1.399862
H33	-3.124717	1.223825	0.044294

9

C1	0.664161	-0.397174	0.455589
H2	0.512441	-0.973557	1.374569
C3	0.214102	-1.262100	-0.745602
H4	0.699647	-0.907749	-1.658131
H5	0.567107	-2.281945	-0.567296
C6	2.158005	-0.094902	0.456222
O7	2.863851	-1.095938	-0.059333
O8	2.662626	0.909923	0.924662
N9	-0.101921	0.821931	0.633399
H10	-0.789855	0.827028	1.373765
C11	-1.298925	-1.259150	-0.964147
H12	-1.605194	-0.244974	-1.246310
H13	-1.522099	-1.885352	-1.834191
C14	-2.116889	-1.763353	0.231125
H15	-1.696710	-1.419810	1.183626
H16	-2.083564	-2.856651	0.263755
C17	-3.578781	-1.351094	0.187466
H18	-4.032255	-1.538837	-0.786983
H19	-4.159532	-1.862469	0.954751
N20	-3.730807	0.115212	0.458753
H21	-4.716878	0.382855	0.483371
H22	-3.311292	0.362242	1.358662
C23	4.295876	-0.953940	-0.046283
H24	4.591052	-0.074811	-0.621659
H25	4.656432	-0.872501	0.980701
H26	4.678940	-1.859037	-0.513174
C27	-0.167782	1.799317	-0.292187
C28	-1.190697	2.876735	-0.057914
H29	-1.948416	2.803201	-0.844049
H30	-1.678504	2.793147	0.914605
H31	-0.710689	3.853960	-0.145591
O32	0.570744	1.803842	-1.290974
H33	-3.273721	0.686601	-0.255938

10

N1	-5.536254	-0.649856	-0.010998
C2	-4.248373	0.043374	-0.313924
H3	-4.261032	0.987329	0.232124
H4	-4.248131	0.252583	-1.384541
C5	-3.069099	-0.823107	0.088758
H6	-3.117774	-1.776415	-0.451074
H7	-3.132570	-1.046654	1.160703
C8	-1.745268	-0.124427	-0.216208
H9	-1.685305	0.095152	-1.289024
H10	-1.716503	0.836587	0.311449
C11	-0.555941	-0.989247	0.195071
H12	-0.646290	-1.979073	-0.264742
H13	-0.553589	-1.129806	1.282766
C14	0.803845	-0.418111	-0.233414
H15	0.816336	-0.315618	-1.320981
C16	0.996333	0.968145	0.375054
N17	1.850559	-1.329055	0.192727
O18	1.340587	1.172125	1.526033
O19	0.714955	1.929886	-0.496095
H20	-6.338499	-0.080782	-0.288693
H21	-5.595796	-1.542489	-0.507525
H22	1.613337	-2.002227	0.912723
C23	0.801044	3.285281	-0.018160
H24	0.552733	3.909389	-0.874220
H25	0.084251	3.443579	0.789633
H26	1.815236	3.493875	0.326441
C27	3.160327	-1.258217	-0.131592
C28	3.597822	-0.197593	-1.102439
H29	3.673955	0.761901	-0.578650
H30	4.582830	-0.457462	-1.489339
H31	2.897780	-0.075766	-1.931923
O32	3.973802	-2.051002	0.375613
H33	-5.619995	-0.846381	0.989483

11

C1	-0.769182	-0.233248	-0.635600
H2	-0.766749	0.060511	-1.687410
C3	0.039250	-1.531543	-0.459844
H4	0.092846	-1.748308	0.614245
H5	-0.514712	-2.354567	-0.918304
C6	-2.220851	-0.494389	-0.269133
O7	-2.541993	-0.108684	0.959284
O8	-2.995542	-1.055385	-1.026654
N9	-0.167345	0.837038	0.129023
H10	2.882900	0.747955	0.094213
C11	1.447365	-1.430451	-1.073534
H12	1.472073	-1.987287	-2.014213
H13	1.661801	-0.389119	-1.343409
C14	2.550512	-1.969982	-0.157392
H15	3.482921	-2.091156	-0.720673
H16	2.272117	-2.965332	0.204678
C17	2.832031	-1.115094	1.069229
H18	1.924874	-0.860100	1.619872
H19	3.520224	-1.618041	1.748011
N20	3.483532	0.179357	0.695571
H21	3.693640	0.734917	1.527183
H22	4.360045	0.015413	0.194340
C23	0.188960	2.029364	-0.388817
C24	0.940128	2.953500	0.531317
H25	1.093346	2.529600	1.525551
H26	1.911145	3.175229	0.079973
H27	0.387772	3.892540	0.617349
O28	-0.079641	2.356781	-1.557420
C29	-3.885566	-0.387915	1.395097
H30	-4.056119	-1.465892	1.408712
H31	-3.954432	0.022108	2.400584
H32	-4.603520	0.100521	0.734394
H33	0.128050	0.623114	1.073122

12

C1	-0.453174	-0.371097	-0.528836
H2	-0.723094	-0.336472	-1.588132
C3	0.457065	-1.578852	-0.261726
H4	0.652660	-1.625948	0.814555
H5	-0.118028	-2.473729	-0.511532
C6	-1.726091	-0.533953	0.291000
O7	-2.650213	-1.198869	-0.389474
O8	-1.860660	-0.156679	1.440367
N9	0.232379	0.871512	-0.175587
H10	1.272121	0.836470	0.095949
C11	1.772688	-1.543381	-1.065779
H12	1.765502	-2.347202	-1.807087
H13	1.837078	-0.613992	-1.642611
C14	3.036403	-1.687007	-0.207694
H15	3.908228	-1.606709	-0.868414
H16	3.072399	-2.687141	0.239730
C17	3.174121	-0.668839	0.922925
H18	2.455041	-0.879659	1.721112
H19	4.173165	-0.766895	1.364900
N20	2.915825	0.702107	0.452189
H21	3.159593	1.368895	1.179893
H22	3.514262	0.910222	-0.344497
C23	-0.331949	2.033265	-0.280191
C24	0.361044	3.295346	0.072250
H25	1.384496	3.110480	0.393802
H26	0.357413	3.958292	-0.797307
H27	-0.193776	3.784571	0.878073
O28	-1.572859	2.057859	-0.709553
C29	-3.866966	-1.516011	0.313615
H30	-4.366423	-0.598058	0.627551
H31	-4.480412	-2.058689	-0.402380
H32	-3.644162	-2.142983	1.178705
H33	-1.932471	2.957890	-0.732626

13

C1	-0.347911	-0.505893	-0.809260
H2	-0.497666	-0.407500	-1.888146
C3	0.755075	-1.539472	-0.534465
H4	0.815479	-1.699573	0.547023
H5	0.419903	-2.483114	-0.970850
C6	-1.658555	-1.024410	-0.234258
O7	-1.877746	-0.635414	1.012868
O8	-2.388139	-1.776144	-0.856038
N9	0.029471	0.799708	-0.268559
H10	1.002746	0.926824	0.175480
C11	2.125968	-1.131332	-1.112673
H12	2.393196	-1.813123	-1.924866
H13	2.058471	-0.139150	-1.572837
C14	3.266318	-1.132085	-0.086172
H15	4.178216	-0.783785	-0.586155
H16	3.462906	-2.156843	0.249724
C17	3.024737	-0.274570	1.155154
H18	2.263783	-0.730188	1.796906
H19	3.950465	-0.234109	1.741901
N20	2.548533	1.072192	0.797270
H21	2.530660	1.663444	1.624204
H22	3.200502	1.503239	0.145033
C23	-0.718253	1.849656	-0.395386
C24	-0.321497	3.175072	0.137078
H25	0.654101	3.130215	0.618605
H26	-0.300381	3.896697	-0.684208
H27	-1.074951	3.501894	0.859239
O28	-1.866144	1.695766	-1.015681
C29	-3.065930	-1.138068	1.652717
H30	-3.028638	-2.227505	1.703904
H31	-3.056304	-0.708808	2.652248
H32	-3.951762	-0.811575	1.105395
H33	-2.370241	2.522602	-1.059182

14

C1	0.416800	-0.400188	0.058242
H2	0.145718	-1.168976	0.783197
C3	-0.018922	-0.852137	-1.349911
H4	0.382857	-0.147749	-2.086219
H5	0.444123	-1.827108	-1.534768
C6	1.922406	-0.250481	0.106880
O7	2.512715	-1.316149	0.596004
O8	2.531734	0.728686	-0.315045
N9	-0.328198	0.789195	0.481299
H10	-1.232601	0.471221	0.954198
C11	-1.538802	-0.943521	-1.516324
H12	-1.972426	0.059570	-1.418476
H13	-1.717535	-1.241476	-2.553529
C14	-2.268321	-1.918833	-0.566124
H15	-1.549220	-2.548649	-0.025197
H16	-2.877107	-2.606486	-1.161581
C17	-3.207514	-1.255129	0.440650
H18	-3.846724	-0.535823	-0.081036
H19	-3.866396	-2.017859	0.874015
N20	-2.485532	-0.526098	1.502185
H21	-3.151140	-0.006945	2.068736
H22	-2.046617	-1.201585	2.125237
C23	3.957778	-1.323034	0.615143
H24	4.341776	-1.234326	-0.401826
H25	4.319568	-0.502935	1.236512
H26	4.229346	-2.282688	1.048231
C27	-0.283929	2.011321	0.031451
C28	-1.367057	2.970389	0.362583
H29	-1.765403	3.377949	-0.570351
H30	-2.167436	2.496225	0.929199
H31	-0.942194	3.797446	0.937241
O32	0.684382	2.486401	-0.701720
H33	1.462237	1.856693	-0.737420

15

C1	0.196295	-0.697063	0.063798
H2	-0.198515	-1.184226	0.962826
C3	-0.500438	-1.278038	-1.169822
H4	0.021373	-0.937844	-2.069848
H5	-0.394538	-2.365970	-1.121333
C6	1.691686	-0.980278	0.093269
O7	2.317053	-0.274684	1.027069
O8	2.236362	-1.804507	-0.616633
N9	-0.115473	0.719656	0.239975
H10	-1.020015	0.865754	0.789592
C11	-1.981282	-0.897025	-1.271543
H12	-2.065563	0.187730	-1.412785
H13	-2.356694	-1.343436	-2.197013
C14	-2.878122	-1.337145	-0.091770
H15	-2.330566	-2.008422	0.583183
H16	-3.715543	-1.925673	-0.479470
C17	-3.479466	-0.193194	0.724284
H18	-3.907312	0.551298	0.045260
H19	-4.301689	-0.583081	1.337054
N20	-2.480354	0.491491	1.567850
H21	-2.909395	1.299537	2.011337
H22	-2.207778	-0.133808	2.324472
C23	3.738939	-0.469538	1.143855
H24	3.956165	-1.512270	1.381176
H25	4.230300	-0.180470	0.213067
H26	4.052202	0.181176	1.957502
C27	0.399791	1.689911	-0.443624
C28	-0.079486	3.085453	-0.311487
H29	-0.435335	3.429754	-1.286659
H30	-0.880984	3.155953	0.422220
H31	0.757795	3.720861	-0.008956
O32	1.383810	1.400875	-1.263884
H33	1.731580	2.193133	-1.700568

16

C1	0.348168	-0.441998	0.213348
H2	-0.014686	-1.063089	1.041350
C3	-0.014222	-1.137211	-1.106142
H4	0.500313	-0.639014	-1.933572
H5	0.365705	-2.160979	-1.052319
C6	1.834992	-0.289131	0.499877
O7	2.551348	-1.239207	-0.081977
O8	2.301547	0.563581	1.233047
N9	-0.355146	0.826686	0.367238
H10	-1.306395	0.699732	0.835193
C11	-1.521553	-1.155871	-1.384682
H12	-1.877671	-0.127860	-1.524632
H13	-1.652756	-1.646364	-2.353744
C14	-2.398000	-1.869199	-0.329172
H15	-1.774524	-2.416529	0.390742
H16	-3.007117	-2.628961	-0.829038
C17	-3.363707	-0.964830	0.436796
H18	-3.891843	-0.316565	-0.269612
H19	-4.120058	-1.588273	0.929830
N20	-2.683982	-0.099071	1.420253
H21	-3.359974	0.541053	1.828710
H22	-2.344464	-0.678658	2.185980
C23	3.963307	-1.254384	0.202881
H24	4.422288	-0.322771	-0.131414
H25	4.126490	-1.397979	1.272252
H26	4.359051	-2.097952	-0.358639
C27	-0.098670	1.918004	-0.280209
C28	-0.963753	3.116078	-0.163904
H29	-1.317713	3.393041	-1.160945
H30	-1.811454	2.926531	0.493329
H31	-0.368336	3.944700	0.229977
O32	0.965113	1.943882	-1.048005
H33	1.083603	2.811840	-1.463153

17

C1	-0.523257	-0.282331	-0.564285
H2	-0.811740	-0.168377	-1.614922
C3	0.342653	-1.545310	-0.413078
H4	0.514011	-1.706319	0.656179
H5	-0.254611	-2.388922	-0.763820
C6	-1.781484	-0.442901	0.282967
O7	-2.653139	-1.246628	-0.308834
O8	-1.952920	0.076495	1.369731
N9	0.232875	0.891956	-0.138055
H10	1.224556	0.735815	0.258838
C11	1.676284	-1.464428	-1.182324
H12	1.646264	-2.152297	-2.032091
H13	1.801567	-0.466749	-1.616916
C14	2.910797	-1.794019	-0.332287
H15	3.803174	-1.623738	-0.946428
H16	2.909986	-2.857390	-0.065855
C17	3.038710	-0.991462	0.962376
H18	2.304632	-1.329434	1.700194
H19	4.029003	-1.174868	1.396459
N20	2.804134	0.445152	0.737479
H21	3.010161	0.964908	1.586840
H22	3.446238	0.790340	0.026536
C23	-0.149971	2.121426	-0.293447
C24	0.674456	3.261842	0.172535
H25	1.576357	2.920977	0.678025
H26	0.941425	3.878707	-0.689658
H27	0.074731	3.870821	0.853460
O28	-1.281584	2.470138	-0.861771
C29	-3.867847	-1.526687	0.414809
H30	-4.407734	-0.597933	0.606128
H31	-4.448376	-2.176626	-0.236272
H32	-3.634911	-2.032729	1.353024
H33	-1.804696	1.737229	-1.222294

18

C1	-0.395281	-0.508409	-0.796537
H2	-0.580839	-0.393924	-1.870500
C3	0.763962	-1.501285	-0.596879
H4	0.844887	-1.708081	0.475281
H5	0.468476	-2.437002	-1.074381
C6	-1.654724	-1.111216	-0.182365
O7	-2.081926	-0.478305	0.897828
O8	-2.184869	-2.100485	-0.655319
N9	-0.033708	0.787566	-0.224689
H10	0.878665	0.833509	0.339686
C11	2.104925	-0.997855	-1.165088
H12	2.358930	-1.571287	-2.061303
H13	2.008883	0.039948	-1.500447
C14	3.274726	-1.092510	-0.176814
H15	4.152862	-0.628905	-0.642031
H16	3.530253	-2.143976	-0.001430
C17	3.030140	-0.443505	1.186445
H18	2.348213	-1.053096	1.787057
H19	3.980850	-0.406780	1.732458
N20	2.425443	0.892987	1.058486
H21	2.371013	1.332760	1.973744
H22	3.024891	1.488085	0.489376
C23	-0.633889	1.919243	-0.431757
C24	-0.166451	3.168393	0.217324
H25	0.771386	3.014903	0.748555
H26	-0.045902	3.943861	-0.542175
H27	-0.934960	3.497714	0.922361
O28	-1.691849	2.074382	-1.192458
C29	-3.261103	-1.007924	1.535778
H30	-3.068897	-2.021569	1.890697
H31	-3.458076	-0.339383	2.370934
H32	-4.095765	-1.001570	0.833071
H33	-2.001672	1.276598	-1.648576

19

C1	0.263865	-0.668819	0.207069
H2	-0.272082	-1.286871	0.929070
C3	-0.167355	-1.080709	-1.212738
H4	0.463158	-0.565520	-1.945008
H5	0.027656	-2.154006	-1.306943
C6	1.728269	-0.996053	0.429463
O7	2.556081	-0.044403	0.004733
O8	2.103498	-2.054418	0.890824
N9	-0.164443	0.699957	0.520294
H10	-1.122561	0.640862	0.995147
C11	-1.640214	-0.784302	-1.513589
H12	-1.800398	0.301070	-1.521970
H13	-1.813263	-1.115269	-2.541802
C14	-2.674647	-1.452013	-0.580426
H15	-2.203463	-2.242401	0.019471
H16	-3.427058	-1.956175	-1.194997
C17	-3.433916	-0.502046	0.347080
H18	-3.777855	0.365659	-0.225092
H19	-4.326526	-1.014321	0.726663
N20	-2.609889	-0.001924	1.464793
H21	-3.141547	0.683976	1.994742
H22	-2.418293	-0.770940	2.104273
C23	3.976515	-0.283446	0.115013
H24	4.233965	-0.464791	1.158686
H25	4.251566	-1.135476	-0.507525
H26	4.445978	0.628068	-0.246855
C27	0.128176	1.830885	-0.054363
C28	-0.712309	3.031419	0.179579
H29	-1.093116	3.379013	-0.784823
H30	-1.545167	2.816114	0.847533
H31	-0.090247	3.824388	0.601944
O32	1.146014	2.017506	-0.853336
H33	1.774523	1.261412	-0.838417

20

N1	5.188522	-1.484769	-0.260487
C2	4.121268	-0.553531	0.122880
H3	4.318323	0.408416	-0.361674
H4	4.100376	-0.365293	1.206949
C5	2.757065	-1.068571	-0.312818
H6	2.592727	-2.063571	0.123067
H7	2.746746	-1.191689	-1.403286
C8	1.623739	-0.136715	0.113082
H9	1.607714	-0.052982	1.207032
H10	1.816707	0.869082	-0.280030
C11	0.267088	-0.634735	-0.381645
H12	0.129845	-1.684251	-0.101078
H13	0.215887	-0.575324	-1.474538
C14	-0.929002	0.140298	0.204610
H15	-0.947006	0.043931	1.291002
C16	-0.856922	1.610569	-0.165075
N17	-2.186682	-0.375925	-0.334530
O18	-1.307734	2.061529	-1.203324
O19	-0.218985	2.318221	0.749997
H20	6.082477	-1.106636	0.040662
H21	5.065802	-2.352433	0.256529
H22	-2.553203	0.069830	-1.172641
C23	0.014171	3.709006	0.448654
H24	0.554945	4.100411	1.307278
H25	0.615861	3.795682	-0.457416
H26	-0.938392	4.226528	0.326973
C27	-2.833060	-1.401601	0.136181
C28	-4.079783	-1.904378	-0.483150
H29	-3.918734	-2.942219	-0.788442
H30	-4.873024	-1.887931	0.269577
H31	-4.370633	-1.304936	-1.344861
O32	-2.333441	-1.980097	1.194876
H33	-2.885387	-2.721035	1.491308

21

C1	-0.654510	0.123741	0.713303
H2	-1.050040	0.054760	1.728678
C3	0.518619	-0.858532	0.559800
H4	1.222754	-0.626664	1.363936
H5	0.134635	-1.866780	0.745999
C6	-0.167014	1.552452	0.540428
O7	-0.707759	2.184158	-0.488693
O8	0.667424	2.034797	1.283506
N9	-1.746186	-0.177040	-0.213349
H10	-1.730951	0.257473	-1.131223
C11	1.207682	-0.790976	-0.803210
H12	0.486300	-1.024746	-1.594192
H13	1.549861	0.234480	-0.995560
C14	2.391903	-1.756997	-0.921122
H15	2.811848	-1.674857	-1.930596
H16	2.028754	-2.785945	-0.807291
C17	3.503778	-1.527729	0.098499
H18	3.129043	-1.746570	1.108795
H19	4.307124	-2.244313	-0.095141
N20	4.068494	-0.175966	-0.002844
H21	3.363750	0.502556	0.277466
H22	4.820838	-0.083247	0.673837
C23	-0.254368	3.529424	-0.741275
H24	-0.503015	4.169514	0.106406
H25	0.822039	3.528385	-0.919342
H26	-0.790058	3.848599	-1.632534
C27	-2.701681	-1.027559	0.025665
C28	-3.758911	-1.320554	-0.967927
H29	-4.731415	-1.110521	-0.513926
H30	-3.631635	-0.726237	-1.871520
H31	-3.719259	-2.385594	-1.213490
O32	-2.691060	-1.614633	1.191510
H33	-3.438560	-2.223456	1.297489

22

N1	5.389482	-1.013934	-0.469159
C2	4.256749	-0.352622	0.188654
H3	4.359098	0.726679	0.034815
H4	4.247462	-0.520737	1.276094
C5	2.931628	-0.821495	-0.395263
H6	2.849962	-1.910642	-0.278562
H7	2.918031	-0.612958	-1.472637
C8	1.733338	-0.149418	0.272150
H9	1.727576	-0.379661	1.345124
H10	1.840863	0.939176	0.181070
C11	0.412760	-0.592963	-0.353997
H12	0.334008	-1.685187	-0.339593
H13	0.363506	-0.269872	-1.399830
C14	-0.820150	-0.049970	0.387465
H15	-0.863523	-0.454324	1.398077
C16	-0.761289	1.464014	0.514729
N17	-2.046719	-0.429590	-0.315723
O18	-0.422262	2.035842	1.533161
O19	-1.070923	2.071708	-0.621067
H20	6.255829	-0.665744	-0.067887
H21	5.360196	-2.006909	-0.249753
H22	-2.306946	0.114341	-1.133918
C23	-1.002439	3.511410	-0.635714
H24	-1.278927	3.800236	-1.647357
H25	-1.707275	3.923433	0.088133
H26	0.014652	3.834383	-0.408762
C27	-2.789996	-1.458394	-0.026834
C28	-3.997362	-1.792335	-0.815513
H29	-3.855929	-2.778501	-1.267167
H30	-4.854568	-1.844299	-0.138492
H31	-4.180527	-1.051220	-1.591707
O32	-2.425862	-2.193036	0.988700
H33	-3.049893	-2.918998	1.146110

23

N1	-5.595237	-0.839356	-0.008919
C2	-4.366733	-0.056435	-0.186914
H3	-4.407251	0.799436	0.494803
H4	-4.274376	0.351533	-1.204783
C5	-3.133826	-0.893179	0.122868
H6	-3.157410	-1.807093	-0.486621
H7	-3.164126	-1.209797	1.173201
C8	-1.834460	-0.139386	-0.154405
H9	-1.784332	0.124103	-1.218121
H10	-1.833730	0.802648	0.408007
C11	-0.612049	-0.973949	0.221777
H12	-0.689335	-1.965556	-0.236807
H13	-0.570244	-1.112905	1.308564
C14	0.719268	-0.369194	-0.249359
H15	0.718894	-0.298198	-1.338946
C16	0.915014	1.024751	0.337287
N17	1.801709	-1.253236	0.179341
O18	1.374898	1.242284	1.442671
O19	0.489238	1.959627	-0.497308
H20	-6.397807	-0.247942	-0.205990
H21	-5.615044	-1.576028	-0.710367
H22	1.569791	-1.985826	0.847510
C23	0.521929	3.318738	-0.018884
H24	0.105792	3.916976	-0.826332
H25	-0.088112	3.410496	0.881214
H26	1.552067	3.614163	0.186088
C27	3.055343	-1.151472	-0.164971
C28	3.566326	-0.109596	-1.083862
H29	3.722948	0.809906	-0.508767
H30	4.519504	-0.423682	-1.509146
H31	2.854303	0.096370	-1.883789
O32	3.852946	-2.030484	0.380645
H33	4.771636	-1.923544	0.088045

24

N1	5.194852	-1.472817	-0.280704
C2	4.129413	-0.542870	0.110493
H3	4.323333	0.420113	-0.373253
H4	4.114480	-0.356734	1.195026
C5	2.763084	-1.057958	-0.318518
H6	2.602468	-2.054474	0.115274
H7	2.745632	-1.177480	-1.409239
C8	1.631903	-0.128591	0.118188
H9	1.624948	-0.046251	1.212324
H10	1.818749	0.877828	-0.275647
C11	0.272481	-0.629391	-0.365326
H12	0.143809	-1.681724	-0.088218
H13	0.207734	-0.567126	-1.457101
C14	-0.920461	0.140621	0.235432
H15	-0.915052	0.072232	1.326380
C16	-0.869834	1.609960	-0.148166
N17	-2.186090	-0.383983	-0.280774
O18	-1.362077	2.047044	-1.172808
O19	-0.205268	2.327652	0.737746
H20	6.090346	-1.094540	0.015639
H21	5.075860	-2.341317	0.235778
H22	-2.570735	0.100247	-1.090182
C23	0.005021	3.718549	0.418193
H24	0.562008	4.123562	1.259846
H25	0.583821	3.802562	-0.502880
H26	-0.955793	4.224391	0.314237
C27	-2.838388	-1.429515	0.140879
C28	-4.099241	-1.866493	-0.500497
H29	-3.956858	-2.878316	-0.888987
H30	-4.881803	-1.900629	0.261632
H31	-4.393687	-1.197423	-1.307996
O32	-2.447506	-2.163588	1.146411
H33	-1.605646	-1.902054	1.552850

25

C1	-0.656009	0.149114	0.765430
H2	-1.026915	0.101417	1.794163
C3	0.536733	-0.808522	0.597218
H4	1.252203	-0.552052	1.383572
H5	0.183560	-1.825002	0.802403
C6	-0.195645	1.585203	0.563779
O7	-0.737687	2.178013	-0.486373
O8	0.624708	2.098023	1.300705
N9	-1.757303	-0.173611	-0.144085
H10	-1.784158	0.326330	-1.029010
C11	1.191319	-0.740882	-0.782100
H12	0.446522	-0.955250	-1.556600
H13	1.546446	0.280183	-0.973732
C14	2.352415	-1.729604	-0.936490
H15	2.752267	-1.645479	-1.953839
H16	1.968779	-2.751385	-0.825282
C17	3.489874	-1.534695	0.061596
H18	3.130087	-1.752178	1.077736
H19	4.272340	-2.268000	-0.153458
N20	4.083548	-0.195895	-0.042541
H21	3.399309	0.496785	0.253167
H22	4.849454	-0.123665	0.621297
C23	-0.299289	3.520756	-0.778796
H24	-0.556322	4.182244	0.049509
H25	0.777372	3.524921	-0.955155
H26	-0.836827	3.807081	-1.679977
C27	-2.671845	-1.085724	0.027749
C28	-3.711982	-1.335386	-0.995410
H29	-4.693329	-1.226674	-0.526954
H30	-3.620565	-0.646271	-1.833826
H31	-3.613104	-2.365712	-1.346991
O32	-2.748177	-1.833373	1.093823
H33	-2.055007	-1.683625	1.756256

26

N1	-5.519571	-1.018326	0.107867
C2	-4.328781	-0.219218	-0.202198
H3	-4.352070	0.680017	0.422555
H4	-4.313055	0.121190	-1.248629
C5	-3.054036	-0.999224	0.084748
H6	-3.059997	-1.930361	-0.498052
H7	-3.039330	-1.285204	1.144201
C8	-1.793742	-0.201482	-0.246625
H9	-1.773992	0.036548	-1.317187
H10	-1.823832	0.753746	0.293271
C11	-0.532824	-0.975599	0.131989
H12	-0.532143	-1.952672	-0.361001
H13	-0.517393	-1.146766	1.215139
C14	0.771310	-0.264626	-0.262562
H15	0.832852	-0.196654	-1.351353
C16	0.800347	1.135296	0.342753
N17	1.896509	-1.052503	0.241891
O18	1.071470	1.364769	1.506222
O19	0.444767	2.051595	-0.543669
H20	-6.349410	-0.459123	-0.069368
H21	-5.568267	-1.799514	-0.542070
H22	1.701889	-1.661452	1.032194
C23	0.292233	3.399843	-0.056055
H24	-0.035334	3.979150	-0.916490
H25	-0.461431	3.423443	0.732752
H26	1.247920	3.772677	0.315532
C27	3.129294	-1.054635	-0.186999
C28	4.160728	-1.919369	0.430305
H29	4.628168	-2.518543	-0.354619
H30	4.928001	-1.275445	0.868912
H31	3.738811	-2.568267	1.196561
O32	3.552616	-0.310707	-1.168518
H33	2.892048	0.271856	-1.575060

27

N1	-5.595922	-0.818809	-0.013968
C2	-4.362830	-0.042454	-0.188787
H3	-4.399790	0.812720	0.494012
H4	-4.266508	0.366392	-1.205937
C5	-3.135010	-0.886475	0.121846
H6	-3.162232	-1.798943	-0.489627
H7	-3.169007	-1.205021	1.171457
C8	-1.831454	-0.138743	-0.151494
H9	-1.779811	0.129575	-1.213932
H10	-1.825835	0.800661	0.415315
C11	-0.612541	-0.980738	0.220269
H12	-0.693916	-1.969740	-0.243213
H13	-0.570179	-1.124593	1.306429
C14	0.718487	-0.376083	-0.250347
H15	0.716996	-0.300410	-1.339409
C16	0.918348	1.013806	0.343960
N17	1.804455	-1.263448	0.171599
O18	1.371091	1.222332	1.454006
O19	0.505984	1.955315	-0.489521
H20	-6.394889	-0.222918	-0.212248
H21	-5.618225	-1.554777	-0.716070
H22	1.560052	-1.998263	0.833416
C23	0.551655	3.312517	-0.006566
H24	0.148774	3.918388	-0.815042
H25	-0.063517	3.408863	0.889513
H26	1.584074	3.594073	0.206421
C27	3.056394	-1.144060	-0.179868
C28	3.542531	-0.088532	-1.094355
H29	3.648473	0.842656	-0.526487
H30	4.517456	-0.372662	-1.487340
H31	2.841447	0.082988	-1.912265
O32	3.967710	-1.956164	0.278971
H33	3.635148	-2.620485	0.905999

28

N1	5.424430	-1.006829	-0.464529
C2	4.286559	-0.357547	0.196311
H3	4.379017	0.723086	0.045630
H4	4.279705	-0.529055	1.283231
C5	2.965436	-0.836859	-0.388125
H6	2.893723	-1.926967	-0.274056
H7	2.949328	-0.625730	-1.464915
C8	1.761382	-0.177100	0.281160
H9	1.759084	-0.406837	1.354199
H10	1.857339	0.912465	0.188773
C11	0.445593	-0.635606	-0.344185
H12	0.372192	-1.727887	-0.319059
H13	0.398027	-0.322718	-1.393190
C14	-0.791758	-0.091864	0.386828
H15	-0.821179	-0.476880	1.405987
C16	-0.740942	1.425216	0.512086
N17	-2.007393	-0.477491	-0.333201
O18	-0.432798	1.998629	1.538955
O19	-1.021188	2.027130	-0.632955
H20	6.288029	-0.653474	-0.061843
H21	5.403085	-2.000932	-0.249339
H22	-2.155520	-0.014862	-1.226803
C23	-0.957010	3.467405	-0.649597
H24	-1.218263	3.752785	-1.666159
H25	-1.674122	3.878613	0.062484
H26	0.055511	3.793598	-0.407231
C27	-2.875769	-1.399737	-0.023469
C28	-4.012280	-1.709156	-0.920450
H29	-3.890954	-2.733131	-1.284875
H30	-4.939116	-1.659805	-0.344596
H31	-4.056309	-1.020756	-1.762962
O32	-2.822184	-2.119424	1.061861
H33	-2.076742	-1.930466	1.652592

29

N1	-5.628497	-0.715349	0.171336
C2	-4.389363	-0.026305	-0.207411
H3	-4.347817	0.923982	0.334875
H4	-4.356750	0.216888	-1.280159
C5	-3.167642	-0.862737	0.145329
H6	-3.232538	-1.830310	-0.370474
H7	-3.172820	-1.072606	1.222389
C8	-1.861375	-0.168088	-0.235141
H9	-1.844052	0.026831	-1.314397
H10	-1.813900	0.805363	0.267188
C11	-0.646995	-1.012138	0.148733
H12	-0.733763	-2.006963	-0.301580
H13	-0.606959	-1.141619	1.236713
C14	0.683950	-0.414555	-0.328102
H15	0.720518	-0.354833	-1.415783
C16	0.940971	0.953238	0.280585
N17	1.790237	-1.313727	0.112754
O18	1.462601	1.103460	1.370991
O19	0.501566	1.926314	-0.492872
H20	-6.423103	-0.131609	-0.074572
H21	-5.717544	-1.558497	-0.391104
H22	1.784904	-1.405498	1.138709
C23	0.611203	3.266477	0.030171
H24	0.199999	3.910510	-0.743768
H25	0.031273	3.352530	0.950258
H26	1.659655	3.505569	0.213279
C27	3.187116	-0.906215	-0.319348
C28	4.250599	-1.695863	0.340407
H29	5.217713	-1.424532	-0.078578
H30	4.227306	-1.483366	1.414928
H31	4.055635	-2.764225	0.206927
O32	3.279552	-0.017911	-1.113501
H33	1.619532	-2.261879	-0.251768

30

N1	-5.581102	-0.709845	-0.001837
C2	-4.321067	-0.038466	-0.342357
H3	-4.329918	0.956329	0.114755
H4	-4.204842	0.111102	-1.426244
C5	-3.124281	-0.822885	0.176838
H6	-3.147855	-1.836388	-0.245832
H7	-3.204655	-0.928475	1.265979
C8	-1.796979	-0.155749	-0.178152
H9	-1.701991	-0.072480	-1.267679
H10	-1.790021	0.865122	0.222462
C11	-0.610397	-0.940938	0.378629
H12	-0.667432	-1.983608	0.047238
H13	-0.632257	-0.934354	1.474540
C14	0.745443	-0.397074	-0.089277
H15	0.850221	-0.498564	-1.170544
C16	0.936800	1.050759	0.335840
N17	1.839133	-1.201082	0.562536
O18	1.352300	1.357205	1.438774
O19	0.573435	1.895608	-0.605556
H20	-6.356762	-0.169726	-0.375122
H21	-5.611239	-1.605223	-0.484130
H22	2.034750	-0.781571	1.486643
C23	0.637147	3.299988	-0.275539
H24	0.308509	3.817538	-1.173605
H25	-0.031972	3.513910	0.559066
H26	1.664110	3.571662	-0.027559
C27	3.135946	-1.310026	-0.211715
C28	3.768002	-0.022811	-0.583800
H29	3.833539	0.633463	0.288559
H30	4.757557	-0.222229	-0.991683
H31	3.159654	0.477701	-1.345600
O32	3.514756	-2.421793	-0.441033
H33	1.516773	-2.162669	0.723571

31

N1	5.091456	-1.504503	-0.255411
C2	4.037100	-0.560126	0.131347
H3	4.238661	0.396290	-0.362165
H4	4.028575	-0.363805	1.214089
C5	2.663452	-1.064581	-0.286684
H6	2.487857	-2.048926	0.168304
H7	2.643484	-1.206245	-1.374633
C8	1.548368	-0.107184	0.129887
H9	1.553222	0.012966	1.220188
H10	1.743432	0.882158	-0.301422
C11	0.177255	-0.608472	-0.321304
H12	0.039470	-1.642326	0.012840
H13	0.112251	-0.601019	-1.415970
C14	-0.983440	0.220531	0.243621
H15	-1.024098	0.158522	1.331277
C16	-0.897002	1.674694	-0.187357
N17	-2.279406	-0.318226	-0.279380
O18	-1.347116	2.086851	-1.240931
O19	-0.253164	2.407361	0.701408
H20	5.991643	-1.132189	0.034239
H21	4.966015	-2.366761	0.269975
H22	-2.240611	-0.398065	-1.303703
C23	-0.014663	3.786841	0.352374
H24	0.535175	4.202837	1.193310
H25	0.579551	3.840423	-0.561136
H26	-0.966281	4.303946	0.222222
C27	-2.713040	-1.647295	0.322899
C28	-3.548927	-2.454976	-0.591479
H29	-2.941964	-2.747477	-1.455679
H30	-3.912450	-3.336961	-0.067430
H31	-4.383186	-1.850614	-0.961341
O32	-2.362576	-1.884353	1.439670
H33	-3.046858	0.340902	-0.080418

32

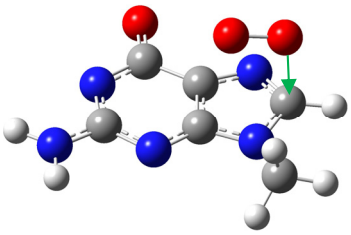
N1	5.324875	-0.714881	-0.508014
C2	4.188804	-0.073144	0.163734
H3	4.261399	1.006568	-0.003375
H4	4.204212	-0.229760	1.252791
C5	2.865141	-0.583102	-0.388339
H6	2.816711	-1.672847	-0.259139
H7	2.821120	-0.385707	-1.466825
C8	1.663788	0.062233	0.299654
H9	1.695529	-0.147562	1.375923
H10	1.726282	1.150465	0.183023
C11	0.346038	-0.449926	-0.278326
H12	0.332425	-1.544329	-0.229727
H13	0.253975	-0.163892	-1.332663
C14	-0.884781	0.060337	0.481812
H15	-0.860081	-0.250817	1.526235
C16	-0.977884	1.577265	0.455477
N17	-2.120637	-0.535312	-0.124103
O18	-0.481800	2.275895	1.316898
O19	-1.610188	2.028552	-0.616254
H20	6.189627	-0.349628	-0.118503
H21	5.316804	-1.707360	-0.284351
H22	-2.131996	-0.376471	-1.139854
C23	-1.723797	3.459945	-0.756238
H24	-2.289172	3.612414	-1.672641
H25	-2.257185	3.874898	0.099904
H26	-0.729725	3.901219	-0.840926
C27	-2.317178	-2.019063	0.166624
C28	-3.035049	-2.732456	-0.911988
H29	-2.414896	-2.715460	-1.815388
H30	-3.230211	-3.758265	-0.605270
H31	-3.969312	-2.210291	-1.141902
O32	-1.902087	-2.432790	1.206968
H33	-2.963070	-0.067616	0.242146

Cartesian coordinates for the structures in Fig. 3, optimized at SMD-ωB97XD/6-31+ G(d,p). For each TS, the vibrational mode corresponding to TS imaginary frequency is indicated by displacement vectors.

[9MG – H]⁻

C1	-1.190857	1.319433	0.000905
C2	0.199251	0.983609	-0.002827
C3	-1.587902	-0.999143	-0.007401
C4	2.327108	0.897920	0.000700
N5	-2.055509	0.262396	-0.002194
N6	1.345055	1.768339	-0.001351
N7	1.904677	-0.406387	0.001114
N8	-0.311909	-1.409633	-0.001908
C9	0.533861	-0.362272	-0.001549
N10	-2.545918	-1.990753	-0.073125
H11	-2.246048	-2.900256	0.249531
H12	-3.464072	-1.718220	0.248224
O13	-1.630190	2.512073	0.007941
H14	3.381136	1.139734	0.001331
C15	2.740766	-1.592440	0.004293
H16	2.550236	-2.191640	0.897058
H17	2.547525	-2.197925	-0.883623
H18	3.784597	-1.278652	0.001477

TS1⁻ (open-shell)

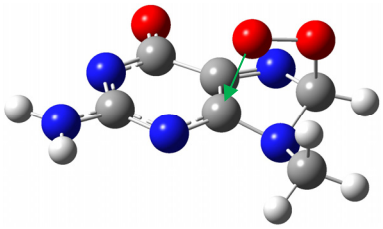


C1	-0.012025	0.858156	-0.438807
C2	0.171463	-0.555115	-0.364376
C3	-1.979028	-0.880704	0.073384
C4	-1.363542	1.365515	-0.221951
C5	2.048589	0.498358	-0.714088
N6	-2.307805	0.429164	0.042906
N7	-0.766108	-1.460083	-0.130682
O8	-1.634286	2.588279	-0.279712
N9	1.479097	-0.759048	-0.672405
N10	-2.983919	-1.732920	0.343847
H11	-3.920397	-1.382832	0.469975
H12	-2.813704	-2.726583	0.345872
N13	1.123806	1.481563	-0.758580
H14	3.077839	0.625888	-1.015621
O15	1.126872	0.335800	1.774253
O16	2.273224	0.686583	1.305106
C17	2.217125	-1.989677	-0.457838
H18	2.293194	-2.204466	0.611562
H19	1.710625	-2.813242	-0.961719
H20	3.214980	-1.874000	-0.880803

[8-OO9MG – H]⁻

C1	-1.516584	1.443926	-0.094996
C2	-0.152981	0.865988	-0.276995
C3	-2.232087	-0.768373	0.164264
C4	1.971672	0.393111	-0.614610
N5	-2.504363	0.554947	0.123795
N6	0.966138	1.451783	-0.458170
N7	1.230053	-0.872411	-0.468930
N8	-1.036179	-1.422512	-0.013874
C9	-0.039678	-0.602361	-0.236585
N10	-3.266174	-1.567613	0.406866
H11	-3.136589	-2.568215	0.439480
H12	-4.184819	-1.173890	0.547160
O13	-1.697934	2.669838	-0.149933
H14	2.381421	0.461810	-1.627907
O15	3.049704	0.501764	0.230054
O16	2.615771	0.429459	1.617264
C17	1.866151	-2.172672	-0.415100
H18	1.933406	-2.521172	0.618958
H19	1.292360	-2.888174	-1.006799
H20	2.868611	-2.085916	-0.833643

TS2⁻



C1	-1.485315	1.331128	-0.156970
C2	-0.049811	0.966826	-0.302503
C3	-1.869114	-0.977258	0.017270
C4	2.061170	0.721182	-0.289679
N5	-2.330886	0.308578	0.036296
N6	0.992776	1.699206	-0.468771
N7	1.549994	-0.532307	-0.799480
N8	-0.614778	-1.443174	-0.163196
C9	0.296355	-0.464614	-0.206418
N10	-2.819019	-1.906000	0.186049
H11	-2.577665	-2.885047	0.181755
H12	-3.784502	-1.628846	0.271457
O13	-1.849844	2.522576	-0.213791
H14	3.039134	1.020120	-0.650913
O15	0.955466	-0.123551	1.504815
O16	2.158937	0.537881	1.150010

C17	2.377352	-1.715952	-0.593757
H18	1.911113	-2.570186	-1.084900
H19	3.349173	-1.541804	-1.057548
H20	2.515844	-1.941481	0.467932

[4,8-OO-9MG – H]$^-$

C1	-1.510809	1.323977	-0.137634
C2	-0.063284	0.991911	-0.237190
C3	-1.836162	-1.000309	0.008767
C4	2.047513	0.767659	-0.261252
N5	-2.335666	0.285966	0.007631
N6	0.960321	1.745959	-0.405071
N7	1.551336	-0.455698	-0.843824
N8	-0.582543	-1.437266	-0.067004
C9	0.352991	-0.426790	-0.038866
N10	-2.801922	-1.935133	0.101082
H11	-2.562049	-2.913850	0.097331
H12	-3.769424	-1.655580	0.091769
O13	-1.892721	2.514608	-0.194902
H14	3.027593	1.107014	-0.579582
O15	2.120535	0.490816	1.165322
O16	0.941110	-0.304781	1.383397
C17	2.420805	-1.622780	-0.673090
H18	1.962108	-2.482893	-1.161363
H19	3.371933	-1.420724	-1.168509
H20	2.611442	-1.867914	0.375702

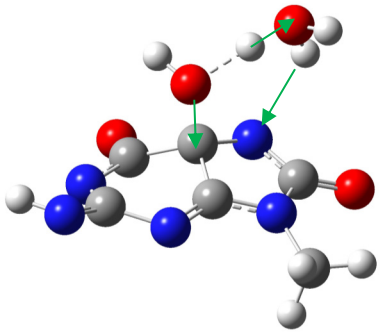
[8-OOH9MG – H]$^-$

C1	-1.554614	1.472626	-0.013309
C2	-0.264787	0.857423	-0.097283
C3	-2.408056	-0.716111	0.098624
C4	1.777183	0.344767	-0.265996
N5	-2.611095	0.614369	0.083307
N6	1.005590	1.395341	-0.213493
N7	1.117859	-0.857178	-0.183186
N8	-1.242805	-1.379850	0.033370
C9	-0.208656	-0.529447	-0.070676
N10	-3.545023	-1.490471	0.142295
H11	-3.416331	-2.440775	0.459702
H12	-4.368334	-1.029582	0.502650
O13	-1.736000	2.727692	-0.030405
H14	3.888712	1.113818	1.146927
O15	3.121140	0.393502	-0.437388
O16	3.760686	0.196445	0.852822
C17	1.685520	-2.192774	-0.231737
H18	1.196755	-2.770873	-1.017671
H19	2.748655	-2.112482	-0.453718
H20	1.552724	-2.695597	0.728097

[9MOG^{ox} – H]$^-$

C1	1.447624	1.333259	-0.003996
C2	0.028077	0.884383	-0.012037
C3	2.021600	-0.975852	0.005045
C4	-2.115823	0.575047	0.000945
N5	2.361120	0.369197	0.008180
N6	-1.062128	1.560686	0.004643
N7	-1.573378	-0.697024	-0.057853
N8	0.685282	-1.476760	-0.030244
C9	-0.210808	-0.567568	-0.036029
N10	2.924721	-1.892452	0.036043
O11	1.706142	2.560876	-0.004900
O12	-3.297832	0.846931	0.044754
C13	-2.321911	-1.938730	0.014549
H14	-1.975969	-2.621729	-0.762123
H15	-2.194282	-2.400782	0.995726
H16	-3.374830	-1.713366	-0.149870
H17	3.836721	-1.435332	0.061188

TS3a$^-$ (water-assisted addition)

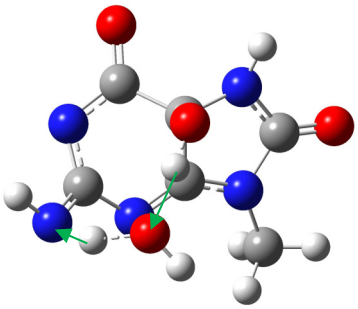


C1	-0.049963	0.645217	-0.138196
C2	-0.142168	-0.836421	0.148805
C3	-2.388557	-0.673650	0.294913
C4	-1.318190	1.031457	-0.920936
C5	1.896000	-0.300116	-0.620563
N6	-2.435423	0.400388	-0.588533
N7	-1.223984	-1.471954	0.417604
O8	-1.257478	1.957455	-1.768710
N9	1.231092	0.852750	-0.729393
N10	1.105589	-1.325223	0.000953
N11	-3.427094	-1.061576	0.955352
O12	2.165871	2.014549	1.651093
H13	2.664894	1.427078	2.242722
H14	2.451285	1.834831	0.725996
O15	-0.159476	1.323805	1.164079
H16	1.156426	1.712002	1.605865
H17	-0.641887	2.157776	1.059307
O18	3.062628	-0.548524	-0.982384
C19	1.449982	-2.731448	0.011667
H20	1.023263	-3.246851	-0.854538
H21	2.535187	-2.823833	-0.013385
H22	1.074468	-3.193326	0.926162
H23	-4.189877	-0.416890	0.749225

[5-OH9MOG – H_{N2}]$^-$

C1	1.336312	-1.208552	-0.419561
C2	0.069001	-0.799612	0.338860
C3	2.056623	1.012180	-0.108182
C4	-2.148885	-0.388403	-0.116498
N5	2.294656	-0.296769	-0.510609
N6	-1.177067	-1.354580	-0.095505
N7	-1.525523	0.855230	0.016936
N8	0.739582	1.550650	-0.051173
C9	-0.175442	0.671937	0.093108
N10	3.009834	1.842676	0.138207
O11	1.429270	-2.388654	-0.834654
H12	1.098193	-0.810171	2.025155
O13	0.217189	-1.074361	1.725184
O14	-3.350961	-0.559786	-0.267157
C15	-2.181710	2.123149	-0.246039
H16	-1.927998	2.835667	0.539665
H17	-1.871773	2.521239	-1.215343
H18	-3.257968	1.956458	-0.246391
H19	-1.425738	-2.310400	0.126910
H20	3.895532	1.344966	0.047896

TS3b$^-$ (water-assisted proton transfer)

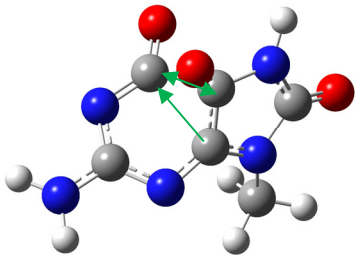


C1	-0.846542	1.670544	-0.420385
C2	0.091054	0.768930	0.419469
C3	-1.863824	-0.317682	-0.822793
C4	2.326464	0.225637	0.241165
N5	-1.896479	1.021948	-0.953880
N6	1.447382	1.216217	0.565246
N7	1.597959	-0.816835	-0.367444
N8	-0.682536	-1.056993	-1.009471
C9	0.292001	-0.484711	-0.403134
N10	-2.918989	-1.031531	-0.467194
O11	-0.661051	2.895427	-0.485459
H12	-1.022824	-0.414194	1.671169
O13	-0.507238	0.479069	1.660777
O14	3.537284	0.218655	0.399504
C15	2.209226	-1.957505	-1.026606
H16	3.187409	-2.128484	-0.579184
H17	1.581247	-2.834578	-0.868654
H18	2.320232	-1.770054	-2.096967
H19	1.705091	1.926150	1.238432
H20	-3.723418	-0.439063	-0.279594
O21	-1.901853	-1.721652	1.729947
H22	-2.556482	-1.590811	0.467083
H23	-1.310024	-2.481895	1.712462

[5-OH9MOG – H_{O6}]$^-$

C1	1.244930	-1.313892	-0.352922
C2	0.001286	-0.854382	0.407806
C3	2.030232	0.845029	-0.097864
C4	-2.192511	-0.336743	-0.128016
N5	2.276832	-0.431008	-0.407069
N6	-1.282703	-1.347470	-0.119159
N7	-1.494699	0.884703	0.009668
N8	0.790179	1.470443	-0.004539
C9	-0.178711	0.624380	0.118211
N10	3.064312	1.666069	0.048893
H11	2.910720	2.646081	0.236244
H12	4.006205	1.310718	-0.026828
O13	1.345455	-2.475580	-0.773502
H14	-1.606022	-2.264617	0.165405
O15	0.189728	-1.089213	1.735898
O16	-3.407004	-0.415274	-0.267313
C17	-2.087039	2.187948	-0.238639
H18	-1.847613	2.533321	-1.247131
H19	-3.166662	2.099668	-0.127516
H20	-1.708633	2.902176	0.493141

TS3c$^-$



C1	0.227571	-0.958919	-0.778596
C2	0.002686	0.445368	-0.589371
C3	-2.134550	0.486613	-0.003366
C4	-0.675098	-0.981575	0.912019
C5	2.174527	0.068033	-0.115110
N6	-1.901650	-0.493429	0.925753
N7	-1.177718	1.072219	-0.714002
O8	-0.113240	-1.748546	1.682865
N9	1.183847	1.043837	-0.222134
N10	-3.402542	0.902050	-0.131543
H11	-4.108632	0.543149	0.491989
H12	-3.612727	1.698628	-0.713572
O13	3.314660	0.258387	0.312395
N14	1.626792	-1.098026	-0.546660

O15	-0.431561	-1.815400	-1.473881
H16	2.085712	-1.989007	-0.413359
C17	1.281139	2.320070	0.470686
H18	1.089907	2.194278	1.539890
H19	2.279819	2.728563	0.320937
H20	0.548297	3.004761	0.045623

[9MSp – H]$^-$

C1	-0.620417	1.470337	-0.173450
C2	0.107909	0.126255	-0.205701
C3	2.246850	-0.149230	-0.349070
C4	0.759041	-0.128345	1.193836
C5	-2.188794	-0.185335	-0.303609
N6	2.068466	-0.281006	1.019016
N7	1.202185	0.064195	-1.125545
O8	0.097693	-0.173888	2.248843
N9	-0.992173	-0.797392	-0.458204
N10	3.504205	-0.216351	-0.831246
H11	4.234029	-0.561742	-0.227475
H12	3.641342	-0.290940	-1.827895
O13	-3.304428	-0.699325	-0.280922
N14	-1.950549	1.189279	-0.192005
O15	-0.105486	2.576610	-0.117414
H16	-2.694581	1.875890	-0.161485
C17	-0.830036	-2.230062	-0.282222
H18	-0.834198	-2.504452	0.777806
H19	-1.638797	-2.750627	-0.795099
H20	0.117714	-2.528093	-0.732730

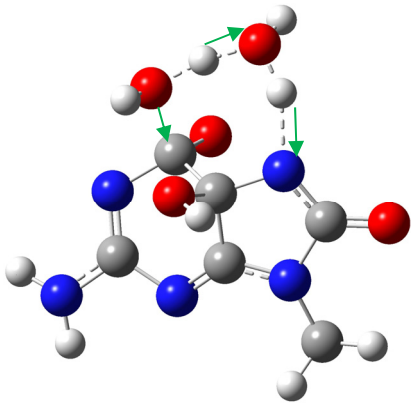
[5-OH9MOG – H_{N7}]$^-$

C1	1.194492	-1.302841	-0.416379
C2	-0.058036	-0.857750	0.349624
C3	1.993427	0.858163	-0.118923
C4	-2.168844	-0.418530	-0.121370
N5	2.220157	-0.419999	-0.466448
N6	-1.312760	-1.420198	-0.016197
N7	-1.509509	0.876562	0.051412
N8	0.773659	1.485018	0.043665
C9	-0.210262	0.637915	0.148619
N10	3.050145	1.655557	-0.004963
H11	2.926560	2.632869	0.216000
H12	3.978808	1.284418	-0.142500
O13	1.281702	-2.449595	-0.873539
H14	1.054209	-0.836156	2.010641
O15	0.173555	-1.134356	1.741567
O16	-3.390045	-0.442357	-0.363568
C17	-2.117669	2.158408	-0.246102
H18	-1.732730	2.913959	0.440323
H19	-1.904767	2.457962	-1.276048
H20	-3.194280	2.066647	-0.109193

[5-OH9MOG – H_{N7}]$^-$·2H_2O

C1	0.183671	0.130824	0.144620
C2	-1.158164	-0.572236	0.164614
C3	-2.183640	1.383917	-0.128050
C4	0.041526	1.358726	-0.766632
C5	0.510807	-2.048925	-0.128771
N6	-1.146701	2.000003	-0.718909
N7	-2.306991	0.035581	0.158338
O8	1.000093	1.759610	-1.436260
N9	-0.908645	-1.875037	0.160628
N10	-3.268687	2.105465	0.125134
H11	-3.285613	3.090446	-0.095827
H12	-4.089614	1.664041	0.513342
O13	0.966460	-3.191417	-0.291239
N14	1.131037	-0.877388	-0.198350
O15	0.424898	0.711878	1.435319
H16	0.558611	-0.012740	2.063755
H17	3.429559	1.233890	0.681089
O18	3.095946	1.822459	1.386358
H19	2.160397	1.568208	1.457322
H20	3.703728	0.444233	-1.458595
O21	3.720256	-0.052957	-0.633072
H22	2.790673	-0.390351	-0.518372
C23	-1.895871	-2.934817	0.140652
H24	-2.603305	-2.791853	0.959005
H25	-2.434713	-2.942378	-0.810542
H26	-1.381013	-3.885368	0.273479

TS3d$^-$ (water-assisted addition)



C1	-0.107482	-0.348918	0.477779
C2	-0.083965	1.125414	0.140048
C3	2.151031	1.001025	-0.066238
C4	0.946172	-0.952784	-0.497597
C5	-2.197437	0.343785	0.066383
N6	2.217819	-0.276537	-0.279847
N7	0.993156	1.810551	-0.054038
O8	0.561796	-1.049674	-1.736654
N9	-1.360995	1.519686	0.034917
N10	3.288598	1.721779	0.157537
H11	4.163751	1.280410	-0.085656

H12	3.232703	2.717237	-0.001185
O13	-3.420759	0.442669	-0.130705
N14	-1.478286	-0.746176	0.316811
O15	0.363703	-0.569086	1.803511
H16	-0.320720	-0.269507	2.415153
H17	0.086606	-2.927345	-0.027049
O18	1.186316	-2.397647	0.026895
H19	1.450281	-2.359223	0.960432
H20	-1.290058	-3.526502	-0.952037
O21	-1.073988	-3.226514	-0.058230
H22	-1.478187	-2.261918	0.057827
C23	-1.810548	2.836302	-0.363611
H24	-1.296977	3.593623	0.230936
H25	-1.610767	3.011986	-1.424803
H26	-2.881850	2.909199	-0.180399

[*gem*-9Mdiol – H]$^-$

C1	-0.078234	-0.716028	0.472593
C2	-0.378124	0.742014	0.165644
C3	1.819727	1.160292	-0.002275
C4	1.153417	-1.055595	-0.386522
C5	-2.237932	-0.512558	0.022480
N6	2.193500	-0.073918	-0.209794
N7	0.512352	1.669210	0.009866
N8	-1.703169	0.840875	0.053914
N9	2.754875	2.116866	0.200105
H10	3.726962	1.897284	0.046063
H11	2.471148	3.083601	0.170182
O12	-3.458014	-0.675600	-0.191757
N13	-1.299633	-1.419953	0.231114
O14	0.360547	-0.845073	1.822661
O15	0.717241	-1.110167	-1.721093
H16	1.494712	-0.968600	-2.277279
H17	2.060938	-2.296185	0.796784
O18	1.658793	-2.335289	-0.080713
C19	-2.429506	2.028576	-0.343614
H20	-2.121960	2.872128	0.276823
H21	-2.242942	2.264216	-1.395713
H22	-3.493707	1.848313	-0.196375
H23	-0.425259	-0.783482	2.380478

LysNH_2

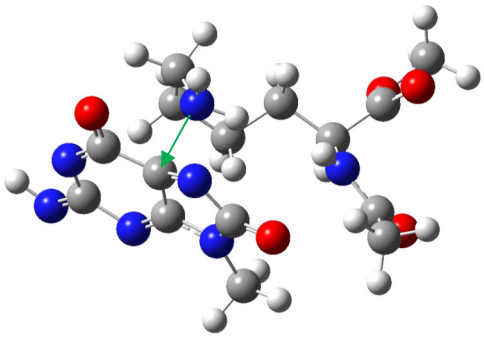
C1	-0.472120	-0.351185	-0.516146
H2	-0.742063	-0.358051	-1.577699
C3	0.439716	-1.549790	-0.210453
H4	0.651786	-1.543678	0.864183
H5	-0.130400	-2.461366	-0.409742
C6	-1.752634	-0.515329	0.287912
O7	-2.710405	-1.096955	-0.430093
O8	-1.877836	-0.224631	1.465315
N9	0.193181	0.891772	-0.179982
H10	1.208859	0.874215	0.032278
C11	1.745224	-1.545450	-1.031900
H12	1.714083	-2.354747	-1.767425
H13	1.818141	-0.620220	-1.613173
C14	3.018879	-1.702933	-0.191200
H15	3.881991	-1.676747	-0.868515
H16	3.028493	-2.688097	0.290312
C17	3.215448	-0.648234	0.897105
H18	2.478974	-0.781648	1.696894
H19	4.203212	-0.800040	1.352922
N20	3.051696	0.713031	0.367346
H21	3.319095	1.392228	1.074006
H22	3.682728	0.848862	-0.419088
C23	-0.435997	2.068934	-0.300910
C24	0.351791	3.302139	0.045509
H25	1.393265	3.083577	0.288815
H26	0.313865	3.998414	-0.796028
H27	-0.122200	3.787330	0.903569
O28	-1.629298	2.143657	-0.661741
C29	-3.936502	-1.402060	0.257444
H30	-4.392542	-0.485992	0.636957
H31	-4.580088	-1.863762	-0.488753
H32	-3.743840	-2.097025	1.076917

weak complex

C1	4.07773300	0.54737700	-0.80559800
C2	3.09666700	-0.55358700	-0.59714400
C3	3.53841400	1.26484800	1.39663300
C4	1.92464900	-2.36481100	-0.52564000
N5	4.25206700	1.38139400	0.21358300
N6	2.88154200	-1.62658100	-1.28249000
N7	1.64539800	-1.71218300	0.66926500
N8	2.60745600	0.22343800	1.68031800
C9	2.41674800	-0.58390800	0.71003000
N10	3.69305900	2.11123900	2.35794700
O11	4.68958000	0.62870000	-1.89937300
O12	1.43830300	-3.42386300	-0.87898700
C13	0.75555300	-2.18058400	1.71393300
H14	1.30077400	-2.26351400	2.65622800
H15	-0.08158700	-1.48885300	1.83377900
H16	0.38058000	-3.16237500	1.42841800
H17	4.37675900	2.80617300	2.05706600
C18	-2.80354300	0.46243800	0.27009200
H19	-2.89718400	0.48281000	1.36047700
C20	-1.88781300	1.60804600	-0.18339400
H21	-1.71305700	1.49740000	-1.26088600
H22	-2.41064500	2.55820400	-0.03844400
C23	-4.19938600	0.64955400	-0.30932800
O24	-4.90906900	1.50760200	0.41706000
O25	-4.61367900	0.11730500	-1.32386000
N26	-2.24536200	-0.80718000	-0.13827500
H27	-1.49771600	-0.80937400	-0.81978400
C28	-0.57067500	1.61861900	0.59309000
H29	-0.78045600	1.86834600	1.63937700
H30	-0.14129500	0.61028300	0.60474100

C31	0.46398400	2.60083800	0.04086400
H32	1.34114800	2.58586400	0.69555600
H33	0.06172500	3.62076900	0.07541600
C34	0.90555700	2.31547100	-1.39466800
H35	0.09948500	2.58046500	-2.09435500
H36	1.75715200	2.95810000	-1.63908800
N37	1.33293000	0.92515700	-1.57312900
H38	1.72804200	0.79701300	-2.50015700
H39	0.54288700	0.28749400	-1.49841300
C40	-2.70272400	-1.98148500	0.33122700
C41	-2.06473200	-3.22634900	-0.21632900
H42	-1.15965200	-3.01999500	-0.79025600
H43	-1.82848500	-3.89990500	0.61014200
H44	-2.79190500	-3.72613000	-0.86354200
O45	-3.62820700	-2.02931100	1.16217800
C46	-6.22435800	1.83549300	-0.06647000
H47	-6.84461200	0.93817500	-0.10209900
H48	-6.62652000	2.54698600	0.65192700
H49	-6.15693100	2.28986500	-1.05657400

TS4a$^-$



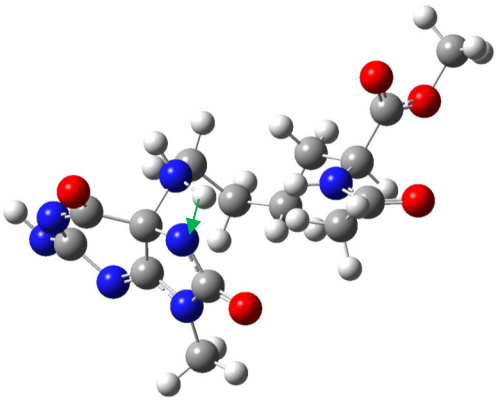
C1	-3.941768	-0.650658	-0.874535
C2	-2.884287	0.398321	-0.737041
C3	-3.552226	-1.178721	1.410735
C4	-1.880935	2.310432	-0.699171
N5	-4.210054	-1.375545	0.204979
N6	-2.713143	1.485439	-1.460616
N7	-1.648293	1.752430	0.567127
N8	-2.662098	-0.098883	1.669015
C9	-2.371979	0.600117	0.639086
N10	-3.748250	-1.964809	2.415464
O11	-4.513564	-0.801654	-1.983311
O12	-1.429506	3.390242	-1.058492
C13	-0.918989	2.373962	1.653334
H14	-1.579690	2.534666	2.508434
H15	-0.079732	1.741810	1.953882
H16	-0.542666	3.334941	1.305436
H17	-4.404299	-2.688977	2.122808
C18	2.797461	-0.468920	0.308035
H19	2.945387	-0.497866	1.392016
C20	1.827599	-1.586723	-0.101376
H21	1.615798	-1.479236	-1.172694
H22	2.323598	-2.552587	0.032582
C23	4.157700	-0.689757	-0.340989
O24	4.868253	-1.591413	0.329254
O25	4.545076	-0.142659	-1.358132
N26	2.253717	0.818604	-0.061830
H27	1.509319	0.848325	-0.746341
C28	0.543832	-1.545282	0.727698
H29	0.789824	-1.775310	1.770259
H30	0.142298	-0.525230	0.734595
C31	-0.538066	-2.515799	0.250940
H32	-1.388348	-2.452400	0.935147
H33	-0.165355	-3.544830	0.312163
C34	-1.016462	-2.291810	-1.182737
H35	-0.259048	-2.644788	-1.894343
H36	-1.922410	-2.877028	-1.365084
N37	-1.331858	-0.886612	-1.474798
H38	-1.633704	-0.792231	-2.441587
H39	-0.516289	-0.286605	-1.357380
C40	2.732741	1.976850	0.426761
C41	2.097213	3.241073	-0.078498
H42	1.205772	3.056564	-0.680725
H43	1.837590	3.872868	0.773814
H44	2.834200	3.776443	-0.684480
O45	3.668876	1.997038	1.246639
C46	6.150254	-1.947130	-0.219926
H47	6.797292	-1.069090	-0.258936
H48	6.559254	-2.690607	0.461268
H49	6.025456	-2.371378	-1.217795

[5-LysNH$_2$-9MOG – H$_{N2}$]$^-$

C1	-3.781756	-0.752956	-0.900441
C2	-2.504603	0.094095	-0.857106
C3	-3.570313	-1.089259	1.433396
C4	-1.839575	2.206375	-0.879255
N5	-4.212795	-1.309762	0.220090
N6	-2.442442	1.290362	-1.638434
N7	-1.598701	1.723459	0.453415
N8	-2.684626	-0.005825	1.636403
C9	-2.241180	0.538972	0.563459
N10	-3.824208	-1.813975	2.470529
O11	-4.320063	-0.928993	-2.022738
O12	-1.518058	3.368995	-1.190951
C13	-1.186771	2.545631	1.569402
H14	-2.042210	2.815210	2.197007
H15	-0.450931	2.007628	2.172067
H16	-0.731464	3.452989	1.174761
H17	-4.495867	-2.530178	2.195006
C18	2.786944	-0.468753	0.344037
H19	2.966600	-0.501131	1.422950
C20	1.793349	-1.576426	-0.036925
H21	1.558567	-1.470930	-1.103711
H22	2.277776	-2.548804	0.089047

C23	4.125798	-0.700473	-0.344453
O24	4.839311	-1.622920	0.293181
O25	4.495202	-0.142055	-1.361977
N26	2.242696	0.824778	-0.003273
H27	1.506983	0.866073	-0.696455
C28	0.536208	-1.507264	0.830606
H29	0.805697	-1.764942	1.860159
H30	0.176792	-0.473012	0.875112
C31	-0.597637	-2.434783	0.391727
H32	-1.412855	-2.360264	1.114612
H33	-0.256953	-3.475473	0.421876
C34	-1.131031	-2.223916	-1.020811
H35	-0.417316	-2.582952	-1.764818
H36	-2.067436	-2.762301	-1.172910
N37	-1.371071	-0.793494	-1.416061
H38	-1.564916	-0.792439	-2.422447
H39	-0.501567	-0.258576	-1.317498
C40	2.718841	1.976459	0.504541
C41	2.064780	3.245951	0.036927
H42	1.207573	3.068956	-0.615418
H43	1.744324	3.818345	0.910719
H44	2.809139	3.839716	-0.501204
O45	3.658532	1.986964	1.320025
C46	6.103322	-1.986510	-0.291843
H47	6.759913	-1.115804	-0.334742
H48	6.519281	-2.744105	0.369277
H49	5.949243	-2.395616	-1.291942

TS4b$^-$



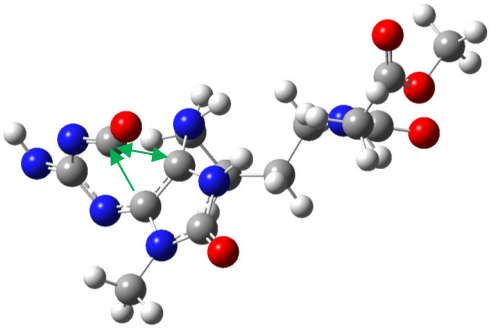
C1	3.491603	-0.069887	1.738618
C2	2.333748	0.175031	0.764227
C3	4.566701	-1.147854	-0.056717
C4	1.358045	1.910132	-0.324806
N5	4.490448	-0.817901	1.291355
N6	1.435578	1.318668	0.904897
N7	2.252350	1.304261	-1.231810
N8	3.945954	-0.335877	-1.041092
C9	2.920941	0.298570	-0.610368
N10	5.291506	-2.121338	-0.490555
O11	3.389883	0.352570	2.915558
O12	0.612531	2.836623	-0.649623
C13	2.490510	1.738704	-2.591659
H14	3.510863	2.115196	-2.700260
H15	2.335870	0.903427	-3.278694
H16	1.783071	2.533788	-2.823970
H17	5.697895	-2.594837	0.316296
C18	-2.989524	-0.324448	-0.420744
H19	-3.298889	-0.055844	-1.435759
C20	-1.842992	-1.343561	-0.487333
H21	-1.508240	-1.541349	0.537374
H22	-2.230809	-2.285018	-0.887999
C23	-4.190662	-0.952399	0.272089
O24	-4.936833	-1.637352	-0.588878
O25	-4.426299	-0.880532	1.465210
N26	-2.553096	0.863898	0.279222
H27	-1.652156	0.852256	0.739891
C28	-0.694127	-0.840980	-1.360743
H29	-1.041972	-0.769478	-2.397069
H30	-0.430683	0.180386	-1.068186
C31	0.556277	-1.720853	-1.331804
H32	1.323826	-1.256723	-1.958702
H33	0.336200	-2.690599	-1.792904
C34	1.117447	-2.042558	0.051830
H35	0.446261	-2.722129	0.580945
H36	2.079472	-2.556182	-0.044101
N37	1.277655	-0.882841	0.962598
H38	1.357077	-1.233248	1.918076
H39	0.647757	0.256007	0.985991
C40	-3.287108	1.990062	0.311595
C41	-2.688227	3.172956	1.018376
H42	-1.754982	2.932870	1.530443
H43	-2.498209	3.956564	0.279436
H44	-3.412985	3.557410	1.739937
O45	-4.405706	2.046688	-0.231322
C46	-6.063616	-2.350582	-0.047498
H47	-6.759641	-1.651439	0.419174
H48	-6.530971	-2.840302	-0.899414
H49	-5.724235	-3.090826	0.679251

[5-LysNH-9MOG – H_{N2}]$^-$

C1	-3.264449	0.056623	-1.782379
C2	-2.150299	0.201246	-0.735187
C3	-4.446479	-1.174798	-0.169614
C4	-1.347553	1.905575	0.609767
N5	-4.292815	-0.722362	-1.471098
N6	-1.484226	1.499470	-0.689625
N7	-2.194225	1.125653	1.396263
N8	-3.866369	-0.471841	0.921102
C9	-2.824819	0.200985	0.613601
N10	-5.209741	-2.167813	0.137498
O11	-3.093802	0.587501	-2.907782

O12	-0.643925	2.819476	1.028037
C13	-2.501629	1.386039	2.787506
H14	-3.509507	1.796328	2.889921
H15	-2.425717	0.456227	3.354634
H16	-1.774939	2.102022	3.169600
H17	-5.579945	-2.558708	-0.728873
C18	2.924573	-0.327473	0.403673
H19	3.235210	-0.015225	1.405929
C20	1.843123	-1.412981	0.517627
H21	1.506981	-1.665705	-0.493856
H22	2.292565	-2.314165	0.945350
C23	4.149860	-0.893147	-0.299319
O24	4.940061	-1.534496	0.556317
O25	4.370643	-0.812437	-1.494812
N26	2.399640	0.814585	-0.312592
H27	1.496556	0.728956	-0.760343
C28	0.673831	-0.947204	1.385086
H29	1.009498	-0.879865	2.426214
H30	0.390718	0.067718	1.093036
C31	-0.562703	-1.841784	1.320591
H32	-1.321117	-1.422934	1.990527
H33	-0.328033	-2.835626	1.721037
C34	-1.147977	-2.062118	-0.080059
H35	-0.522198	-2.778530	-0.619068
H36	-2.134774	-2.536204	0.019927
N37	-1.178138	-0.875103	-0.947502
H38	-1.259088	-1.186928	-1.909310
H39	-0.686270	1.647892	-1.295935
C40	3.037530	1.996703	-0.361492
C41	2.338671	3.115820	-1.081410
H42	1.399505	2.803609	-1.542279
H43	2.136814	3.916229	-0.364385
H44	3.006973	3.511663	-1.850212
O45	4.150917	2.154285	0.172268
C46	6.097654	-2.189130	0.006138
H47	6.752766	-1.455680	-0.467167
H48	6.596820	-2.652902	0.854524
H49	5.791135	-2.947063	-0.716967

TS4c⁻



C1	3.401511	0.099544	1.661311
C2	1.776880	-0.014567	0.265789
C3	4.217335	-1.696442	0.415685
C4	2.091809	2.007053	-0.720645
N5	4.141819	-0.938249	1.618104
N6	1.278946	1.276583	0.098852
N7	3.059638	1.139453	-1.171081
N8	3.752295	-1.133718	-0.729025
C9	2.920792	-0.103027	-0.537487
N10	4.808380	-2.855640	0.428258
O11	3.140471	1.055072	2.360093
O12	1.981915	3.211273	-0.994519
C13	4.268459	1.564267	-1.850456
H14	5.114754	1.568073	-1.158233
H15	4.484075	0.894686	-2.683468
H16	4.109529	2.571018	-2.235134
H17	5.134237	-3.034279	1.375679
C18	-3.178161	-0.201480	-0.458654
H19	-3.460836	0.132264	-1.462035
C20	-2.174128	-1.359065	-0.566535
H21	-1.860608	-1.625572	0.449968
H22	-2.686333	-2.232471	-0.981351
C23	-4.443258	-0.682692	0.237970
O24	-5.271945	-1.267355	-0.621418
O25	-4.661946	-0.588727	1.432882
N26	-2.580623	0.900684	0.262967
H27	-1.702449	0.744689	0.739980
C28	-0.977723	-0.989725	-1.445967
H29	-1.318764	-0.898833	-2.483316
H30	-0.603578	-0.000904	-1.161951
C31	0.183012	-1.984111	-1.386203
H32	0.982420	-1.615398	-2.039725
H33	-0.126065	-2.956677	-1.788824
C34	0.747704	-2.230335	0.016975
H35	0.058556	-2.837588	0.608141
H36	1.675202	-2.803868	-0.066009
N37	1.009034	-1.028721	0.824166
H38	0.164180	-0.654517	1.239348
H39	0.510598	1.681201	0.617508
C40	-3.155795	2.113845	0.338038
C41	-2.411000	3.175500	1.097883
H42	-1.463475	2.820517	1.507979
H43	-2.219564	4.015228	0.424717
H44	-3.045686	3.534168	1.912408
O45	-4.252680	2.343364	-0.203023
C46	-6.471684	-1.845972	-0.076024
H47	-7.077125	-1.072771	0.400120
H48	-6.999102	-2.271385	-0.927416
H49	-6.217415	-2.626098	0.643742

[5-LysNH-9MSp – H_{N2}]⁻

C1	3.901394	-1.002141	0.993727
C2	2.093741	0.663101	0.330049
C3	3.822857	-1.942852	-0.983979
C4	3.657228	2.306378	0.408260

N5	4.159069	-2.137423	0.385470
N6	2.298714	1.959196	0.581011
N7	4.277897	1.219995	-0.067135
N8	3.387650	-0.695307	-1.298735
C9	3.408718	0.024784	-0.084308
N10	3.921687	-2.911781	-1.861178
O11	4.016773	-0.691757	2.206964
O12	4.107707	3.421448	0.656468
C13	5.717988	1.105572	-0.173443
H14	6.164422	0.819668	0.784234
H15	5.949529	0.347946	-0.923709
H16	6.134193	2.059171	-0.499091
H17	4.264385	-3.738136	-1.376111
C18	-3.732510	-0.272252	-0.423749
H19	-4.126123	-0.625192	-1.381803
C20	-2.414970	-0.995881	-0.116207
H21	-2.023779	-0.606831	0.832020
H22	-2.635480	-2.057072	0.037878
C23	-4.756986	-0.620878	0.649113
O24	-5.391501	-1.752404	0.357729
O25	-4.946996	0.019796	1.667608
N26	-3.522495	1.157676	-0.485896
H27	-2.634731	1.532118	-0.178066
C28	-1.385515	-0.849061	-1.238333
H29	-1.836896	-1.181331	-2.179697
H30	-1.124823	0.206692	-1.377753
C31	-0.112024	-1.664412	-1.001961
H32	0.571301	-1.525094	-1.844982
H33	-0.359404	-2.731389	-0.960278
C34	0.630827	-1.343805	0.291089
H35	0.036171	-1.617203	1.165697
H36	1.557736	-1.910590	0.344161
N37	0.934274	0.084587	0.444708
H38	0.149385	0.679894	0.698497
C39	-4.504783	2.007734	-0.838145
C40	-4.181425	3.474721	-0.813146
H41	-3.129053	3.672882	-0.602749
H42	-4.449390	3.912618	-1.777486
H43	-4.797117	3.950848	-0.044791
O44	-5.630930	1.590577	-1.163288
C45	-6.325625	-2.244578	1.335736
H46	-7.121281	-1.514533	1.494384
H47	-6.731417	-3.161038	0.912449
H48	-5.810509	-2.453762	2.274968
H49	1.601398	2.621874	0.902428

[5-LysNH-9MSp – H_{N3}]$^-$

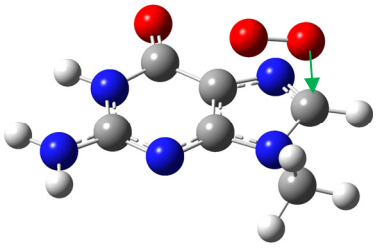
C1	3.947527	-0.909309	1.019632
C2	2.084525	0.738211	0.407791
C3	3.751855	-1.898654	-0.873936
C4	3.549455	2.334207	0.356047
N5	4.173323	-2.084070	0.433709
N6	2.224442	2.028587	0.637169
N7	4.203754	1.261204	-0.176972
N8	3.292864	-0.724689	-1.248948
C9	3.375696	0.073663	-0.055261
N10	3.776386	-2.965908	-1.704858
O11	4.152780	-0.579263	2.203839
O12	4.067655	3.445643	0.545709
C13	5.647276	1.177595	-0.268934
H14	6.111471	1.020987	0.711575
H15	5.910784	0.349194	-0.929778
H16	6.036452	2.098437	-0.704910
H17	4.348757	-3.753623	-1.440255
C18	-3.705478	-0.256987	-0.409561
H19	-4.062902	-0.593454	-1.387649
C20	-2.398945	-0.984424	-0.066374
H21	-2.036729	-0.602893	0.896296
H22	-2.624219	-2.046855	0.072224
C23	-4.771198	-0.625643	0.615233
O24	-5.397925	-1.747477	0.273086
O25	-4.999433	-0.007834	1.639947
N26	-3.494658	1.173970	-0.440367
H27	-2.618118	1.543349	-0.096038
C28	-1.335571	-0.828332	-1.154759
H29	-1.758619	-1.154397	-2.111731
H30	-1.073567	0.229145	-1.276975
C31	-0.066088	-1.639061	-0.883839
H32	0.641300	-1.480882	-1.703533
H33	-0.307386	-2.708676	-0.863226
C34	0.634737	-1.311497	0.433483
H35	0.009962	-1.597259	1.283746
H36	1.554404	-1.888314	0.521523
N37	0.935466	0.107549	0.597647
H38	0.158695	0.700813	0.867228
H39	3.661513	-2.793993	-2.692993
C40	-4.462970	2.029134	-0.817201
C41	-4.140012	3.495245	-0.763830
H42	-3.103352	3.690440	-0.484098
H43	-4.341343	3.937892	-1.742321
H44	-4.804904	3.969101	-0.036388
O45	-5.576679	1.616950	-1.188689
C46	-6.378062	-2.253405	1.197755
H47	-7.181561	-1.525875	1.325334
H48	-6.760047	-3.165113	0.743196
H49	-5.909319	-2.473123	2.158499

Cartesian coordinates for the structures in Fig. 4, optimized at SMD-ωB97XD/6-31+ G(d,p). For each TS, the vibrational mode corresponding to TS imaginary frequency is indicated by displacement vectors.

9MG

C1	-1.130432	1.366537	0.000875
C2	0.241414	0.997063	-0.001077
H3	-2.959548	0.438671	-0.004438
C4	-1.546751	-1.064071	-0.001877
C5	2.359148	0.896134	0.000086
N6	-1.963105	0.243970	0.000419
N7	1.385500	1.773749	-0.000548
N8	1.925935	-0.405795	0.000059
N9	-0.276917	-1.415763	0.000943
C10	0.562575	-0.354584	-0.000815
N11	-2.515236	-2.005900	-0.054389
H12	-2.233634	-2.954567	0.148069
H13	-3.461809	-1.753510	0.194714
O14	-1.629272	2.503642	0.003123
H15	3.414849	1.128636	0.000417
C16	2.757222	-1.598271	0.002873
H17	2.562901	-2.191816	0.897670
H18	2.558060	-2.199230	-0.885866
H19	3.801056	-1.286002	-0.001323

TS1 (open-shell)

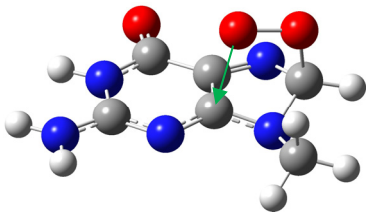


C1	0.032083	0.872266	-0.436413
C2	0.210123	-0.544415	-0.356655
C3	-1.937193	-0.957048	0.063092
C4	-1.300976	1.404796	-0.229445
C5	2.090588	0.508742	-0.656792
N6	-2.217524	0.392359	0.026130
N7	-0.725232	-1.469402	-0.132564
O8	-1.644787	2.580972	-0.265254
N9	1.508335	-0.750533	-0.659967
N10	-2.958283	-1.769437	0.312877
H11	-3.898807	-1.422297	0.437699
H12	-2.791231	-2.765352	0.337371
N13	1.163365	1.496915	-0.736905
H14	-3.175039	0.693067	0.188150
H15	3.118503	0.633908	-0.963124
O16	1.135117	0.314434	1.747346
O17	2.268672	0.688153	1.259029
C18	2.239658	-1.988487	-0.448595
H19	2.328924	-2.193000	0.621277
H20	1.714855	-2.807586	-0.939615
H21	3.230462	-1.881645	-0.888865

8-OO9MG

C1	-1.450682	1.480298	-0.105006
C2	-0.109610	0.871849	-0.278785
H3	-3.368030	0.866198	0.232606
C4	-2.201441	-0.843688	0.156671
C5	2.006837	0.390281	-0.612394
N6	-2.419700	0.519845	0.103899
N7	1.009074	1.456072	-0.451017
N8	1.251419	-0.874673	-0.447927
N9	-1.009608	-1.433944	-0.016483
C10	-0.009568	-0.597927	-0.234729
N11	-3.252852	-1.597693	0.393129
H12	-3.135321	-2.601971	0.429172
H13	-4.176152	-1.204949	0.525440
O14	-1.698293	2.668670	-0.138105
H15	2.387970	0.445345	-1.637967
O16	2.660228	0.439575	1.602473
O17	3.089472	0.491335	0.212332
C18	1.881606	-2.180882	-0.401300
H19	1.940539	-2.527991	0.632851
H20	1.303413	-2.887382	-0.998241
H21	2.885151	-2.092722	-0.815417

TS2



C1	-1.395695	1.385846	-0.179603
C2	0.006755	0.952357	-0.345583
C3	-1.857133	-1.022523	0.029683
C4	2.103484	0.665684	-0.336370
N5	-2.235727	0.313049	0.028309
N6	1.060048	1.654390	-0.556619
N7	1.556318	-0.607562	-0.750015
N8	-0.613304	-1.458307	-0.137104
C9	0.298657	-0.487948	-0.249950
N10	-2.836521	-1.895774	0.199862
H11	-2.615032	-2.881828	0.205231
H12	-3.801330	-1.607193	0.292767
O13	-1.798965	2.534761	-0.214076
H14	3.082407	0.909496	-0.732279

O15	1.004905	0.031056	1.568665
O16	2.214075	0.590227	1.113709
H17	-3.220526	0.534122	0.153001
C18	2.348239	-1.810764	-0.532083
H19	1.857579	-2.655067	-1.015676
H20	3.325673	-1.664153	-0.991704
H21	2.469558	-2.020205	0.534684

4,8-OO-9MG

C1	-1.450621	1.372863	-0.146483
C2	-0.021560	1.003510	-0.242667
C3	-1.794619	-1.063377	0.006591
C4	2.080411	0.762232	-0.254745
N5	-2.241967	0.266714	0.006010
N6	1.000738	1.754002	-0.406261
N7	1.577940	-0.454183	-0.841210
N8	-0.547238	-1.442997	-0.065643
C9	0.388234	-0.418340	-0.027893
N10	-2.778996	-1.962504	0.088417
H11	-2.542131	-2.943254	0.108014
H12	-3.752147	-1.694265	0.074487
O13	-1.892986	2.509844	-0.197009
H14	3.064659	1.096082	-0.564116
O15	2.130510	0.492070	1.171158
O16	0.950725	-0.306138	1.376104
H17	-3.240132	0.438216	0.087546
C18	2.444529	-1.625963	-0.671972
H19	1.984814	-2.481810	-1.165635
H20	3.395726	-1.420743	-1.165009
H21	2.631643	-1.873215	0.376496

8-H-8-OOH9MG

C1	-1.532661	1.438400	-0.128479
C2	-0.169773	0.858001	-0.318492
C3	-2.239144	-0.769677	0.178684
C4	1.941119	0.377420	-0.650750
N5	-2.514236	0.550101	0.119604
N6	0.948391	1.440836	-0.517093
N7	1.218232	-0.880239	-0.517782
N8	-1.041438	-1.427059	-0.022311
C9	-0.055402	-0.611445	-0.267178
N10	-3.256574	-1.569678	0.468414
H11	-3.116512	-2.568225	0.523850
H12	-4.173026	-1.179875	0.635008
O13	-1.712720	2.661431	-0.202793
H14	2.437592	0.450309	-1.621877
O15	2.474254	0.350964	1.587958
O16	2.993263	0.497999	0.267147
H17	2.437801	1.268822	1.902106
C18	1.859769	-2.181563	-0.473984
H19	1.955384	-2.526463	0.558549
H20	1.267682	-2.896492	-1.047183
H21	2.848640	-2.095769	-0.923581

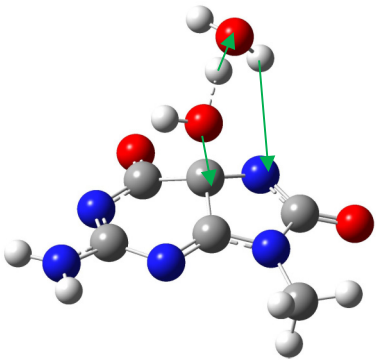
8-OOH9MG

C1	-1.491802	1.502970	-0.015551
C2	-0.224219	0.865433	-0.105411
C3	-2.374318	-0.796945	0.099522
C4	1.808994	0.351890	-0.268097
N5	-2.525697	0.568645	0.086033
N6	1.040667	1.403190	-0.222096
N7	1.145399	-0.849558	-0.183209
N8	-1.199269	-1.394798	0.030153
C9	-0.174440	-0.523245	-0.074345
N10	-3.503012	-1.529537	0.152351
H11	-3.408886	-2.520030	0.322988
H12	-4.382320	-1.092798	0.388602
O13	-1.748037	2.715827	-0.019603
H14	3.928697	1.109129	1.140014
O15	3.151264	0.396674	-0.439496
O16	3.783475	0.193007	0.848774
H17	-3.461719	0.957335	0.151233
C18	1.713405	-2.188069	-0.215897
H19	1.216325	-2.774915	-0.989096
H20	2.773851	-2.107866	-0.448737
H21	1.588098	-2.672712	0.753635

9MOG^{ox}

C1	1.366246	1.418465	-0.005306
C2	-0.042711	0.918912	-0.008393
C3	1.989472	-0.828454	0.004111
C4	-2.170404	0.527968	0.004456
N5	2.325627	0.466716	0.004816
N6	-1.149277	1.557580	0.005670
N7	-1.571514	-0.732983	-0.038393
N8	0.712490	-1.415132	-0.017134
C9	-0.232510	-0.548002	-0.023577
N10	2.962706	-1.718533	0.026361
H11	2.747519	-2.706397	0.026404
H12	3.927114	-1.414151	0.044691
O13	1.595988	2.629737	-0.009841
O14	-3.353627	0.751804	0.038051
C15	-2.276930	-2.004508	-0.000842
H16	-1.908407	-2.647631	-0.800422
H17	-2.127567	-2.486354	0.966745
H18	-3.336760	-1.807623	-0.155024

TS3a (water-assisted addition)

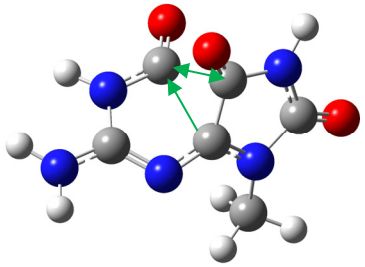


C1	-0.201119	0.485214	0.013710
C2	0.191336	-0.961985	-0.188853
C3	2.356128	-0.431138	-0.029932
C4	0.914898	1.201710	0.783319
C5	-1.969919	-0.770360	0.381273
N6	2.171940	0.741651	0.602550
N7	1.409703	-1.396049	-0.321933
O8	0.657871	2.209186	1.453147
N9	-1.513975	0.467269	0.544583
N10	-0.935322	-1.658461	-0.141464
N11	3.601448	-0.764119	-0.342974
H12	4.364391	-0.141926	-0.118200
H13	3.791821	-1.654354	-0.779491
O14	-1.727268	3.105064	-0.966629
H15	-2.281118	2.802511	-0.223256
H16	-1.228793	3.881457	-0.659519
O17	-0.271948	1.123797	-1.305396
H18	-1.054880	2.316892	-1.164142
H19	0.603703	1.287804	-1.690049
O20	-3.091300	-1.234702	0.634862
C21	-1.056618	-3.100907	-0.217557
H22	-2.098409	-3.347139	-0.418947
H23	-0.435140	-3.472882	-1.032819
H24	-0.745216	-3.566351	0.721458

5-OH9MOG

C1	1.255012	-1.302843	-0.396633
C2	-0.010686	-0.839311	0.335534
C3	2.031697	0.859953	-0.112548
C4	-2.195484	-0.323543	-0.141278
N5	2.274934	-0.417638	-0.434032
N6	-1.269046	-1.332236	-0.129154
N7	-1.500670	0.898640	-0.005062
N8	0.788095	1.483382	-0.017885
C9	-0.184084	0.647506	0.096857
N10	3.061868	1.672130	0.050181
H11	2.910993	2.651119	0.249362
H12	4.003889	1.313695	-0.021317
O13	1.328918	-2.455591	-0.827954
H14	-1.564982	-2.275783	0.091598
H15	0.960909	-0.861773	2.064225
O16	0.095433	-1.123342	1.718290
O17	-3.399192	-0.422986	-0.289009
C18	-2.101062	2.205218	-0.220706
H19	-1.773455	2.618942	-1.176546
H20	-3.182861	2.082530	-0.224275
H21	-1.814379	2.874796	0.590653

TS3b



C1	0.270653	-0.949591	-0.814160
C2	0.046624	0.460192	-0.523034
C3	-2.132186	0.551633	-0.075561
C4	-0.635986	-0.994072	0.883370
C5	2.221799	0.038483	-0.110748
N6	-1.908219	-0.510103	0.788030
N7	-1.114921	1.119622	-0.676143
O8	-0.223864	-1.769438	1.712820
N9	1.225541	1.026968	-0.155206
N10	-3.379586	0.985552	-0.206863
H11	-4.143177	0.547273	0.288072
H12	-3.564205	1.790807	-0.787799
O13	3.366910	0.214420	0.282599
N14	1.650732	-1.113588	-0.557800
O15	-0.407923	-1.740119	-1.528429
H16	2.133436	-2.002575	-0.573088
H17	-2.627583	-0.805875	1.443300
C18	1.363556	2.297887	0.544172
H19	1.188085	2.165644	1.614335
H20	2.370226	2.678103	0.377266
H21	0.640651	3.001371	0.133631

9MSp

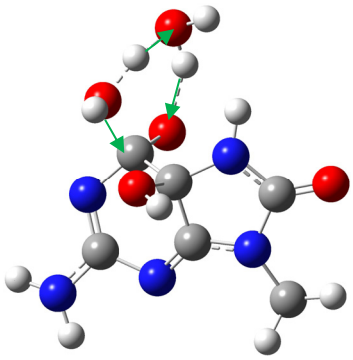
C1	-0.653471	1.478850	-0.141064
C2	0.068841	0.118736	-0.188150
C3	2.228522	-0.130786	-0.458636
C4	0.720052	-0.140238	1.197818
C5	-2.227485	-0.171388	-0.302805
N6	2.040653	-0.258330	0.921341
N7	1.141055	0.073942	-1.144713
O8	0.158171	-0.221441	2.275054
N9	-1.028853	-0.794614	-0.433889
N10	3.465519	-0.219216	-0.945047

H11	4.250092	-0.407192	-0.338968
H12	3.615733	-0.154956	-1.940758
O13	-3.341053	-0.679435	-0.306326
N14	-1.980959	1.201943	-0.180964
O15	-0.119602	2.570274	-0.069044
H16	-2.721285	1.893680	-0.163627
H17	2.767731	-0.451062	1.601189
C18	-0.877194	-2.233413	-0.287401
H19	-0.881491	-2.528609	0.766518
H20	-1.693692	-2.732637	-0.808460
H21	0.065297	-2.531046	-0.749035

5-OH9MOG·2H2O

C1	0.160723	0.085297	0.207981
C2	-1.278398	-0.382150	0.117614
C3	-1.932749	1.745226	-0.062772
C4	0.281525	1.381788	-0.605973
C5	0.040970	-2.176282	-0.208739
N6	-0.773965	2.211795	-0.549627
N7	-2.292650	0.409293	0.092851
O8	1.331729	1.649811	-1.200642
N9	-1.276693	-1.723266	0.041407
N10	-2.894271	2.609538	0.205308
H11	-2.734460	3.599867	0.081196
H12	-3.797919	2.281840	0.517669
O13	0.347394	-3.341743	-0.377215
N14	0.850895	-1.077810	-0.263616
O15	0.502906	0.458298	1.525930
H16	0.264995	-0.251928	2.141501
H17	1.855702	-1.173307	-0.173012
H18	3.653240	0.400431	0.775355
O19	3.437296	0.431787	1.727654
H20	2.470085	0.496662	1.744608
H21	2.935111	0.805626	-1.186041
O22	3.832735	0.437844	-1.061568
H23	3.784837	-0.466029	-1.393112
C24	-2.456615	-2.564218	-0.080564
H25	-2.902921	-2.447311	-1.070477
H26	-2.156046	-3.599491	0.071992
H27	-3.175055	-2.279142	0.687517

TS3c (water-assisted addition)



C1	0.060446	-0.256356	0.660463
C2	-0.833767	0.837455	0.107200
C3	0.999327	2.103531	-0.194009
C4	1.318670	-0.213952	-0.253591
C5	-2.047491	-1.058297	0.134683
N6	1.853103	1.129330	-0.252856
N7	-0.414010	1.999407	-0.229850
O8	1.128640	-0.751578	-1.443269
N9	-2.088486	0.340333	-0.017546
N10	1.417572	3.390300	-0.134197
H11	2.394554	3.585860	-0.295869
H12	0.751769	4.119598	-0.340115
O13	-2.985388	-1.808321	-0.092882
N14	-0.804066	-1.394956	0.571176
O15	0.481130	0.010896	1.978597
H16	-0.284410	0.010388	2.568853
H17	-0.479298	-2.351970	0.550152
H18	2.229226	-2.174605	0.041526
O19	2.369856	-1.051056	0.477095
H20	2.249987	-0.981538	1.438985
H21	1.430588	-2.307090	-1.289656
O22	1.935886	-3.020572	-0.759634
H23	1.290994	-3.641334	-0.392715
C24	-3.211354	1.050376	-0.603357
H25	-3.054557	1.200135	-1.674339
H26	-4.113383	0.462097	-0.442229
H27	-3.320240	2.016062	-0.109266

***gem*-9Mdiol**

C1	-0.033625	-0.705369	0.466121
C2	-0.364872	0.742974	0.143876
C3	1.836811	1.178640	0.006687
C4	1.207075	-1.042137	-0.385625
C5	-2.281246	-0.436163	-0.001595
N6	2.227341	-0.050834	-0.185752
N7	0.510342	1.665094	-0.018297
N8	-1.708449	0.850359	0.028336
N9	2.739191	2.153360	0.213185
H10	3.725045	1.943954	0.182487

H11	2.437732	3.113543	0.266453
O12	-3.472952	-0.660140	-0.147808
N13	-1.275328	-1.345052	0.131458
O14	0.340350	-0.888185	1.807986
H15	-1.474996	-2.304041	0.384791
O16	0.765796	-1.095039	-1.715000
H17	1.542055	-0.975715	-2.278565
H18	2.197644	-2.261283	0.757832
O19	1.704702	-2.317828	-0.071047
H20	-0.379079	-0.603832	2.388281
C21	-2.426196	2.060441	-0.333796
H22	-2.222836	2.326842	-1.373570
H23	-3.491560	1.877441	-0.202212
H24	-2.116541	2.871823	0.324948

$LysNH_3^+$

N1	-5.541400	-0.702935	0.108660
C2	-4.272147	-0.003797	-0.255529
H3	-4.264558	0.940959	0.289215
H4	-4.323904	0.203849	-1.325077
C5	-3.070358	-0.863022	0.093342
H6	-3.130755	-1.812362	-0.452142
H7	-3.089524	-1.096160	1.164942
C8	-1.765931	-0.147443	-0.253752
H9	-1.746221	0.081467	-1.326110
H10	-1.730488	0.809763	0.280285
C11	-0.551585	-0.999242	0.109454
H12	-0.639793	-1.982122	-0.365948
H13	-0.517709	-1.160076	1.193796
C14	0.784878	-0.395462	-0.343073
H15	0.777437	-0.259263	-1.427951
C16	0.986957	0.974213	0.295589
N17	1.864751	-1.286167	0.029386
O18	1.372587	1.148694	1.438556
O19	0.640396	1.958733	-0.525983
H20	-6.357708	-0.136636	-0.131122
H21	-5.620978	-1.595325	-0.385360
H22	1.653806	-2.079091	0.620822
C23	0.712371	3.296123	0.000711
H24	0.370254	3.942923	-0.804604
H25	0.060488	3.392383	0.870837
H26	1.743085	3.534657	0.268882
C27	3.150678	-0.998068	-0.246706
C28	4.190781	-1.944943	0.279325
H29	4.886300	-2.195255	-0.524579
H30	4.753351	-1.432407	1.065487
H31	3.760662	-2.859590	0.690868
O32	3.454128	0.019563	-0.894642
H33	-5.577956	-0.900073	1.111814

Weak Complex of 9MOGOX with $LysNH_3^+$

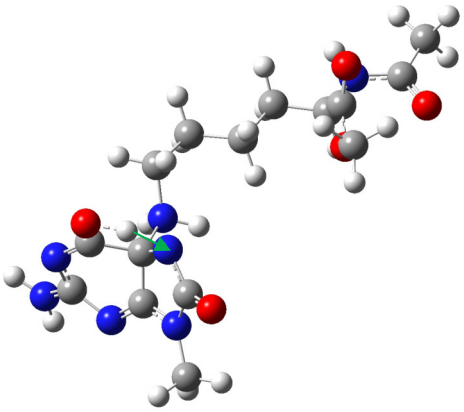
C1	3.989202	1.160689	-0.146511
C2	3.049945	0.107871	-0.640893
C3	4.848801	-0.491651	1.252521
C4	1.577402	-1.178890	-1.572116
N5	4.859642	0.771866	0.801703
N6	2.124801	0.164577	-1.519316
N7	2.261135	-1.999902	-0.672123
N8	4.034564	-1.565173	0.859467
C9	3.190273	-1.241202	-0.050355
N10	5.709577	-0.811442	2.196399
H11	5.737563	-1.753201	2.564311
H12	6.346089	-0.113443	2.558513
O13	3.942825	2.306879	-0.610909
O14	0.678421	-1.509167	-2.300793
C15	1.992387	-3.411031	-0.440059
H16	2.923538	-3.972271	-0.524546
H17	1.557123	-3.552226	0.550531
H18	1.294082	-3.752141	-1.202505
N19	1.259507	3.128247	-1.160838
C20	0.858626	3.103137	0.277289
H21	1.310278	3.982380	0.736346
H22	1.311951	2.210607	0.713579
C23	-0.648901	3.098102	0.452251
H24	-1.084759	3.948198	-0.086932
H25	-0.841439	3.267051	1.517212
C26	-1.318547	1.791976	0.022702
H27	-1.196792	1.626086	-1.054770
H28	-0.817888	0.958210	0.531823
C29	-2.806020	1.805620	0.365922
H30	-3.286897	2.664690	-0.114579
H31	-2.932166	1.922576	1.449168
C32	-3.563556	0.549529	-0.081722
H33	-3.500858	0.445840	-1.168511
C34	-2.925803	-0.686877	0.541457
N35	-4.950559	0.660493	0.321902
O36	-3.071726	-1.023201	1.704120
O37	-2.139099	-1.324267	-0.317565
H38	2.285191	3.029792	-1.227230
H39	0.857509	2.342844	-1.677122
H40	-5.229535	1.455718	0.880933
C41	-1.405016	-2.452307	0.191958
H42	-0.884744	-2.867548	-0.667288
H43	-0.695536	-2.120687	0.952180
H44	-2.092754	-3.188759	0.611186
C45	-5.845299	-0.312619	0.069185
C46	-7.239418	-0.113112	0.591148
H47	-7.948613	-0.240245	-0.230206
H48	-7.443916	-0.887948	1.335321
H49	-7.382701	0.867923	1.047373
O50	-5.518061	-1.335799	-0.558606
H51	0.961272	3.994925	-1.611794

5-$LysNH_2^+$-9MOG′

C1	-3.868775	-1.001801	0.976813
C2	-2.734943	-0.129328	0.461380

C3	-4.833376	-0.882297	-1.090167
C4	-2.084780	1.950479	0.751910
N5	-4.810766	-1.401660	0.194465
N6	-2.117135	0.765887	1.360633
N7	-2.805523	1.902360	-0.533989
N8	-4.253964	0.282433	-1.484412
C9	-3.340945	0.708757	-0.650596
N10	-5.572658	-1.529234	-1.954862
H11	-5.658041	-1.188618	-2.904430
H12	-6.072897	-2.363701	-1.675952
O13	-3.885873	-1.358087	2.233870
O14	-1.583520	3.012050	1.119099
C15	-3.093227	3.063327	-1.355781
H16	-3.109883	2.765962	-2.404298
H17	-4.057855	3.493510	-1.076619
H18	-2.304174	3.796413	-1.195463
N19	-1.678719	-1.049470	-0.158196
C20	-1.018706	-1.993476	0.813395
H21	-1.701757	-2.832035	0.950258
H22	-0.914789	-1.448590	1.752375
C23	0.339612	-2.442102	0.300735
H24	0.226756	-3.038590	-0.610933
H25	0.742195	-3.106746	1.072442
C26	1.299515	-1.273999	0.065598
H27	1.045107	-0.753481	-0.866452
H28	1.180604	-0.548326	0.880457
C29	2.755010	-1.726528	-0.009417
H30	2.858061	-2.547800	-0.726555
H31	3.073152	-2.099404	0.971382
C32	3.709705	-0.606816	-0.451420
H33	3.483154	-0.321797	-1.482590
C34	3.496907	0.624172	0.422595
N35	5.076367	-1.072438	-0.363966
O36	3.980898	0.778402	1.530277
O37	2.653748	1.480751	-0.143438
H38	-3.154852	-0.949995	2.730361
H39	-0.970621	-0.415862	-0.547140
H40	5.256832	-1.971059	0.063023
C41	2.215700	2.593589	0.657401
H42	1.525522	3.148877	0.025488
H43	1.704988	2.229478	1.551105
H44	3.067465	3.217592	0.933134
C45	6.113423	-0.302383	-0.742282
C46	7.491239	-0.876661	-0.576504
H47	8.007242	-0.834791	-1.538881
H48	8.044797	-0.252494	0.130369
H49	7.479621	-1.906133	-0.214914
O50	5.929345	0.837435	-1.205752
H51	-2.048794	-1.591568	-0.948298

TS4



C1	3.849153	-0.670285	-1.219263
C2	2.832063	-0.021708	-0.294592
C3	4.732932	-1.621447	0.619688
C4	2.819818	2.174749	-0.001652
N5	4.681078	-1.558463	-0.756744
N6	2.461004	1.207421	-0.890529
N7	3.403648	1.575190	1.193769
N8	4.439655	-0.570965	1.468299
C9	3.616828	0.287888	0.942638
N10	5.248502	-2.698864	1.154242
H11	5.372706	-2.762701	2.156895
H12	5.547914	-3.465593	0.565098
O13	3.810692	-0.116416	-2.367548
O14	2.733745	3.384143	-0.112837
C15	4.062202	2.363374	2.223084
H16	4.078811	1.788762	3.148420
H17	5.082013	2.607285	1.916399
H18	3.491699	3.278552	2.372371
N19	1.649561	-0.903956	-0.019933
C20	0.939186	-1.393878	-1.257423
H21	1.585181	-2.154491	-1.698254
H22	0.859026	-0.543550	-1.935438
C23	-0.427605	-1.956296	-0.907800
H24	-0.325915	-2.725100	-0.132680
H25	-0.787786	-2.462543	-1.809388
C26	-1.439511	-0.891718	-0.483559
H27	-1.109673	-0.381057	0.429739
H28	-1.496653	-0.129720	-1.270054
C29	-2.816594	-1.501080	-0.232573
H30	-2.730934	-2.321316	0.488465
H31	-3.214454	-1.920561	-1.164426
C32	-3.831567	-0.500355	0.336144
H33	-3.467163	-0.112445	1.291580
C34	-3.985513	0.680616	-0.615231
N35	-5.104110	-1.161790	0.533754
O36	-4.660951	0.664335	-1.629503
O37	-3.242883	1.715105	-0.237912
H38	3.119159	0.807766	-2.024144

H39	1.004563	-0.348570	0.555892
H40	-5.212668	-2.112607	0.207428
C41	-3.208509	2.846415	-1.126688
H42	-2.542960	3.565143	-0.652967
H43	-2.814863	2.544641	-2.099138
H44	-4.209367	3.267493	-1.236071
C45	-6.164246	-0.516424	1.054094
C46	-7.439550	-1.295985	1.199340
H47	-7.735480	-1.288308	2.251602
H48	-8.222776	-0.793582	0.625658
H49	-7.345753	-2.327936	0.857329
O50	-6.081136	0.676119	1.398990
H51	1.909749	-1.719061	0.548944

5-LysNH$_2^+$-9MOG

C1	-3.851047	-0.919761	1.231700
C2	-2.851760	-0.049506	0.442195
C3	-4.928413	-1.246365	-0.789296
C4	-2.380549	2.192886	0.224529
N5	-4.738290	-1.605341	0.487086
N6	-2.320294	1.110631	1.061746
N7	-3.149387	1.811888	-0.899382
N8	-4.525980	-0.048172	-1.381605
C9	-3.592704	0.553281	-0.735825
N10	-5.649003	-2.029529	-1.567522
H11	-5.854356	-1.753226	-2.518036
H12	-6.020080	-2.898256	-1.206545
O13	-3.749203	-0.990487	2.453579
O14	-1.909521	3.296453	0.403737
C15	-3.651493	2.756060	-1.886159
H16	-3.607967	2.295527	-2.872783
H17	-4.679779	3.036013	-1.648287
H18	-3.012140	3.636879	-1.866299
N19	-1.732008	-0.944999	-0.063231
C20	-1.000516	-1.724144	1.003852
H21	-1.648060	-2.557656	1.274165
H22	-0.877344	-1.067015	1.865919
C23	0.347601	-2.203730	0.493591
H24	0.213739	-2.808205	-0.410838
H25	0.736381	-2.872642	1.268614
C26	1.346754	-1.072549	0.247296
H27	1.042068	-0.463823	-0.613250
H28	1.350819	-0.410426	1.121771
C29	2.750708	-1.615343	-0.009117
H30	2.720016	-2.356727	-0.814993
H31	3.122658	-2.119541	0.890759
C32	3.756397	-0.532964	-0.424334
H33	3.428267	-0.068157	-1.358394
C34	3.816183	0.558323	0.638583
N35	5.061307	-1.131043	-0.611301
O36	4.440750	0.471702	1.681502
O37	3.050191	1.595487	0.319011
H38	-1.725995	1.097460	1.881425
H39	-1.069871	-0.338790	-0.563590
H40	5.189263	-2.104479	-0.369514
C41	2.923631	2.637313	1.303585
H42	2.249531	3.369386	0.863500
H43	2.498507	2.231437	2.223515
H44	3.898361	3.086530	1.501407
C45	6.122202	-0.402959	-1.005919
C46	7.434296	-1.119730	-1.144963
H47	7.818100	-0.956137	-2.154995
H48	8.145697	-0.682797	-0.438870
H49	7.352196	-2.191433	-0.956807
O50	6.010775	0.814056	-1.239800
H51	-2.086101	-1.610511	-0.760946

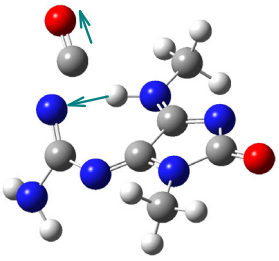
Cartesian coordinates for the structures in Fig. 5, optimized at SMD-ωB97XD/6-31+ G(d,p). For each TS, the vibrational mode corresponding to TS imaginary frequency is indicated by displacement vectors.

Fig. 5a

[5-MeNH-9MSp – H]⁻

C1	-0.880763	-0.316619	1.183945
C2	0.871567	0.944202	-0.138934
C3	-2.330311	0.048980	-0.352577
C4	1.994222	-0.890181	-0.316567
N5	-2.193626	-0.183336	1.006631
N6	2.105675	0.493019	-0.176456
N7	0.693339	-1.272588	-0.502612
N8	-1.258850	0.082168	-1.118453
C9	-0.177311	-0.150754	-0.202135
N10	-3.579268	0.199577	-0.847013
H11	-3.679525	0.555189	-1.786120
O12	-0.257674	-0.540849	2.240261
O13	2.955794	-1.671238	-0.301600
C14	0.251480	-2.642250	-0.323404
H15	0.297620	-2.951829	0.726972
H16	-0.777326	-2.727653	-0.679074
H17	0.876730	-3.306809	-0.920896
H18	-4.323177	0.400661	-0.196040
N19	0.524340	2.215035	-0.039948
H20	-0.464387	2.428691	-0.058221
C21	1.483746	3.304999	0.001456
H22	0.934374	4.241401	0.084326
H23	2.146539	3.204500	0.864149
H24	2.087143	3.325168	-0.910118

[TSco – H]⁻



C1	-1.778221	0.307005	1.846761
C2	0.442977	0.883662	-0.432010
C3	-1.806710	-1.269940	-0.482565
C4	2.479424	0.351177	0.068649
N5	-2.521508	-0.349366	0.027854
N6	1.662497	1.386676	-0.344739
N7	1.749436	-0.820816	0.244737
N8	-0.427710	-1.532222	-0.193524
C9	0.434930	-0.597684	-0.106237
N10	-2.287678	-2.291241	-1.317817
H11	-1.602453	-2.690700	-1.948320
O12	-2.554474	1.086446	2.247376
O13	3.690122	0.437125	0.269463
C14	2.299359	-2.108990	0.606097
H15	1.789696	-2.502240	1.488209
H16	2.195941	-2.819052	-0.218254
H17	3.356365	-1.973589	0.832638
H18	-3.151311	-2.041660	-1.782056
N19	-0.630483	1.551387	-0.790124
H20	-1.521947	1.058346	-0.627465
C21	-0.599176	2.966201	-1.112630
H22	-1.597811	3.263511	-1.429586
H23	-0.308135	3.558609	-0.239867
H24	0.107105	3.158677	-1.923112

[IMG – H]⁻

C1	0.195952	0.993182	0.027874
C2	-2.245735	-0.894859	0.069489
C3	2.226395	0.186110	-0.010640
N4	-2.957972	-0.870765	1.144317
N5	1.524000	1.335517	0.012400
N6	1.372838	-0.941999	-0.013442
N7	-0.915094	-1.328626	0.026097
C8	0.076809	-0.517368	0.012695
N9	-2.820630	-0.694215	-1.161311
H10	-2.198878	-0.366808	-1.888019
O11	3.463242	0.061219	-0.030502
C12	1.793748	-2.325093	-0.022153
H13	1.425562	-2.842389	0.867747
H14	1.420082	-2.835664	-0.913522
H15	2.882788	-2.352523	-0.026029
H16	-3.713645	-0.219956	-1.135623
N17	-0.838107	1.753326	0.049681
H18	-2.370279	-1.118788	1.937129
C19	-0.575679	3.183874	0.058469
H20	-1.523616	3.725415	0.070302
H21	0.000284	3.490055	0.940528
H22	-0.012420	3.503177	-0.827084

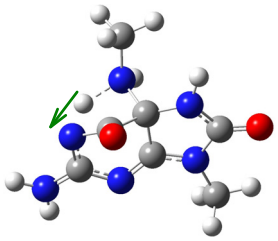
Fig. 5b

5-MeNH₂⁺-9MOG

C1	1.252159	0.761487	-0.920948
C2	0.018346	0.656343	-0.000008
C3	1.861029	-1.301865	-0.072323
C4	-2.235301	0.283088	-0.267609
N5	2.188023	-0.187689	-0.740373
N6	-1.217603	1.179056	-0.452175
N7	-1.650891	-0.935298	0.151376
N8	0.570030	-1.744333	0.217462
C9	-0.313035	-0.813561	0.159246
N10	2.820876	-2.136722	0.273760

H11	2.596868	-3.012516	0.726159
O12	1.343296	1.708890	-1.696913
O13	-3.421338	0.456287	-0.455201
C14	-2.380712	-2.191978	0.228221
H15	-2.260372	-2.753955	-0.700090
H16	-1.998844	-2.769057	1.069744
H17	-3.432716	-1.963922	0.390845
H18	3.784496	-1.912828	0.063817
N19	0.384901	1.231049	1.359657
H20	1.125826	0.667651	1.794761
C21	0.827150	2.659677	1.346787
H22	0.937447	2.966840	2.384974
H23	1.782282	2.729739	0.831016
H24	0.068100	3.265979	0.855838
H25	-0.441801	1.145537	1.964289
H26	-1.382128	2.153527	-0.672577

[TS$_{HT1}$ + H]$^+$

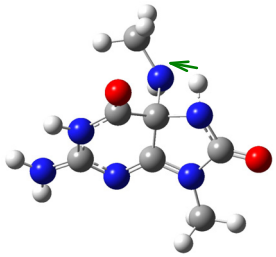


C1	-1.110371	-0.736675	-1.027974
C2	0.051297	-0.734522	-0.022106
C3	-1.937435	1.139661	0.054165
C4	2.285763	-0.216428	-0.172796
N5	-2.201262	-0.167267	-0.307051
N6	1.349214	-1.187334	-0.373391
N7	1.588703	0.986796	0.137682
N8	-0.672594	1.659002	0.204395
C9	0.274836	0.771685	0.137075
N10	-2.946368	1.927149	0.313432
H11	-2.786786	2.869292	0.649141
O12	-1.120705	-1.127720	-2.160899
O13	3.490995	-0.304049	-0.265527
C14	2.239352	2.282642	0.271564
H15	2.053723	2.886664	-0.618032
H16	1.850579	2.784927	1.156972
H17	3.307539	2.109018	0.387945
H18	-3.894208	1.594340	0.188688
N19	-0.588758	-1.266121	1.201157
H20	-0.160704	-0.867294	2.036758
C21	-0.623293	-2.737815	1.281807
H22	-1.197974	-3.006763	2.167484
H23	-1.122781	-3.139390	0.397621
H24	0.382109	-3.157240	1.363715
H25	-1.787680	-0.731948	0.739589
H26	1.610427	-2.164315	-0.422447

5-MeNH$_2^+$-9MOG_HT1

C1	-1.189248	-0.885776	-0.826523
C2	0.043171	-0.700416	0.054728
C3	-1.877181	1.294184	-0.000821
C4	2.253594	-0.202867	-0.319384
N5	-2.138664	0.104378	-0.629554
N6	1.280708	-1.132271	-0.538402
N7	1.608967	0.985504	0.132726
N8	-0.623106	1.693402	0.321209
C9	0.297171	0.781636	0.198052
N10	-2.872404	2.112698	0.223259
H11	-2.683980	3.017302	0.637667
O12	-1.392168	-1.847056	-1.535351
O13	3.448797	-0.300437	-0.503421
C14	2.278051	2.276040	0.213765
H15	2.138088	2.827605	-0.717802
H16	1.861679	2.834979	1.050552
H17	3.337888	2.095507	0.384236
H18	-3.825548	1.873212	-0.024145
N19	-0.164825	-1.279352	1.381415
H20	-0.860875	-0.735231	1.886985
C21	-0.566247	-2.691554	1.385723
H22	-0.596376	-3.019354	2.425440
H23	-1.549397	-2.873145	0.936255
H24	0.179503	-3.296909	0.866646
H25	-3.059751	-0.049216	-1.034709
H26	1.535128	-2.112792	-0.568754

[TS$_{HT2}$ + H]$^+$



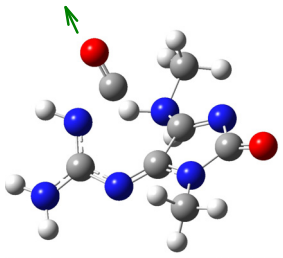
C1	1.189268	0.785138	-0.901472
C2	-0.044737	0.699998	-0.013671
C3	1.760641	-1.399634	0.011395
C4	-2.261689	0.381727	-0.295627
N5	2.070453	-0.257081	-0.687125
N6	-1.283535	1.322546	-0.436907
N7	-1.684716	-0.883999	0.095721
N8	0.496543	-1.717915	0.361034
C9	-0.372267	-0.757404	0.192432
N10	2.725891	-2.248083	0.259058
H11	2.508587	-3.122880	0.720627
O12	1.430663	1.693549	-1.663260
O13	-3.463786	0.518123	-0.435823
C14	-2.428456	-2.128416	0.197016

H15	-2.080340	-2.829080	-0.563803
H16	-2.291016	-2.556934	1.190364
H17	-3.480834	-1.901869	0.036158
H18	3.683657	-2.061561	-0.013912
N19	0.119238	1.475670	1.265927
H20	0.092438	0.866259	2.084805
C21	1.212519	2.458923	1.384898
H22	1.079647	2.966278	2.339697
H23	2.191402	1.975900	1.371524
H24	1.136860	3.189595	0.580547
H25	2.987079	-0.180461	-1.123106
H26	-1.001281	1.881426	0.715976

5-MeNH$_2$$^+$-9MOG_HT2

C1	-1.157344	0.838644	0.878408
C2	0.088141	0.692970	-0.005430
C3	-1.841516	-1.327013	-0.015711
C4	2.220758	0.283424	0.345835
N5	-2.089461	-0.159288	0.675827
N6	1.298241	1.228009	0.483102
N7	1.618236	-0.975418	-0.141694
N8	-0.609120	-1.705001	-0.394400
C9	0.323987	-0.794861	-0.227371
N10	-2.855639	-2.127163	-0.239680
H11	-2.689574	-3.014889	-0.696965
O12	-1.344320	1.757277	1.643316
O13	3.427898	0.311187	0.587397
C14	2.321092	-2.242848	-0.221419
H15	2.195055	-2.798978	0.710297
H16	1.926200	-2.820516	-1.056867
H17	3.377126	-2.034814	-0.385208
H18	-3.797434	-1.890165	0.048182
N19	-0.243419	1.341963	-1.356189
H20	-0.976464	0.830086	-1.861851
C21	-0.625240	2.783095	-1.283487
H22	-0.626249	3.165840	-2.302514
H23	-1.621555	2.867001	-0.854175
H24	0.110284	3.309948	-0.679962
H25	-2.989765	-0.042648	1.136384
H26	0.612619	1.259253	-1.916742

[TS$_{CO}$ + H]$^+$



C1	-1.091568	0.588426	1.450877
C2	0.483555	0.831160	-0.462943
C3	-1.943488	-1.149885	-0.345451
C4	2.425166	0.076726	0.056442
N5	-2.289478	-0.016926	0.258719
N6	1.682016	1.237614	-0.278547
N7	1.606476	-1.046012	-0.039350
N8	-0.630823	-1.495767	-0.501586
C9	0.333497	-0.658086	-0.325484
N10	-2.830507	-2.053908	-0.757214
H11	-2.507292	-2.925996	-1.151740
O12	-1.608000	1.033765	2.403380
O13	3.593897	0.071597	0.373178
C14	2.012379	-2.403333	0.287842
H15	1.485986	-2.744090	1.180894
H16	1.791952	-3.064298	-0.550942
H17	3.085119	-2.395345	0.473285
H18	-3.822135	-1.888133	-0.659218
N19	-0.512202	1.692449	-1.062143
H20	-1.451410	1.345981	-0.776483
C21	-0.368387	3.147396	-0.746268
H22	-1.212896	3.651552	-1.211062
H23	-0.393628	3.268288	0.335552
H24	0.569156	3.508227	-1.161178
H25	-3.262496	0.023030	0.561795
H26	-0.454832	1.561303	-2.082610

[IMG + H]$^+$

C1	0.313949	0.979981	-0.036320
C2	-2.198436	-0.887079	0.043227
C3	2.285126	0.098808	0.012193
N4	-2.675034	-0.532431	1.225812
N5	1.590931	1.292649	-0.001392
N6	1.391892	-0.995628	-0.022059
N7	-0.900953	-1.296995	-0.065516
C8	0.125149	-0.530962	-0.030261
N9	-2.977592	-0.959062	-1.021112
H10	-2.584480	-1.236221	-1.909922
O11	3.495809	-0.032602	0.049686
C12	1.771676	-2.396059	-0.003615
H13	1.369733	-2.883095	0.886727
H14	1.399199	-2.895850	-0.899556
H15	2.859154	-2.448093	0.015057
H16	-3.964717	-0.744381	-0.961376
N17	-0.670184	1.848763	-0.086415
H18	-2.059890	-0.512033	2.027847
C19	-0.438964	3.287428	-0.098460
H20	-1.406943	3.782472	-0.133712
H21	0.094307	3.591754	0.804491
H22	0.145915	3.571028	-0.975979
H23	-3.654709	-0.309115	1.348972
H24	-1.628460	1.530576	-0.125851