Transnitrosylation Products of the Dipeptide Cysteinyl-Cysteine: An Examination

by Tandem Mass Spectrometry and Density Functional Theory

Electronic Supplementary Information (ESI)

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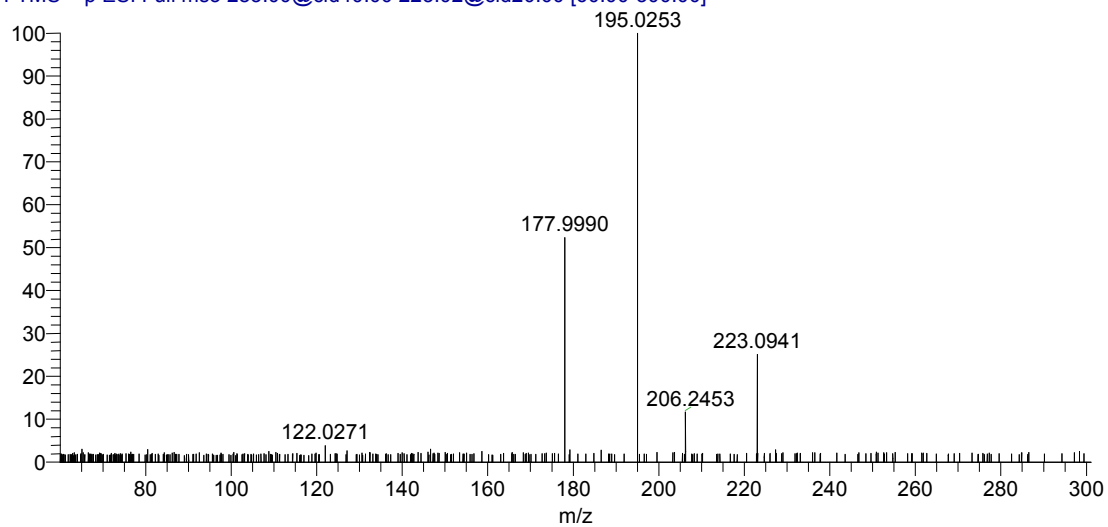
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Contents

a)

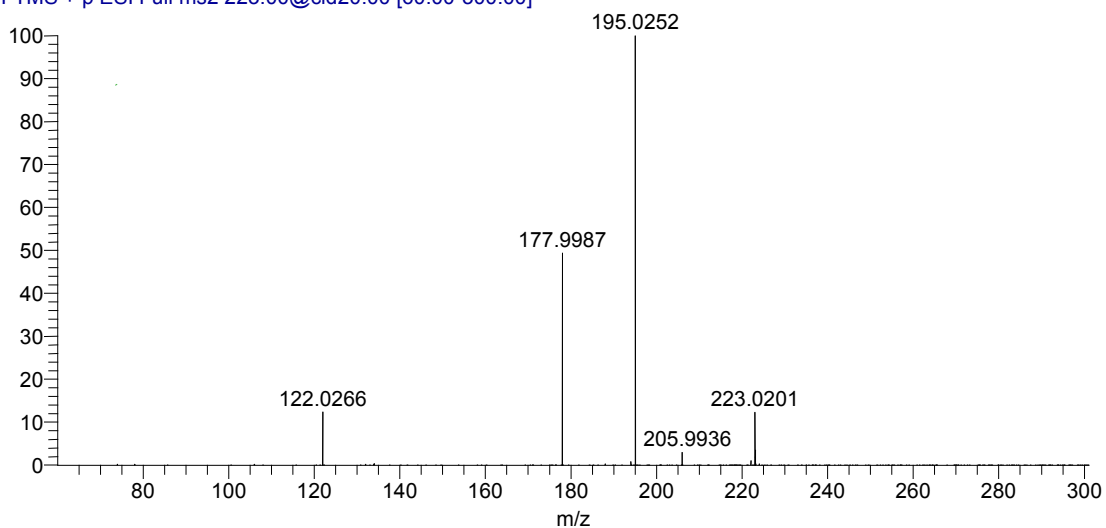T: FTMS + p ESI Full ms3 283.00@cid40.00 223.02@cid20.00 [60.00-300.00]
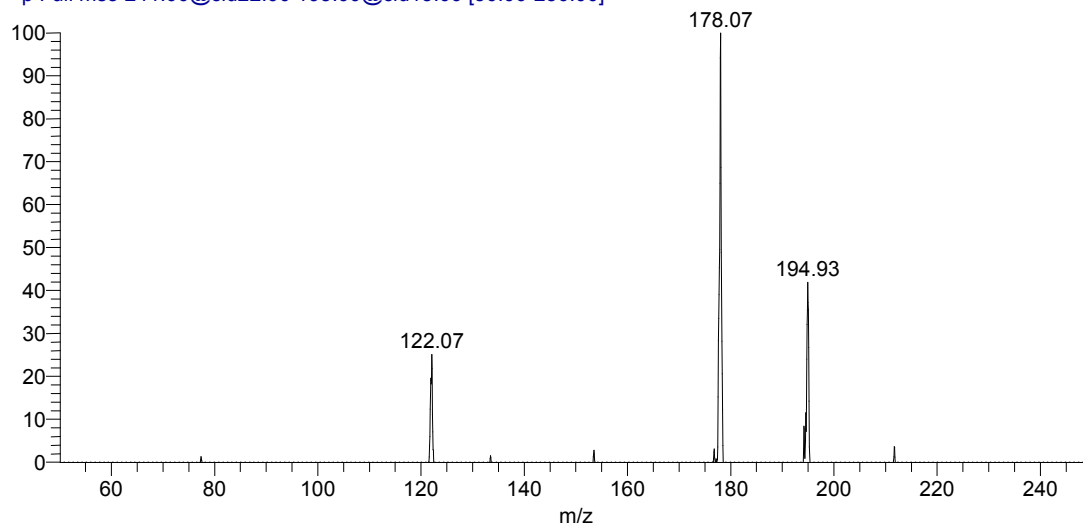
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Figure S1. a) HR-(+)ESI MS^3 mass spectrum (CE 20 eV) obtained in the Orbitrap selecting the precursor ion of [CySNO-CySNO+H]$^+$ (*m/z* 283). b) HR-ESI(+) CID mass spectrum (CE 20 eV) obtained in the Orbitrap selecting the precursor ion of [ox-(Cys-Cys)+H]$^+$ (*m/z* 223).

a)

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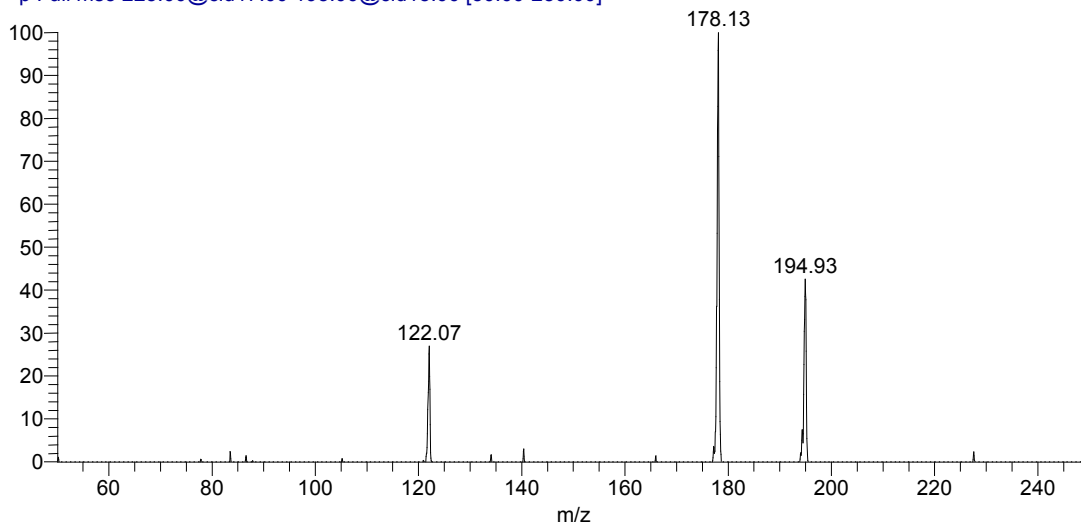
Figure S2. ESI(+)- CID MS^3 mass spectra (CE 15 eV) obtained in the LCQ selecting the precursor ion of *m/z* 195.00 a) after dissociation of [(CyS)$_2$+H]$^+$ (*m/z* 241) and b) after dissociation of [ox-(Cys-Cys)+H]$^+$ (*m/z* 223).

a)

T: ITMS + p ESI Full ms2 122.00@cid20.00 [50.00-150.00]

b)
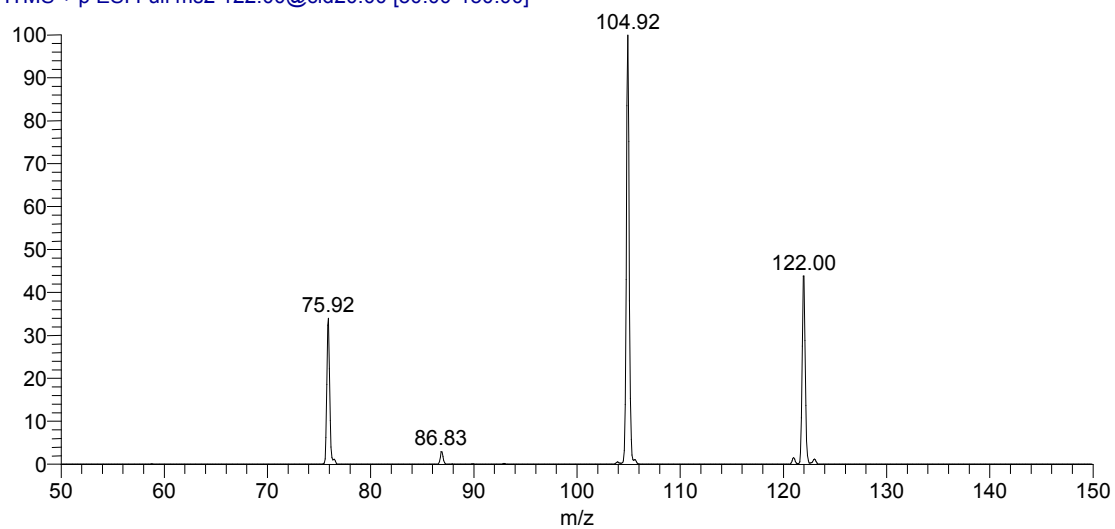
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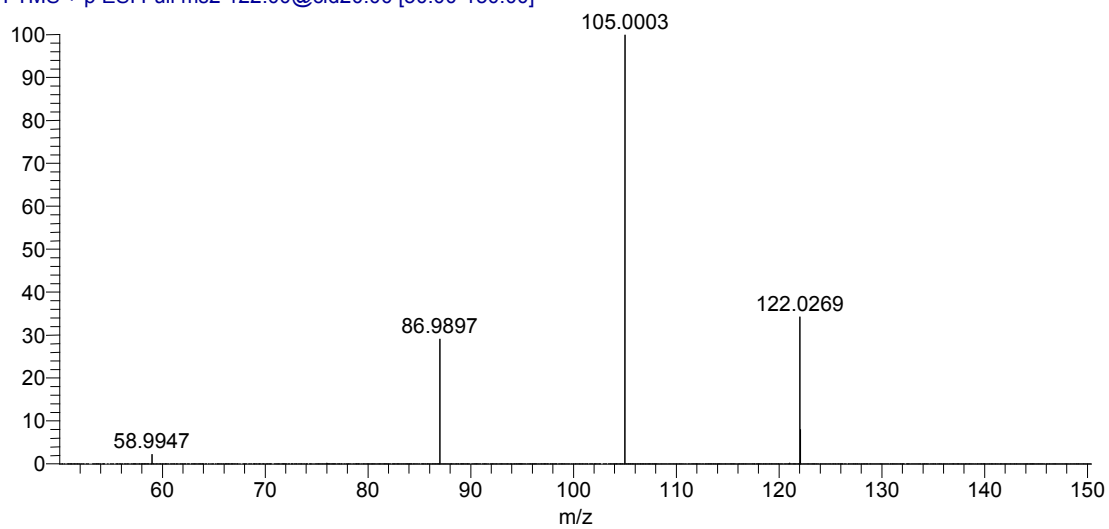
Figure S3. ESI(+)-CID mass spectra (CE 20 eV) obtained in the Orbitrap selecting the precursor ion of [Cys+H]$^+$ (*m/z* 122) with both low a) and high b) resolution and accuracy.

a)

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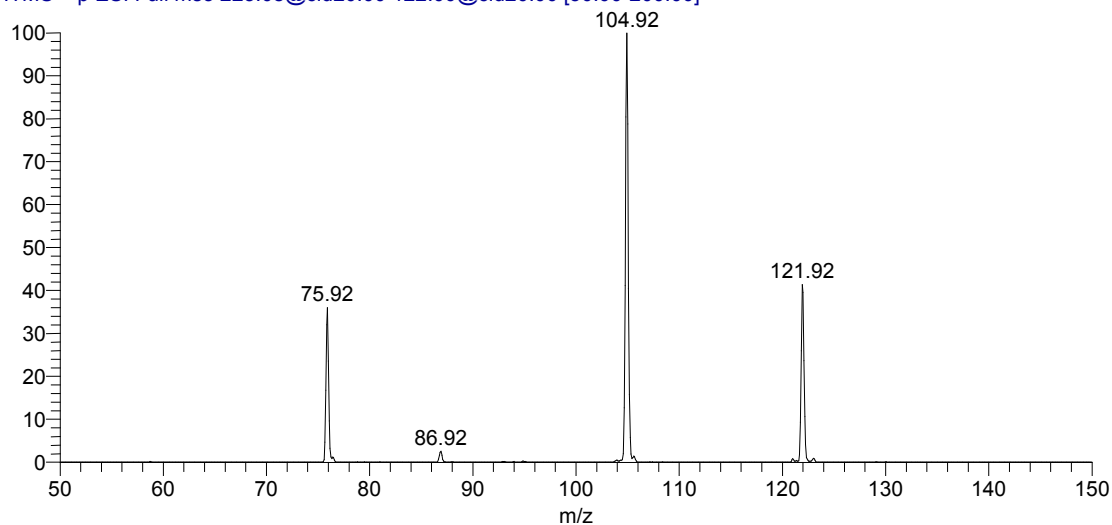
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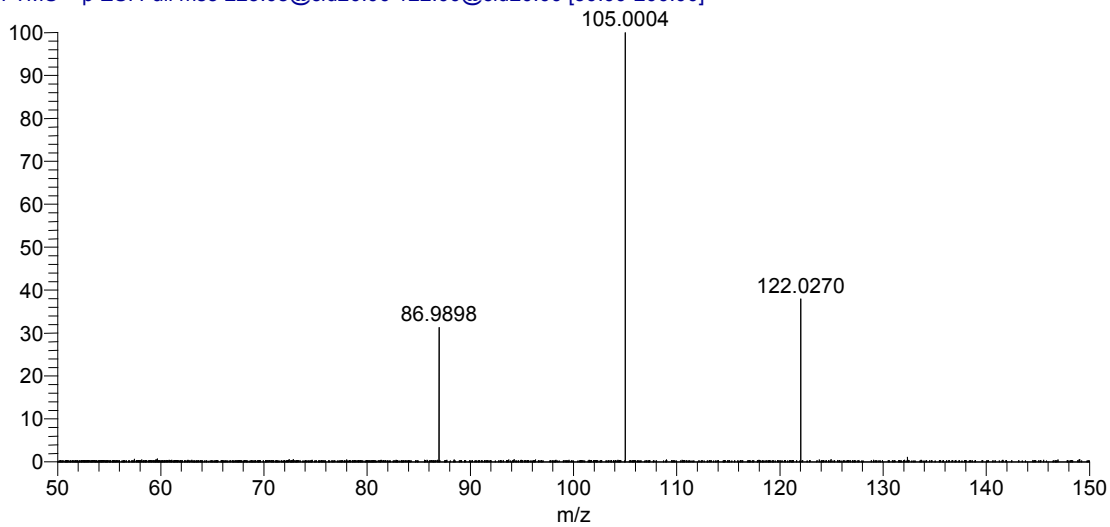
Figure S4. ESI(+)-CID MS[3] (CE 20 eV) mass spectrum obtained in the Orbitrap selecting the precursor ion of m/z 122.00 after dissociation of [ox-(Cys-Cys)+H][+] (m/z 223) with both low a) and high b) resolution and accuracy.

There is a difference between the conditions in the collision cell when using the ion trap (low resolution) (Figures S3a and S4a) and the Orbitrap (high resolution) (Figures S3b and S4b), namely the pressure. Therefore, the activation conditions of the ions are not the same. Taking that into account, it is not surprising to obtain differences in the product ion abundances. The ion of m/z 75.92 may be a product ion obtained from some of the other ions seen in the spectrum and the ion activation conditions may not be enough to produce it at high resolution.

+MS2 (228.00)
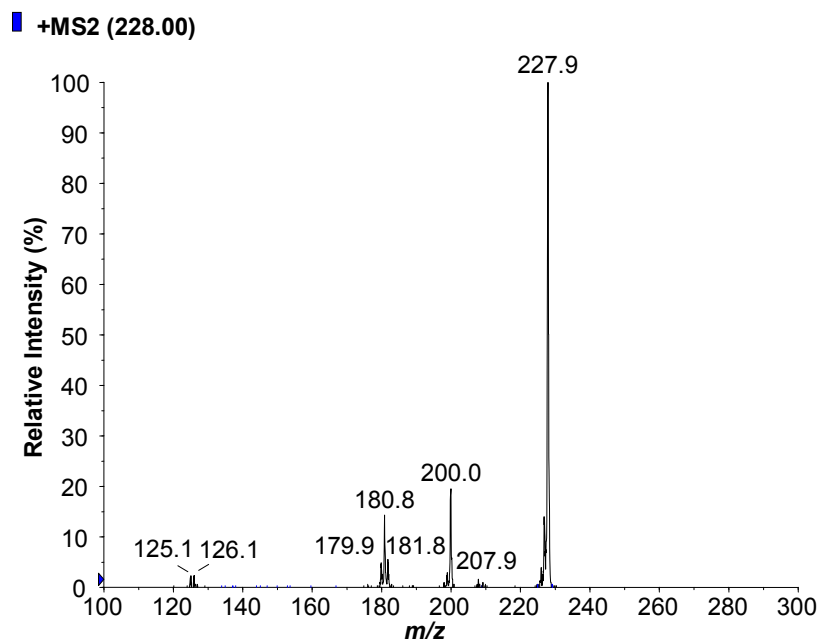
Figure S5. ESI(+)-CID mass spectrum obtained in the 2000-Qtrap selecting the precursor ion of [ox-(Cys-Cys)-d_4+D]$^+$ (m/z 228).

a)

b)

Figure S6. a) ESI(+)-CID mass spectrum (CE 22 eV) obtained in the LCQ selecting the precursor ion of protonated cystine-d_4 (*m/z* 241). b) CID MS^3 (CE 15 eV) selecting the precursor ion of *m/z* 199.00.

a)

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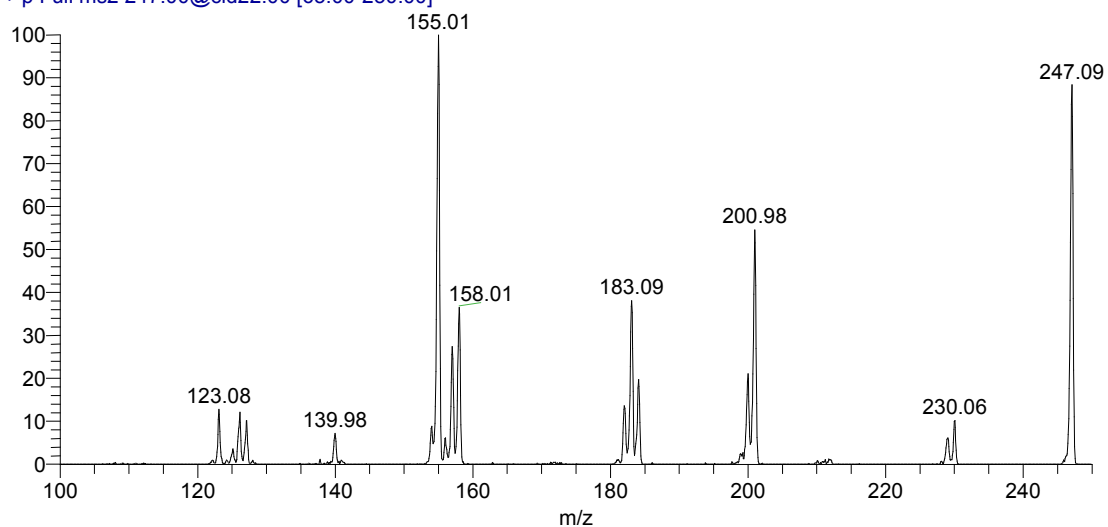
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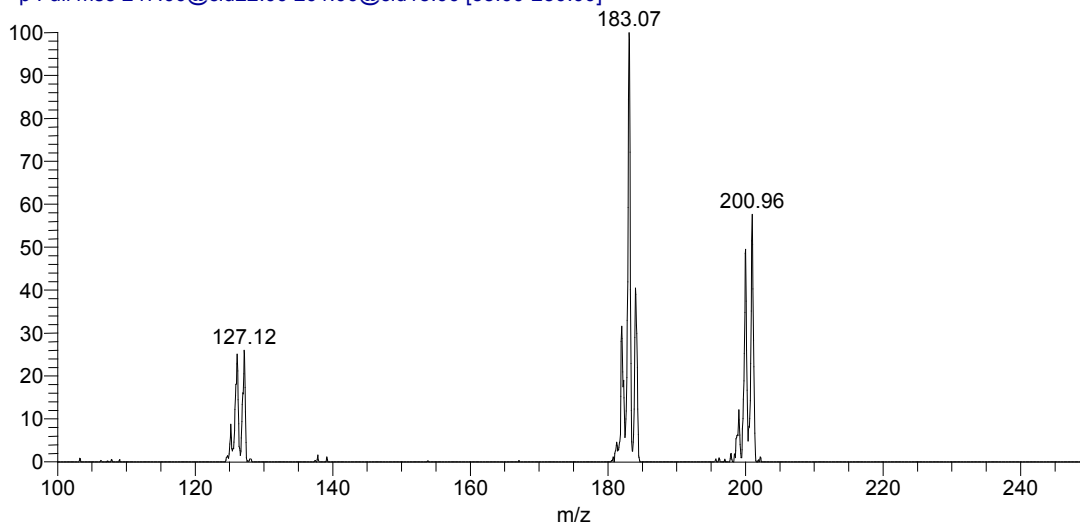
Figure S7. a) ESI (+)-CID mass spectrum (CE 22 eV) obtained in the LCQ selecting the precursor ion of protonated cystine-d_6 (*m/z* 243). b) CID MS^3 (CE 15 eV) selecting the precursor ion of *m/z* 201.00.
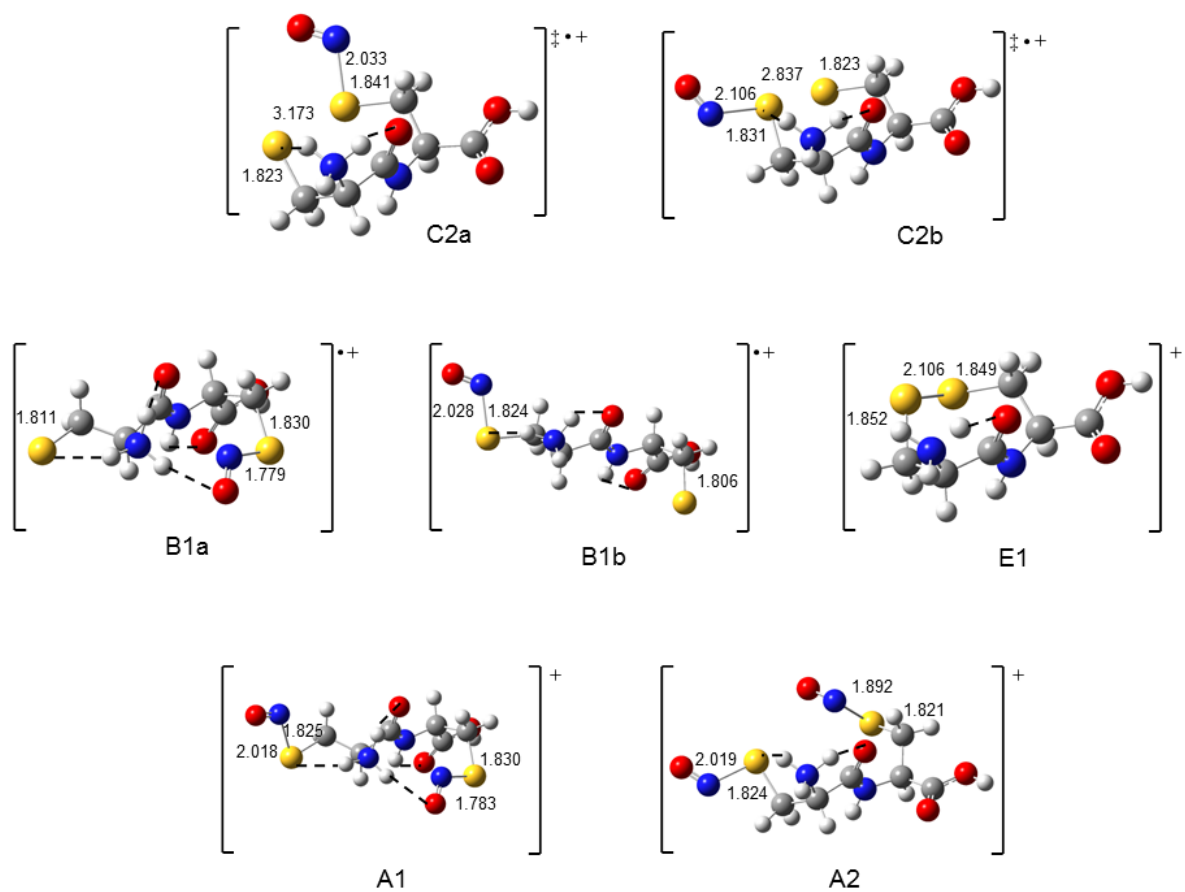
Figure S8. Optimized structures of [CySNO-CySNO+H]$^+$ (A1-A2), the radical cations [CyS$^•$-CySNO+H]$^+$ (B1a) and [CySNO-CyS$^•$+H]$^+$ (B1b) and the transition state structures (C2a and C2b) leading to formation of [ox-(Cys-Cys)+H]$^+$ (E1). Relevant distances for bonds involving the sulfur atoms are given in Å.
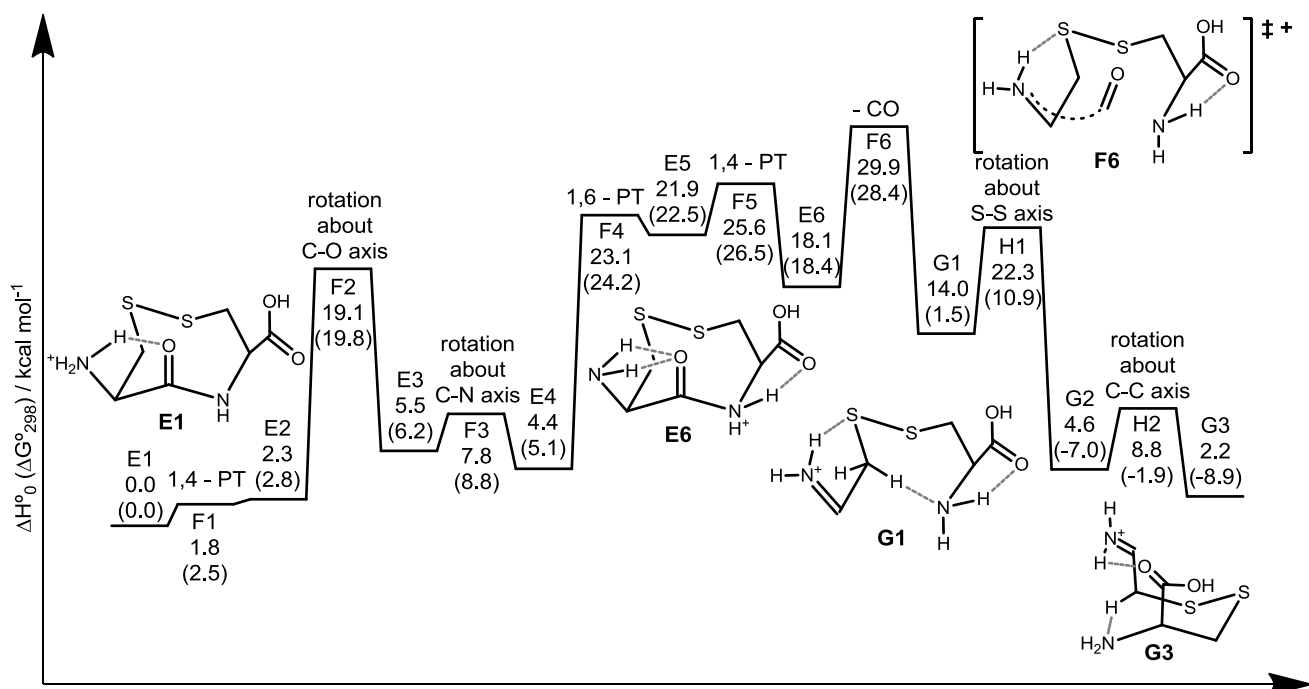
Figure S9. Fragmentation pathway for the loss of CO starting from structure **E1**. The energetic contribution of the CO molecule lost from structure **G1** onwards is considered although not shown for simplicity in the diagram. The enthalpies at 0K (ΔH°_0) and free energies at 298K (ΔG°_{298}, in parentheses) are given in kcal mol^{-1} relative to structure **E1**. Transition state structures **Fn** are associated with rearrangements and dissociation of protonated ox-(Cys-Cys), *m/z* 223; structures **Hn** are transition states associated with rearrangements and dissociation of the *m/z* 195 ion.
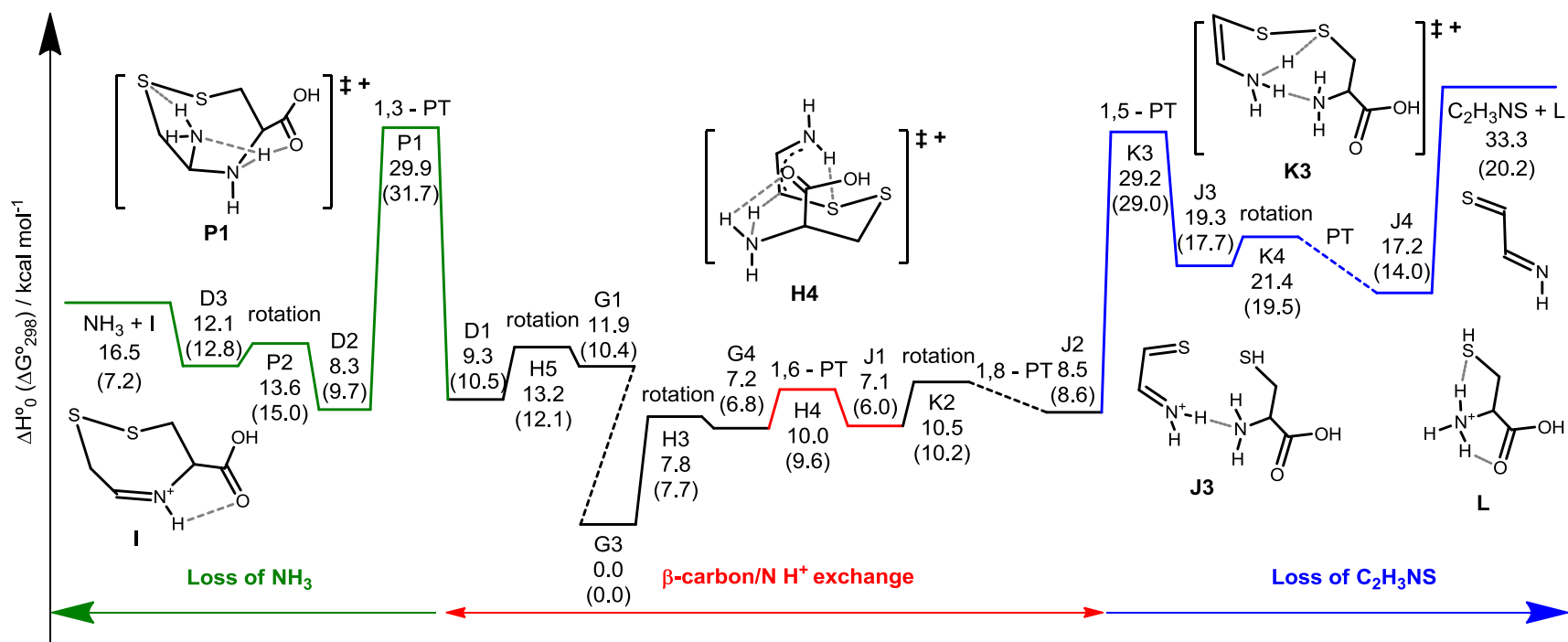
Figure S10. Energy barriers and pathways after the loss of CO starting from the structure **G3**: proton exchange between the β-carbon and the nitrogen (middle in red); loss of ammonia (left side in green) and loss of C_2H_3NS (right side in blue). The enthalpies at 0K ($\Delta H°_0$) and free energies at 298K ($\Delta G°_{298}$, in parentheses) are given in kcal mol^{-1} relative to structure **G3**. The interconversion steps between structures **G1** and **G3** are shown in Figure S9. Proton transfers (PT) that occur with trivial energy barriers are omitted. **P1** and **K3** are the critical transition states leading to product ions **I** and **L** respectively.

4. Total energies of calculated structures

Table S1. Total electronic energies and unscaled zero-point vibrational energies (ZPVE) at the UB3LYP-6-311++G(d,p) level (all data in hartrees)

Structure	Electronic energy	ZPVE
A1	-1626.7155512	0.2022544
A2	-1626.7074182	0.2014062
NO	-129.9316566	0.00451
B1a	-1496.7409555	0.1945265
B1b	-1496.7381876	0.1934034
B2a	-1496.7334583	0.1939715
B2b	-1496.7322455	0.1933981
C2a	-1496.7323868	0.1936459
C2b	-1496.7262677	0.1933211
E1	-1366.8251065	0.1880665
E2	-1366.8207582	0.1873304
E3	-1366.8153852	0.1870877
E4	-1366.817142	0. 1871719
E5	-1366.7889097	0.1867531
E6	-1366.7948972	0.1867039
F1	-1366.8184777	0.1843216
F2	-1366.7920325	0.1854346
F3	-1366.8111421	0.1864675
F4	-1366.7863407	0.1861738
F5	-1366.7791376	0.1829587
F6	-1366.771983	0.1825235
CO	-113.3490503	0.0050387
G1	-1253.444685	0.1740044
G2	-1253.4609771	0.1752697

G3	-1253.465333	0.1757346
G4	-1253.4525797	0.1744234
H1	-1253.4308659	0.1734022
H2	-1253.4542308	0.1752241
H3	-1253.4511668	0.1739896
H4	-1253.4443912	0.1707908
H5	-1253.442274	0.1737388
D1	-1253.4534325	0.1786555
D2	-1253.455114	0.1787513
D3	-1253.4483819	0.1781089
P1	-1253.4188401	0.1768857
P2	-1253.4453187	0.1774722
I	-1196.8517304	0.1368107
NH3	-56.582722	0.0342648
J1	-1253.4535447	0.1752628
J2	-1253.45213	0.1760985
J3	-1253.4302477	0.1714224
J4	-1253.4331714	0.1709986
K2	-1253.4483327	0.1755392
K3	-1253.4134717	0.1704385
K4	-1253.4249367	0.1695195
L	-722.4259278	0.1219837
C2H3NS	-530.9805622	0.0480119

10. Cartesian coordinates of calculated structures

B3LYP/6-311++G(d,p) fully optimized geometries, given in standard XYZ format: coordinates are Cartesian coordinates in the usual order, units are ångstroms, first line is molecule name, second line indicates total number of atoms.

```
A1
28
C        0.08449       -0.30541        0.56228
O        0.19314       -0.04056        1.75077
C        1.26744        0.05174       -0.36790
C        2.42710       -0.94692       -0.22095
N        1.70430        1.41731        0.10596
H        0.96968        0.15479       -1.41145
H        2.68222        1.57502       -0.18231
H        1.10236        2.16391       -0.26642
H        2.12343       -1.89698       -0.66147
H        2.65035       -1.11897        0.83880
S        3.96856       -0.37616       -1.01378
N        5.00062       -0.55138        0.71192
O        6.12551       -0.35385        0.65837
H        1.62060        1.41731        1.13541
N       -0.99578       -0.84122       -0.02535
C       -2.27653       -0.99868        0.65077
H       -1.01102       -1.05506       -1.01796
C       -3.19848       -1.71868       -0.33519
C       -2.86173        0.34830        1.14777
H       -2.16090       -1.63528        1.53415
O       -4.38703       -1.97688        0.21402
O       -2.87398       -2.00153       -1.45972
H       -2.22216        0.75561        1.92931
H       -3.85680        0.18570        1.56189
S       -3.04399        1.63247       -0.14381
H       -4.94655       -2.43481       -0.43469
N       -1.32432        2.10026       -0.10848
O       -0.94413        2.91421       -0.90253

A2
28
C        0.29672       -1.09204        0.21408
O        0.66083       -1.11157        1.38468
C       -1.04991       -1.79411       -0.12994
C       -2.06429       -1.01081       -0.97996
N       -1.61203       -2.13405        1.22359
H       -0.80137       -2.73421       -0.62971
H       -1.96982       -3.08604        1.29991
H       -2.35160       -1.45313        1.46036
H       -2.87432       -1.67535       -1.30409
H       -1.57739       -0.64219       -1.88305
S       -2.84892        0.37907       -0.09762
N       -4.69130       -0.35576       -0.47469
O       -5.57707        0.29142       -0.15445
H       -0.79900       -1.97157        1.87309
N        0.98838       -0.55645       -0.79952
C        2.38298       -0.12974       -0.65818
H        0.63511       -0.66045       -1.73828
C        3.24317       -1.34855       -0.26111
C        2.56492        1.09648        0.25683
H        2.71840        0.14541       -1.66224
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O        2.85663       -2.48583       -0.29553
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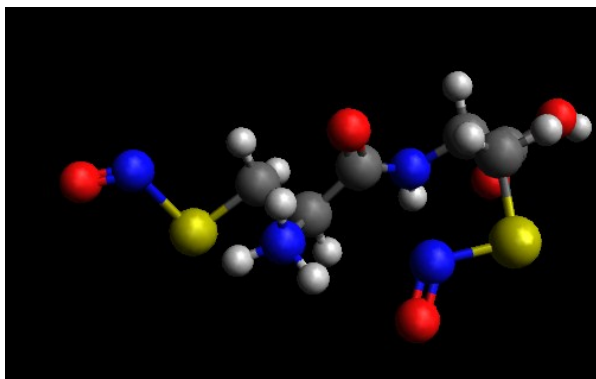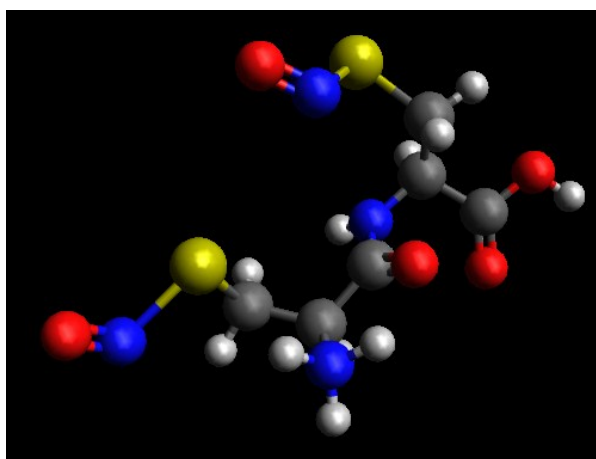
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H          2.12782          0.91966          1.24119
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H          5.01392         -1.76293          0.25592
N          0.31809          2.54087          0.75777
O         -0.46287          3.40387          0.65923


B1a
26
C          0.64577         -0.39712          0.67890
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C          1.90822         -0.14910         -0.17872
C          3.00267         -1.19628          0.10793
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H         -3.30876          0.40698          1.40017
S         -2.28521          1.73623         -0.28815
H         -4.45258         -2.19011         -0.60011
N         -0.54387          2.07305         -0.15366
O         -0.04874          2.82410         -0.94793


B1b
26
C          0.05654         -0.63464          0.37986
O          0.04926         -1.24629          1.44718
C         -1.20057         -0.74605         -0.52172
C         -2.11136          0.48949         -0.35747
N         -1.90225         -1.97807         -0.01502
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H         -2.92377         -1.84427         -0.08192
H         -1.64491         -2.81938         -0.53446
H         -1.64804          1.33064         -0.87273
H         -2.21140          0.75658          0.70187
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C          2.91390          1.62035         -0.00403
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O          4.02890          1.99473          0.62516
O          2.46550          2.14257         -0.99338
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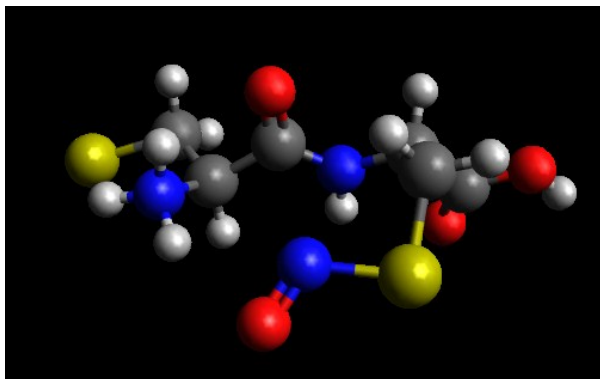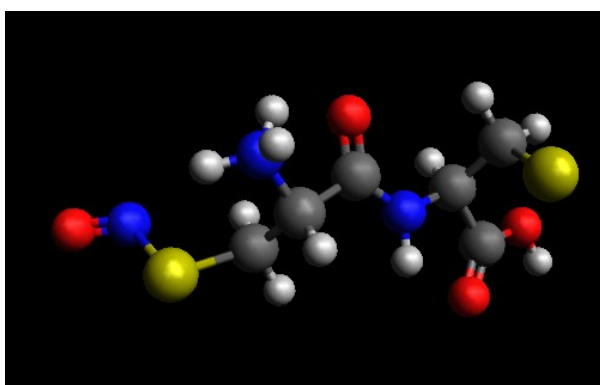
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B2a
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N	-1.73662	-2.35328	1.29891
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H	-2.13742	-3.26753	1.50818
H	-2.46746	-1.61353	1.31499
H	-2.86960	-2.39405	-1.24651
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S	-2.79100	-0.12115	-0.54563
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N	0.81900	-0.88683	-0.83649
C	1.81381	0.17577	-0.75025
H	0.59154	-1.24277	-1.75147
C	3.09120	-0.34365	-0.06037
C	1.26409	1.46799	-0.10447
H	2.10455	0.40287	-1.77960
O	3.91313	0.67557	0.23390
O	3.32626	-1.50158	0.13766
H	1.97372	2.27385	-0.28713
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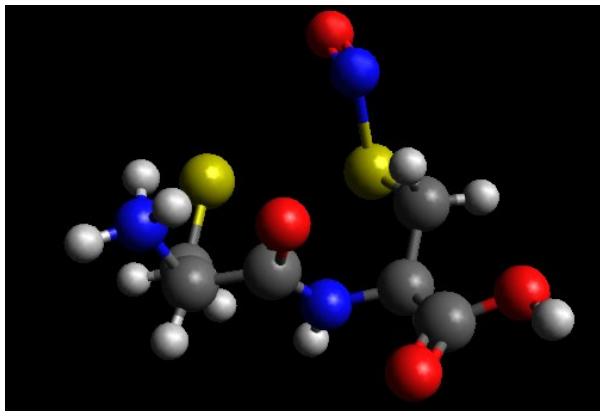
B2b
26

C	0.31793	-0.80149	0.14694
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C	-2.03929	-0.55103	-1.00405
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H	-0.77583	-2.31080	-0.93821
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H	-2.85561	-1.15266	-1.42138
H	-1.55592	-0.04369	-1.83899
S	-2.80668	0.68572	0.09496
N	-4.65790	0.03022	-0.37318
O	-5.53573	0.62392	0.05470
H	-0.77373	-1.89879	1.66783
N	1.02405	-0.16617	-0.79197
C	2.38945	0.31523	-0.57144
H	0.67872	-0.15005	-1.73906
C	3.31320	-0.89041	-0.30824
C	2.48471	1.42423	0.49683
H	2.71609	0.74252	-1.52301
O	4.53979	-0.47708	0.03801
O	2.98625	-2.03912	-0.43915
H	3.52320	1.75507	0.58015
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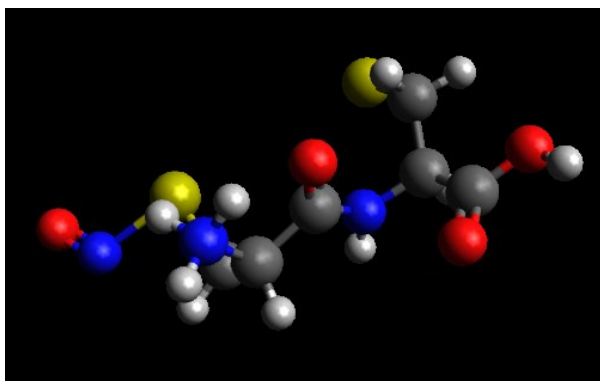
C2a
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| C | 0.19206 | -1.49953 | 0.16356 |

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C     -2.09185    -1.73005    -1.01998
N     -1.58596    -2.71543     1.20887
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C      3.05047    -0.31022    -0.12839
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H      1.95260     0.57368    -1.71123
O      3.80793     0.70897     0.30545
O      3.37232    -1.46405    -0.12120
H      1.76569     2.23849     0.03658
H      0.98498     1.09598     1.14767
S     -0.52890     1.83944    -0.59721
H      4.65669     0.35533     0.61763
N     -0.74937     3.40068     0.68581
O     -1.73035     3.97992     0.60131

C2b
26
C      0.50419     1.16934     0.13371
O      0.78284     1.36677    -1.04621
C     -0.83551     1.75402     0.66101
C     -1.80515     0.66458     1.15401
N     -1.38016     2.47648    -0.54543
H     -0.65921     2.49080     1.44771
H     -1.63468     3.44855    -0.37047
H     -2.17731     1.96949    -0.94475
H     -2.76371     1.11082     1.44082
H     -1.39334     0.18977     2.04448
S     -2.15469    -0.62916    -0.09297
N     -4.19237    -0.09605    -0.11274
O     -4.89218    -0.73535    -0.74266
H     -0.58351     2.39462    -1.23980
N      1.21668     0.42907     0.98296
C      2.21581    -0.53412     0.51321
H      0.87310     0.29864     1.92192
C      3.43793     0.20247    -0.05844
C      1.57695    -1.57400    -0.43503
H      2.57417    -1.05669     1.40403
O      4.21240    -0.65123    -0.74827
O      3.68703     1.35953     0.13004
H      2.28443    -2.38447    -0.62672
H      1.33940    -1.13225    -1.40441
S      0.07620    -2.34784     0.25254
H      5.00155    -0.17533    -1.05361

E1
24
C      0.21708    -1.20258     0.16368
O     -0.13616    -1.51200    -0.96876
C      1.68726    -1.48561     0.56517
C      2.44314    -0.16288     0.80178
N      2.22166    -2.23759    -0.63412
H      1.76321    -2.13876     1.43691
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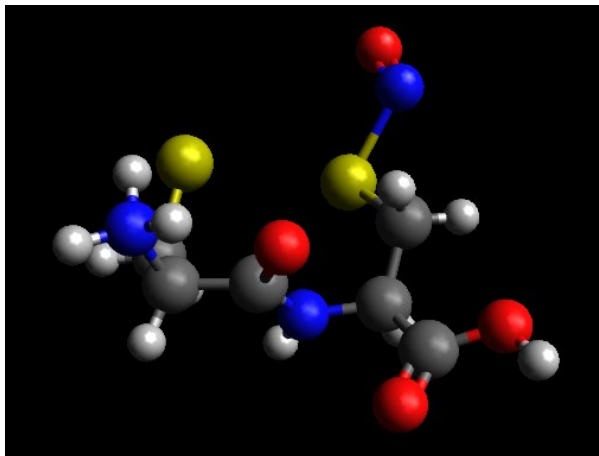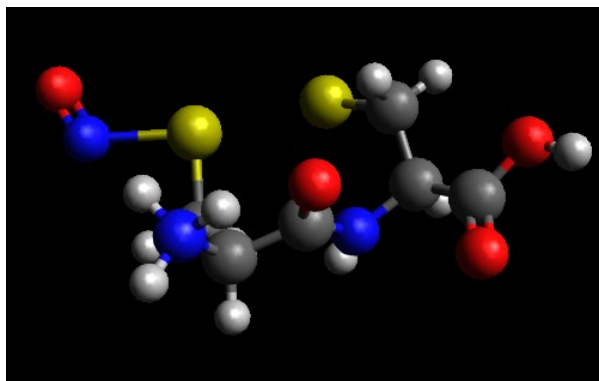
H	2.51122	-3.19244	-0.41824
H	2.99357	-1.75180	-1.09613
H	3.52312	-0.33921	0.82314
H	2.17464	0.24529	1.77650
S	2.16413	1.13250	-0.49273
H	1.38463	-2.24402	-1.28594
N	-0.51285	-0.50254	1.03810
C	-1.56785	0.40322	0.57938
H	-0.11468	-0.30123	1.94294
C	-2.79580	-0.38805	0.09693
C	-1.00978	1.41548	-0.44615
H	-1.90239	0.95243	1.46360
O	-3.61176	0.41296	-0.60842
O	-3.01029	-1.53553	0.36116
H	-1.73208	2.21685	-0.60718
H	-0.80397	0.95029	-1.40872
S	0.51502	2.27207	0.15310
H	-4.40391	-0.09060	-0.85699
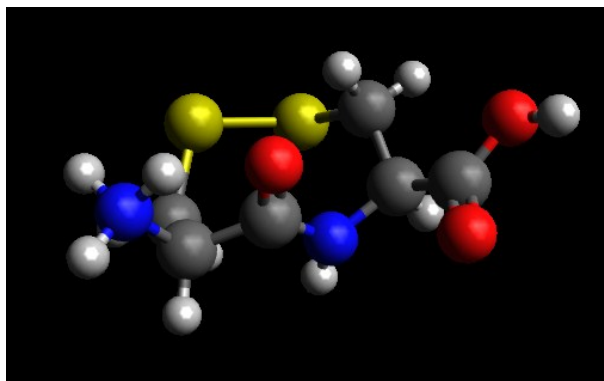
E2
24

C	0.28296	-1.17565	0.22175
O	-0.09179	-1.47601	-0.96333
C	1.74125	-1.49062	0.56712
C	2.46211	-0.12685	0.75642
N	2.24082	-2.27569	-0.56260
H	1.79147	-2.05465	1.50359
H	2.44296	-3.24017	-0.32332
H	3.05670	-1.87065	-1.00883
H	3.54233	-0.28981	0.72701
H	2.22833	0.30533	1.72978
S	2.11343	1.14487	-0.54877
H	0.72302	-1.95985	-1.34143
N	-0.48214	-0.48826	1.02714
C	-1.57707	0.39148	0.57953
H	-0.10455	-0.28956	1.94408
C	-2.77356	-0.43579	0.08232
C	-1.04089	1.43512	-0.42727
H	-1.91882	0.91456	1.47576
O	-3.68842	0.37904	-0.45862
O	-2.87224	-1.62300	0.20186
H	-1.78094	2.22744	-0.54800
H	-0.85314	0.99981	-1.40782
S	0.49110	2.28785	0.16190
H	-4.45995	-0.14462	-0.73127
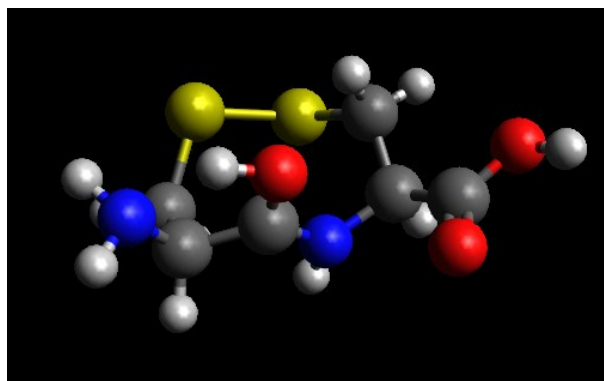
E3
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C	0.34929	-1.23903	0.26117
O	-0.06186	-1.79256	-0.81037
C	1.81211	-1.39689	0.64009
C	2.45223	0.03333	0.72069
N	2.43984	-2.35692	-0.22624
H	1.83003	-1.81102	1.65741
H	3.33332	-2.67157	0.12980
H	2.54023	-2.04413	-1.18538
H	3.53638	-0.08649	0.67437
H	2.22425	0.54202	1.65999
S	2.02638	1.17698	-0.66867
H	-1.07338	-1.71677	-0.92168
N	-0.42861	-0.47665	1.02210
C	-1.55545	0.37774	0.58096
H	0.02056	-0.11796	1.85533
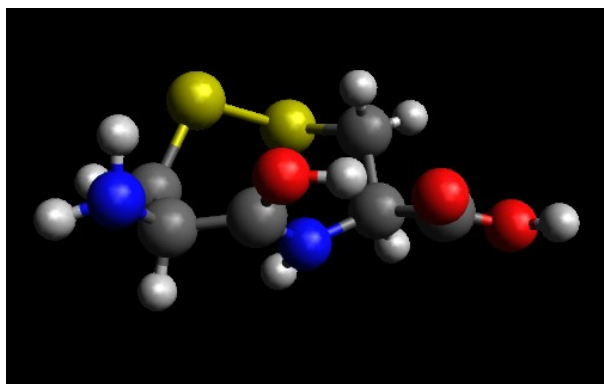
C	-2.71482	-0.43042	0.00782
C	-1.08292	1.43207	-0.45645
H	-1.90752	0.88701	1.47696
O	-3.88386	0.08935	0.31853
O	-2.56925	-1.40692	-0.70758
H	-1.86071	2.19108	-0.56800
H	-0.90325	0.98360	-1.43435
S	0.43237	2.34219	0.06042
H	-4.60151	-0.40723	-0.11370

E4
24
C	0.34384	-1.24198	0.28045
O	-0.08185	-1.85308	-0.75711
C	1.82694	-1.39633	0.64287
C	2.45714	0.02379	0.73179
N	2.58301	-2.24063	-0.23863
H	1.86251	-1.83654	1.64823
H	2.55009	-1.94496	-1.20831
H	2.32817	-3.21919	-0.18288
H	3.53942	-0.10448	0.68401
H	2.22507	0.53217	1.66856
S	2.02798	1.16143	-0.66297
H	-1.09476	-1.77093	-0.86521
N	-0.42581	-0.45397	1.02062
C	-1.55972	0.39031	0.57371
H	0.04546	-0.05130	1.82181
C	-2.71765	-0.42311	0.00839
C	-1.08249	1.43854	-0.46764
H	-1.91396	0.90527	1.46587
O	-3.88340	0.12456	0.27966
O	-2.57725	-1.42840	-0.66809
H	-1.85563	2.20146	-0.58353
H	-0.90194	0.98412	-1.44275
S	0.43755	2.34174	0.05135
H	-4.60166	-0.37591	-0.14698
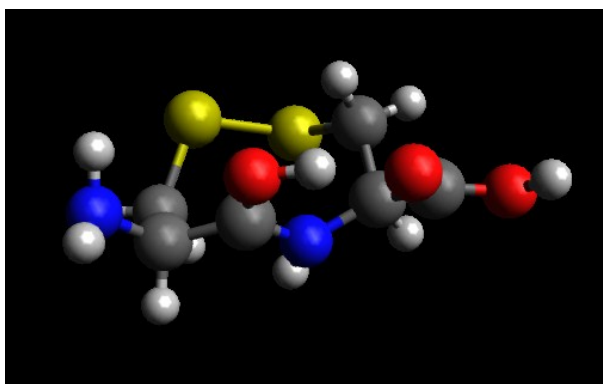
E5
24
C	0.03494	1.17104	0.23067
O	0.74571	1.38135	-0.74213
C	-1.37003	1.75698	0.42652
C	-2.37540	0.59454	0.64426
N	-1.80796	2.61796	-0.64285
H	-1.35408	2.34360	1.35420
H	-1.74202	2.16759	-1.55023
H	-1.28514	3.48488	-0.68448
H	-3.37749	1.01015	0.52531
H	-2.31421	0.15981	1.64317
S	-2.28536	-0.77668	-0.59411
N	0.52518	0.29282	1.18980
C	1.39703	-0.72776	0.61166
H	-0.12156	-0.05984	1.88441
C	2.53758	0.02794	-0.02831
C	0.68272	-1.70178	-0.36184
H	1.84597	-1.29273	1.43806
O	3.06353	-0.43859	-1.09977
O	3.17145	0.97174	0.58478
H	1.26285	-2.62135	-0.45876
H	0.56963	-1.26129	-1.35064
S	-0.98281	-2.20571	0.23986
H	3.82823	0.08534	-1.40452
H	2.67141	1.28478	1.36204
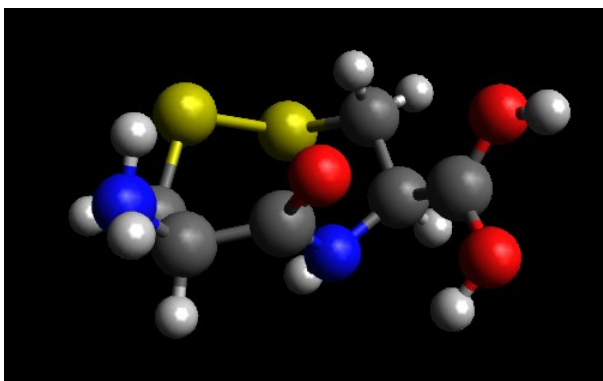
E6
24
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C      0.26479    -1.30446    -0.02008
O     -0.29488    -1.59518    -1.01241
C      1.71331    -1.56052     0.41196
C      2.41848    -0.22912     0.77297
N      2.46542    -2.29263    -0.56623
H      1.65787    -2.16440     1.33015
H      2.53232    -1.81267    -1.45807
H      2.11967    -3.23200    -0.72330
H      3.48715    -0.44652     0.81738
H      2.12677     0.16730     1.74729
S      2.22287     1.10649    -0.48524
N     -0.61913    -0.55612     1.07584
C     -1.56132     0.49501     0.52162
H     -0.02924    -0.14458     1.80159
C     -2.80786    -0.28020     0.06515
C     -0.89702     1.44018    -0.48008
H     -1.87865     1.07584     1.39433
O     -3.54217     0.41401    -0.78954
O     -3.06339    -1.36656     0.51936
H     -1.59884     2.24739    -0.69504
H     -0.64720     0.95552    -1.42202
S      0.60911     2.24816     0.22261
H     -4.34934    -0.08177    -1.01123
H     -1.23498    -1.28088     1.48495
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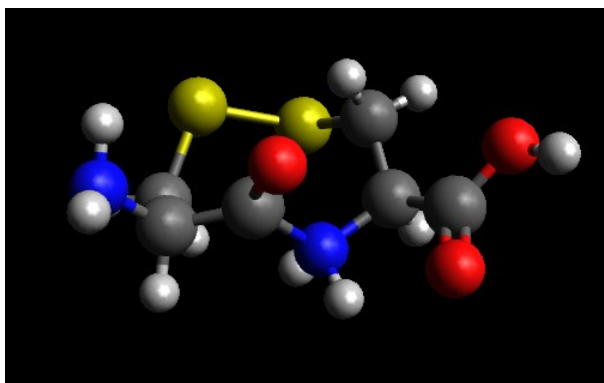
F1
24
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C      0.24166    -1.18477     0.23614
O     -0.09343    -1.52256    -0.92760
C      1.71273    -1.50027     0.57473
C      2.46978    -0.16713     0.77482
N      2.13313    -2.25421    -0.63155
H      1.79976    -2.12333     1.46765
H      2.36653    -3.22593    -0.44664
H      2.89601    -1.81748    -1.14325
H      3.54737    -0.35026     0.75133
H      2.24019     0.25854     1.75225
S      2.15492     1.11683    -0.52599
H      0.93692    -2.05224    -1.20383
N     -0.50628    -0.47451     1.05131
C     -1.57395     0.41890     0.57770
H     -0.11682    -0.25587     1.95769
C     -2.78410    -0.39004     0.08307
C     -1.00736     1.43076    -0.44477
H     -1.91714     0.96693     1.45865
O     -3.65441     0.42669    -0.52788
O     -2.93289    -1.56452     0.26039
H     -1.72950     2.23369    -0.59854
H     -0.80918     0.96833    -1.41074
S      0.52797     2.27211     0.15239
H     -4.43508    -0.08598    -0.79466
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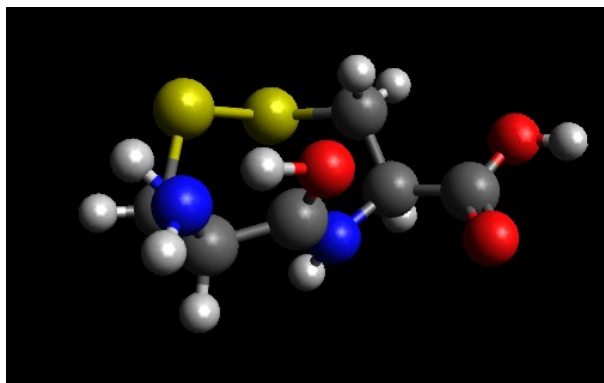
F2
24
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C      0.33221    -1.15675     0.20304
O     -0.06923    -1.37208    -1.03014
C      1.76425    -1.46408     0.58722
C      2.48829    -0.06588     0.67981
N      2.29876    -2.44472    -0.32290
H      1.76769    -1.89790     1.59369
H      3.11434    -2.91220     0.05325
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H	2.51865	-2.06636	-1.23825
H	3.56016	-0.23787	0.55927
H	2.33500	0.40061	1.65510
S	2.05684	1.17506	-0.62855
H	-0.53426	-2.21754	-1.15409
N	-0.42109	-0.46595	1.00485
C	-1.56718	0.37244	0.59740
H	-0.03096	-0.25000	1.91611
C	-2.72503	-0.48749	0.07386
C	-1.08307	1.45865	-0.39667
H	-1.91558	0.85974	1.50980
O	-3.78031	0.29052	-0.16733
O	-2.67951	-1.67862	-0.08307
H	-1.84146	2.24045	-0.46052
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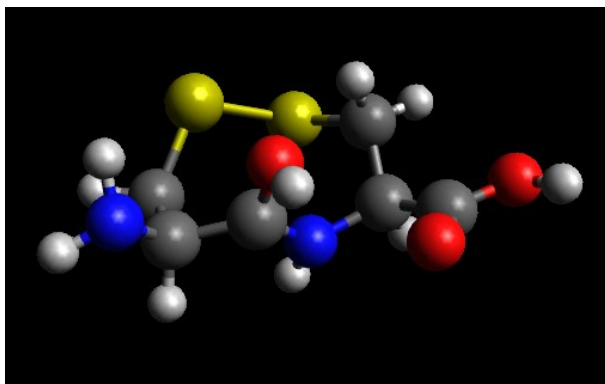
F3
24

C	0.34176	-1.22923	0.27336
O	-0.08024	-1.80149	-0.78745
C	1.79360	-1.40117	0.66349
C	2.45271	0.01008	0.71979
N	2.48243	-2.34309	-0.18462
H	1.77648	-1.77485	1.70316
H	3.36838	-2.00551	-0.53374
H	1.93054	-2.71923	-0.94318
H	3.53687	-0.11896	0.68589
H	2.23024	0.52835	1.65423
S	2.03279	1.14341	-0.68077
H	-1.09831	-1.72446	-0.89284
N	-0.43505	-0.46499	1.03213
C	-1.55422	0.39404	0.58183
H	0.01978	-0.10067	1.86068
C	-2.71380	-0.41089	0.00595
C	-1.06888	1.44263	-0.45735
H	-1.90886	0.90854	1.47381
O	-3.88088	0.12333	0.29239
O	-2.56901	-1.40076	-0.69335
H	-1.83738	2.21100	-0.56838
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S	0.45968	2.33363	0.05508
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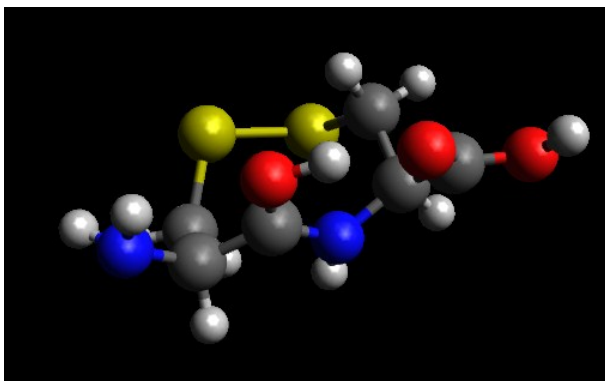
F4
24

C	-0.21736	1.25442	0.12714
O	0.32730	1.57619	-0.91112
C	-1.68410	1.56206	0.46836
C	-2.44453	0.23689	0.73625
N	-2.36365	2.34466	-0.53517
H	-1.69740	2.12807	1.40911
H	-2.24939	1.94971	-1.46366
H	-2.03277	3.30202	-0.56640
H	-3.51101	0.46717	0.71641
H	-2.21403	-0.19928	1.70919
S	-2.21435	-1.07380	-0.54531
H	2.18171	1.95481	0.44742
N	0.52105	0.52771	1.07259
C	1.47223	-0.45720	0.57760
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S21
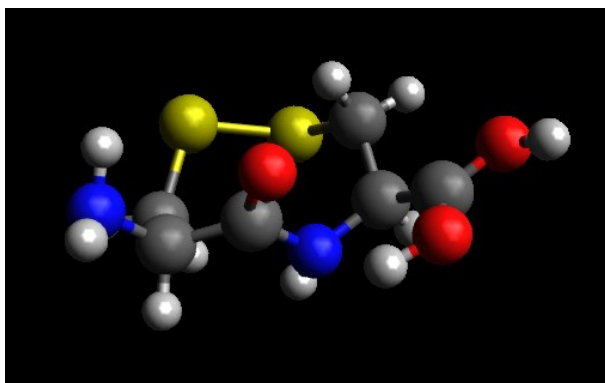
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H       1.60326    -2.28061    -0.62019
H       0.67178    -0.98872    -1.40449
S      -0.64539    -2.26505     0.18111
H       4.39941    -0.05709    -0.76982

F5
24
C       0.23043    -1.27104    -0.04517
O      -0.21179    -1.46412    -1.13823
C       1.65547    -1.57267     0.43123
C       2.36137    -0.25294     0.84071
N       2.44454    -2.29170    -0.53467
H       1.57576    -2.18844     1.33831
H       2.48626    -1.81299    -1.42918
H       2.10292    -3.23200    -0.69722
H       3.42305    -0.48232     0.94605
H       2.00761     0.14818     1.79166
S       2.26095     1.09139    -0.42046
N      -0.68431    -0.67862     0.95729
C      -1.50208     0.48788     0.49143
H      -0.24574    -0.50643     1.85799
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C      -0.85820     1.45031    -0.51443
H      -1.76381     1.05888     1.38971
O      -3.68563     0.44483    -0.58746
O      -2.90095    -1.39191     0.44779
H      -1.56579     2.25738    -0.71731
H      -0.60803     0.96788    -1.45694
S       0.63661     2.26102     0.19964
H      -4.47636    -0.09395    -0.77739
H      -1.80554    -1.45500     0.92034

F6
24
C      -0.52104     1.65979     0.03982
O       0.06760     2.27716    -0.71024
C      -2.51356     1.36300     0.41607
C      -2.52949    -0.07642     0.84565
N      -3.14483     1.72619    -0.69629
H      -2.52559     2.10330     1.21110
H      -3.24576     1.07478    -1.46598
H      -3.32193     2.69988    -0.90210
H      -3.55501    -0.29937     1.15949
H      -1.87650    -0.23174     1.70023
S      -2.09434    -1.28611    -0.48716
N       0.95233     0.49133     1.30714
C       1.81613    -0.43533     0.55844
H       0.48681     0.01308     2.07125
C       2.98259     0.37529    -0.01841
C       1.05690    -1.22523    -0.52042
H       2.27926    -1.15968     1.24241
O       3.71600    -0.35026    -0.86984
O       3.21373     1.51362     0.29513
H       1.73172    -1.94691    -0.98039
H       0.66531    -0.58138    -1.30748
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H       1.52046     1.25221     1.67984
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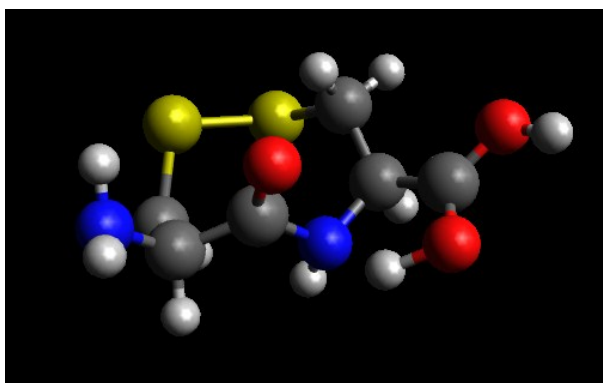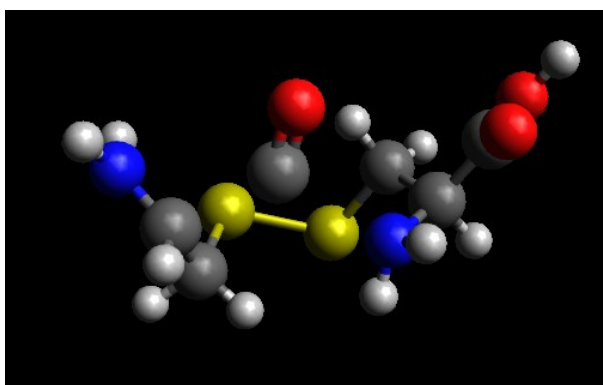
G1
22
C	3.07785	-1.39008	0.41336
C	2.23438	-0.28619	0.83651
N	3.33695	-1.68427	-0.82137
H	3.49961	-2.05185	1.16735
H	2.98022	-1.10051	-1.57689
H	3.88889	-2.49744	-1.07243
H	2.56286	0.09922	1.80442
H	1.19604	-0.72437	0.98140
S	2.02310	1.03421	-0.42831
N	-0.70475	-1.12617	0.83283
C	-1.67000	-0.06625	0.50471
H	-0.95489	-1.53840	1.72861
C	-2.94624	-0.66832	-0.10474
C	-1.10117	0.96071	-0.49103
H	-1.94667	0.46058	1.42021
O	-3.96688	0.19960	-0.07452
O	-2.99991	-1.77569	-0.57471
H	-1.87386	1.68716	-0.75242
H	-0.75980	0.48483	-1.41203
S	0.27148	1.98148	0.19154
H	-4.74316	-0.21002	-0.49049
H	-0.82263	-1.87762	0.15132
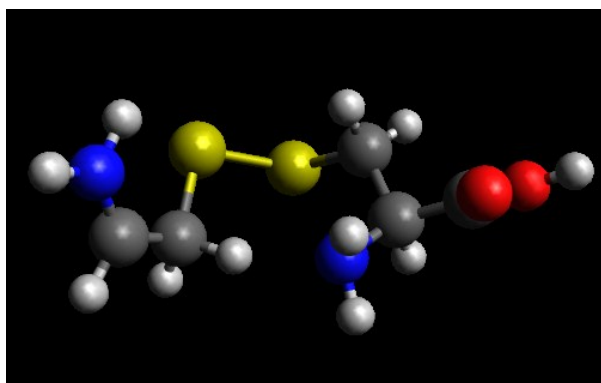
G2
22
C	-2.68569	1.31259	0.39732
N	-1.93011	1.95256	-0.42701
C	-2.12115	0.37455	1.37091
S	-2.02509	-1.31266	0.50971
S	-0.92884	-0.99954	-1.21930
C	0.84120	-1.00700	-0.71213
C	1.30938	0.18818	0.13464
C	2.83944	0.14621	0.29900
O	3.56823	1.04274	-0.02956
N	0.86741	1.48249	-0.41196
O	3.23583	-1.00266	0.86590
H	-3.76352	1.41252	0.30024
H	-0.86820	1.83403	-0.41651
H	-2.34510	2.53078	-1.15125
H	-2.79693	0.19371	2.20614
H	-1.13942	0.66712	1.73284
H	1.37503	2.22274	0.07262
H	0.89914	0.07749	1.14360
H	1.06420	-1.94062	-0.19930
H	1.35695	-1.02495	-1.67888
H	4.20201	-0.99032	0.96573
H	1.18611	1.55947	-1.37824
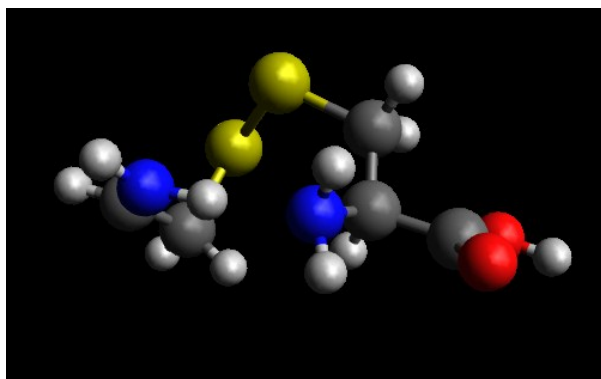
G3
22
C	-2.23356	1.56522	-0.03220
C	-2.09083	0.49505	0.95459
N	-1.21657	2.20035	-0.51117
H	-3.21195	1.80102	-0.44235
H	-0.24809	2.01535	-0.19526
H	-2.96681	0.41731	1.59931
H	-1.15618	0.52545	1.51852
S	-2.11735	-1.10024	-0.04257
H	-1.33558	2.87862	-1.25632
N	0.88410	-0.19372	1.93487
C	1.71769	-0.62088	0.81245
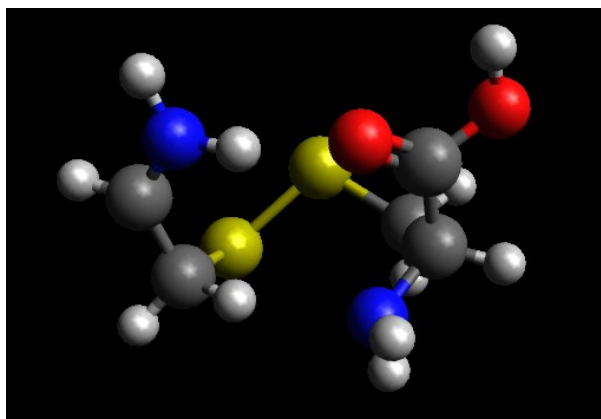
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H        0.71080       -0.98476        2.54959
C        2.10500        0.58978       -0.03035
C        0.99370       -1.67185       -0.05681
H        2.65988       -1.09163        1.12573
O        3.19318        0.34934       -0.75678
O        1.50200        1.64370       -0.06389
H        0.60598       -2.47408        0.57279
H        1.70126       -2.11433       -0.76226
S       -0.36445       -1.07112       -1.15663
H        3.39907        1.12667       -1.30207
H        1.36426        0.50745        2.49282

G4
22
C       -1.83120        1.60831        0.40147
C       -1.68464        0.32484        1.10134
N       -2.19459        1.72576       -0.82606
H       -1.60970        2.52378        0.94438
H       -2.40781        0.88933       -1.37005
H       -2.41212        0.28547        1.92309
H       -0.68291        0.30858        1.57994
S       -1.88166       -1.21413        0.12441
H       -2.25761        2.62840       -1.28415
N        1.19648       -0.35143        1.93477
C        1.88480       -0.46526        0.64864
H        1.25132       -1.23124        2.44028
C        1.81366        0.87572       -0.08242
C        1.26909       -1.58735       -0.21723
H        2.95007       -0.71133        0.75435
O        2.71889        0.93158       -1.06424
O        1.03661        1.76777        0.17154
H        1.07231       -2.47118        0.39202
H        1.97429       -1.87293       -1.00168
S       -0.23858       -1.17574       -1.19333
H        2.64091        1.78259       -1.52441
H        1.63767        0.35396        2.51861

H1
22
C       -2.10134        1.88842       -0.30086
C       -1.79041        0.97270        0.79871
N       -2.62309        1.50028       -1.41359
H       -1.86868        2.94666       -0.19581
H       -2.88873        0.51280       -1.50141
H       -2.81853        2.13816       -2.17793
H       -2.21411        1.37219        1.72857
H       -0.67716        0.96651        1.01182
S       -2.35589       -0.74168        0.58903
N        1.00892        0.27717        1.55206
C        1.64683       -0.44018        0.44360
H        0.83106       -0.34442        2.33415
C        2.84065        0.37947       -0.05877
C        0.66841       -0.69034       -0.72211
H        2.04262       -1.41002        0.76216
O        3.47579       -0.24282       -1.06264
O        3.15900        1.44882        0.39245
H        1.18238       -1.21115       -1.53451
H        0.29728        0.25026       -1.13600
S       -0.71364       -1.83891       -0.36401
H        4.23705        0.29508       -1.33478
H        1.62527        1.02281        1.87217
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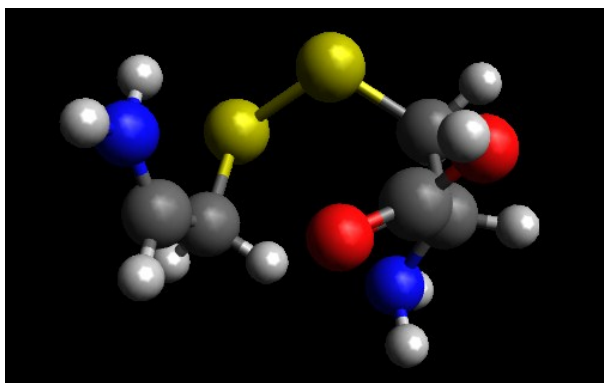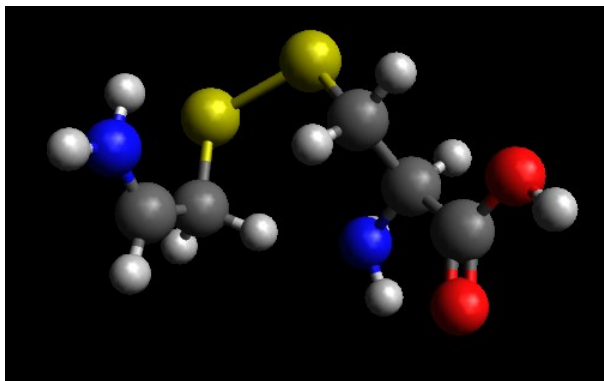
H2
22
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C    -2.82829     1.30815     0.14029
N    -1.86591     1.97922    -0.39445
C    -2.55820     0.24568     1.11167
S    -2.31175    -1.31485     0.07948
S    -0.61078    -0.93514    -1.04419
C     0.77955    -1.11933     0.15242
C     1.50437     0.19625     0.61124
C     2.94704     0.16854     0.08753
O     3.35246     0.89588    -0.78116
N     0.85656     1.45963     0.20553
O     3.67003    -0.78008     0.69631
H    -3.84234     1.48086    -0.20984
H    -0.85357     1.79200    -0.12661
H    -2.05881     2.64269    -1.13808
H    -3.42257     0.02246     1.73592
H    -1.67735     0.42357     1.72475
H     1.17839     2.18870     0.84054
H     1.55090     0.17188     1.70146
H     0.39387    -1.66354     1.01315
H     1.48487    -1.78486    -0.34633
H     4.56618    -0.78932     0.32119
H     1.25966     1.72134    -0.69845
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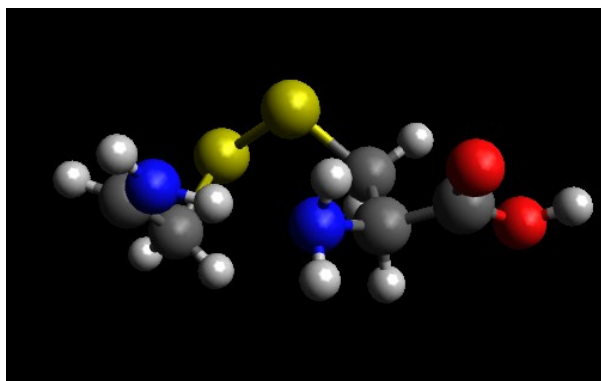
H3
22
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C    -2.04173     1.69090     0.25665
C    -1.91843     0.41774     0.97170
N    -1.62809     1.90171    -0.94377
H    -2.46247     2.54663     0.78199
H    -1.16954     1.15492    -1.47043
H    -2.67711     0.35095     1.75470
H    -0.91659     0.42255     1.48008
S    -2.00393    -1.15728     0.02825
H    -1.67435     2.82254    -1.36625
N     0.89737    -0.23936     1.95600
C     1.74838    -0.54036     0.80257
H     0.83017    -1.05392     2.56057
C     1.97788     0.73613    -0.00265
C     1.13442    -1.63856    -0.08553
H     2.74146    -0.90907     1.09589
O     2.95309     0.56139    -0.90436
O     1.35788     1.76245     0.13711
H     0.82000    -2.49027     0.51996
H     1.87978    -1.99108    -0.80206
S    -0.27936    -1.15355    -1.17010
H     3.08344     1.38658    -1.39832
H     1.30218     0.51129     2.50933
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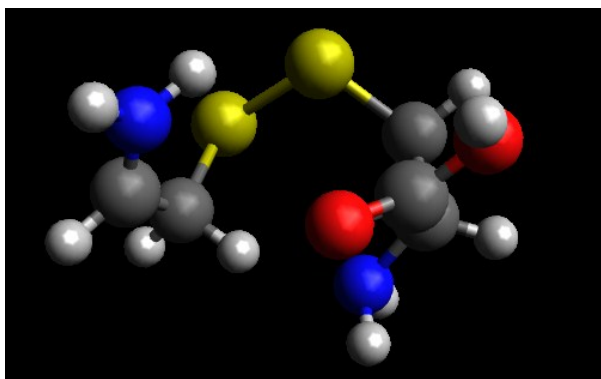
H4
22
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C    -2.14084     1.61910     0.12889
C    -1.85592     0.46966     0.89443
N    -2.18162     1.68593    -1.18056
H    -2.28068     2.56346     0.65029
H    -2.10536     0.84688    -1.74404
H    -2.30342     0.48729     1.88832
H    -0.53062     0.51981     1.28459
S    -1.96737    -1.18121     0.15638
H    -2.31566     2.56468    -1.66043
N     0.71104     0.35349     1.78551
C     1.69378    -0.31532     0.89302
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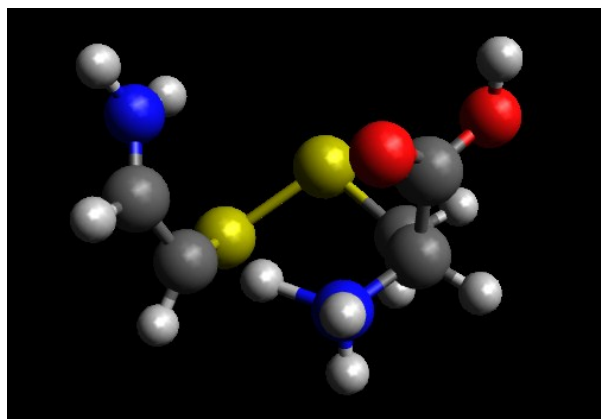
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H      0.61160     -0.15959      2.66053
C      2.14550      0.72422     -0.13408
C      1.13665     -1.59837      0.26607
H      2.58307     -0.58929      1.47495
O      2.97780      0.19205     -1.02999
O      1.80558      1.87935     -0.09579
H      0.77479     -2.28379      1.03470
H      1.93721     -2.09962     -0.28103
S     -0.19078     -1.33588     -0.98018
H      3.27408      0.88341     -1.64443
H      1.03752      1.29742      1.99886
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H5
22
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C     -2.63426      1.65613      0.34756
C     -2.49653      0.27245      0.83571
N     -2.41484      2.00514     -0.86898
H     -2.93020      2.43693      1.04618
H     -2.13035      1.28620     -1.54136
H     -2.49430      2.96785     -1.18169
H     -3.38115      0.01682      1.42969
H     -1.62823      0.28806      1.51079
S     -2.18637     -0.97497     -0.48232
N      0.67615      1.04529      0.93666
C      1.58594     -0.03953      0.54897
H      0.92535      1.36273      1.86996
C      2.88039      0.52074     -0.06187
C      0.95919     -0.99578     -0.48401
H      1.85434     -0.62276      1.43239
O      3.86454     -0.38895     -0.07075
O      2.97552      1.63646     -0.50703
H      1.68931     -1.75281     -0.77975
H      0.64406     -0.46663     -1.38502
S     -0.46332     -1.97335      0.15662
H      4.65066     -0.00059     -0.48863
H      0.87747      1.84014      0.32904
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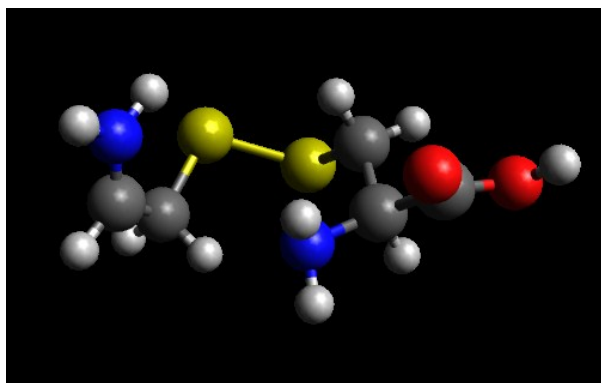
D1
22
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C     -0.27624      1.67738      0.22140
C     -1.78990      1.46434      0.33915
N      0.25790      1.58688     -1.07088
H     -0.01274      2.61721      0.71044
H     -0.38877      1.28617     -1.78885
H      0.86720      2.33777     -1.36067
H     -2.27960      2.34054     -0.09554
H     -2.10105      1.40136      1.38439
S     -2.45818      0.04214     -0.60079
N      0.45284      0.61500      1.20240
C      1.08439     -0.62441      0.61811
H     -0.21446      0.32770      1.92201
C      2.41352     -0.17318      0.00318
C      0.16301     -1.47641     -0.26514
H      1.36265     -1.21928      1.49596
O      2.88166     -1.05709     -0.86959
O      2.96694      0.83666      0.35944
H      0.54987     -2.49669     -0.27490
H      0.13112     -1.12175     -1.29166
S     -1.55641     -1.58429      0.38150
H      3.75921     -0.77582     -1.17965
H      1.22725      1.12119      1.64739
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S26
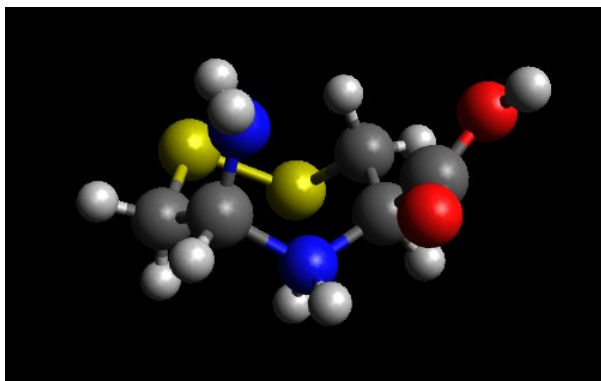
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D2
22
C        -0.47084        1.56648        0.67676
C        -1.95349        1.16027        0.61751
N        -0.03066        2.02901       -0.74441
H        -0.40697        2.46262        1.29626
H        -0.53962        1.46233       -1.43925
H        -0.23849        3.01433       -0.91677
H        -2.57030        2.03011        0.36662
H        -2.24305        0.80836        1.60695
S        -2.37693       -0.10234       -0.63438
N         0.42808        0.61974        1.25337
C         1.11206       -0.52107        0.64680
H         0.99819        1.03387        1.97633
C         2.38536       -0.07982       -0.09313
C         0.31598       -1.40487       -0.34668
H         1.41924       -1.15774        1.47904
O         3.36088       -0.97075       -0.00961
O         2.47888        0.96538       -0.71488
H         0.83347       -2.36331       -0.42747
H         0.28756       -0.97369       -1.34942
S        -1.40456       -1.79239        0.13473
H         4.13168       -0.67020       -0.52146
H         0.99776        1.84479       -0.85061


D3
22
C        -1.73754        0.65307        1.09121
S        -2.37519       -0.61011       -0.08724
S        -0.87943       -2.08087       -0.02870
C         0.58791       -1.20542       -0.68064
C         1.08583       -0.06451        0.23062
C         2.59916        0.17762        0.07266
O         3.08467        1.26934       -0.07889
C        -0.79697        1.67580        0.44761
N        -1.56545        2.23490       -0.82414
N         0.46074        1.23732       -0.02219
O         3.29091       -0.95964        0.16619
H        -0.71821        2.55777        1.09159
H        -1.88593        1.40592       -1.35250
H        -2.37563        2.81761       -0.59305
H        -2.61634        1.17053        1.48619
H        -1.24504        0.16226        1.93094
H         1.18033        1.95637       -0.00547
H         0.96462       -0.38565        1.27371
H         1.33975       -1.99665       -0.72127
H         0.40766       -0.84457       -1.69428
H         4.23968       -0.76104        0.10244
H        -0.91893        2.77059       -1.40623


P1
22
C        -0.44166        1.67672        0.39873
C        -1.92404        1.25974        0.51188
N         0.05142        1.90680       -0.95125
H        -0.36447        2.61931        0.94979
H        -0.47442        1.37099       -1.63795
H        -0.01332        2.88368       -1.21474
H        -2.54497        2.11102        0.21452
H        -2.17408        1.00852        1.54439
S        -2.46757       -0.09973       -0.58166
N         0.53216        0.79861        1.10756
C         1.05077       -0.47501        0.62294
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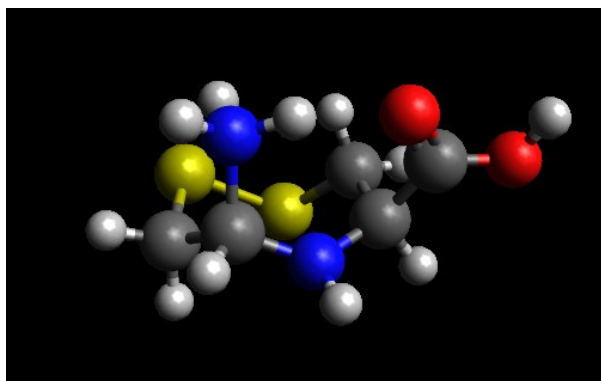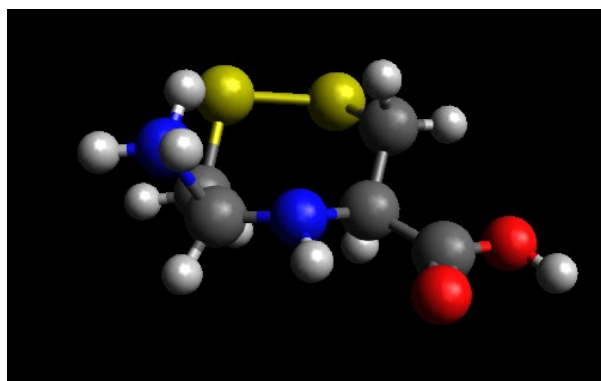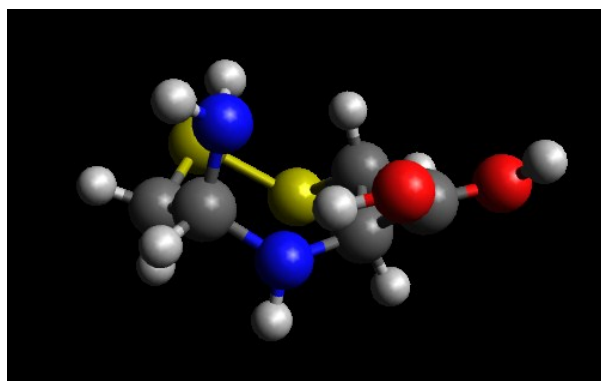

S27

H	0.32370	0.74731	2.09664
C	2.40561	-0.20766	-0.00253
C	0.23469	-1.39749	-0.33845
H	1.27301	-1.08370	1.50676
O	3.13893	-1.20253	-0.35716
O	2.82668	0.97418	-0.17593
H	0.74231	-2.36273	-0.40072
H	0.17334	-0.98287	-1.34418
S	-1.45619	-1.72567	0.26395
H	3.99041	-0.92900	-0.74795
H	2.08662	1.57481	0.13192

P2
22

C	-1.97716	0.88143	0.86412
S	-2.47761	-0.39116	-0.35312
S	-1.12815	-1.92720	0.08355
C	0.44533	-1.18974	-0.49194
C	1.14462	-0.26471	0.51976
C	2.57185	0.01393	0.00540
O	2.96329	1.10306	-0.33166
C	-0.67420	1.63099	0.56190
N	-0.80205	2.12221	-1.02165
N	0.55288	1.04649	0.82215
O	3.30259	-1.10267	-0.01667
H	-0.69416	2.59354	1.07424
H	0.12747	2.36247	-1.37191
H	-1.19056	1.33538	-1.56137
H	-2.80430	1.59716	0.88606
H	-1.89401	0.43295	1.85450
H	1.28164	1.72558	1.00008
H	1.24879	-0.83025	1.45218
H	1.10226	-2.04859	-0.64477
H	0.29517	-0.72077	-1.46753
H	4.19497	-0.89747	-0.34102
H	-1.42048	2.92835	-1.13967
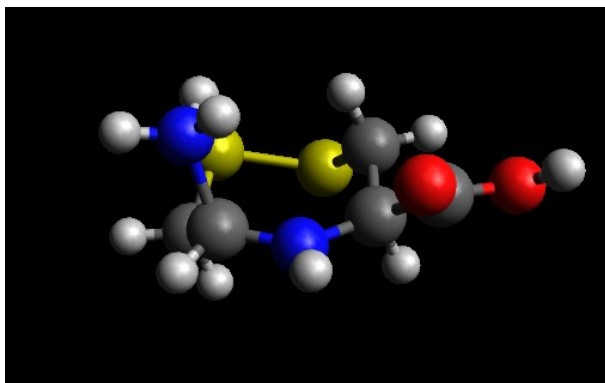
I
18

C	-1.82563	1.30649	0.76378
S	-2.52973	0.04384	-0.40425
S	-1.36349	-1.61257	0.14288
C	0.29539	-1.14188	-0.48125
C	0.97606	0.00300	0.29513
C	2.49111	0.04938	0.02211
O	3.01803	0.98435	-0.52446
C	-0.65695	1.89978	0.07598
N	0.49223	1.34401	-0.10581
O	3.08900	-1.05060	0.45645
H	-0.76027	2.88681	-0.37034
H	-2.58884	2.06404	0.93782
H	-1.57177	0.81130	1.70231
H	1.22019	1.86173	-0.61459
H	0.82184	-0.12870	1.36975
H	0.89115	-2.04542	-0.33540
H	0.25437	-0.92292	-1.54965
H	4.04315	-1.00600	0.27232
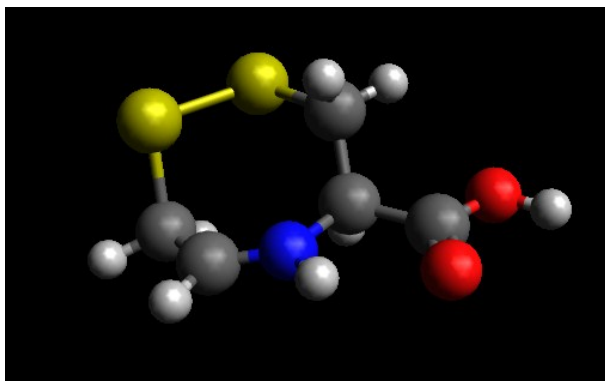
J1
22

C	-2.80037	1.37592	0.08133
C	-2.20612	0.40453	0.84718
N	-3.06172	1.31791	-1.22976

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H      -3.07682     2.31175     0.55995
H      -2.93578     0.45455    -1.73974
H      -2.20450     0.53722     1.92358
H      -0.15653     0.80611     1.00064
S      -1.95894    -1.24451     0.25858
H      -3.55609     2.06422    -1.69071
N       0.80693     0.96074     1.39045
C       1.81007    -0.06222     0.90830
H       0.72991     0.97812     2.40829
C       2.56597     0.63606    -0.23279
C       1.16112    -1.39772     0.53840
H       2.53030    -0.21585     1.71860
O       3.36753    -0.19881    -0.87551
O       2.44062     1.81611    -0.44750
H       0.69994    -1.86306     1.41105
H       1.94504    -2.06435     0.17641
S      -0.09291    -1.24287    -0.79889
H       3.85780     0.27898    -1.56615
H       1.13071     1.88198     1.04787


J2
22
C      -2.20236     1.76084    -0.16166
C      -2.78277     0.58797     0.08625
N      -0.77051     1.92349    -0.42676
H      -2.77035     2.67997    -0.15437
H      -0.45459     1.41942    -1.26162
H      -3.84926     0.61448     0.29817
H      -0.17656     1.51367     0.38561
S      -2.26466    -1.09652     0.12422
H      -0.51928     2.90470    -0.54890
N       0.65918     0.69432     1.60098
C       1.57287    -0.29657     1.00387
H       0.04718     0.24012     2.27574
C       2.35076     0.37138    -0.13200
C       0.81453    -1.53619     0.49847
H       2.31180    -0.66316     1.72717
O       3.39748    -0.36998    -0.49785
O       2.04206     1.42227    -0.64219
H       0.29745    -2.02873     1.32365
H       1.52999    -2.25000     0.08644
S      -0.40570    -1.27572    -0.86712
H       3.86297     0.06517    -1.23122
H       1.19117     1.39269     2.11680


J3
22
C      -2.44895     1.61485    -0.44053
C      -2.86207     0.25090    -0.62346
N      -1.41850     1.98366     0.25294
H      -3.01425     2.39699    -0.94284
H       0.43274    -1.10087    -1.62540
H      -3.55445     0.07709    -1.44300
H      -0.75835     1.31700     0.72353
S      -2.33114    -0.99691     0.30145
H      -1.16382     2.96349     0.29363
N       0.62086     0.46666     1.68492
C       1.76570    -0.04149     0.91774
H       0.25289    -0.25691     2.29629
C       2.04601     0.90632    -0.25219
C       1.60480    -1.50335     0.47052
H       2.68958    -0.04353     1.51462
O       3.09974     0.48885    -0.96875
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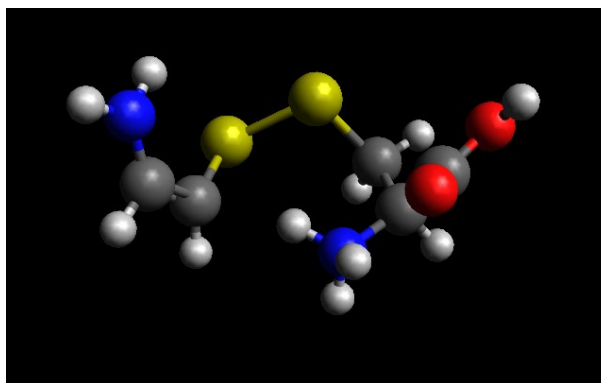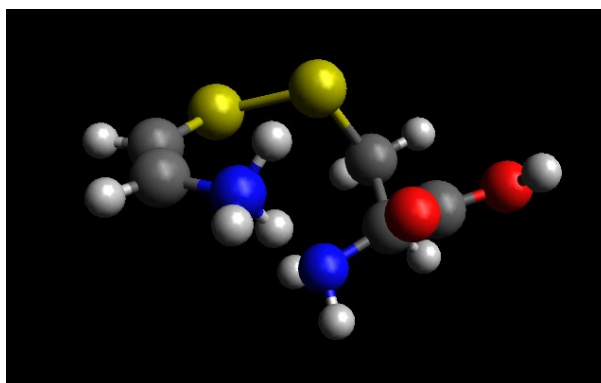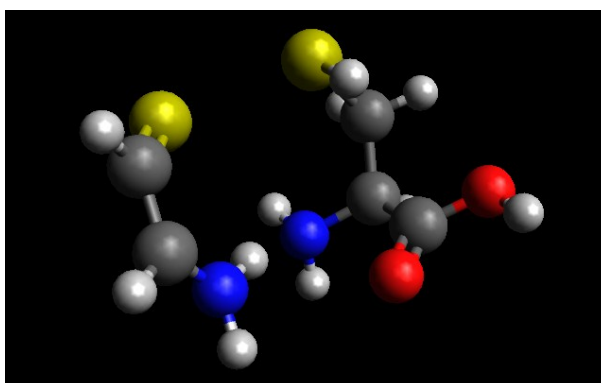

S29

O	1.41736	1.90651	-0.49139
H	1.48561	-2.14457	1.34602
H	2.50990	-1.82046	-0.04706
S	0.18861	-1.96728	-0.61733
H	3.28677	1.13554	-1.66848
H	0.92752	1.22480	2.29024

J4
22

C	2.89646	-1.12875	-0.56402
C	2.99139	0.04072	0.31686
N	1.76805	-1.66740	-0.85591
H	3.84132	-1.51462	-0.95208
H	-3.26525	1.10808	1.43690
H	2.04832	0.45724	0.66892
H	0.20375	-1.36699	-0.32398
S	4.41969	0.68614	0.73690
H	1.88943	-2.47066	-1.47476
N	-0.83749	-1.32197	-0.00551
C	-1.66852	-0.38178	-0.82334
H	-0.87857	-1.02565	0.97759
C	-1.05956	1.00940	-0.65291
C	-3.15224	-0.43921	-0.41004
H	-1.57416	-0.67857	-1.87145
O	-1.66259	1.89023	-1.44871
O	-0.16582	1.24874	0.11712
H	-3.56326	-1.42011	-0.65839
H	-3.71063	0.30066	-0.98121
S	-3.44677	-0.22859	1.39042
H	-1.26706	2.76939	-1.32420
H	-1.22239	-2.26780	-0.05102
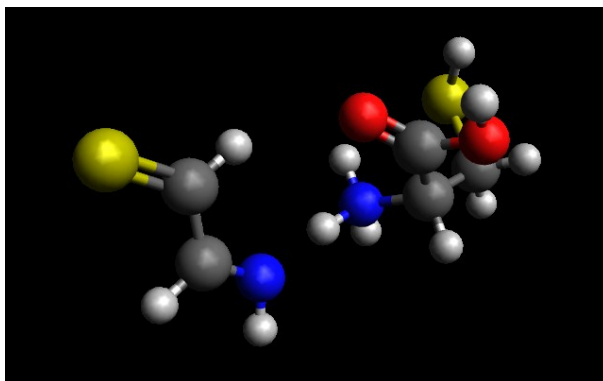
K2
22

C	-2.53540	1.48049	0.22441
C	-2.62881	0.24696	0.76120
N	-1.95023	1.79552	-0.98946
H	-2.85389	2.33414	0.81591
H	-1.96950	1.06464	-1.69324
H	-3.04731	0.12677	1.75266
H	0.15602	1.57016	1.57841
S	-2.27795	-1.28739	-0.05909
H	-2.20226	2.69742	-1.37248
N	0.71285	1.35409	0.74987
C	1.56607	0.12488	0.93200
H	1.32287	2.14446	0.49938
C	2.72046	0.29147	-0.06846
C	0.74487	-1.16461	0.80100
H	2.00622	0.17705	1.93312
O	3.42803	-0.82222	-0.19115
O	2.93680	1.34271	-0.61566
H	0.07303	-1.28223	1.65192
H	1.43218	-2.00998	0.78672
S	-0.25989	-1.17842	-0.74614
H	4.17655	-0.67420	-0.79421
H	0.05144	1.21835	-0.04375
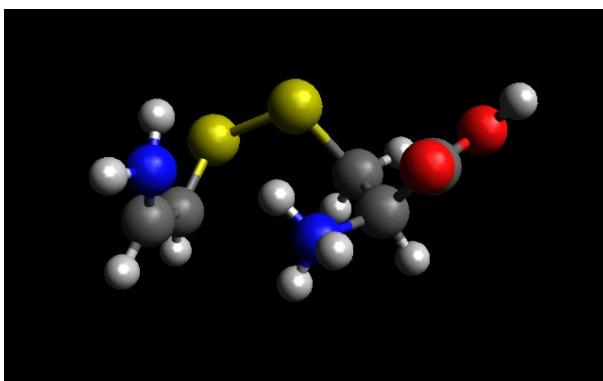
K3
22

C	-2.29025	1.66655	-0.37092
C	-2.97259	0.51170	-0.19397
N	-0.93586	1.78533	-0.10364
H	-2.76666	2.50289	-0.87085
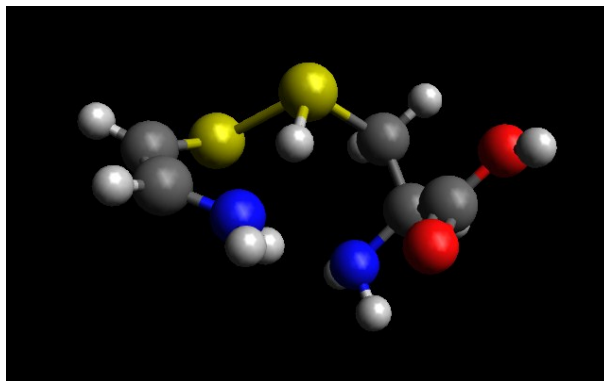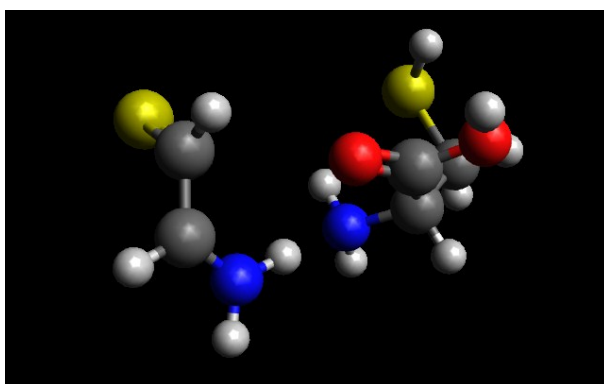
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H    -0.34901     0.40744    -0.81295
H    -3.99773     0.41564    -0.52534
H    -0.56299     1.37961     0.77060
S    -2.22530    -0.94106     0.42859
H    -0.51649     2.68492    -0.30912
N     0.85196     0.31692     1.76166
C     1.68645    -0.49417     0.87750
H     0.50082    -0.23875     2.53654
C     2.40902     0.42735    -0.11221
C     0.88594    -1.59445     0.16660
H     2.48332    -1.03714     1.40977
O     3.18839    -0.27805    -0.94463
O     2.29301     1.62431    -0.12739
H     0.41695    -2.26470     0.88919
H     1.53630    -2.18476    -0.47912
S    -0.48678    -1.03766    -0.95790
H     3.66927     0.33212    -1.52774
H     1.40411     1.07462     2.15596


K4
22
C     2.91138    -0.97747     0.31568
C     2.67096     0.04099    -0.72874
N     2.06480    -1.28372     1.22491
H     3.88823    -1.46317     0.32829
H    -2.43971     1.46576    -1.36104
H     2.32465    -0.31101    -1.70008
H     1.06240    -0.86540     1.27761
S     3.03472     1.57627    -0.38163
H     2.34089    -1.94579     1.94544
N    -0.46288    -0.16513     1.49062
C    -1.59942    -0.73913     0.74623
H    -0.34465     0.80230     1.17749
C    -1.11161    -1.20011    -0.62633
C    -2.82140     0.20104     0.65308
H    -1.92296    -1.64882     1.26614
O    -2.11885    -1.65961    -1.37486
O     0.04100    -1.17800    -0.99160
H    -3.18601     0.40809     1.66074
H    -3.62993    -0.27060     0.09800
S    -2.44137     1.84890    -0.06727
H    -1.76919    -1.97345    -2.22442
H    -0.70735    -0.10979     2.47766


L
15
H    -1.29976    -1.20662    -1.28108
H    -0.78158     1.62822    -0.51709
N     0.03254     1.77837     0.11467
C     0.31667     0.45752     0.78597
H    -0.17619     2.53331     0.77068
C     1.40244    -0.20064    -0.08013
C    -0.97678    -0.36126     0.95834
H     0.75896     0.66184     1.76501
O     1.62974    -1.45107     0.28975
O     1.96383     0.40471    -0.95760
H    -1.58933     0.07456     1.74945
H    -0.71941    -1.37437     1.26100
S    -2.05169    -0.37257    -0.53031
H     2.35587    -1.82961    -0.23584
H     0.84818     2.02235    -0.47209
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