Supporting Information:

Chemiluminescent Detection of Enzymatically-Produced Hydrogen Sulfide: Substrate Hydrogen Bonding Influences Selectivity for H_2S over Biological Thiols

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Selectivity Data

Table S1. Selectivity of CLSS-1 and CLSS-2 with 33 equiv. of selected biologically-relevant reactive sulfur, oxygen, and nitrogen species.

	Normalized Luminescence (CL/CL_0)	
Reactant	CLSS-1	CLSS-2
Blank	1.0 ± 0.1	1.0 ± 0.3
H_2S	128 ± 16	45 ± 3
Cys	81 ± 5	1.5 ± 0.03
GSH	94 ± 12	3.7 ± 0.9
Hcy	57 ± 3	3.3 ± 0.5
NAC	37 ± 19	3.3 ± 0.4
Toluenethiol (TolSH)	0.8 ± 0.1	1.9 ± 0.4
2-mercaptoethanol (2-ME)	6.6 ± 3.2	1.7 ± 0.08
$S_2O_3^{2-}$	5.9 ± 1.1	2.2 ± 0.6
SO_4^{2-}	0.8 ± 0.3	1.5 ± 0.3
NO_2^-	0.9 ± 0.2	3.2 ± 0.6
SNAP (NO)	0.05 ± 0.01	1.5 ± 0.5
$ONOO^-$	0.6 ± 0.2	4.0 ± 0.2
HNO	9.1 ± 0.2	3.3 ± 0.2

Photoactivation of Azides

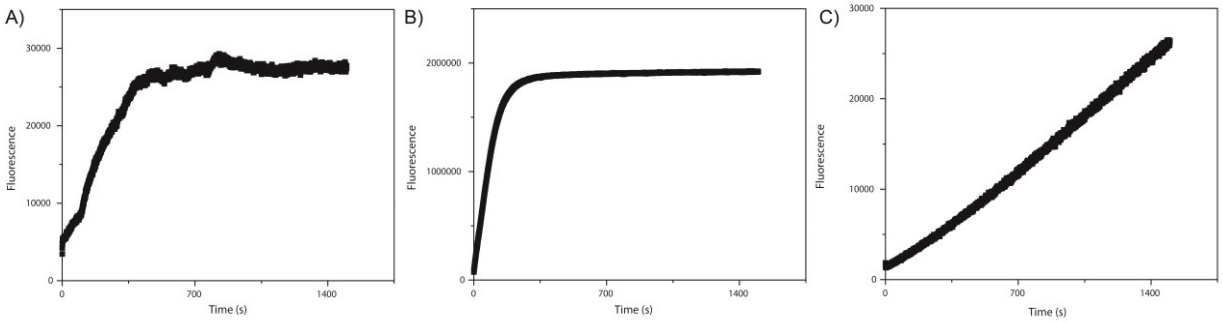

Figure S1. Photoactivation of (a) HSN2 (λ_{ex}= 435 nm, λ_{em}= 550 nm), (b) C-7Az (λ_{ex}= 340 nm, λ_{em}=445 nm), and (c) DNS-Az (λ_{ex}= 340 nm, λ_{em}= 510 nm). Measurements performed on 5 μM probe in pH 7.4 PIPES buffer (50 mM PIPES, 100 mM KCl, pH 7.4). Slits: excitation= 5 nm, emission= 1.4 nm.

NMR Spectra

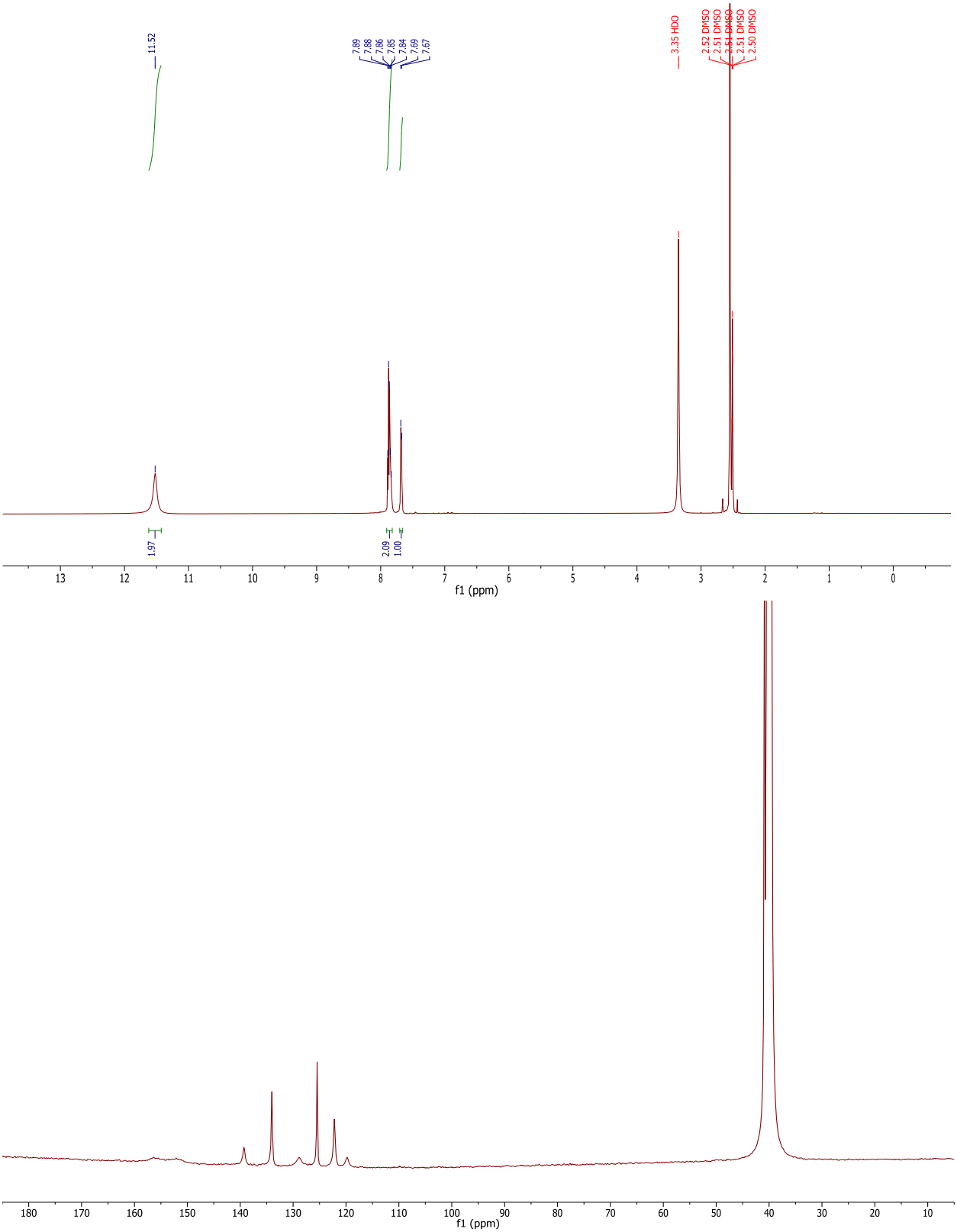

Figure S2. ^{1}H (600 MHz, DMSO) and $^{13}C\{^{1}H\}$ (150 MHz, DMSO) NMR spectra of CLSS-1.

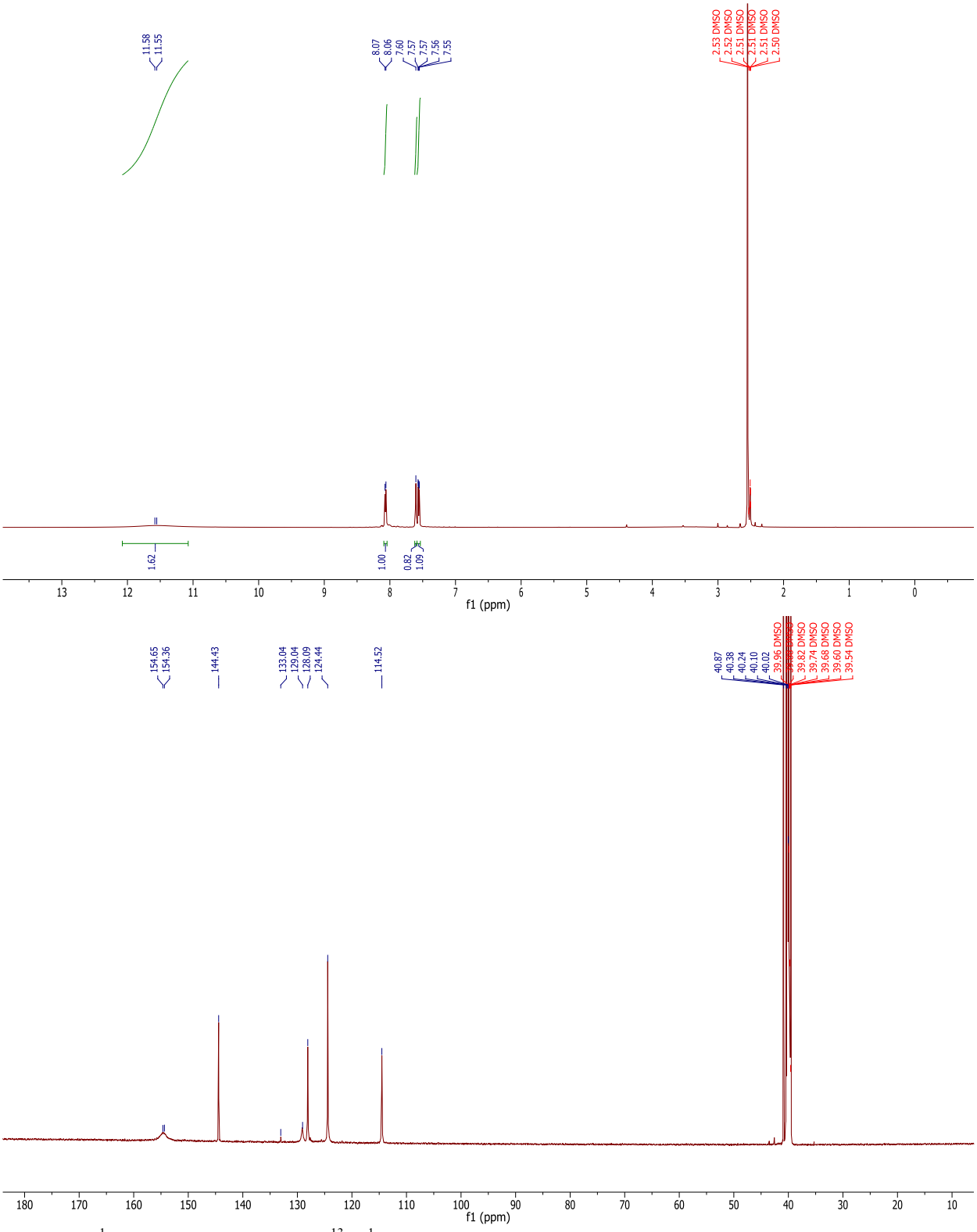

Figure S3. ^{1}H (600 MHz, DMSO) and $^{13}C\{^{1}H\}$ (150 MHz, DMSO) NMR spectra of CLSS-2.

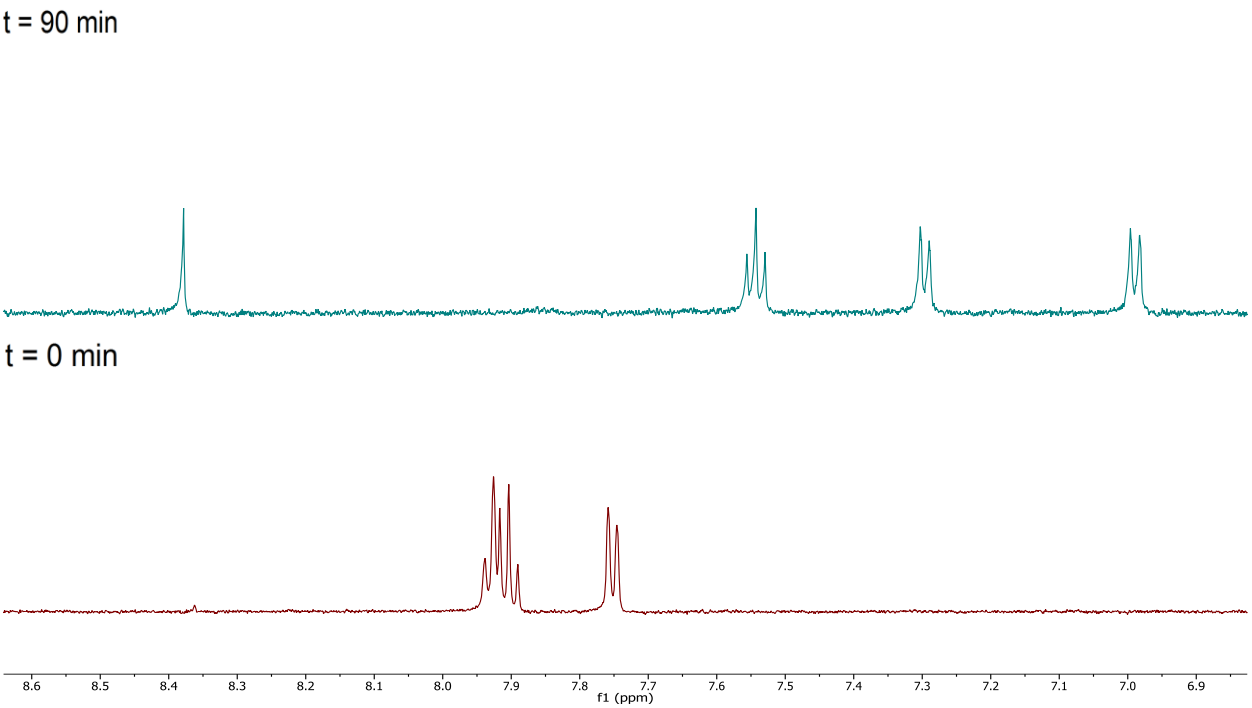

Figure S4. ^{1}H NMR spectra (600 MHz, 1% DMSO in D_2O) of CLSS-1 before (bottom) and 90 min after (top) reaction with H_2S showing clean conversion to the parent amine.

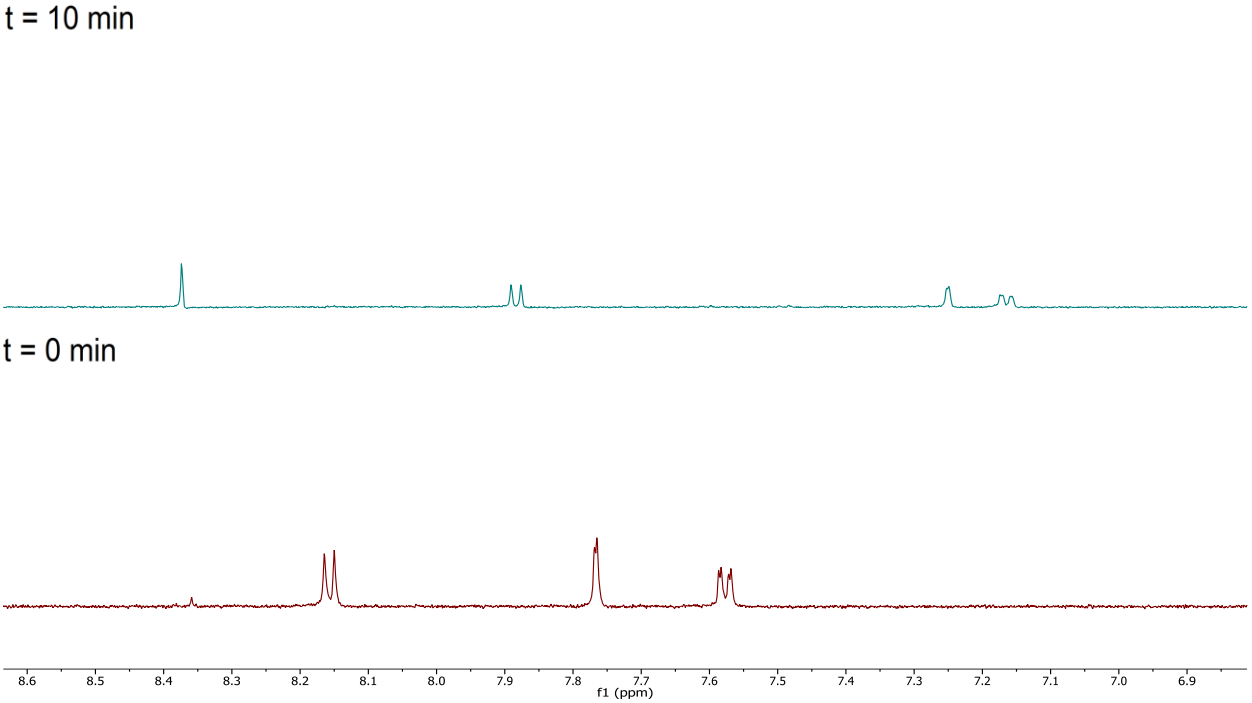

Figure S5. ^{1}H NMR spectra (600 MHz, 1% DMSO in D_2O) of CLSS-2 before (bottom) and 10 min after (top) reaction with H_2S showing clean conversion to the parent amine.

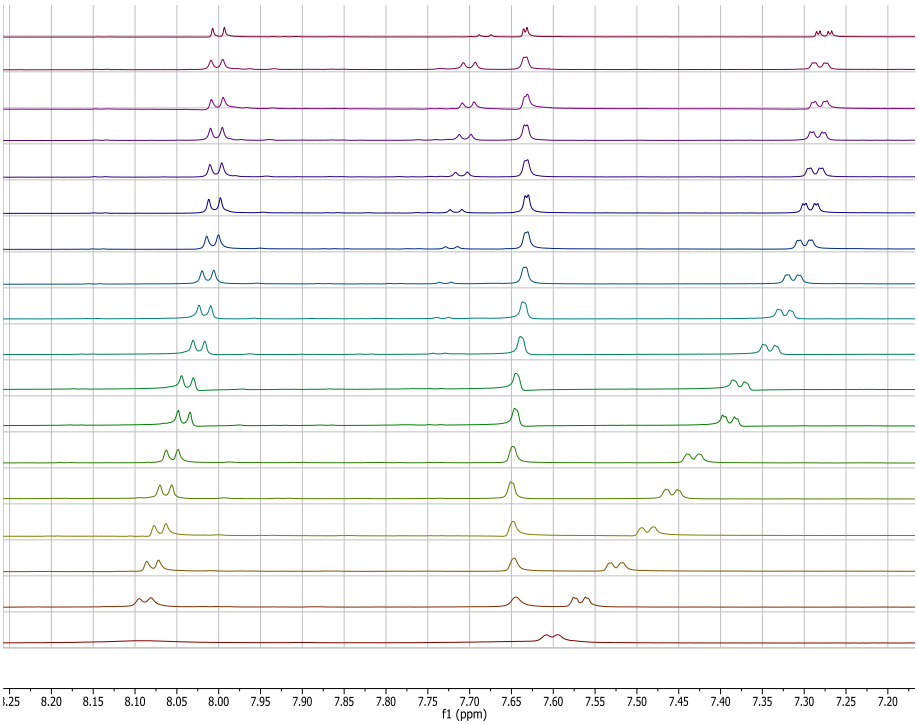

Figure S6. Representative titration of 10 mM CLSS-2 with 0-200 mM TBA-Ser.

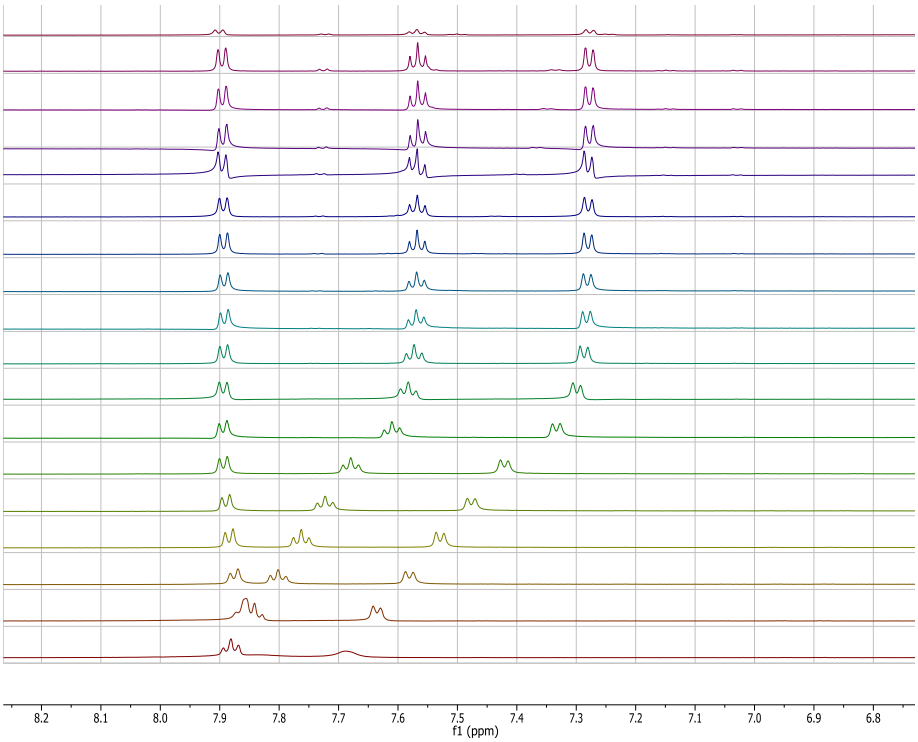

Figure S7. Representative titration of 10 mM CLSS-1 with 0-200 mM TBA-Val

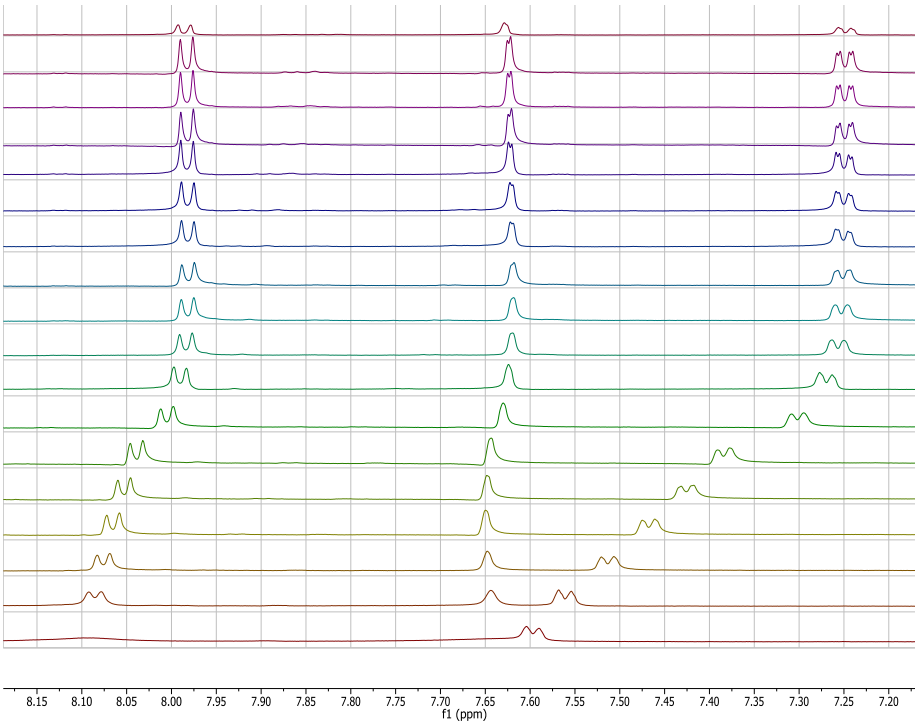

Figure S8. Representative titration of 10 mM CLSS-2 with 0-200 mM TBA-Val

Tabulated NMR Titration Data

Table S2. Tabulated titration data for CLSS-1 with TBA-Ser.

		Run 1		Run 2		Run 3	
[CLSS-1] (M)	[TBA-Ser] (M)	Proton 1 (ppm)	Proton 2 (ppm)	Proton 1 (ppm)	Proton 2 (ppm)	Proton 1 (ppm)	Proton 2 (ppm)
0.010091	0	7.883	7.687	7.881	7.685	7.898	7.694
0.010091	0.001353	7.847	7.643	7.841	7.636	7.84	7.634
0.010091	0.002688	7.818	7.602	7.805	7.587	7.803	7.583
0.010091	0.004006	7.789	7.563	7.775	7.548	7.772	7.542
0.010091	0.005307	7.766	7.533	7.751	7.514	7.748	7.51
0.010091	0.006591	7.746	7.507	7.731	7.485	7.727	7.482
0.010091	0.00973	7.707	7.457	7.691	7.437	7.69	7.434
0.010091	0.01277	7.681	7.423	7.667	7.405	7.665	7.403
0.010091	0.018575	7.649	7.383	7.636	7.367	7.636	7.366
0.010091	0.024038	7.633	7.361	7.621	7.348	7.62	7.346
0.010091	0.029189	7.622	7.348	7.612	7.335	7.611	7.335
0.010091	0.040865	7.607	7.329	7.602	7.318	7.598	7.319
0.010091	0.051081	7.6	7.32	7.591	7.31	7.591	7.31
0.010091	0.068108	7.593	7.311	7.586	7.303	7.585	7.302
0.010091	0.08173	7.589	7.307	7.584	7.299	7.583	7.298
0.010091	0.092874	7.587	7.303	7.582	7.297	7.581	7.296
0.010091	0.102162	7.587	7.302	7.58	7.296	7.579	7.294
0.010091	0.204324	7.579	7.287	7.576	7.288	7.577	7.287

Table S3. Tabulated titration data for CLSS-2 with TBA-Ser.

		Run 1		Run 2		Run 3	
[CLSS-2] (M)	[TBA-Ser] (M)	Proton 1 (ppm)	Proton 2 (ppm)	Proton 1 (ppm)	Proton 2 (ppm)	Proton 1 (ppm)	Proton 2 (ppm)
0.010091	0	7.598	8.094	7.599	8.109	7.601	8.093
0.010091	0.001339	7.577	8.088	7.568	8.087	7.567	8.088
0.010091	0.00266	7.542	8.082	7.515	8.074	7.525	8.077
0.010091	0.003964	7.509	8.075	7.47	8.063	7.487	8.07
0.010091	0.005252	7.482	8.069	7.438	8.054	7.458	8.063
0.010091	0.006522	7.455	8.061	7.416	8.048	7.432	8.056
0.010091	0.009628					7.389	8.042
0.010091	0.012636	7.383	8.039	7.354	8.026	7.377	8.036
0.010091	0.01838	7.35	8.027	7.326	8.016	7.341	8.024
0.010091	0.023786	7.33	8.021	7.313	8.011	7.323	8.018
0.010091	0.028883	7.321	8.016	7.304	8.006	7.313	8.014
0.010091	0.040437	7.304	8.009	7.294	8.004	7.299	8.007
0.010091	0.050546	7.297	8.008	7.288	8.003	7.292	8.005
0.010091	0.067395	7.291	8.004	7.283	7.999	7.286	8.004
0.010091	0.080874	7.287	8.003	7.28	7.999	7.2835	8.003
0.010091	0.091902			7.278	7.999	7.2815	8.002
0.010091	0.101092			7.277	7.998	7.28	8.002
0.010091	0.202184	7.275	7.999	7.276	7.998	7.275	8.001

Table S4. Tabulated titration data for CLSS-1 with TBA-Val

		Run 1		Run 2		Run 3	
[CLSS-1] (M)	[TBA-Val] (M)	Proton 1 (ppm)	Proton 2 (ppm)	Proton 1 (ppm)	Proton 2 (ppm)	Proton 1 (ppm)	Proton 2 (ppm)
0.010091	0	7.881	7.685	7.884	7.686	7.883	7.684
0.010091	0.001427	7.841	7.635	7.843	7.638	7.838	7.629
0.010091	0.002835	7.801	7.581	7.802	7.582	7.796	7.573
0.010091	0.004225	7.762	7.528	7.765	7.532	7.755	7.518
0.010091	0.005597	7.722	7.475	7.728	7.483	7.716	7.468
0.010091	0.006951	7.679	7.422	7.686	7.43	7.675	7.414
0.010091	0.01026	7.609	7.332	7.61	7.333	7.606	7.329
0.010091	0.013467	7.581	7.298	7.582	7.3	7.583	7.299
0.010091	0.019588	7.571	7.285	7.573	7.288	7.575	7.289
0.010091	0.025349	7.569	7.282	7.57	7.283	7.573	7.287
0.010091	0.030781	7.569	7.282	7.569	7.282	7.571	7.284
0.010091	0.043093	7.568	7.281	7.567	7.28	7.571	7.283
0.010091	0.053867	7.567	7.279	7.567	7.28	7.571	7.282
0.010091	0.071822	7.567	7.279	7.567	7.279	7.571	7.282
0.010091	0.086187	7.566	7.277	7.567	7.279	7.571	7.282
0.010091	0.097939	7.566	7.277	7.567	7.279	7.571	7.282
0.010091	0.107733	7.566	7.277	7.567	7.279		
0.010091	0.215466	7.566	7.277	7.567	7.279	7.568	7.277

Table S5. Tabulated titration data for CLSS-2 with TBA-Val.

		Run 1		Run 2		Run 3	
[CLSS-2] (M)	[TBA-Val] (M)	Proton 1 (ppm)	Proton 2 (ppm)	Proton 1 (ppm)	Proton 2 (ppm)	Proton 1 (ppm)	Proton 2 (ppm)
0.010152	0	8.101	7.598	8.103	7.6	8.092	7.597
0.010152	0.001367	8.088	7.563	8.088	7.564	8.084	7.559
0.010152	0.002715	8.079	7.519	8.082	7.521	8.075	7.513
0.010152	0.004046	8.067	7.476	8.067	7.476	8.066	7.467
0.010152	0.00536	8.058	7.433	8.056	7.433	8.053	7.424
0.010152	0.006657	8.04	7.382	8.04	7.386	8.039	7.382
0.010152	0.009827	8.005	7.298	8.005	7.304	8.003	7.3
0.010152	0.012897	7.993	7.271	7.991	7.269	7.99	7.268
0.010152	0.01876	7.986	7.258	7.983	7.256	7.984	7.256
0.010152	0.024277	7.986	7.257	7.982	7.254	7.981	7.252
0.010152	0.02948			7.982	7.252	7.981	7.252
0.010152	0.041271	7.985	7.253	7.982	7.252	7.981	7.251
0.010152	0.051589	7.985	7.253	7.982	7.252	7.981	7.251
0.010152	0.068786	7.985	7.253	7.982	7.252	7.981	7.25
0.010152	0.082543	7.985	7.252	7.982	7.25	7.981	7.249
0.010152	0.093799	7.984	7.252	7.982	7.25	7.981	7.249
0.010152	0.103178	7.984	7.252	7.982	7.25	7.981	7.248
0.010152	0.206357	7.984	7.252	7.982	7.25	7.981	7.248

MS Data

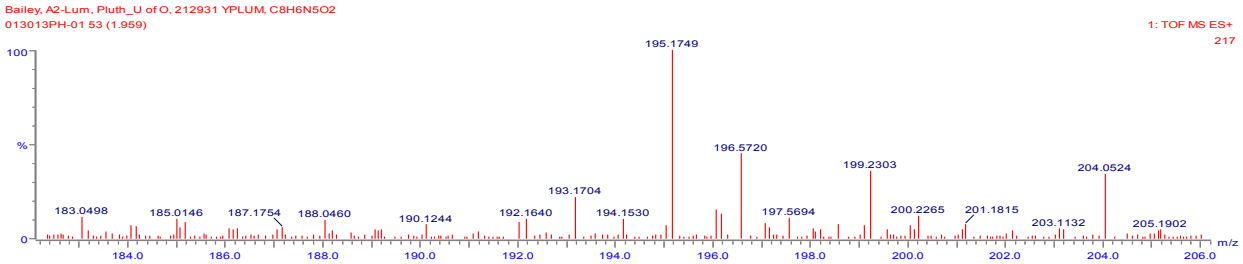

Figure S9. High resolution ESI mass spectrum of CLSS-1.

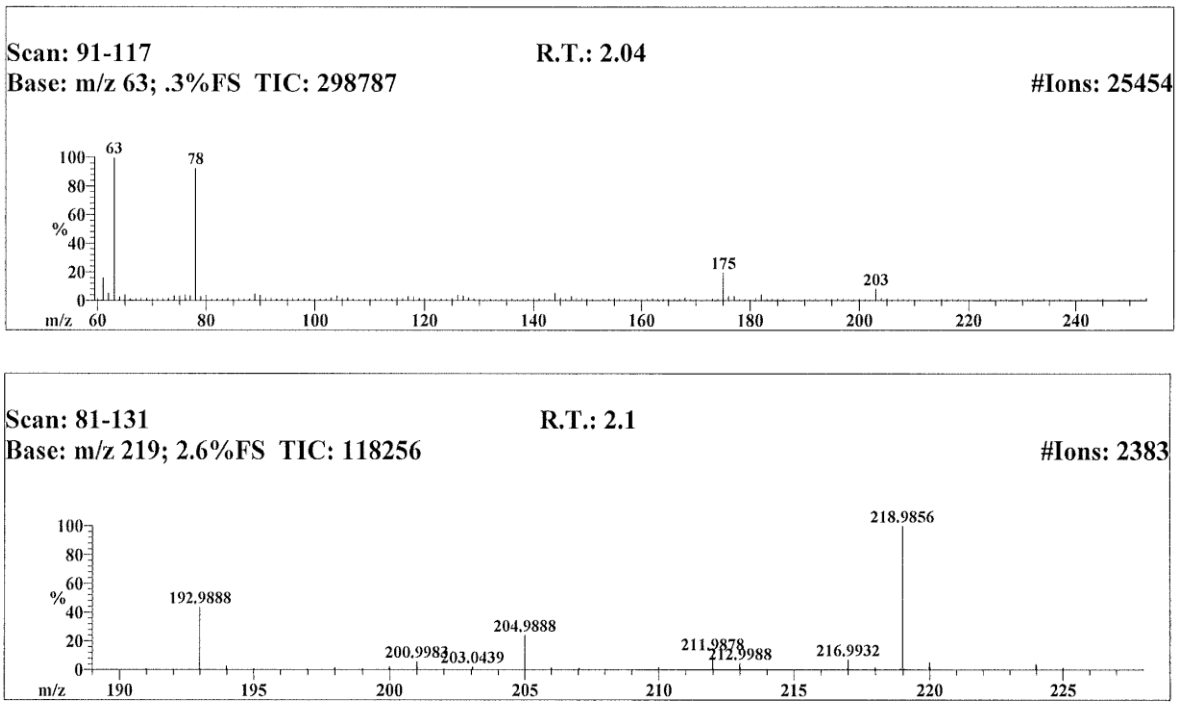

Figure S10. Low resolution (top) and high resolution (bottom) EI mass spectra of CLSS-2.

UV-Vis Data

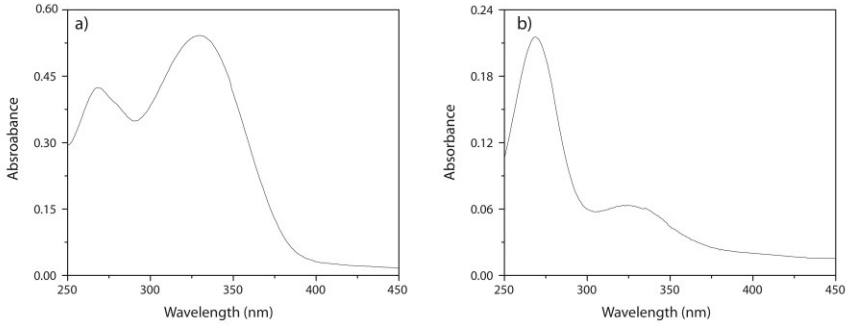

Figure S11. UV-Vis spectra of a) CLSS-1 and b) CLSS-2, measured at 33 μM in pH 7.4 PIPES buffer, 37 ^{o}C.

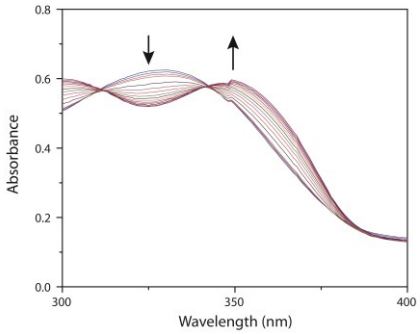

Figure S12. UV-Vis spectrum of CLSS-1 during the H_2S mediated reduction. pH 7.4 PIPES buffer, 37 ^{o}C, 1 hr.

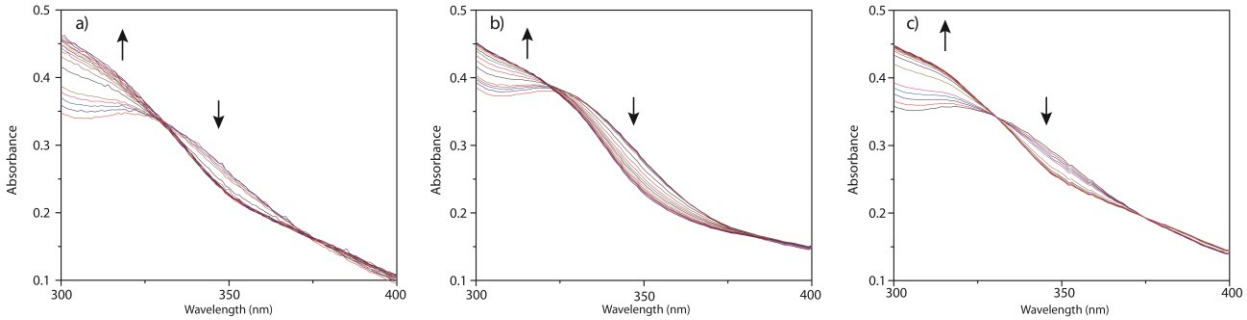

Figure S13. pH dependent H_2S reduction of CLSS-2. The spectra show 50 μM CLSS-2 being reduced by 33 equiv. H_2S in a) pH 7.0 PIPES buffer, b) pH 7.4 PIPES buffer, and c) pH 8.0 tris buffer at 37 ^{o}C over the course of 1 hr.

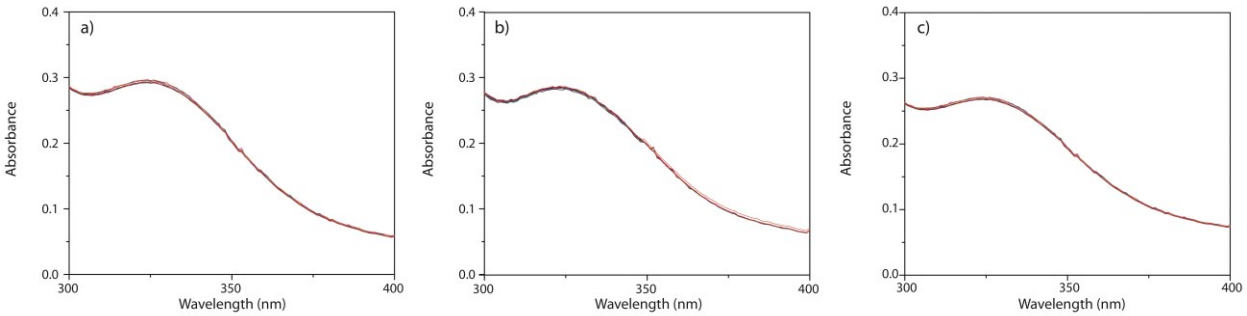

Figure S14. pH dependent reaction of CLSS-2 with cysteine. The spectra show 33 equiv. L-cysteine does not react with 50 μM CLSS-2 in a) pH 7.0 PIPES buffer, b) pH 7.4 PIPES buffer, or c) pH 8.0 tris buffer at 37 ^{o}C over the course of 1 hr.

DFT Calculations

Optimized Geometries

Cysteine
Calculated Enthalpy: -721.974543 Hartree
Zero Point Energy: 0.10770 Hartree
Lowest Frequency: 56.7 cm^{-1}
Coordinates:

Atom	x	y	z
N	-1.40186600	1.66348600	-0.05516900
H	-1.26669800	2.45430400	-0.67462700
H	-1.36440400	2.00878100	0.90013700
C	-0.40155600	0.61171400	-0.29509000
H	-0.17542600	0.61187900	-1.36607500
C	0.90929300	0.80374700	0.48509000
C	-1.07049000	-0.75149100	-0.02307600
H	1.20901600	1.84843300	0.39725000
H	0.76905600	0.58167500	1.54419900
S	2.36112600	-0.13352500	-0.14831200
O	-0.47125500	-1.79236500	0.13524000
H	1.84767900	-1.36334600	0.04928500
O	-2.40307200	-0.69553100	-0.00901300
H	-2.61303000	0.26961600	-0.10235800

Luminol Azide (CLSS-1)
Calculated Enthalpy: -732.08227 Hartree
Zero Point Energy: 0.13547 Hartree
Lowest Frequency: 46.9 cm^{-1}
Coordinates:

Atom	x	y	z
C	0.35420000	2.59415900	0.00000600
C	-0.94958100	2.12718700	0.00001000
C	-1.19372700	0.75023900	0.00001100
C	-0.13097600	-0.18091400	0.00001400
C	1.19421200	0.32610000	0.00000900
C	1.42412800	1.69793200	0.00000500
H	0.55441400	3.65852000	0.00000000
H	-1.79170500	2.80620000	0.00001000
C	-2.58692400	0.26986500	0.00000500
C	-0.48581700	-1.59696100	0.00001200
H	2.43954400	2.07592900	-0.00000300
N	-1.70674900	-2.02071800	-0.00002600
N	-2.70089900	-1.09157600	-0.00005600
O	0.44541300	-2.57594800	0.00005700
O	-3.58294300	0.99863700	0.00000900
N	2.24150100	-0.62726600	-0.00000200
N	3.41812500	-0.25101900	-0.00002900
N	4.52536000	-0.03613600	-0.00002200
H	-3.63363200	-1.48335400	-0.00006300
H	1.33715100	-2.17744700	0.00004400

Luminol Azide – Cysteine (CLSS-1/Cys; N_3-H bond)
Calculated Enthalpy: -1454.066548 Hartree

Zero Point Energy: 0.245206 Hartree
Lowest Frequency: 13.8 cm^{-1}
Coordinates:

Atom	x	y	z
C	-4.82580600	-1.01615500	-0.06144100
C	-4.46905700	0.31492900	-0.22493500
C	-3.12841600	0.68652200	-0.13186900
C	-2.11563200	-0.27016600	0.11832500
C	-2.49338200	-1.63274600	0.21334300
C	-3.84511300	-1.97873500	0.15276200
H	-5.86568900	-1.31430200	-0.11650700
H	-5.20975500	1.07887300	-0.41919800
C	-2.79734600	2.12191200	-0.31637500
C	-0.73649200	0.19832500	0.35807800
H	-4.10976500	-3.02349100	0.25587800
N	-0.50854100	1.51134000	0.18530100
H	0.44565700	1.89768200	0.35655700
N	-1.48252100	2.42213800	-0.16799500
H	-1.16477900	3.37506500	-0.28682400
O	0.19099500	-0.55070400	0.73566200
O	-3.62229300	2.99198400	-0.59906300
N	-1.62709800	-2.73515200	0.43264400
N	-0.57001900	-2.86411200	-0.18251700
N	0.40221800	-3.15526700	-0.67915400
O	2.00989700	2.42809800	0.61518400
C	3.07782800	2.06164000	0.04191800
C	3.59045600	0.63223600	0.39280500
O	3.77578200	2.69544000	-0.76240700
N	2.76301400	0.04554000	1.50053200
H	4.60862900	0.71764400	0.77393300
C	3.57125100	-0.27764400	-0.83616300
H	1.77059800	-0.13585500	1.19655300
H	2.57047800	-0.35285200	-1.26094900
H	4.22439900	0.16394600	-1.58540700
S	4.19957000	-1.98815900	-0.52702300
H	3.00104000	-2.58534500	-0.36769000
H	3.17105300	-0.83541200	1.82322800
H	2.72084600	0.69394200	2.28742200

Luminol Azide – Cysteine (CLSS-1/Cys; No N_3-H bond)
Calculated Enthalpy: -1454.063897 Hartree
Zero Point Energy: 0.245530 Hartree
Lowest Frequency: 12.1 cm^{-1}

Coordinates:

Atom	x	y	z
C	-5.07376700	0.63752700	0.13156500
C	-4.55917800	-0.64086400	0.29597300
C	-3.18394000	-0.84896000	0.19978800
C	-2.29330300	0.22250600	-0.05183000
C	-2.83238800	1.52994300	-0.14281400
C	-4.21599700	1.71095800	-0.08202400
H	-6.14195200	0.80820200	0.18671800
H	-5.20235100	-1.48818800	0.49201900
C	-2.68186400	-2.23365300	0.38533900

C	-0.87043100	-0.07764800	-0.30991800
H	-4.60361400	2.71678300	-0.18304000
N	-0.48652300	-1.35509000	-0.13818000
H	0.48669700	-1.64095300	-0.37472700
N	-1.34411800	-2.37716300	0.21339300
H	-0.90984700	-3.27961400	0.35558200
O	-0.04478600	0.77357700	-0.70589400
O	-3.39275100	-3.19365300	0.68629000
N	-2.10396400	2.72856300	-0.35491800
N	-1.06908800	2.97203900	0.26552800
N	-0.13819400	3.36548400	0.76971900
O	2.07572100	-2.03303600	-0.77541600
C	3.13406300	-1.52156300	-0.30650400
C	3.50964600	-0.11306000	-0.85852300
O	3.91355300	-2.01204700	0.52609900
N	2.43834500	0.32383500	-1.82700100
H	4.43157000	-0.20062700	-1.43556400
C	3.67570900	0.95511500	0.23059700
H	1.51890800	0.50866700	-1.34852400
H	3.66188300	1.95068600	-0.21608200
H	2.86261600	0.90049800	0.95526500
S	5.28746500	0.86520300	1.10619600
H	5.18099100	-0.44677400	1.41013200
H	2.71587600	1.15665800	-2.34896800
H	2.25938100	-0.43279400	-2.49025500

Luminol Azide Trimer [$(CLSS\text{-}1)_3$]
Calculated Enthalpy: -2196.276923 Hartree
Zero Point Energy: 0.409041 Hartree
Lowest Frequency: 13.0 cm^{-1}

Coordinates:

Atom	x	y	z
C	-4.77132500	5.00404100	-0.00159300
C	-4.55234100	3.63728300	-0.00073800
C	-3.24240000	3.15077600	0.00003700
C	-2.12368300	4.02287700	-0.00014000
C	-2.37605800	5.42230500	-0.00093100
C	-3.69282800	5.88611900	-0.00164700
H	-5.78016800	5.39827100	-0.00217600
H	-5.37187400	2.93168700	-0.00061200
C	-3.03206400	1.69801700	0.00117100
C	-0.80346500	3.39969500	0.00051700
H	-3.88267800	6.95287100	-0.00222200
N	-0.64085600	2.10985200	0.00176800
N	-1.74170300	1.30876500	0.00229900
O	0.28435400	4.17025800	-0.00025400
O	-3.95382600	0.85257500	0.00128300
N	-1.28169500	6.31096000	-0.00087500
N	-1.49523800	7.52391500	-0.00175000
N	-1.52826500	8.65512700	-0.00244400
H	1.12498800	3.63170800	0.00005200
H	-1.55452800	0.29716000	0.00277500
N	-1.50828400	-1.60987100	0.00232200

C	-2.54371600	-2.39587600	0.00069500
N	-0.26396000	-2.16219800	0.00313700
C	-2.42297000	-3.85056700	-0.00028800
O	-3.75514700	-1.83964000	-0.00015600
C	0.04449100	-3.47434100	0.00210800
H	0.51783600	-1.49354800	0.00353800
C	-1.10827800	-4.38311700	0.00039200
C	-3.50879600	-4.76854500	-0.00186200
H	-3.70918300	-0.84229100	0.00048300
O	1.23757800	-3.84974600	0.00272200
C	-0.87472700	-5.76082700	-0.00054500
C	-3.25220500	-6.14085100	-0.00276800
N	-4.82545100	-4.26437200	-0.00246100
C	-1.94897200	-6.63373000	-0.00213000
H	0.14604100	-6.11798300	0.00002300
H	-4.08076500	-6.83901700	-0.00396900
N	-5.76967800	-5.05522300	-0.00359200
H	-1.78596900	-7.70453600	-0.00286300
N	-6.73314600	-5.64887200	-0.00462000
N	2.14887000	-0.49979000	0.00243100
C	3.34716900	-1.00402100	0.00155100
N	2.00581100	0.85409800	0.00238200
C	4.54712700	-0.17255100	0.00064000
O	3.47012500	-2.33133100	0.00125000
C	2.98819800	1.77679600	0.00087900
H	1.03625100	1.19787500	0.00274700
C	4.35145500	1.23245200	-0.00016000
C	5.88515800	-0.65401900	0.00027200
H	2.58321700	-2.78961800	0.00175200
O	2.71657500	2.99770800	0.00060500
C	5.42791800	2.12337400	-0.00173600
C	6.94542700	0.25426900	-0.00143600
N	6.10689100	-2.04628500	0.00174900
C	6.72096000	1.62936000	-0.00250200
H	5.22696300	3.18599000	-0.00226800
H	7.96442000	-0.11422800	-0.00181400
N	7.26376400	-2.46872100	0.00162400
H	7.56693200	2.30577000	-0.00386200
N	8.25962400	-3.00627500	0.00175900

Isoluminol Azide (CLSS-2)
Calculated Enthalpy: -732.088312 Hartree
Zero Point Energy: 0.134688 Hartree
Lowest Frequency: 53.4 cm^{-1}

Coordinates:

Atom	x	y	z
C	1.57997700	-1.14733000	0.01396300
C	0.28900100	-1.64579800	0.02037300
C	-0.80958100	-0.77889300	0.01245400
C	-0.58917300	0.61055100	-0.00850200
C	0.70805900	1.11720100	-0.01408100
C	1.79314800	0.24252500	-0.00404900
H	2.41953900	-1.83217100	0.02249200
H	0.11419200	-2.71385400	0.03262200

C	-2.17792700	-1.33478700	0.00413200
C	-1.72990800	1.55877500	-0.00482900
N	-2.95568900	0.96964200	-0.04195100
H	-3.77769900	1.54299200	0.09549900
N	-3.17126800	-0.40192600	0.04364700
H	-4.12650300	-0.69653400	-0.11191400
O	-1.61623700	2.78450000	0.02155100
O	-2.44451200	-2.53746100	-0.02656900
H	0.86782400	2.18712900	-0.02686600
N	3.07179100	0.84223700	-0.01260500
N	4.07229400	0.11824000	-0.00380800
N	5.06959300	-0.41352600	0.00207900

Isoluminol Azide – Cysteine (CLSS-2 /Cys)
Calculated Enthalpy: -1454.075989 Hartree
Zero Point Energy: 0.245238 Hartree
Lowest Frequency: 21.8 cm^{-1}

Coordinates:

Atom	x	y	z
C	-4.42835800	0.60307700	-0.30380400
C	-3.64173800	1.73866800	-0.33998100
C	-2.25921100	1.65031900	-0.13073600
C	-1.68010100	0.39310500	0.11626400
C	-2.47027500	-0.75648500	0.15369200
C	-3.84378100	-0.65150200	-0.05650800
H	-5.49762300	0.66256900	-0.46377600
H	-4.08292800	2.70860700	-0.52962900
C	-1.42999200	2.87014500	-0.17306300
C	-0.22660900	0.27602300	0.34696900
N	0.47208300	1.41995700	0.28725700
H	1.50376300	1.41831900	0.44577600
N	-0.10264100	2.65394200	0.04607400
H	0.54208200	3.43282300	0.02602600
O	0.33711500	-0.81536600	0.58571300
O	-1.86051600	4.00579100	-0.38471600
O	3.14288500	1.36518800	0.75404300
C	4.09748300	0.64538900	0.33720000
C	4.06106900	-0.85328200	0.75506900
O	5.08012300	0.98702600	-0.33541600
N	2.86427500	-1.11141900	1.63323400
H	4.93526300	-1.03729100	1.38449500
C	4.12843900	-1.82980200	-0.41757300
H	1.94030800	-0.98466500	1.14195900
H	5.10349400	-1.70493800	-0.88529700
H	4.05762100	-2.86178600	-0.07174000
S	2.93162000	-1.56305200	-1.79257700
H	1.80725900	-1.93088200	-1.14521200
H	2.88912700	-2.04948900	2.03701400
H	2.86257600	-0.43719500	2.40050700
N	-4.73157200	-1.75024200	-0.03911000
N	-4.27613300	-2.87729400	0.17976900
N	-3.99922600	-3.95687700	0.36588300
H	-1.99278200	-1.70876300	0.34718400

Isoluminol Azide Trimer [$(CLSS\text{-}2)_3$]
Calculated Enthalpy: -2196.305164 Hartree
Zero Point Energy: 0.409167 Hartree
Lowest Frequency: 10.2 cm^{-1}

Coordinates:

Atom	x	y	z
C	5.19845400	-4.53825300	-0.10318600
C	3.82601600	-4.41709500	-0.03570600
C	3.23091800	-3.14851500	0.03279900
C	4.04797500	-1.99765300	0.03312100
C	5.44106400	-2.11957500	-0.03509900
C	6.01127900	-3.38723800	-0.10494000
H	5.66939900	-5.51170900	-0.15743900
H	3.19372000	-5.29543500	-0.03613000
C	1.77860200	-2.99503600	0.09525300
C	3.39293500	-0.70193800	0.09833800
N	2.10424300	-0.57884500	0.15667300
N	1.34686600	-1.71307400	0.16074000
O	4.16663200	0.38683100	0.09241900
O	0.95793400	-3.94039600	0.09026700
H	3.63390300	1.23139100	0.11854400
H	0.33020600	-1.55766100	0.18207800
N	-1.55367500	-1.53194700	0.13829100
C	-2.30437000	-2.58698300	0.08686500
N	-2.15784900	-0.30935800	0.14299500
C	-3.75449800	-2.50726100	0.03237100
O	-1.74773100	-3.80107800	0.07915200
C	-3.48437900	-0.04289900	0.08515700
H	-1.51465600	0.49326500	0.16379500
C	-4.34339500	-1.22446500	0.03339600
C	-4.55671900	-3.65328300	-0.02551900
H	-0.74953200	-3.76152600	0.09538000
O	-3.89288800	1.14046200	0.07860500
C	-5.74017600	-1.10651400	-0.02263700
C	-5.94020400	-3.51419000	-0.08351800
C	-6.53137900	-2.23512800	-0.07943600
H	-6.18531100	-0.12002100	-0.02146700
H	-7.61039500	-2.15695200	-0.12375900
N	-0.54903100	2.11107600	0.13372000
C	-1.08731200	3.28828600	0.07238700
N	0.81170500	2.02394600	0.16236900
C	-0.29319800	4.50462200	0.02734500
O	-2.41678700	3.41279000	0.04520100
C	1.70585600	3.04018500	0.11699700
H	1.18600600	1.06608100	0.18778300
C	1.11187200	4.37438400	0.05295700
C	-0.88457200	5.77168000	-0.04428600
H	-2.88238100	2.52912900	0.06813400
O	2.93505300	2.80322600	0.13021900
C	1.91226200	5.52570500	0.00883400
C	-0.07253100	6.90095200	-0.09092600
C	1.33050500	6.77459500	-0.06107800
H	2.98905300	5.41895600	0.02919600
H	1.93770900	7.67036700	-0.09660000

N	7.40127400	-3.62617500	-0.18225200
N	8.17177800	-2.66082400	-0.20022800
N	8.98742800	-1.87940300	-0.22545200
N	-6.84152900	-4.59970200	-0.15097700
N	-6.38827900	-5.74866300	-0.17097000
N	-6.11661000	-6.84506100	-0.19644200
H	6.05012000	-1.22507800	-0.03436400
H	-4.08617300	-4.62781900	-0.02769300
N	-0.56147100	8.22378800	-0.17063900
N	-1.78239800	8.40574200	-0.21765100
N	-2.86669800	8.71937100	-0.26744700
H	-1.96372900	5.85025100	-0.06400800