

Supporting Information for

Topomeric Aza/Thia Cryptands: Synthesis and Structural Analysis of *In/Out* Isomerism

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General Information All reactions were carried out under an inert atmosphere of nitrogen in dry solvents, unless otherwise noted. Toluene was distilled with sodium and benzophenone and collected when the purple ketyl radical was persistent, then stored over 4 Å molecular sieves for 48 hours. All other reagents were used as supplied. Analytical thin-layer chromatography (TLC) was performed using Merck Silica gel 60 F₂₅₄ precoated aluminum plates. Flash chromatography was performed using 40-63 µm Silica-gel 60 (Merck). Melting points were measured on an electrothermal Mel-Temp, and are uncorrected. Infrared (IR) spectra were recorded on JASCO FT/IR-4600 with an ATR attachment using zinc-selenide as the refractive support. ¹H, ¹³C, gCOSY, gHSQC, gHMBC, and variable temperature NMR spectra were recorded on a Varian-400 MHz or Varian-500 MHz spectrometer. Chemical shifts were reported in ppm on the δ scale relative to CHCl₃ (δ = 7.26 for ¹H NMR), CDCl₃ (δ = 77.0 for ¹³C NMR) as internal references. High resolution mass spectra were measured on a Bruker micrOTOF II and analyzed with Bruker Compass Data Analysis 4.0 software.

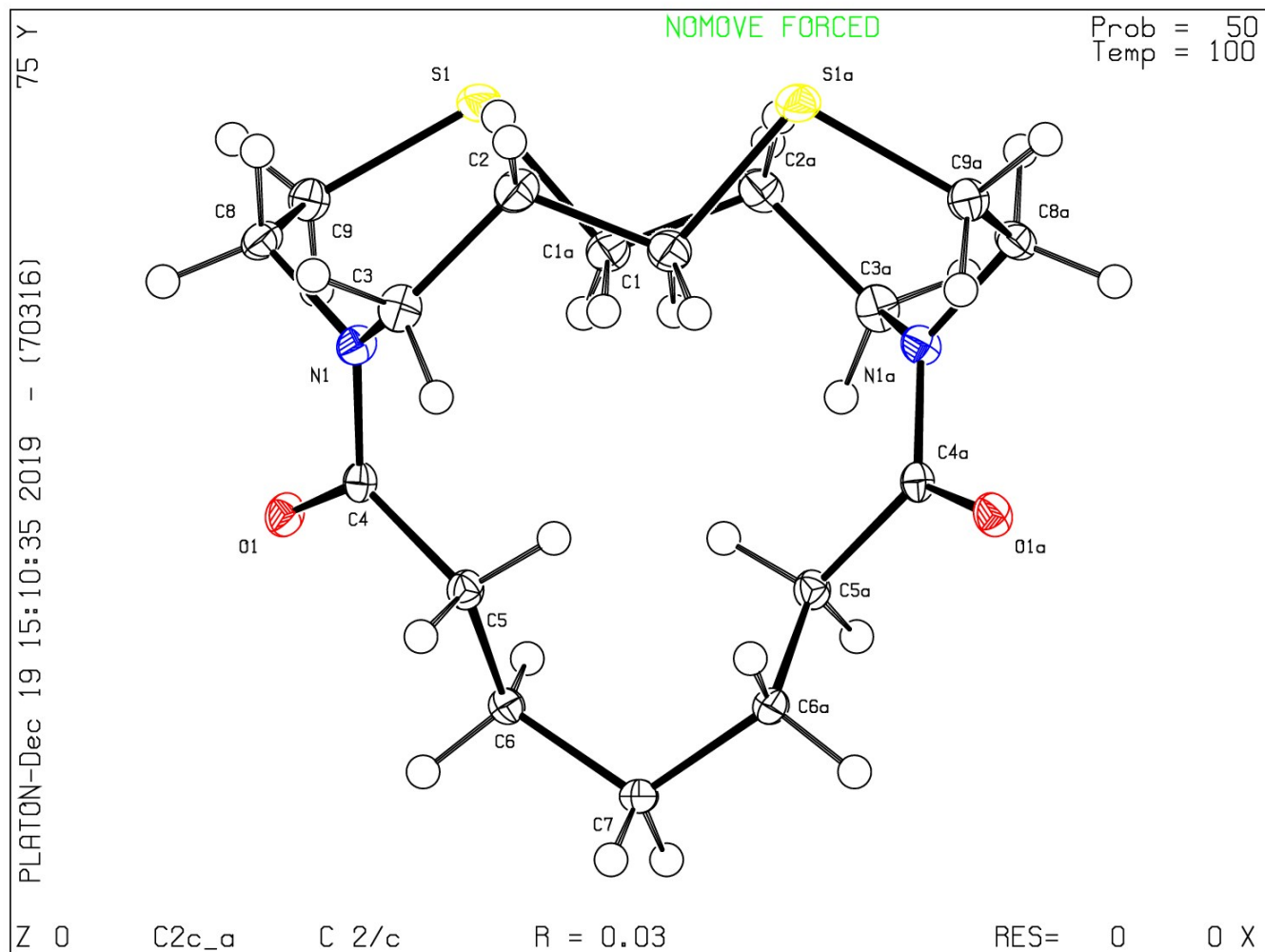


Figure S1. Ellipsoid plot for compound **L1** with ellipsoid contour at 50% probability

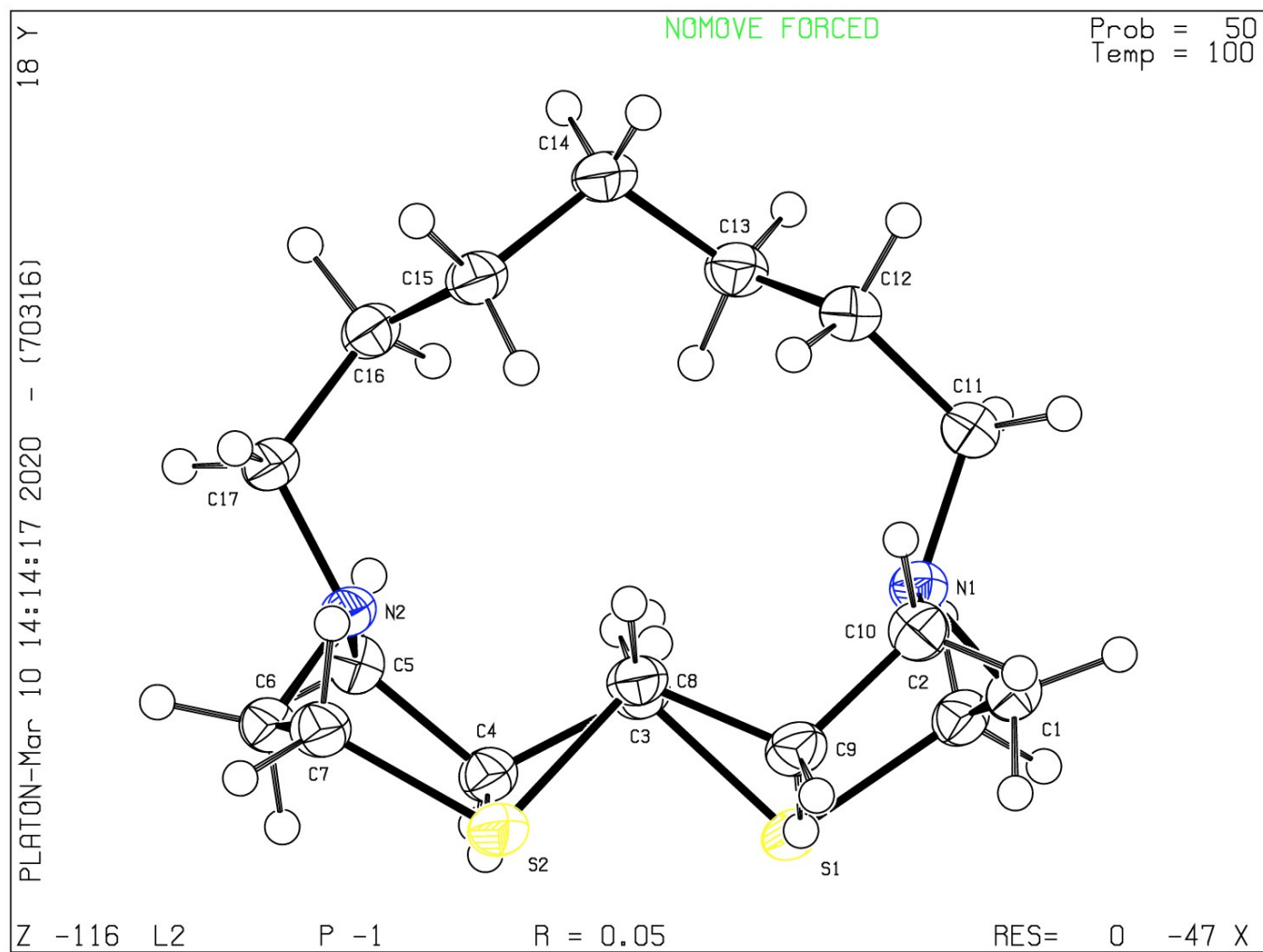


Figure S2. Ellipsoid plot for compound **L2** with ellipsoid contour at 50% probability

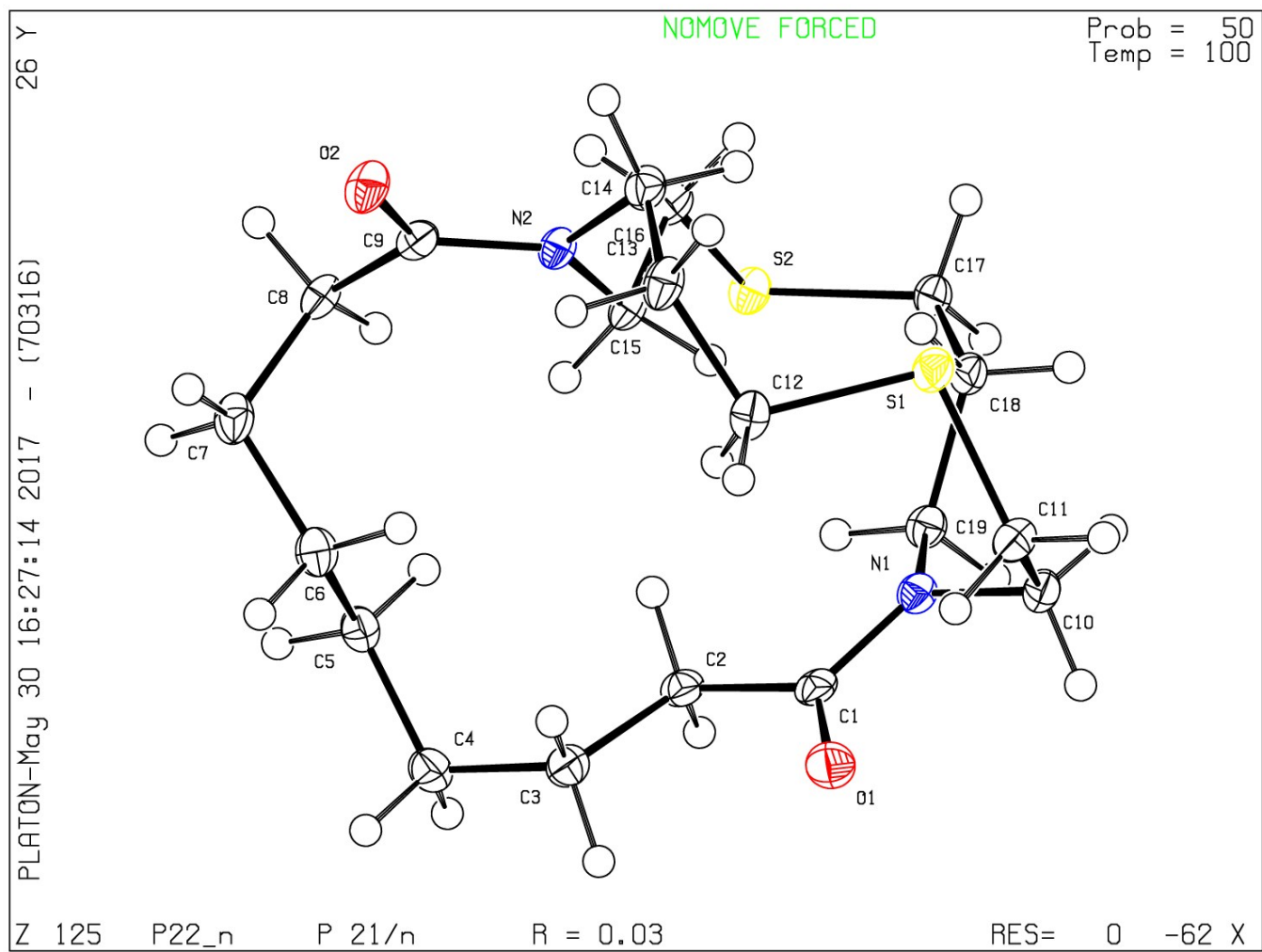
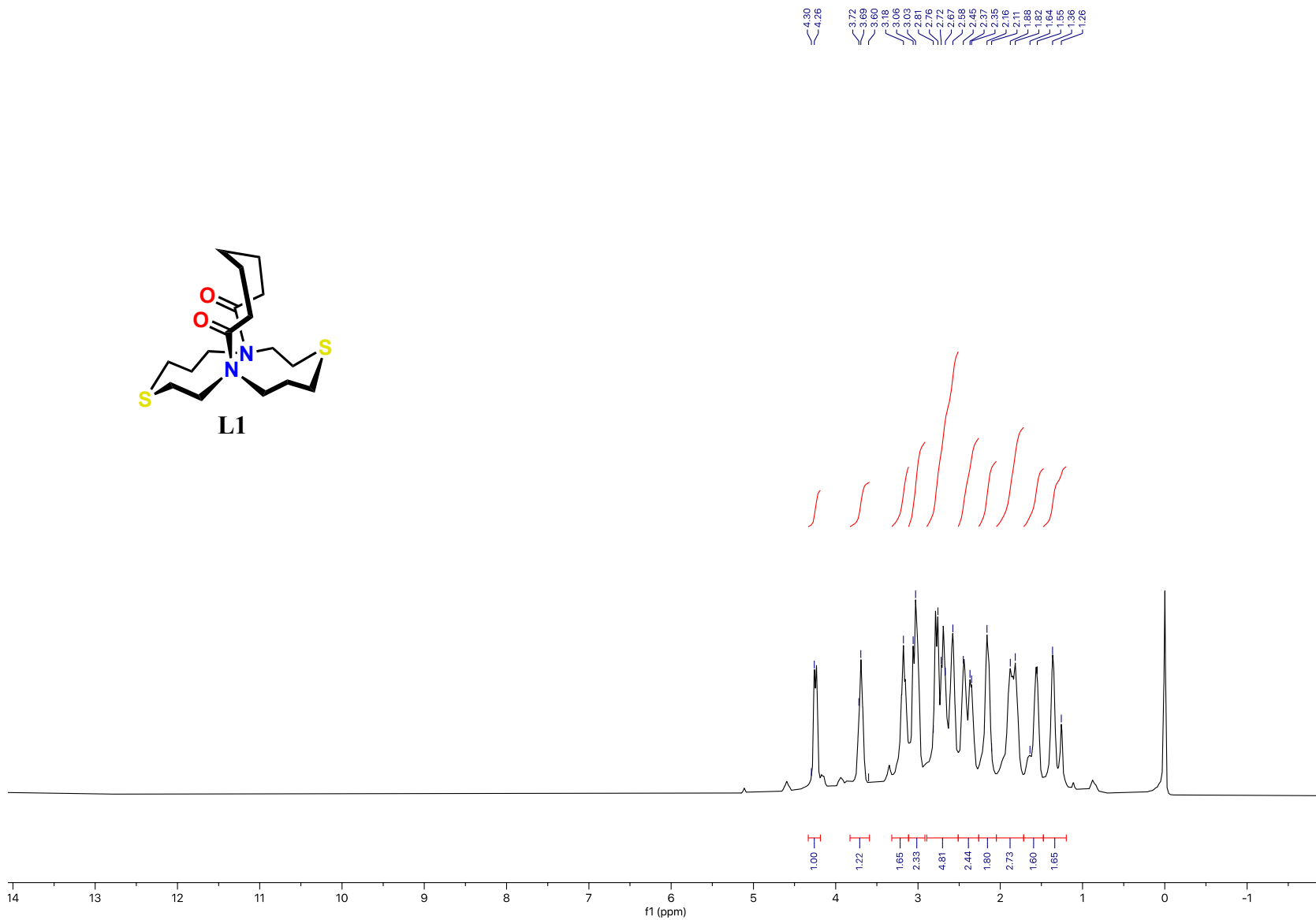
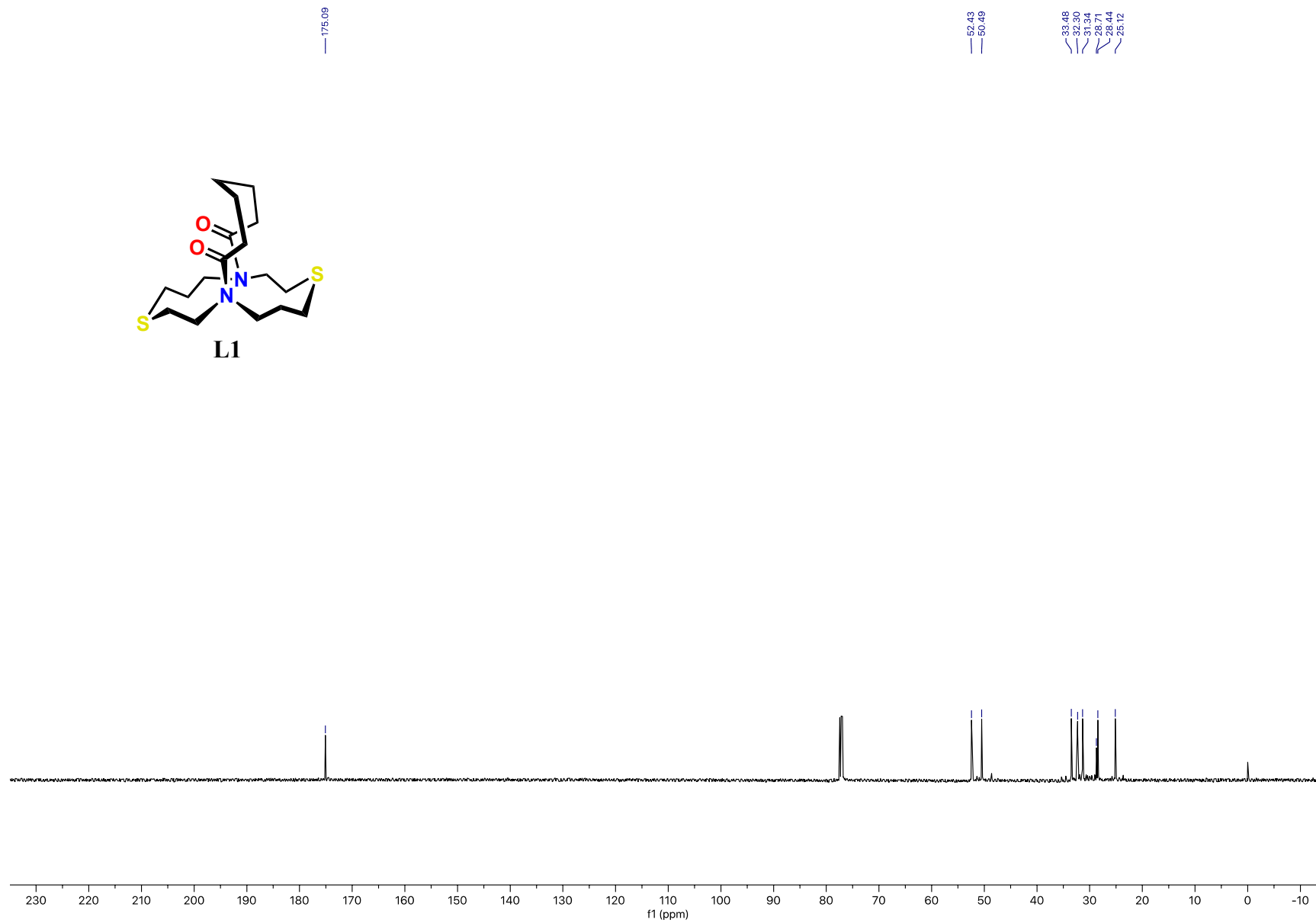
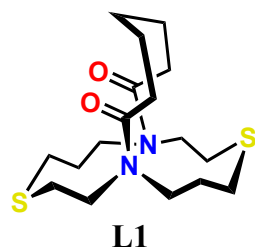


Figure S3 Ellipsoid plot for compound L3 with ellipsoid contour at 50% probability





Elemental Composition Report

Page 1

Multiple Mass Analysis: 2 mass(es) processed

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

21 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

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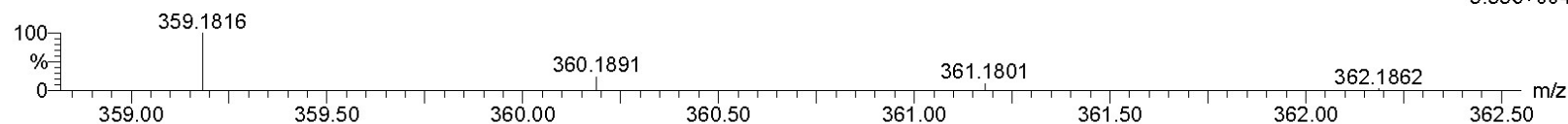
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it-01-cryptamide-c7

it-01-cryptamide-c7d 27 (1.053) Cm (27:31)

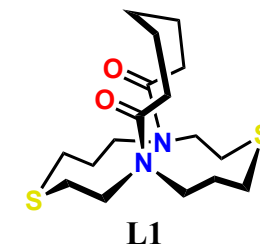
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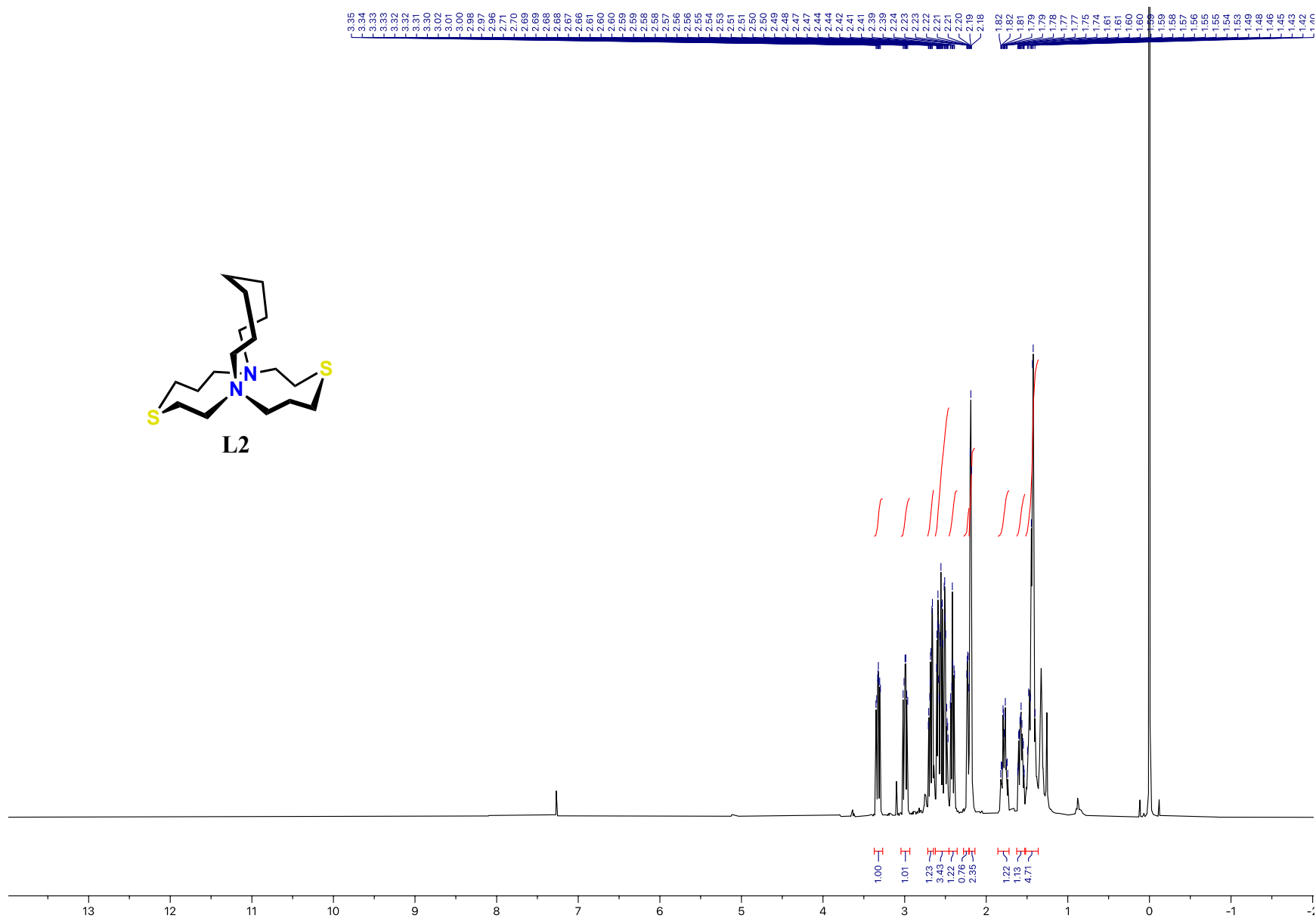
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5.35e+004

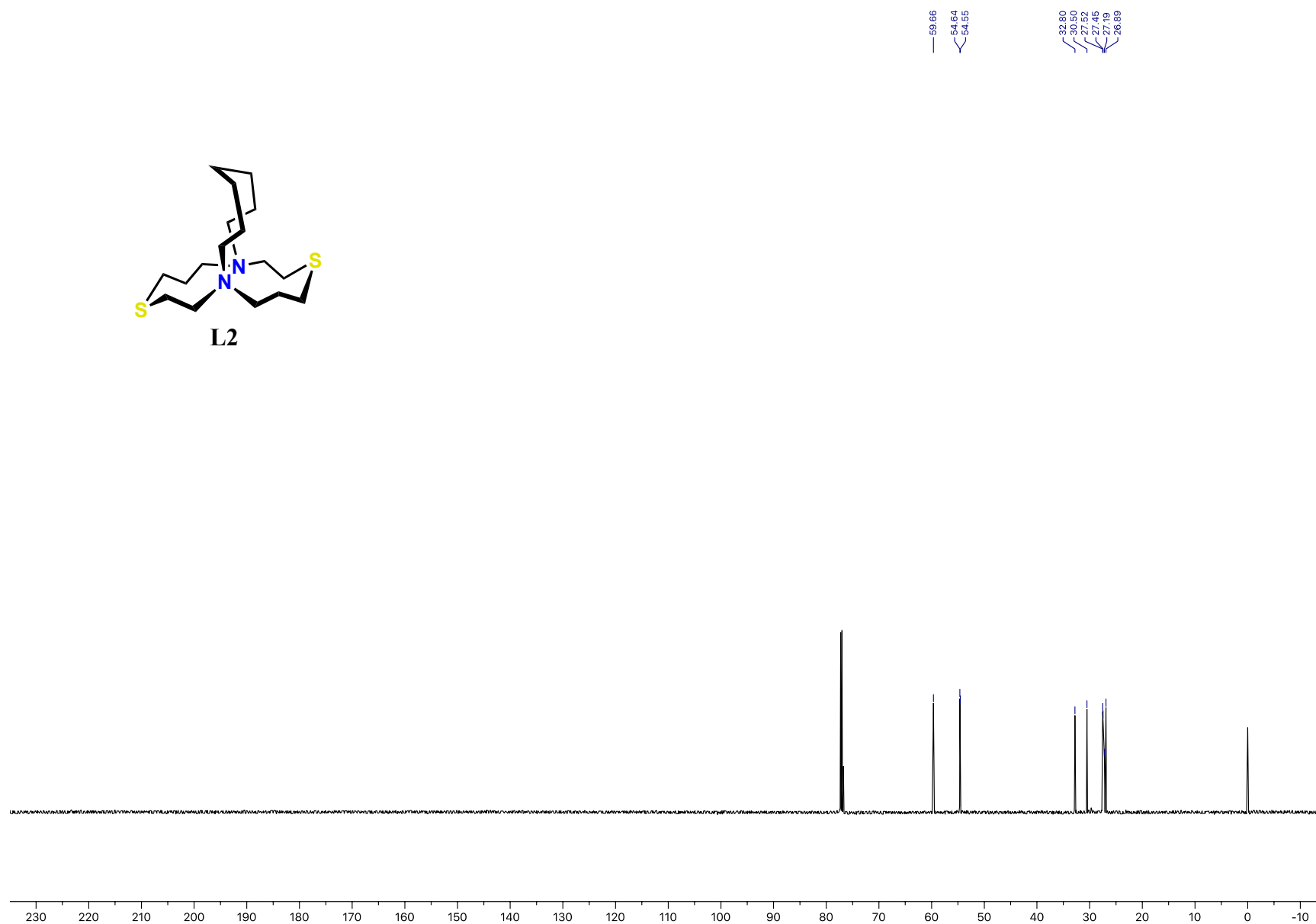
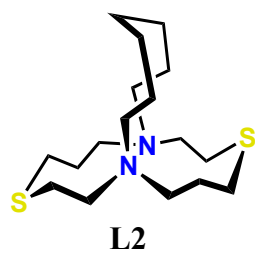


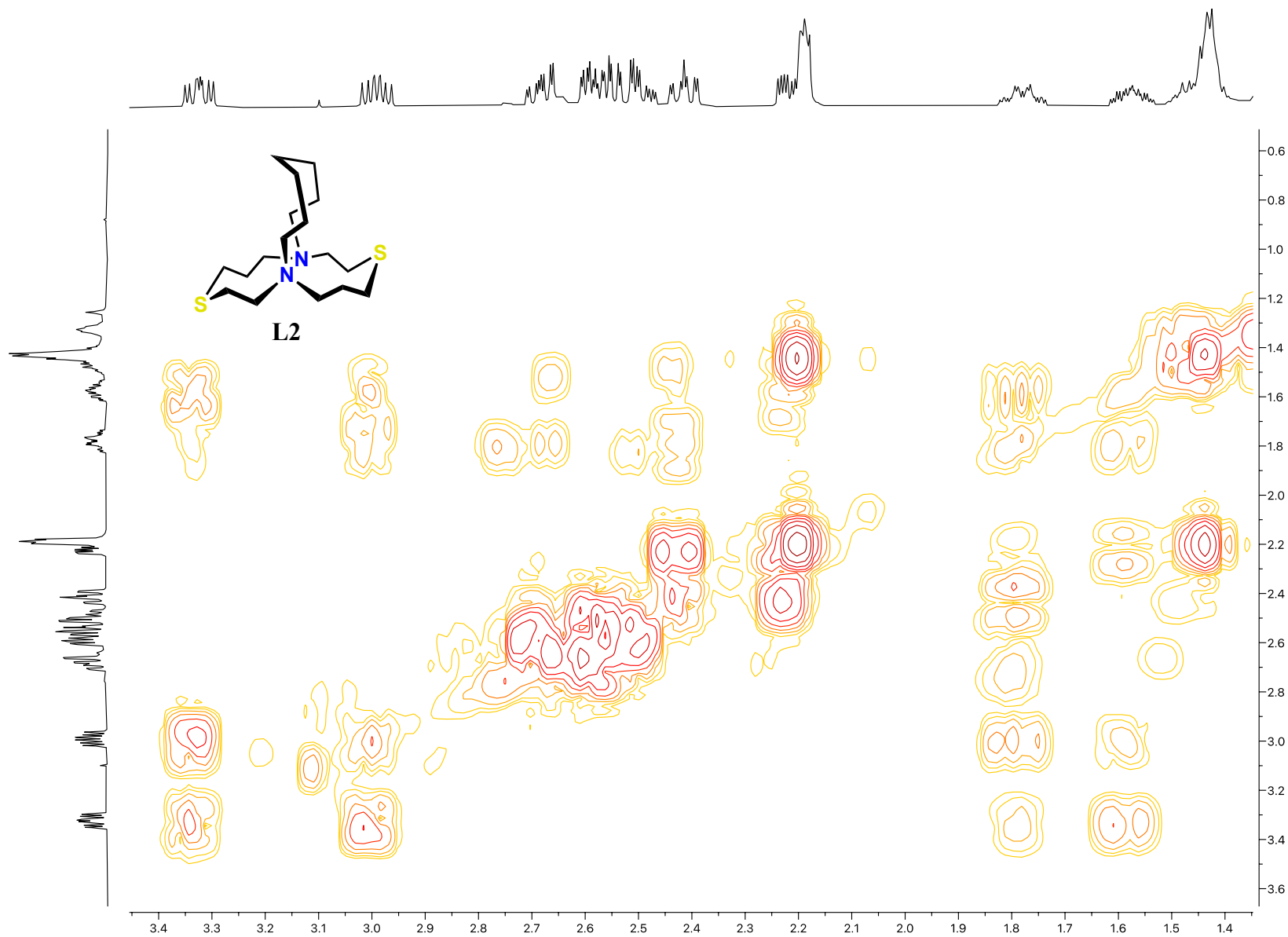
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Maximum: 100.00 5.0 10.0 100.0

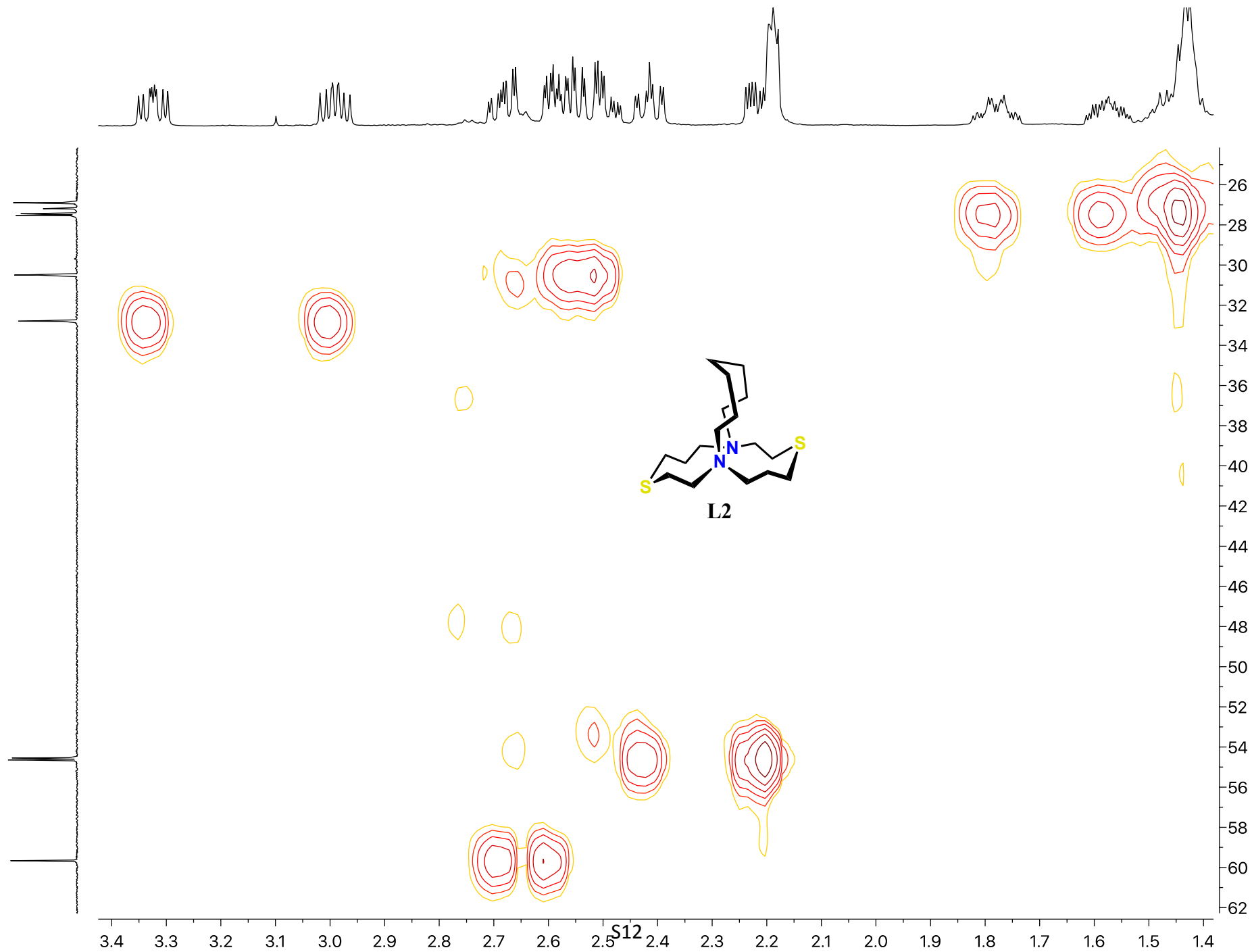
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
359.1816	100.00	359.1827	-1.1	-3.1	3.5	21.0	0.0	C17 H31 N2 O2 S2

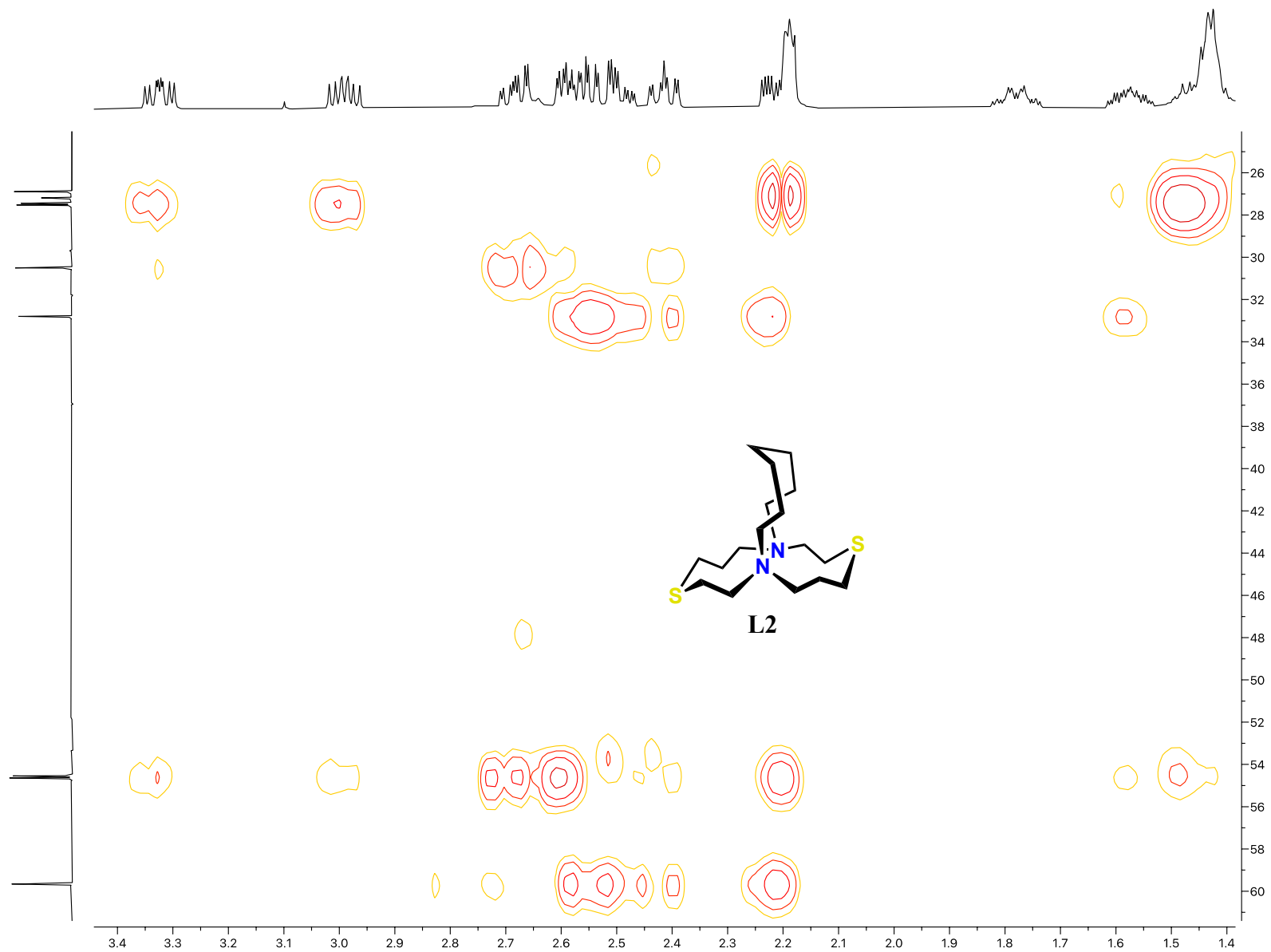












S13

Elemental Composition Report

Page 1

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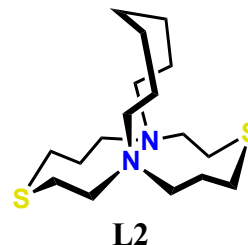
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

16 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 9-17 H: 10-35 N: 0-2 S: 0-2 Na: 0-1

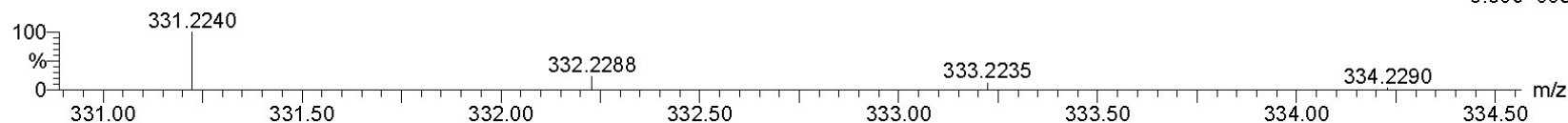


it-01-cryptamine-c7-070617

5.00000000

it-01-cryptamine-c7-070617 12 (0.484) Cm (11:14)

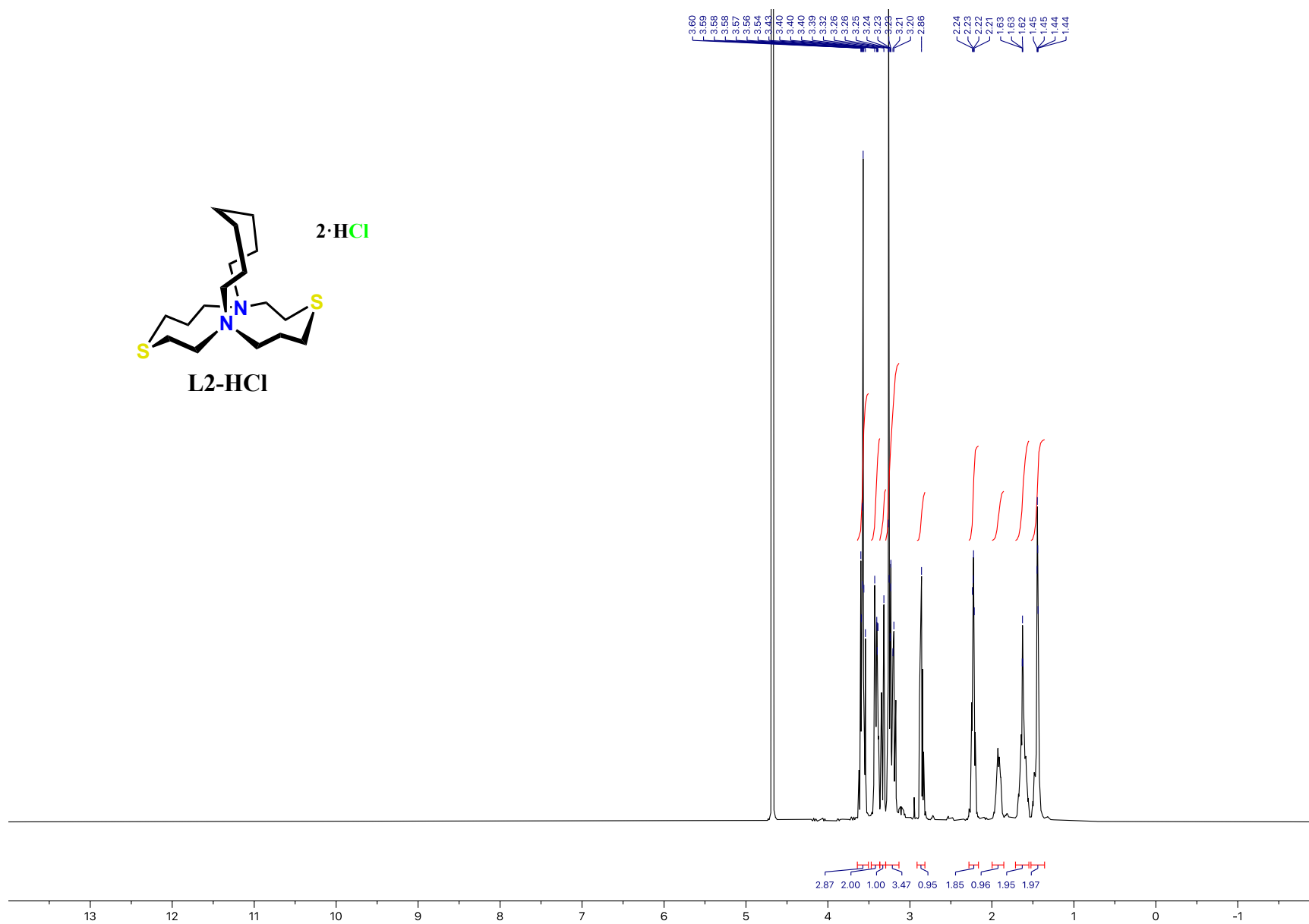
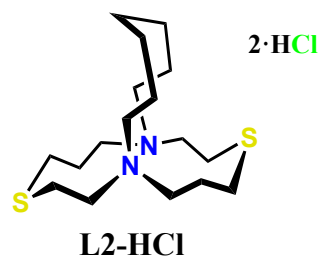
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8.80e+005

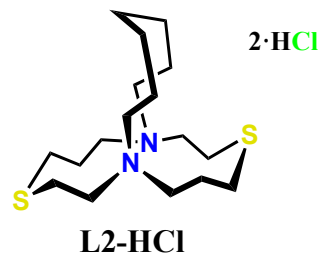


Minimum: 25.00
Maximum: 100.00

5.0 10.0 -1.5 100.0

Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
331.2240	100.00	331.2242	-0.2	-0.6	1.5	25.1	0.0	C17 H35 N2 S2



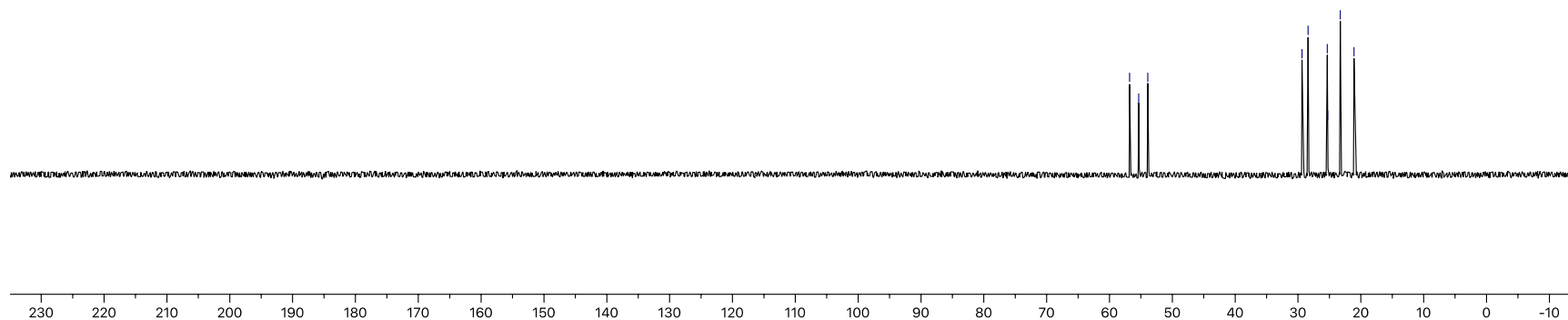


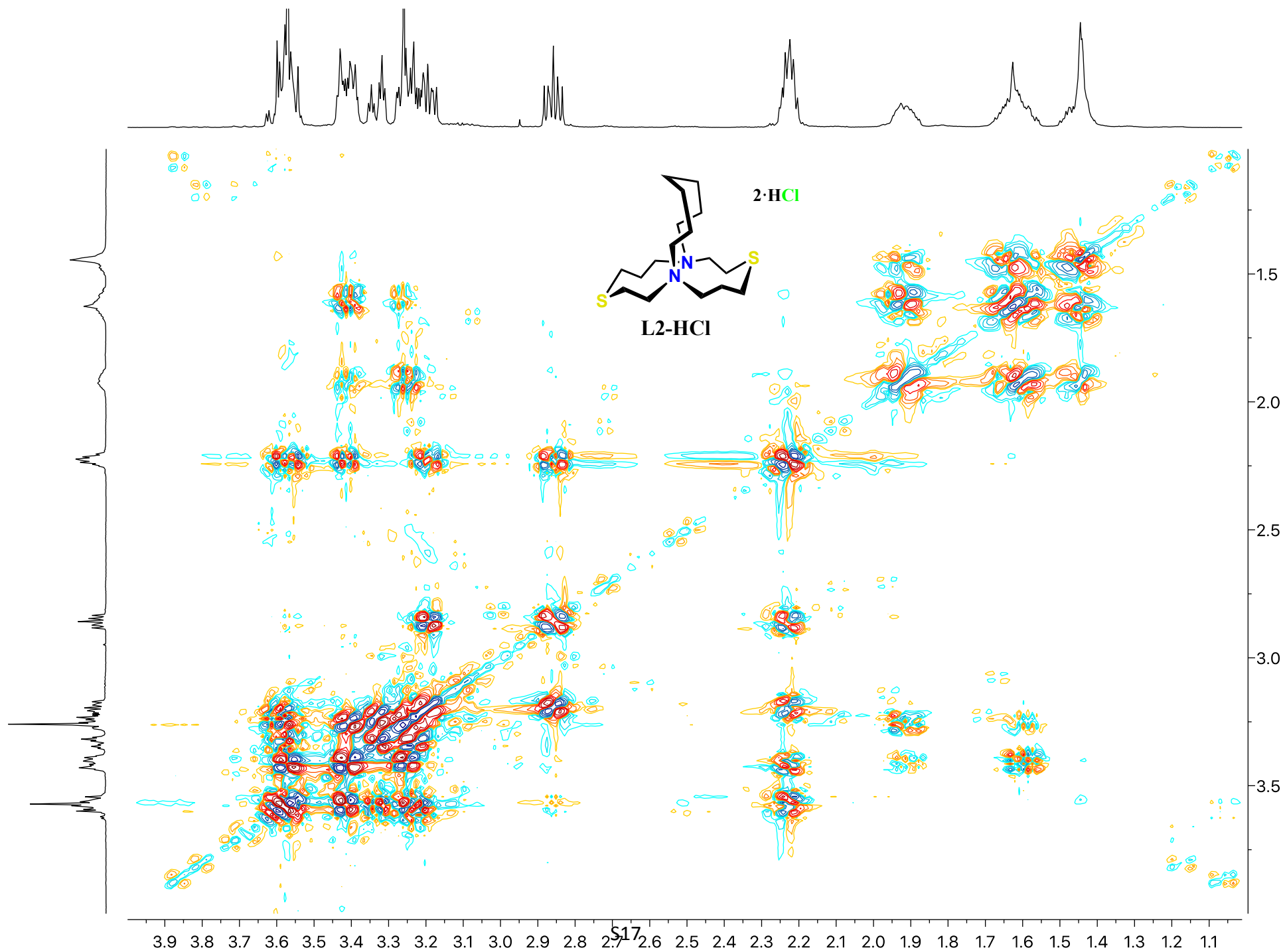
2·HCl

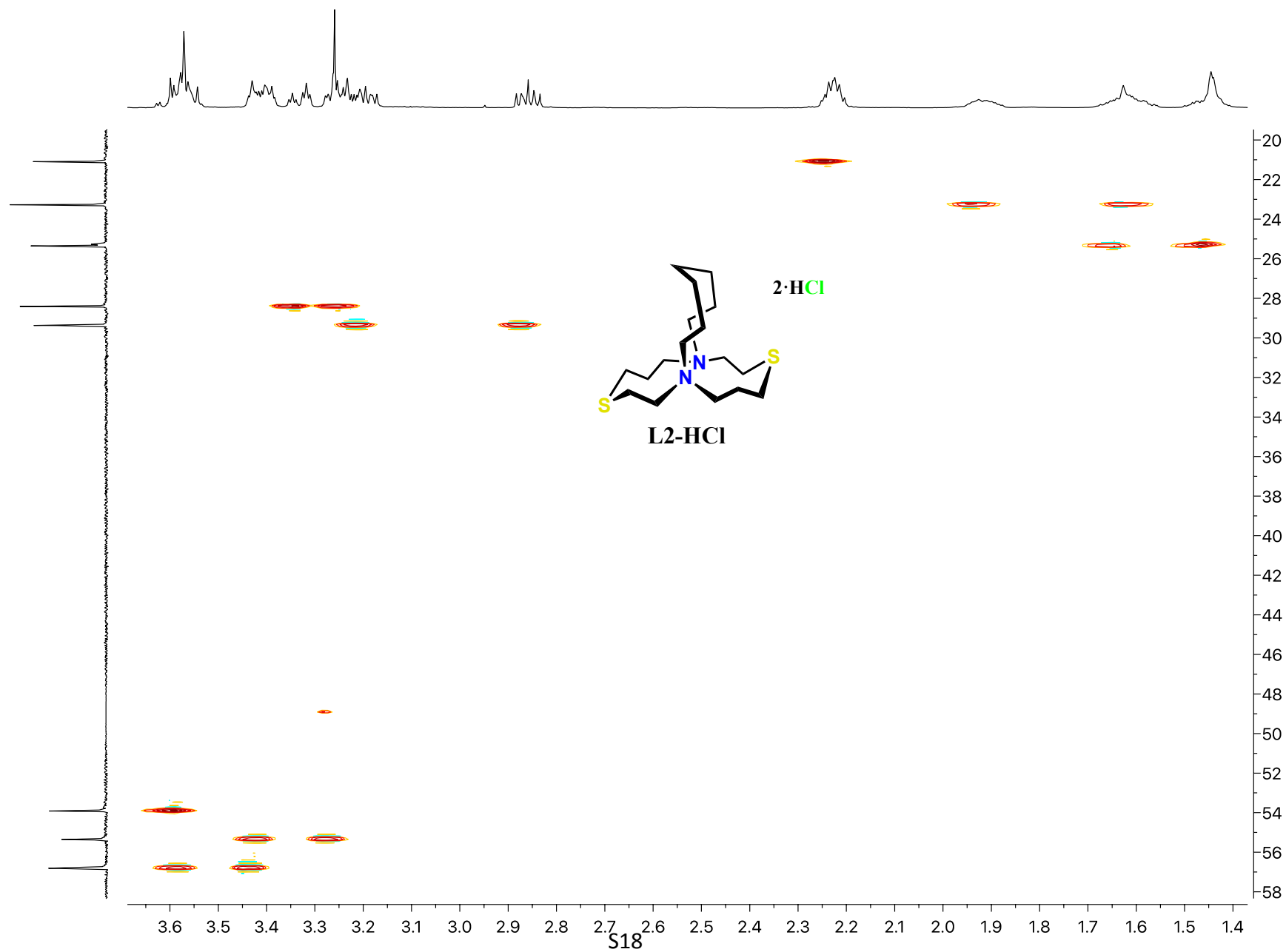
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55.36
53.91

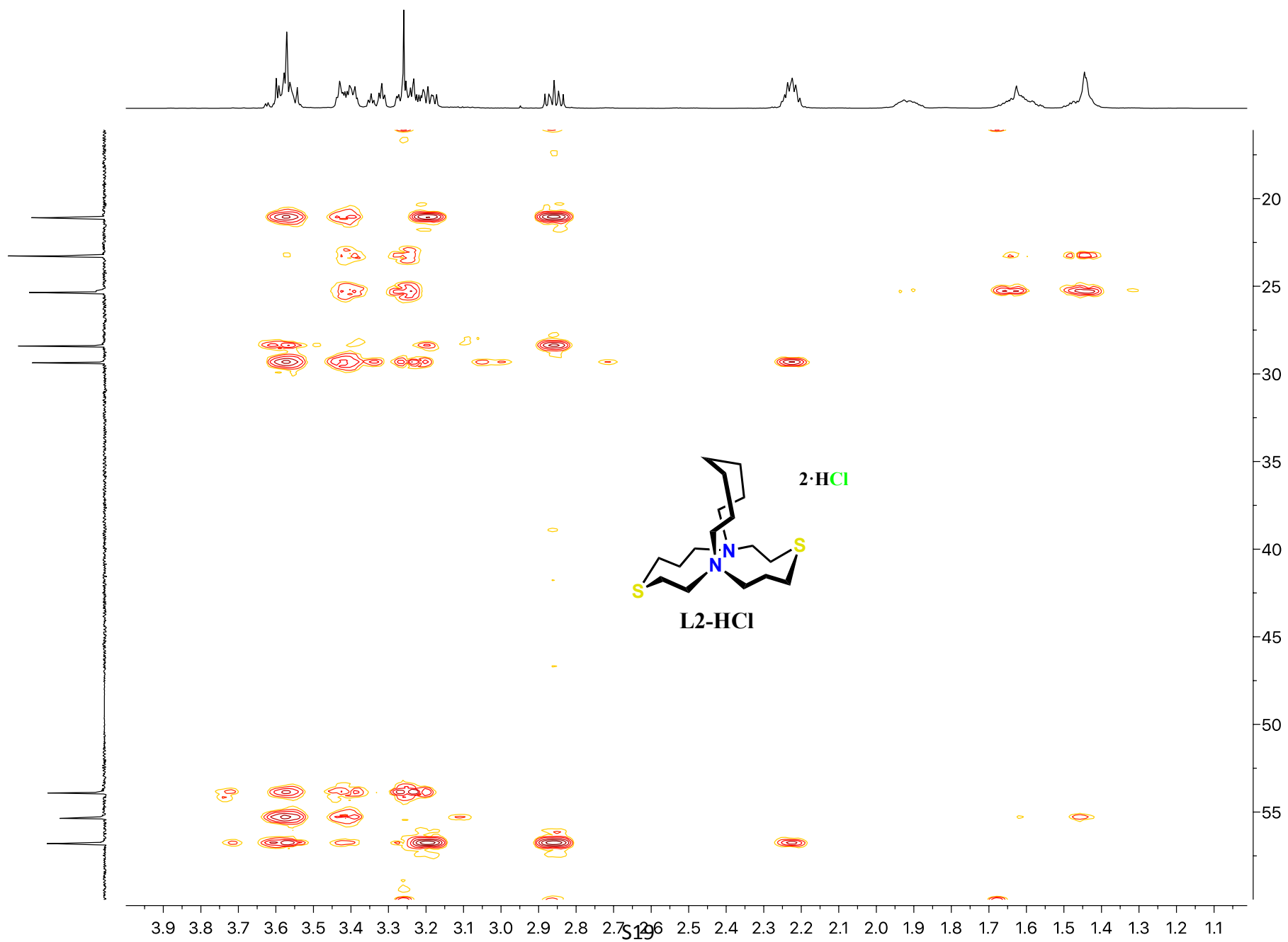
29.37
28.41
25.95
25.25
23.27
21.09

20.00
19.00
18.00









Elemental Composition Report

Page 1

Multiple Mass Analysis: 2 mass(es) processed

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

16 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

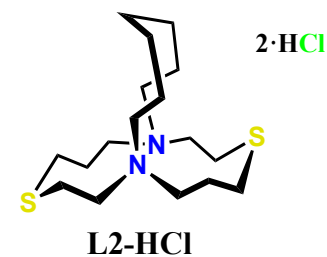
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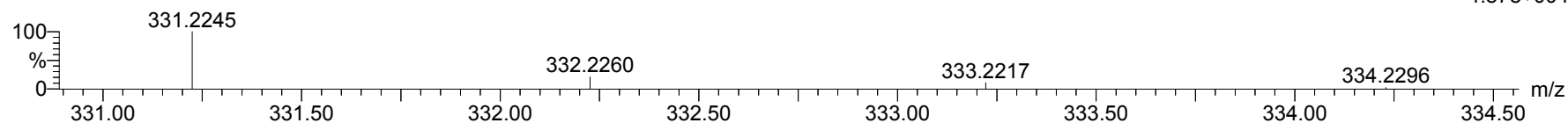
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it-01-cryptamine-c7-2hcl-070617 20 (0.775) Cm (20:21)



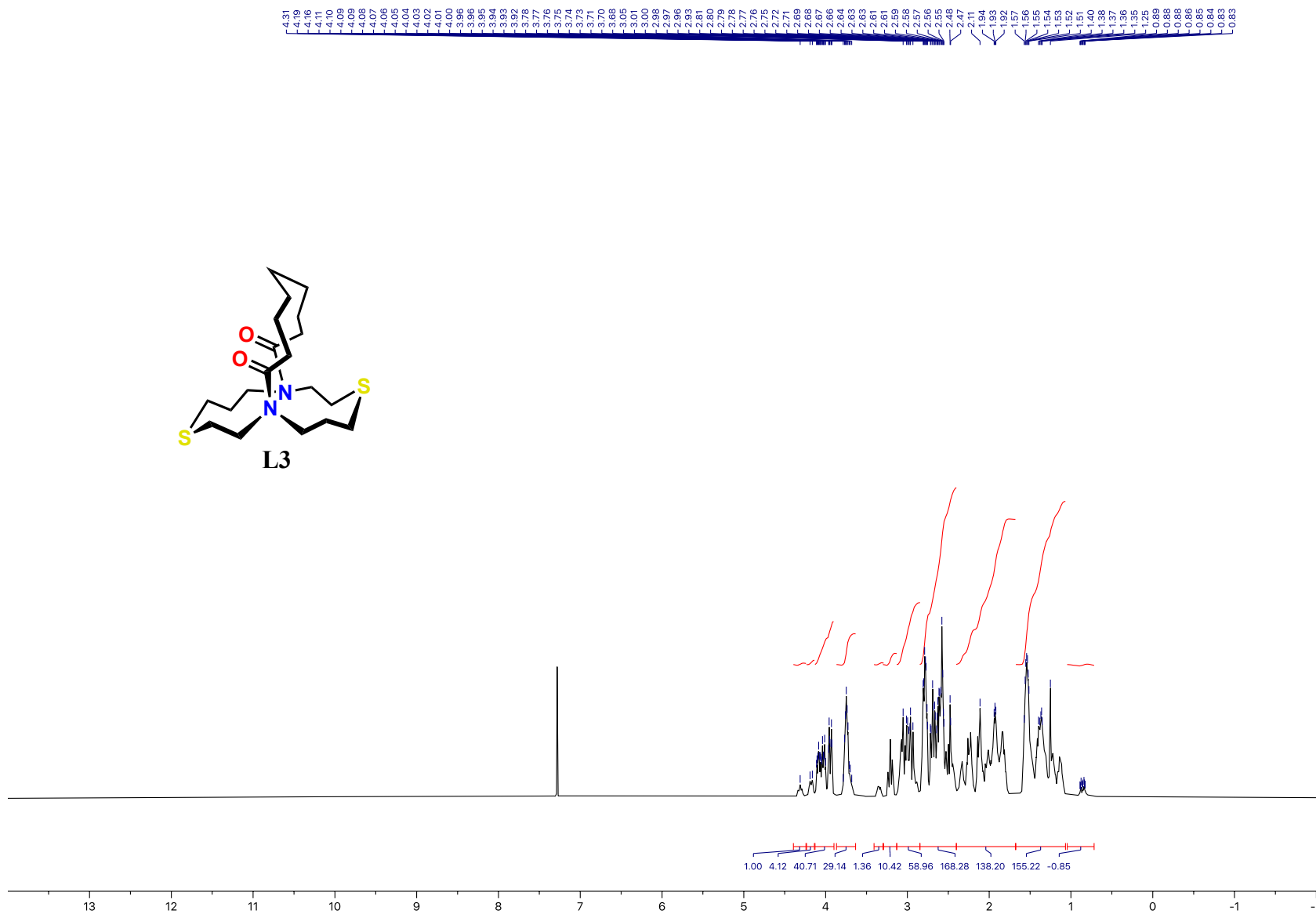
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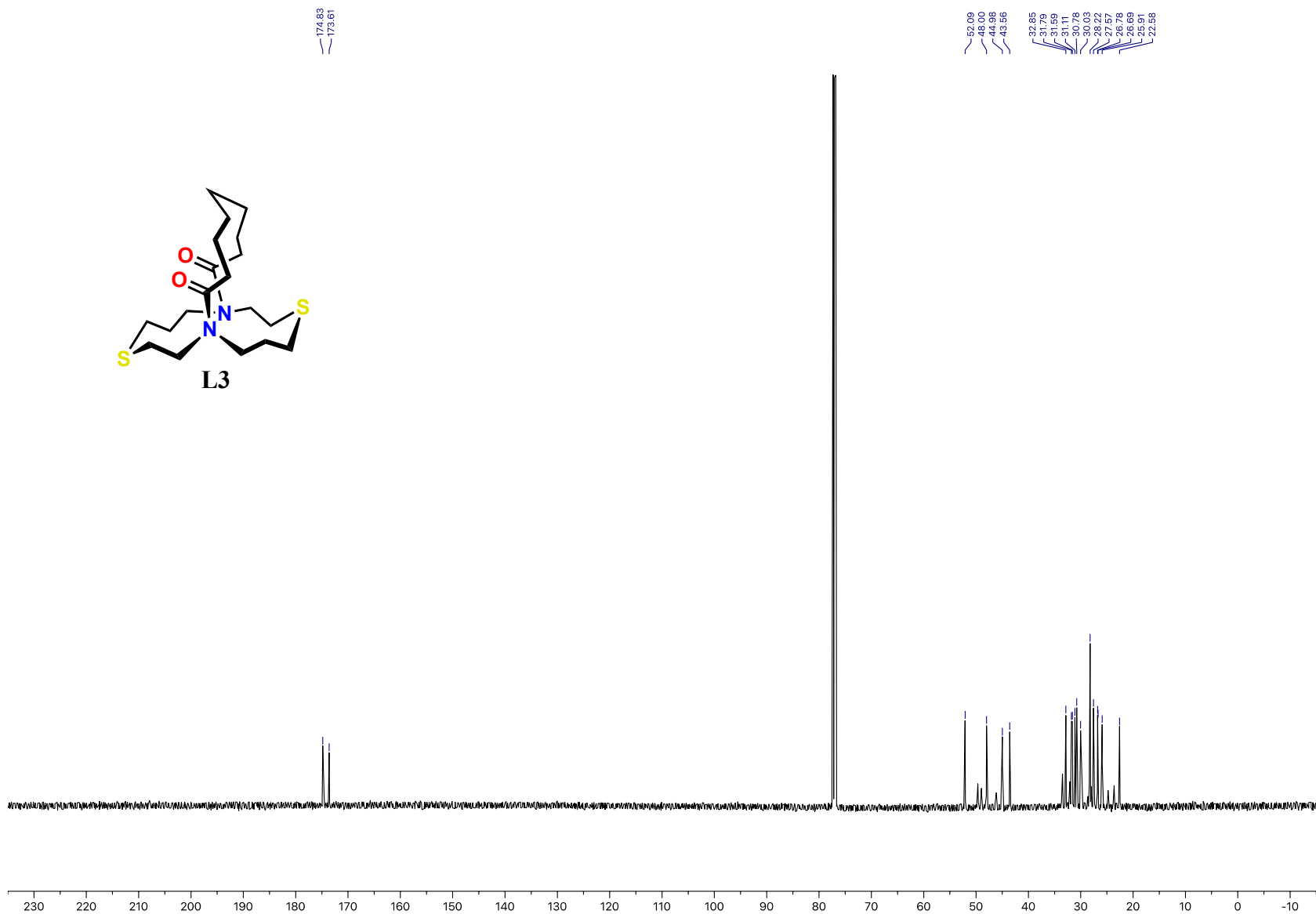
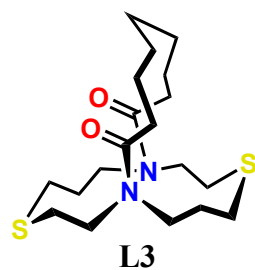


Minimum: 25.00
Maximum: 100.00

5.0 10.0 -1.5 100.0

Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
331.2245	100.00	331.2242	0.3	0.9	1.5	14.3	0.0	C17 H35 N2 S2





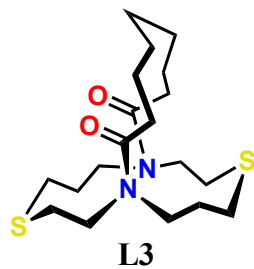
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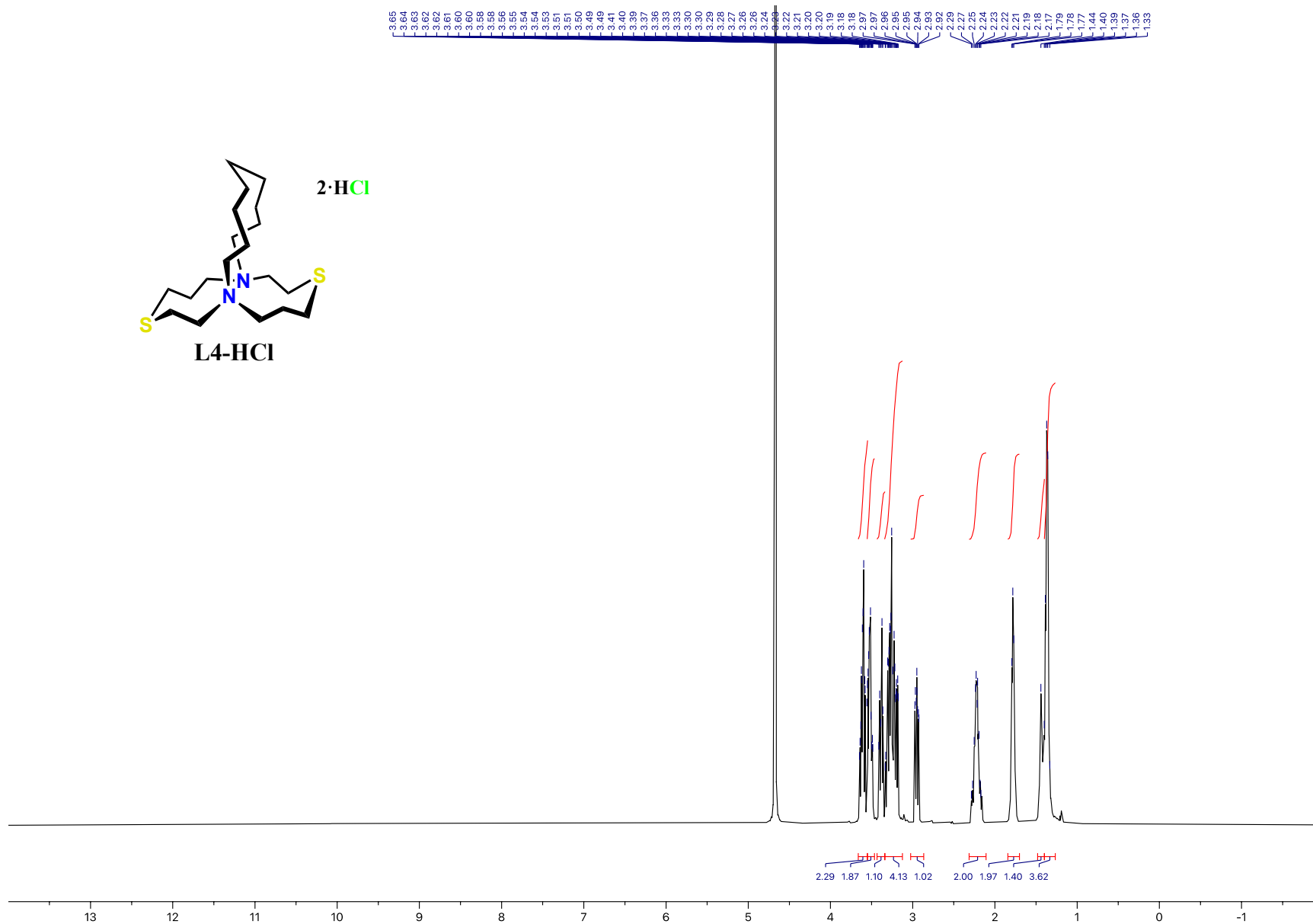
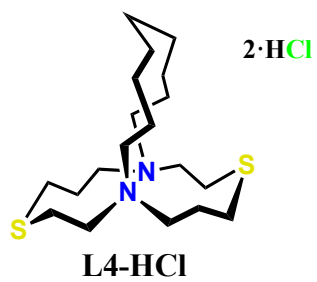
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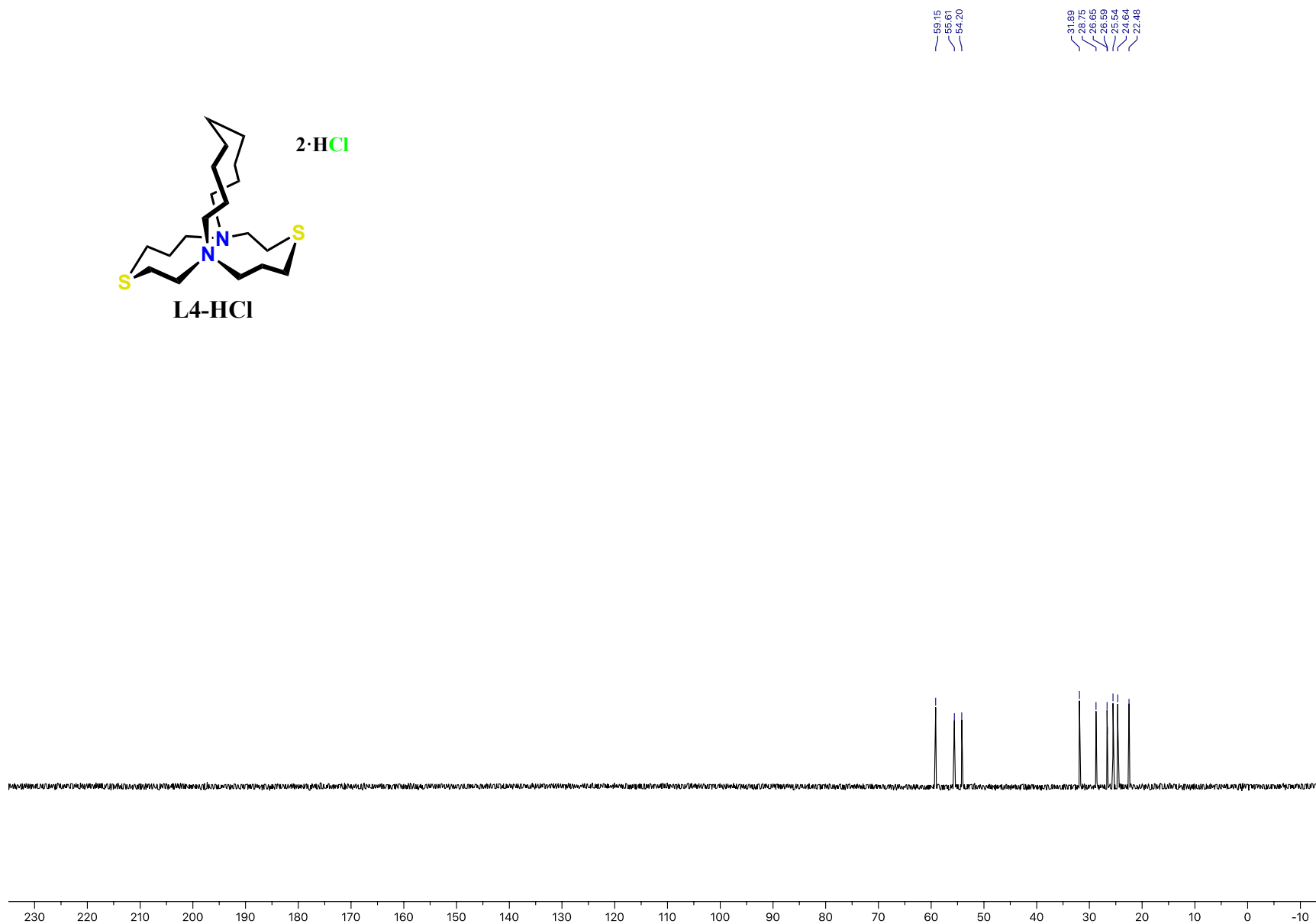
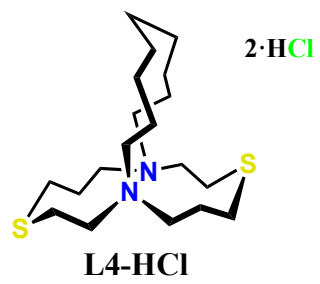
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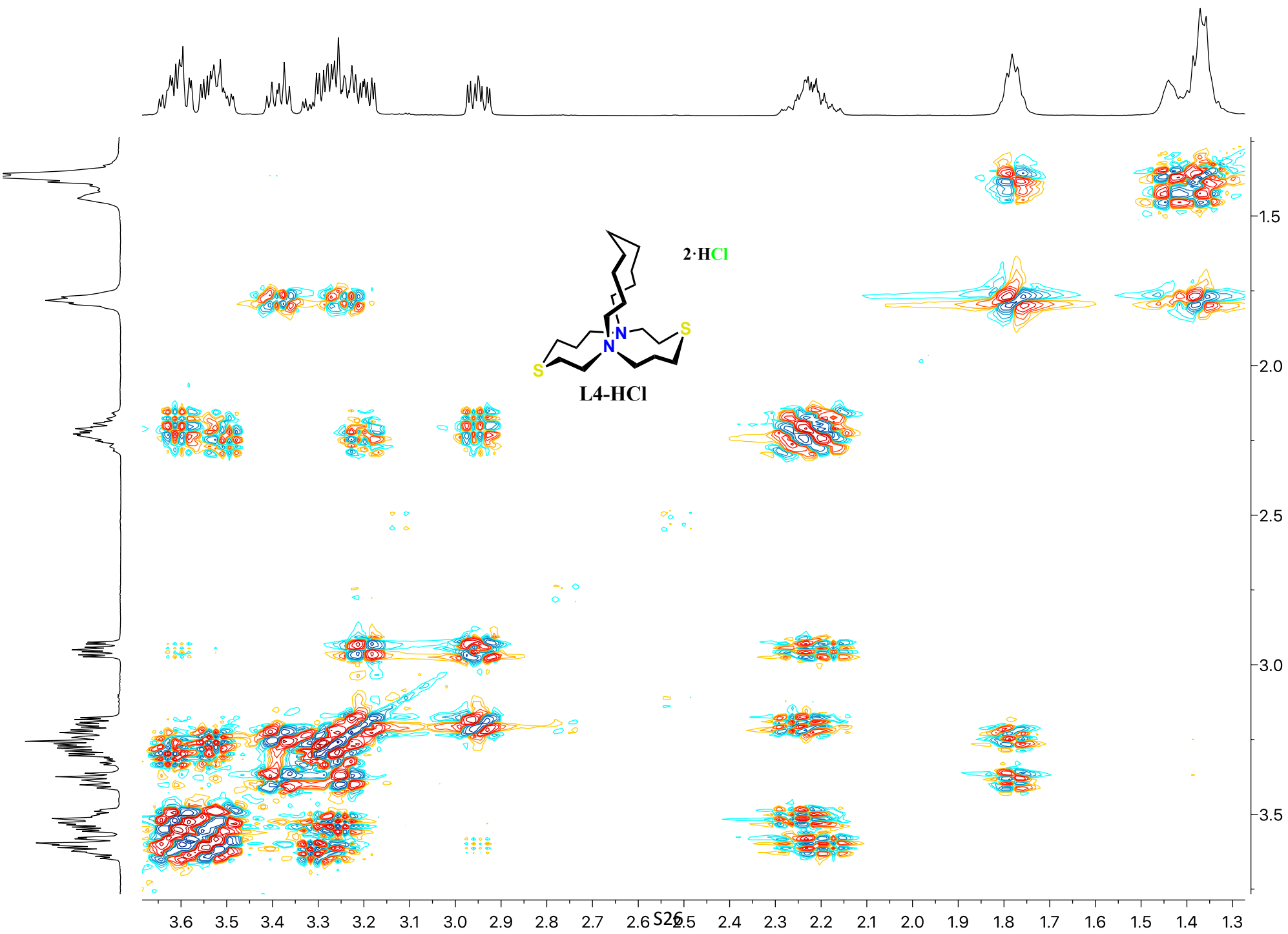
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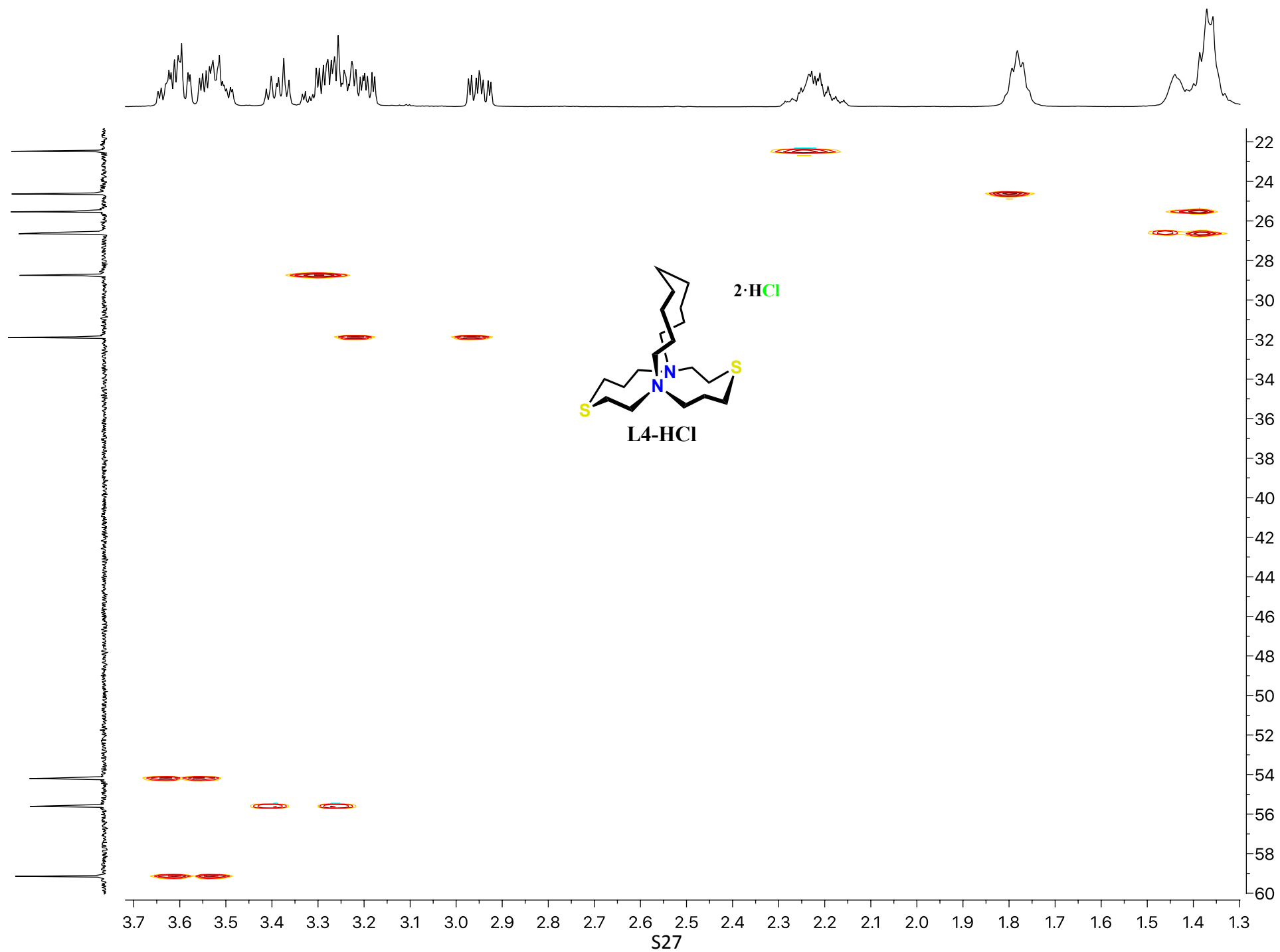
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384.1896	159805	1.017	384.1900	-1.0	-0.4	C ₁₉ H ₃₂ O ₂ N ₂ S ₂
384.9825	17239	0.110				
385.1983	595745	3.791	385.1978	1.4	0.5	C ₁₉ H ₃₃ O ₂ N ₂ S ₂
386.2060	15716773	100.000	386.2056	1.0	0.4	C ₁₉ H ₃₄ O ₂ N ₂ S ₂
386.3476	120047	0.764				
386.5181	20909	0.133				
387.2087	3544066	22.550				
387.3636	44778	0.285				
387.9932	44359	0.282				
388.2042	1804057	11.479				
389.2061	347220	2.209				
390.2025	79193	0.504				
391.2100	19330	0.123				
391.9870	41261	0.263				
396.9749	27102	0.172				
399.9801	49760	0.317				
401.9814	26325	0.167				
402.2011	16997	0.108				
402.9798	83722	0.533				
405.9784	343341	2.185				
406.9891	75056	0.478				
408.9737	98920	0.629				
410.3923	16364	0.104				
411.9734	137097	0.872				
420.9727	121502	0.773				
421.9761	66376	0.422				
422.9868	31337	0.199				
423.9744	470282	2.992				
425.9812	74595	0.475				
426.9925	17436	0.111				
430.3902	31282	0.199				
437.9874	48012	0.305				
441.9805	37435	0.238				
444.9804	88582	0.564				
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450.9788	96130	0.612				
451.9725	22067	0.140				

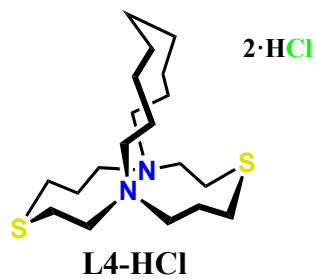
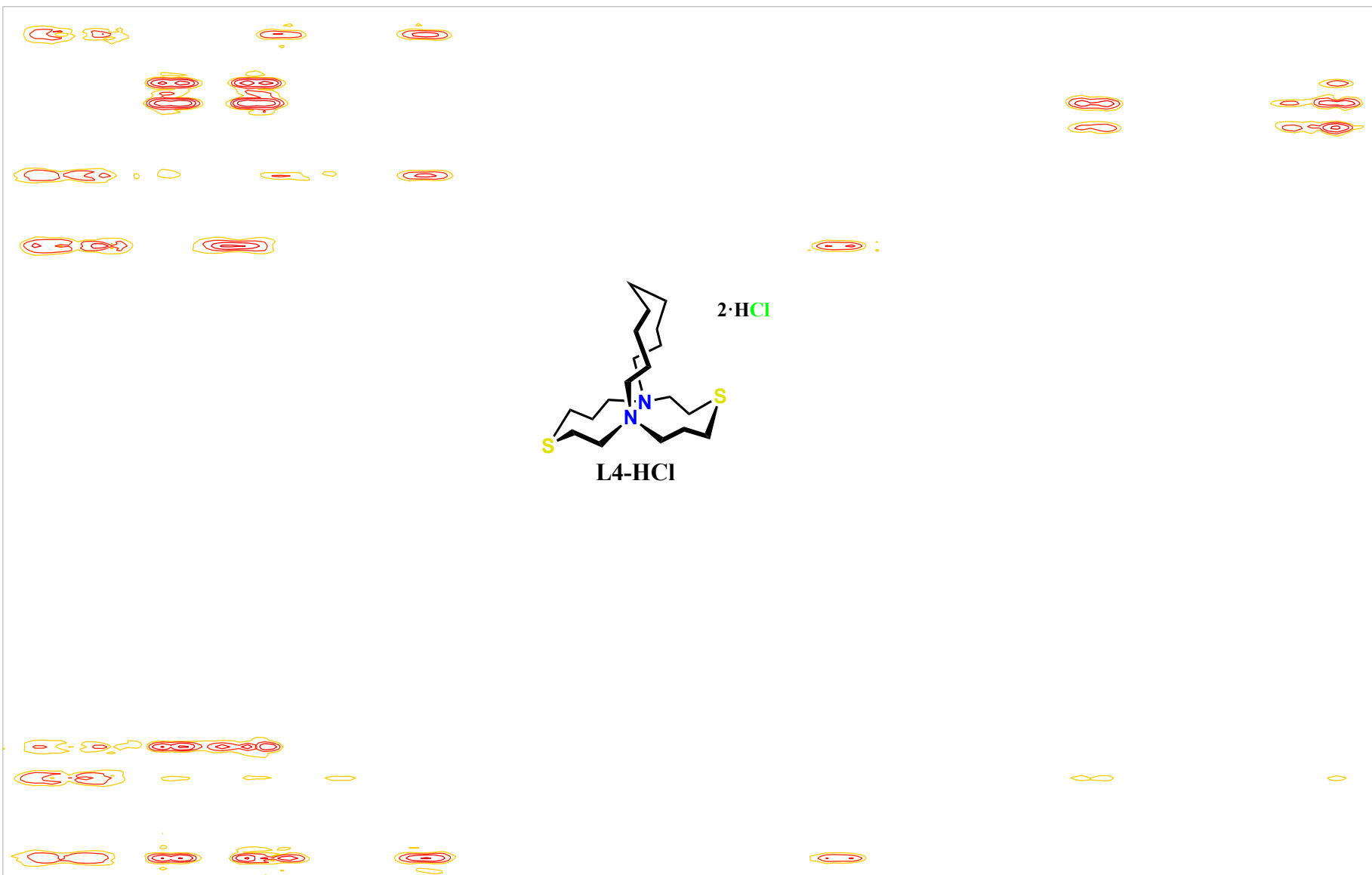
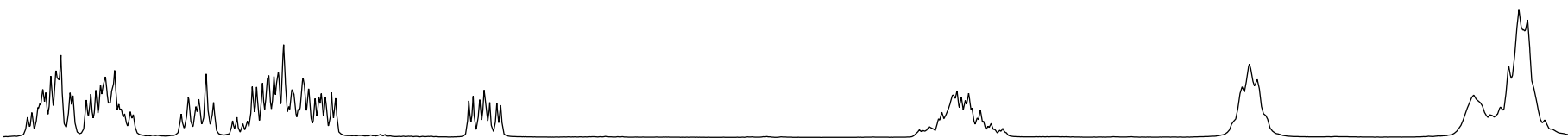












S28

Elemental Composition Report

Page 1

Multiple Mass Analysis: 2 mass(es) processed

Tolerance = 8.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

68 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

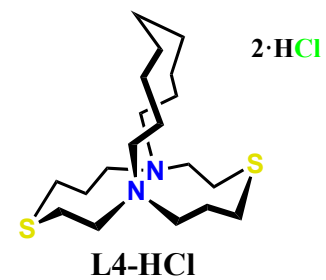
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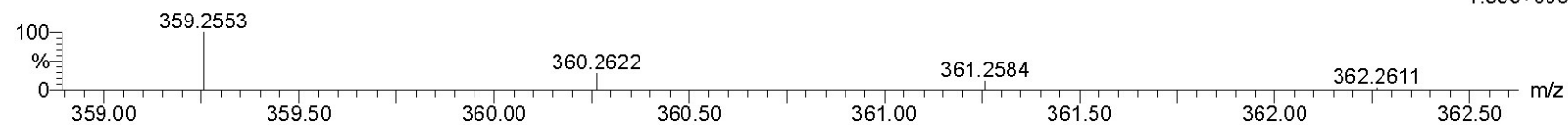
it-01-cryptamine-c9

it-01-cryptamine-c9 10 (0.396) Cm (9:11)

5.00000000



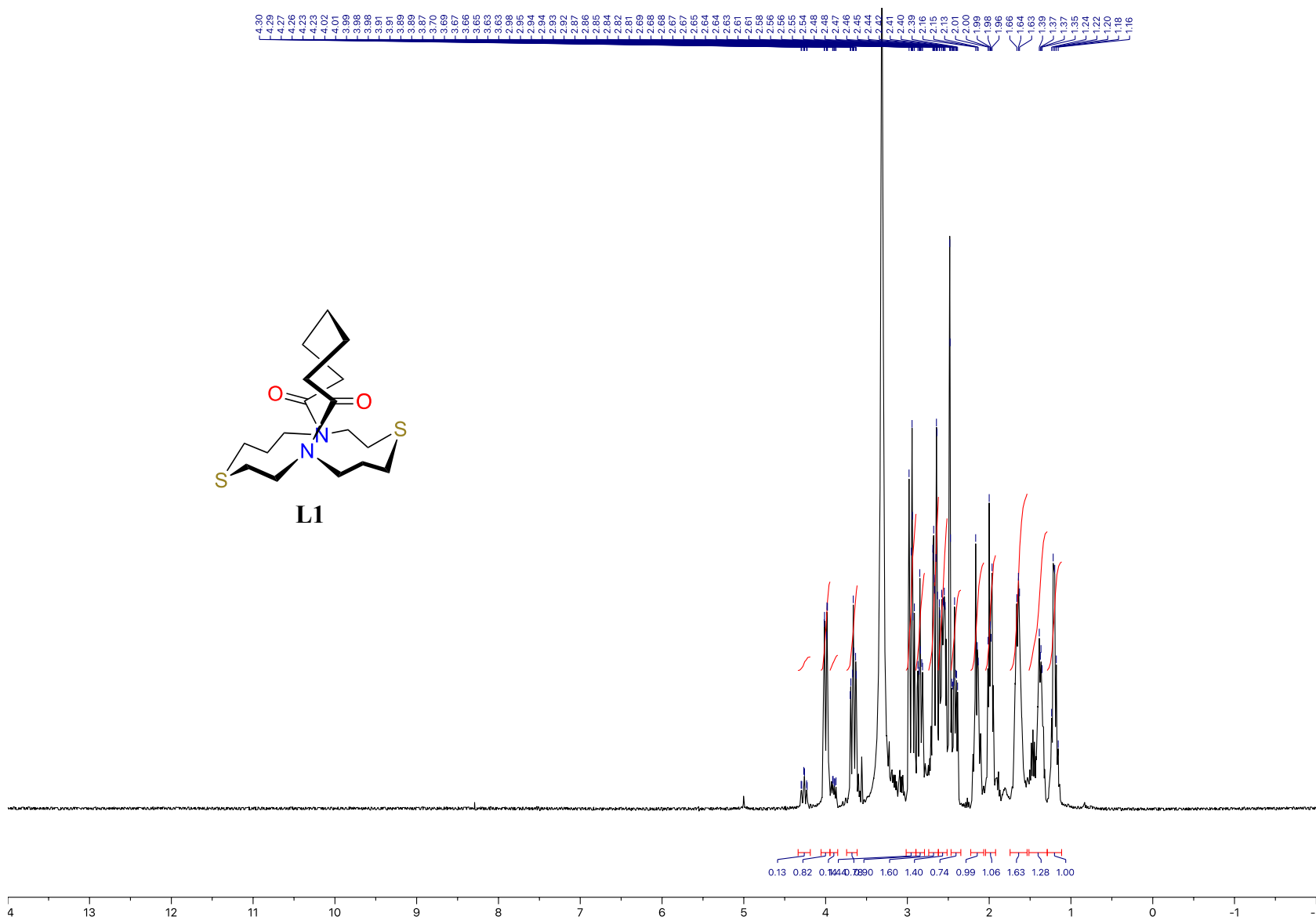
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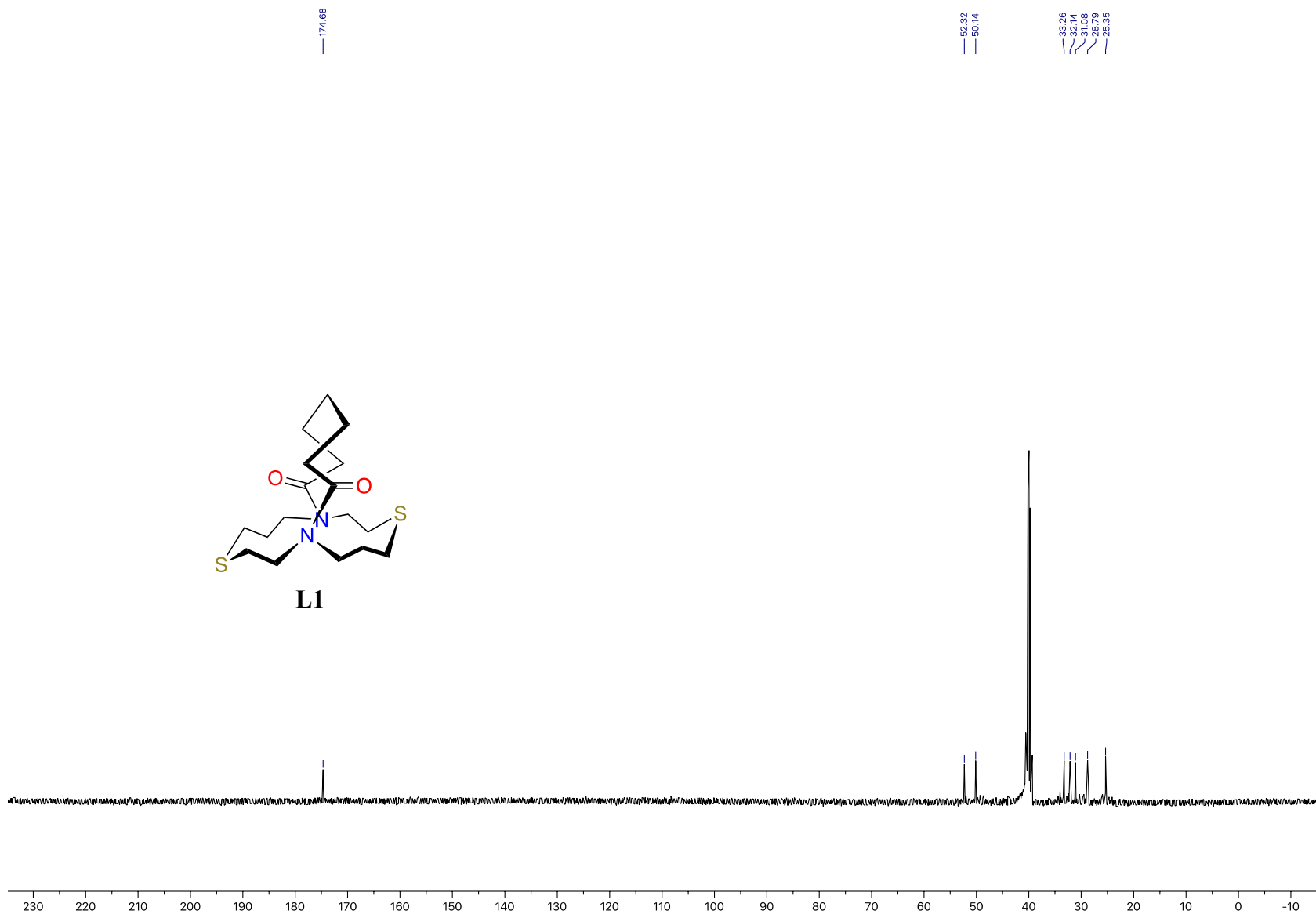


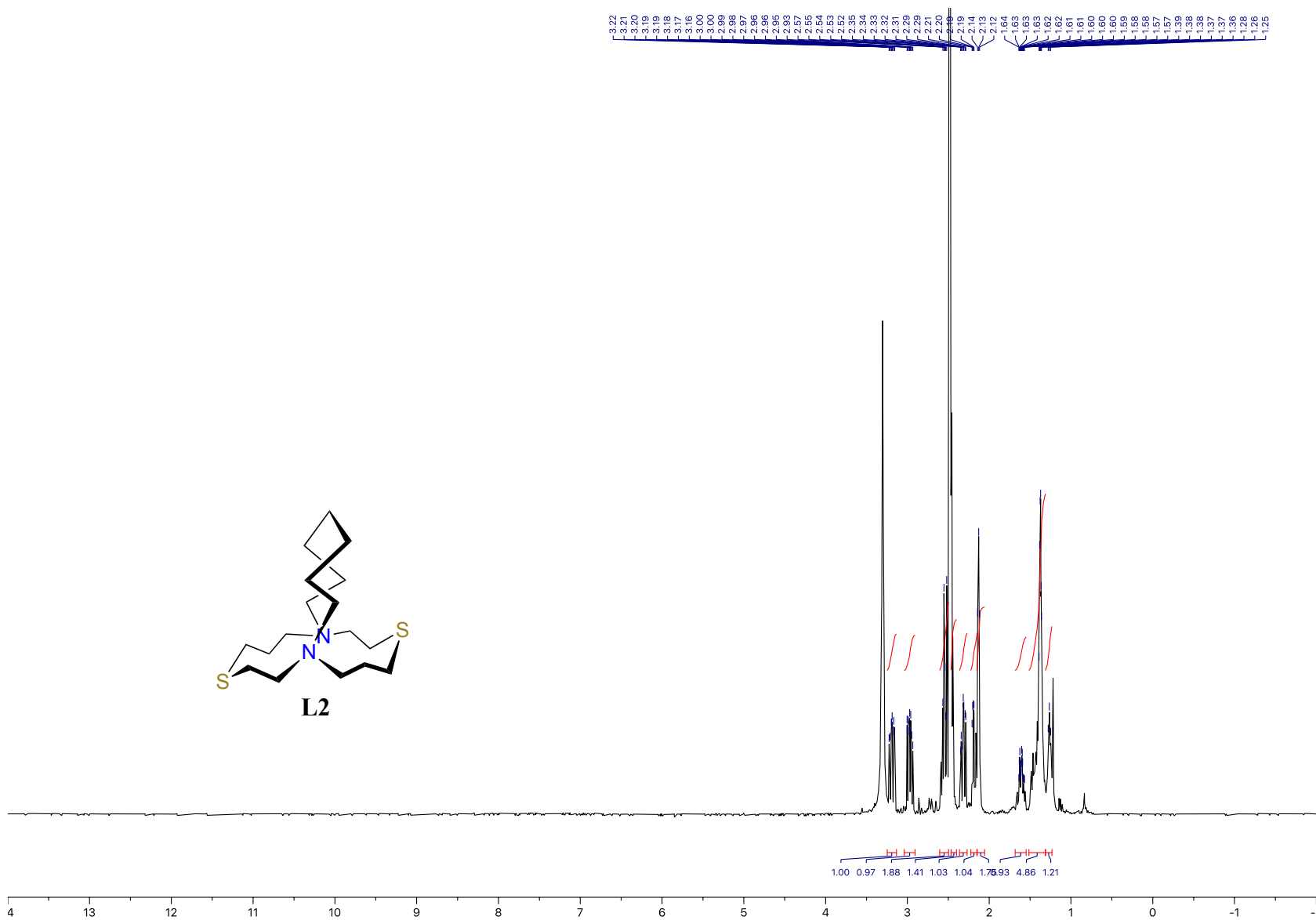
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Maximum: 100.00

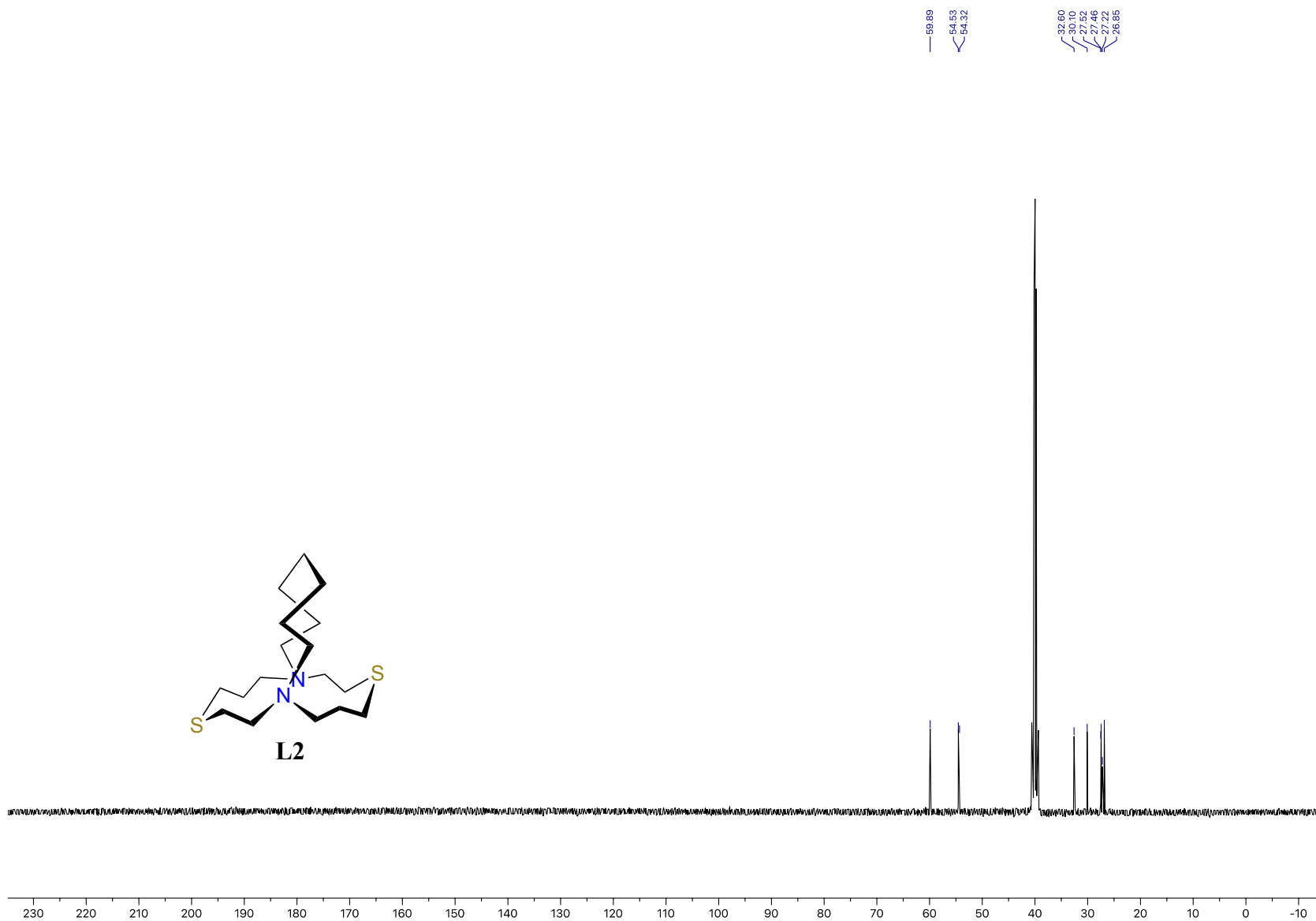
-1.5
100.0

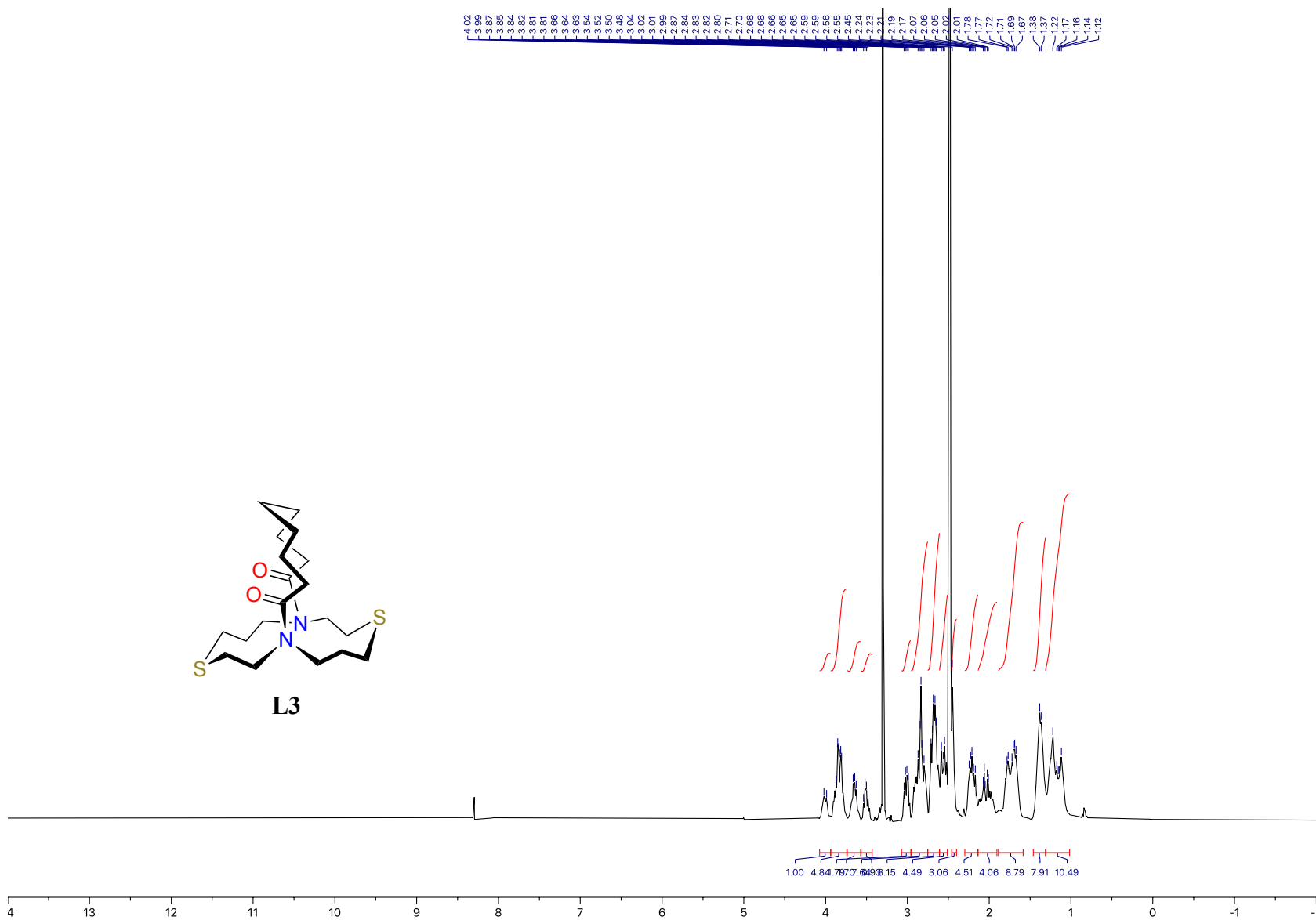
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
359.2553	100.00	359.2555	-0.2	-0.6	1.5	34.7	0.0	C19 H39 N2 S2
360.2622	27.86	---						

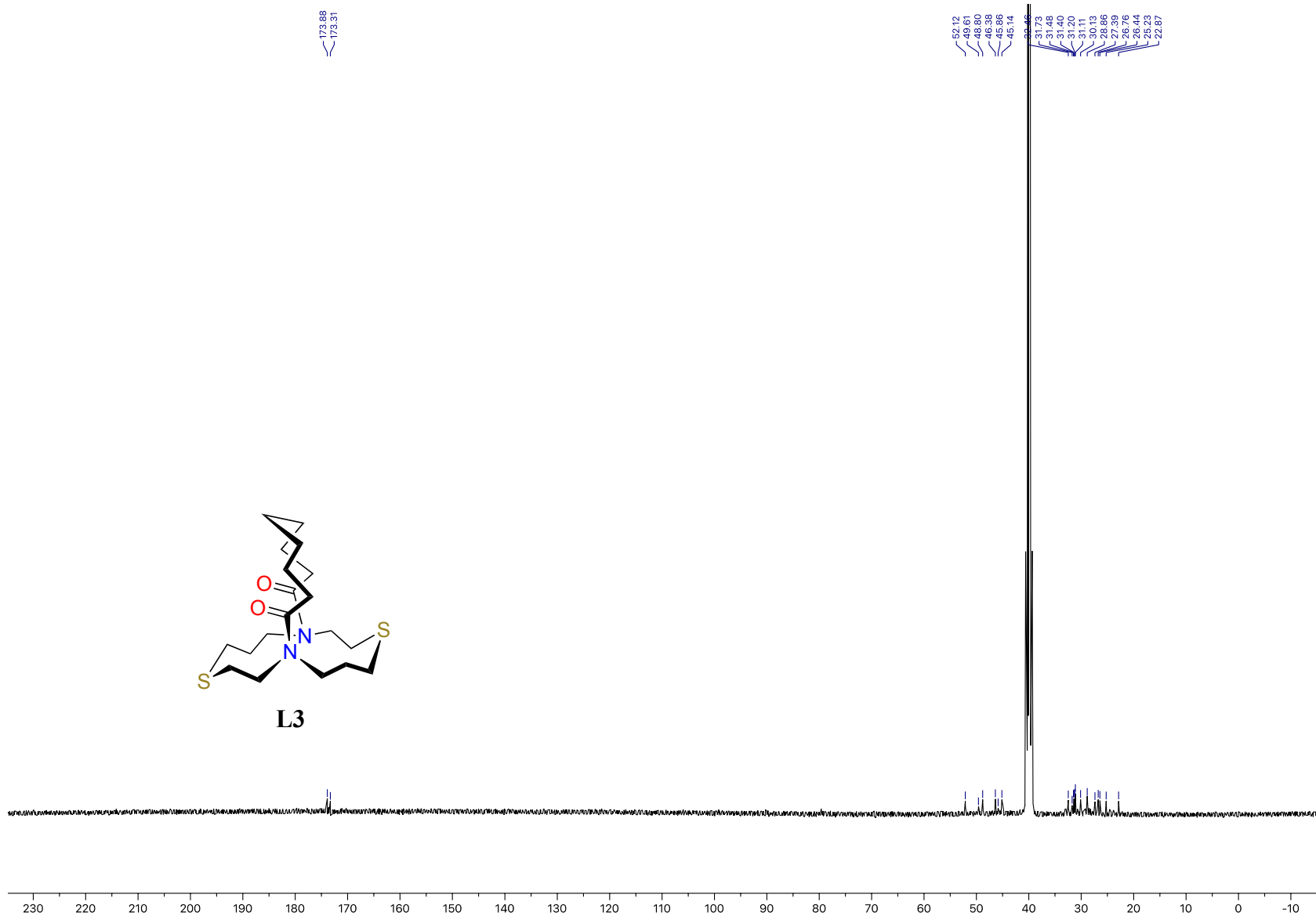


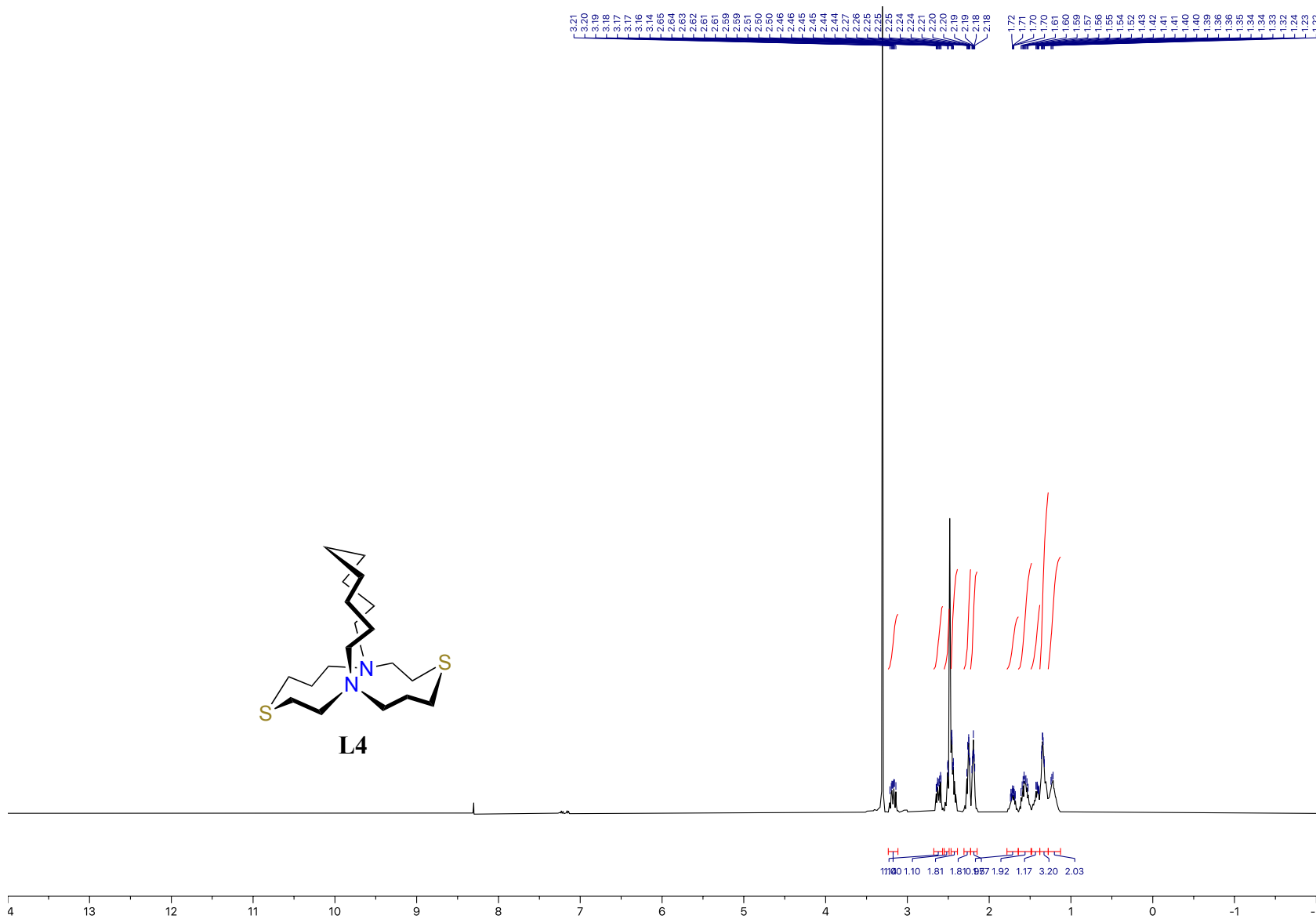


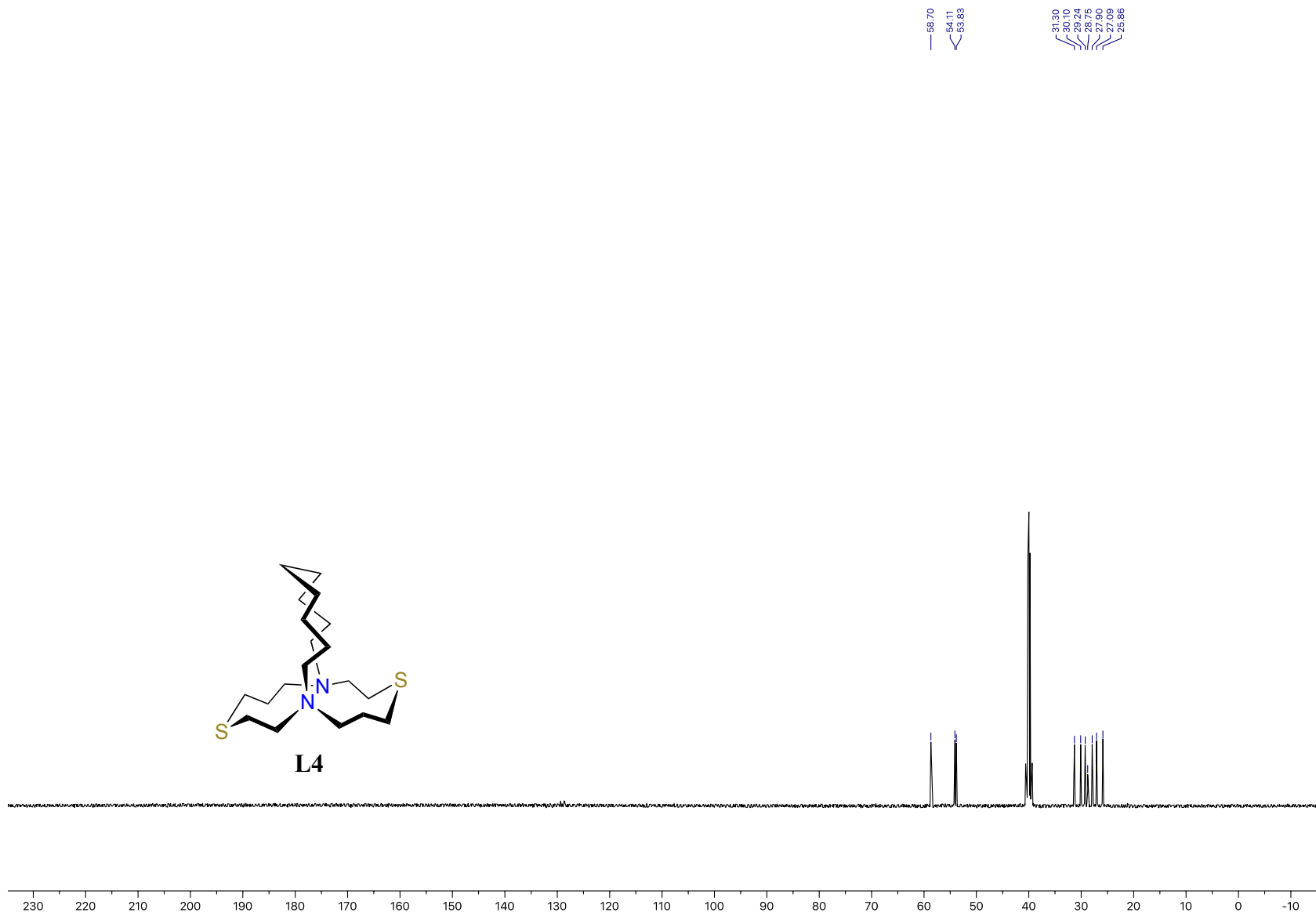


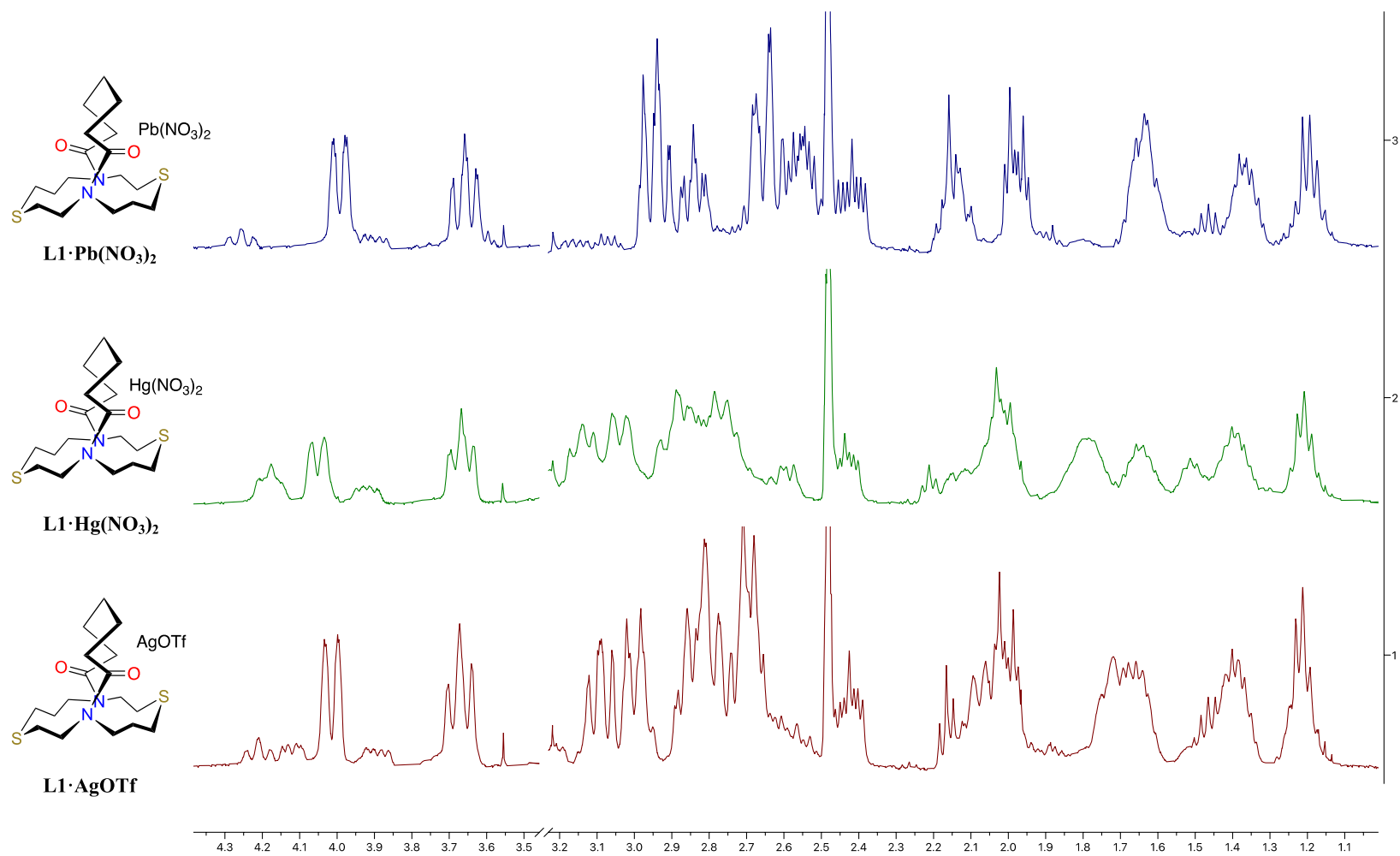




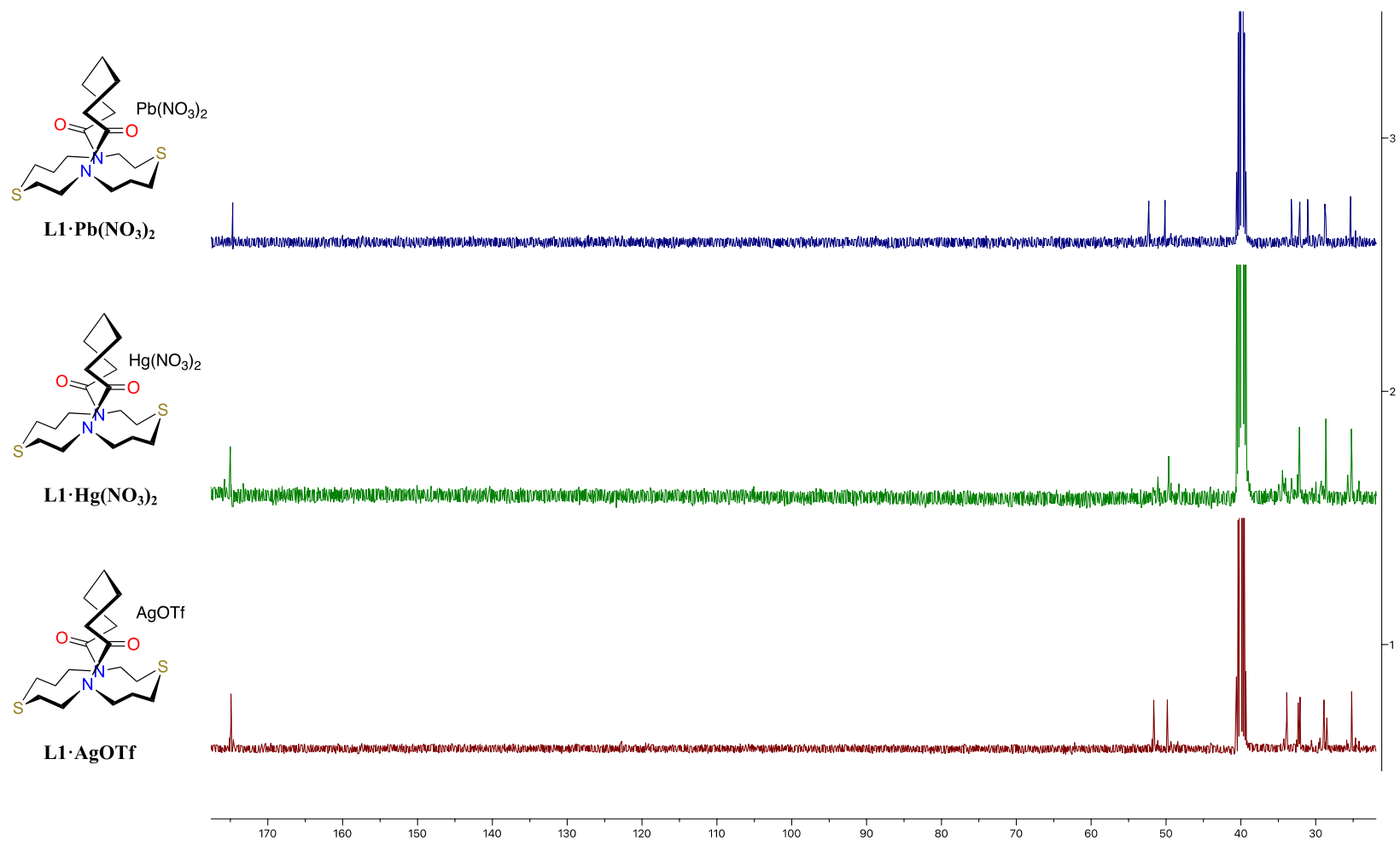


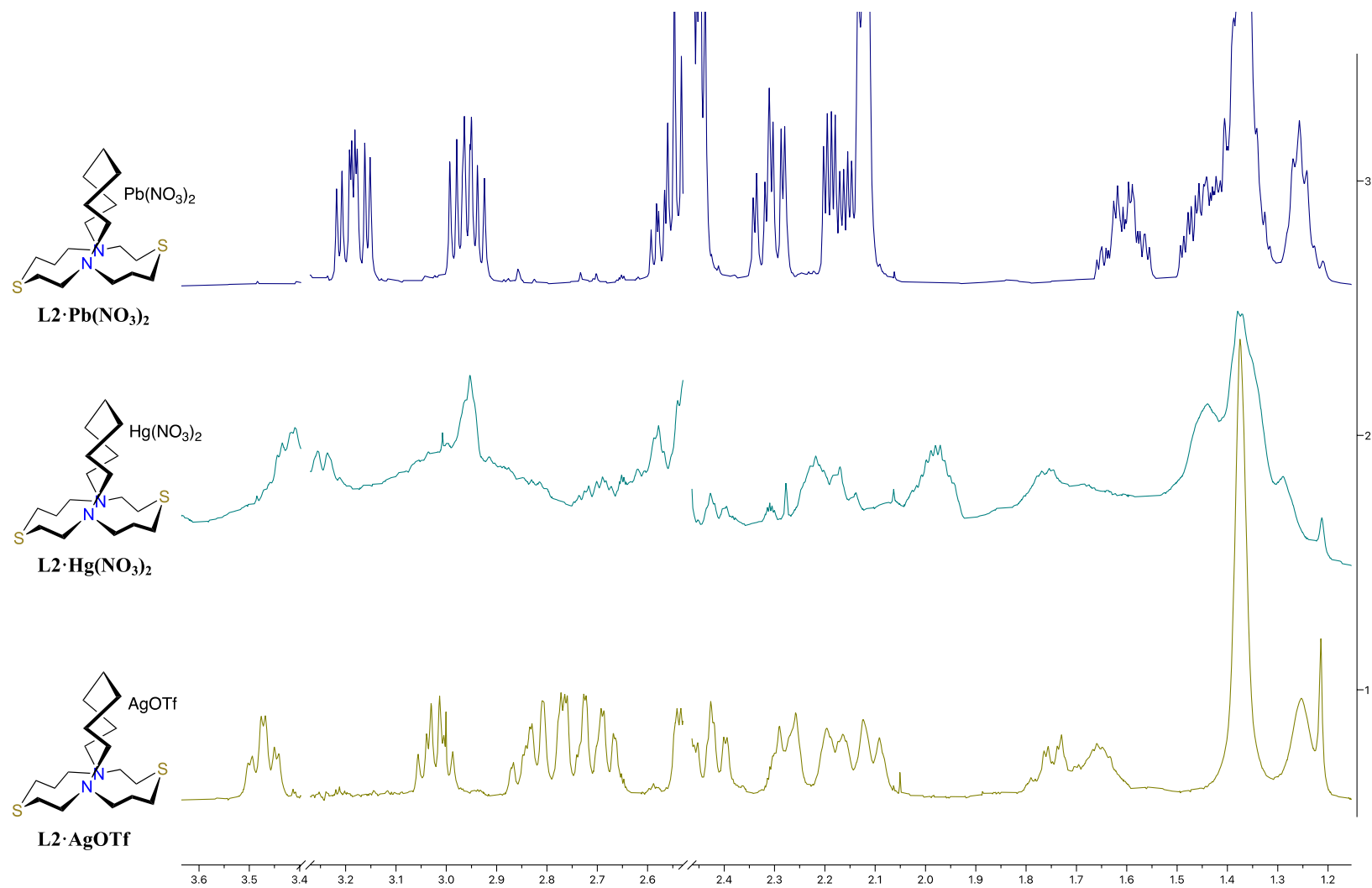




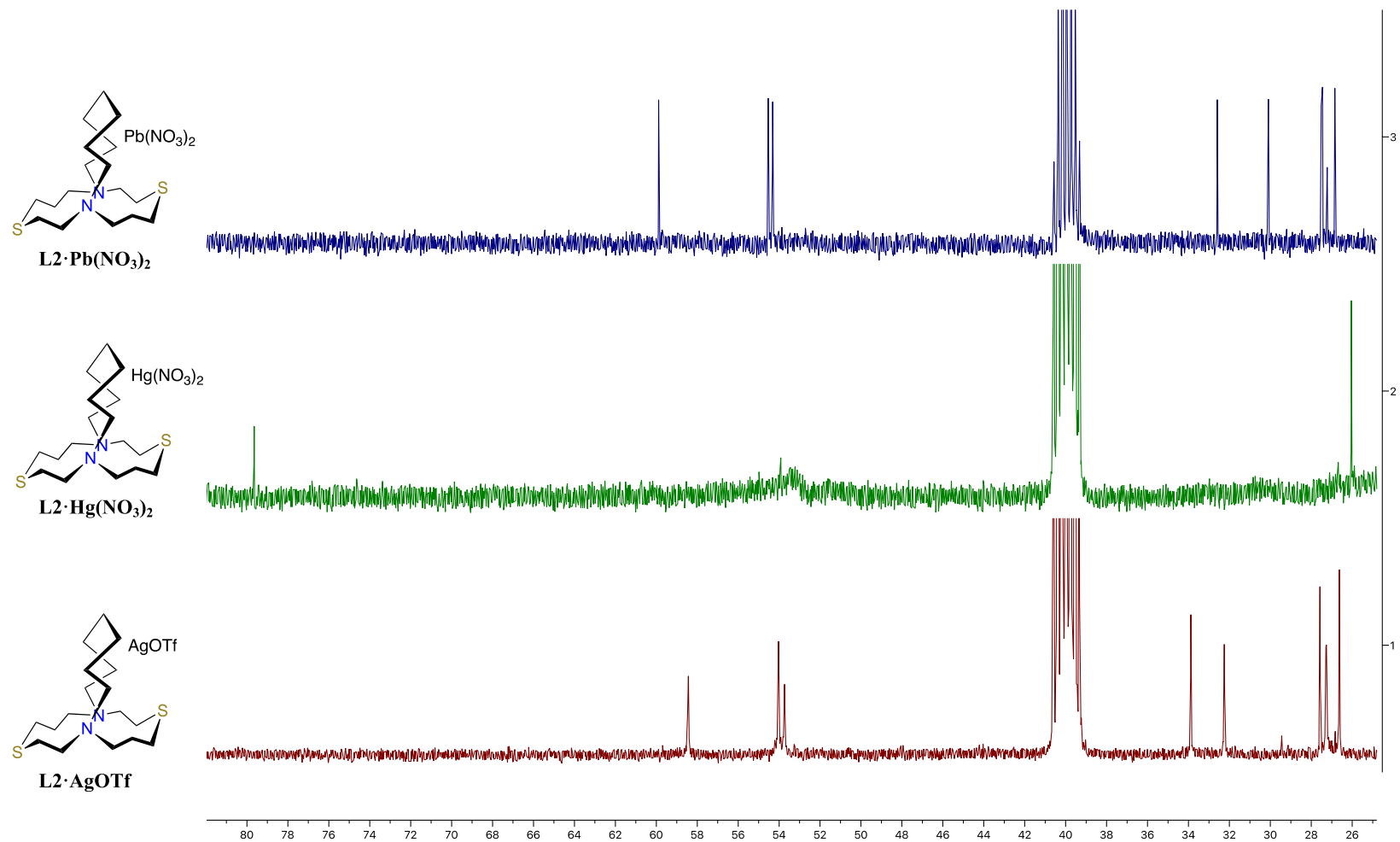


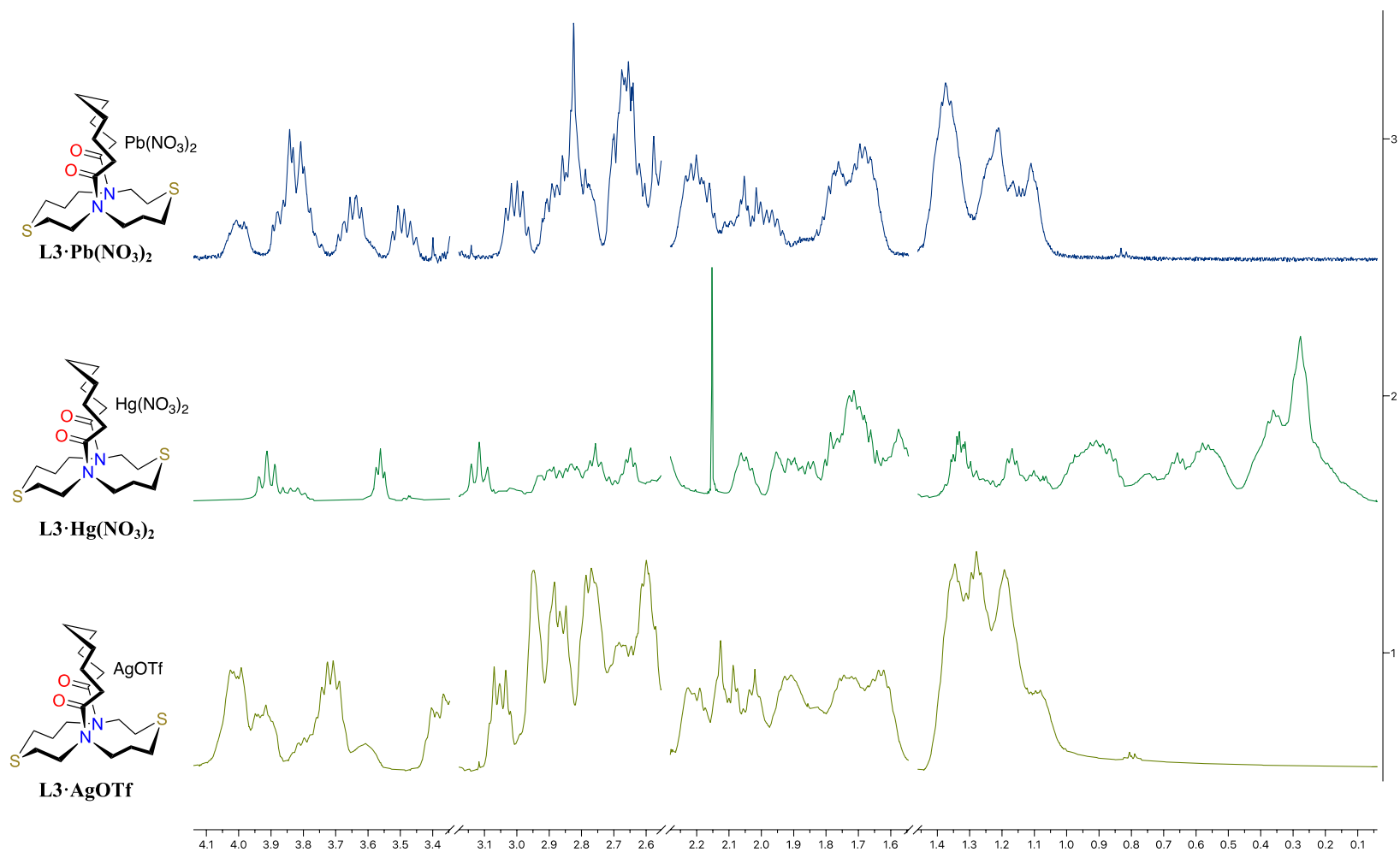
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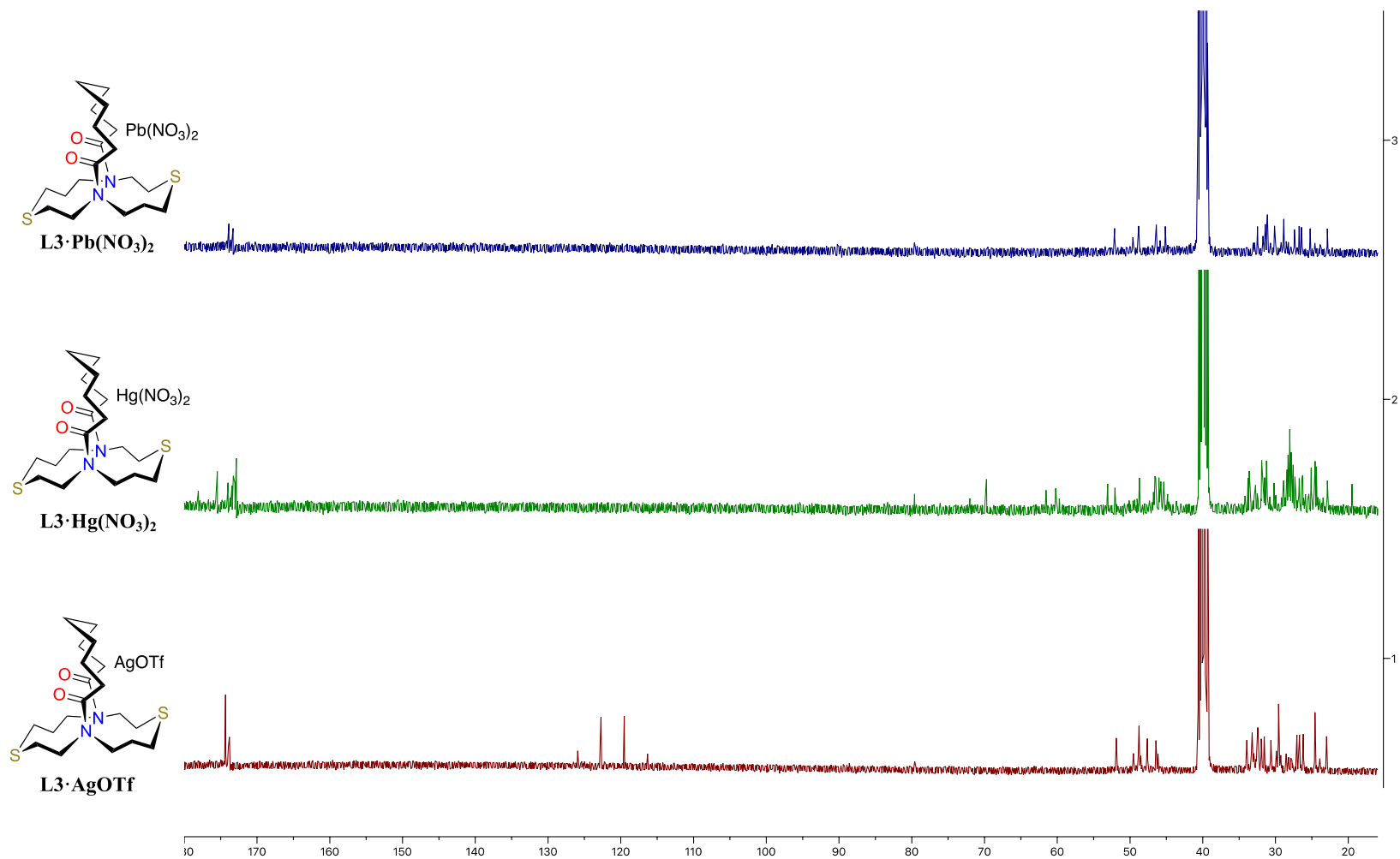


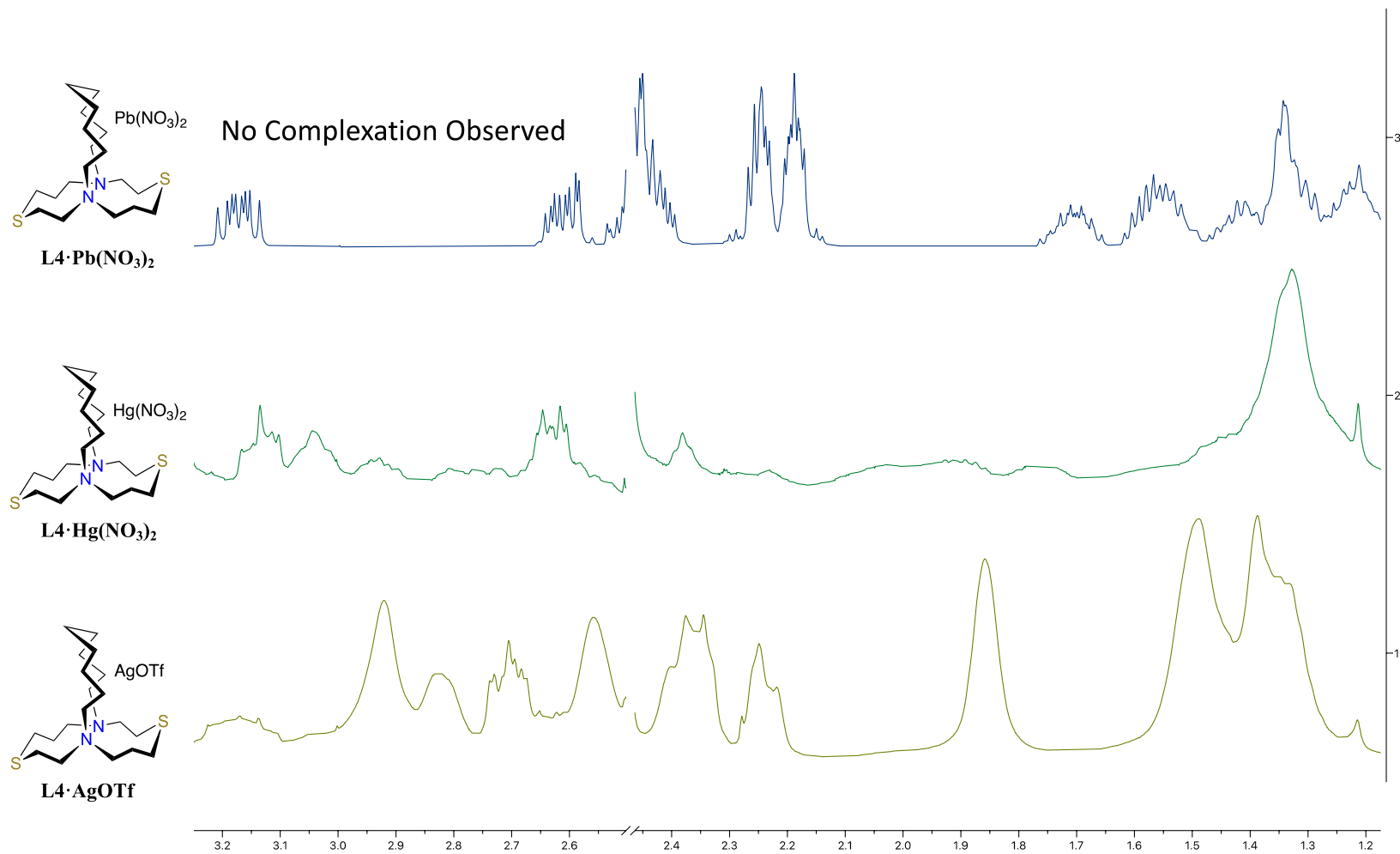
* HOD and DMSO removed from spectra for clarity



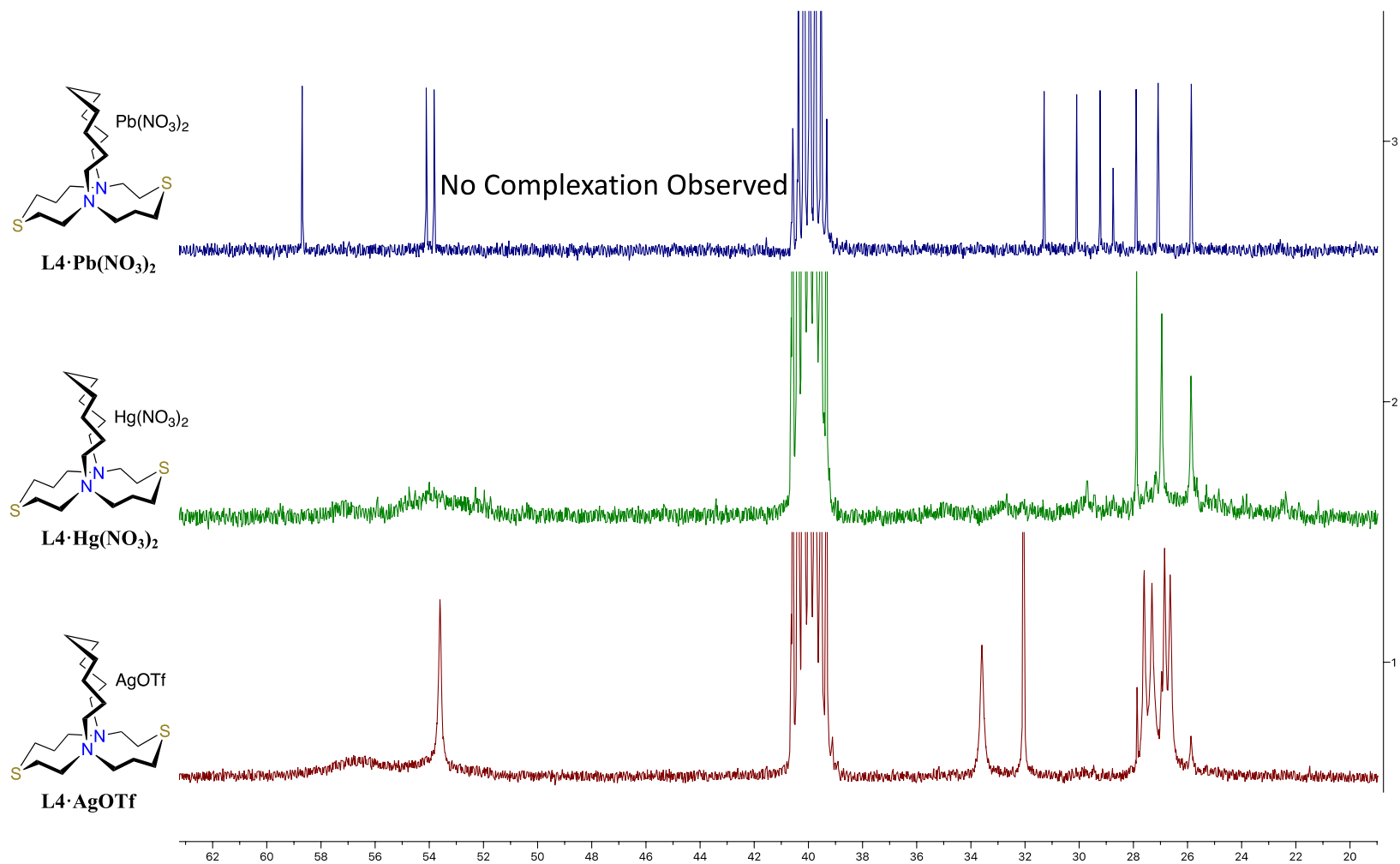


* HOD and DMSO removed from spectra for clarity





* HOD and DMSO removed from spectra for clarity



Computational Data

Table S3. Absolute electronic energies (E, at the PCM chloroform-wB97X-D/def2-TZVP//B97D/def2-TZVP level of theory) for the structures in Figure 9 (in hartrees).

Molecule	Conformer	E (Hartree)
L1	7_Amide_73	-1722.357943
L2	7_Amine_39	-1574.246736
L3	9_Amide_5	-1800.991588
L4	9_Amine_621	-1652.886841
L6	8_Amide_19	-1761.675734
L7	8_Amine_111	-1613.567194

Table S4. Absolute and relative (with respect to their respective low-lying conformer) electronic energies (E, at the PCM chloroform-wB97X-D/def2-TZVP//B97D/def2-TZVP level of theory) for the structures in Figure 10 (in hartrees).

Molecule	E (Hartree)	ΔE (kcal/mol)
T1	-1722.3284019	18.5
T2	-1800.9489641	26.7
T3	-1761.6434817	20.2
LR1 (7_Amide_170)	-1722.35700366	0.6
LR3 (9_Amide_111)	-1800.99117755	0.3
LR6 (8_Amide_121)	-1761.67221048	2.2

Table S5. Absolute and relative (with respect to their respective low-lying conformer) electronic energies (E, at the PCM chloroform-wB97X-D/def2-TZVP//B97D/def2-TZVP level of theory) for the conformers of L1

Conformer	E (Hartree)	ΔE (kcal/mol)
7_Amide_73	-1722.35794342	0.0
7_Amide_190	-1722.35754838	0.2
7_Amide_170	-1722.35700366	0.6
7_Amide_224	-1722.35643471	0.9
7_Amide_116	-1722.35633330	1.0
7_Amide_109	-1722.35633278	1.0
7_Amide_145	-1722.35615264	1.1
7_Amide_210	-1722.35406298	2.4
7_Amide_108	-1722.35401273	2.5
7_Amide_64	-1722.35378181	2.6
7_Amide_26	-1722.35368733	2.7
7_Amide_151	-1722.35359350	2.7
7_Amide_240	-1722.35358241	2.7
7_Amide_32	-1722.35356476	2.7
7_Amide_1	-1722.35347950	2.8
7_Amide_77	-1722.35333236	2.9
7_Amide_231	-1722.35303997	3.1
7_Amide_95	-1722.35289713	3.2
7_Amide_111	-1722.35287615	3.2
7_Amide_51	-1722.35262159	3.3
7_Amide_46	-1722.35261153	3.3
7_Amide_84	-1722.35219507	3.6
7_Amide_98	-1722.35208934	3.7
7_Amide_223	-1722.35206864	3.7
7_Amide_121	-1722.35202704	3.7

7_Amide_101	-1722.35167512	3.9
7_Amide_48	-1722.35162263	4.0
7_Amide_40	-1722.35162022	4.0
7_Amide_47	-1722.35145318	4.1
7_Amide_243	-1722.35141411	4.1
7_Amide_159	-1722.35138079	4.1
7_Amide_92	-1722.35118747	4.2
7_Amide_118	-1722.35115711	4.3
7_Amide_82	-1722.35111586	4.3
7_Amide_200	-1722.35109643	4.3
7_Amide_232	-1722.35109555	4.3
7_Amide_104	-1722.35104523	4.3
7_Amide_106	-1722.35097125	4.4
7_Amide_156	-1722.35095965	4.4
7_Amide_185	-1722.35082726	4.5
7_Amide_23	-1722.35081346	4.5
7_Amide_11	-1722.35033160	4.8
7_Amide_149	-1722.35032949	4.8
7_Amide_183	-1722.35005403	5.0
7_Amide_65	-1722.35002363	5.0
7_Amide_238	-1722.34996640	5.0
7_Amide_178	-1722.34994733	5.0
7_Amide_69	-1722.34991230	5.0
7_Amide_58	-1722.34989520	5.1
7_Amide_93	-1722.34989083	5.1
7_Amide_57	-1722.34989043	5.1
7_Amide_119	-1722.34987996	5.1
7_Amide_172	-1722.34962768	5.2
7_Amide_72	-1722.34956956	5.3
7_Amide_228	-1722.34948898	5.3

7_Amide_147	-1722.34938124	5.4
7_Amide_139	-1722.34934646	5.4
7_Amide_142	-1722.34928713	5.4
7_Amide_191	-1722.34923359	5.5
7_Amide_211	-1722.34920601	5.5
7_Amide_80	-1722.34920584	5.5
7_Amide_123	-1722.34896729	5.6
7_Amide_29	-1722.34889951	5.7
7_Amide_204	-1722.34889636	5.7
7_Amide_167	-1722.34882299	5.7
7_Amide_31	-1722.34882294	5.7
7_Amide_158	-1722.34865270	5.8
7_Amide_246	-1722.34865270	5.8
7_Amide_181	-1722.34857906	5.9
7_Amide_91	-1722.34837337	6.0
7_Amide_22	-1722.34835182	6.0
7_Amide_117	-1722.34833768	6.0
7_Amide_171	-1722.34831912	6.0
7_Amide_34	-1722.34828131	6.1
7_Amide_179	-1722.34825398	6.1
7_Amide_27	-1722.34800979	6.2
7_Amide_155	-1722.34798789	6.2
7_Amide_44	-1722.34791826	6.3
7_Amide_83	-1722.34790097	6.3
7_Amide_148	-1722.34782691	6.3
7_Amide_53	-1722.34770569	6.4
7_Amide_13	-1722.34764960	6.5
7_Amide_131	-1722.34744526	6.6
7_Amide_197	-1722.34741357	6.6
7_Amide_124	-1722.34738583	6.6

7_Amide_78	-1722.34734695	6.6
7_Amide_230	-1722.34723748	6.7
7_Amide_244	-1722.34714959	6.8
7_Amide_222	-1722.34713717	6.8
7_Amide_239	-1722.34698178	6.9
7_Amide_234	-1722.34694609	6.9
7_Amide_235	-1722.34689161	6.9
7_Amide_59	-1722.34685150	7.0
7_Amide_50	-1722.34681044	7.0
7_Amide_127	-1722.34679526	7.0
7_Amide_33	-1722.34669391	7.1
7_Amide_166	-1722.34654674	7.2
7_Amide_226	-1722.34654414	7.2
7_Amide_79	-1722.34653880	7.2
7_Amide_189	-1722.34652151	7.2
7_Amide_218	-1722.34644480	7.2
7_Amide_36	-1722.34640202	7.2
7_Amide_154	-1722.34636826	7.3
7_Amide_125	-1722.34631843	7.3
7_Amide_74	-1722.34625838	7.3
7_Amide_42	-1722.34620063	7.4
7_Amide_99	-1722.34612005	7.4
7_Amide_7	-1722.34598679	7.5
7_Amide_28	-1722.34588598	7.6
7_Amide_3	-1722.34575070	7.7
7_Amide_56	-1722.34574861	7.7
7_Amide_81	-1722.34571621	7.7
7_Amide_161	-1722.34563345	7.7
7_Amide_207	-1722.34557600	7.8
7_Amide_60	-1722.34556887	7.8

7_Amide_96	-1722.34556615	7.8
7_Amide_242	-1722.34555182	7.8
7_Amide_233	-1722.34554336	7.8
7_Amide_85	-1722.34553847	7.8
7_Amide_182	-1722.34553840	7.8
7_Amide_86	-1722.34551525	7.8
7_Amide_194	-1722.34551279	7.8
7_Amide_157	-1722.34542513	7.9
7_Amide_180	-1722.34535506	7.9
7_Amide_241	-1722.34534092	7.9
7_Amide_24	-1722.34518565	8.0
7_Amide_229	-1722.34514329	8.0
7_Amide_10	-1722.34513908	8.0
7_Amide_153	-1722.34498543	8.1
7_Amide_176	-1722.34498464	8.1
7_Amide_12	-1722.34492426	8.2
7_Amide_237	-1722.34479933	8.2
7_Amide_162	-1722.34479109	8.3
7_Amide_120	-1722.34471027	8.3
7_Amide_146	-1722.34465811	8.3
7_Amide_25	-1722.34453416	8.4
7_Amide_136	-1722.34452809	8.4
7_Amide_186	-1722.34452514	8.4
7_Amide_196	-1722.34444034	8.5
7_Amide_39	-1722.34433711	8.5
7_Amide_213	-1722.34429456	8.6
7_Amide_209	-1722.34407048	8.7
7_Amide_177	-1722.34407027	8.7
7_Amide_66	-1722.34403423	8.7
7_Amide_20	-1722.34402222	8.7

7_Amide_140	-1722.34395076	8.8
7_Amide_150	-1722.34394064	8.8
7_Amide_206	-1722.34388827	8.8
7_Amide_14	-1722.34365427	9.0
7_Amide_192	-1722.34363697	9.0
7_Amide_76	-1722.34357721	9.0
7_Amide_184	-1722.34350918	9.1
7_Amide_216	-1722.34342828	9.1
7_Amide_163	-1722.34341060	9.1
7_Amide_87	-1722.34341049	9.1
7_Amide_245	-1722.34337721	9.1
7_Amide_103	-1722.34337267	9.1
7_Amide_107	-1722.34334525	9.2
7_Amide_54	-1722.34330108	9.2
7_Amide_160	-1722.34320437	9.2
7_Amide_49	-1722.34320019	9.3
7_Amide_67	-1722.34318643	9.3
7_Amide_70	-1722.34303215	9.4
7_Amide_225	-1722.34283459	9.5
7_Amide_144	-1722.34272326	9.6
7_Amide_201	-1722.34254318	9.7
7_Amide_134	-1722.34252898	9.7
7_Amide_38	-1722.34249586	9.7
7_Amide_6	-1722.34231456	9.8
7_Amide_137	-1722.34229292	9.8
7_Amide_52	-1722.34213116	9.9
7_Amide_187	-1722.34205552	10.0
7_Amide_122	-1722.34183092	10.1
7_Amide_71	-1722.34180657	10.1
7_Amide_215	-1722.34178134	10.1

7_Amide_5	-1722.34166892	10.2
7_Amide_141	-1722.34159837	10.3
7_Amide_220	-1722.34155128	10.3
7_Amide_168	-1722.34154628	10.3
7_Amide_4	-1722.34146809	10.3
7_Amide_173	-1722.34146339	10.3
7_Amide_115	-1722.34143599	10.4
7_Amide_113	-1722.34131235	10.4
7_Amide_227	-1722.34124632	10.5
7_Amide_110	-1722.34087851	10.7
7_Amide_89	-1722.34082898	10.7
7_Amide_75	-1722.34076684	10.8
7_Amide_219	-1722.34071102	10.8
7_Amide_21	-1722.34059764	10.9
7_Amide_126	-1722.34059196	10.9
7_Amide_138	-1722.34057469	10.9
7_Amide_175	-1722.34024575	11.1
7_Amide_112	-1722.34018070	11.1
7_Amide_203	-1722.34005304	11.2
7_Amide_217	-1722.33994553	11.3
7_Amide_221	-1722.33980250	11.4
7_Amide_195	-1722.33939107	11.6
7_Amide_128	-1722.33922700	11.7
7_Amide_188	-1722.33919072	11.8
7_Amide_236	-1722.33896432	11.9
7_Amide_97	-1722.33892507	11.9
7_Amide_41	-1722.33871543	12.1
7_Amide_133	-1722.33839120	12.3
7_Amide_214	-1722.33814526	12.4
7_Amide_102	-1722.33806135	12.5

7_Amide_212	-1722.33791418	12.6
7_Amide_114	-1722.33770382	12.7
7_Amide_100	-1722.33763074	12.7
7_Amide_2	-1722.33749643	12.8
7_Amide_17	-1722.33711958	13.1
7_Amide_193	-1722.33705186	13.1
7_Amide_15	-1722.33674733	13.3
7_Amide_132	-1722.33671049	13.3
7_Amide_143	-1722.33637394	13.5
7_Amide_198	-1722.33617182	13.7
7_Amide_61	-1722.33616717	13.7
7_Amide_8	-1722.33614845	13.7
7_Amide_129	-1722.33590801	13.8
7_Amide_35	-1722.33518456	14.3
7_Amide_37	-1722.33497754	14.4
7_Amide_169	-1722.33489676	14.5
7_Amide_152	-1722.33488499	14.5
7_Amide_63	-1722.33417178	14.9
7_Amide_16	-1722.33411489	15.0
7_Amide_165	-1722.33373041	15.2
7_Amide_88	-1722.33333673	15.4
7_Amide_68	-1722.33307003	15.6
7_Amide_90	-1722.33286157	15.7
7_Amide_202	-1722.33259389	15.9
7_Amide_18	-1722.33156686	16.6
7_Amide_205	-1722.33121461	16.8
7_Amide_199	-1722.32896416	18.2
7_Amide_62	-1722.32428092	21.1

Table S6. Absolute and relative (with respect to their respective low-lying conformer) electronic energies (E, at the PCM chloroform-wB97X-D/def2-TZVP//B97D/def2-TZVP level of theory) for the conformers of L2

Conformer	E (Hartree)	ΔE (kcal/mol)
7_Amine_39	-1574.24673622	0.0
7_Amine_242	-1574.24623292	0.3
7_Amine_231	-1574.24561108	0.7
7_Amine_190	-1574.24559578	0.7
7_Amine_143	-1574.24538924	0.8
7_Amine_156	-1574.24449358	1.4
7_Amine_83	-1574.24446109	1.4
7_Amine_194	-1574.24356132	2.0
7_Amine_86	-1574.24356042	2.0
7_Amine_72	-1574.24337810	2.1
7_Amine_32	-1574.24334394	2.1
7_Amine_111	-1574.24331235	2.1
7_Amine_230	-1574.24327595	2.2
7_Amine_109	-1574.24298807	2.4
7_Amine_116	-1574.24298807	2.4
7_Amine_108	-1574.24281238	2.5
7_Amine_150	-1574.24277824	2.5
7_Amine_188	-1574.24268253	2.5
7_Amine_91	-1574.24244833	2.7
7_Amine_197	-1574.24241551	2.7
7_Amine_129	-1574.24238506	2.7
7_Amine_240	-1574.24211581	2.9
7_Amine_119	-1574.24207017	2.9
7_Amine_49	-1574.24195227	3.0
7_Amine_142	-1574.24175831	3.1

7_Amine_217	-1574.24132973	3.4
7_Amine_146	-1574.24121762	3.5
7_Amine_153	-1574.24111434	3.5
7_Amine_134	-1574.24103340	3.6
7_Amine_148	-1574.24095624	3.6
7_Amine_180	-1574.24088094	3.7
7_Amine_65	-1574.24063177	3.8
7_Amine_185	-1574.24057334	3.9
7_Amine_64	-1574.24056973	3.9
7_Amine_151	-1574.24035738	4.0
7_Amine_73	-1574.24024560	4.1
7_Amine_183	-1574.24016609	4.1
7_Amine_196	-1574.24000765	4.2
7_Amine_93	-1574.23968257	4.4
7_Amine_36	-1574.23941971	4.6
7_Amine_100	-1574.23939035	4.6
7_Amine_131	-1574.23924320	4.7
7_Amine_123	-1574.23921804	4.7
7_Amine_170	-1574.23920611	4.7
7_Amine_238	-1574.23915684	4.8
7_Amine_162	-1574.23915619	4.8
7_Amine_40	-1574.23889465	4.9
7_Amine_37	-1574.23883057	5.0
7_Amine_171	-1574.23874405	5.0
7_Amine_7	-1574.23874336	5.0
7_Amine_169	-1574.23870178	5.0
7_Amine_66	-1574.23859573	5.1
7_Amine_159	-1574.23833061	5.3
7_Amine_27	-1574.23831060	5.3
7_Amine_115	-1574.23822066	5.3

7_Amine_181	-1574.23818066	5.4
7_Amine_239	-1574.23806279	5.4
7_Amine_210	-1574.23805707	5.4
7_Amine_201	-1574.23787731	5.6
7_Amine_79	-1574.23783001	5.6
7_Amine_132	-1574.23781787	5.6
7_Amine_76	-1574.23780548	5.6
7_Amine_158	-1574.23776690	5.6
7_Amine_246	-1574.23776689	5.6
7_Amine_163	-1574.23760495	5.7
7_Amine_87	-1574.23760282	5.7
7_Amine_138	-1574.23751690	5.8
7_Amine_166	-1574.23744932	5.8
7_Amine_233	-1574.23717133	6.0
7_Amine_182	-1574.23716974	6.0
7_Amine_245	-1574.23715982	6.0
7_Amine_10	-1574.23710459	6.0
7_Amine_229	-1574.23710454	6.0
7_Amine_243	-1574.23709956	6.0
7_Amine_75	-1574.23704483	6.1
7_Amine_62	-1574.23704385	6.1
7_Amine_31	-1574.23693322	6.2
7_Amine_74	-1574.23685893	6.2
7_Amine_60	-1574.23668152	6.3
7_Amine_92	-1574.23657666	6.4
7_Amine_186	-1574.23657566	6.4
7_Amine_99	-1574.23636409	6.5
7_Amine_120	-1574.23631539	6.5
7_Amine_178	-1574.23607905	6.7
7_Amine_97	-1574.23607341	6.7

7_Amine_136	-1574.23603978	6.7
7_Amine_237	-1574.23598919	6.7
7_Amine_20	-1574.23568561	6.9
7_Amine_107	-1574.23564038	7.0
7_Amine_216	-1574.23557614	7.0
7_Amine_56	-1574.23551881	7.0
7_Amine_44	-1574.23551856	7.0
7_Amine_104	-1574.23538884	7.1
7_Amine_228	-1574.23536406	7.1
7_Amine_23	-1574.23517160	7.3
7_Amine_12	-1574.23514244	7.3
7_Amine_145	-1574.23505467	7.3
7_Amine_106	-1574.23499892	7.4
7_Amine_139	-1574.23494835	7.4
7_Amine_220	-1574.23481052	7.5
7_Amine_122	-1574.23478743	7.5
7_Amine_101	-1574.23471528	7.5
7_Amine_1	-1574.23467576	7.6
7_Amine_127	-1574.23460696	7.6
7_Amine_192	-1574.23460008	7.6
7_Amine_121	-1574.23449448	7.7
7_Amine_90	-1574.23446007	7.7
7_Amine_154	-1574.23440133	7.7
7_Amine_118	-1574.23418688	7.9
7_Amine_227	-1574.23412470	7.9
7_Amine_128	-1574.23400270	8.0
7_Amine_168	-1574.23400012	8.0
7_Amine_209	-1574.23391114	8.0
7_Amine_204	-1574.23389631	8.1
7_Amine_29	-1574.23389604	8.1

7_Amine_15	-1574.23386797	8.1
7_Amine_26	-1574.23379756	8.1
7_Amine_18	-1574.23340280	8.4
7_Amine_244	-1574.23340171	8.4
7_Amine_96	-1574.23338529	8.4
7_Amine_124	-1574.23336084	8.4
7_Amine_172	-1574.23335348	8.4
7_Amine_8	-1574.23328708	8.4
7_Amine_241	-1574.23327482	8.4
7_Amine_67	-1574.23326979	8.5
7_Amine_38	-1574.23325572	8.5
7_Amine_77	-1574.23323364	8.5
7_Amine_110	-1574.23307504	8.6
7_Amine_46	-1574.23305358	8.6
7_Amine_47	-1574.23282960	8.7
7_Amine_179	-1574.23281493	8.7
7_Amine_113	-1574.23277604	8.8
7_Amine_133	-1574.23273114	8.8
7_Amine_173	-1574.23271262	8.8
7_Amine_59	-1574.23269213	8.8
7_Amine_21	-1574.23266574	8.8
7_Amine_177	-1574.23251604	8.9
7_Amine_184	-1574.23243807	9.0
7_Amine_161	-1574.23220601	9.1
7_Amine_78	-1574.23214830	9.2
7_Amine_211	-1574.23197056	9.3
7_Amine_80	-1574.23196971	9.3
7_Amine_35	-1574.23171766	9.4
7_Amine_6	-1574.23154828	9.5
7_Amine_187	-1574.23142325	9.6

7_Amine_195	-1574.23133695	9.7
7_Amine_11	-1574.23124022	9.7
7_Amine_34	-1574.23121989	9.7
7_Amine_223	-1574.23109025	9.8
7_Amine_53	-1574.23108844	9.8
7_Amine_112	-1574.23090585	9.9
7_Amine_125	-1574.23085902	10.0
7_Amine_50	-1574.23070060	10.1
7_Amine_5	-1574.23068963	10.1
7_Amine_203	-1574.23065383	10.1
7_Amine_200	-1574.23063462	10.1
7_Amine_165	-1574.23062957	10.1
7_Amine_232	-1574.23059160	10.1
7_Amine_213	-1574.23056914	10.1
7_Amine_28	-1574.23050430	10.2
7_Amine_152	-1574.23047515	10.2
7_Amine_205	-1574.23044046	10.2
7_Amine_103	-1574.23039270	10.3
7_Amine_198	-1574.23014644	10.4
7_Amine_14	-1574.23012574	10.4
7_Amine_176	-1574.23005022	10.5
7_Amine_69	-1574.23000163	10.5
7_Amine_226	-1574.22995850	10.5
7_Amine_126	-1574.22995145	10.5
7_Amine_155	-1574.22991841	10.6
7_Amine_84	-1574.22960161	10.8
7_Amine_147	-1574.22954093	10.8
7_Amine_63	-1574.22930670	10.9
7_Amine_61	-1574.22929612	10.9
7_Amine_160	-1574.22928008	11.0

7_Amine_88	-1574.22899293	11.1
7_Amine_189	-1574.22886960	11.2
7_Amine_16	-1574.22868403	11.3
7_Amine_236	-1574.22843254	11.5
7_Amine_234	-1574.22811119	11.7
7_Amine_214	-1574.22798590	11.8
7_Amine_218	-1574.22796130	11.8
7_Amine_206	-1574.22795175	11.8
7_Amine_51	-1574.22780759	11.9
7_Amine_102	-1574.22770313	11.9
7_Amine_41	-1574.22750114	12.1
7_Amine_2	-1574.22749550	12.1
7_Amine_207	-1574.22729782	12.2
7_Amine_221	-1574.22716961	12.3
7_Amine_219	-1574.22704063	12.4
7_Amine_222	-1574.22700427	12.4
7_Amine_58	-1574.22687967	12.5
7_Amine_3	-1574.22685084	12.5
7_Amine_117	-1574.22679125	12.5
7_Amine_202	-1574.22671548	12.6
7_Amine_140	-1574.22639007	12.8
7_Amine_4	-1574.22633081	12.8
7_Amine_33	-1574.22628226	12.8

Table S7. Absolute and relative (with respect to their respective low-lying conformer) electronic energies (E , at the PCM chloroform-wB97X-D/def2-TZVP//B97D/def2-TZVP level of theory) for the conformers of L3

Conformer	E (Hartree)	ΔE (kcal/mol)
9_Amide_5	-1800.99158872	0.0
9_Amide_111	-1800.99117755	0.3

7_Amine_54	-1574.22624467	12.9
7_Amine_175	-1574.22609866	13.0
7_Amine_157	-1574.22606052	13.0
7_Amine_17	-1574.22585334	13.1
7_Amine_225	-1574.22517927	13.5
7_Amine_98	-1574.22506830	13.6
7_Amine_57	-1574.22487783	13.7
7_Amine_70	-1574.22449837	14.0
7_Amine_137	-1574.22424920	14.1
7_Amine_81	-1574.22422086	14.1
7_Amine_235	-1574.22388984	14.3
7_Amine_22	-1574.22353657	14.6
7_Amine_144	-1574.22300127	14.9
7_Amine_42	-1574.22296506	14.9
7_Amine_24	-1574.22284230	15.0
7_Amine_68	-1574.22242676	15.3
7_Amine_13	-1574.22185209	15.6
7_Amine_25	-1574.22169013	15.7
7_Amine_193	-1574.21968083	17.0
7_Amine_212	-1574.21884305	17.5
7_Amine_52	-1574.21849886	17.7
7_Amine_199	-1574.20852981	24.0

9_Amide_47	-1800.99068586	0.6
9_Amide_17	-1800.99041829	0.7
9_Amide_2	-1800.99024254	0.8
9_Amide_137	-1800.99021870	0.9
9_Amide_1	-1800.99006334	1.0
9_Amide_16	-1800.98931170	1.4
9_Amide_107	-1800.98917811	1.5

9_Amide_34	-1800.98916989	1.5
9_Amide_63	-1800.98909426	1.6
9_Amide_117	-1800.98877613	1.8
9_Amide_130	-1800.98836570	2.0
9_Amide_108	-1800.98827310	2.1
9_Amide_11	-1800.98823282	2.1
9_Amide_150	-1800.98811694	2.2
9_Amide_110	-1800.98794910	2.3
9_Amide_27	-1800.98779418	2.4
9_Amide_3	-1800.98762576	2.5
9_Amide_159	-1800.98748325	2.6
9_Amide_151	-1800.98746650	2.6
9_Amide_7	-1800.98744382	2.6
9_Amide_9	-1800.98739047	2.6
9_Amide_93	-1800.98720452	2.8
9_Amide_28	-1800.98716474	2.8
9_Amide_162	-1800.98715920	2.8
9_Amide_40	-1800.98705247	2.8
9_Amide_65	-1800.98701810	2.9
9_Amide_14	-1800.98697569	2.9
9_Amide_21	-1800.98685570	3.0
9_Amide_55	-1800.98668696	3.1
9_Amide_139	-1800.98663151	3.1
9_Amide_30	-1800.98661021	3.1
9_Amide_95	-1800.98647167	3.2
9_Amide_132	-1800.98645090	3.2
9_Amide_22	-1800.98644271	3.2
9_Amide_128	-1800.98638914	3.3
9_Amide_109	-1800.98637959	3.3
9_Amide_45	-1800.98629270	3.3

9_Amide_31	-1800.98629042	3.3
9_Amide_114	-1800.98622172	3.4
9_Amide_115	-1800.98618751	3.4
9_Amide_41	-1800.98602281	3.5
9_Amide_19	-1800.98600481	3.5
9_Amide_33	-1800.98591517	3.6
9_Amide_133	-1800.98588746	3.6
9_Amide_43	-1800.98579948	3.6
9_Amide_37	-1800.98576423	3.7
9_Amide_4	-1800.98574220	3.7
9_Amide_38	-1800.98567503	3.7
9_Amide_171	-1800.98566614	3.7
9_Amide_124	-1800.98565158	3.7
9_Amide_197	-1800.98564367	3.7
9_Amide_90	-1800.98561181	3.8
9_Amide_36	-1800.98554345	3.8
9_Amide_59	-1800.98552624	3.8
9_Amide_10	-1800.98551292	3.8
9_Amide_149	-1800.98550484	3.8
9_Amide_156	-1800.98549701	3.8
9_Amide_155	-1800.98537887	3.9
9_Amide_51	-1800.98534578	3.9
9_Amide_20	-1800.98531473	3.9
9_Amide_119	-1800.98530223	3.9
9_Amide_167	-1800.98526819	4.0
9_Amide_146	-1800.98524422	4.0
9_Amide_138	-1800.98519834	4.0
9_Amide_164	-1800.98516468	4.0
9_Amide_58	-1800.98508795	4.1
9_Amide_147	-1800.98505915	4.1

9_Amide_64	-1800.98505410	4.1
9_Amide_127	-1800.98502738	4.1
9_Amide_18	-1800.98490347	4.2
9_Amide_120	-1800.98488807	4.2
9_Amide_92	-1800.98485498	4.2
9_Amide_50	-1800.98484700	4.2
9_Amide_116	-1800.98475564	4.3
9_Amide_72	-1800.98474609	4.3
9_Amide_61	-1800.98470057	4.3
9_Amide_125	-1800.98469966	4.3
9_Amide_181	-1800.98468385	4.3
9_Amide_202	-1800.98466674	4.3
9_Amide_13	-1800.98461801	4.4
9_Amide_158	-1800.98460300	4.4
9_Amide_74	-1800.98445682	4.5
9_Amide_42	-1800.98445438	4.5
9_Amide_160	-1800.98438353	4.5
9_Amide_121	-1800.98436012	4.5
9_Amide_142	-1800.98432248	4.6
9_Amide_122	-1800.98432088	4.6
9_Amide_80	-1800.98430707	4.6
9_Amide_189	-1800.98421176	4.6
9_Amide_24	-1800.98417443	4.7
9_Amide_123	-1800.98411251	4.7
9_Amide_165	-1800.98401480	4.8
9_Amide_211	-1800.98392232	4.8
9_Amide_113	-1800.98383967	4.9
9_Amide_89	-1800.98376249	4.9
9_Amide_83	-1800.98373957	4.9
9_Amide_135	-1800.98370672	4.9

9_Amide_136	-1800.98370101	4.9
9_Amide_106	-1800.98369782	5.0
9_Amide_8	-1800.98368928	5.0
9_Amide_66	-1800.98362385	5.0
9_Amide_191	-1800.98362158	5.0
9_Amide_29	-1800.98354200	5.0
9_Amide_87	-1800.98351401	5.1
9_Amide_53	-1800.98348087	5.1
9_Amide_91	-1800.98348084	5.1
9_Amide_179	-1800.98347407	5.1
9_Amide_140	-1800.98338683	5.1
9_Amide_25	-1800.98337382	5.2
9_Amide_201	-1800.98337301	5.2
9_Amide_129	-1800.98334170	5.2
9_Amide_60	-1800.98321437	5.3
9_Amide_26	-1800.98320281	5.3
9_Amide_56	-1800.98316444	5.3
9_Amide_57	-1800.98300048	5.4
9_Amide_35	-1800.98295609	5.4
9_Amide_46	-1800.98290911	5.4
9_Amide_79	-1800.98288256	5.5
9_Amide_153	-1800.98287780	5.5
9_Amide_178	-1800.98283086	5.5
9_Amide_195	-1800.98280183	5.5
9_Amide_184	-1800.98273863	5.6
9_Amide_174	-1800.98272586	5.6
9_Amide_15	-1800.98269738	5.6
9_Amide_177	-1800.98266883	5.6
9_Amide_154	-1800.98263097	5.6
9_Amide_118	-1800.98250680	5.7

9_Amide_183	-1800.98241251	5.8
9_Amide_73	-1800.98239684	5.8
9_Amide_82	-1800.98237902	5.8
9_Amide_169	-1800.98235865	5.8
9_Amide_207	-1800.98231336	5.8
9_Amide_180	-1800.98224963	5.9
9_Amide_186	-1800.98223428	5.9
9_Amide_84	-1800.98223148	5.9
9_Amide_173	-1800.98222313	5.9
9_Amide_112	-1800.98209568	6.0
9_Amide_148	-1800.98186266	6.1
9_Amide_67	-1800.98183725	6.1
9_Amide_99	-1800.98183102	6.1
9_Amide_94	-1800.98178335	6.2
9_Amide_141	-1800.98176030	6.2
9_Amide_32	-1800.98171064	6.2
9_Amide_96	-1800.98166335	6.2
9_Amide_152	-1800.98162470	6.3
9_Amide_44	-1800.98154557	6.3
9_Amide_71	-1800.98152982	6.3
9_Amide_6	-1800.98139160	6.4
9_Amide_76	-1800.98123207	6.5
9_Amide_86	-1800.98112211	6.6
9_Amide_12	-1800.98101136	6.6
9_Amide_168	-1800.98095790	6.7
9_Amide_203	-1800.98088403	6.7
9_Amide_68	-1800.98075537	6.8
9_Amide_200	-1800.98075242	6.8
9_Amide_144	-1800.98069924	6.8
9_Amide_194	-1800.98059328	6.9

9_Amide_105	-1800.98053017	6.9
9_Amide_206	-1800.98046951	7.0
9_Amide_126	-1800.98037114	7.0
9_Amide_52	-1800.98036895	7.0
9_Amide_77	-1800.98034288	7.1
9_Amide_78	-1800.98031245	7.1
9_Amide_163	-1800.98017929	7.2
9_Amide_54	-1800.98008440	7.2
9_Amide_69	-1800.98007722	7.2
9_Amide_131	-1800.97984275	7.4
9_Amide_62	-1800.97969321	7.5
9_Amide_185	-1800.97968691	7.5
9_Amide_198	-1800.97964325	7.5
9_Amide_157	-1800.97963188	7.5
9_Amide_23	-1800.97961677	7.5
9_Amide_101	-1800.97959125	7.5
9_Amide_196	-1800.97957226	7.5
9_Amide_204	-1800.97952664	7.6
9_Amide_205	-1800.97947577	7.6
9_Amide_166	-1800.97936113	7.7
9_Amide_143	-1800.97930634	7.7
9_Amide_100	-1800.97927331	7.7
9_Amide_39	-1800.97923695	7.8
9_Amide_88	-1800.97916790	7.8
9_Amide_175	-1800.97913735	7.8
9_Amide_48	-1800.97912701	7.8
9_Amide_182	-1800.97892472	7.9
9_Amide_187	-1800.97890824	8.0
9_Amide_75	-1800.97886508	8.0
9_Amide_103	-1800.97864508	8.1

9_Amide_188	-1800.97864000	8.1
9_Amide_104	-1800.97863187	8.1
9_Amide_209	-1800.97836497	8.3
9_Amide_81	-1800.97834447	8.3
9_Amide_134	-1800.97833108	8.3
9_Amide_190	-1800.97818833	8.4
9_Amide_172	-1800.97816552	8.4
9_Amide_145	-1800.97800657	8.5
9_Amide_98	-1800.97767622	8.7
9_Amide_192	-1800.97755894	8.8
9_Amide_199	-1800.97700603	9.2
9_Amide_85	-1800.97698171	9.2
9_Amide_176	-1800.97649214	9.5
9_Amide_97	-1800.97612364	9.7
9_Amide_49	-1800.97608097	9.7
9_Amide_70	-1800.97597942	9.8
9_Amide_193	-1800.97558596	10.0
9_Amide_102	-1800.97552567	10.1
9_Amide_170	-1800.97495492	10.4
9_Amide_161	-1800.97493335	10.5
9_Amide_210	-1800.97448836	10.7
9_Amide_208	-1800.97379268	11.2

Table S8. Absolute and relative (with respect to their respective low-lying conformer) electronic energies (E, at the PCM chloroform-wB97X-D/def2-TZVP//B97D/def2-TZVP level of theory) for the conformers of L4

Conformer	E (Hartree)	ΔE (kcal/mol)
9_Amine_621	-1652.8868409	0.0
9_Amine_3	-1652.8855444	0.8

9_Amine_7	-1652.8850320	1.1
9_Amine_2	-1652.8848215	1.3
9_Amine_1	-1652.8842018	1.7
9_Amine_9	-1652.8831658	2.3
9_Amine_6	-1652.8823590	2.8
9_Amine_19	-1652.8820501	3.0
9_Amine_8	-1652.8820379	3.0
9_Amine_15	-1652.8818721	3.1
9_Amine_17	-1652.8814931	3.4
9_Amine_22	-1652.8809926	3.7
9_Amine_14	-1652.8808355	3.8
9_Amine_4	-1652.8805402	4.0
9_Amine_16	-1652.8803810	4.1
9_Amine_27	-1652.8803753	4.1
9_Amine_25	-1652.8799414	4.3
9_Amine_13	-1652.8798888	4.4
9_Amine_38	-1652.8798472	4.4
9_Amine_37	-1652.8798471	4.4
9_Amine_18	-1652.8792268	4.8
9_Amine_5	-1652.8791552	4.8
9_Amine_36	-1652.8791484	4.8
9_Amine_23	-1652.8790717	4.9
9_Amine_40	-1652.8790353	4.9
9_Amine_12	-1652.8790289	4.9
9_Amine_21	-1652.8790147	4.9
9_Amine_41	-1652.8789704	4.9
9_Amine_24	-1652.8788469	5.0
9_Amine_28	-1652.8786012	5.2
9_Amine_64	-1652.8784702	5.3
9_Amine_30	-1652.8783961	5.3

9_Amine_10	-1652.8782679	5.4
9_Amine_11	-1652.8782255	5.4
9_Amine_46	-1652.8782199	5.4
9_Amine_29	-1652.8782105	5.4
9_Amine_125	-1652.8779108	5.6
9_Amine_26	-1652.8778520	5.6
9_Amine_78	-1652.8776058	5.8
9_Amine_31	-1652.8775080	5.9
9_Amine_35	-1652.8774880	5.9
9_Amine_70	-1652.8774813	5.9
9_Amine_53	-1652.8774362	5.9
9_Amine_33	-1652.8773410	6.0
9_Amine_43	-1652.8773040	6.0
9_Amine_620	-1652.8772251	6.0
9_Amine_62	-1652.8772012	6.0
9_Amine_32	-1652.8771766	6.1
9_Amine_49	-1652.8771304	6.1
9_Amine_34	-1652.8768715	6.3
9_Amine_51	-1652.8768539	6.3
9_Amine_20	-1652.8767202	6.4
9_Amine_56	-1652.8766443	6.4
9_Amine_59	-1652.8765904	6.4
9_Amine_102	-1652.8765703	6.4
9_Amine_123	-1652.8765595	6.5
9_Amine_39	-1652.8765382	6.5
9_Amine_86	-1652.8765336	6.5
9_Amine_112	-1652.8764756	6.5
9_Amine_81	-1652.8764687	6.5
9_Amine_50	-1652.8764588	6.5
9_Amine_83	-1652.8764246	6.5

9_Amine_69	-1652.8763828	6.6
9_Amine_91	-1652.8762918	6.6
9_Amine_77	-1652.8762290	6.7
9_Amine_120	-1652.8762123	6.7
9_Amine_54	-1652.8761681	6.7
9_Amine_58	-1652.8761383	6.7
9_Amine_48	-1652.8760437	6.8
9_Amine_155	-1652.8759594	6.8
9_Amine_47	-1652.8759184	6.9
9_Amine_66	-1652.8759005	6.9
9_Amine_113	-1652.8758894	6.9
9_Amine_116	-1652.8758862	6.9
9_Amine_88	-1652.8758459	6.9
9_Amine_76	-1652.8757678	6.9
9_Amine_97	-1652.8757659	6.9
9_Amine_133	-1652.8756350	7.0
9_Amine_93	-1652.8755249	7.1
9_Amine_87	-1652.8755076	7.1
9_Amine_67	-1652.8754807	7.1
9_Amine_157	-1652.8753978	7.2
9_Amine_61	-1652.8752832	7.3
9_Amine_44	-1652.8752319	7.3
9_Amine_55	-1652.8752214	7.3
9_Amine_72	-1652.8752082	7.3
9_Amine_57	-1652.8751238	7.4
9_Amine_114	-1652.8750249	7.4
9_Amine_126	-1652.8749140	7.5
9_Amine_159	-1652.8748935	7.5
9_Amine_96	-1652.8748874	7.5
9_Amine_89	-1652.8748357	7.5

9_Amine_202	-1652.8748027	7.6
9_Amine_68	-1652.8747811	7.6
9_Amine_269	-1652.8747681	7.6
9_Amine_130	-1652.8747164	7.6
9_Amine_140	-1652.8746582	7.6
9_Amine_357	-1652.8746420	7.7
9_Amine_161	-1652.8746240	7.7
9_Amine_101	-1652.8745496	7.7
9_Amine_107	-1652.8744887	7.8
9_Amine_100	-1652.8744691	7.8
9_Amine_134	-1652.8743953	7.8
9_Amine_90	-1652.8743535	7.8
9_Amine_105	-1652.8743207	7.9
9_Amine_106	-1652.8742583	7.9
9_Amine_45	-1652.8742530	7.9
9_Amine_79	-1652.8741689	8.0
9_Amine_152	-1652.8741491	8.0
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9_Amine_367	-1652.8646780	13.9
9_Amine_521	-1652.8646259	13.9
9_Amine_585	-1652.8646163	13.9

9_Amine_469	-1652.8646070	14.0
9_Amine_535	-1652.8645377	14.0
9_Amine_416	-1652.8644609	14.0
9_Amine_491	-1652.8643940	14.1
9_Amine_541	-1652.8643857	14.1
9_Amine_547	-1652.8643584	14.1
9_Amine_310	-1652.8643294	14.1
9_Amine_139	-1652.8642808	14.2
9_Amine_614	-1652.8642723	14.2
9_Amine_519	-1652.8642531	14.2
9_Amine_397	-1652.8642458	14.2
9_Amine_344	-1652.8642442	14.2
9_Amine_556	-1652.8642425	14.2
9_Amine_312	-1652.8641922	14.2
9_Amine_591	-1652.8641591	14.2
9_Amine_435	-1652.8641187	14.3
9_Amine_566	-1652.8640853	14.3
9_Amine_577	-1652.8640776	14.3
9_Amine_590	-1652.8640773	14.3
9_Amine_573	-1652.8640405	14.3
9_Amine_364	-1652.8640314	14.3
9_Amine_412	-1652.8640026	14.3
9_Amine_419	-1652.8639973	14.3
9_Amine_376	-1652.8639512	14.4
9_Amine_537	-1652.8639402	14.4
9_Amine_387	-1652.8639153	14.4
9_Amine_389	-1652.8638931	14.4
9_Amine_525	-1652.8638863	14.4
9_Amine_548	-1652.8638711	14.4
9_Amine_401	-1652.8638526	14.4

9_Amine_582	-1652.8638103	14.5
9_Amine_424	-1652.8637908	14.5
9_Amine_405	-1652.8637858	14.5
9_Amine_542	-1652.8637700	14.5
9_Amine_602	-1652.8637694	14.5
9_Amine_533	-1652.8637650	14.5
9_Amine_352	-1652.8637399	14.5
9_Amine_578	-1652.8637258	14.5
9_Amine_446	-1652.8636007	14.6
9_Amine_348	-1652.8636003	14.6
9_Amine_430	-1652.8635301	14.6
9_Amine_586	-1652.8634923	14.7
9_Amine_433	-1652.8634890	14.7
9_Amine_439	-1652.8634710	14.7
9_Amine_324	-1652.8634321	14.7
9_Amine_601	-1652.8634099	14.7
9_Amine_355	-1652.8633973	14.7
9_Amine_505	-1652.8633650	14.7
9_Amine_539	-1652.8632634	14.8
9_Amine_531	-1652.8632589	14.8
9_Amine_404	-1652.8632053	14.8
9_Amine_503	-1652.8631927	14.8
9_Amine_517	-1652.8630262	14.9
9_Amine_567	-1652.8629260	15.0
9_Amine_540	-1652.8628408	15.1
9_Amine_545	-1652.8628326	15.1
9_Amine_507	-1652.8628257	15.1
9_Amine_592	-1652.8628200	15.1
9_Amine_553	-1652.8627199	15.1
9_Amine_543	-1652.8627099	15.1

9_Amine_492	-1652.8626961	15.2
9_Amine_610	-1652.8626794	15.2
9_Amine_587	-1652.8626618	15.2
9_Amine_462	-1652.8625266	15.3
9_Amine_307	-1652.8623145	15.4
9_Amine_398	-1652.8623004	15.4
9_Amine_604	-1652.8622462	15.4
9_Amine_421	-1652.8622175	15.5
9_Amine_452	-1652.8621973	15.5
9_Amine_417	-1652.8621959	15.5
9_Amine_554	-1652.8621861	15.5
9_Amine_473	-1652.8621777	15.5
9_Amine_447	-1652.8621664	15.5
9_Amine_522	-1652.8621425	15.5
9_Amine_612	-1652.8621352	15.5
9_Amine_489	-1652.8621316	15.5
9_Amine_475	-1652.8621301	15.5
9_Amine_616	-1652.8618740	15.7
9_Amine_496	-1652.8617464	15.7
9_Amine_485	-1652.8616722	15.8
9_Amine_565	-1652.8616087	15.8
9_Amine_309	-1652.8614638	15.9
9_Amine_550	-1652.8614609	15.9
9_Amine_551	-1652.8613555	16.0
9_Amine_383	-1652.8613381	16.0
9_Amine_571	-1652.8612480	16.1
9_Amine_511	-1652.8612359	16.1
9_Amine_538	-1652.8612277	16.1
9_Amine_611	-1652.8611833	16.1
9_Amine_608	-1652.8610522	16.2

9_Amine_392	-1652.8609930	16.2
9_Amine_596	-1652.8609454	16.2
9_Amine_617	-1652.8608793	16.3
9_Amine_454	-1652.8607622	16.4
9_Amine_593	-1652.8607106	16.4
9_Amine_479	-1652.8606793	16.4
9_Amine_390	-1652.8606269	16.4
9_Amine_461	-1652.8602415	16.7
9_Amine_526	-1652.8599391	16.9
9_Amine_618	-1652.8593630	17.2
9_Amine_549	-1652.8591262	17.4
9_Amine_581	-1652.8591117	17.4
9_Amine_499	-1652.8590878	17.4
9_Amine_508	-1652.8586443	17.7
9_Amine_467	-1652.8582014	18.0
9_Amine_532	-1652.8580532	18.1
9_Amine_607	-1652.8577338	18.3
9_Amine_544	-1652.8556591	19.6

Table S9. Absolute and relative (with respect to their respective low-lying conformer) electronic energies (E, at the PCM chloroform-wB97X-D/def2-TZVP//B97D/def2-TZVP level of theory) for the conformers of L6

Conformer	E (Hartree)	ΔE (kcal/mol)
8_Amide_19	-1761.67573396	0.0
8_Amide_72	-1761.67523256	0.3
8_Amide_121	-1761.67221048	2.2
8_Amide_136	-1761.67217551	2.2
8_Amide_164	-1761.67204180	2.3
8_Amide_49	-1761.67183821	2.4

8_Amide_56	-1761.67147319	2.7
8_Amide_103	-1761.67137391	2.7
8_Amide_47	-1761.67112250	2.9
8_Amide_167	-1761.67090777	3.0
8_Amide_137	-1761.67088883	3.0
8_Amide_219	-1761.67085183	3.1
8_Amide_197	-1761.67069824	3.2
8_Amide_208	-1761.67049412	3.3
8_Amide_168	-1761.67049407	3.3
8_Amide_50	-1761.67038998	3.4
8_Amide_40	-1761.67020656	3.5
8_Amide_127	-1761.67010719	3.5
8_Amide_16	-1761.67010077	3.5
8_Amide_156	-1761.66998759	3.6
8_Amide_38	-1761.66998759	3.6
8_Amide_177	-1761.66988148	3.7
8_Amide_215	-1761.66977210	3.7
8_Amide_165	-1761.66971849	3.8
8_Amide_17	-1761.66967331	3.8
8_Amide_110	-1761.66960529	3.8
8_Amide_153	-1761.66941990	4.0
8_Amide_37	-1761.66936581	4.0
8_Amide_146	-1761.66931510	4.0
8_Amide_163	-1761.66914359	4.1
8_Amide_64	-1761.66913637	4.1
8_Amide_92	-1761.66905441	4.2
8_Amide_32	-1761.66900683	4.2
8_Amide_14	-1761.66895574	4.3
8_Amide_204	-1761.66892338	4.3
8_Amide_179	-1761.66884190	4.3

8_Amide_185	-1761.66858752	4.5
8_Amide_188	-1761.66840171	4.6
8_Amide_186	-1761.66839787	4.6
8_Amide_175	-1761.66834163	4.6
8_Amide_28	-1761.66830529	4.7
8_Amide_15	-1761.66817775	4.7
8_Amide_154	-1761.66817123	4.7
8_Amide_21	-1761.66809830	4.8
8_Amide_5	-1761.66802237	4.8
8_Amide_13	-1761.66786965	4.9
8_Amide_20	-1761.66781175	5.0
8_Amide_54	-1761.66769850	5.0
8_Amide_142	-1761.66768572	5.1
8_Amide_147	-1761.66762331	5.1
8_Amide_70	-1761.66754634	5.1
8_Amide_90	-1761.66747927	5.2
8_Amide_187	-1761.66747678	5.2
8_Amide_212	-1761.66732046	5.3
8_Amide_114	-1761.66730546	5.3
8_Amide_155	-1761.66728380	5.3
8_Amide_71	-1761.66711337	5.4
8_Amide_209	-1761.66711205	5.4
8_Amide_83	-1761.66710373	5.4
8_Amide_31	-1761.66698679	5.5
8_Amide_159	-1761.66688248	5.6
8_Amide_200	-1761.66678524	5.6
8_Amide_139	-1761.66675021	5.6
8_Amide_170	-1761.66670368	5.7
8_Amide_132	-1761.66664575	5.7
8_Amide_33	-1761.66662633	5.7

8_Amide_149	-1761.66661186	5.7
8_Amide_63	-1761.66657421	5.7
8_Amide_30	-1761.66644789	5.8
8_Amide_220	-1761.66643112	5.8
8_Amide_27	-1761.66642490	5.8
8_Amide_206	-1761.66641289	5.8
8_Amide_120	-1761.66640153	5.9
8_Amide_65	-1761.66638194	5.9
8_Amide_126	-1761.66629853	5.9
8_Amide_75	-1761.66628359	5.9
8_Amide_8	-1761.66607618	6.1
8_Amide_82	-1761.66605004	6.1
8_Amide_166	-1761.66598607	6.1
8_Amide_26	-1761.66593215	6.2
8_Amide_101	-1761.66582618	6.2
8_Amide_58	-1761.66582467	6.2
8_Amide_213	-1761.66569539	6.3
8_Amide_41	-1761.66556814	6.4
8_Amide_69	-1761.66555913	6.4
8_Amide_152	-1761.66548692	6.4
8_Amide_134	-1761.66532319	6.5
8_Amide_93	-1761.66525910	6.6
8_Amide_36	-1761.66516055	6.6
8_Amide_35	-1761.66509775	6.7
8_Amide_102	-1761.66477313	6.9
8_Amide_80	-1761.66471893	6.9
8_Amide_23	-1761.66466100	6.9
8_Amide_1	-1761.66461828	7.0
8_Amide_145	-1761.66455944	7.0
8_Amide_18	-1761.66455627	7.0

8_Amide_207	-1761.66420414	7.2
8_Amide_162	-1761.66419712	7.2
8_Amide_129	-1761.66416641	7.3
8_Amide_96	-1761.66414954	7.3
8_Amide_88	-1761.66406469	7.3
8_Amide_118	-1761.66406388	7.3
8_Amide_68	-1761.66403295	7.3
8_Amide_169	-1761.66393646	7.4
8_Amide_143	-1761.66391916	7.4
8_Amide_100	-1761.66375999	7.5
8_Amide_43	-1761.66375998	7.5
8_Amide_124	-1761.66374923	7.5
8_Amide_111	-1761.66373455	7.5
8_Amide_34	-1761.66357342	7.6
8_Amide_73	-1761.66356665	7.6
8_Amide_105	-1761.66356612	7.6
8_Amide_53	-1761.66350085	7.7
8_Amide_178	-1761.66341191	7.7
8_Amide_94	-1761.66332832	7.8
8_Amide_181	-1761.66311919	7.9
8_Amide_135	-1761.66307643	7.9
8_Amide_61	-1761.66303464	8.0
8_Amide_194	-1761.66296268	8.0
8_Amide_98	-1761.66291149	8.0
8_Amide_24	-1761.66289653	8.1
8_Amide_42	-1761.66289565	8.1
8_Amide_205	-1761.66287234	8.1
8_Amide_151	-1761.66275033	8.1
8_Amide_184	-1761.66268489	8.2
8_Amide_22	-1761.66265687	8.2

8_Amide_39	-1761.66260618	8.2
8_Amide_161	-1761.66259459	8.2
8_Amide_173	-1761.66249134	8.3
8_Amide_91	-1761.66249134	8.3
8_Amide_113	-1761.66244562	8.3
8_Amide_221	-1761.66242411	8.4
8_Amide_141	-1761.66236101	8.4
8_Amide_183	-1761.66216987	8.5
8_Amide_190	-1761.66215448	8.5
8_Amide_116	-1761.66214553	8.5
8_Amide_174	-1761.66214453	8.5
8_Amide_76	-1761.66206538	8.6
8_Amide_44	-1761.66203058	8.6
8_Amide_45	-1761.66197220	8.6
8_Amide_57	-1761.66190088	8.7
8_Amide_217	-1761.66187941	8.7
8_Amide_198	-1761.66180956	8.7
8_Amide_140	-1761.66176181	8.8
8_Amide_79	-1761.66174159	8.8
8_Amide_81	-1761.66170952	8.8
8_Amide_123	-1761.66159277	8.9
8_Amide_85	-1761.66143345	9.0
8_Amide_192	-1761.66131572	9.0
8_Amide_51	-1761.66130930	9.1
8_Amide_67	-1761.66125299	9.1
8_Amide_97	-1761.66117739	9.1
8_Amide_196	-1761.66116947	9.1
8_Amide_148	-1761.66116565	9.1
8_Amide_144	-1761.66104661	9.2
8_Amide_84	-1761.66098791	9.3

8_Amide_128	-1761.66095931	9.3
8_Amide_201	-1761.66095296	9.3
8_Amide_55	-1761.66080564	9.4
8_Amide_87	-1761.66068026	9.4
8_Amide_6	-1761.66053936	9.5
8_Amide_199	-1761.66043688	9.6
8_Amide_171	-1761.66039818	9.6
8_Amide_60	-1761.66037728	9.6
8_Amide_119	-1761.66037337	9.6
8_Amide_160	-1761.66034474	9.7
8_Amide_12	-1761.65987056	10.0
8_Amide_138	-1761.65975585	10.0
8_Amide_52	-1761.65953911	10.2
8_Amide_48	-1761.65947550	10.2
8_Amide_25	-1761.65933165	10.3
8_Amide_115	-1761.65928727	10.3
8_Amide_66	-1761.65917913	10.4
8_Amide_195	-1761.65913668	10.4
8_Amide_203	-1761.65904977	10.5
8_Amide_46	-1761.65902253	10.5
8_Amide_78	-1761.65899914	10.5
8_Amide_122	-1761.65891203	10.6
8_Amide_158	-1761.65891013	10.6
8_Amide_133	-1761.65889970	10.6
8_Amide_180	-1761.65888408	10.6
8_Amide_104	-1761.65880255	10.6
8_Amide_211	-1761.65875981	10.7
8_Amide_125	-1761.65875092	10.7
8_Amide_176	-1761.65869214	10.7
8_Amide_130	-1761.65857987	10.8

8_Amide_29	-1761.65840450	10.9
8_Amide_107	-1761.65835709	10.9
8_Amide_214	-1761.65832517	10.9
8_Amide_191	-1761.65831946	10.9
8_Amide_99	-1761.65825920	11.0
8_Amide_210	-1761.65823688	11.0
8_Amide_218	-1761.65818966	11.0
8_Amide_11	-1761.65816804	11.0
8_Amide_131	-1761.65808151	11.1
8_Amide_59	-1761.65803724	11.1
8_Amide_4	-1761.65797758	11.1
8_Amide_7	-1761.65761765	11.4
8_Amide_189	-1761.65759255	11.4
8_Amide_95	-1761.65738706	11.5
8_Amide_112	-1761.65676043	11.9
8_Amide_150	-1761.65667697	12.0
8_Amide_172	-1761.65616734	12.3
8_Amide_202	-1761.65586362	12.5
8_Amide_157	-1761.65584372	12.5
8_Amide_10	-1761.65545368	12.7
8_Amide_193	-1761.65541937	12.7
8_Amide_2	-1761.65517736	12.9
8_Amide_216	-1761.65501009	13.0
8_Amide_74	-1761.65484575	13.1
8_Amide_106	-1761.65378923	13.8
8_Amide_109	-1761.65291669	14.3
8_Amide_9	-1761.65281372	14.4
8_Amide_62	-1761.65276612	14.4
8_Amide_182	-1761.65255535	14.5
8_Amide_108	-1761.65094239	15.6

8_Amide_117	-1761.65089627	15.6
8_Amide_89	-1761.64771713	17.6
8_Amide_86	-1761.64713532	17.9

Table S10. Absolute and relative (with respect to their respective low-lying conformer) electronic energies (E, at the PCM chloroform-wB97X-D/def2-TZVP//B97D/def2-TZVP level of theory) for the conformers of L7

Conformer	E (Hartree)	ΔE (kcal/mol)
8_Amine_111	-1613.56719371	0.0
8_Amine_60	-1613.56415153	1.9
8_Amine_103	-1613.56339747	2.4
8_Amine_97	-1613.56276597	2.8
8_Amine_21	-1613.56274339	2.8
8_Amine_31	-1613.56265702	2.8
8_Amine_35	-1613.56261948	2.9
8_Amine_155	-1613.56226234	3.1
8_Amine_156	-1613.56193080	3.3
8_Amine_100	-1613.56163156	3.5
8_Amine_75	-1613.56099483	3.9
8_Amine_133	-1613.56076434	4.0
8_Amine_126	-1613.56045952	4.2
8_Amine_121	-1613.56032034	4.3
8_Amine_118	-1613.55949719	4.8
8_Amine_58	-1613.55934604	4.9
8_Amine_137	-1613.55934337	4.9
8_Amine_122	-1613.55934000	4.9
8_Amine_136	-1613.55873507	5.3
8_Amine_76	-1613.55857581	5.4
8_Amine_144	-1613.55857297	5.4

8_Amine_120	-1613.55834075	5.6
8_Amine_140	-1613.55805160	5.7
8_Amine_187	-1613.55769603	6.0
8_Amine_2	-1613.55754311	6.1
8_Amine_125	-1613.55747811	6.1
8_Amine_10	-1613.55742885	6.1
8_Amine_104	-1613.55737467	6.2
8_Amine_188	-1613.55718038	6.3
8_Amine_177	-1613.55669260	6.6
8_Amine_13	-1613.55668944	6.6
8_Amine_166	-1613.55660938	6.6
8_Amine_88	-1613.55650745	6.7
8_Amine_71	-1613.55646529	6.7
8_Amine_171	-1613.55627287	6.9
8_Amine_173	-1613.55619420	6.9
8_Amine_98	-1613.55581985	7.1
8_Amine_129	-1613.55581923	7.1
8_Amine_116	-1613.55572081	7.2
8_Amine_159	-1613.55568366	7.2
8_Amine_114	-1613.55552507	7.3
8_Amine_175	-1613.55535706	7.4
8_Amine_119	-1613.55532852	7.4
8_Amine_167	-1613.55531162	7.5
8_Amine_157	-1613.55524836	7.5
8_Amine_20	-1613.55520358	7.5
8_Amine_67	-1613.55511076	7.6
8_Amine_4	-1613.55493701	7.7
8_Amine_32	-1613.55480554	7.8
8_Amine_17	-1613.55467447	7.9
8_Amine_52	-1613.55465774	7.9

8_Amine_102	-1613.55395069	8.3
8_Amine_112	-1613.55374004	8.4
8_Amine_86	-1613.55372262	8.5
8_Amine_165	-1613.55367443	8.5
8_Amine_110	-1613.55363257	8.5
8_Amine_108	-1613.55355607	8.6
8_Amine_37	-1613.55343841	8.6
8_Amine_54	-1613.55324115	8.8
8_Amine_130	-1613.55321355	8.8
8_Amine_22	-1613.55297223	8.9
8_Amine_107	-1613.55280788	9.0
8_Amine_138	-1613.55278310	9.0
8_Amine_101	-1613.55265827	9.1
8_Amine_48	-1613.55265485	9.1
8_Amine_160	-1613.55264048	9.1
8_Amine_8	-1613.55262091	9.1
8_Amine_6	-1613.55256361	9.2
8_Amine_117	-1613.55222012	9.4
8_Amine_16	-1613.55215794	9.4
8_Amine_150	-1613.55207168	9.5
8_Amine_134	-1613.55190004	9.6
8_Amine_151	-1613.55184066	9.6
8_Amine_162	-1613.55178601	9.7
8_Amine_43	-1613.55168873	9.7
8_Amine_135	-1613.55163762	9.8
8_Amine_181	-1613.55155429	9.8
8_Amine_44	-1613.55149785	9.8
8_Amine_33	-1613.55142783	9.9
8_Amine_59	-1613.55130931	10.0
8_Amine_73	-1613.55125470	10.0

8_Amine_57	-1613.55120841	10.0
8_Amine_183	-1613.55114762	10.1
8_Amine_9	-1613.55113893	10.1
8_Amine_12	-1613.55113623	10.1
8_Amine_42	-1613.55111887	10.1
8_Amine_109	-1613.55105761	10.1
8_Amine_158	-1613.55103387	10.1
8_Amine_164	-1613.55103079	10.1
8_Amine_87	-1613.55102979	10.1
8_Amine_27	-1613.55096470	10.2
8_Amine_36	-1613.55073297	10.3
8_Amine_123	-1613.55071573	10.3
8_Amine_147	-1613.55067989	10.4
8_Amine_115	-1613.55028171	10.6
8_Amine_38	-1613.55000267	10.8
8_Amine_168	-1613.54995741	10.8
8_Amine_113	-1613.54993022	10.8
8_Amine_179	-1613.54985375	10.9
8_Amine_105	-1613.54975778	10.9
8_Amine_178	-1613.54966960	11.0
8_Amine_55	-1613.54954883	11.1
8_Amine_79	-1613.54942473	11.2
8_Amine_7	-1613.54940673	11.2
8_Amine_40	-1613.54918314	11.3
8_Amine_19	-1613.54917034	11.3
8_Amine_189	-1613.54908018	11.4
8_Amine_143	-1613.54899829	11.4
8_Amine_70	-1613.54879573	11.5
8_Amine_186	-1613.54871248	11.6
8_Amine_154	-1613.54869254	11.6

8_Amine_148	-1613.54862471	11.7
8_Amine_132	-1613.54845966	11.8
8_Amine_163	-1613.54845962	11.8
8_Amine_124	-1613.54845589	11.8
8_Amine_172	-1613.54821189	11.9
8_Amine_182	-1613.54815127	11.9
8_Amine_49	-1613.54800450	12.0
8_Amine_169	-1613.54788088	12.1
8_Amine_127	-1613.54776121	12.2
8_Amine_11	-1613.54765148	12.3
8_Amine_41	-1613.54756892	12.3
8_Amine_99	-1613.54744087	12.4
8_Amine_61	-1613.54737287	12.4
8_Amine_184	-1613.54736702	12.4
8_Amine_46	-1613.54709302	12.6
8_Amine_1	-1613.54704482	12.6
8_Amine_50	-1613.54698181	12.7
8_Amine_142	-1613.54698023	12.7
8_Amine_180	-1613.54694676	12.7
8_Amine_170	-1613.54694668	12.7
8_Amine_161	-1613.54685512	12.8
8_Amine_51	-1613.54660448	12.9
8_Amine_74	-1613.54647302	13.0
8_Amine_72	-1613.54641269	13.0
8_Amine_65	-1613.54635626	13.1
8_Amine_131	-1613.54623465	13.2
8_Amine_23	-1613.54591756	13.4
8_Amine_26	-1613.54587655	13.4
8_Amine_141	-1613.54577880	13.4
8_Amine_92	-1613.54577495	13.4

8_Amine_176	-1613.54565791	13.5
8_Amine_85	-1613.54553298	13.6
8_Amine_149	-1613.54495930	14.0
8_Amine_28	-1613.54490392	14.0
8_Amine_25	-1613.54479641	14.1
8_Amine_30	-1613.54479493	14.1
8_Amine_69	-1613.54476721	14.1
8_Amine_152	-1613.54476357	14.1
8_Amine_64	-1613.54457725	14.2
8_Amine_128	-1613.54456396	14.2
8_Amine_106	-1613.54436566	14.3
8_Amine_95	-1613.54430746	14.4
8_Amine_91	-1613.54418332	14.4
8_Amine_62	-1613.54404560	14.5
8_Amine_153	-1613.54401011	14.5
8_Amine_174	-1613.54398282	14.6
8_Amine_90	-1613.54395299	14.6
8_Amine_15	-1613.54393627	14.6
8_Amine_5	-1613.54342238	14.9
8_Amine_81	-1613.54315035	15.1
8_Amine_66	-1613.54275520	15.3
8_Amine_185	-1613.54268867	15.4
8_Amine_3	-1613.54265799	15.4
8_Amine_139	-1613.54257108	15.5

8_Amine_83	-1613.54233198	15.6
8_Amine_82	-1613.54225337	15.7
8_Amine_24	-1613.54217925	15.7
8_Amine_39	-1613.54205748	15.8
8_Amine_93	-1613.54200732	15.8
8_Amine_56	-1613.54194736	15.8
8_Amine_18	-1613.54169707	16.0
8_Amine_53	-1613.54164509	16.0
8_Amine_63	-1613.54146242	16.1
8_Amine_45	-1613.54091504	16.5
8_Amine_89	-1613.54076480	16.6
8_Amine_77	-1613.54035734	16.8
8_Amine_145	-1613.53989280	17.1
8_Amine_14	-1613.53982095	17.2
8_Amine_68	-1613.53980933	17.2
8_Amine_146	-1613.53980293	17.2
8_Amine_84	-1613.53939090	17.4
8_Amine_96	-1613.53862698	17.9
8_Amine_47	-1613.53837895	18.1
8_Amine_34	-1613.53831828	18.1
8_Amine_80	-1613.53830870	18.1
8_Amine_29	-1613.53772583	18.5
8_Amine_78	-1613.53770024	18.5
8_Amine_94	-1613.53668337	19.1

**PCM-ChloroformB97-D/def2-TZVP Optimized Cartesian
Coordinates for the molecules in Table S3 and S4**

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7_Amide_73

C	-2.5373120	1.3441650	-0.6739570
O	-3.0682290	1.9754680	0.2488300
C	-1.6686080	2.0893430	-1.6841250
C	-0.1356940	3.3193730	-0.0056070
C	1.8265100	2.2069370	1.2204410
C	2.5320550	1.2278190	0.2721630
O	3.0185410	1.6070440	-0.7972870
N	2.6366260	-0.0839890	0.6681400
C	2.3383780	-0.5610400	2.0311230
C	3.4564590	-0.9824780	-0.1681170
C	1.0984680	-1.4619840	2.1117740
C	-0.2117630	-0.6763790	2.0240870
S	-1.6255540	-1.8420740	1.9863930
C	-3.0273140	-0.7005120	1.6904870
C	-3.5595190	-0.6522980	0.2515130
N	-2.6767760	-0.0242090	-0.7513700
C	-2.3936490	-0.8475340	-1.9415080
C	-1.2897460	-1.8976940	-1.7499470
C	2.8812310	-1.3791750	-1.5355810
H	-2.1534280	3.0605700	-1.8388500
H	-1.6120220	1.5912720	-2.6549210
H	-0.8051020	3.0043970	0.8054930
H	-0.5038740	4.2962220	-0.3509710
H	1.0101120	1.7102990	1.7553180
H	2.5719240	2.4759570	1.9841620
H	2.2366050	0.2906190	2.7074600
H	3.2119720	-1.1286660	2.3767010
H	4.4209240	-0.4891310	-0.3601900
H	3.6455320	-1.8885740	0.4150280

H	1.1491260	-2.2033380	1.3035480
H	1.1308480	-2.0063430	3.0653690
H	-0.3200910	-0.0153520	2.8940950
H	-0.2424890	-0.0549990	1.1245080
H	-2.7376060	0.2983910	2.0249750
H	-3.8483470	-1.0443640	2.3313050
H	-4.5086690	-0.0973310	0.2756810
H	-3.7668010	-1.6713990	-0.0886270
H	-2.1350720	-0.2019720	-2.7817040
H	-3.3261170	-1.3609290	-2.2142130
H	-1.3077050	-2.5574910	-2.6285030
H	-1.5072510	-2.5059050	-0.8635590
H	2.6315830	-0.4877060	-2.1172400
H	3.6711560	-1.9201710	-2.0710450
C	0.0850050	-1.2490190	-1.6128000
H	0.1248990	-0.6510670	-0.7031360
H	0.2851470	-0.5907350	-2.4678050
S	1.4258240	-2.4928600	-1.5382470
C	1.2889260	3.4817950	0.5475370
H	1.2801750	4.2839320	1.2965580
H	1.9761550	3.7864520	-0.2513720
C	-0.2305000	2.3209410	-1.1624010
H	0.3855120	2.6782780	-1.9976250
H	0.1995590	1.3617760	-0.8609920

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7_Amine_39

C	-1.3766490	1.1246900	-1.8452570
C	-0.5901060	1.9571560	-0.8304520
C	1.3251320	3.6527420	-0.5530500
C	2.6968710	1.4353580	-0.4689840
C	2.3656710	1.0363330	0.9765630

N	1.8502970	-0.3335760	1.1156120
C	1.3387450	-0.5627840	2.4775730
C	2.8634240	-1.3385570	0.7605070
C	-0.0167890	0.1034100	2.7683450
C	-1.1305930	-0.5097490	1.9217220
S	-2.7486370	0.3077710	2.2043590
C	-3.6838210	-0.2731180	0.7332470
C	-3.3631270	0.4477380	-0.5857800
N	-2.0972810	0.0322130	-1.1891200
C	-2.2233770	-1.1906590	-1.9811890
C	-0.8736890	-1.8704470	-2.2914840
C	2.2940130	-2.7114810	0.3681600
H	0.0548040	1.2679980	-0.2767810
H	-1.2727550	2.3984730	-0.0911880
H	0.9680350	3.6077420	0.4864950
H	1.4725210	4.7176440	-0.7785670
H	3.6830210	1.0459580	-0.7513610
H	1.9721090	0.9648360	-1.1446600
H	2.0821740	-0.2224010	3.2283720
H	1.2208050	-1.6435430	2.6225630
H	3.4505490	-0.9675060	-0.0844510
H	3.5728580	-1.4900000	1.6038400
H	-0.2298840	-0.0248200	3.8389200
H	0.0335630	1.1838180	2.5848790
H	-0.9091790	-0.3881250	0.8646860
H	-1.2286320	-1.5817330	2.1419780
H	-4.7387140	-0.1079880	0.9861280
H	-3.5331300	-1.3552300	0.6326110
H	-3.3228980	1.5248920	-0.3888840
H	-4.2097350	0.2802090	-1.2863110
H	-2.7680440	-1.0108820	-2.9326630
H	-2.8313000	-1.8934900	-1.3963440
H	-0.3264480	-1.3125770	-3.0624540

H	-1.0865070	-2.8627620	-2.7121510
H	3.1123840	-3.4418280	0.3797380
H	1.5393860	-3.0544220	1.0865610
C	-0.0181880	-1.9807000	-1.0314410
H	-0.5672600	-2.5134700	-0.2442920
H	0.2277560	-0.9887740	-0.6556340
S	1.5704600	-2.8454570	-1.3149040
C	0.2436420	3.0672690	-1.4862370
H	0.7307610	2.6724360	-2.3922130
H	-0.4315680	3.8654110	-1.8245530
C	2.6974000	2.9599650	-0.6785850
H	3.0899520	3.1655820	-1.6848500
H	3.3985320	3.4222870	0.0327790
H	3.2595180	1.1909980	1.6184170
H	1.5931140	1.7128180	1.3535330
H	-2.0578250	1.7698740	-2.4371470
H	-0.6596140	0.6980870	-2.5556820

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9_Amide_5

C	-3.0540350	-1.4078310	0.2508460
O	-3.8319850	-2.2987760	-0.1096870
C	-3.5453270	0.0192640	0.4554520
C	-3.5296150	2.3254630	-0.6700190
C	-2.2056360	2.9628790	-0.2130380
C	-1.1758390	3.0583940	-1.3490990
C	1.0705700	2.7602210	-0.1296360
C	1.8137510	1.7434910	-1.0093060
O	1.7590980	1.7976360	-2.2422340
N	2.5604870	0.7754280	-0.3782980
C	2.9078210	0.8245150	1.0514060
C	3.4196610	-0.0788270	-1.2147410
C	2.6785270	-0.5061140	1.8017380
C	2.0535160	-0.3135780	3.1910050

S	0.4111890	0.5078260	3.2315560
C	-0.6628350	-0.7400700	2.4348880
C	-0.7566530	-0.6472840	0.9020910
N	-1.7098460	-1.6368860	0.3907500
C	-1.1812660	-2.9765790	0.1013520
C	-0.8971150	-3.1759000	-1.3955740
C	2.7032790	-1.0741420	-2.1394780
H	-3.0025850	0.5387180	1.2525690
H	-4.5971470	-0.0362240	0.7528580
H	-4.3227510	2.5366310	0.0617030
H	-3.8349260	2.7995110	-1.6139690
H	-1.7900610	2.3948930	0.6336460
H	-2.3981370	3.9764640	0.1668970
H	-1.6210010	3.6555680	-2.1578230
H	-0.9749020	2.0658310	-1.7731340
H	0.5078510	2.2320660	0.6518780
H	1.8298160	3.3525020	0.4012690
H	2.3098010	1.6006680	1.5252830
H	3.9620810	1.1266000	1.1421940
H	4.0340920	0.5644330	-1.8625740
H	4.0936570	-0.6196680	-0.5427670
H	2.0526240	-1.1680100	1.1978460
H	3.6327570	-1.0337150	1.9387190
H	1.9617480	-1.2801130	3.7011980
H	2.6862850	0.3328410	3.8132800
H	-1.6612350	-0.5902070	2.8626660
H	-0.3197390	-1.7378640	2.7347210
H	0.2123240	-0.8470890	0.4407350
H	-1.0490820	0.3586890	0.5961190
H	-1.9111140	-3.7223110	0.4300350
H	-0.2650570	-3.1065770	0.6878010
H	-1.8439810	-3.0649040	-1.9384260
H	-0.5486020	-4.2061120	-1.5527080

H	1.9924040	-0.5423730	-2.7742590
H	3.4653470	-1.5282000	-2.7842930
C	0.1056470	-2.1843620	-1.9929850
H	-0.2064010	-1.1532170	-1.7903820
H	0.1615700	-2.3192090	-3.0788460
S	1.7928660	-2.4293670	-1.2971480
C	-3.4246580	0.8048870	-0.8724120
H	-2.4657830	0.5684660	-1.3531860
H	-4.2076850	0.4476260	-1.5519180
C	0.1542120	3.6990400	-0.9234560
H	0.6944660	4.0463320	-1.8113810
H	-0.0569170	4.5811360	-0.3022820

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9_Amine_621

C	-3.6129220	0.9652170	0.1278870
C	-1.9374070	2.6750670	-0.8027170
C	-1.1079860	3.9265380	-0.4708480
C	0.1086030	3.6747230	0.4341300
C	2.3677140	2.5287970	0.6980950
N	2.6900590	0.0279050	0.5494770
C	2.5815610	-0.2777860	1.9854170
C	3.4755130	-1.0185630	-0.1162460
C	1.4411130	-1.2559930	2.2923770
C	0.0695800	-0.5955200	2.1223470
S	-1.3302040	-1.6419190	2.6680510
C	-1.6778520	-2.6441860	1.1690420
C	-2.7599550	-2.0523170	0.2575440
N	-2.2618650	-1.0080240	-0.6513460
C	-1.7098320	-1.6343750	-1.8643180
C	-0.7978570	-0.7123410	-2.6834720
C	3.2558730	-1.1394760	-1.6269580
H	-4.4816960	1.5607980	-0.1910260
H	-3.9068730	0.4465350	1.0502210

H	-2.7987960	2.9822070	-1.4155030
H	-1.3405310	1.9962060	-1.4252230
H	-1.7627190	4.6659360	0.0145150
H	-0.7609350	4.3789550	-1.4122400
H	-0.2322620	3.3774580	1.4367600
H	0.6567140	4.6208680	0.5589330
H	2.1355640	2.4948770	1.7714710
H	2.9390920	3.4558320	0.5441880
H	2.3896820	0.6481590	2.5375360
H	3.5391960	-0.6793470	2.3744200
H	4.5618980	-0.8553710	0.0629830
H	3.2230570	-1.9837820	0.3365630
H	1.5476320	-1.6056070	3.3280750
H	1.5111990	-2.1396670	1.6444860
H	0.0143520	0.3122270	2.7374420
H	-0.1141270	-0.3058090	1.0842510
H	-2.0104760	-3.6221380	1.5378310
H	-0.7372640	-2.7966020	0.6268640
H	-3.5486370	-1.6324600	0.8900200
H	-3.2269670	-2.8760580	-0.3235760
H	-1.1282600	-2.5122940	-1.5557120
H	-2.5319640	-2.0097790	-2.5084460
H	-1.2933930	0.2511870	-2.8556650
H	-0.6446380	-1.1622560	-3.6743050
H	3.3527330	-0.1708860	-2.1323180
H	4.0302210	-1.8005560	-2.0355640
C	0.5518670	-0.4341610	-2.0199760
H	1.0585460	0.4047410	-2.5110160
H	0.4220170	-0.1861840	-0.9658210
S	1.6681770	-1.8878640	-2.1432070
C	-3.3337580	-0.0540850	-0.9827830
H	-3.0460700	0.4942730	-1.8848090
H	-4.2695060	-0.5954780	-1.2335860

C	3.2754530	1.3559580	0.3062260
H	4.2503180	1.4500200	0.8308870
H	3.4880510	1.4368390	-0.7672900
C	1.0603850	2.5975510	-0.0949540
H	0.5636770	1.6245680	-0.0460650
H	1.2858760	2.7829580	-1.1567480
C	-2.4418690	1.9132040	0.4318880
H	-1.6175870	1.3418100	0.8732780
H	-2.7713880	2.6356700	1.1936630

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8_Amide_19

C	2.9608410	0.4716560	0.1494520
O	3.4137150	0.7958340	-0.9527140
C	2.7513410	1.5063020	1.2671920
C	1.4044870	3.5122480	0.3610420
C	0.5907560	2.5863060	-0.5500710
C	-1.7240630	2.2442520	-1.5416470
C	-2.4467350	1.6406130	-0.3280880
O	-2.6056380	2.3060340	0.7016520
N	-2.9255410	0.3592460	-0.4143730
C	-3.0111310	-0.4147840	-1.6641340
C	-3.6970650	-0.1522150	0.7319420
C	-2.0341850	-1.5964180	-1.7237650
C	-0.5762060	-1.1472430	-1.8358380
S	0.5242070	-2.6095820	-1.7345250
C	2.1859440	-1.8452190	-1.8787760
C	3.0356040	-1.8359420	-0.5981480
N	2.6626490	-0.8407460	0.4227520
C	2.3942480	-1.3658220	1.7716050
C	1.0043220	-1.9952320	1.9233370
C	-2.9084570	-0.4031110	2.0265880
H	3.5584930	1.3429830	1.9965180
H	1.8144720	1.3030300	1.8000880

H	1.5488130	4.4813850	-0.1390650
H	0.8034580	3.7123160	1.2611190
H	0.2912440	1.7008610	0.0302190
H	1.2158270	2.2179860	-1.3735070
H	-1.2513120	1.4699540	-2.1535980
H	-2.4948630	2.7195190	-2.1671640
H	-2.8633370	0.2497060	-2.5183730
H	-4.0367570	-0.7988420	-1.7424690
H	-4.4854890	0.5760360	0.9728330
H	-4.1775620	-1.0827400	0.4144660
H	-2.1633440	-2.2048480	-0.8198420
H	-2.2991130	-2.2171320	-2.5904380
H	-0.4012490	-0.6416320	-2.7943260
H	-0.3270510	-0.4491450	-1.0317910
H	2.0681910	-0.8294610	-2.2631720
H	2.7338470	-2.4255140	-2.6309870
H	4.0747930	-1.6448000	-0.9029310
H	2.9954860	-2.8223880	-0.1256370
H	2.5268250	-0.5712190	2.5079050
H	3.1545270	-2.1295410	1.9886960
H	0.9798820	-2.5372700	2.8784770
H	0.8510680	-2.7245490	1.1179960
H	-2.3603110	0.4957060	2.3177360
H	-3.6399070	-0.6213200	2.8143200
C	-0.1166290	-0.9549860	1.8937730
H	-0.0683120	-0.3659540	0.9729770
H	-0.0290490	-0.2690410	2.7461980
S	-1.7355190	-1.8101610	1.9978790
C	-0.6658130	3.2679370	-1.1129270
H	-1.1022730	3.9310440	-0.3566210
H	-0.3901640	3.8895070	-1.9750260
C	2.7812480	2.9634510	0.7746850
H	3.1841660	3.5962700	1.5758660

H	3.4745750	3.0297740	-0.0716110
58			
8_Amine_111			
C	1.6511460	2.7284710	0.4612370
C	-0.3662250	3.6750140	-0.8201090
C	-1.3685960	3.6117210	0.3490210
C	-2.8967430	1.7954990	-0.6509190
N	-2.3146580	-0.6622900	-0.7063450
C	-1.9185250	-0.7665540	-2.1185090
C	-2.6914450	-1.9833110	-0.1670970
C	-0.6486330	-1.5952270	-2.3517160
C	0.5873420	-0.8994670	-1.7836310
S	2.0544410	-1.9893910	-1.8772620
C	3.3672280	-0.8551650	-1.2892610
C	3.4099860	-0.6111680	0.2239920
N	2.4015320	0.3373160	0.7184500
C	2.1699420	0.1188680	2.1567710
C	1.1898170	-1.0319210	2.4291140
C	-1.6313300	-2.6309660	0.7377900
H	1.0595300	2.6081680	1.3777810
H	2.0769390	3.7425200	0.4984110
H	-0.9087650	3.5711570	-1.7699490
H	0.0954180	4.6737620	-0.8335170
H	-2.1443750	4.3759390	0.1906110
H	-0.8511430	3.8800120	1.2806330
H	-2.3496050	1.9363270	-1.5905880
H	-3.7836150	2.4429050	-0.7167560
H	-1.7461650	0.2419600	-2.5101890
H	-2.7457330	-1.2092560	-2.7132240
H	-3.6205760	-1.8966090	0.4096680
H	-2.9055590	-2.6877030	-0.9931990
H	-0.5294070	-1.7440300	-3.4330400
H	-0.7677530	-2.5927070	-1.9094690

H	0.7999910	0.0135960	-2.3530630	C	-0.4227200	3.5791610	0.1585530
H	0.4349870	-0.6137460	-0.7421800	C	1.7031530	2.4024700	0.9291410
H	3.2802650	0.0864570	-1.8448960	C	2.5227870	1.4109260	0.0934930
H	4.3063690	-1.3324420	-1.5952940	O	3.0052550	1.7332890	-0.9965940
H	4.4307210	-0.2604010	0.4930230	N	2.7281650	0.1589370	0.6156390
H	3.2655510	-1.5730840	0.7277280	C	2.4013990	-0.2218970	2.0028240
H	3.1296920	-0.0650170	2.6810210	C	3.6716580	-0.7294220	-0.0920410
H	1.7536630	1.0375300	2.5877990	C	1.2467140	-1.2277620	2.1355520
H	1.2856690	-1.3471310	3.4767410	C	-0.1441770	-0.6060540	1.9645370
H	1.4436420	-1.8998890	1.8067680	S	-1.4135200	-1.8855440	2.3205750
H	-1.8945070	-3.6857100	0.8895700	C	-2.9554060	-1.1473360	1.6572280
H	-0.6368260	-2.5968760	0.2812160	C	-3.1630790	-1.3053860	0.1455440
C	-0.2514860	-0.5985510	2.1540490	N	-2.3974390	-0.3107140	-0.6418120
H	-0.5247440	0.2346950	2.8133640	C	-2.0614520	-0.8127510	-2.0011340
H	-0.3676980	-0.2577430	1.1239110	C	-0.8910920	-1.8030390	-1.9712080
S	-1.5104050	-1.9027880	2.4190140	C	3.2434140	-1.2485330	-1.4712060
C	2.8123170	1.7266930	0.4498020	H	-2.5078310	1.9858410	0.9237480
H	3.5920980	2.0400010	1.1749740	H	-3.0973920	3.0302410	-0.3858370
H	3.2792990	1.7614070	-0.5426020	H	-0.7598510	3.5665180	1.2068600
C	-3.3808420	0.3434410	-0.5321070	H	-0.8130640	4.5047450	-0.2861630
H	-4.2041750	0.1684110	-1.2564220	H	0.9005280	1.8711380	1.4517910
H	-3.7993690	0.2075670	0.4729690	H	2.3782270	2.7682130	1.7163670
C	-2.0289290	2.2373760	0.5323610	H	2.1931780	0.6729220	2.5937040
H	-1.2526680	1.4863610	0.6968270	H	3.3047780	-0.6719700	2.4344980
H	-2.6478450	2.2472310	1.4414210	H	4.6197100	-0.1874850	-0.2321900
C	0.7408810	2.6103300	-0.7662330	H	3.8604350	-1.5849250	0.5630670
H	0.2979670	1.6096090	-0.7884660	H	1.3844940	-2.0326110	1.4023350
H	1.3605970	2.6959120	-1.6716870	H	1.3207580	-1.6745930	3.1375650
53				H	-0.2776990	0.2331470	2.6608630
T1				H	-0.3133700	-0.2471770	0.9478920
C	-3.1562860	0.9350480	-0.7661530	H	-3.0104500	-0.0944910	1.9606480
O	-4.2557010	0.9763770	-1.2808310	H	-3.7579310	-1.6802590	2.1821340
C	-2.4863760	2.1467470	-0.1672710	H	-4.2411270	-1.2383660	-0.0842570

H	-2.8353630	-2.3061360	-0.1505150
H	-1.7860020	0.0491490	-2.6239460
H	-2.9427360	-1.2811790	-2.4710240
H	-0.8772350	-2.3543480	-2.9206850
H	-1.0520240	-2.5412720	-1.1751150
H	3.0691650	-0.4166850	-2.1577390
H	4.0769480	-1.8447650	-1.8629750
C	0.4529650	-1.1031090	-1.7665270
H	0.4158110	-0.4414370	-0.8998210
H	0.7078270	-0.4995040	-2.6467470
S	1.7794020	-2.3409830	-1.5128680
C	1.1124540	3.5910720	0.1364110
H	1.4693670	4.5335230	0.5685880
H	1.4760690	3.5583800	-0.8974880
C	-1.0201360	2.3669930	-0.5702230
H	-0.9375280	2.5084000	-1.6562120
H	-0.4562300	1.4617550	-0.3251400
S9			
T2			
C	3.2987020	1.6174010	0.1264890
O	4.4871710	1.8319300	0.2739800
C	2.2872980	2.7441860	0.1314410
C	-0.0315680	3.6501800	-0.2296930
C	-1.4077620	3.5394260	-0.9075240
C	-1.9575570	2.1074040	-0.8574400
C	-3.9983220	0.5414260	-0.9509240
C	-3.6205810	-0.1616050	0.3548430
O	-4.3075920	0.0311710	1.3665520
N	-2.5179110	-0.9759300	0.3912450
C	-1.5523020	-1.1526490	-0.6986660
C	-2.1758280	-1.6196390	1.6651160
C	-1.4975420	-2.5679430	-1.2790370
C	-0.4150880	-2.6984760	-2.3628450

S	1.3197380	-2.5779410	-1.7611550
C	1.6871500	-0.7879620	-1.9881080
C	2.9715550	-0.3425600	-1.2546980
N	2.7575700	0.2659330	0.0844670
C	3.2867890	-0.4996040	1.2343650
C	2.5374270	-1.7933630	1.5683640
C	-1.4241460	-0.7369440	2.6787900
H	2.8083560	3.6772460	-0.1132250
H	2.0084640	2.8119520	1.1988680
H	0.3857320	4.6545140	-0.3927110
H	-0.1754030	3.5404090	0.8563490
H	-1.3458900	3.8724820	-1.9541920
H	-2.1030510	4.2235370	-0.3994290
H	-1.6483040	1.6374350	0.0867090
H	-1.4758240	1.5306810	-1.6561850
H	-3.6621070	-0.0017030	-1.8406790
H	-5.0935620	0.5543930	-0.9705880
H	-0.5731970	-0.8612890	-0.3116380
H	-1.7806220	-0.4623260	-1.5060820
H	-3.1054610	-1.9398210	2.1476280
H	-1.5876340	-2.5141690	1.4441410
H	-1.3079860	-3.3078020	-0.4919030
H	-2.4718830	-2.8117480	-1.7279290
H	-0.4879430	-3.6825740	-2.8387950
H	-0.5499790	-1.9425950	-3.1475360
H	0.8460060	-0.1907300	-1.6321310
H	1.8059690	-0.6100090	-3.0638740
H	3.4653140	0.3907590	-1.9063660
H	3.6828510	-1.1782000	-1.1669140
H	3.2275630	0.1657500	2.1047790
H	4.3514850	-0.7527020	1.0919890
H	3.0074490	-2.1642180	2.4886370
H	2.7383400	-2.5392910	0.7883730

H	-2.0076210	0.1679430	2.8776510
H	-1.3407640	-1.3063710	3.6147540
C	1.0030450	-1.7631260	1.7559860
H	0.7268940	-2.4689280	2.5493480
H	0.5410120	-2.1103460	0.8293850
S	0.2417960	-0.1445600	2.1906140
C	0.9896540	2.5864910	-0.6652570
H	1.1872640	2.6586790	-1.7449460
H	0.5860440	1.5902770	-0.4627230
C	-3.4789020	1.9993190	-0.9862780
H	-3.8152730	2.4659170	-1.9228850
H	-3.9471580	2.5562510	-0.1630120
56			
T3			
C	3.5813610	0.9284750	0.1160390
O	4.7817700	0.9219050	0.3012950
C	2.8048920	2.1505460	-0.2965420
C	0.6560020	3.4248580	0.2721890
C	-0.3598260	2.4610590	-0.3429220
C	-2.6000740	2.0511920	-1.4207560
C	-3.1167340	1.2178640	-0.2430170
O	-3.5062410	1.7926100	0.7804640
N	-3.0949940	-0.1525550	-0.3151430
C	-3.0074990	-0.9265730	-1.5646590
C	-3.5837380	-0.8838120	0.8675460
C	-1.7839520	-1.8458720	-1.6575170
C	-0.4538740	-1.0942030	-1.7718480
S	0.8796400	-2.3362240	-1.9843670
C	2.4311240	-1.3504470	-1.9905460
C	3.2034470	-1.3353830	-0.6605020
N	2.7526320	-0.2695640	0.2663630
C	2.7359180	-0.7149770	1.6827170
C	1.5188690	-1.6030140	1.9697540

C	-2.6561730	-0.8422180	2.0939860
H	2.1975500	1.8550040	-1.1620580
H	3.4981970	2.9425830	-0.5994100
H	0.9841710	4.1652250	-0.4730830
H	0.1723080	3.9813410	1.0870290
H	-0.6627420	1.7509700	0.4387970
H	0.1162820	1.8620900	-1.1316000
H	-2.0968990	1.4454530	-2.1794500
H	-3.4708560	2.5255170	-1.8941000
H	-3.0404910	-0.2492920	-2.4197390
H	-3.9118040	-1.5484950	-1.6268760
H	-4.5475380	-0.4513630	1.1704660
H	-3.7550790	-1.9224080	0.5680990
H	-1.7544970	-2.4959940	-0.7746010
H	-1.9250290	-2.4852460	-2.5404600
H	-0.4599730	-0.4231450	-2.6410280
H	-0.2662630	-0.5009420	-0.8748130
H	2.1984010	-0.3335280	-2.3269310
H	3.0611280	-1.8164860	-2.7582550
H	4.2800680	-1.2306040	-0.8744320
H	3.0799000	-2.3049610	-0.1671740
H	2.6973290	0.1760350	2.3227580
H	3.6633300	-1.2551470	1.9387240
H	1.6613570	-2.0910800	2.9429040
H	1.4661400	-2.3958430	1.2119380
H	-2.2953640	0.1755930	2.2604800
H	-3.2500110	-1.1316490	2.9691440
C	0.2087990	-0.8091420	1.9726630
H	0.1471570	-0.1927650	1.0721120
H	0.1623800	-0.1498090	2.8488580
S	-1.2088550	-1.9723850	2.0278390
C	-1.6120680	3.1208850	-0.9213870
H	-2.0997790	3.7367130	-0.1565860

H	-1.3409310	3.7775040	-1.7593740
C	1.8675400	2.6607460	0.8282310
H	1.4932040	1.8108540	1.4115510
H	2.4539930	3.2904270	1.5083700

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LR1 (7_Amide_170)

C	2.1766850	2.0666970	-0.2446480
O	2.9361780	2.3241230	-1.1860020
C	0.9735490	2.9597730	0.0409020
C	-1.5690550	3.1232800	-0.0980330
C	-3.1676170	1.1268770	-0.3818930
C	-2.4431090	0.1331820	-1.2986880
O	-2.0725390	0.4718660	-2.4246410
N	-2.2578530	-1.1558430	-0.8408470
C	-1.7101950	-2.1560960	-1.7755250
C	-2.8112730	-1.6807560	0.4118780
C	-0.2731400	-2.6199480	-1.4862010
C	0.7412460	-1.4736360	-1.4576220
S	2.3916030	-2.1694750	-1.0533550
C	3.4703800	-0.6913380	-1.0606170
C	3.5492800	0.1282350	0.2385390
N	2.3528790	0.9372120	0.5222830
C	1.6571350	0.7344420	1.8041740
C	1.3506860	-0.7293550	2.1502850
C	-1.8031640	-1.8938950	1.5592380
H	1.1545610	3.9022990	-0.4854400
H	0.8792260	3.1908010	1.1097850
H	-1.4299080	4.1715730	-0.4004950
H	-1.6622630	3.1197460	0.9992760
H	-4.2432800	0.9240940	-0.4974310
H	-2.9232230	0.9413790	0.6680630
H	-1.7503690	-1.7221360	-2.7770440
H	-2.3712000	-3.0332110	-1.7525470

H	-3.6416670	-1.0542070	0.7477680
H	-3.2425600	-2.6653820	0.1847460
H	-0.2348500	-3.1802690	-0.5434260
H	-0.0018520	-3.3321110	-2.2777050
H	0.7886780	-0.9742610	-2.4321880
H	0.4595470	-0.7270300	-0.7086370
H	3.1786120	-0.0456780	-1.8931000
H	4.4737880	-1.0804330	-1.2744050
H	4.4140780	0.8005950	0.1453720
H	3.7232660	-0.5372920	1.0878820
H	0.7044560	1.2614700	1.7572370
H	2.2455910	1.1817650	2.6221480
H	2.2393920	-1.2246840	2.5626000
H	1.0837910	-1.2833650	1.2459520
H	-2.2154840	-2.6440960	2.2454670
H	-0.8589480	-2.2756220	1.1653310
C	0.2203120	-0.8285580	3.1837540
H	0.3941290	-0.1424410	4.0224990
H	0.1553450	-1.8428540	3.5939280
S	-1.4308260	-0.3739370	2.5204400
C	-0.3249170	2.3163650	-0.4814160
H	-0.2615220	2.2126600	-1.5705290
H	-0.4172370	1.3009350	-0.0761210
C	-2.8757310	2.5992190	-0.7172240
H	-3.7081440	3.2088490	-0.3421480
H	-2.8451300	2.7190820	-1.8065220

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LR2 (9_Amide_111)

C	-1.4590430	2.0398620	-0.2192330
O	-1.5923810	2.6663950	0.8377340
C	-0.2002870	2.1959460	-1.0735100
C	2.2137900	2.9655510	-1.2170340
C	3.5361110	3.0852140	-0.4328090

C	3.7555260	1.9697770	0.6113320	H	-1.0780760	0.8192880	2.4587410
C	3.4964730	-0.5267940	1.1672750	H	-3.2066820	1.4755330	2.1843370
C	2.8281990	-1.7933650	0.6428390	H	-4.6833050	0.5384000	1.8961130
O	3.4992070	-2.7426100	0.2186150	H	-4.1625210	2.1145560	0.0759530
N	1.4594850	-1.8029630	0.5907330	H	-4.3568490	0.4335070	-0.4447090
C	0.5813690	-0.7492690	1.1078650	H	-1.5919500	0.9606750	-2.5696550
C	0.7845730	-2.9610910	0.0031510	H	-3.3235930	1.2669740	-2.5477990
C	0.0001200	-1.0752140	2.4910090	H	-2.8754810	-0.9604380	-3.3286610
C	-1.2275090	-0.2093020	2.8053050	H	-3.7768180	-1.0511620	-1.8203080
S	-2.7340760	-0.8583930	1.9552010	H	1.7856620	-2.9193830	-1.9111270
C	-3.6455710	0.6861210	1.5734590	H	0.2884070	-3.8793870	-1.8837060
C	-3.6961410	1.1166090	0.0949240	C	-1.7782680	-1.7601730	-1.6376800
N	-2.4280870	1.1639930	-0.6525460	H	-2.0869550	-2.7917620	-1.8493370
C	-2.5161700	0.7046750	-2.0531130	H	-1.7581380	-1.6241300	-0.5517770
C	-2.7975820	-0.7944760	-2.2455990	S	-0.0886420	-1.5310680	-2.3188220
C	0.7585260	-2.9507130	-1.5333280	C	0.9587860	2.8660470	-0.3319560
H	-0.4601310	2.7760580	-1.9724570	H	0.6609860	3.8582280	0.0263160
H	0.1259530	1.2094970	-1.4289220	H	1.1718060	2.2745900	0.5649740
H	2.1168710	3.8254750	-1.8942910	C	3.4951390	0.5598580	0.0687070
H	2.2695050	2.0782430	-1.8627040	H	4.2342090	0.3002620	-0.7012110
H	3.5762260	4.0564160	0.0814310	H	2.5191900	0.5414960	-0.4279920
H	4.3656490	3.0748650	-1.1543840	56			
H	3.0884030	2.1386490	1.4686760	LR3 (8_Amide_121)			
H	4.7797170	2.0361680	1.0043080	C	-1.5294970	-1.2726390	-1.5390130
H	2.9841740	-0.1467330	2.0603110	O	-1.4270260	-0.8435490	-2.6920360
H	4.5191340	-0.7892990	1.4540110	C	-0.5180250	-2.2853440	-0.9965780
H	-0.2320510	-0.6110800	0.3909640	C	1.9797830	-2.8129320	-0.8628780
H	1.1143590	0.2002510	1.1503980	C	3.4008220	-2.3667670	-1.2573760
H	1.3033110	-3.8746590	0.3160850	C	3.6802220	-0.4261110	0.4602970
H	-0.2344780	-2.9951930	0.4020140	C	3.1936910	1.0176070	0.5651370
H	-0.2634710	-2.1402990	2.5417190	O	3.9833970	1.9537910	0.3954380
H	0.7670330	-0.9056500	3.2593120	N	1.8533470	1.2340090	0.7634720
H	-1.4192540	-0.1916630	3.8835790	C	1.3327210	2.6076550	0.7512300

C	0.8677160	0.1821930	1.0158890
C	0.9539180	3.0879330	-0.6602290
C	-0.1387060	2.2824350	-1.3737240
S	-1.7703820	2.4406600	-0.5258940
C	-2.8536560	1.5328490	-1.6995260
C	-3.4475360	0.1960520	-1.2178870
N	-2.5079440	-0.8047480	-0.6863860
C	-3.0404120	-1.6358430	0.4136310
C	-3.3308490	-0.8955080	1.7279950
C	0.6430820	-0.0626220	2.5134590
H	-0.8875160	-3.3012260	-1.2006450
H	-0.4321810	-2.1924310	0.0916790
H	1.8844770	-3.8950980	-1.0295150
H	1.8389080	-2.6691350	0.2188420
H	3.5599370	-2.5879630	-2.3228210
H	4.1311610	-2.9669310	-0.6956270
H	4.6996970	-0.4460460	0.8575040
H	3.0839650	-1.1144570	1.0662320
H	2.0981960	3.2740060	1.1578350
H	0.4609600	2.6392440	1.4154930
H	-0.0715840	0.4871670	0.5508530
H	1.1697420	-0.7410580	0.5333810
H	0.6503560	4.1419170	-0.5931460
H	1.8561500	3.0484390	-1.2842660
H	-0.2648000	2.6622070	-2.3937040
H	0.1319370	1.2235550	-1.4424970
H	-2.2766550	1.3840930	-2.6131010
H	-3.7011440	2.1897690	-1.9292420
H	-3.9931460	-0.2312780	-2.0743980
H	-4.1772370	0.3997700	-0.4301860
H	-2.3415630	-2.4476590	0.6117350
H	-3.9790580	-2.0979840	0.0690220
H	-3.7075990	-1.6471160	2.4355650

H	-4.1481050	-0.1753490	1.5874510
H	1.5294670	-0.5249180	2.9634010
H	0.4516310	0.8829250	3.0349630
C	-2.1562330	-0.1271200	2.3356860
H	-2.4948480	0.4169220	3.2251010
H	-1.7921190	0.6031440	1.6072630
S	-0.7478050	-1.2124780	2.8186570
C	0.8685180	-2.0777590	-1.6266710
H	0.8617990	-2.3865320	-2.6780730
H	1.0704080	-1.0010850	-1.6340020
C	3.6907150	-0.8713730	-1.0326240
H	2.9634440	-0.2760840	-1.5980610
H	4.6698840	-0.6247100	-1.4589730

XYZ coordinates for metal complexes of L2

62

Cu⁺(L4)

C	2.4715070	2.2941660	0.3595130
C	0.2431220	3.6004600	0.4947310
C	-1.0237280	3.9942950	-0.2841350
C	-1.9252320	2.8156310	-0.6944820
C	-3.6239080	1.0723780	0.1461760
N	-2.1970220	-1.0716280	0.1765860
C	-2.1640820	-2.4286280	-0.4213570
C	-2.4604500	-1.1932590	1.6211730
C	-1.8115250	-2.5329450	-1.9107150
C	-0.3442850	-2.2886200	-2.2786820
S	0.0725430	-0.4987100	-2.2385670
C	1.8636620	-0.5434350	-2.6253940
C	2.7603150	-0.9729380	-1.4582820
N	2.6100440	-0.1301870	-0.2611930
C	3.2467600	-0.7785410	0.9104470
C	2.4160050	-1.8971810	1.5653550
C	-1.2383120	-1.6436730	2.4239800

H	2.2488930	1.9090810	1.3649570
H	3.1312070	3.1614540	0.4933790
H	0.7720440	4.5115780	0.8066180
H	-0.0292190	3.0653780	1.4158780
H	-0.7244660	4.5463510	-1.1864300
H	-1.6183340	4.6876850	0.3267290
H	-1.3782050	2.1212130	-1.3472220
H	-2.7576150	3.2096990	-1.2943600
H	-4.3173190	1.5636030	-0.5501540
H	-4.2218500	0.8408930	1.0364980
H	-3.1554570	-2.8998490	-0.2800000
H	-1.4378670	-3.0314130	0.1372280
H	-2.7753620	-0.2246180	2.0125700
H	-3.2813950	-1.9069740	1.8211310
H	-2.4671990	-1.9000860	-2.5194550
H	-2.0361230	-3.5679310	-2.2005830
H	0.3200980	-2.8239680	-1.5900390
H	-0.1477120	-2.6350500	-3.2999920
H	2.0997720	0.4696100	-2.9655010
H	2.0069120	-1.2186400	-3.4766600
H	3.8077530	-0.9711940	-1.8136180
H	2.5170980	-2.0056680	-1.1826530
H	4.2387980	-1.1661010	0.6187510
H	3.4274470	0.0034840	1.6568490
H	3.1045860	-2.6617260	1.9503940
H	1.7772850	-2.3925170	0.8212550
H	-1.5148910	-1.7542480	3.4778220
H	-0.8293730	-2.5937410	2.0671710
C	1.5691480	-1.4200430	2.7491380
H	1.1770810	-2.2652540	3.3248050
H	2.1764710	-0.8115910	3.4289000
S	0.1050070	-0.3797460	2.3181510
C	3.2081670	1.2212350	-0.4509960

H	4.2791370	1.1866360	-0.1903210
H	3.1566240	1.4912060	-1.5112270
C	-3.1964980	-0.2306540	-0.5404420
H	-2.7622660	0.0078350	-1.5174740
H	-4.1090950	-0.8270240	-0.7270610
C	-2.5056990	2.0618510	0.5088290
H	-1.7009980	1.5425160	1.0483310
H	-2.9161560	2.7996390	1.2126190
C	1.1794970	2.7269940	-0.3366100
H	0.6284390	1.8190340	-0.6412440
H	1.4309880	3.2427750	-1.2759420
Cu	0.1435010	-0.1791950	0.0412930
123			
Cu ⁺ (L4) ₂			
C	-6.0488820	-2.8747500	-1.3144180
C	-6.7963200	-0.4347240	-1.4958930
C	-7.6463150	0.6734360	-0.8571220
C	-7.0935510	1.2150000	0.4696180
C	-5.2504010	2.5664900	1.5888010
N	-2.7284160	2.2732550	1.5497550
C	-2.5202100	1.9186710	2.9663260
C	-1.5227740	2.8911030	0.9909110
C	-1.5757020	0.7440370	3.2465450
C	-2.0682920	-0.6408630	2.8104210
S	-2.0000280	-0.7876660	0.9876400
C	-2.0917660	-2.5991360	0.6634980
C	-3.3084630	-2.9933880	-0.1874610
N	-3.6361570	-2.0925810	-1.2944410
C	-2.5152040	-1.7245460	-2.1668540
C	-2.7264530	-0.3627540	-2.8529240
C	-1.4888340	3.0156970	-0.5385990
H	-6.7990740	-3.1964520	-2.0501490
H	-5.9301340	-3.7116060	-0.6137860

H	-7.2959910	-0.7743010	-2.4153640
H	-5.8224540	-0.0275860	-1.7993260
H	-8.6621310	0.2885010	-0.6879710
H	-7.7385150	1.5073410	-1.5684460
H	-7.1311930	0.4301810	1.2386210
H	-7.7519980	2.0234230	0.8188500
H	-5.3150700	1.9435680	2.4914700
H	-5.9775430	3.3784790	1.7319480
H	-3.4964650	1.6710540	3.3959660
H	-2.1465520	2.8018940	3.5260300
H	-1.3798630	3.9135510	1.4060560
H	-0.6503800	2.3035580	1.2945300
H	-1.4296720	0.7096660	4.3349690
H	-0.5903570	0.9219920	2.8053150
H	-1.4409050	-1.4228850	3.2525640
H	-3.1064950	-0.8038180	3.1250710
H	-2.1350640	-3.1239530	1.6238470
H	-1.1595670	-2.8811820	0.1713620
H	-4.1878330	-3.0345300	0.4639820
H	-3.1198150	-4.0311410	-0.5409430
H	-1.5962410	-1.6646100	-1.5797380
H	-2.3353460	-2.4924970	-2.9449220
H	-3.6749000	-0.3783350	-3.4034260
H	-1.9402350	-0.2234310	-3.6075220
H	-2.4231390	3.4142720	-0.9464690
H	-0.6970350	3.7253760	-0.8072370
C	-2.7812990	0.8412960	-1.8987900
H	-3.3090150	1.6768600	-2.3719060
H	-3.2869330	0.5782420	-0.9685730
S	-1.1023360	1.5033080	-1.5121790
C	-4.7473870	-2.6408360	-2.0904420
H	-4.9532580	-1.9347740	-2.9014260
H	-4.4355230	-3.5942780	-2.5655340

C	-3.8695300	3.2141460	1.4622160
H	-3.7492470	4.0072720	2.2280540
H	-3.8331940	3.7170830	0.4893250
C	-5.6591300	1.7453470	0.3640070
H	-4.9615580	0.9100350	0.2313180
H	-5.5710890	2.3792280	-0.5331500
C	-6.5689680	-1.6378910	-0.5717660
H	-5.8588710	-1.3583850	0.2181040
H	-7.5144550	-1.8989350	-0.0748560
Cu	-0.0000260	-0.0008680	0.0423600
C	6.0483460	2.8756500	-1.3141420
C	6.7969100	0.4359700	-1.4958910
C	7.6468340	-0.6721100	-0.8569210
C	7.0937000	-1.2138970	0.4695620
C	5.2506950	-2.5657690	1.5882790
N	2.7286100	-2.2735300	1.5494430
C	2.5201270	-1.9194070	2.9661170
C	1.5231650	-2.8917650	0.9904830
C	1.5755480	-0.7448710	3.2464160
C	2.0680160	0.6400950	2.8104480
S	1.9998210	0.7872850	0.9877480
C	2.0915440	2.5987390	0.6639420
C	3.3081990	2.9932300	-0.1870130
N	3.6359090	2.0927060	-1.2942300
C	2.5149070	1.7246970	-2.1665960
C	2.7261680	0.3630040	-2.8528700
C	1.4891520	-3.0159770	-0.5390570
H	6.7983920	3.1978500	-2.0498050
H	5.9291760	3.7123140	-0.6133530
H	7.2969160	0.7757730	-2.4151000
H	5.8232280	0.0287160	-1.7997700
H	8.6625160	-0.2870130	-0.6873420
H	7.7394450	-1.5059240	-1.5683020

H	7.1309090	-0.4291440	1.2386570
H	7.7522130	-2.0222100	0.8189270
H	5.3149660	-1.9426660	2.4908490
H	5.9781520	-3.3774330	1.7316390
H	3.4962750	-1.6719110	3.3960710
H	2.1463710	-2.8028230	3.5254450
H	1.3807670	-3.9143650	1.4053350
H	0.6505620	-2.3046610	1.2943980
H	1.4295330	-0.7105190	4.3348550
H	0.5902060	-0.9229160	2.8051930
H	1.4404740	1.4219570	3.2526430
H	3.1061630	0.8031020	3.1252660
H	2.1348930	3.1234510	1.6243490
H	1.1593620	2.8809990	0.1718600
H	4.1876000	3.0343150	0.4644060
H	3.1194560	4.0310230	-0.5402980
H	1.5959340	1.6646510	-1.5794850
H	2.3349630	2.4927170	-2.9445710
H	3.6745050	0.3786000	-3.4035680
H	1.9397760	0.2237520	-3.6072990
H	2.4235150	-3.4142350	-0.9471530
H	0.6975550	-3.7258500	-0.8077970
C	2.7812200	-0.8411790	-1.8989010
H	3.3089450	-1.6766430	-2.3721640
H	3.2868270	-0.5783040	-0.9686220
S	1.1023220	-1.5034950	-1.5122450
C	4.7469740	2.6412770	-2.0902220
H	4.9530750	1.9352290	-2.9011640
H	4.4348450	3.5946220	-2.5653350
C	3.8700610	-3.2139510	1.4616140
H	3.7501770	-4.0073000	2.2272680
H	3.8337860	-3.7166510	0.4885970
C	5.6594320	-1.7445860	0.3634860

H	4.9616640	-0.9094700	0.2305770
H	5.5718460	-2.3785530	-0.5336530
C	6.5690240	1.6389390	-0.5716690
H	5.8590970	1.3590440	0.2182150
H	7.5144290	1.9003830	-0.0748050
62			
Ag ⁺ (L4)			
C	-3.5961470	0.8298880	-0.6213550
C	-2.0717730	2.7070100	0.2716650
C	-1.2322400	3.9404740	-0.1071040
C	0.1011740	3.6194150	-0.8015590
C	2.3519080	2.4121460	-0.6427940
N	2.5975700	-0.0566850	-0.1251160
C	3.1754970	-1.0141720	0.8529390
C	2.9586310	-0.5172140	-1.4884950
C	2.7255990	-0.9080240	2.3161650
C	1.3182650	-1.4424000	2.6402850
S	0.0586480	-0.1063930	2.5718360
C	-1.4875460	-1.0567400	2.8043800
C	-1.9811840	-1.8669330	1.5955720
N	-2.1766880	-1.0995280	0.3466930
C	-2.4498770	-2.0350070	-0.7732350
C	-1.2323990	-2.8624290	-1.2496040
C	2.0250080	-1.5946800	-2.0468050
H	-3.8741060	0.2928970	-1.5366660
H	-4.5027990	1.3673850	-0.3097190
H	-1.5143120	2.0777540	0.9801860
H	-2.9693860	3.0488150	0.8073730
H	-1.0348030	4.5322060	0.7978800
H	-1.8348050	4.5743110	-0.7724030
H	0.5308510	4.5452590	-1.2073740
H	-0.0842070	2.9636880	-1.6648070
H	3.0382950	3.2393520	-0.8624810

H	2.0196630	2.0309200	-1.6174630
H	4.2769800	-0.9186550	0.8270250
H	2.9382120	-2.0267220	0.5034410
H	2.9605400	0.3378340	-2.1706080
H	3.9877490	-0.9174490	-1.4889010
H	2.8486200	0.1112990	2.7023820
H	3.4365870	-1.5218830	2.8839970
H	1.0369180	-2.2365540	1.9381070
H	1.2920170	-1.8514300	3.6566310
H	-2.2263700	-0.3176260	3.1278710
H	-1.3336720	-1.7446470	3.6440400
H	-2.9326320	-2.3485160	1.8906040
H	-1.2636890	-2.6689650	1.3964040
H	-3.2734030	-2.7118340	-0.4839090
H	-2.8129970	-1.4399870	-1.6149350
H	-1.5480040	-3.9053250	-1.3853670
H	-0.4448680	-2.8766490	-0.4847910
H	2.4730790	-2.0424260	-2.9405110
H	1.8439270	-2.3849140	-1.3096600
C	-0.6326180	-2.3944400	-2.5835220
H	-0.0001930	-3.1745650	-3.0224030
H	-1.4269920	-2.1739550	-3.3061410
S	0.3988160	-0.8709370	-2.5250520
C	-3.3063130	-0.1462290	0.5257630
H	-4.2235630	-0.7270260	0.7357410
H	-3.0903540	0.4496160	1.4162510
C	3.1295810	1.3165910	0.1053970
H	3.0805220	1.5197940	1.1800070
H	4.1972050	1.3330310	-0.1766600
C	1.1283440	2.9480720	0.1170340
H	1.4517730	3.6516120	0.8972810
H	0.6447880	2.1218460	0.6603700
C	-2.5116280	1.8706500	-0.9396900

H	-2.9146320	2.5475660	-1.7062870
H	-1.6443500	1.3849070	-1.4087500
Ag	0.0458110	-0.0690650	-0.0579910
123			
Ag ⁺ (L4) ₂			
C	-5.1682630	2.9019890	2.5147160
C	-6.0985210	2.5219770	0.1580840
C	-7.2602310	1.8915810	-0.6255110
C	-7.2000800	0.3611220	-0.7266120
C	-5.9652330	-1.6698700	-1.6271860
N	-3.5042700	-2.1435130	-1.3119720
C	-2.2569940	-2.3347020	-2.0430220
C	-3.7135860	-2.9912580	-0.1345960
C	-1.9182490	-1.1443430	-2.9794010
C	-2.3808620	0.2582800	-2.5274990
S	-2.1845620	0.5175120	-0.7288410
C	-1.9852750	2.3183590	-0.4816470
C	-1.7055640	2.5228670	1.0177130
N	-2.8452850	2.1250950	1.8503120
C	-2.4737290	1.5157060	3.1312600
C	-1.7714520	0.1540250	3.0063700
C	-2.5228480	-3.4112200	0.7360330
H	-5.1294530	2.4782210	3.5266320
H	-5.7203270	3.8484400	2.6052300
H	-5.1591820	2.3759360	-0.3928460
H	-6.2647560	3.6082580	0.2123370
H	-7.2808290	2.3170350	-1.6396310
H	-8.2055570	2.1784230	-0.1431120
H	-8.0646150	0.0103050	-1.3082690
H	-7.3009630	-0.0803400	0.2754680
H	-6.7719130	-1.8913690	-2.3396210
H	-6.2297370	-2.1960170	-0.6999290
H	-2.2512230	-3.2632750	-2.6495860

H	-1.4475130	-2.4286600	-1.3163100
H	-4.4550620	-2.4967320	0.5047100
H	-4.1653360	-3.9617740	-0.4354500
H	-2.3612660	-1.3077910	-3.9699980
H	-0.8315240	-1.1437700	-3.1172830
H	-1.8109950	1.0248520	-3.0648530
H	-3.4461440	0.3958070	-2.7378860
H	-2.9205970	2.8120920	-0.7701800
H	-1.1647460	2.7174240	-1.0883200
H	-1.4309150	3.5834330	1.1806600
H	-0.8247770	1.9266220	1.2807560
H	-1.8202650	2.1869520	3.7268070
H	-3.3927860	1.3791360	3.7101430
H	-1.4921900	-0.1778430	4.0140270
H	-0.8268750	0.2892530	2.4635650
H	-2.9305220	-4.0848690	1.4988220
H	-1.7922880	-3.9866610	0.1554850
C	-2.6197860	-0.9320240	2.3153730
H	-3.2914340	-1.4178000	3.0328860
H	-3.2065500	-0.4993490	1.5015140
S	-1.4743540	-2.1866770	1.6237660
C	-3.7638490	3.2647420	2.0241950
H	-3.3159330	4.0119170	2.7110840
H	-3.8614910	3.7537140	1.0476000
C	-4.6677770	-2.2329860	-2.2105800
H	-4.4322580	-1.6729480	-3.1234840
H	-4.8240320	-3.2896510	-2.5126670
C	-5.9130730	-0.1621590	-1.3702510
H	-5.7478890	0.3578530	-2.3281210
H	-5.0498340	0.0701770	-0.7338430
C	-5.9425270	1.9626370	1.5810150
H	-6.9386840	1.7908170	2.0131080
H	-5.4409360	0.9869200	1.5389960

Ag	0.0001040	-0.5163670	-0.0001670
C	5.1685110	2.9019540	-2.5144920
C	6.0987680	2.5217500	-0.1579000
C	7.2603670	1.8911400	0.6256800
C	7.2000120	0.3606790	0.7266420
C	5.9649140	-1.6702350	1.6270460
N	3.5039220	-2.1436040	1.3119670
C	2.2566640	-2.3347580	2.0430450
C	3.7131550	-2.9913420	0.1345780
C	1.9180110	-1.1443990	2.9794440
C	2.3807790	0.2581980	2.5275890
S	2.1847180	0.5175300	0.7289080
C	1.9853780	2.3183860	0.4817920
C	1.7057610	2.5229840	-1.0175780
N	2.8455010	2.1252010	-1.8501420
C	2.4740000	1.5159780	-3.1311800
C	1.7716500	0.1543110	-3.0065200
C	2.5223730	-3.4110720	-0.7361140
H	5.1296160	2.4782310	-3.5264250
H	5.7206480	3.8483650	-2.6049840
H	5.1594010	2.3758140	0.3930080
H	6.2651620	3.6080100	-0.2120930
H	7.2809940	2.3165100	1.6398350
H	8.2057420	2.1778990	0.1433270
H	8.0645250	0.0096940	1.3082310
H	7.3007930	-0.0807070	-0.2754830
H	6.7716400	-1.8919500	2.3393610
H	6.2292090	-2.1963220	0.6996920
H	2.2508590	-3.2633680	2.6495510
H	1.4471470	-2.4286460	1.3163650
H	4.4547630	-2.4969280	-0.5046640
H	4.1647110	-3.9619470	0.4354330
H	2.3609890	-1.3079080	3.9700500

H	0.8312860	-1.1437410	3.1172960
H	1.8109120	1.0248070	3.0648900
H	3.4460460	0.3956470	2.7381090
H	2.9206580	2.8121400	0.7704230
H	1.1647920	2.7173990	1.0884180
H	1.4311630	3.5835710	-1.1804850
H	0.8249620	1.9267890	-1.2806960
H	1.8206220	2.1873280	-3.7267040
H	3.3931020	1.3794290	-3.7100000
H	1.4925740	-0.1774680	-4.0142570
H	0.8269670	0.2895260	-2.4638930
H	2.9299610	-4.0848320	-1.4988520
H	1.7916580	-3.9863460	-0.1556010
C	2.6198260	-0.9318240	-2.3154430
H	3.2915040	-1.4176620	-3.0328830

H	3.2065350	-0.4992080	-1.5015120
S	1.4741860	-2.1863670	-1.6239800
C	3.7641540	3.2647930	-2.0238860
H	3.3162920	4.0120810	-2.7106880
H	3.8618570	3.7536480	-1.0472380
C	4.6674450	-2.2331970	2.2105340
H	4.4320270	-1.6731340	3.1234510
H	4.8235960	-3.2898830	2.5126030
C	5.9129620	-0.1624850	1.3702890
H	5.7479060	0.3574390	2.3282290
H	5.0497230	0.0700510	0.7339560
C	5.9427280	1.9624990	-1.5808610
H	6.9388660	1.7906340	-2.0129790
H	5.4410630	0.9868180	-1.5388950