

Supplementary Material

Synthesis of sulfanylidene-diazaspirocycloalkanones in a three-component Mannich-type reaction catalyzed with lactic acid

Tadeusz S. Jagodziński*, Jacek G. Sośnicki, Łukasz Struk

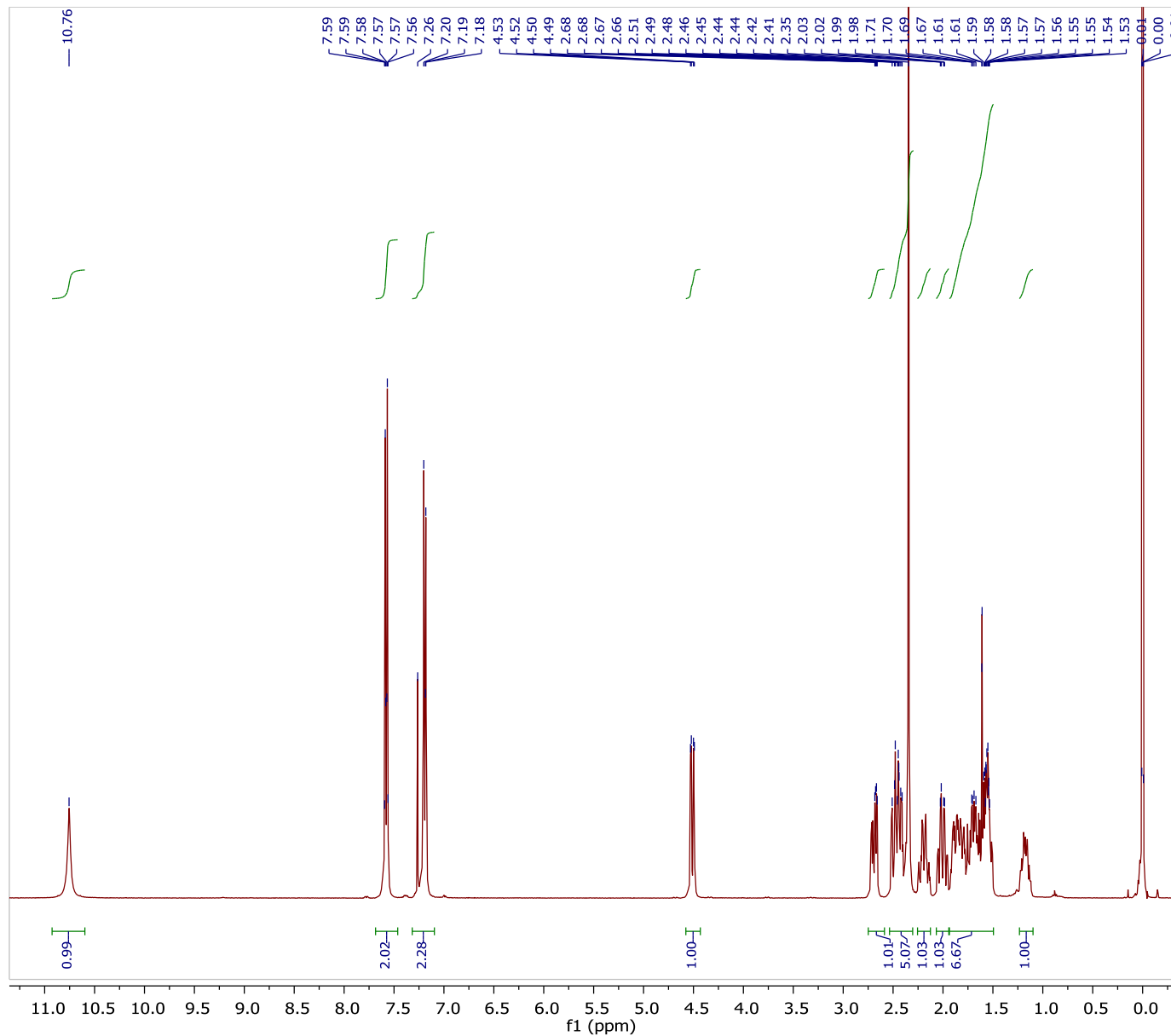
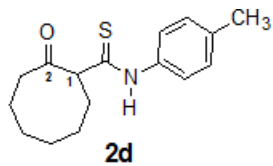
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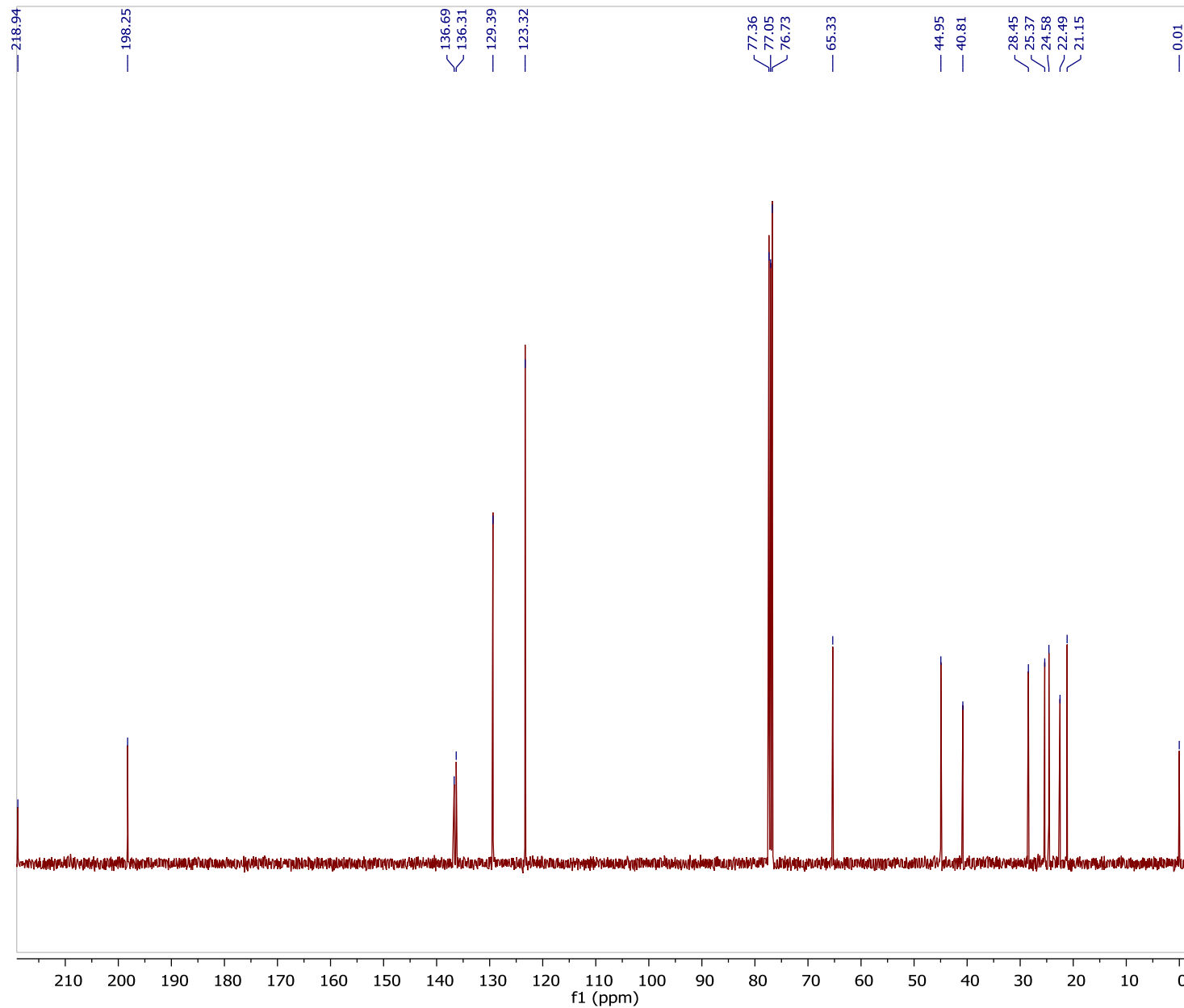
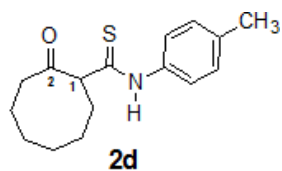
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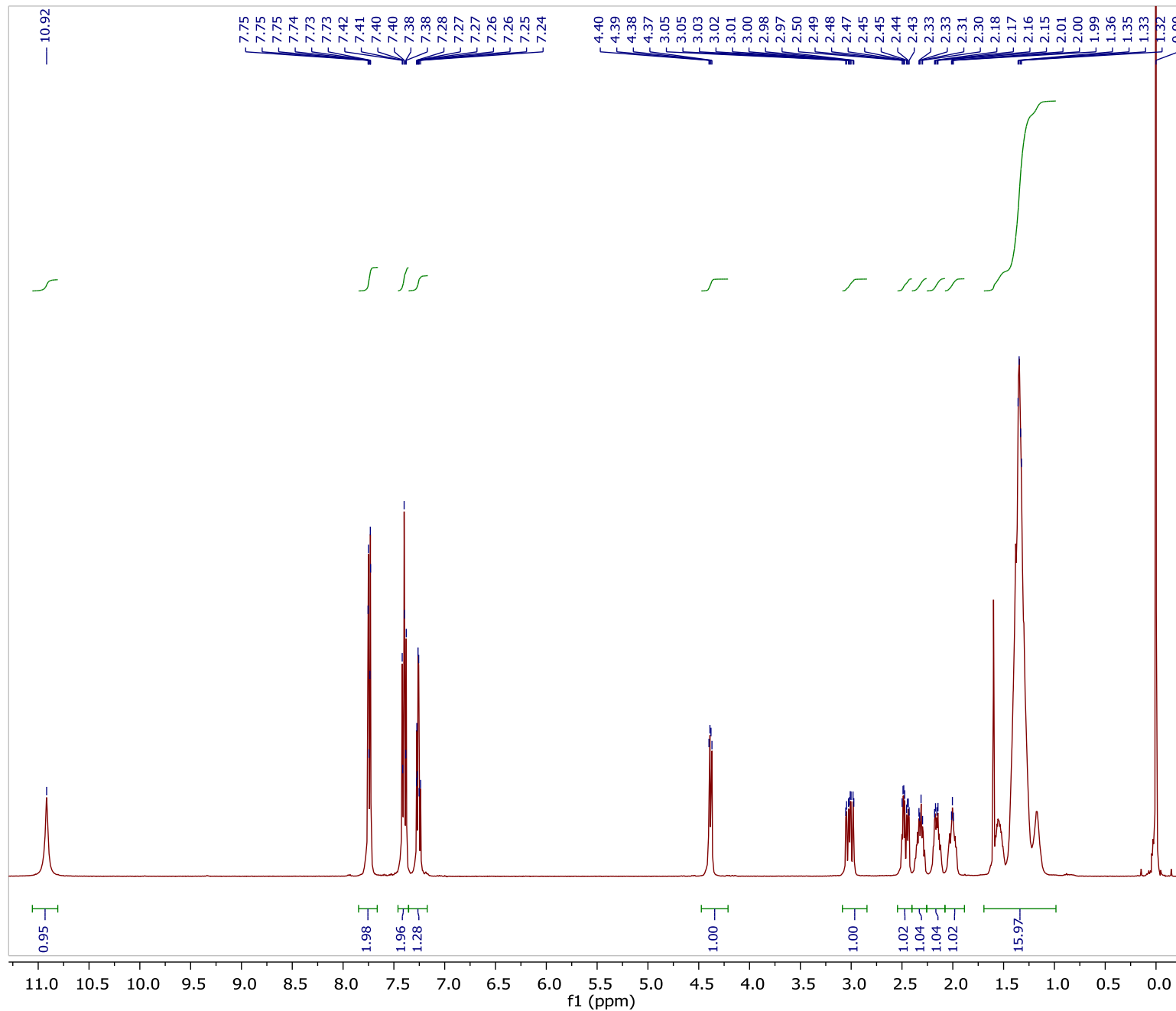
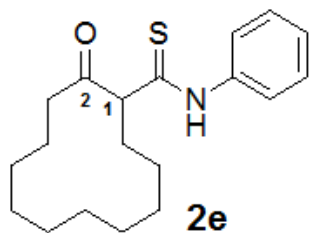
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Spectrometer Frequency	400.13
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Acquired Size	65536
Spectral Size	32768



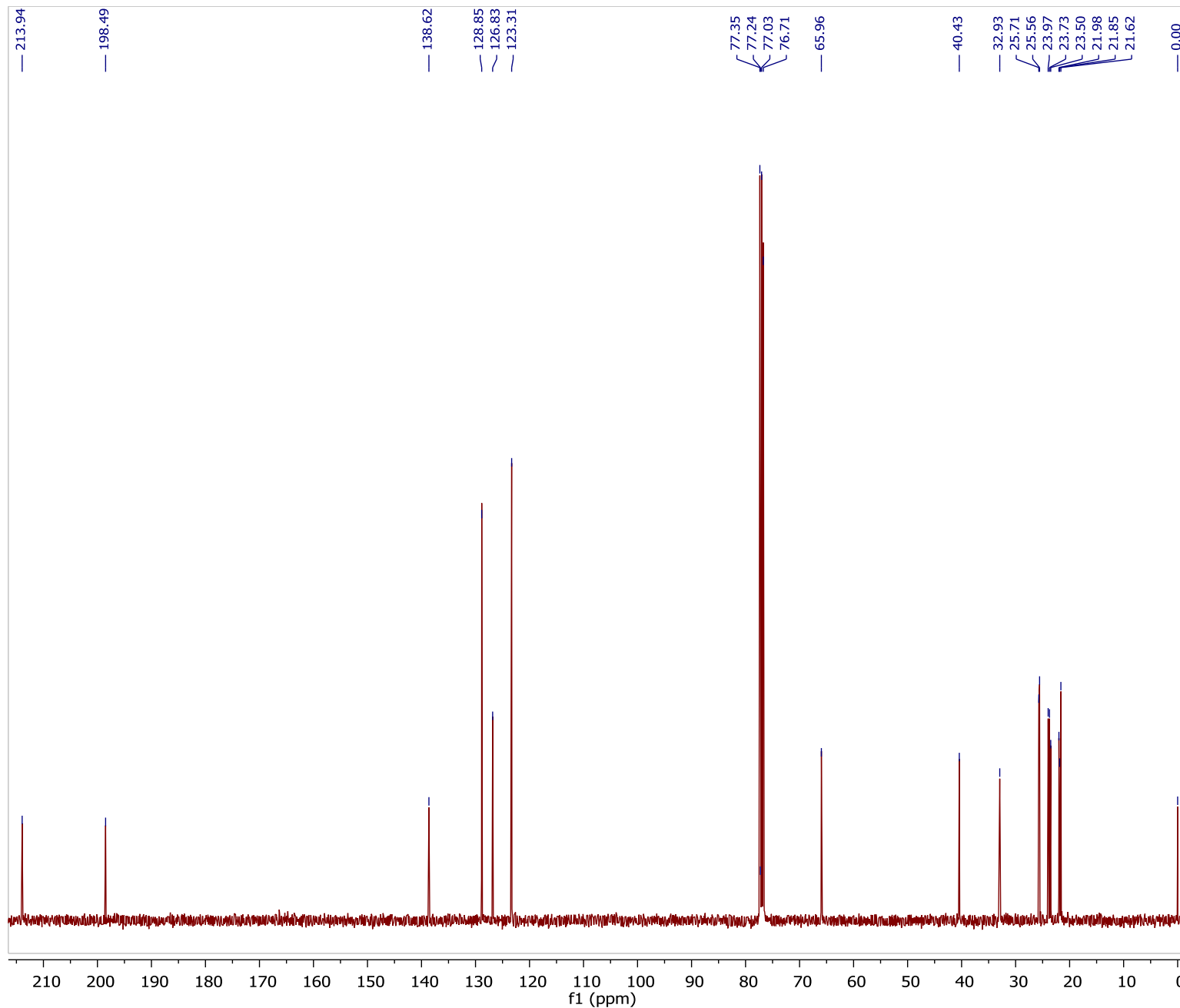
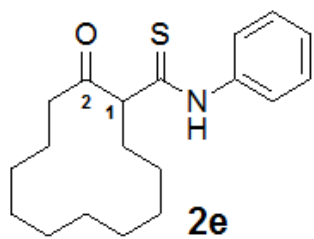
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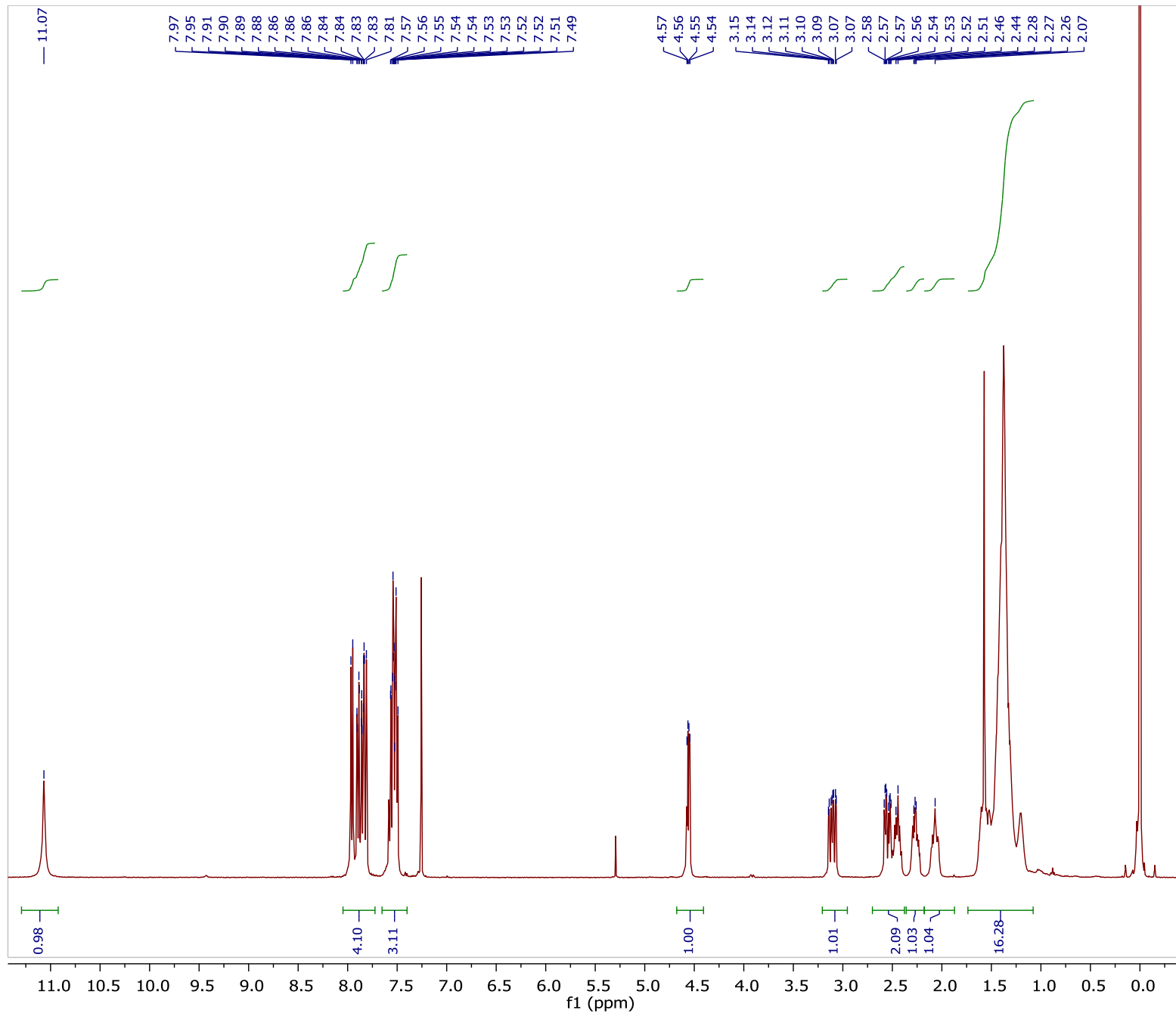
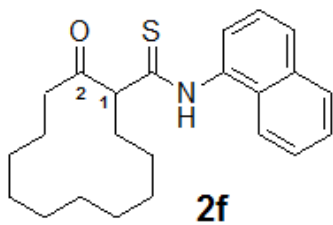
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Spectral Size	32768



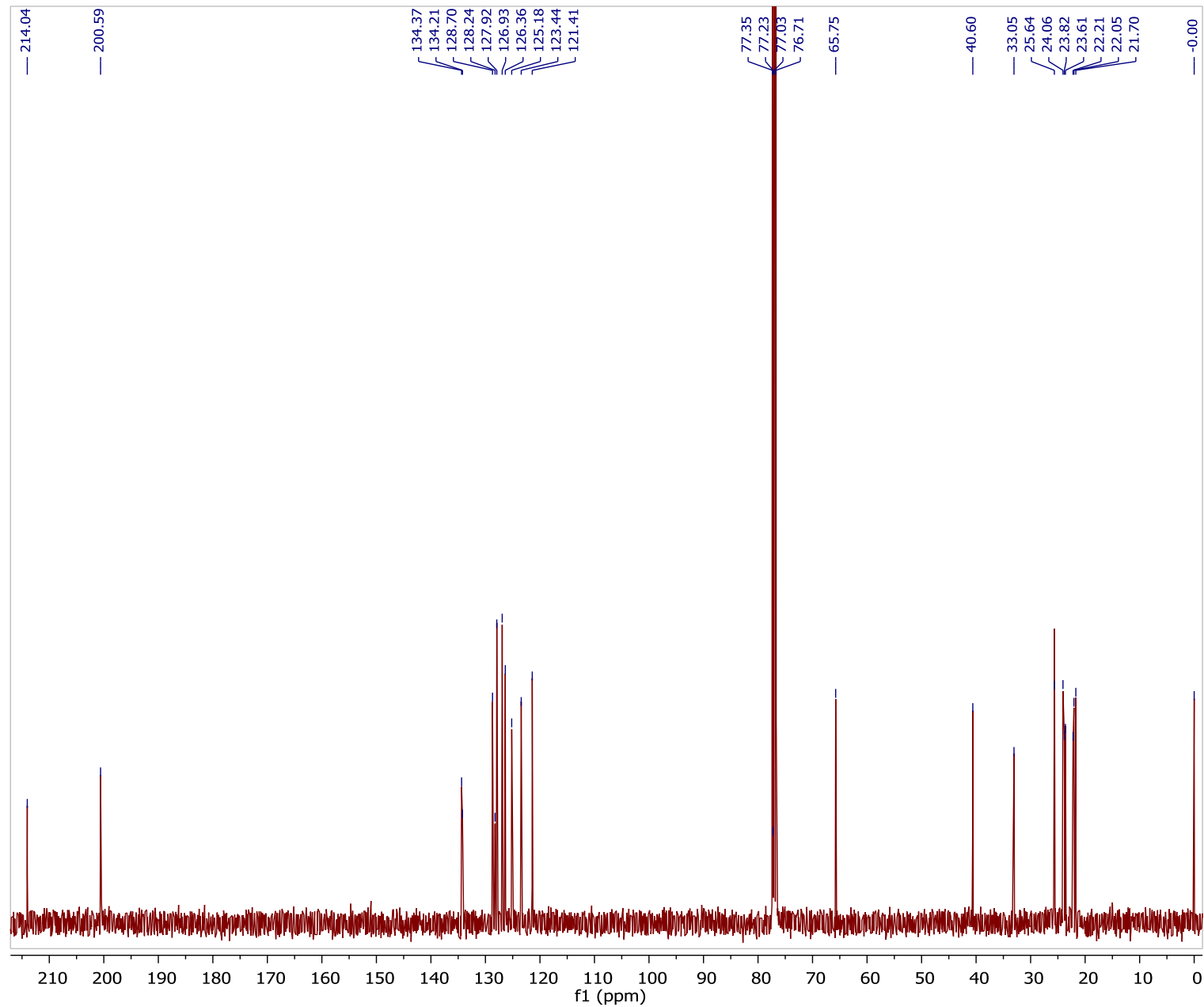
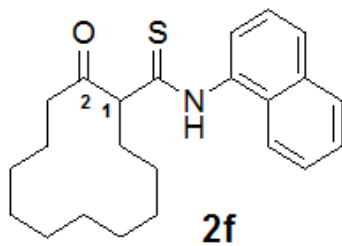
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Spectral Size	16384



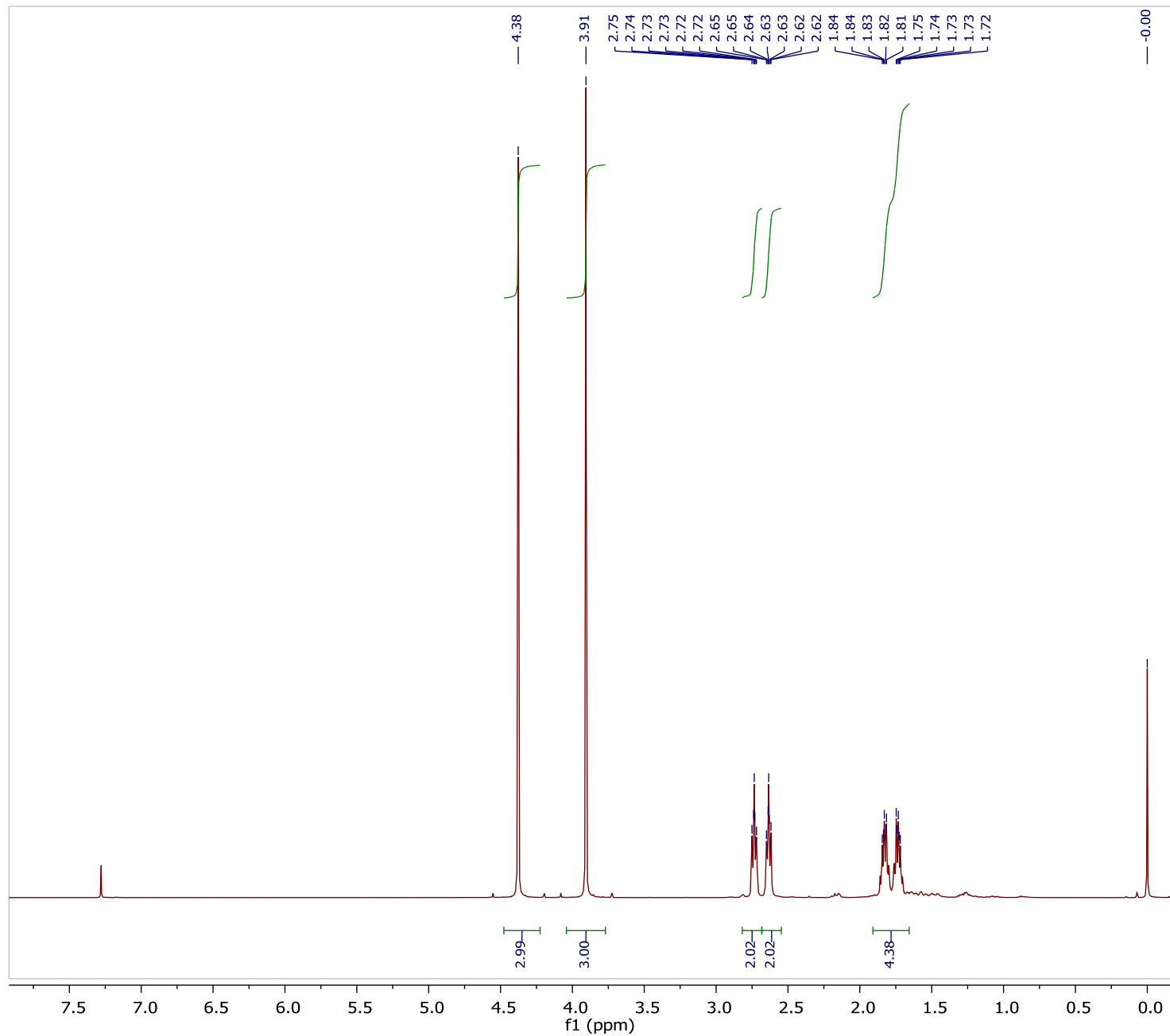
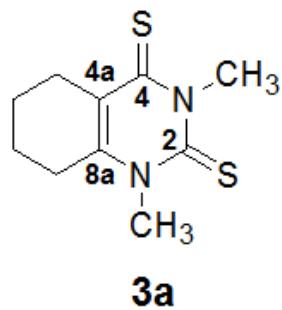
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Spectral Size	32768



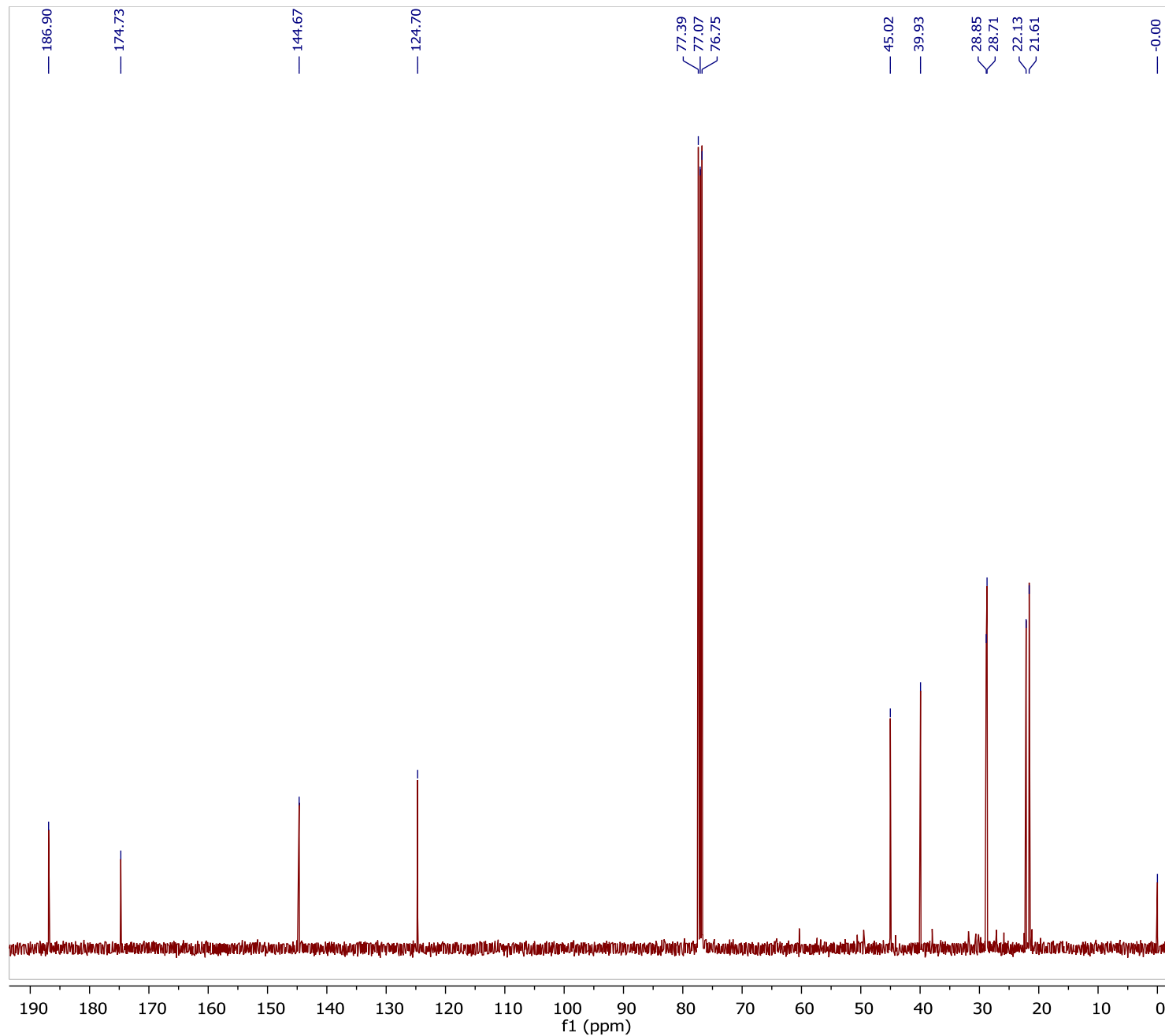
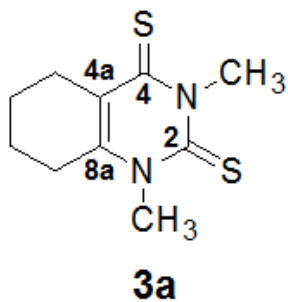
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Spectral Size	16384



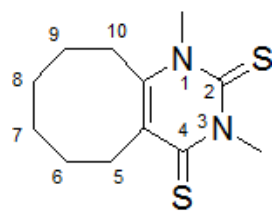
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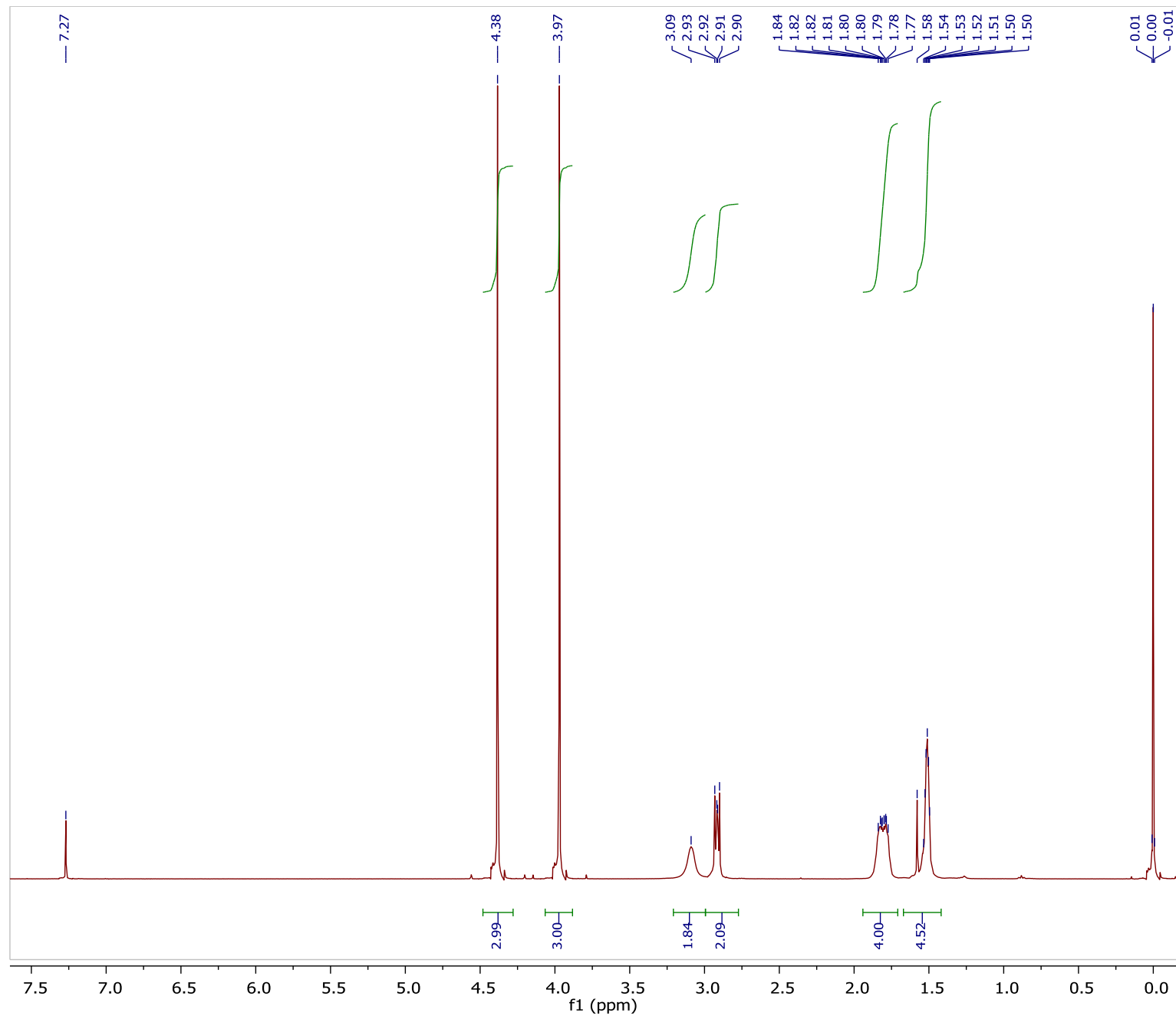
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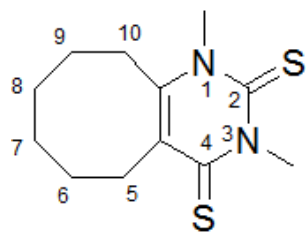
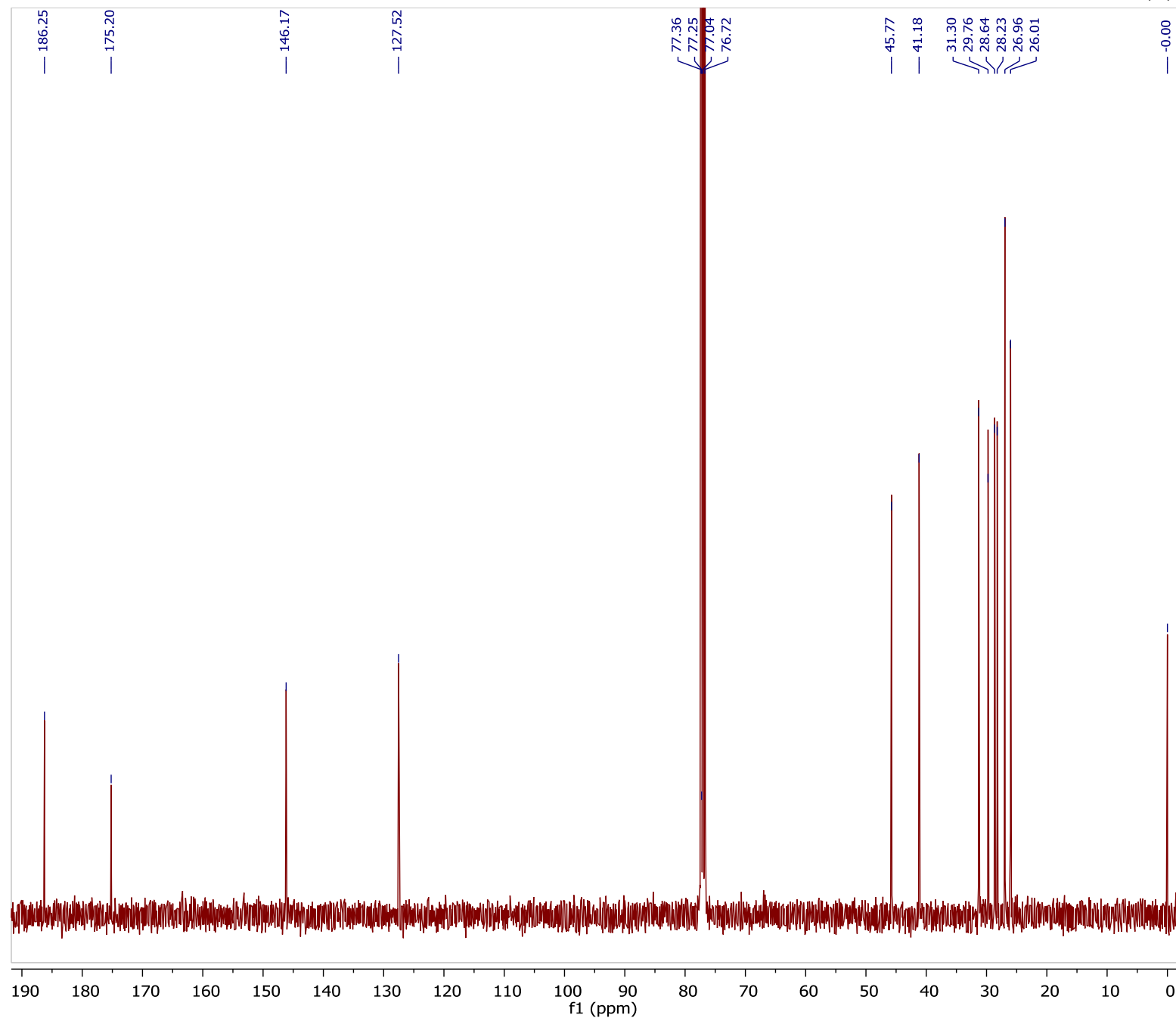
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Spectral Size	32768



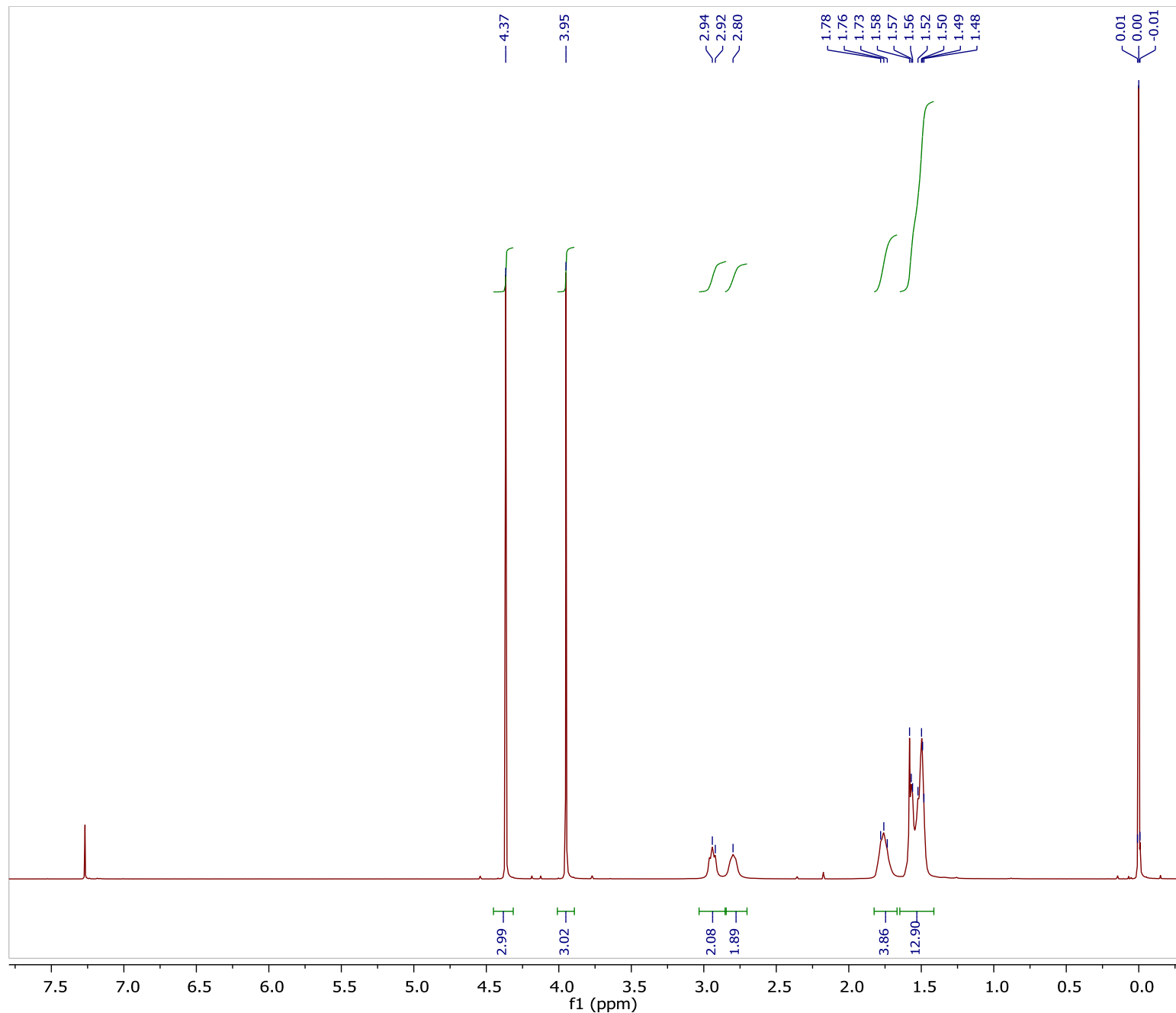
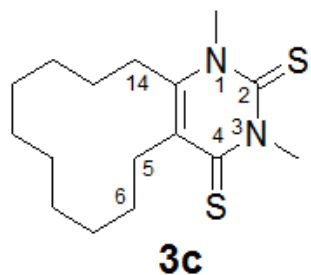
3b



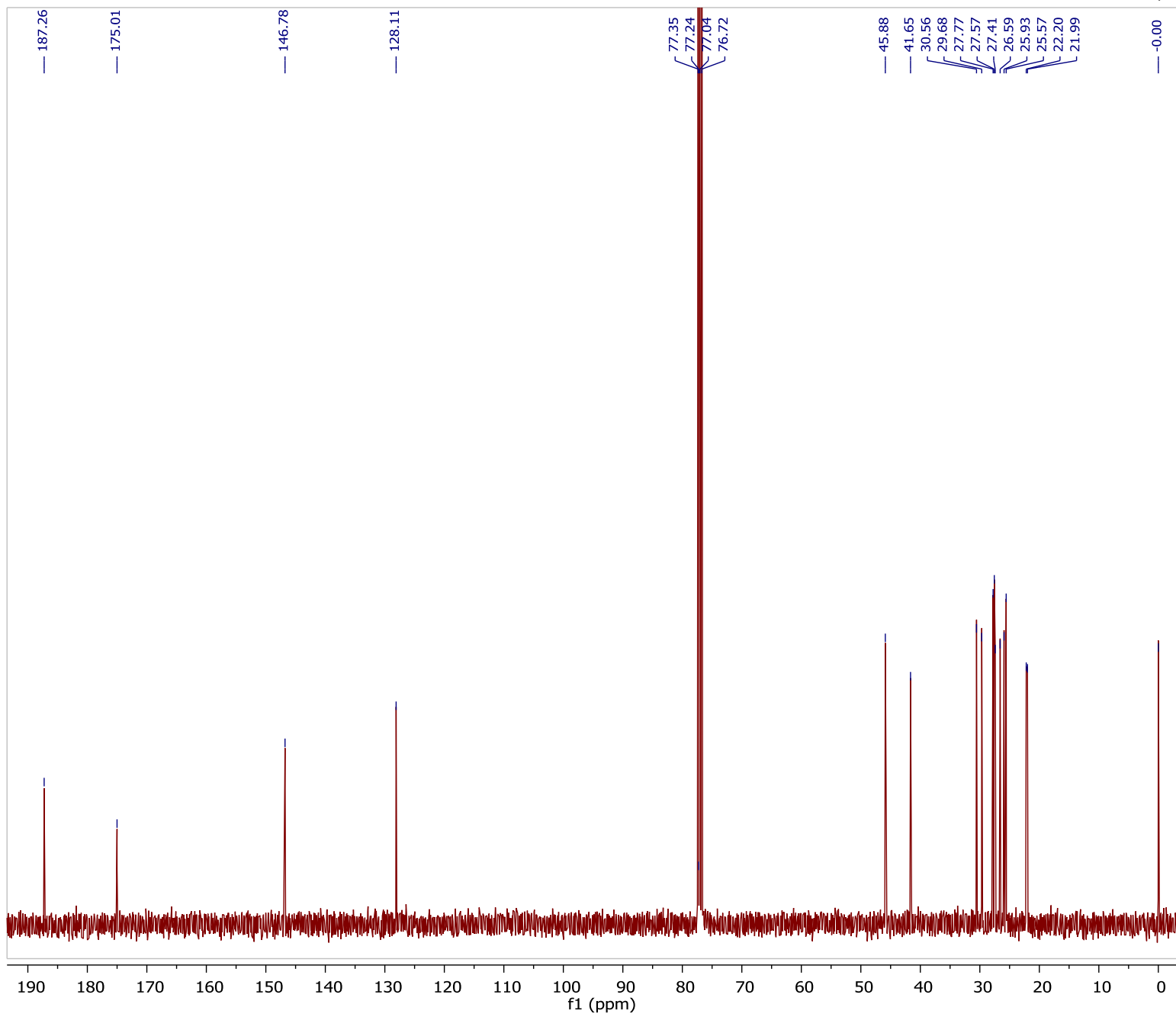
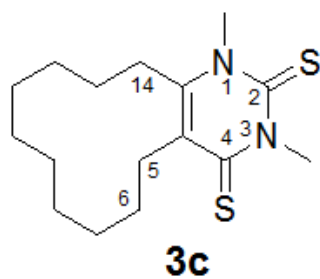
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**3b**

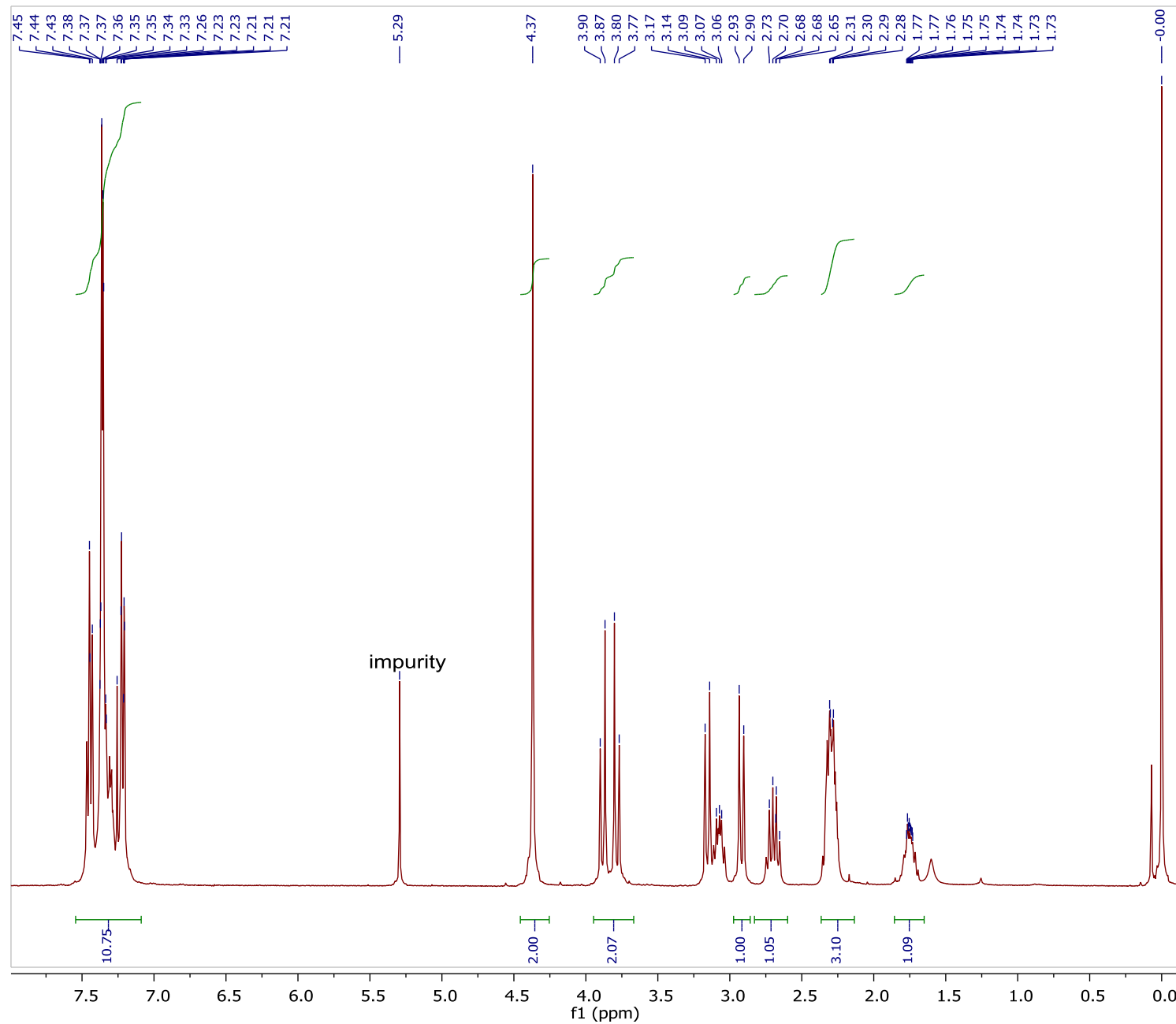
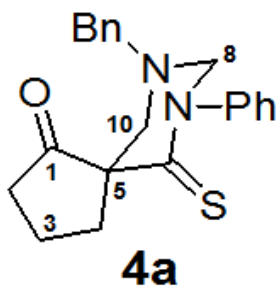
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Spectral Size	65536



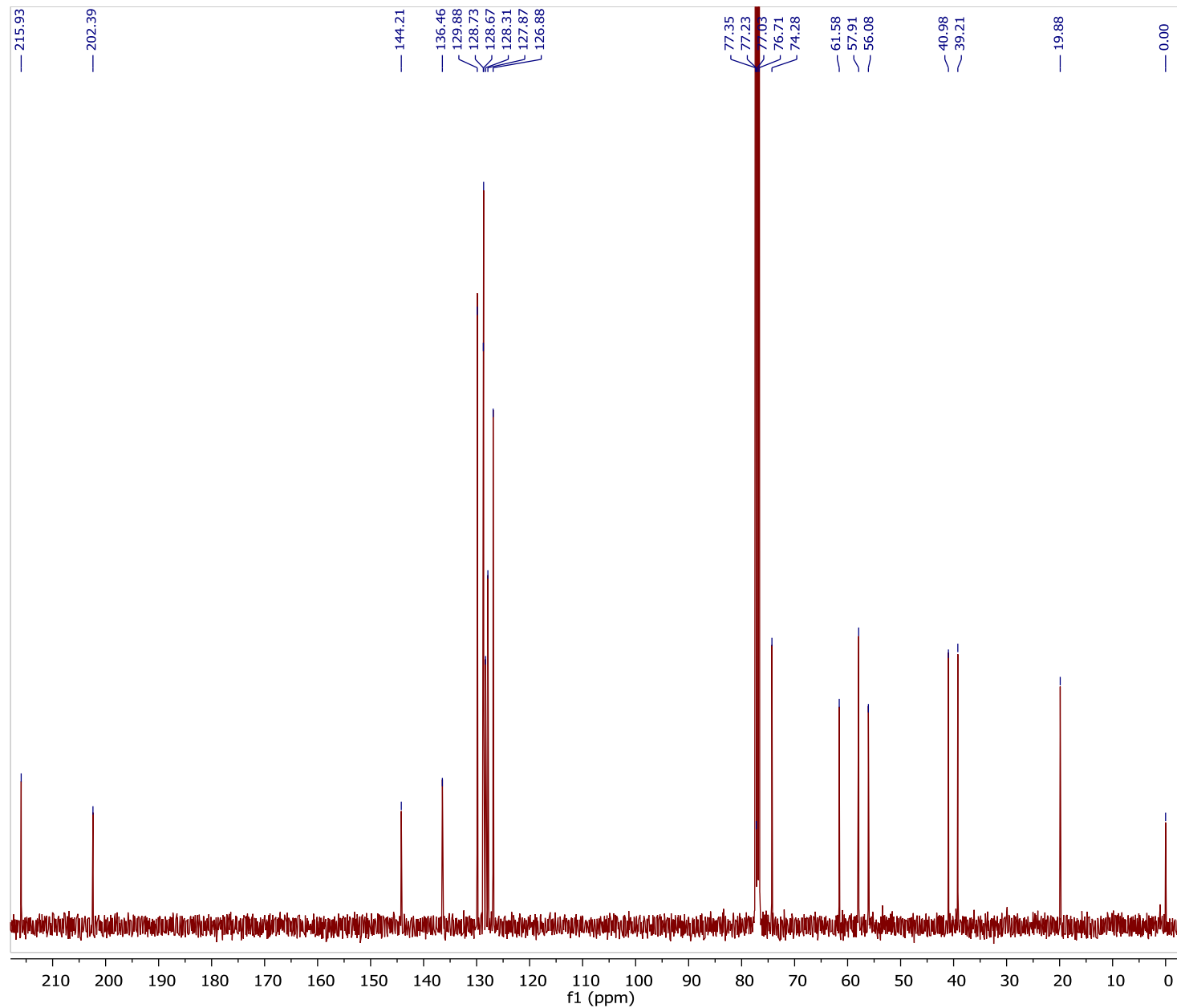
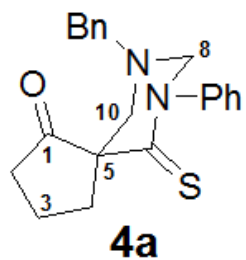
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Spectral Size	32768



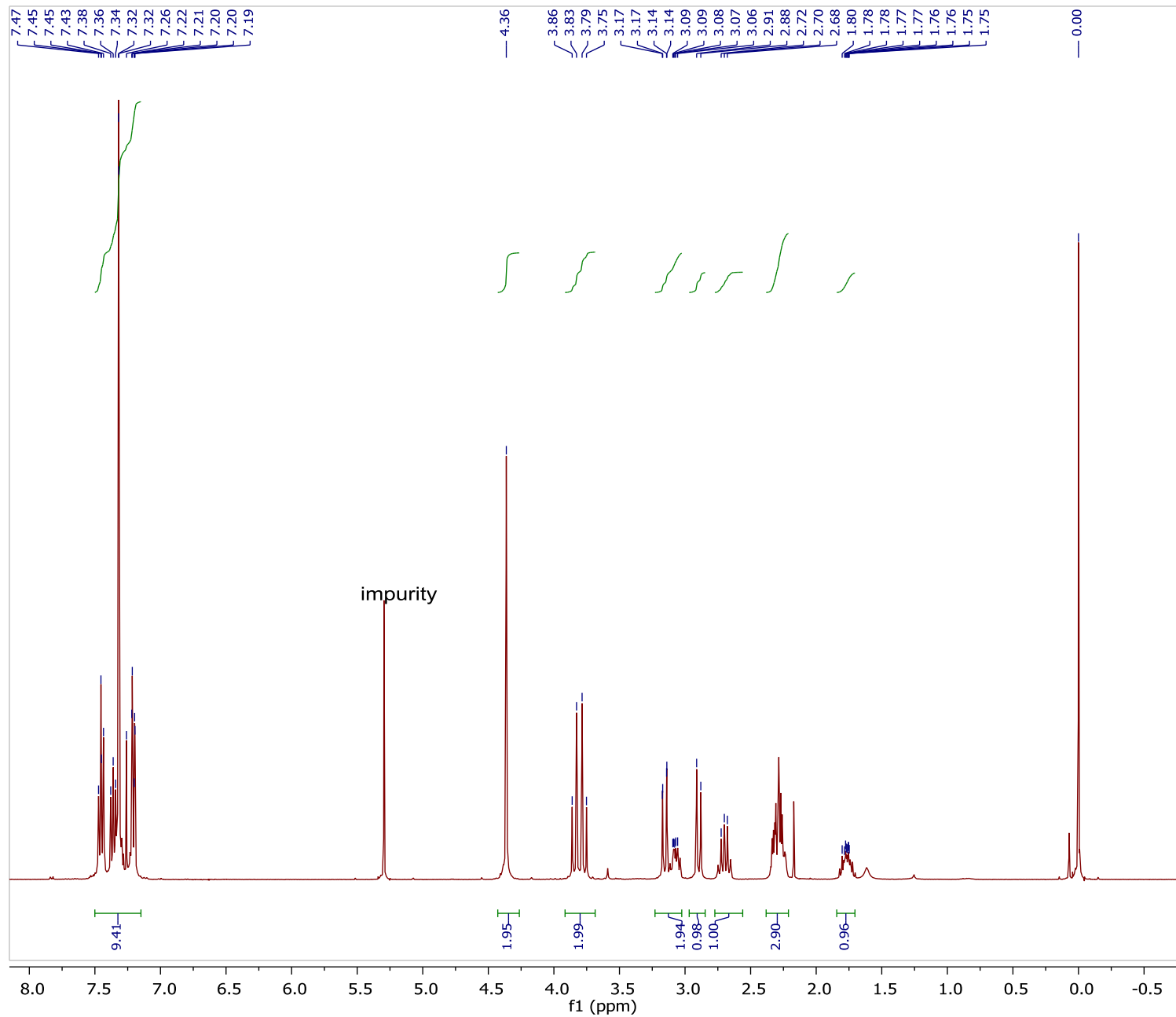
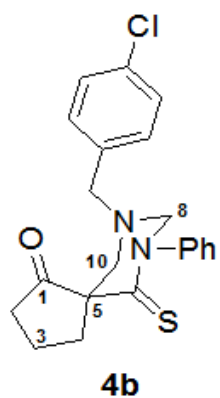
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Spectral Size	65536



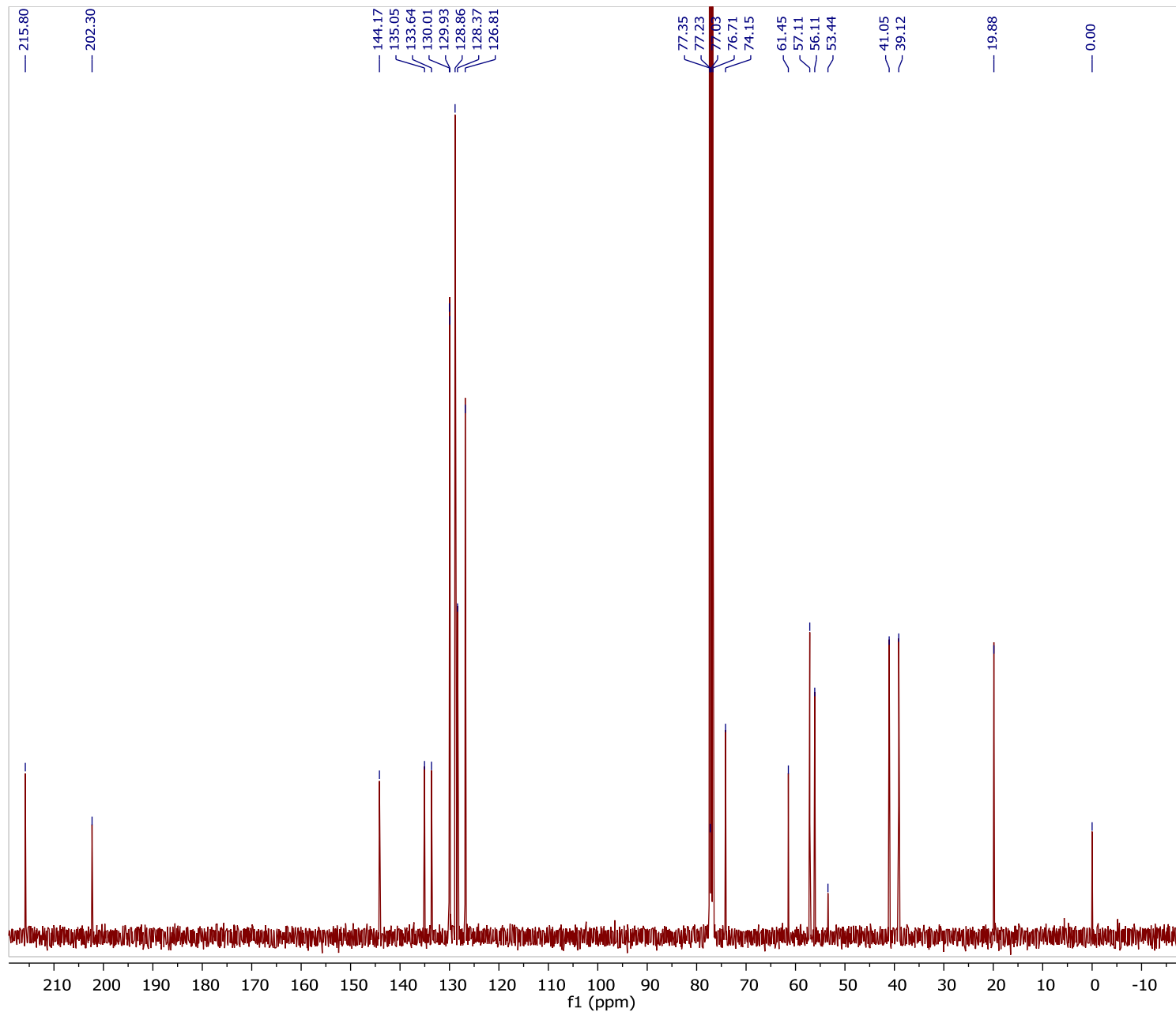
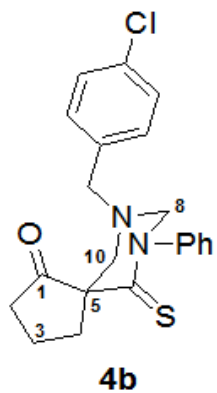
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Spectral Size	16384



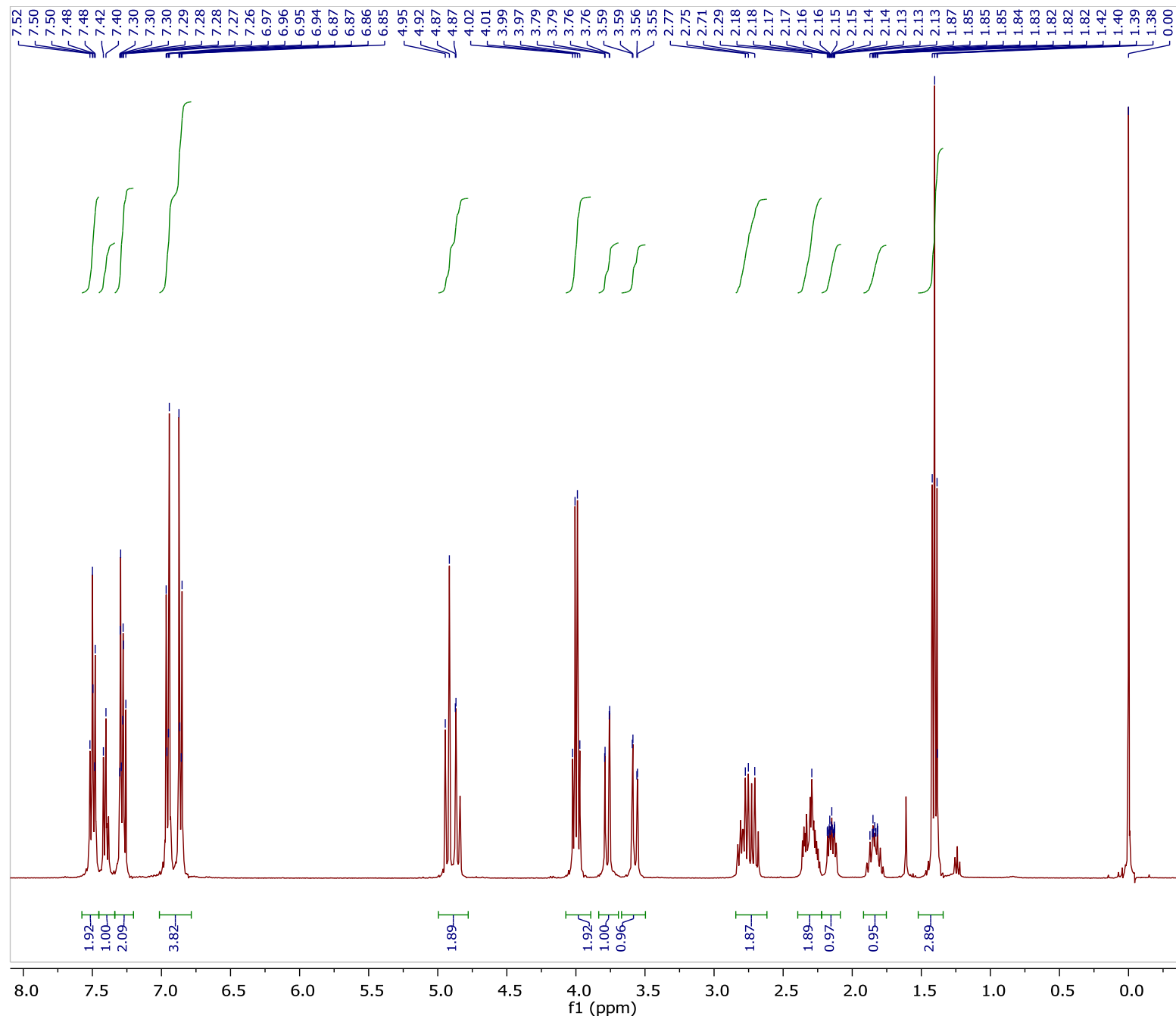
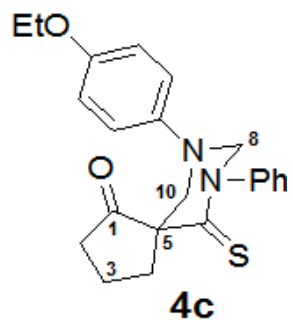
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Spectral Size	65536



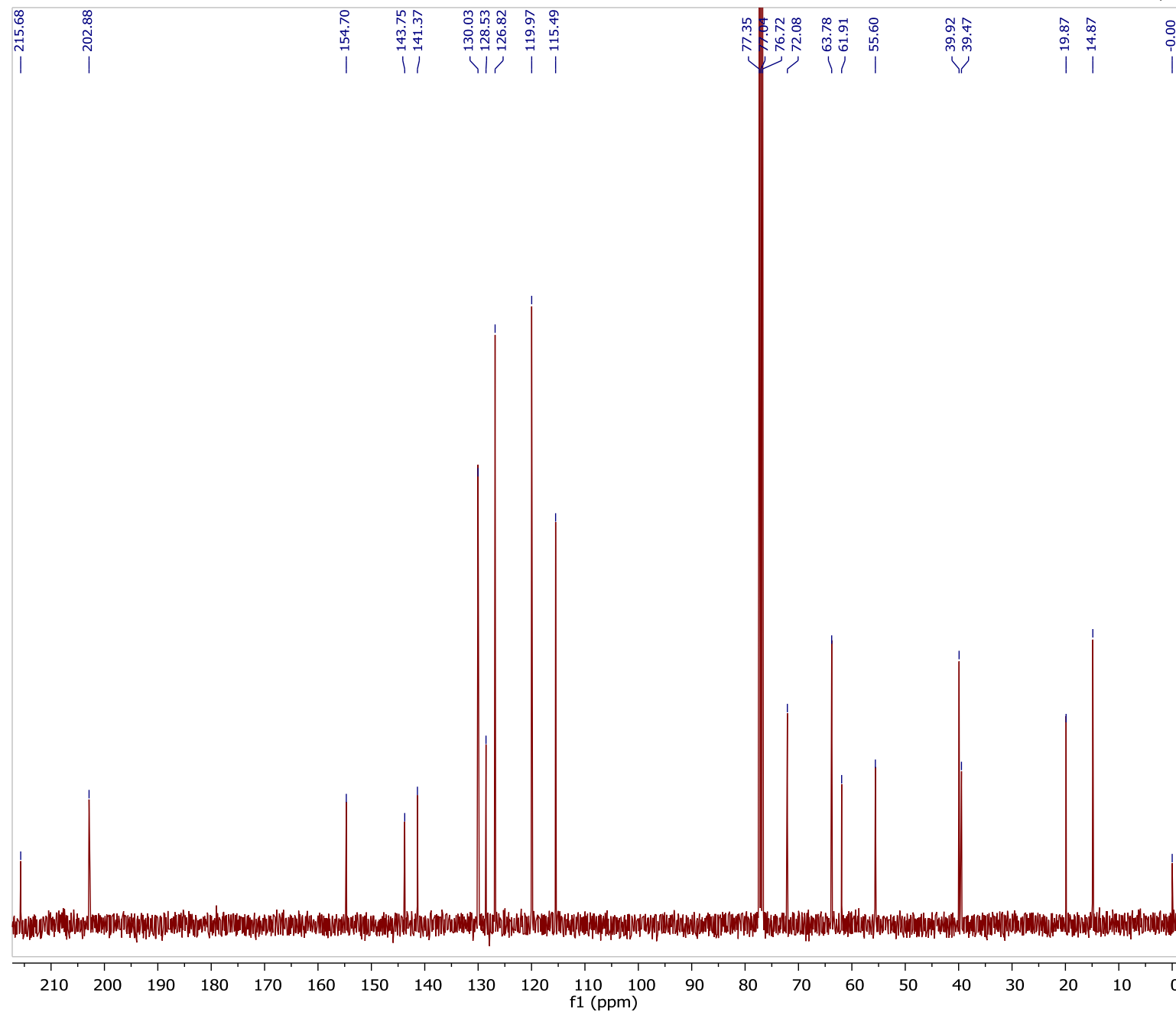
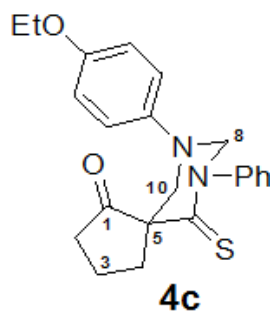
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Spectral Size	16384



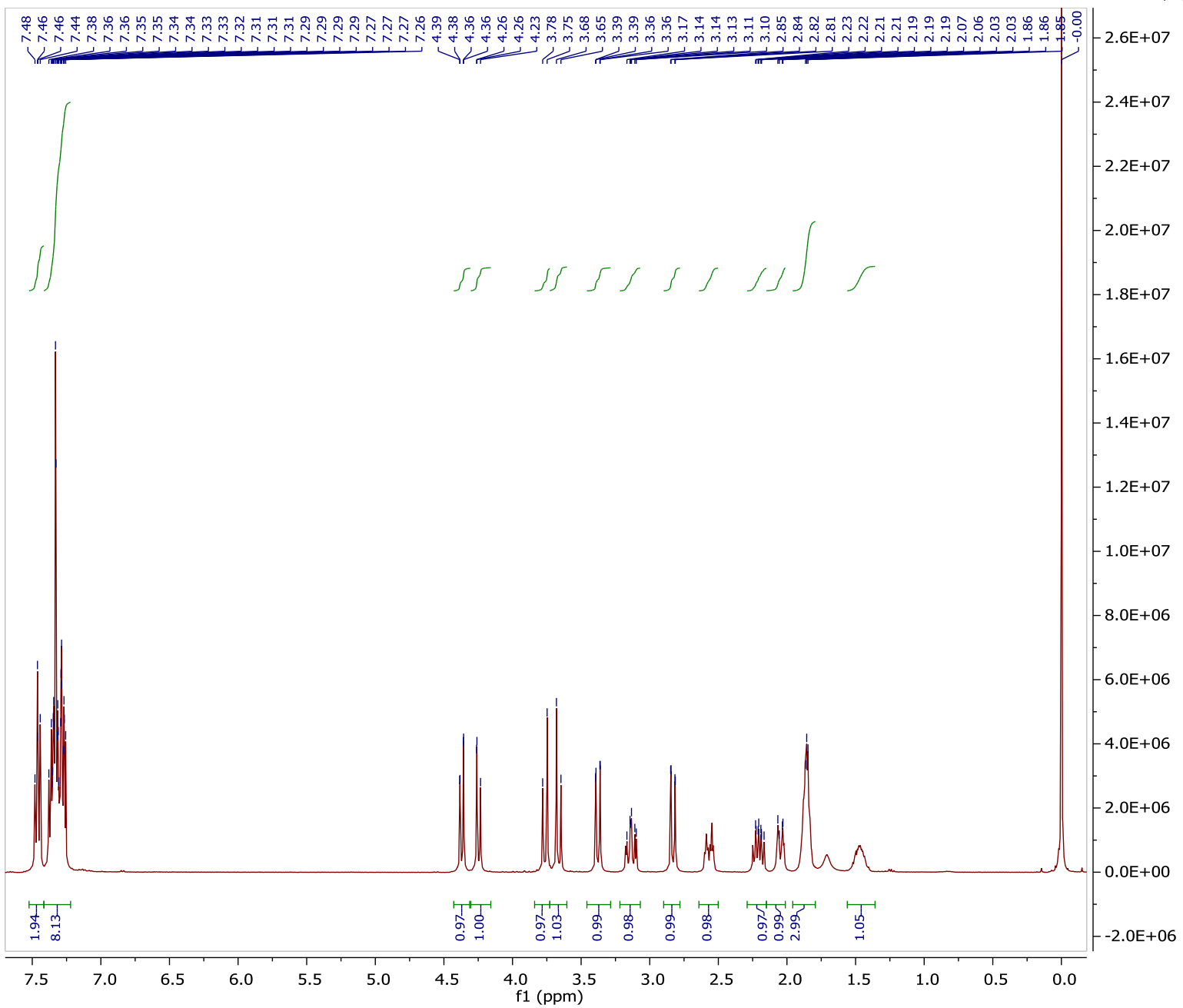
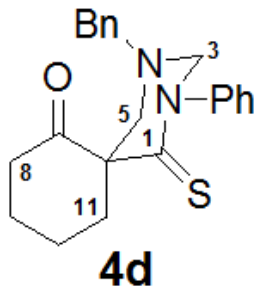
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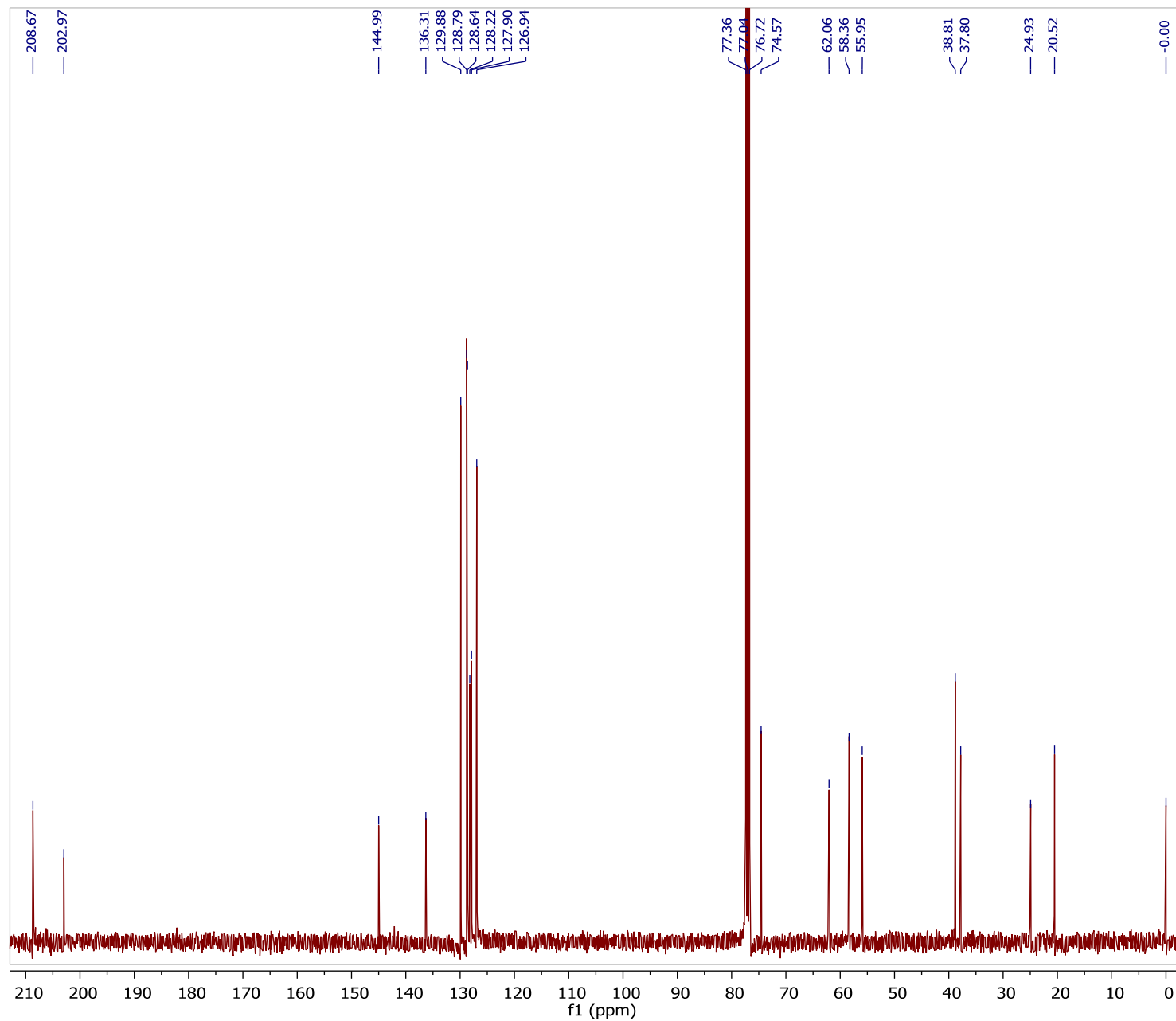
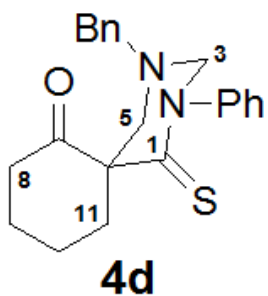
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Spectral Size	16384



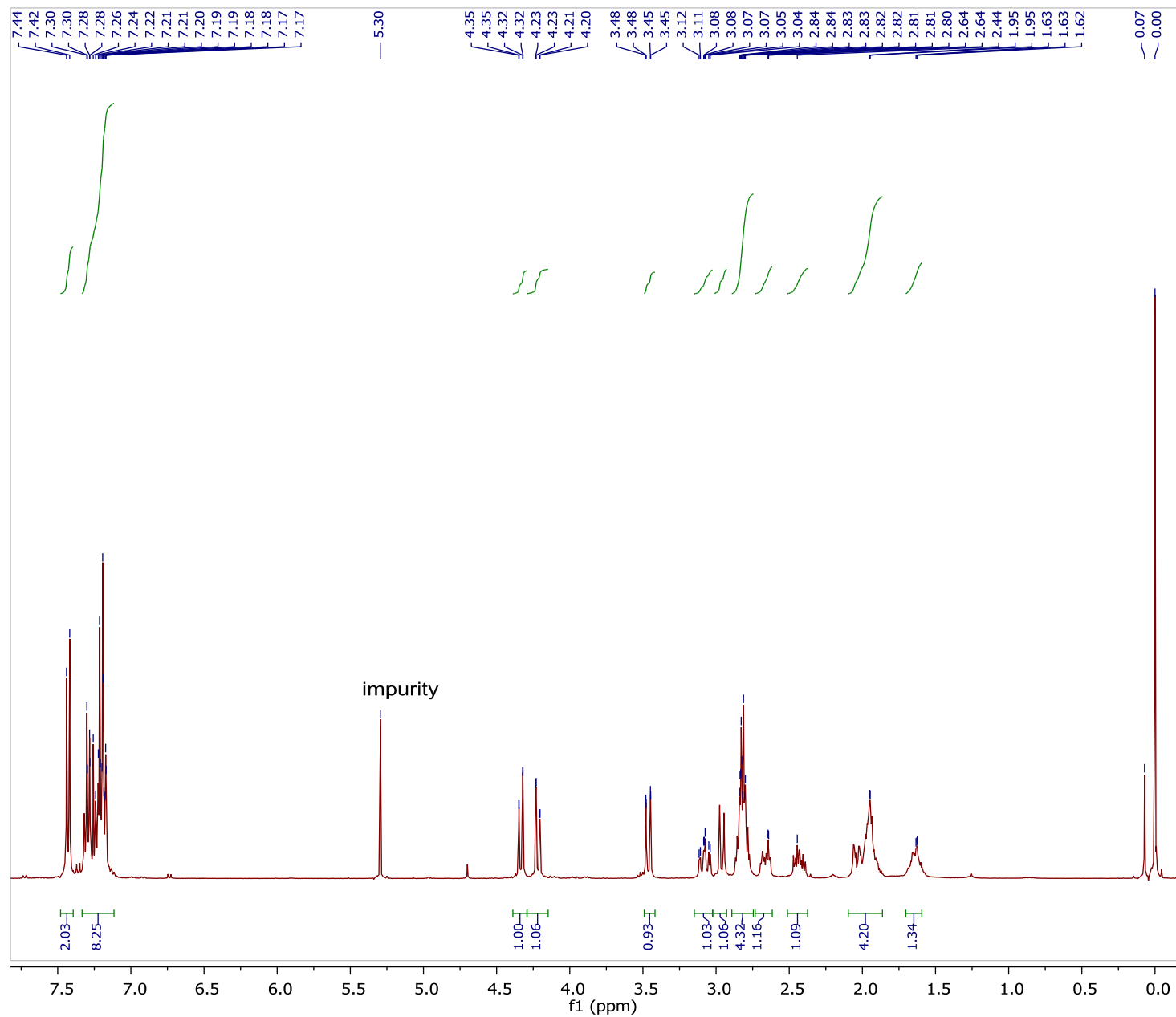
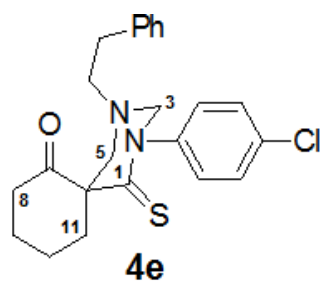
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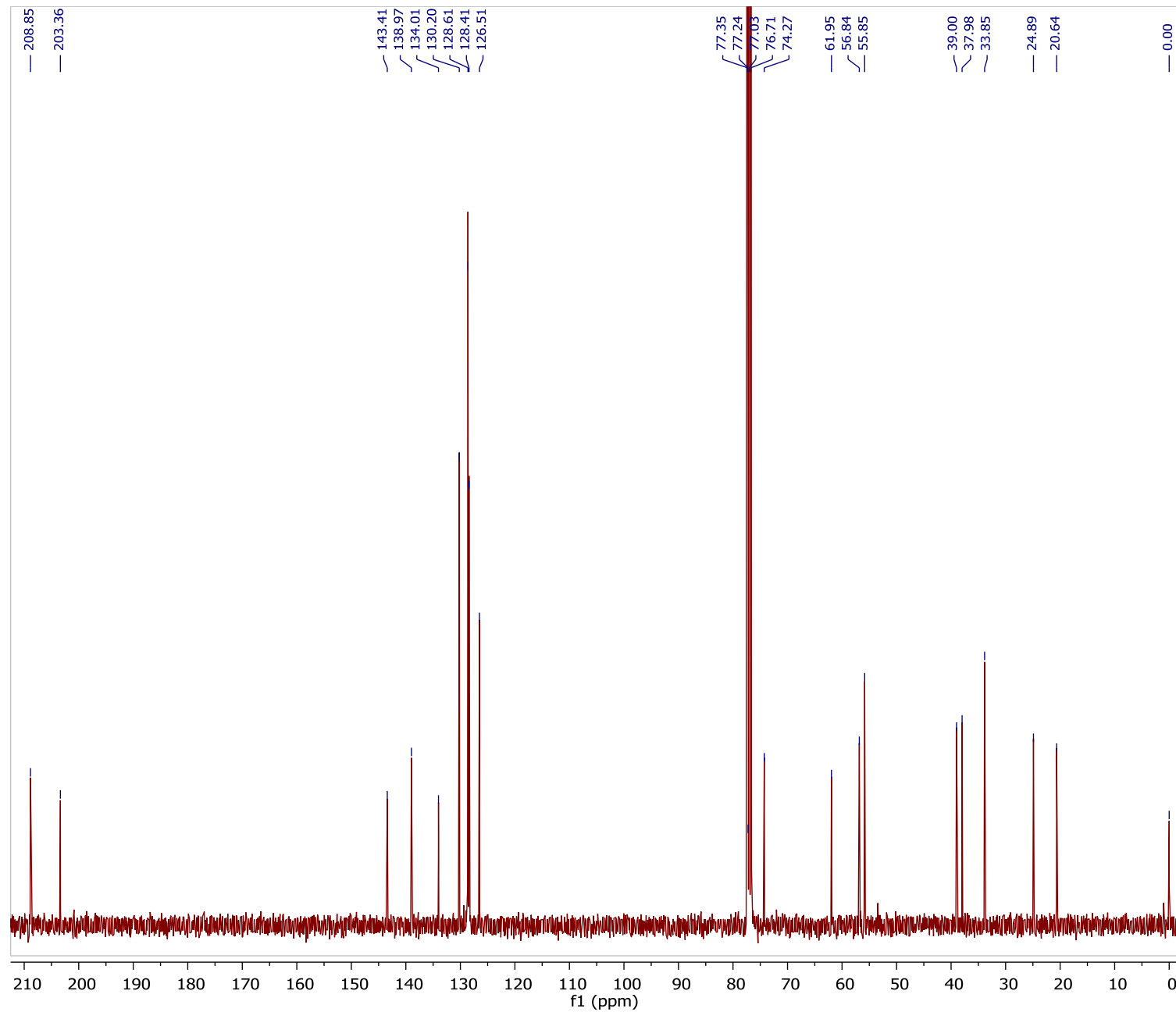
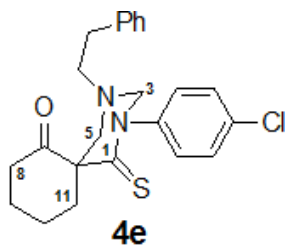
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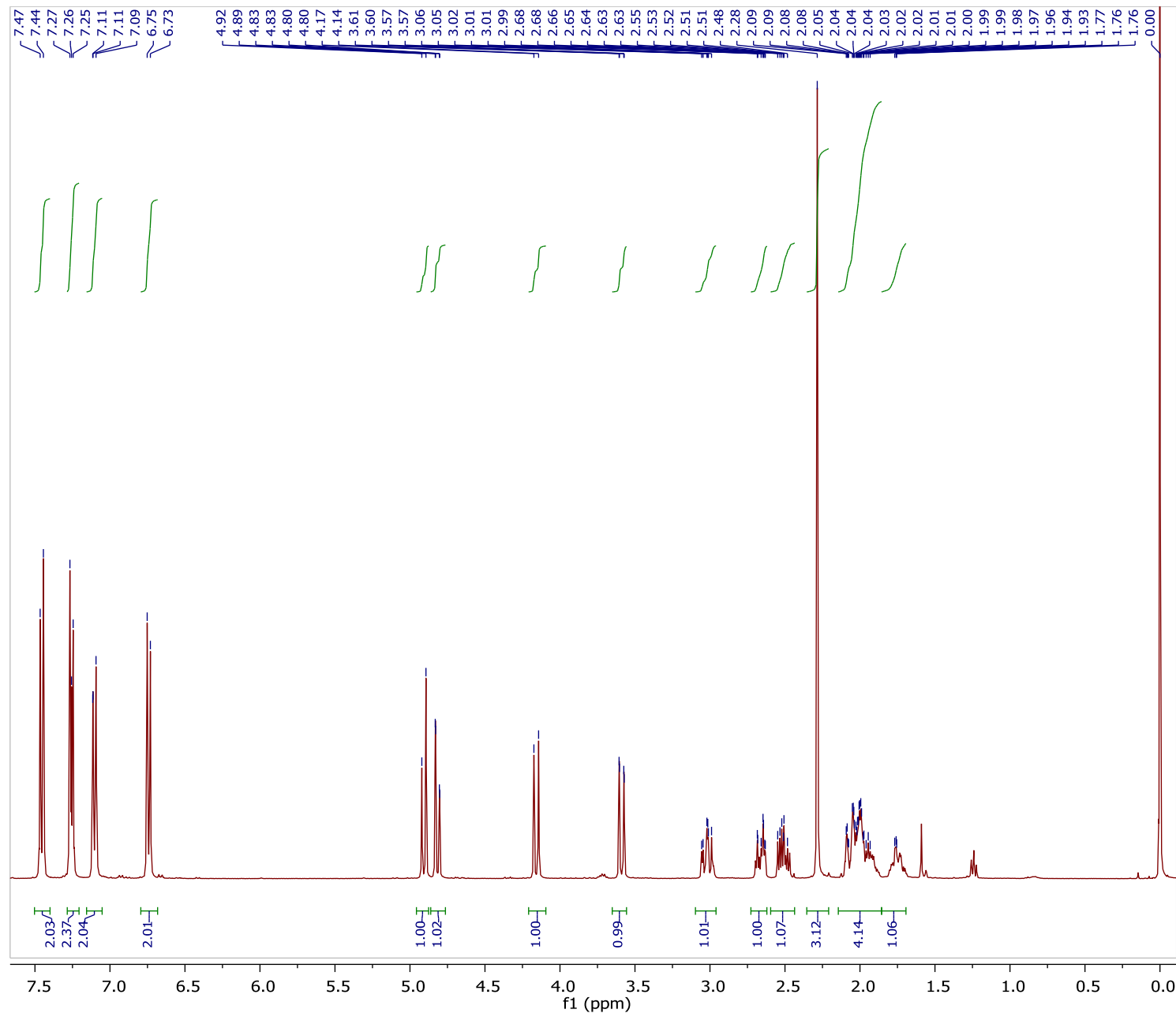
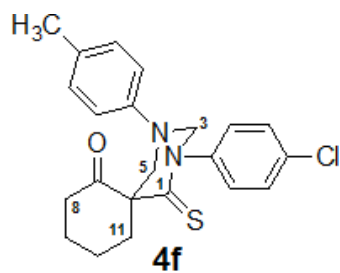
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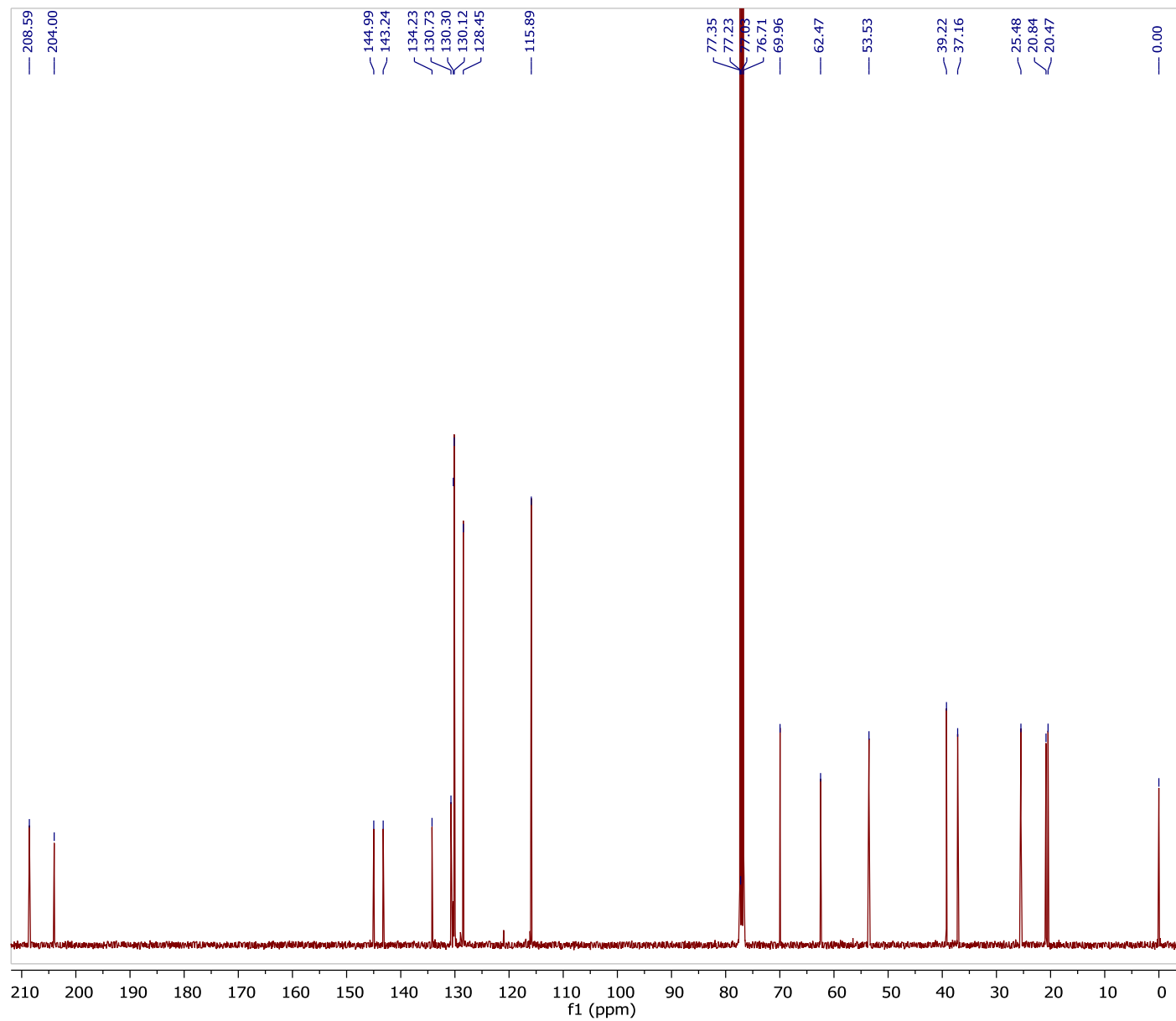
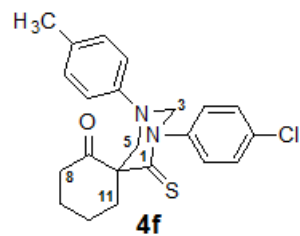
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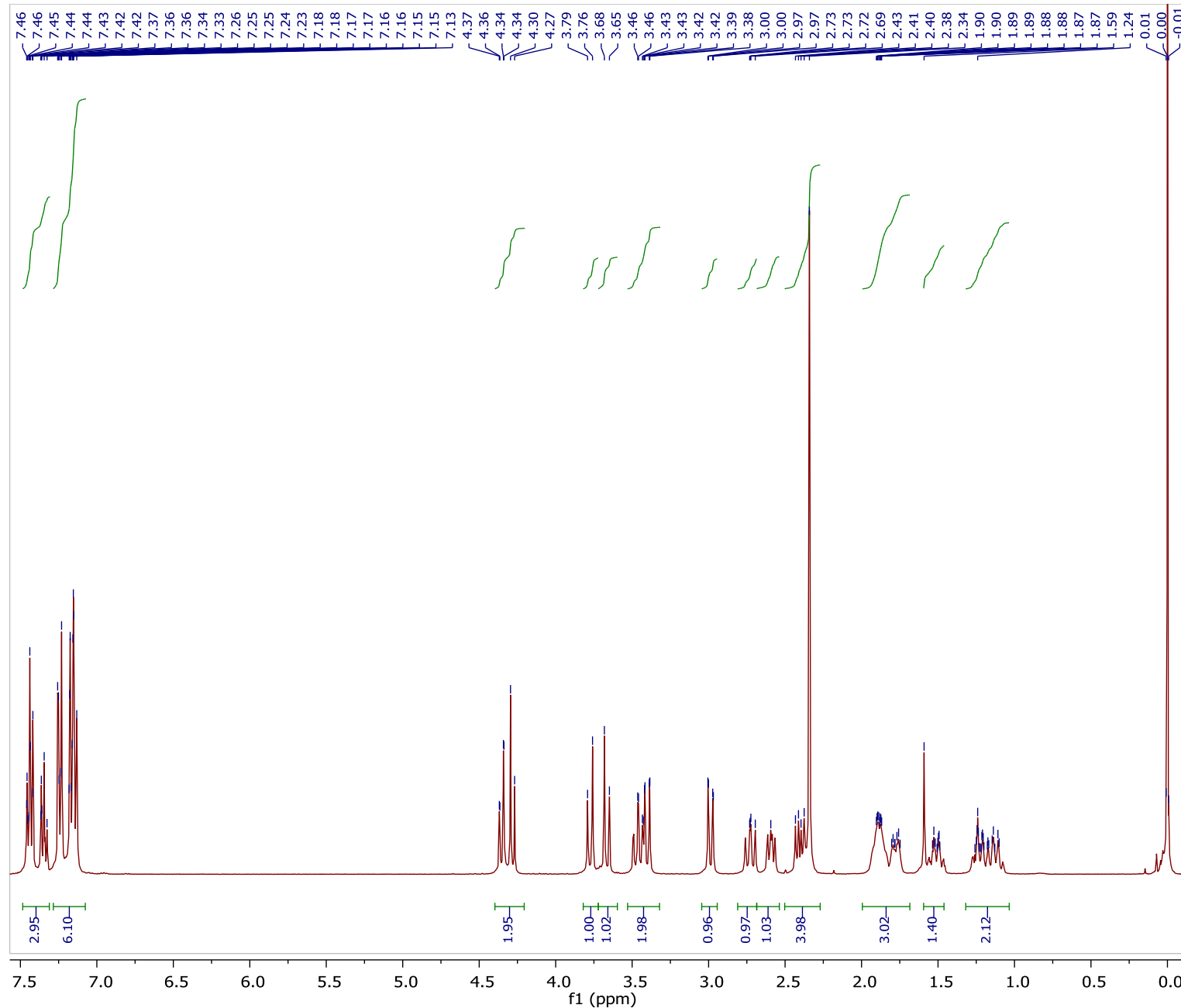
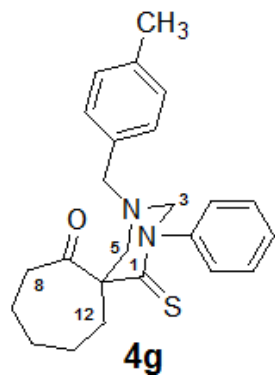
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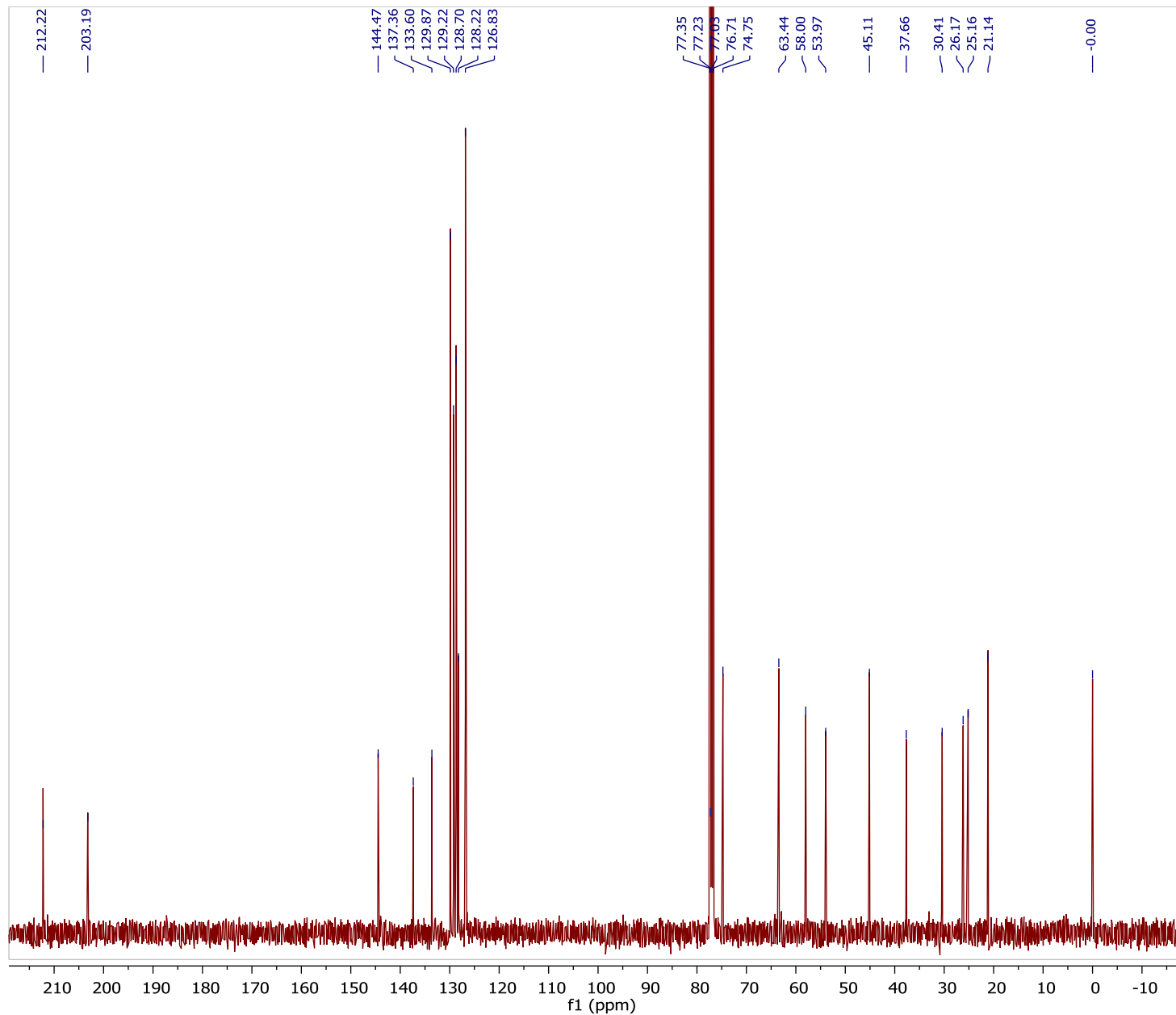
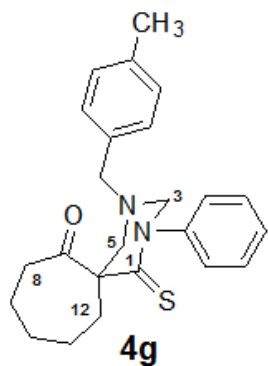
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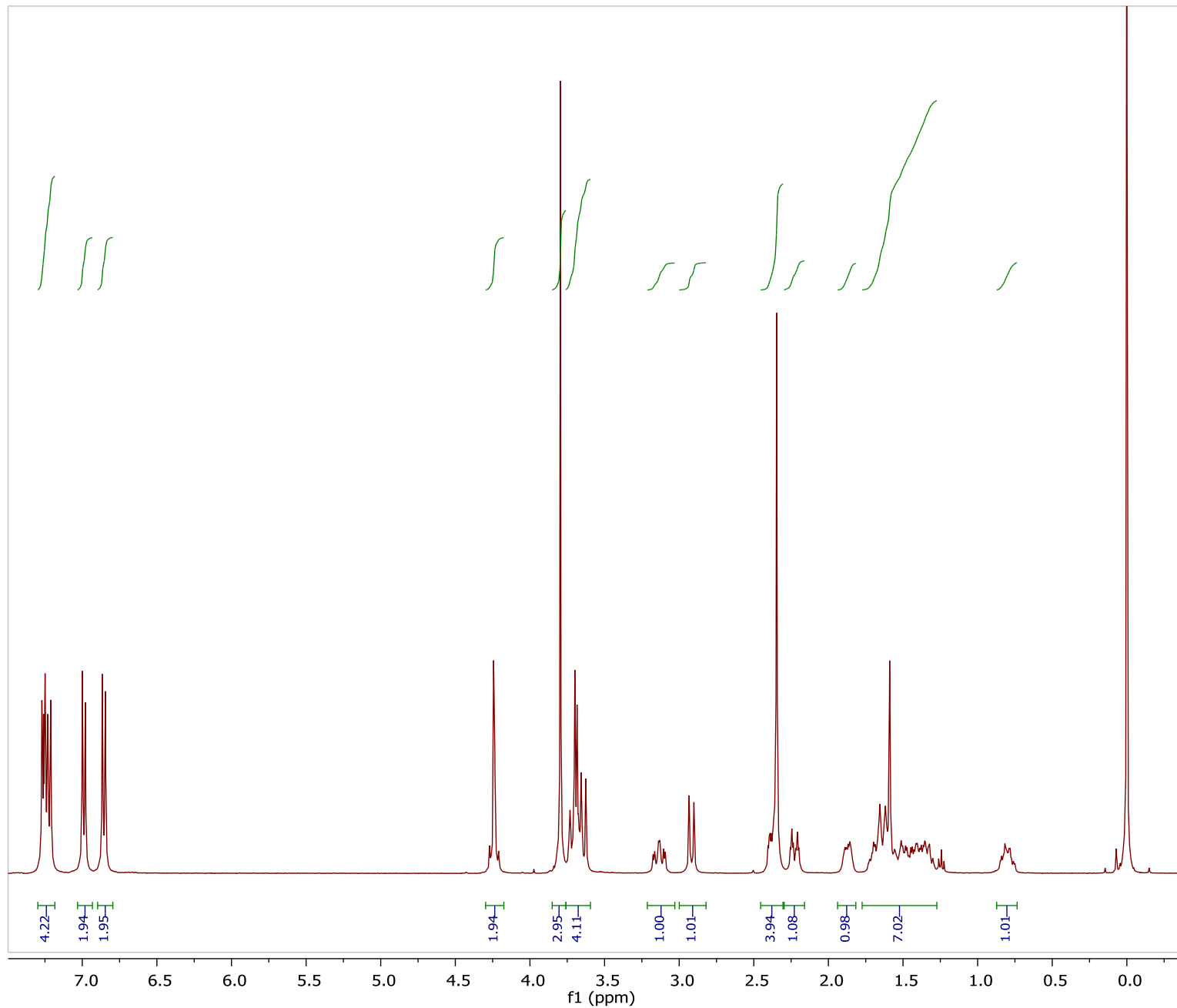
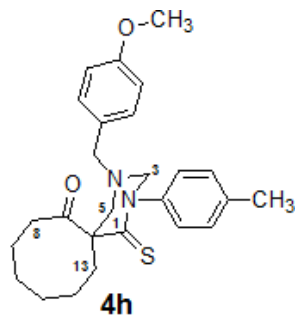
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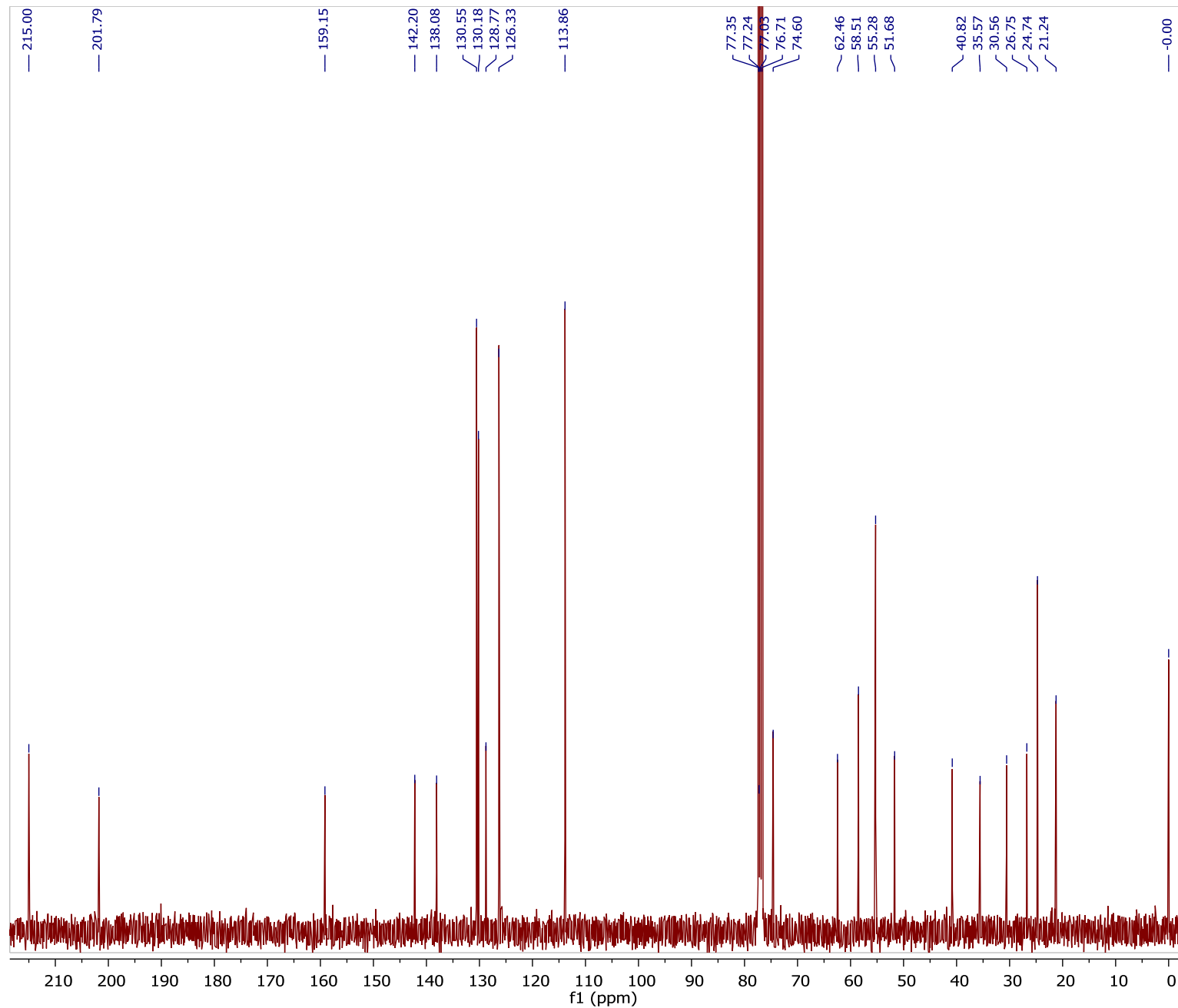
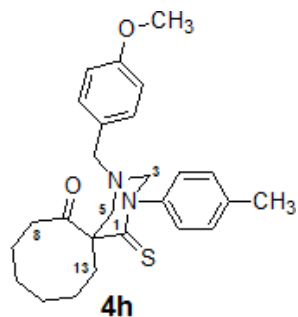
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Nucleus	¹³ C
Acquired Size	16384
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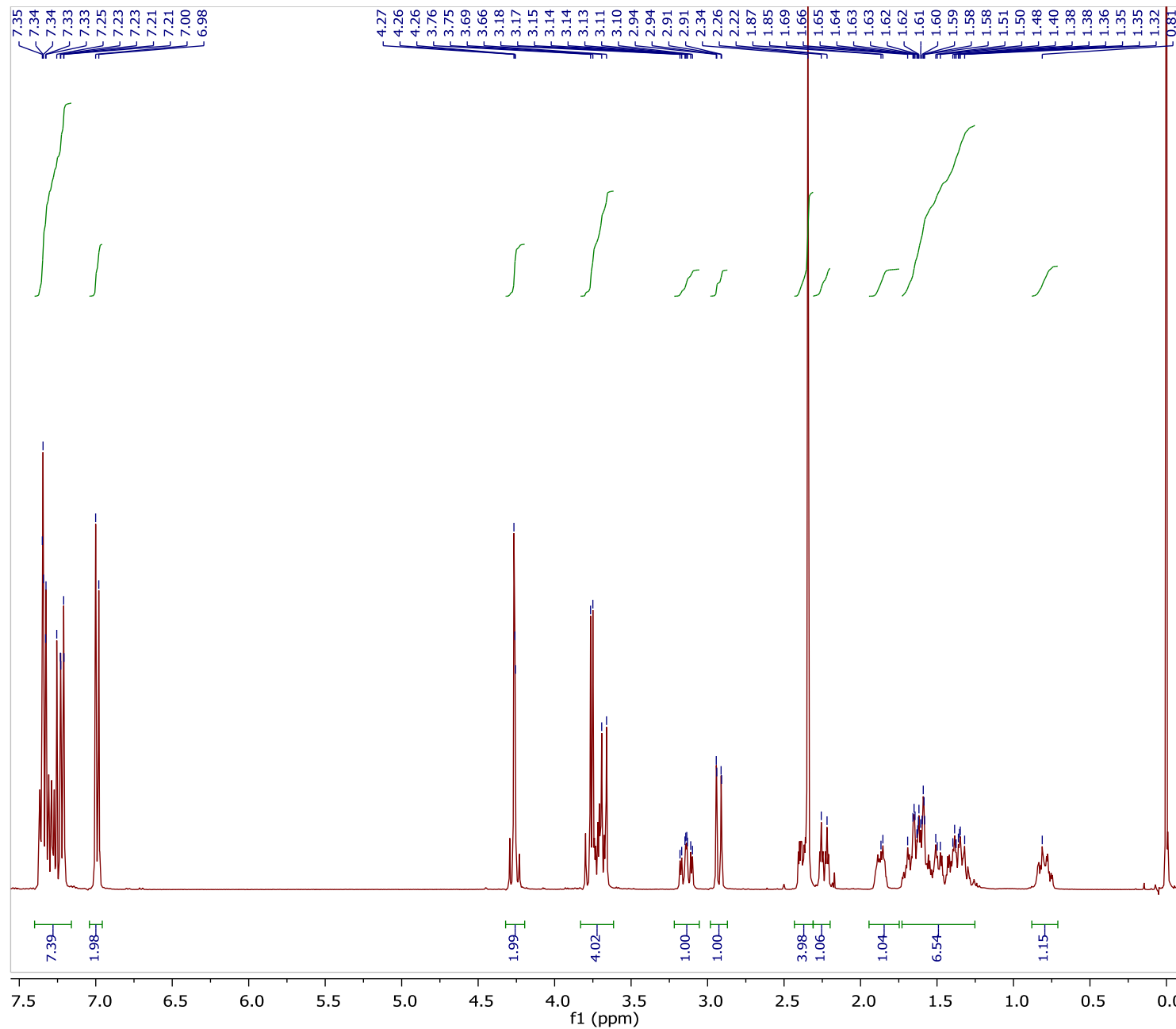
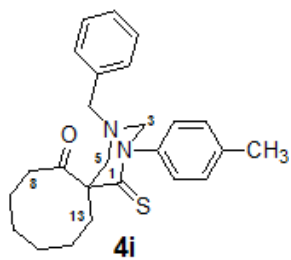
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Spectral Width	8003.2
Nucleus	¹ H
Acquired Size	32768
Spectral Size	32768



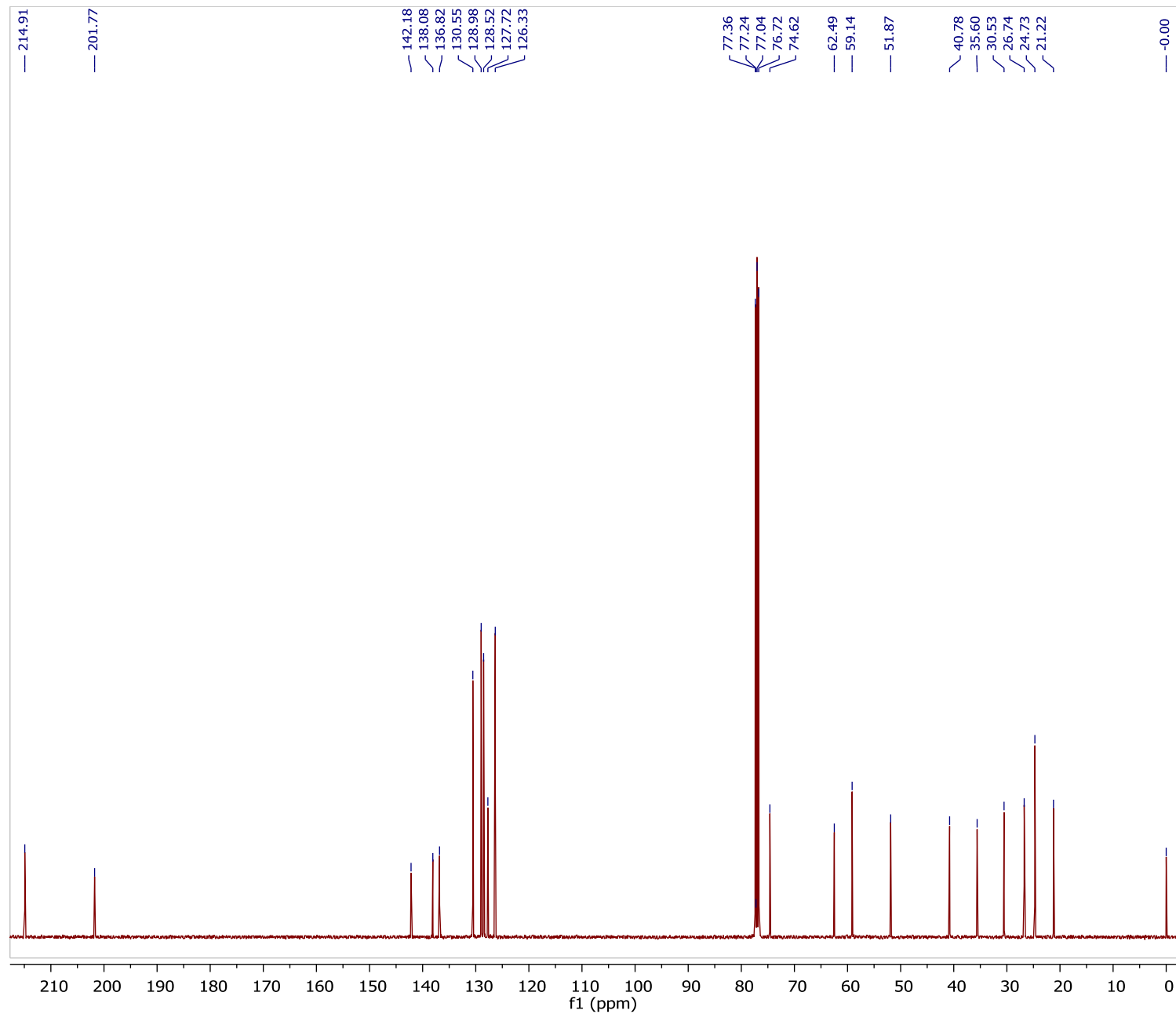
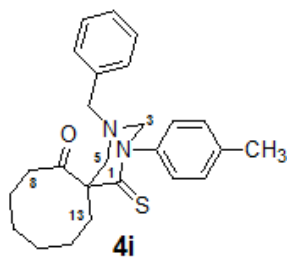
Parameter	Value
Solvent	CDCl ₃
Pulse Sequence	zgpg30
Number of Scans	5120
Receiver Gain	13004.0
Relaxation Delay	1.0000
Pulse Width	9.2000
Acquisition Time	0.6833
Spectrometer Frequency	100.61
Spectral Width	23980.8
Nucleus	¹³ C
Acquired Size	16384
Spectral Size	16384



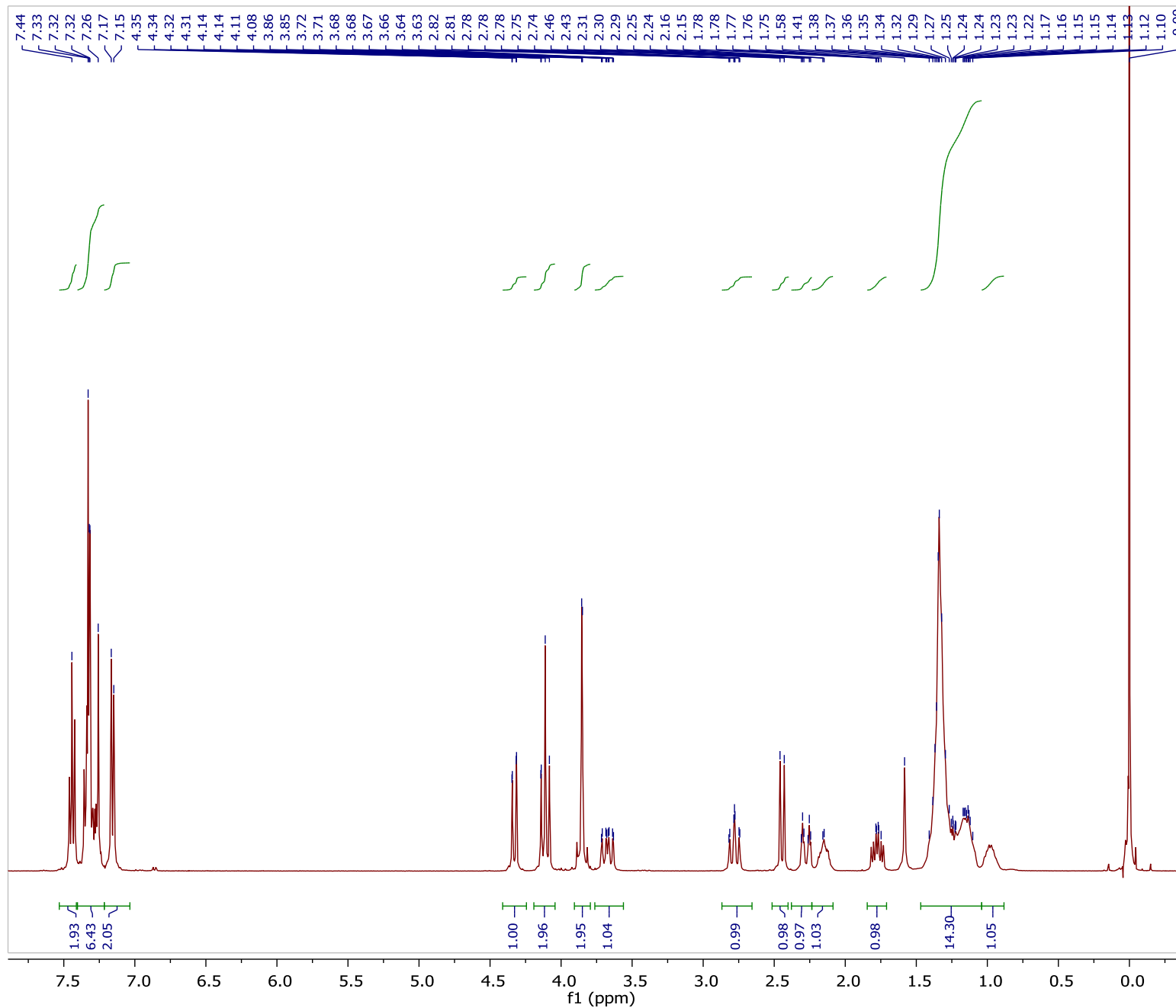
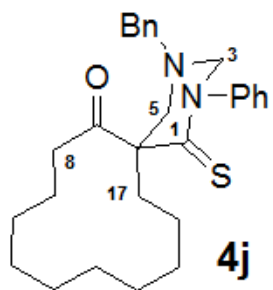
Parameter	Value
Solvent	CDCl ₃
Pulse Sequence	zg30
Number of Scans	16
Receiver Gain	77.8
Relaxation Delay	1.0000
Pulse Width	14.0000
Acquisition Time	8.1789
Spectrometer Frequency	400.20
Spectral Width	8012.8
Nucleus	¹ H
Acquired Size	65536
Spectral Size	131072



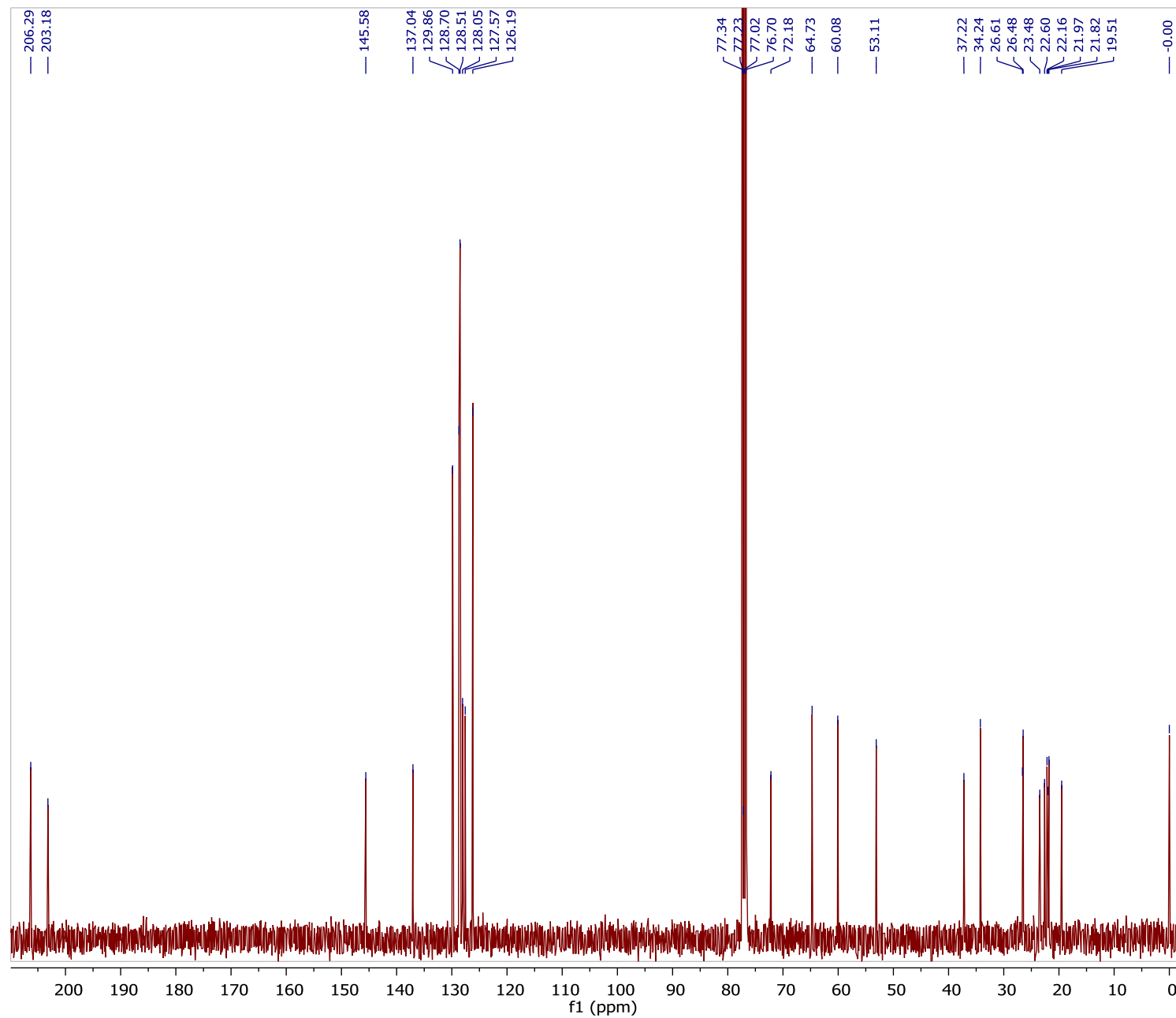
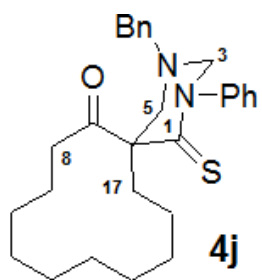
Parameter	Value
Solvent	CDCl ₃
Pulse Sequence	zgpg30
Number of Scans	2048
Receiver Gain	194.7
Relaxation Delay	2.0000
Pulse Width	10.0000
Acquisition Time	1.3631
Spectrometer Frequency	100.63
Spectral Width	24038.5
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	32768



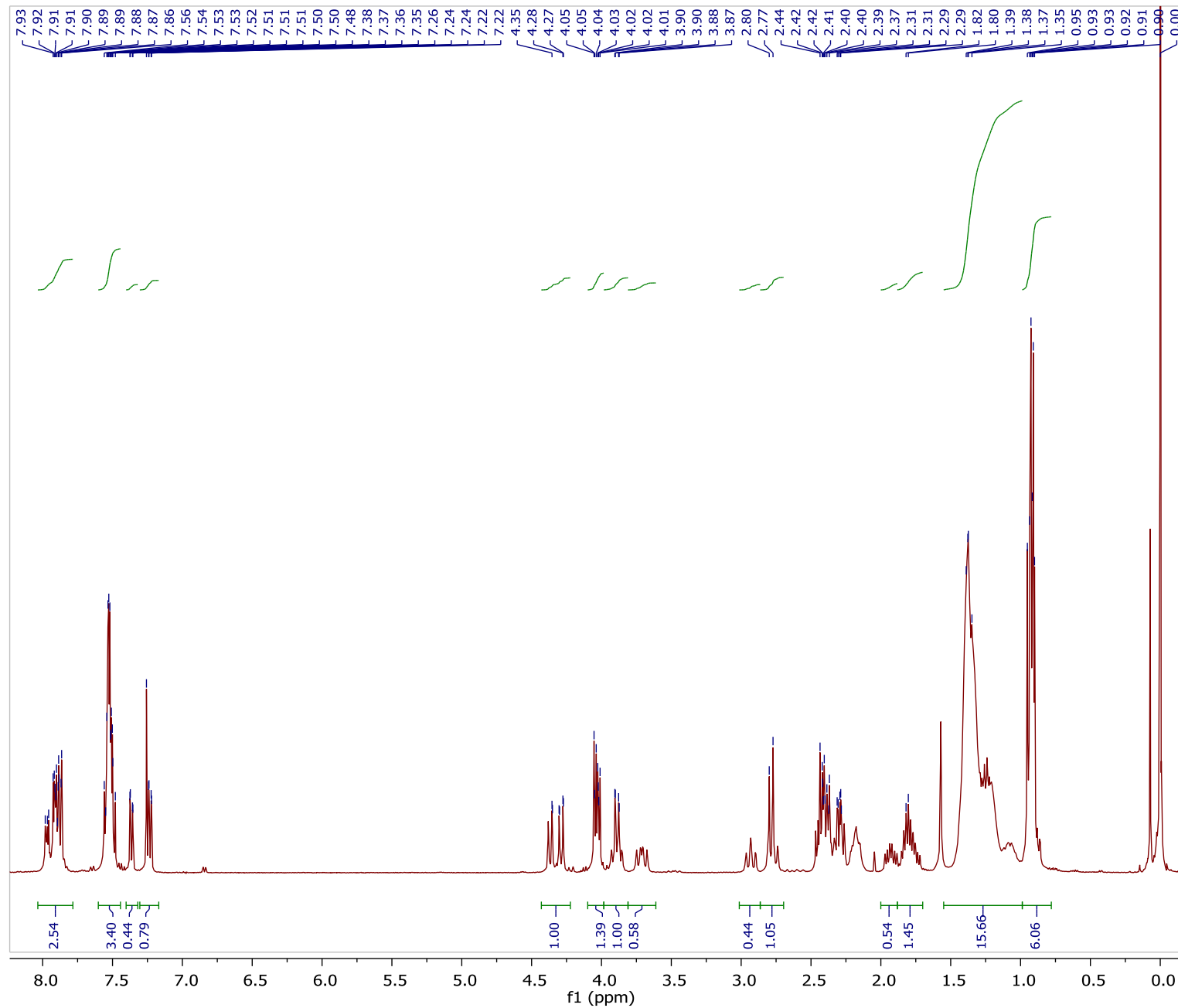
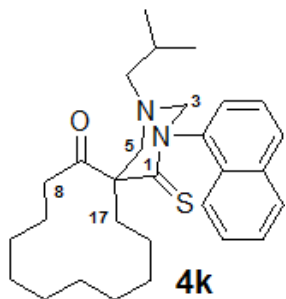
Parameter	Value
Solvent	CDCl3
Pulse Sequence	zg30
Number of Scans	32
Receiver Gain	256.0
Relaxation Delay	1.0000
Pulse Width	7.8000
Acquisition Time	8.1888
Spectrometer Frequency	400.13
Spectral Width	8003.2
Nucleus	1H
Acquired Size	65536
Spectral Size	32768



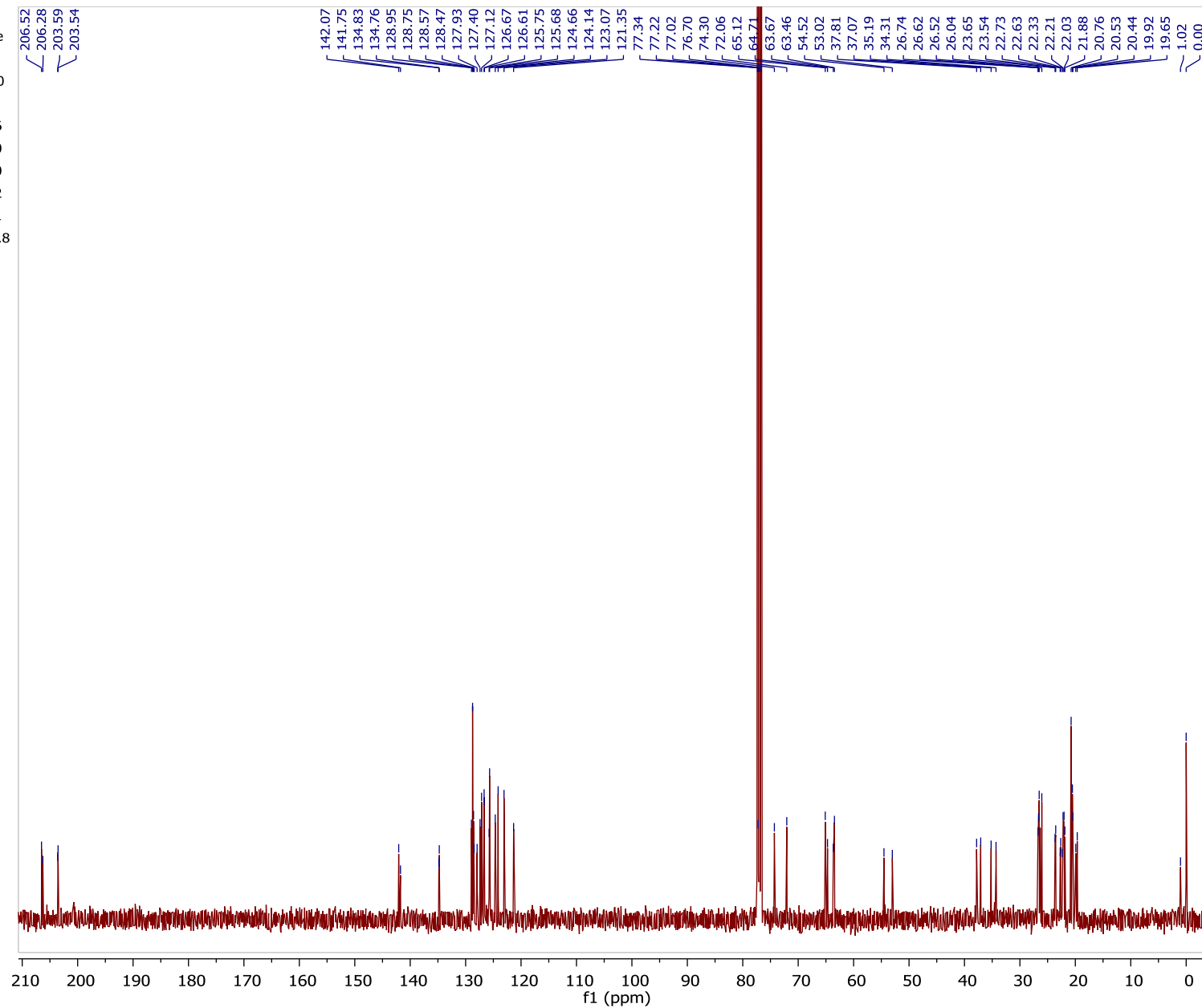
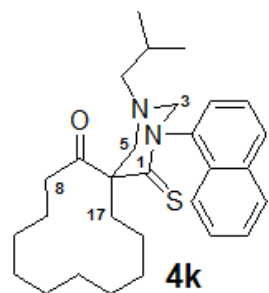
Parameter	Value
Solvent	CDCl ₃
Pulse Sequence	zgpg30
Number of Scans	4096
Receiver Gain	13004.0
Relaxation Delay	1.0000
Pulse Width	9.2000
Acquisition Time	0.6833
Spectrometer Frequency	100.61
Spectral Width	23980.8
Nucleus	¹³ C
Acquired Size	16384
Spectral Size	16384



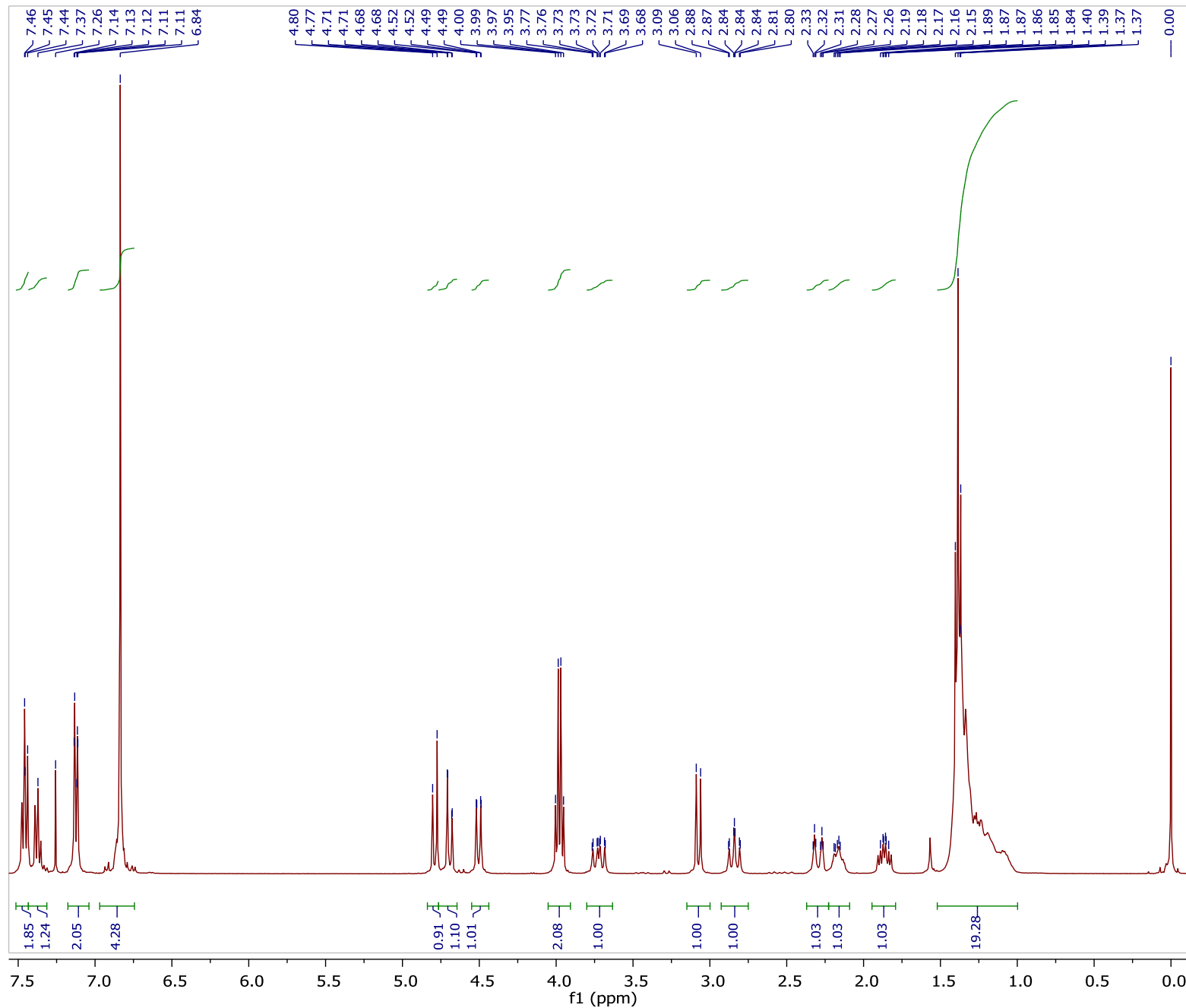
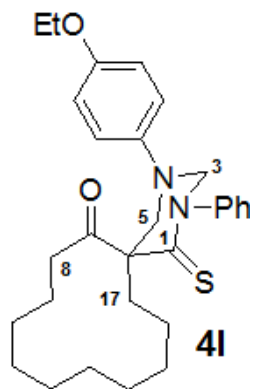
Parameter	Value
Solvent	CDCl ₃
Pulse Sequence	zg30
Number of Scans	16
Receiver Gain	181.0
Relaxation Delay	1.0000
Pulse Width	7.8000
Acquisition Time	4.0944
Spectrometer Frequency	400.13
Spectral Width	8003.2
Nucleus	¹ H
Acquired Size	32768
Spectral Size	32768



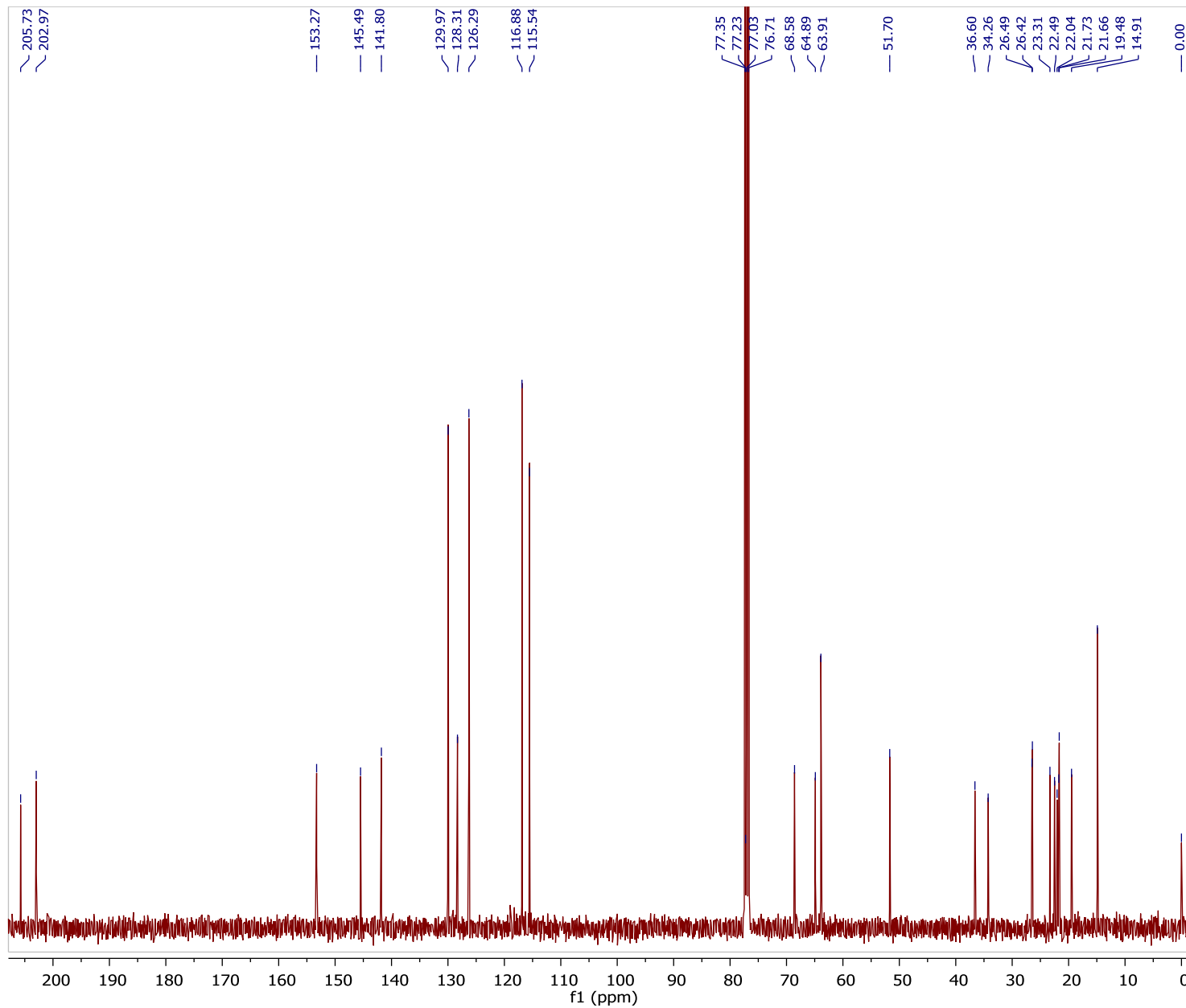
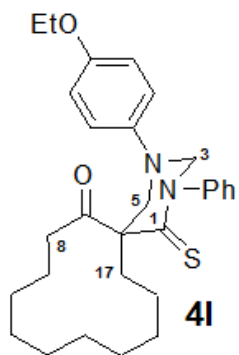
Parameter	Value
Solvent	CDCl ₃
Pulse Sequence	zgpg30
Number of Scans	5120
Receiver Gain	5792.6
Relaxation Delay	1.0000
Pulse Width	9.2000
Acquisition Time	0.6832
Spectrometer Frequency	100.61
Spectral Width	23980.8
Nucleus	¹³ C
Acquired Size	16384
Spectral Size	16384



Parameter	Value
Solvent	CDCl3
Pulse Sequence	zg30
Number of Scans	16
Receiver Gain	128.0
Relaxation Delay	1.0000
Pulse Width	7.8000
Acquisition Time	8.1888
Spectrometer Frequency	400.13
Spectral Width	8003.2
Nucleus	1H
Acquired Size	65536
Spectral Size	65536



Parameter	Value
Solvent	CDCl ₃
Pulse Sequence	zgpg30
Number of Scans	4096
Receiver Gain	10321.3
Relaxation Delay	1.0000
Pulse Width	9.2000
Acquisition Time	0.6833
Spectrometer Frequency	100.61
Spectral Width	23980.8
Nucleus	¹³ C
Acquired Size	16384
Spectral Size	16384



EURO EA

Elemental Analyzer



Method Filename : D:\Program Files\Callidus 2E3\Method\CHNS211.mth

Summarize Result : Percent

Configuration: C H N S

Date: 29/10/2015

Sample Name	N %	C %	H %	S %	Weight
blk	0	0	0	0	0
blk	0	0	0	0	0
blk	0	0	0	0	0
bps	0	0	0	0	1.921
BBOT	6.51	72.53	6.09	7.44	1.731
BBOT	6.476	72.546	6.142	7.454	1.556
BBOT	6.567	72.447	6.107	7.417	1.452
bbot	6.458	72.586	6.365	7.515	1.745

General Paper

				<i>Arkivoc 2017, v, S1-S45</i>	
21_15 2d	5.026	69.335	7.797	11.75	1.681
21_15 2d	4.973	69.667	8.009	11.834	1.641
22_15 2c	5.488	67.41	7.287	13.273	1.662
22_15 2c	5.549	67.913	7.076	12.843	1.626
26_15 3b	10.991	56.618	7.456	25.328	1.58
26_15 3b	10.756	56.773	7.648	25.803	1.766
16a_15 3a	12.001	53.37	6.073	28.16	1.761
16a_15 3a	12.205	53.041	6.684	28.669	1.891
16_15 4c	6.069	66.249	6.873	13.432	1.413
16_15 4c	5.883	66.386	6.748	13.931	1.739
27_15 2b	5.21	58.52	5.421	12.02	1.543
27_15 2b	5.35	58.401	5.55	12.32	1.459

EURO EA

Elemental Analyzer



Method Filename : D:\Program Files\Callidus 2E3\Method\CHNS212.mth

Summarize Result : Percent

Configuration: C H N S

Date: 18/12/2015

blk 1	0	0	0	0	0
blk 2	0	0.01	0	0	0
blk 3	0	0.029	0	0	0
bps	6.696	74.588	3.887	5.955	1.105
BBOT	6.515	72.644	5.88	7.462	1.847
BBOT	6.506	72.417	6.316	7.418	1.741
bbot	6.528	72.27	6.853	7.493	1.765
30_15 2f	3.756	74.995	8.097	8.586	1.362
30_15 2f	3.72	75.388	7.743	8.674	1.365

General Paper

				<i>Arkivoc 2017, v, S1-S45</i>	
30_15 hept 2f	3.769	75.314	8.136	8.793	1.395
30_15 hept 2f	3.861	75.521	8.317	8.523	1.48
63_15 4g	7.109	73.548	7.457	8.219	1.906
63_15 4g	7.157	73.17	7.697	8.401	1.852
50_15 4j	5.965	74.415	8.785	7.299	1.825
50_15 4j	6.294	74.756	8.477	6.913	1.652
28_15 2e	4.383	72.074	9.072	10.176	1.704
28_15 2e	4.338	71.771	8.803	10.206	1.896
57_15 4h	6.436	0	7.519	7.553	1.975
57_15 4h	6.421	71.819	7.716	7.303	1.762
21_15 2d	5.02	69.304	7.893	11.51	1.419
21_15 2d	5.00	69.555	8.044	12.052	1.645
23_15 4d	7.581	72.296	7.001	8.954	1.576
23_15 4d	7.627	73.201	6.98	9.084	1.452

EURO EA

Elemental Analyzer



Method Filename : D:\Program Files\Callidus 2E3\Method\CHNS213.mth

Summarize Result : Percent

Configuration: C H N S

Date: 29/01/2016

blk 1	0	0	0	0	0
blk 2	0	0.002	0	0	0
blk 3	0	0.028	0	0	0
bps	6.449	72.422	3.435	6.358	1.521
BBOT	6.488	72.205	5.632	7.369	1.68
BBOT	6.52	72.485	6.209	7.387	1.797
BBOT	6.522	72.903	6.494	7.568	1.805
bbot	6.453	72.279	6.511	7.31	1.834

General Paper

				<i>Arkivoc 2017, v, S1-S45</i>	
TJ1_16 4c	7.445	69.352	6.354	8.479	1.731
TJ1_16 4c	7.279	69.128	6.716	8.296	1.621
TJ62_15 4k	6.14	74.793	9.08	7.44	1.752
TJ62_15 4k	6.553	74.355	8.74	7.25	1.516
TJ60_15 4l	5.76	72.446	8.108	7.091	1.863
TJ60_15 4l	5.703	72.315	8.436	6.519	1.723
TJ5_16 4e	6.844	66.782	6.099	7.944	1.784
TJ5_16 4e	6.003	66.543	5.995	7.11	0.693
TJ2_16 4a	8.012	71.47	6.872	8.35	1.556
TJ2_16 4a	7.891	72.204	6.482	8.912	1.745
8_15 4i	7.062	73.63	7.81	7.67	1.847
8_15 4i	7.16	73.582	7.773	7.91	1.741

EURO EA

Elemental Analyzer



Method Filename : D:\Program Files\Callidus 2E3\Method\CHNS215.mth

Summarize Result : Percent

Configuration: C H N S

Date: 28/02/2017

Sample Name	N %	C %	H %	S %	Weight
BBOT	6.555	72.779	5.709	7.389	1.726
BBOT	6.467	72.005	6.052	7.398	1.524
BBOT	6.509	72.812	6.128	7.535	1.42
bbot	6.539	72.893	6.433	7.647	1.762
TJ3_16 4b	7.287	66.083	5.789	8.766	1.768
TJ3_16 4b	7.248	65.607	5.732	8.639	1.633
TJ17_17 4f	6.98	66.483	6.278	8.387	1.935
TJ17_17 4f	6.998	66.652	6.259	8.373	1.743
TJ8_16 4i	6.93	74.018	8.086	7.966	1.582
TJ8_16 4i	6.927	73.737	8.097	7.958	1.717

EURO EA

Elemental Analyzer



Method Filename : D:\Program Files\Callidus 2E3\Method\CHNS216.mth

Summarize Result : Percent

Configuration: C H N S

Date: 03/03/2017

BBOT	6.491	72.217	5.866	7.492	1.797
BBOT	6.489	72.115	6.111	7.474	1.95
BBOT	6.55	73.269	6.31	7.355	1.808
bbot	6.561	72.748	6.297	7.513	1.795
TJ29_15 3c	8.924	61.849	8.764	20.468	1.5
TJ29_15 3c	9.243	61.459	8.243	20.913	1.417