Electronic Supporting Information

Cyclohepta[*b*]thiophenes as potential antiproliferative agents: Design, synthesis, *in vitro* and *in vivo* anticancer evaluation

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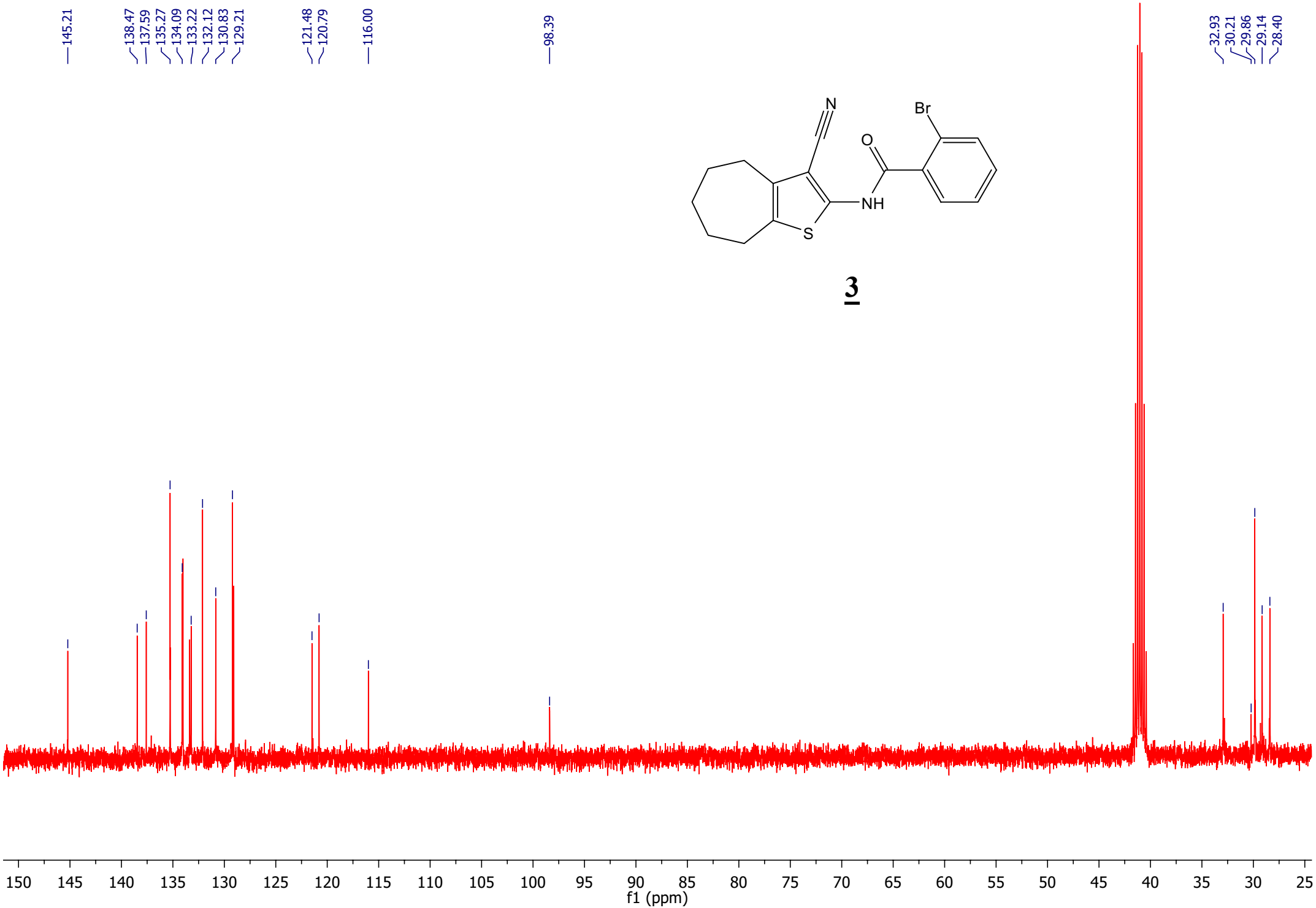


Figure S-1.^{13}CNMR of compound 3

Elemental Composition Report

Single Mass Analysis

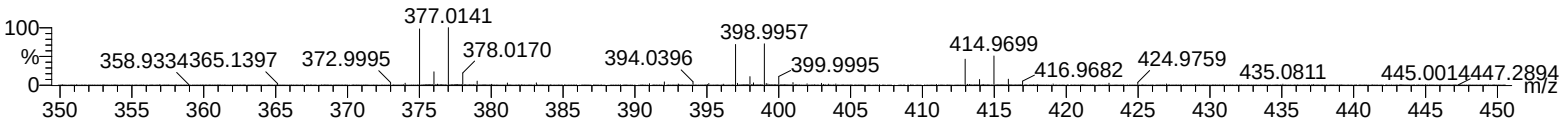
Tolerance = 5.0 mDa / DBE: min = -5.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions
1162 formula(e) evaluated with 15 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 1-100 H: 1-200 N: 0-5 O: 0-12 S: 0-1 Br: 0-1

Salem/Abdelrahman
T03261906 17 (0.611) Cm (16:24)

Sample #40

1: TOF MS ES+
4.84e+004



Minimum:				-5.0			
Maximum:		5.0	15.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
375.0154	375.0154	0.0	0.0	22.5	971.7	28.2	C21 H3 N4 O4
	375.0151	0.3	0.8	2.5	959.2	15.6	C8 H16 N4 O8 Br
	375.0167	-1.3	-3.5	10.5	943.5	0.0	C17 H16 N2 O S Br
	375.0141	1.3	3.5	17.5	971.7	28.2	C20 H7 O8
	375.0138	1.6	4.3	-2.5	959.7	16.2	C7 H20 O12 Br
	375.0134	2.0	5.3	8.5	963.4	19.8	C12 H11 N2 O10 S
	375.0175	-2.1	-5.6	12.5	964.5	20.9	C17 H11 O8 S
	375.0133	2.1	5.6	15.5	955.8	12.3	C20 H12 N2 O Br
	375.0126	2.8	7.5	6.5	951.2	7.7	C12 H16 N4 O3 S Br
	375.0185	-3.1	-8.3	-2.5	955.9	12.4	C5 H20 N4 O8 S Br
	375.0188	-3.4	-9.1	17.5	964.3	20.7	C18 H7 N4 O4 S
	375.0192	-3.8	-10.1	6.5	957.6	14.1	C13 H16 N2 O6 Br
	375.0116	3.8	10.1	21.5	965.4	21.8	C24 H7 O3 S
	375.0113	4.1	10.9	1.5	953.1	9.6	C11 H20 O7 S Br
	375.0195	-4.1	-10.9	26.5	972.3	28.8	C26 H3 N2 O2

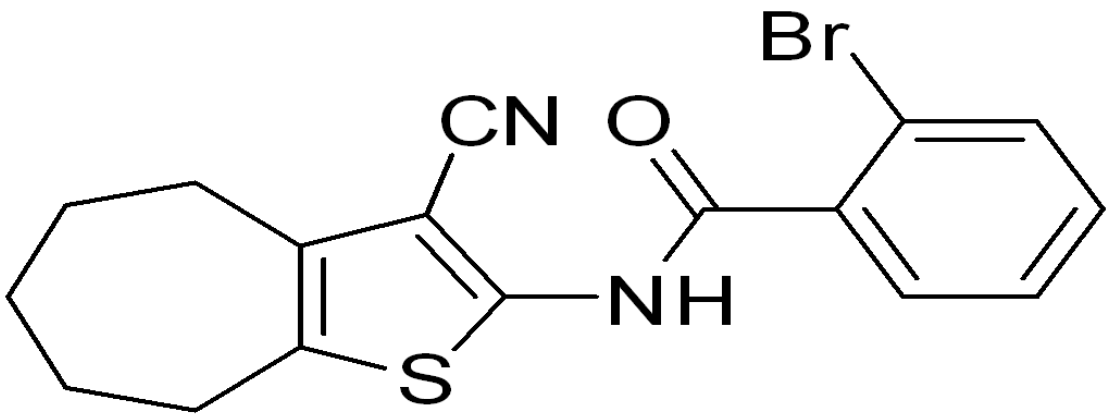


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Figure S-2. HRMS of compound 3

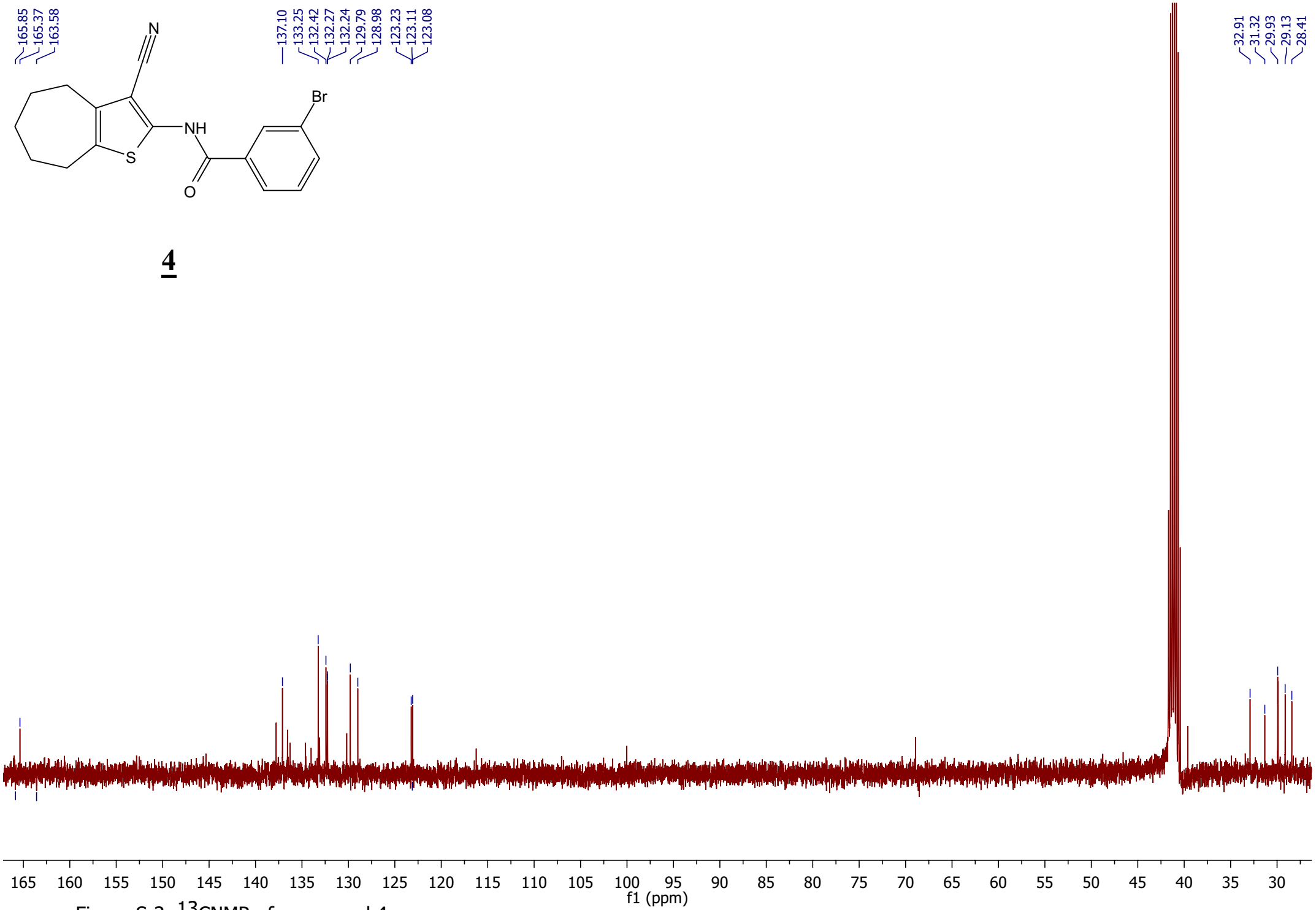


Figure S-3. ^{13}CNMR of compound 4

Elemental Composition Report

Single Mass Analysis

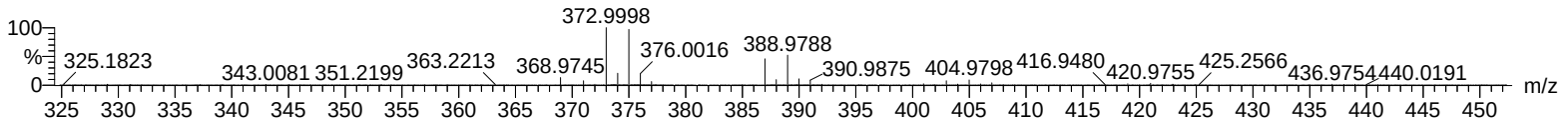
Tolerance = 5.0 mDa / DBE: min = -5.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions
1158 formula(e) evaluated with 15 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 1-100 H: 1-200 N: 0-5 O: 0-12 S: 0-1 Br: 0-1

Salem/Abdelrahman
T03261914 9 (0.322) Cm (4:13)

Sample #41

1: TOF MS ES-
4.21e+004



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
Minimum:				-5.0			
Maximum:		5.0	15.0	100.0			
372.9998	372.9998	0.0	0.0	23.5	928.9	33.7	C21 H N4 O4
	372.9995	0.3	0.8	3.5	916.0	20.8	C8 H14 N4 O8 Br
	373.0010	-1.2	-3.2	11.5	895.2	0.0	C17 H14 N2 O S Br
	372.9984	1.4	3.8	18.5	928.9	33.7	C20 H5 O8
	372.9982	1.6	4.3	-1.5	916.4	21.2	C7 H18 O12 Br
	373.0018	-2.0	-5.4	13.5	922.4	27.2	C17 H9 O8 S
	372.9978	2.0	5.4	9.5	921.6	26.5	C12 H9 N2 O10 S
	372.9976	2.2	5.9	16.5	912.9	17.7	C20 H10 N2 O Br
	372.9970	2.8	7.5	7.5	905.0	9.8	C12 H14 N4 O3 S Br
	373.0029	-3.1	-8.3	-1.5	911.7	16.6	C5 H18 N4 O8 S Br
	373.0032	-3.4	-9.1	18.5	922.3	27.1	C18 H5 N4 O4 S
	373.0035	-3.7	-9.9	7.5	913.8	18.6	C13 H14 N2 O6 Br
	372.9959	3.9	10.5	22.5	923.3	28.1	C24 H5 O3 S
	373.0038	-4.0	-10.7	27.5	929.5	34.3	C26 H N2 O2
	372.9957	4.1	11.0	2.5	906.1	11.0	C11 H18 O7 S Br

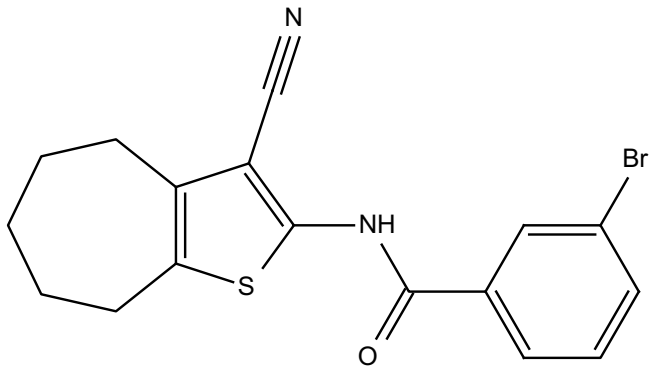


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Figure S-4. HRMS of compound 4

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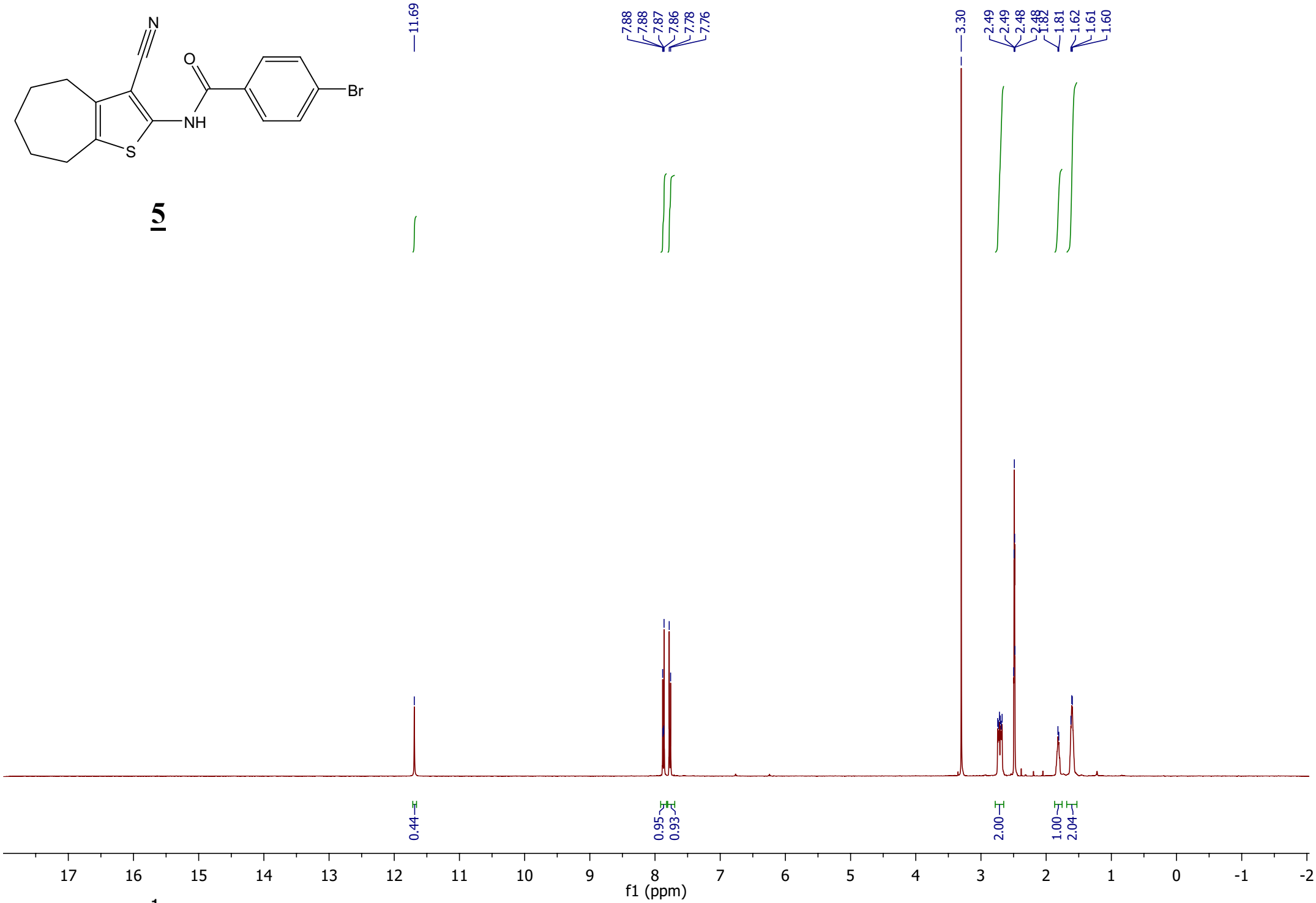


Figure S-5. ^{1}HNMR of compound 5

Elemental Composition Report

Single Mass Analysis

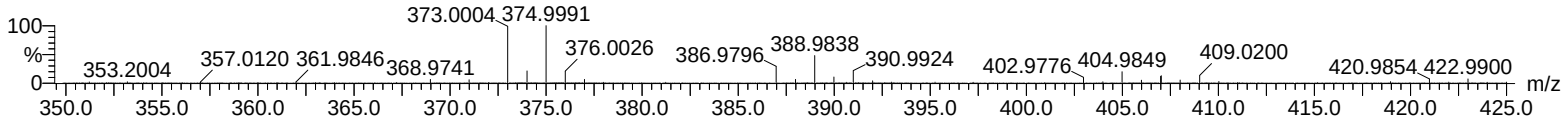
Tolerance = 5.0 mDa / DBE: min = -5.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions
1158 formula(e) evaluated with 15 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 1-100 H: 1-200 N: 0-5 O: 0-12 S: 0-1 Br: 0-1

Salem/Abdelrahman
T03261912 23 (0.803) Cm (5:26)

Sample #42

1: TOF MS ES-
4.62e+004



Minimum:				-5.0			
Maximum:		5.0	15.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
373.0004	373.0010	-0.6	-1.6	11.5	990.8	0.0	C17 H14 N2 O S Br
	372.9998	0.6	1.6	23.5	1027.4	36.7	C21 H N4 O4
	372.9995	0.9	2.4	3.5	1015.5	24.7	C8 H14 N4 O8 Br
	373.0018	-1.4	-3.8	13.5	1021.7	31.0	C17 H9 O8 S
	372.9984	2.0	5.4	18.5	1027.4	36.6	C20 H5 O8
	372.9982	2.2	5.9	-1.5	1016.0	25.2	C7 H18 O12 Br
	373.0029	-2.5	-6.7	-1.5	1010.1	19.3	C5 H18 N4 O8 S Br
	372.9978	2.6	7.0	9.5	1021.2	30.4	C12 H9 N2 O10 S
	373.0032	-2.8	-7.5	18.5	1021.6	30.8	C18 H5 N4 O4 S
	372.9976	2.8	7.5	16.5	1011.9	21.1	C20 H10 N2 O Br
	373.0035	-3.1	-8.3	7.5	1013.2	22.5	C13 H14 N2 O6 Br
	373.0038	-3.4	-9.1	27.5	1028.0	37.2	C26 H N2 O2
	372.9970	3.4	9.1	7.5	1003.4	12.6	C12 H14 N4 O3 S Br
	372.9959	4.5	12.1	22.5	1022.5	31.7	C24 H5 O3 S
	372.9957	4.7	12.6	2.5	1004.9	14.2	C11 H18 O7 S Br

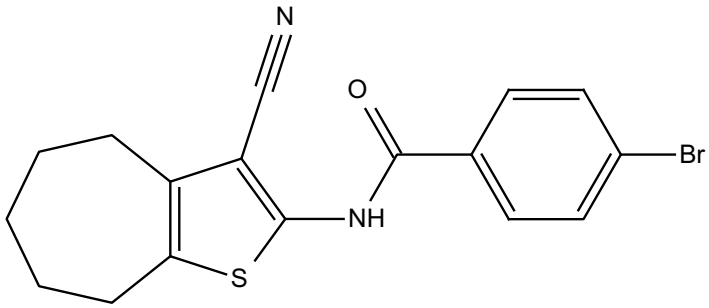


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Figure S-6. HRMS of compound 5

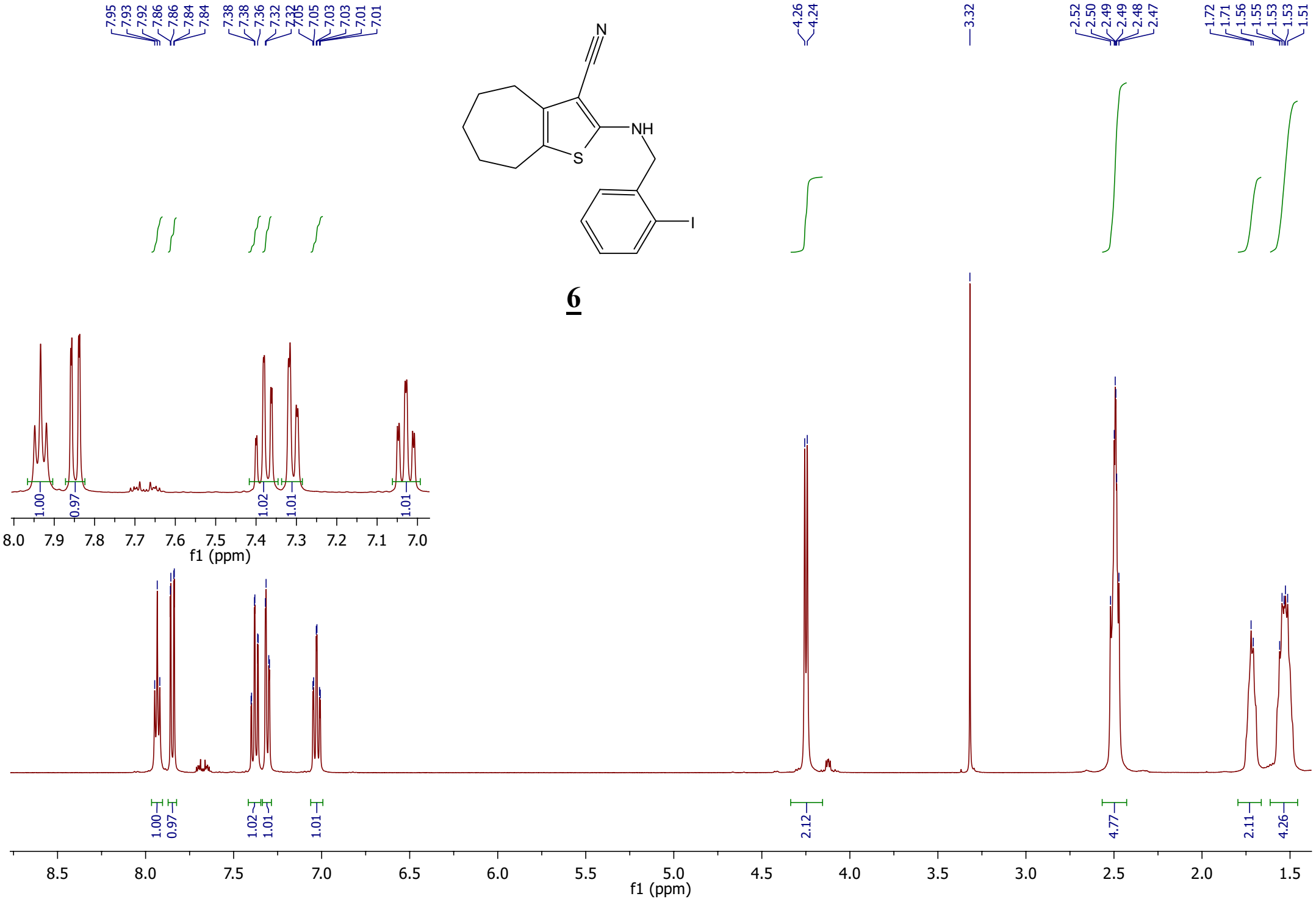


Figure S-7. ^{1}HNMR of compound 6

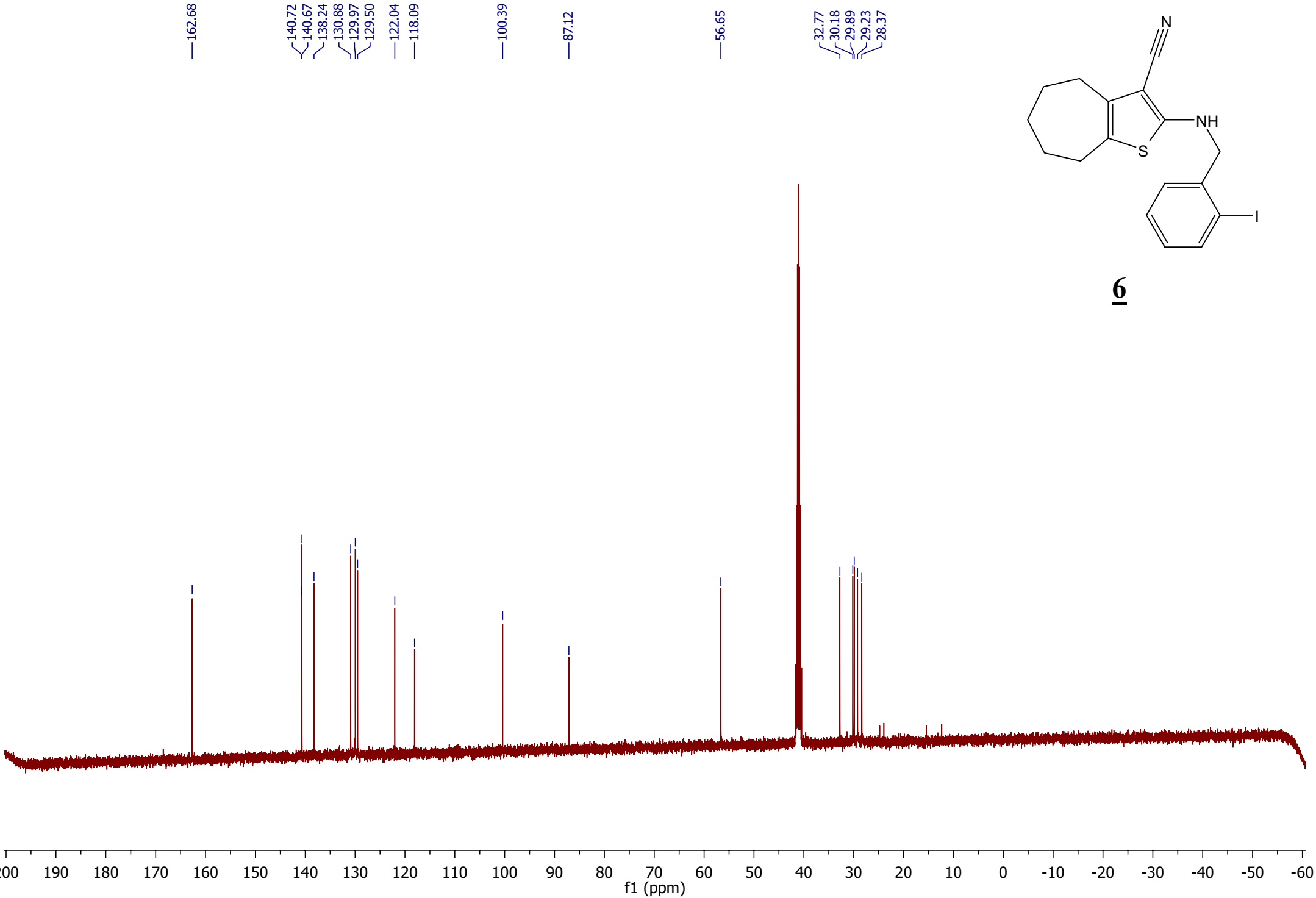


Figure S-8. ^{13}CNMR of compound 6

Elemental Composition Report

Single Mass Analysis

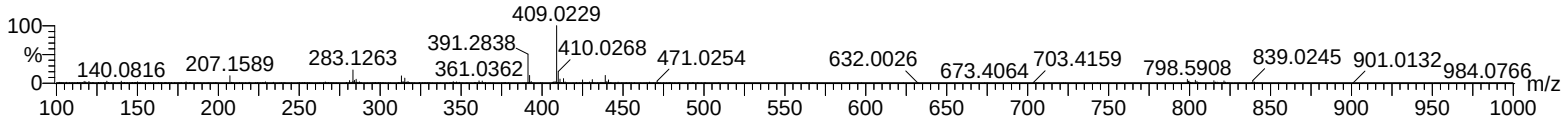
Tolerance = 5.0 mDa / DBE: min = -5.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions
221 formula(e) evaluated with 4 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 1-100 H: 1-200 N: 0-6 O: 0-10 S: 1-1 I: 1-1

Salem/Abdelrahman
T01281947a 12 (0.433) Cm (6:23)

Sample #12

1: TOF MS ES+
9.47e+004



Minimum:				-5.0			
Maximum:		5.0	15.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
409.0230	409.0235	-0.5	-1.2	9.5	844.0	0.0	C17 H18 N2 S I
	409.0254	-2.4	-5.9	-3.5	856.6	12.6	C5 H22 N4 O7 S I
	409.0195	3.5	8.6	5.5	851.3	7.2	C12 H18 N4 O2 S I
	409.0182	4.8	11.7	0.5	852.4	8.3	C11 H22 O6 S I

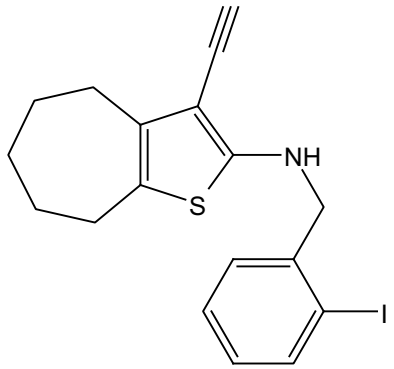


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Figure S-9. HRMS of compound 6

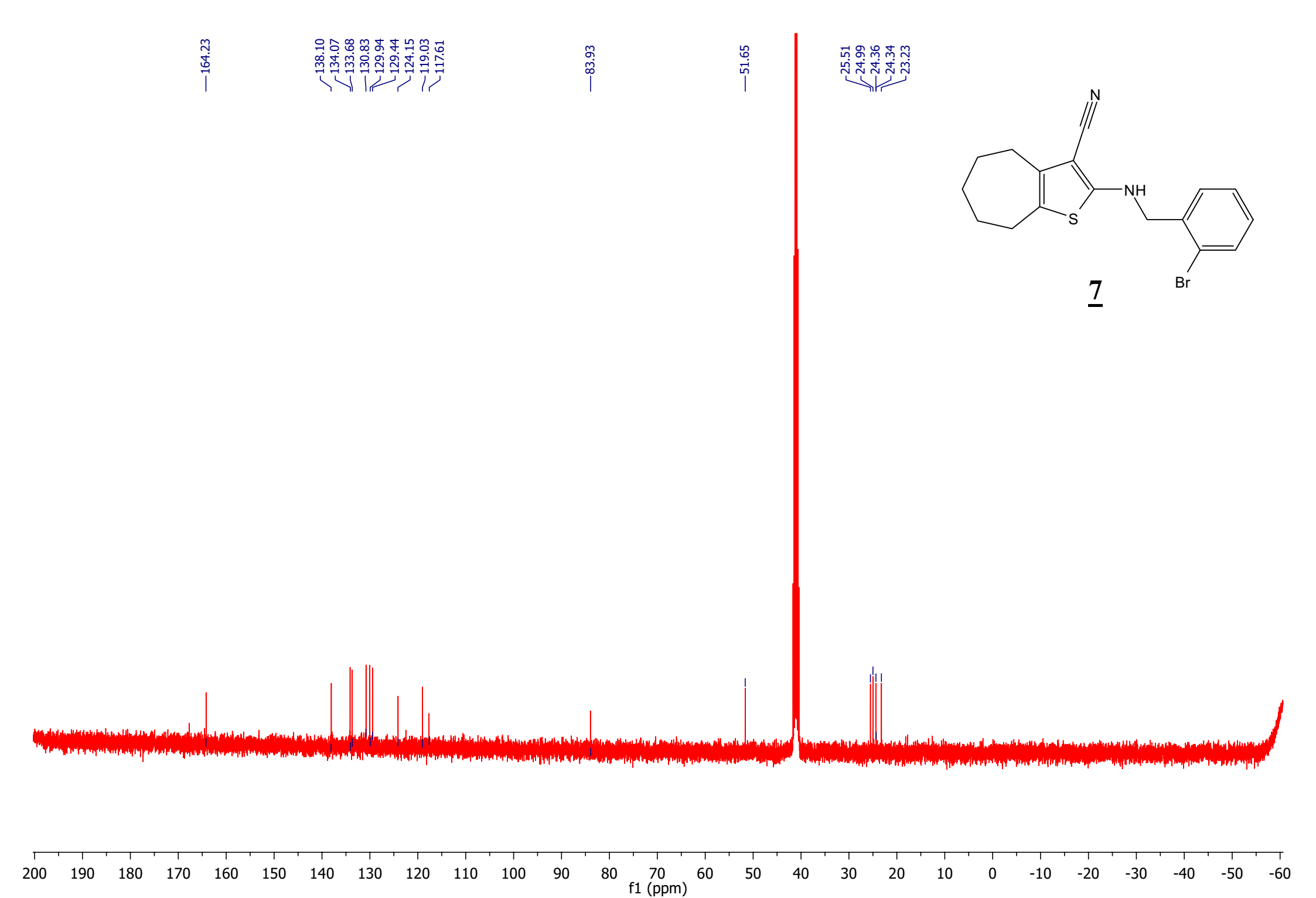


Figure S-10. ^{13}CNMR of compound 7

Elemental Composition Report

Single Mass Analysis

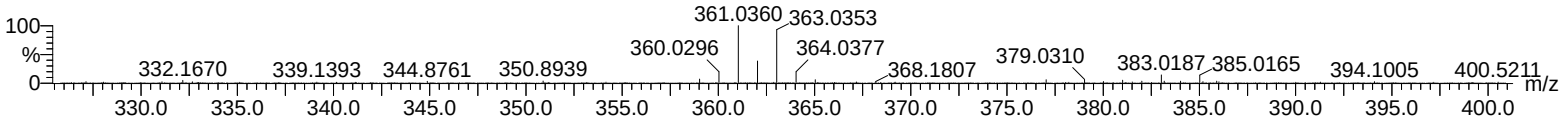
Tolerance = 5.0 mDa / DBE: min = -5.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions
539 formula(e) evaluated with 9 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 1-100 H: 1-200 N: 0-6 O: 0-10 S: 1-1 Br: 0-1

Salem/Abdelrahman
T01281939 5 (0.178) Cm (4:10)

Sample #10

1: TOF MS ES+
6.27e+003



Minimum:				-5.0			
Maximum:		5.0	15.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
361.0361	361.0355	0.6	1.7	12.5	544.8	7.4	C13 H9 N6 O5 S
	361.0374	-1.3	-3.6	9.5	537.8	0.4	C17 H18 N2 S Br
	361.0342	1.9	5.3	7.5	544.9	7.5	C12 H13 N2 O9 S
	361.0382	-2.1	-5.8	11.5	545.0	7.6	C17 H13 O7 S
	361.0334	2.7	7.5	5.5	538.9	1.5	C12 H18 N4 O2 S Br
	361.0393	-3.2	-8.9	-3.5	540.8	3.4	C5 H22 N4 O7 S Br
	361.0395	-3.4	-9.4	16.5	544.9	7.5	C18 H9 N4 O3 S
	361.0323	3.8	10.5	20.5	544.7	7.2	C24 H9 O2 S
	361.0320	4.1	11.4	0.5	540.0	2.6	C11 H22 O6 S Br

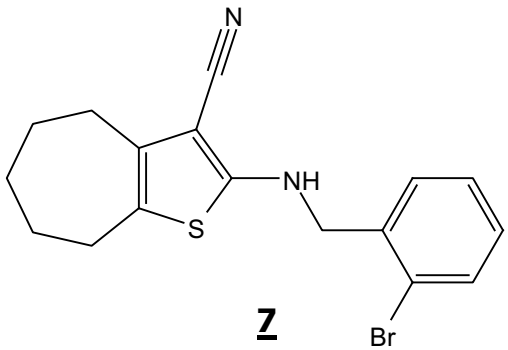


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Figure S-11. HRMS of compound 7

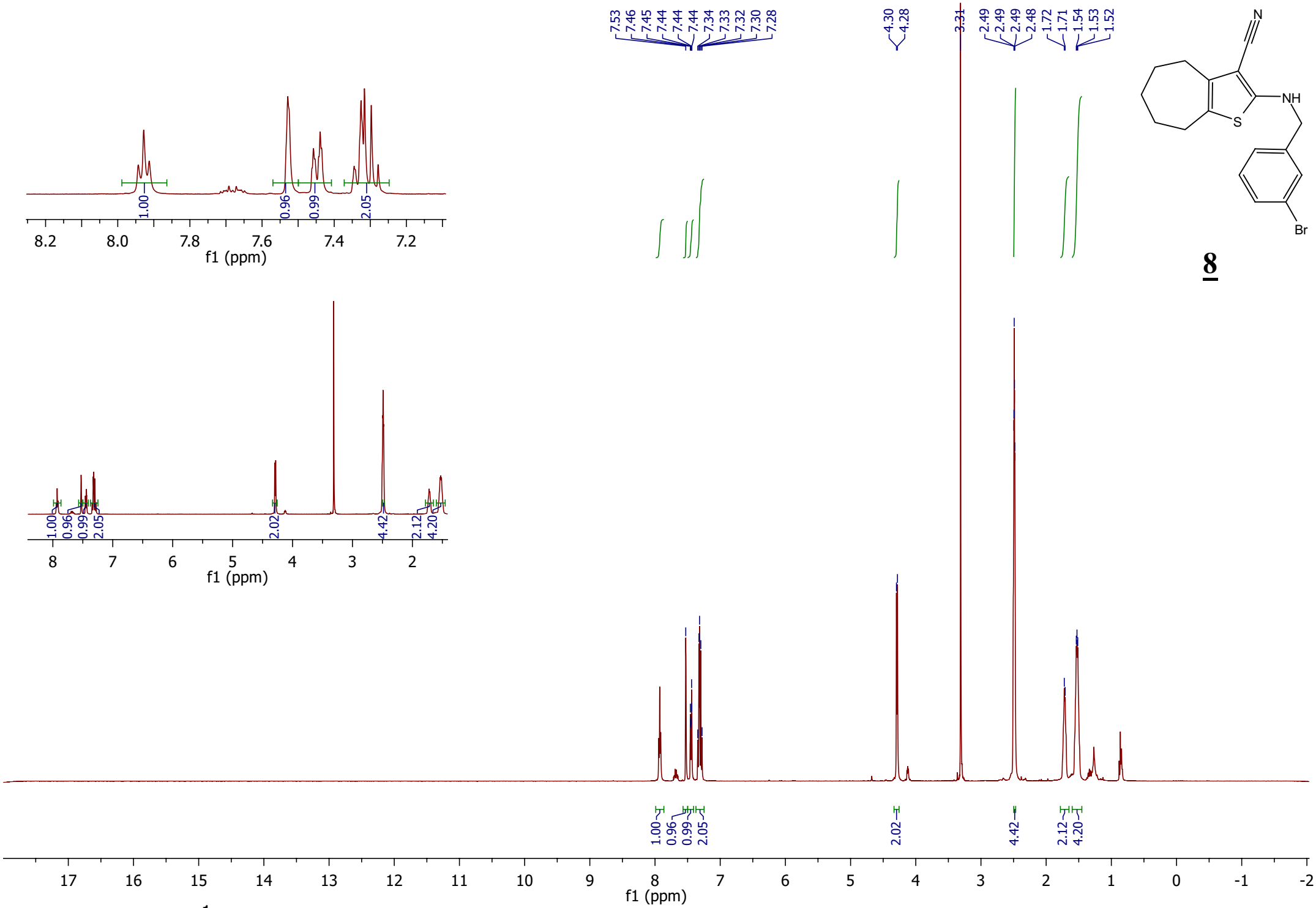


Figure S-12. ^{1}HNMR of compound 8

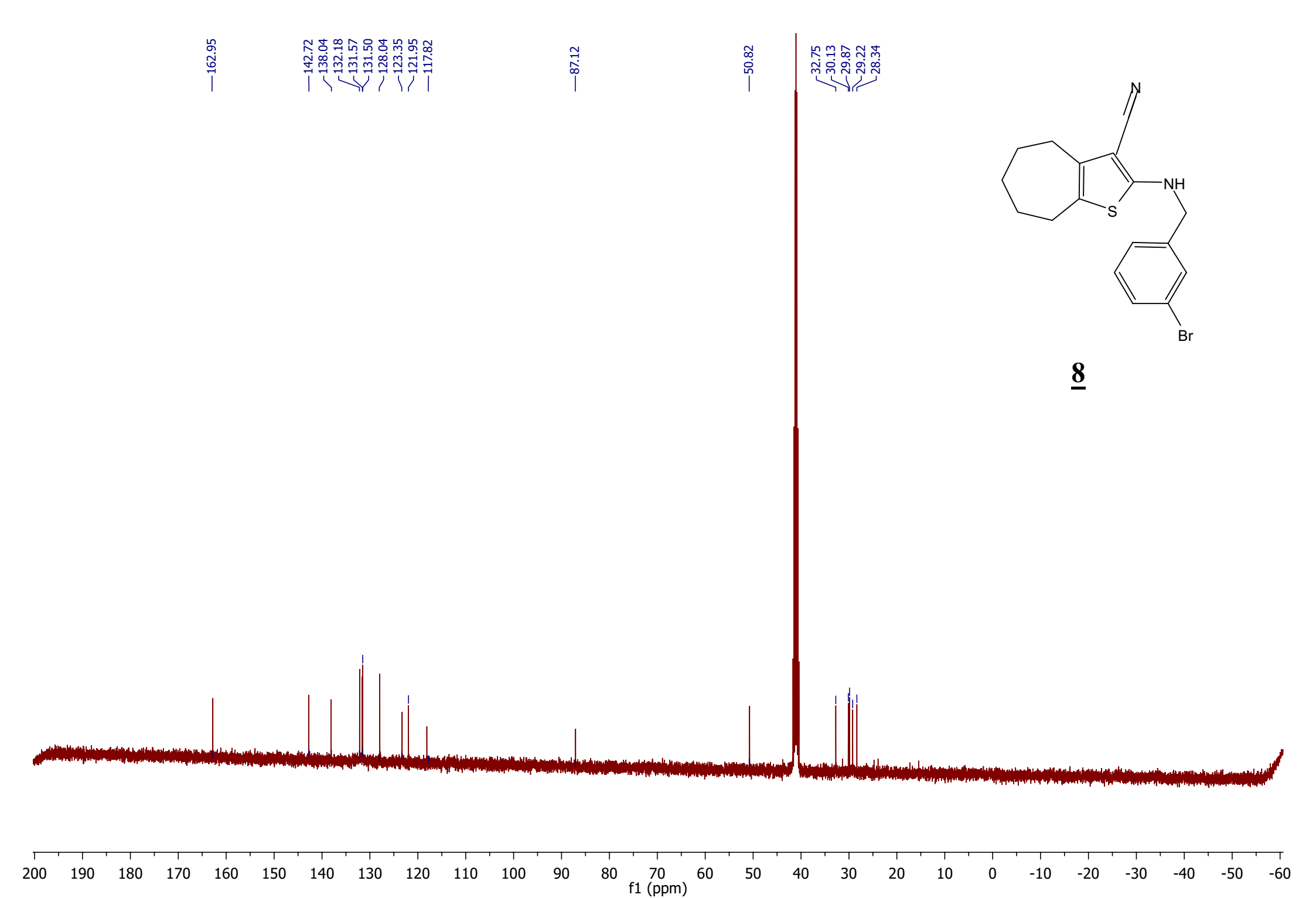


Figure S-13. ^{13}CNMR of compound 8

Elemental Composition Report

Single Mass Analysis

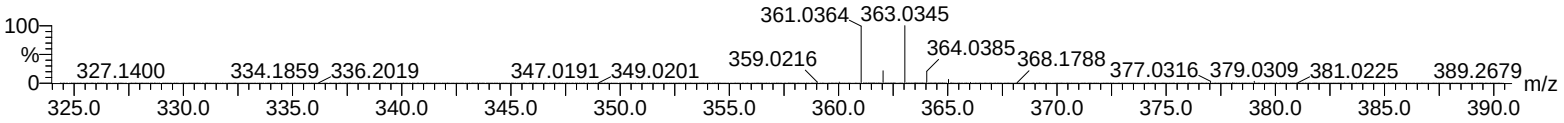
Tolerance = 5.0 mDa / DBE: min = -5.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions
539 formula(e) evaluated with 9 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 1-100 H: 1-200 N: 0-6 O: 0-10 S: 1-1 Br: 0-1

Salem/Abdelrahman
T01281934c 19 (0.679) Cm (5:22)

Sample #9

1: TOF MS ES+
1.30e+005



Minimum:				-5.0			
Maximum:		5.0	15.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
361.0363	361.0355	0.8	2.2	12.5	1041.0	28.2	C13 H9 N6 O5 S
	361.0374	-1.1	-3.0	9.5	1012.8	0.0	C17 H18 N2 S Br
	361.0382	-1.9	-5.3	11.5	1041.7	29.0	C17 H13 O7 S
	361.0342	2.1	5.8	7.5	1041.0	28.2	C12 H13 N2 O9 S
	361.0334	2.9	8.0	5.5	1024.5	11.7	C12 H18 N4 O2 S Br
	361.0393	-3.0	-8.3	-3.5	1031.0	18.2	C5 H22 N4 O7 S Br
	361.0395	-3.2	-8.9	16.5	1041.7	28.9	C18 H9 N4 O3 S
	361.0323	4.0	11.1	20.5	1042.6	29.9	C24 H9 O2 S
	361.0320	4.3	11.9	0.5	1025.5	12.8	C11 H22 O6 S Br

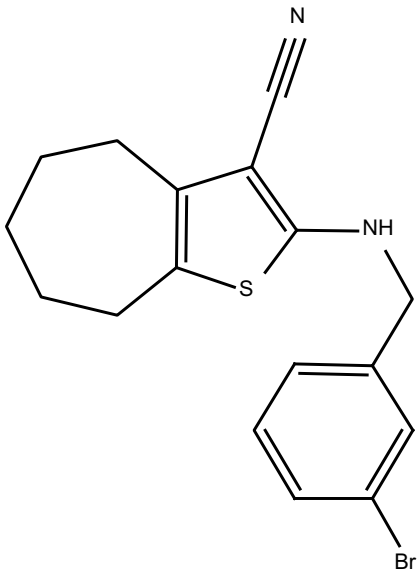


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Figure S-14. HRMS of compound 8

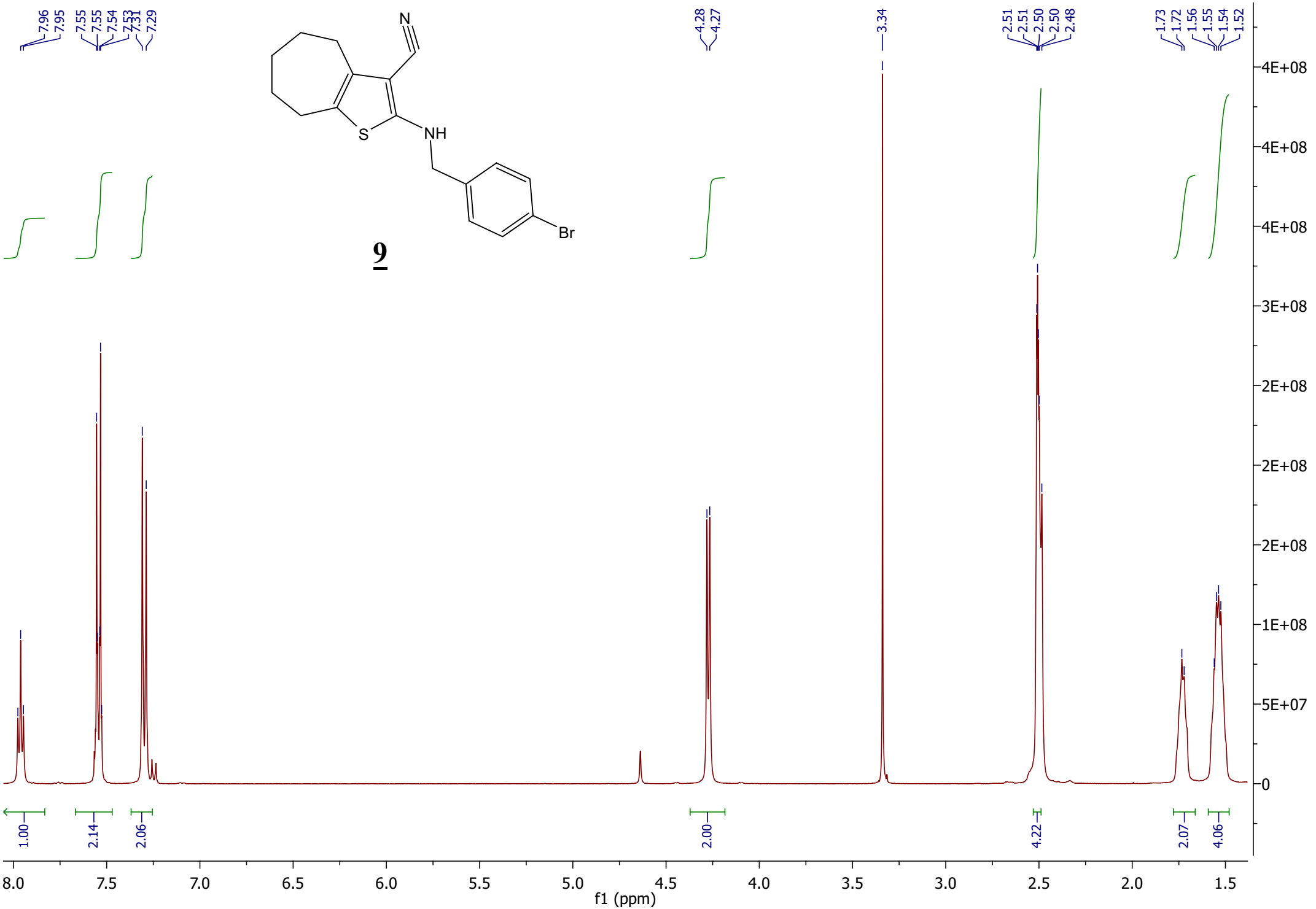


Figure S-15. ^{1}HNMR of compound 9

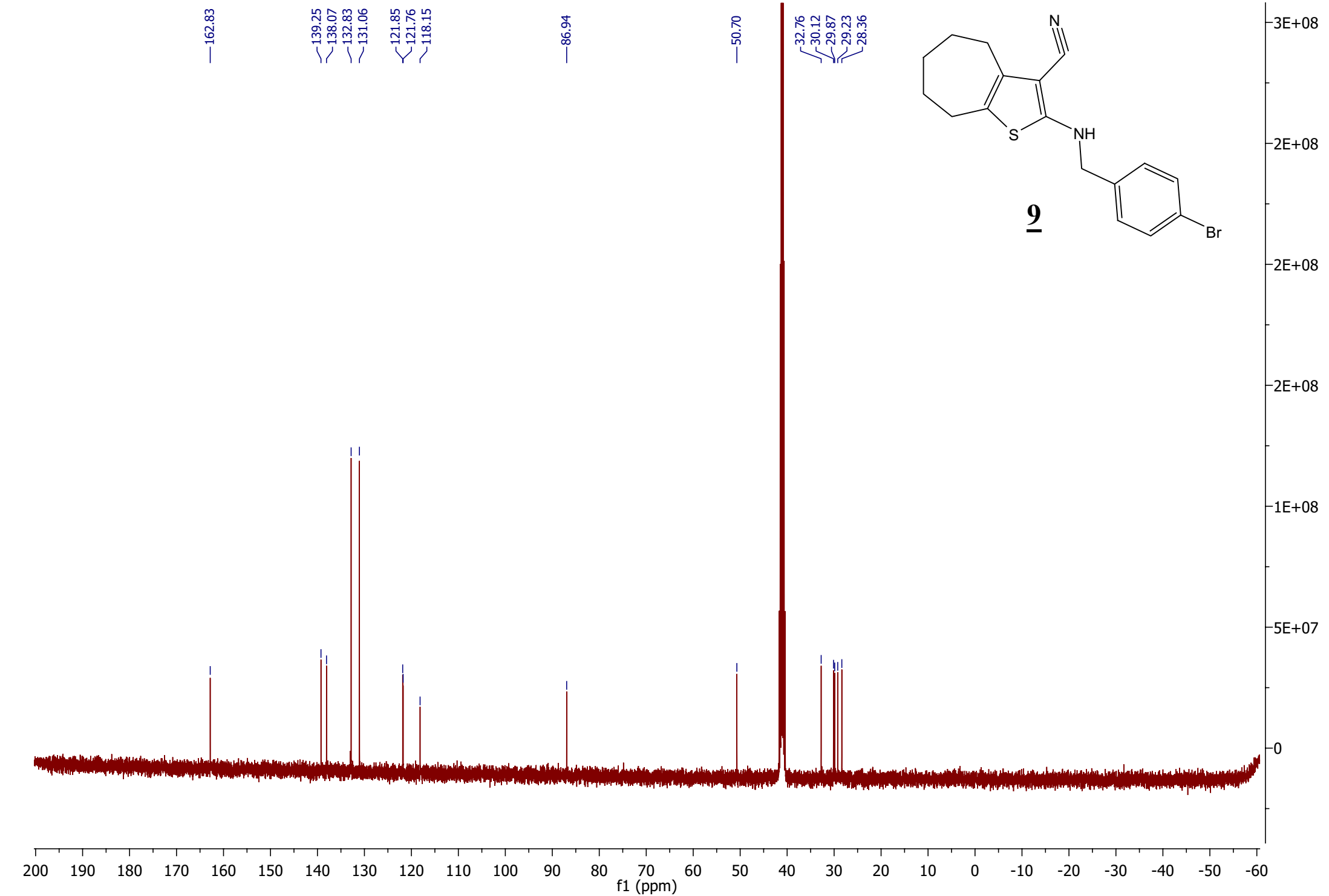


Figure S-16. ^{13}CNMR of compound 9

Elemental Composition Report

Single Mass Analysis

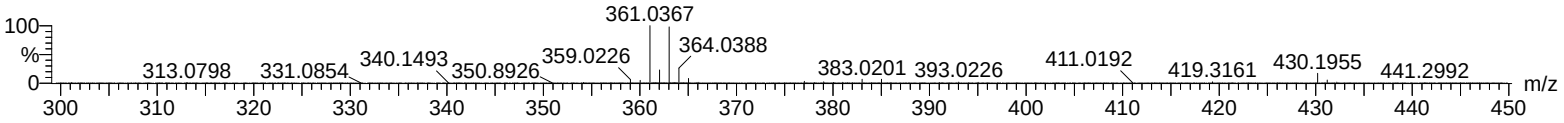
Tolerance = 5.0 mDa / DBE: min = -5.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions
384 formula(e) evaluated with 6 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 1-100 H: 1-200 N: 0-6 O: 0-6 S: 1-1 Br: 0-1

Salem/Abdelrahman
T01311907a 10 (0.356) Cm (9:16)

Sample #16

1: TOF MS ES+
2.88e+004



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
Minimum:				-5.0			
Maximum:		5.0	15.0	100.0			
361.0366	361.0374	-0.8	-2.2	9.5	744.4	0.0	C17 H18 N2 S Br
	361.0355	1.1	3.0	12.5	759.5	15.1	C13 H9 N6 O5 S
	361.0395	-2.9	-8.0	16.5	760.2	15.9	C18 H9 N4 O3 S
	361.0334	3.2	8.9	5.5	749.0	4.6	C12 H18 N4 O2 S Br
	361.0323	4.3	11.9	20.5	761.2	16.8	C24 H9 O2 S
	361.0320	4.6	12.7	0.5	750.4	6.0	C11 H22 O6 S Br

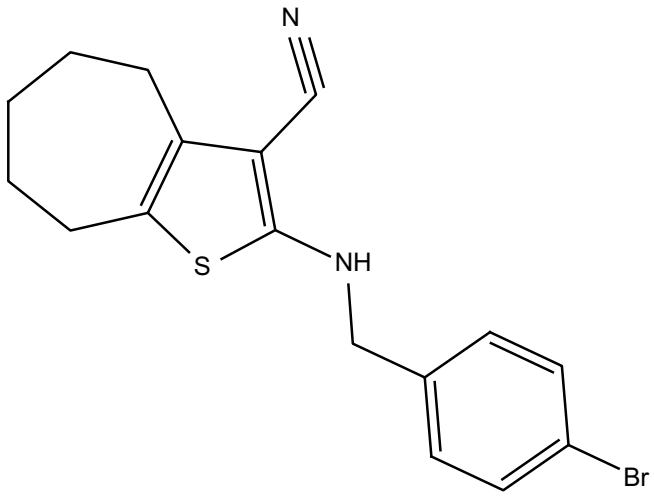


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Figure S-17. HRMS of compound 9

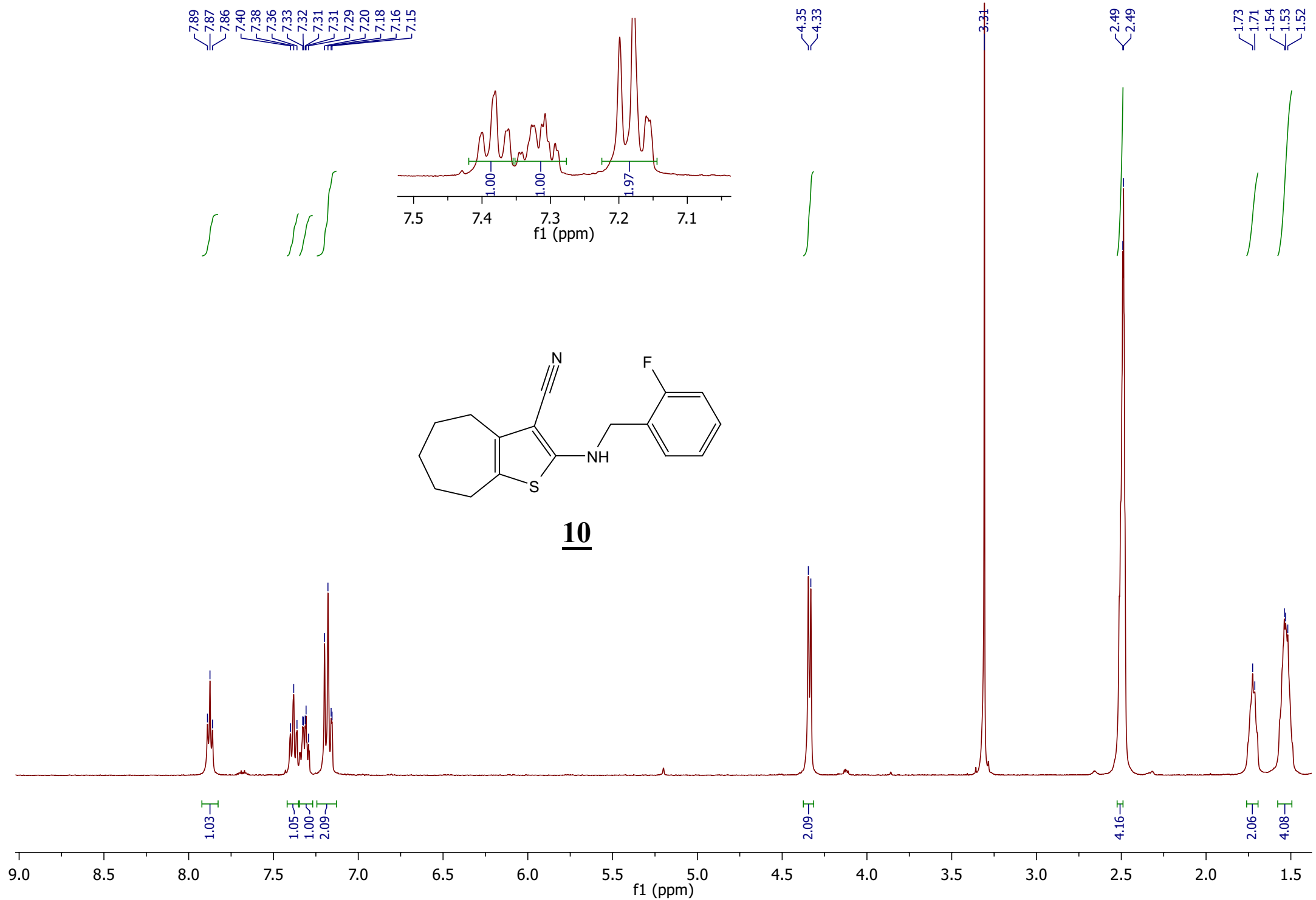


Figure S-18. ^{1}HNMR of compound 10

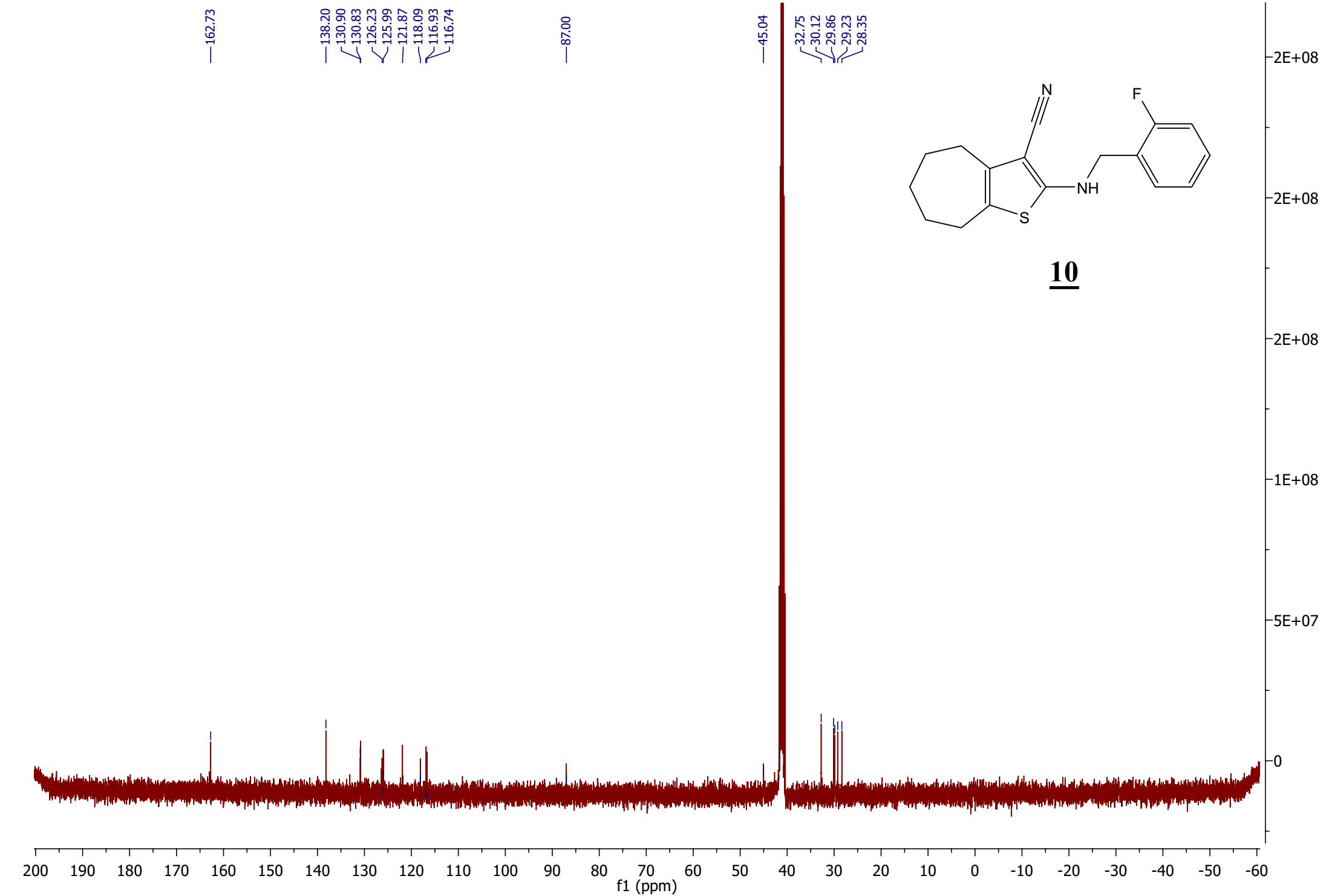


Figure S-19. ^{13}CNMR of compound 10

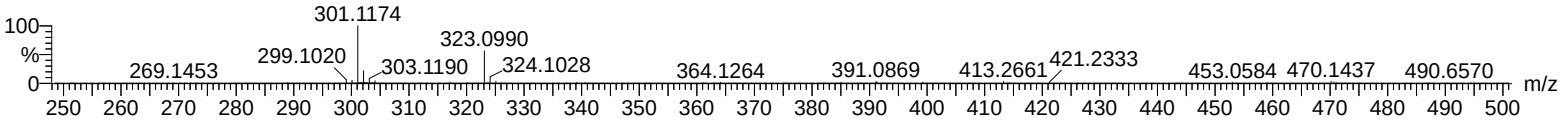
Elemental Composition Report

Single Mass Analysis

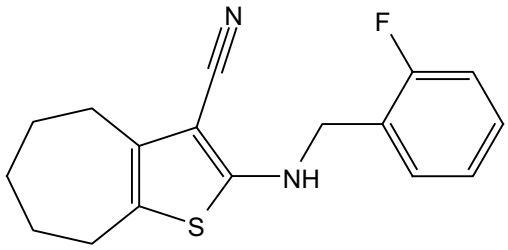
Tolerance = 5.0 mDa / DBE: min = -5.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions
478 formula(e) evaluated with 8 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 1-100 H: 1-200 N: 0-6 O: 0-10 F: 0-1 S: 1-1

Salem/Abdelrahman Sample #15
T01311904a 9 (0.322) Cm (9:14) 1: TOF MS ES+
3.33e+004



Minimum:				-5.0			
Maximum:		5.0	15.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
301.1171	301.1168	0.3	1.0	-4.5	805.2	5.6	C7 H25 O10 S
	301.1175	-0.4	-1.3	9.5	799.9	0.2	C17 H18 N2 F S
	301.1182	-1.1	-3.7	0.5	804.4	4.7	C8 H21 N4 O6 S
	301.1193	-2.2	-7.3	-3.5	805.9	6.2	C5 H22 N4 O7 F S
	301.1142	2.9	9.6	-3.5	807.0	7.3	C3 H21 N6 O8 S
	301.1135	3.6	12.0	5.5	803.3	3.6	C12 H18 N4 O2 F S
	301.1123	4.8	15.9	9.5	801.5	1.8	C15 H17 N4 O S
	301.1121	5.0	16.6	0.5	803.8	4.2	C11 H22 O6 F S



10

Figure S-20. HRMS of compound 10

11

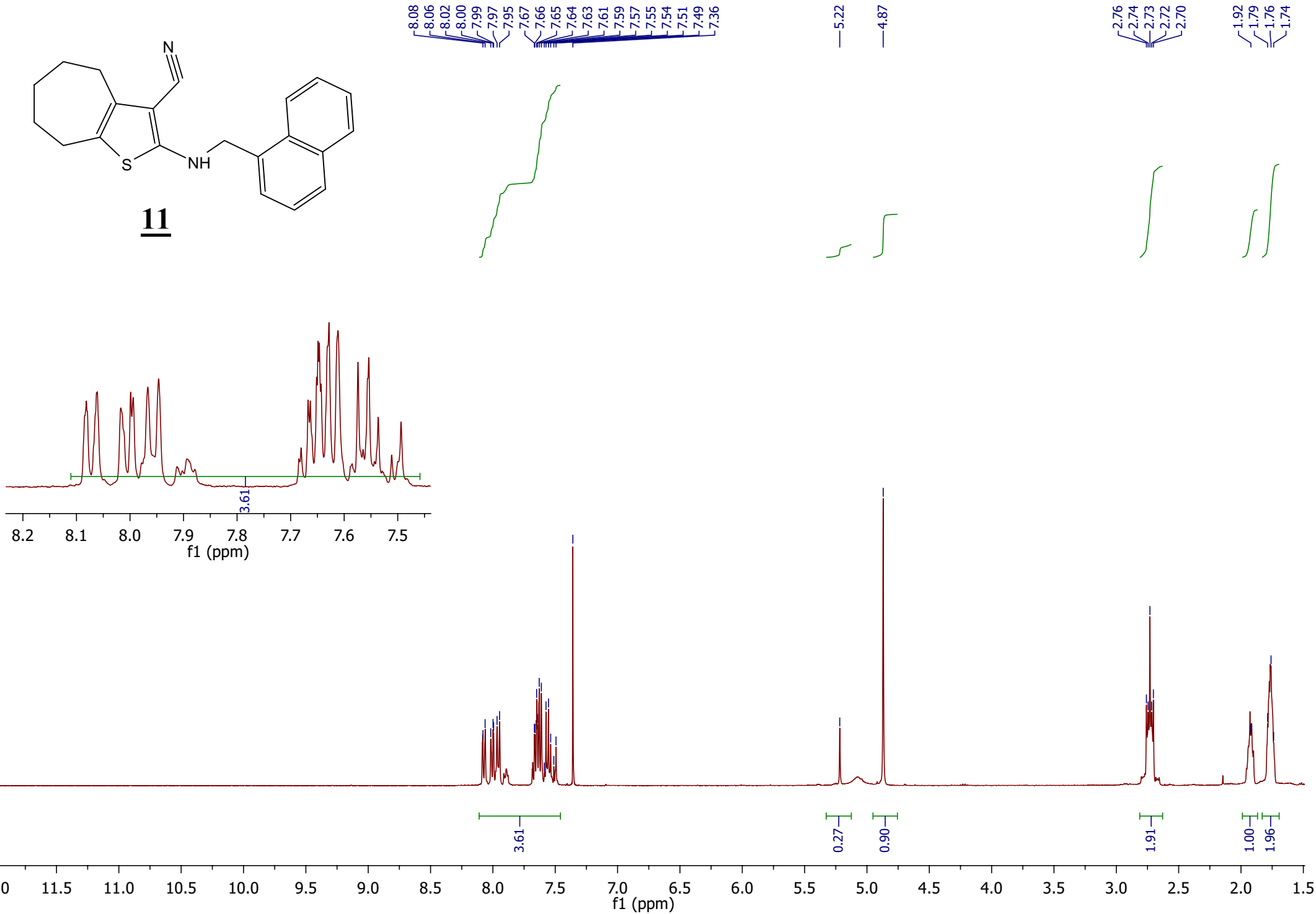


Figure S-21. ^{1}HNMR of compound 11

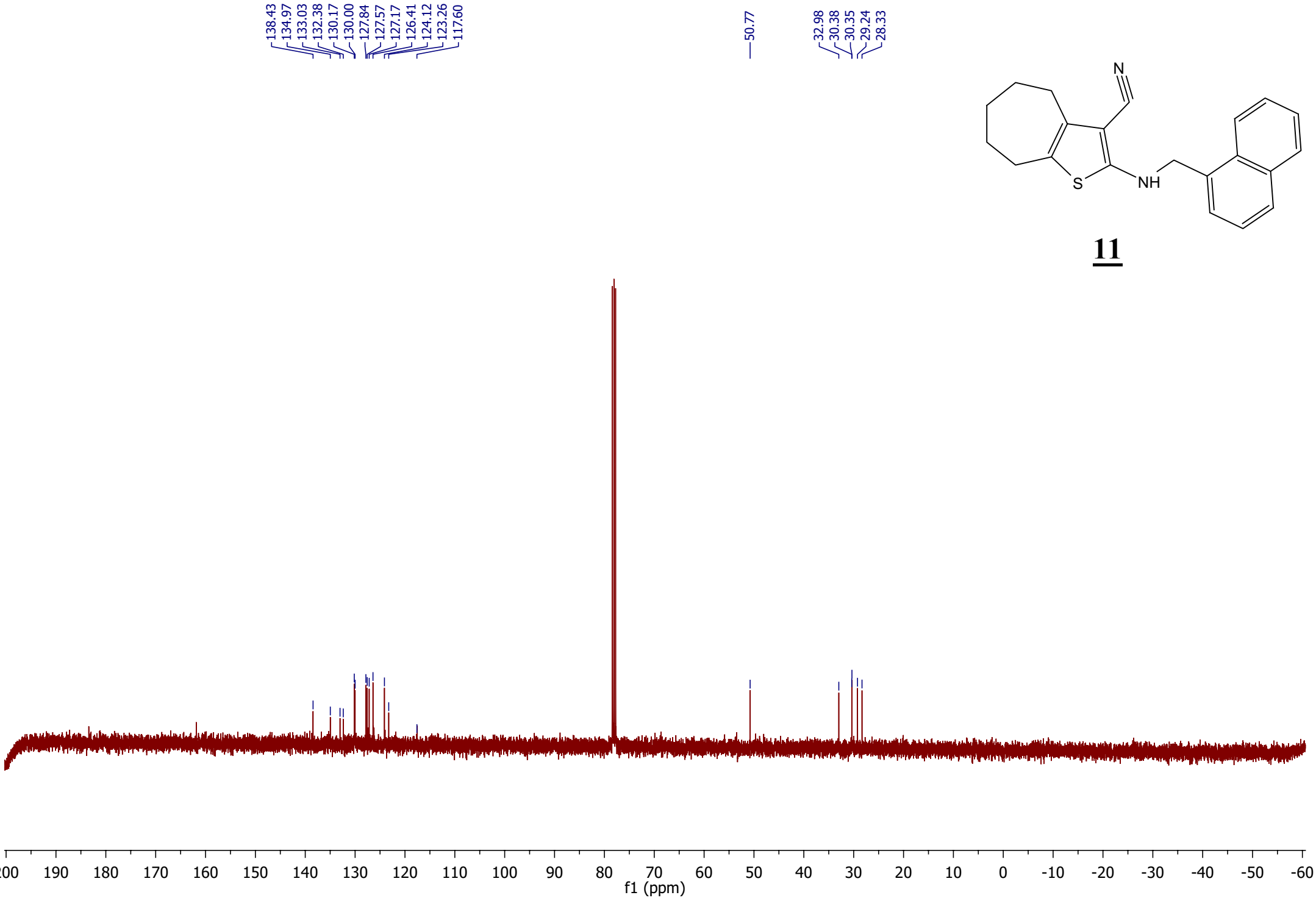


Figure S-22. ^{13}CNMR of compound 11

Elemental Composition Report

Single Mass Analysis

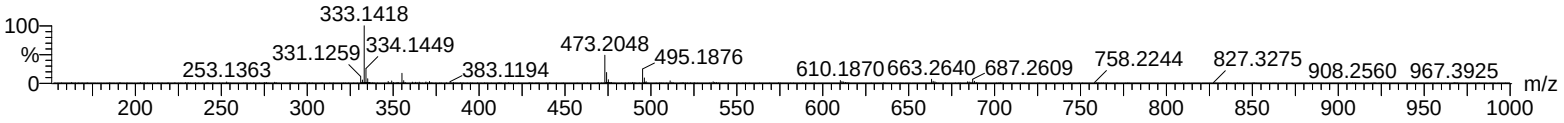
Tolerance = 5.0 mDa / DBE: min = -5.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions
835 formula(e) evaluated with 11 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 1-100 H: 1-200 N: 0-5 O: 0-12 S: 0-2

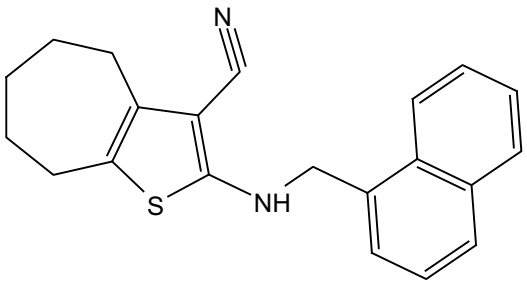
Salem/Abdelrahman
T03251908a 9 (0.322) Cm (8:15)

Sample #38

1: TOF MS ES+
3.77e+004



Minimum:				-5.0			
Maximum:		5.0	15.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
333.1418	333.1419	-0.1	-0.3	3.5	861.3	12.2	C13 H25 N4 O2 S2
	333.1425	-0.7	-2.1	12.5	849.0	0.0	C21 H21 N2 S
	333.1410	0.8	2.4	4.5	872.1	23.1	C12 H21 N4 O7
	333.1406	1.2	3.6	-1.5	862.9	13.9	C12 H29 O6 S2
	333.1397	2.1	6.3	-0.5	872.6	23.6	C11 H25 O11
	333.1444	-2.6	-7.8	-0.5	863.2	14.1	C9 H25 N4 O7 S
	333.1392	2.6	7.8	17.5	870.9	21.9	C24 H17 N2
	333.1450	-3.2	-9.6	8.5	871.1	22.1	C17 H21 N2 O5
	333.1385	3.3	9.9	8.5	857.0	7.9	C16 H21 N4 O2 S
	333.1459	-4.1	-12.3	7.5	859.5	10.5	C18 H25 N2 S2
	333.1372	4.6	13.8	3.5	860.9	11.9	C15 H25 O6 S



11

Figure S-23. HRMS of compound 11

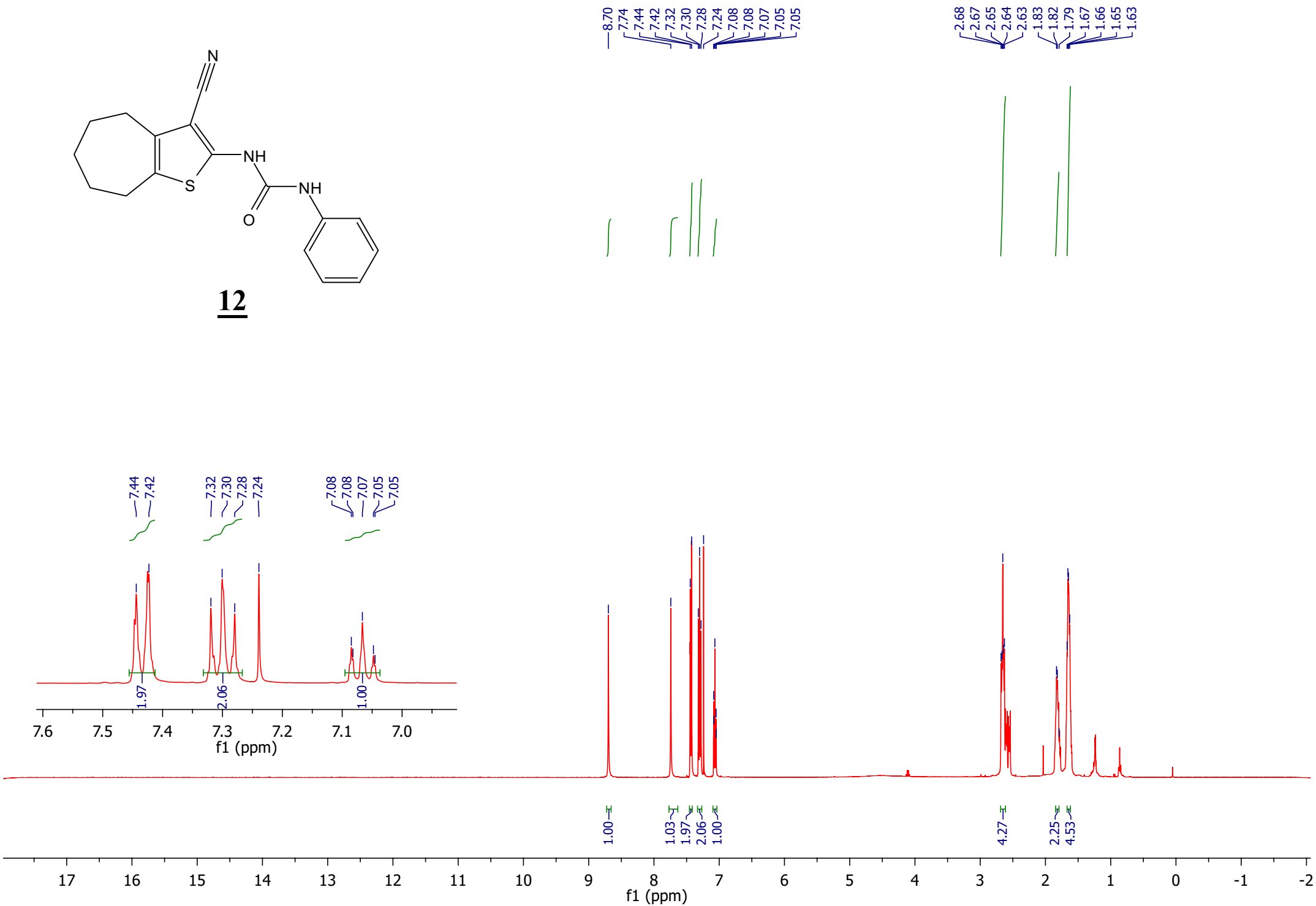


Figure S-24. ^{1}HNMR of compound 12

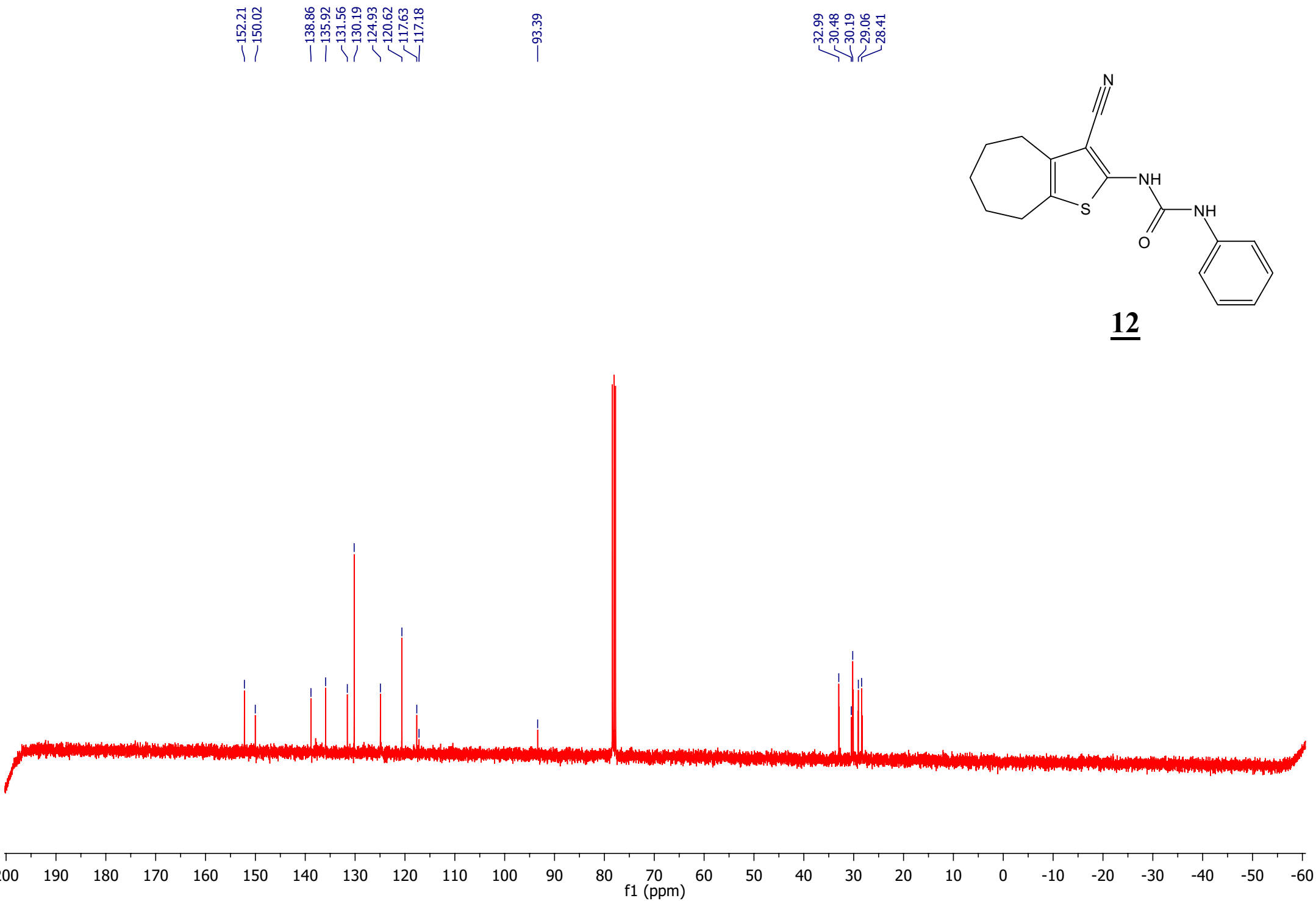


Figure S-25. ^{13}CNMR of compound 12

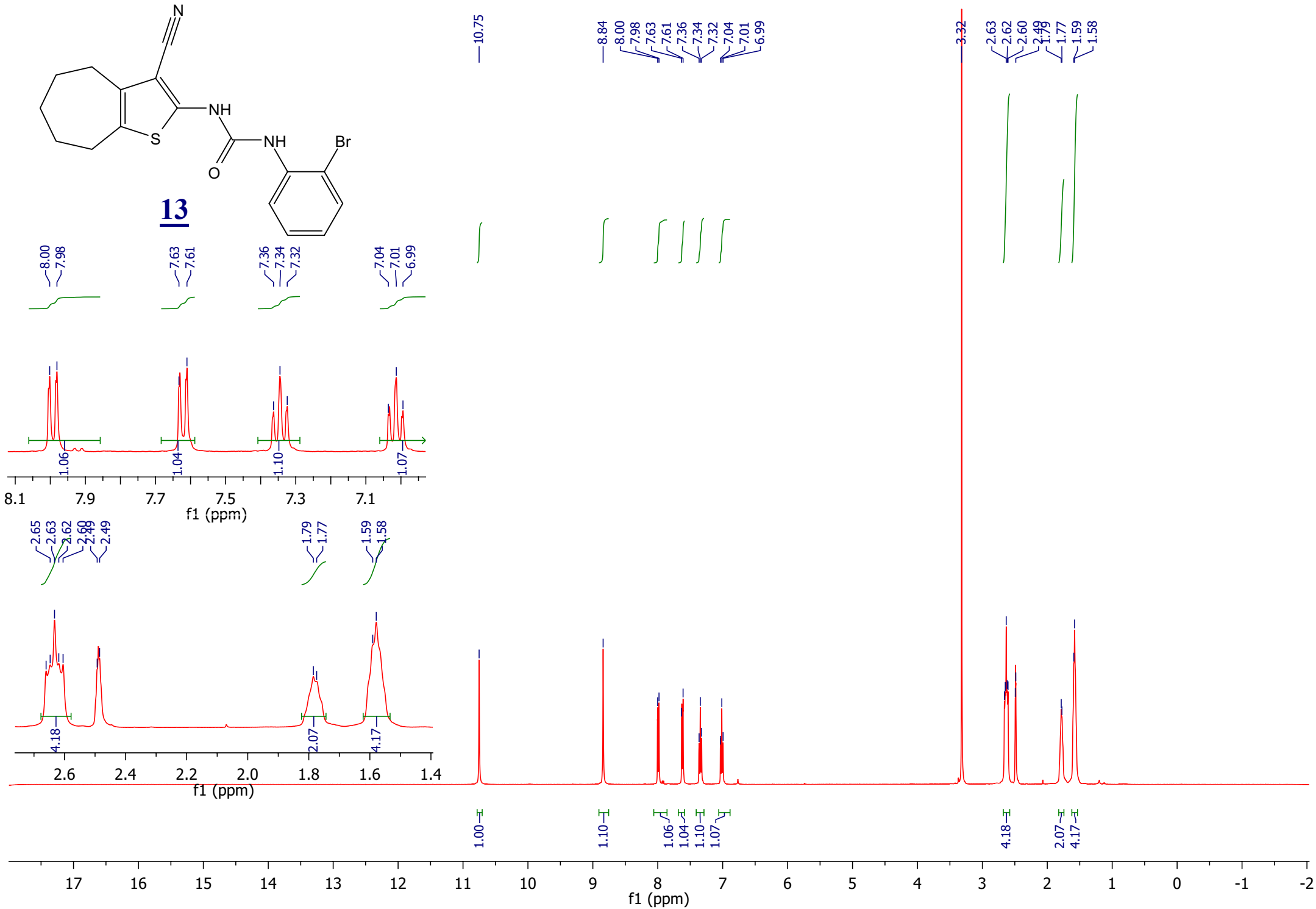


Figure S-26. ^{1}HNMR of compound 13

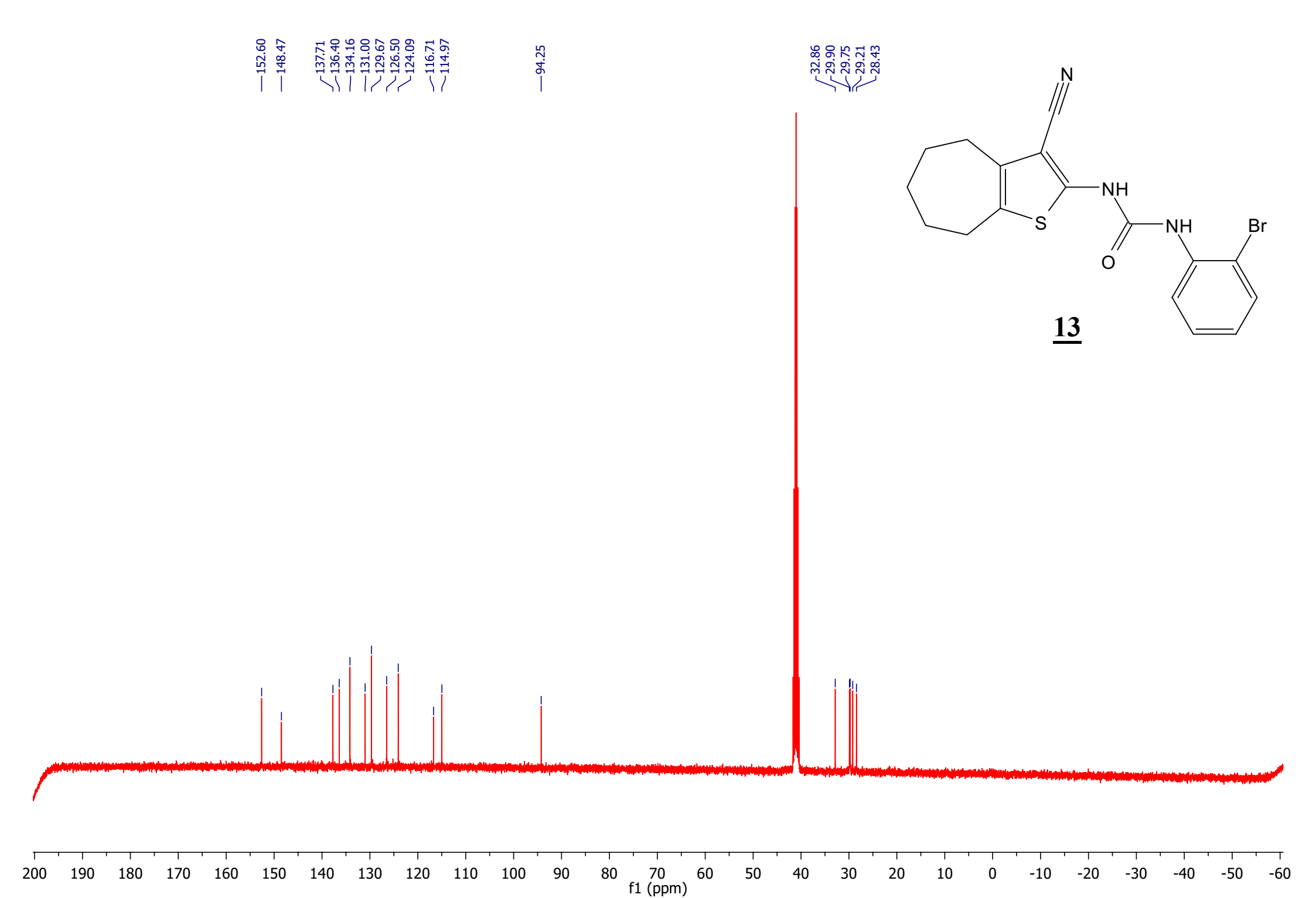


Figure S-27. ^{13}CNMR of compound 13

Elemental Composition Report

Single Mass Analysis

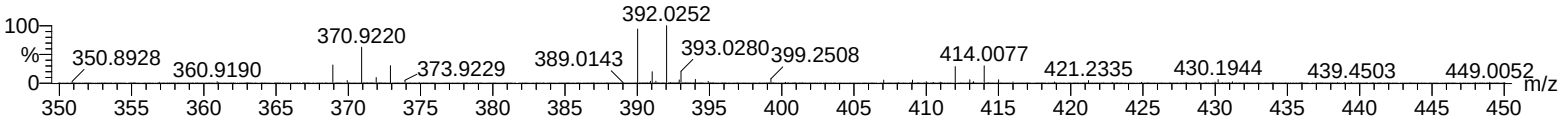
Tolerance = 5.0 mDa / DBE: min = -5.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions
416 formula(e) evaluated with 3 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 1-100 H: 1-200 N: 0-6 O: 0-6 S: 1-1 Br: 0-1

Salem/Abdelrahman
T01311943a 7 (0.255) Cm (5:13)

Sample #25

1: TOF MS ES+
1.39e+004



Minimum:				-5.0			
Maximum:		5.0	15.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
390.0275	390.0276	-0.1	-0.3	10.5	579.4	0.0	C17 H17 N3 O S Br
	390.0297	-2.2	-5.6	17.5	613.7	34.4	C18 H8 N5 O4 S
	390.0235	4.0	10.3	6.5	593.6	14.3	C12 H17 N5 O3 S Br

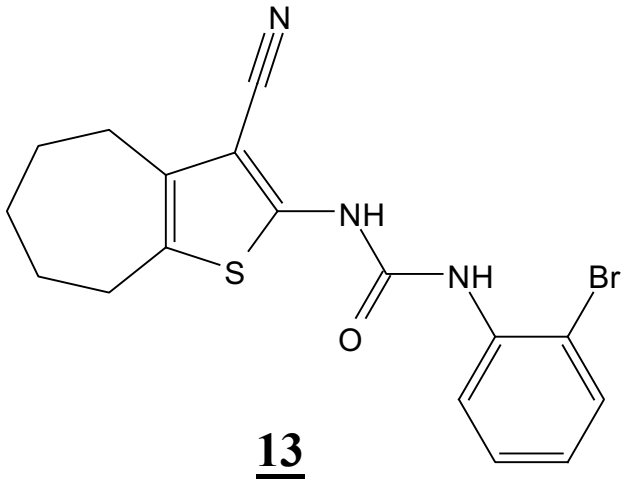


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Figure S-28. HRMS of compound 13

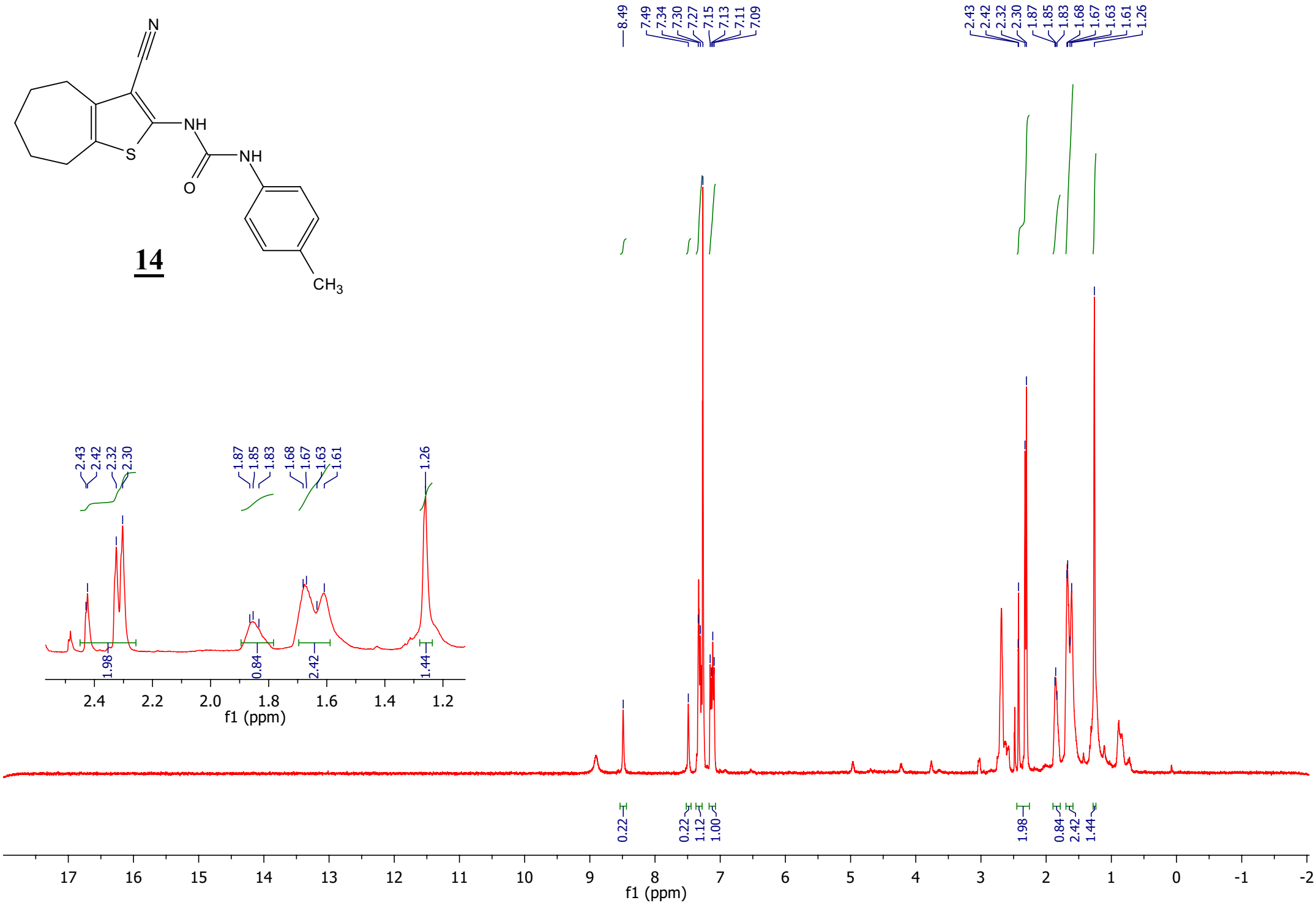


Figure S-29. ^{1}HNMR of compound 14

Elemental Composition Report

Single Mass Analysis

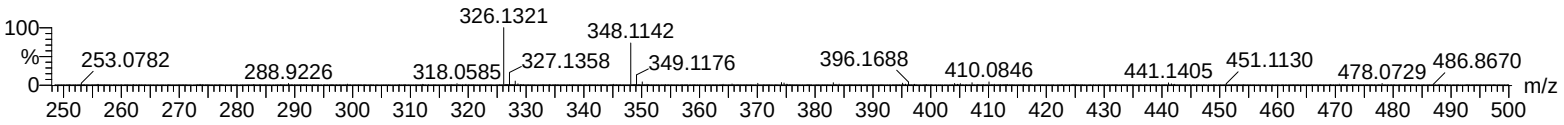
Tolerance = 5.0 mDa / DBE: min = -5.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions
339 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 1-100 H: 1-200 N: 0-6 O: 0-6 S: 1-1 Br: 0-1

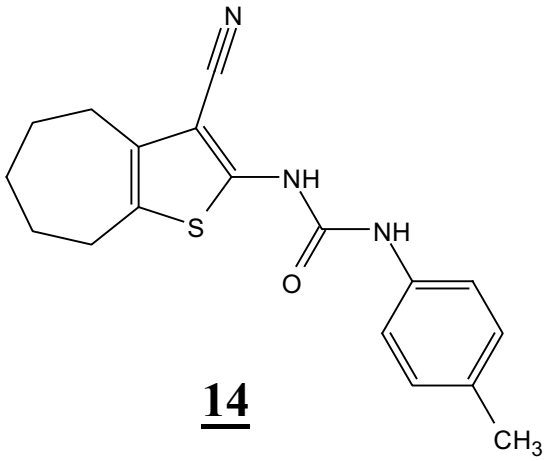
Salem/Abdelrahman
T01311970a 7 (0.255) Cm (5:13)

Sample #32

1: TOF MS ES+
4.27e+004



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
Minimum:				-5.0			
Maximum:		5.0	15.0	100.0			
326.1320	326.1327	-0.7	-2.1	10.5	730.1	0.0	C18 H20 N3 O S
	326.1287	3.3	10.1	6.5	740.9	10.9	C13 H20 N5 O3 S



14

Figure S-30. HRMS of compound 14

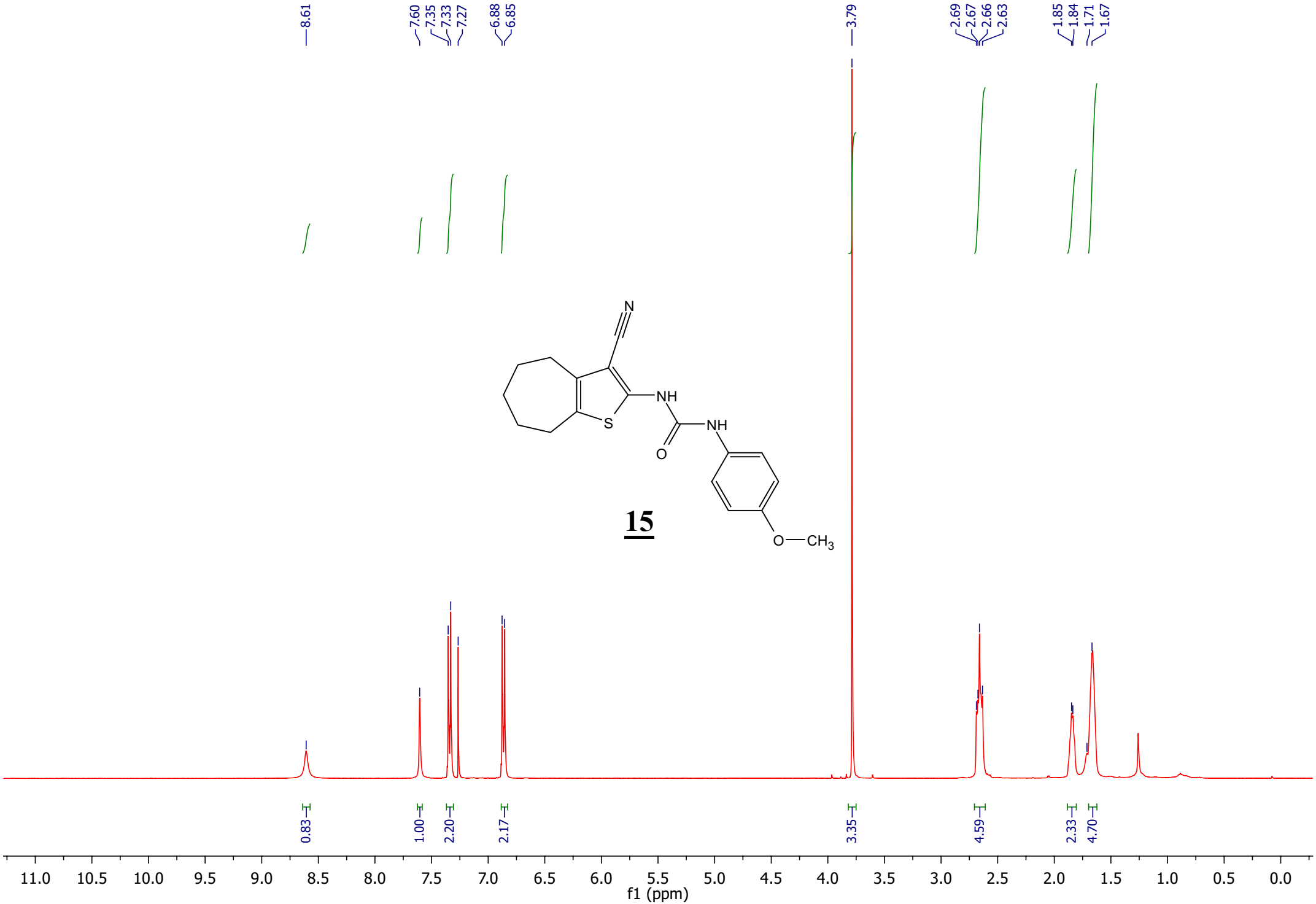


Figure S-31. ^{1}HNMR of compound 15

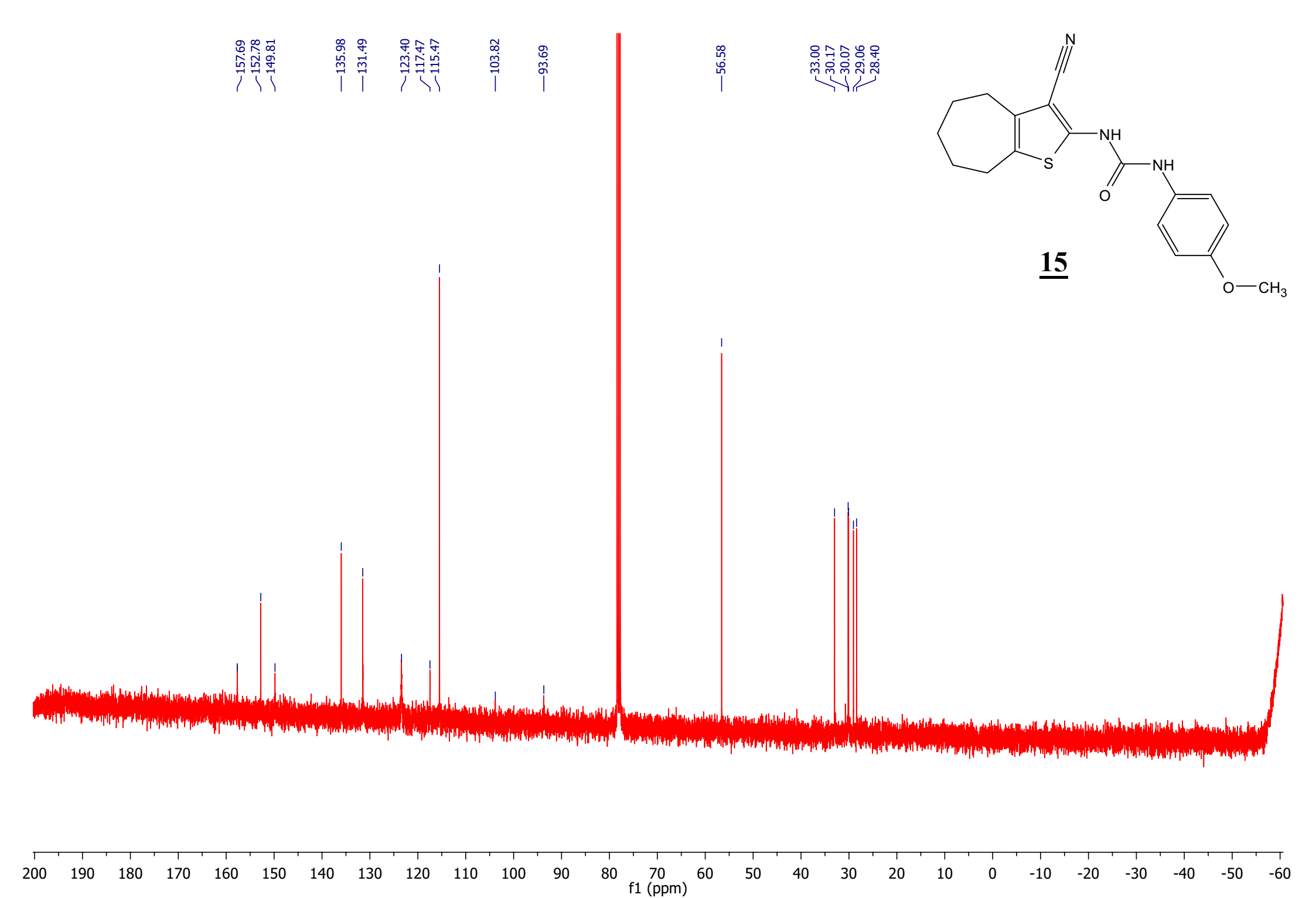


Figure S-32. ^{13}CNMR of compound 15

Elemental Composition Report

Single Mass Analysis

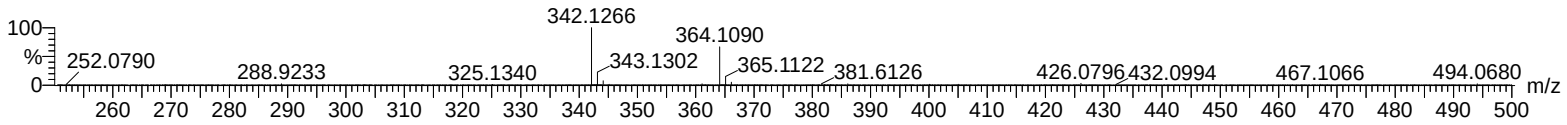
Tolerance = 5.0 mDa / DBE: min = -5.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions
359 formula(e) evaluated with 3 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 1-100 H: 1-200 N: 0-6 O: 0-6 S: 1-1 Br: 0-1

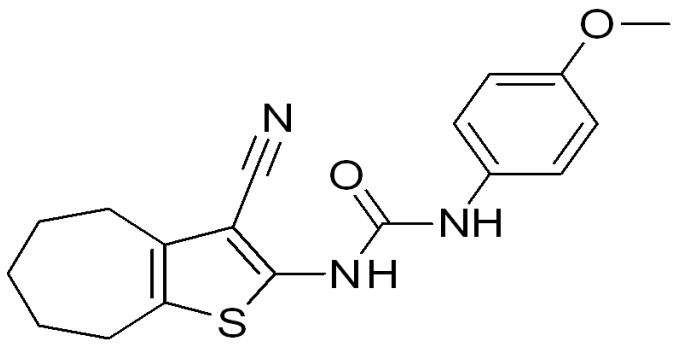
Salem/Abdelrahman
T01311947 7 (0.255) Cm (4:12)

Sample #26

1: TOF MS ES+
3.74e+004



Minimum:				-5.0			
Maximum:		5.0	15.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
342.1267	342.1276	-0.9	-2.6	10.5	656.1	0.0	C18 H20 N3 O2 S
	342.1236	3.1	9.1	6.5	667.2	11.0	C13 H20 N5 O4 S
	342.1316	-4.9	-14.3	14.5	665.9	9.7	C23 H20 N S



Chemical Formula: $C_{18}H_{19}N_3O_2S$

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Figure S-33. HRMS of compound 15

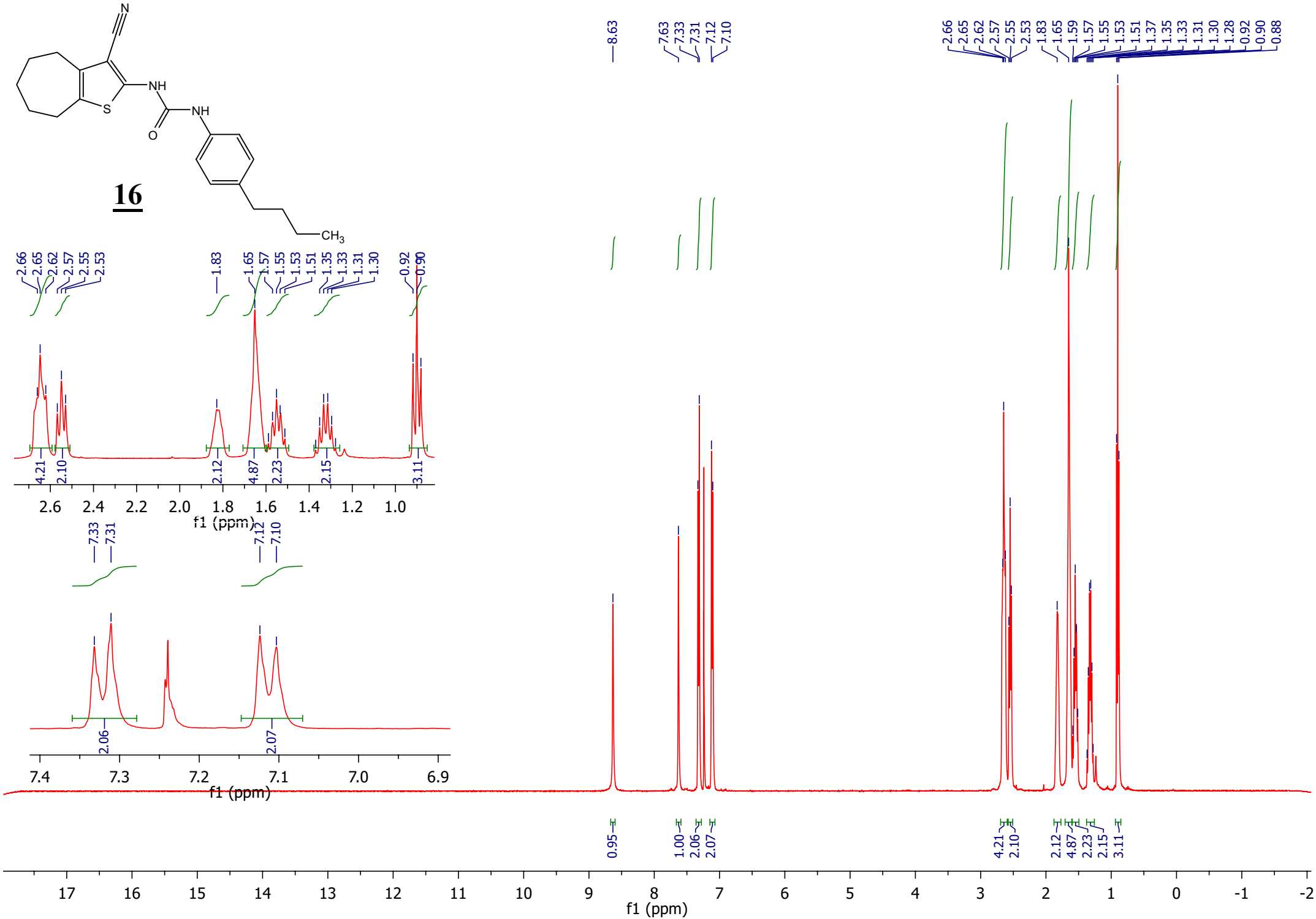


Figure S-34. ^{1}HNMR of compound 16

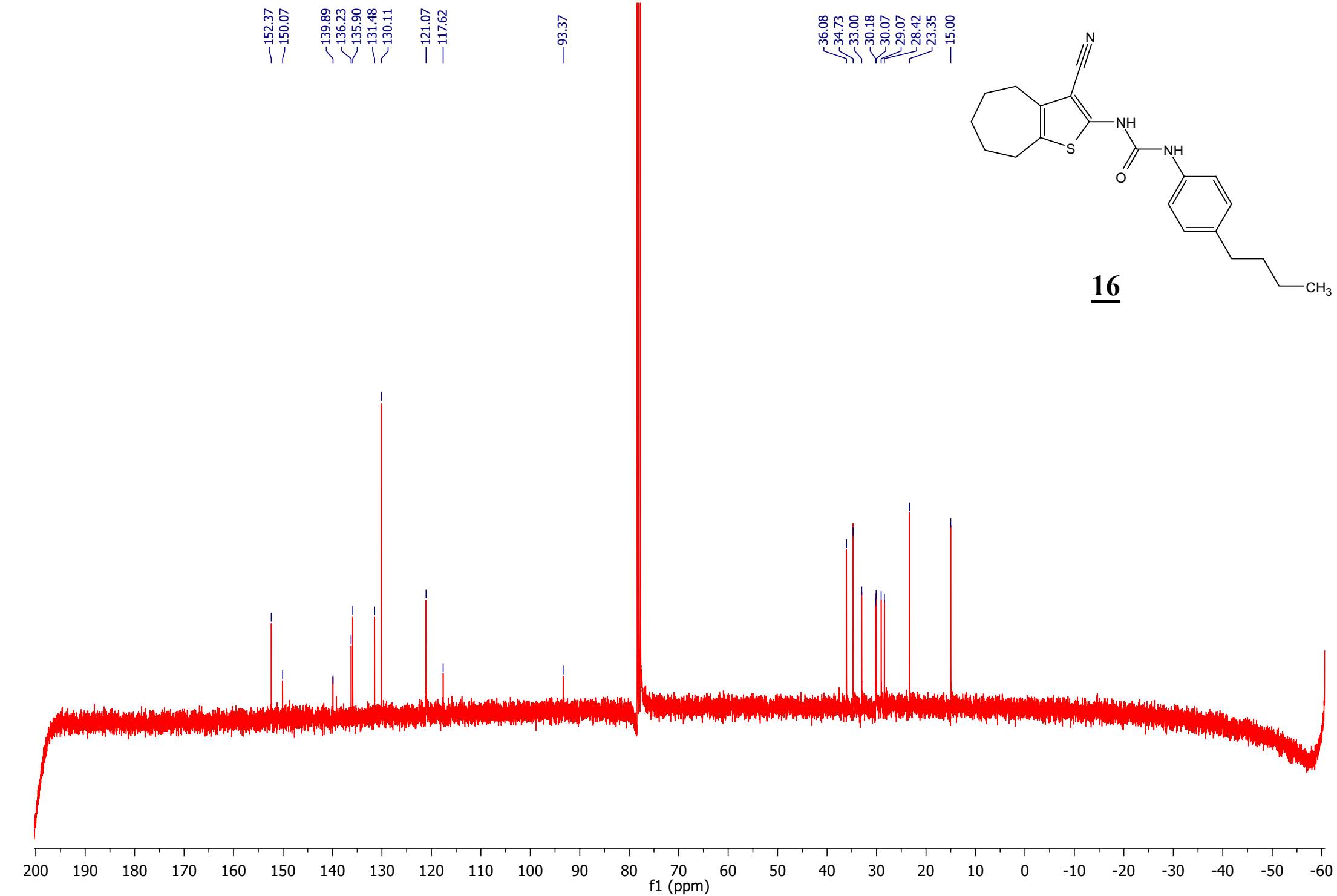


Figure S-35. ^{13}CNMR of compound 16

Elemental Composition Report

Single Mass Analysis

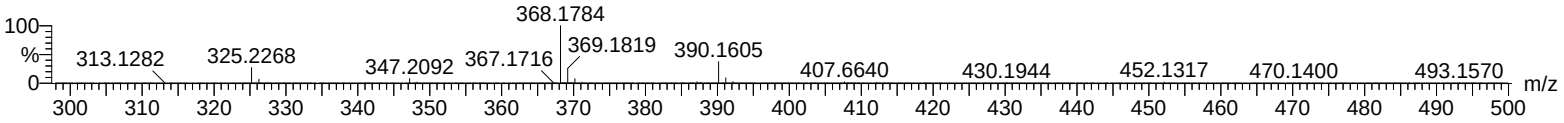
Tolerance = 5.0 mDa / DBE: min = -5.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions
388 formula(e) evaluated with 3 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 1-100 H: 1-200 N: 0-6 O: 0-6 S: 1-1 Br: 0-1

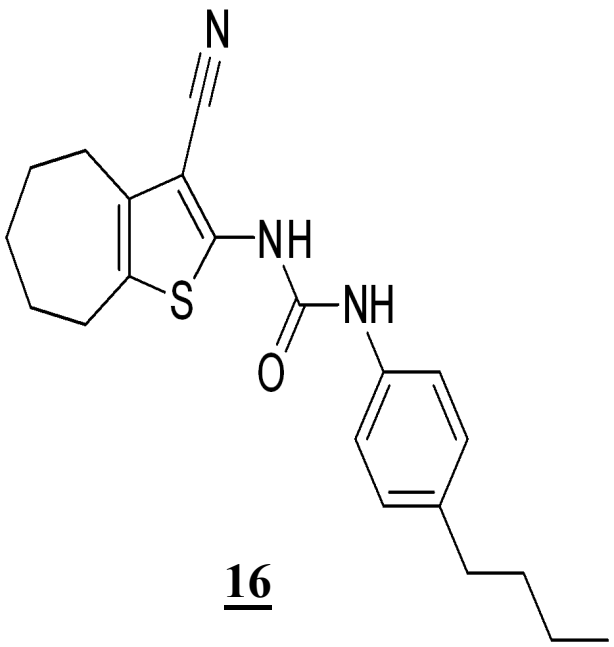
Salem/Abdelrahman
T01311951 7 (0.255) Cm (6:16)

Sample #27

1: TOF MS ES+
4.42e+004



Minimum:				-5.0			
Maximum:		5.0	15.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
368.1784	368.1797	-1.3	-3.5	10.5	666.0	0.0	C21 H26 N3 O S
	368.1756	2.8	7.6	6.5	679.8	13.8	C16 H26 N5 O3 S
	368.1735	4.9	13.3	-0.5	700.0	34.1	C15 H35 N3 S Br



16

Chemical Formula: $C_{21}H_{25}N_3OS$

Figure S-36. HRMS of compound 16

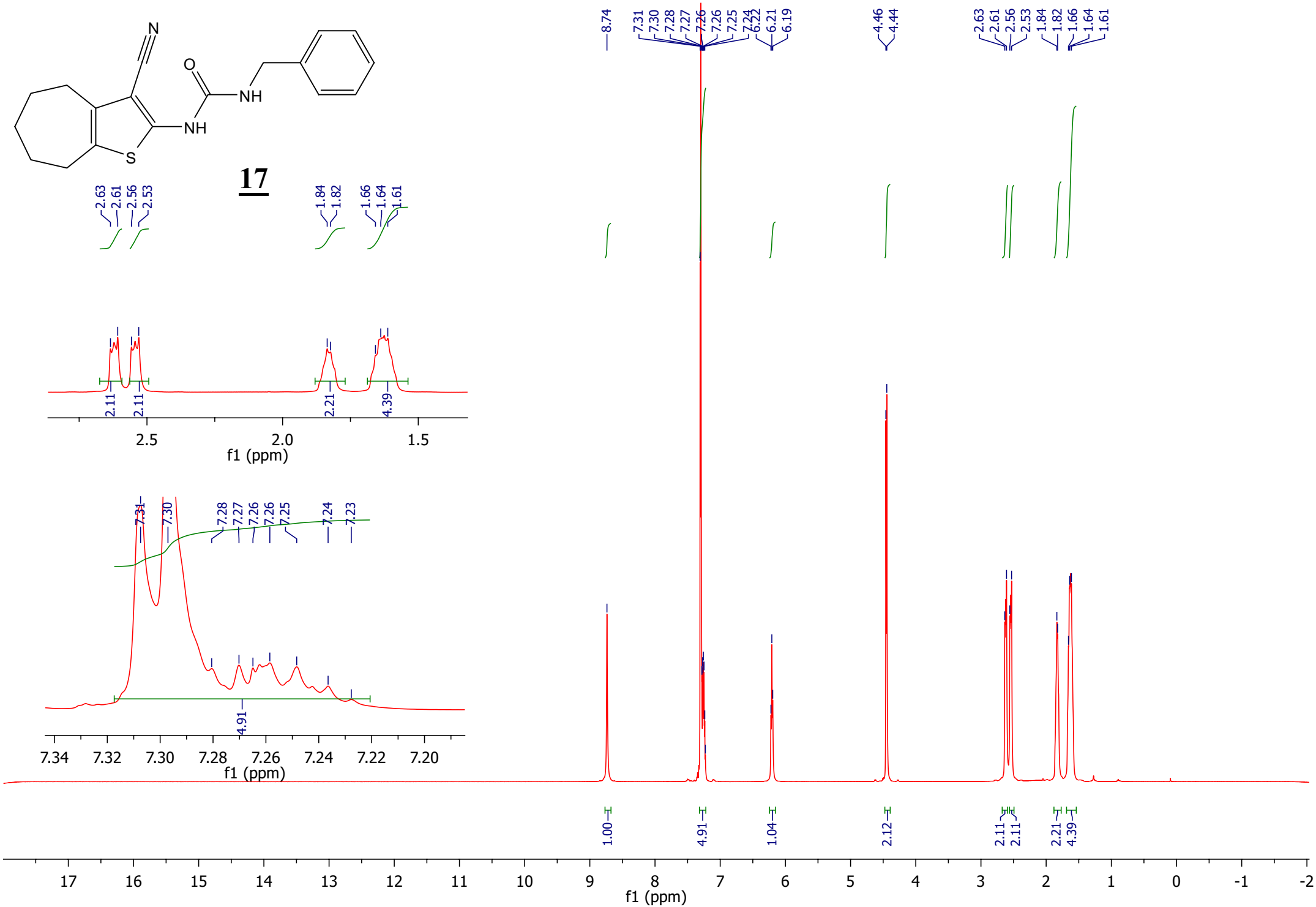


Figure S-37. ^{1}HNMR of compound 17

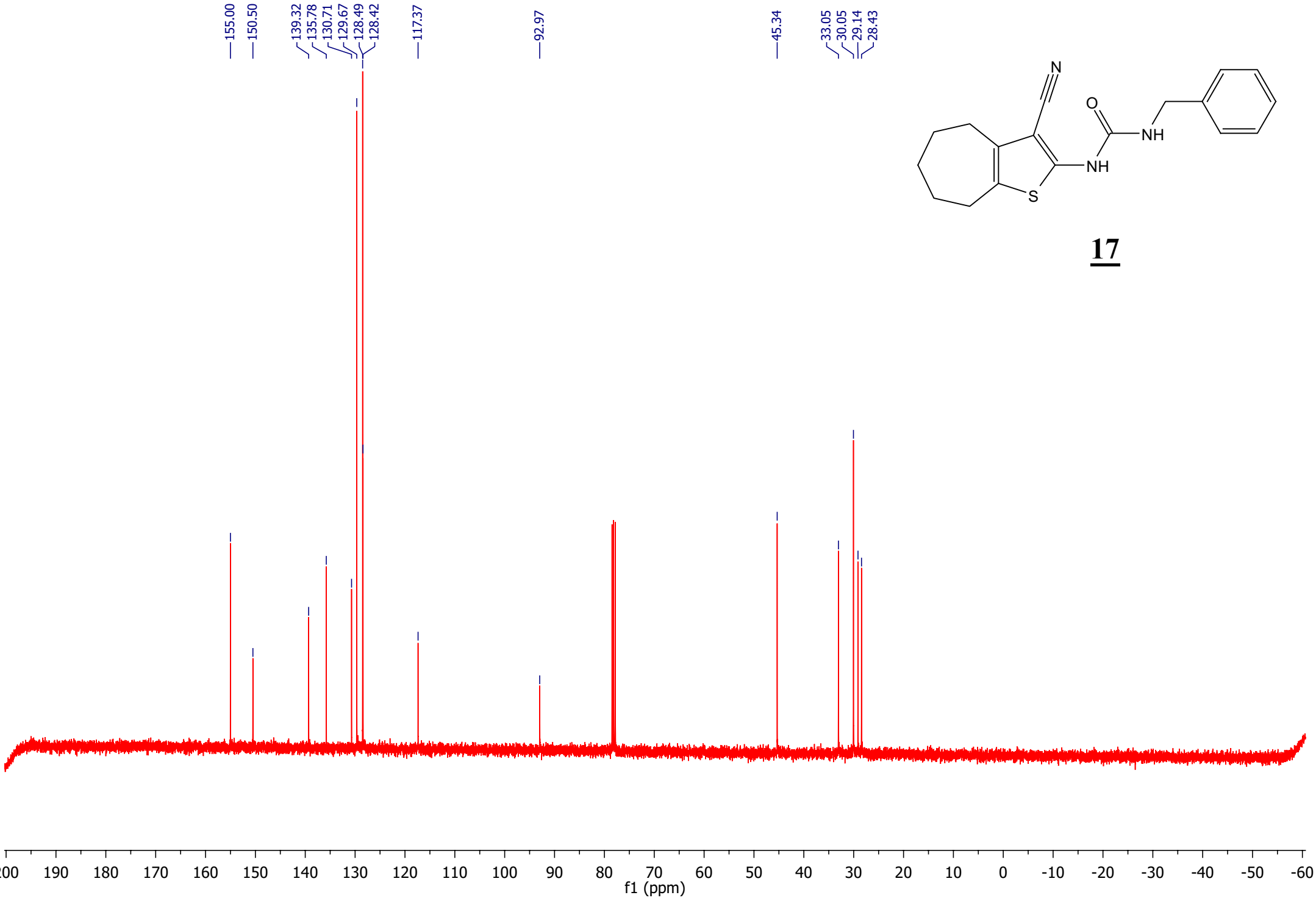


Figure S-38. ^{13}CNMR of compound 17

Elemental Composition Report

Single Mass Analysis

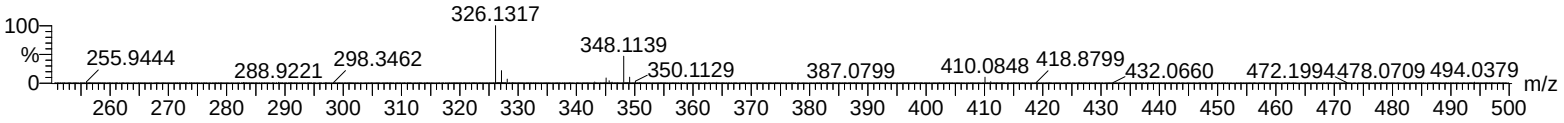
Tolerance = 5.0 mDa / DBE: min = -5.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions
339 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 1-100 H: 1-200 N: 0-6 O: 0-6 S: 1-1 Br: 0-1

Salem/Abdelrahman
T01311962 7 (0.255) Cm (4:12)

Sample #30

1: TOF MS ES+
4.48e+004



Minimum:				-5.0			
Maximum:		5.0	15.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
326.1317	326.1327	-1.0	-3.1	10.5	675.9	0.0	C18 H20 N3 O S
	326.1287	3.0	9.2	6.5	689.9	14.0	C13 H20 N5 O3 S

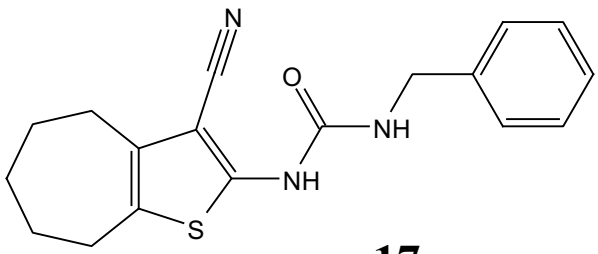


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Figure S-39. HRMS of compound 17