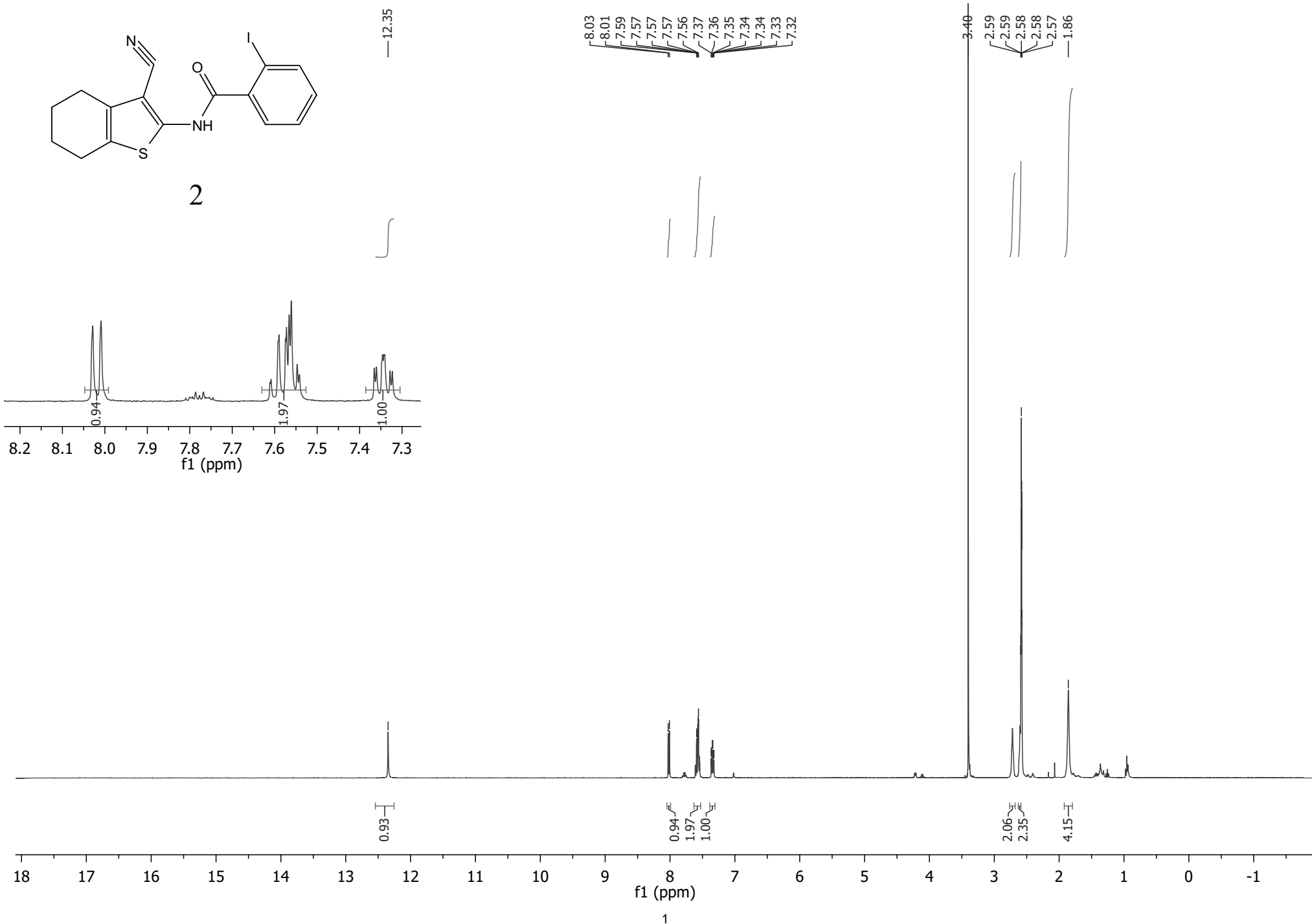
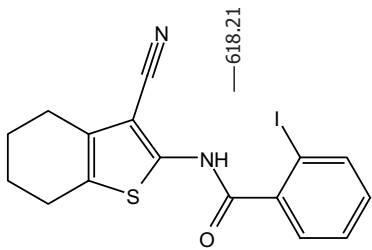
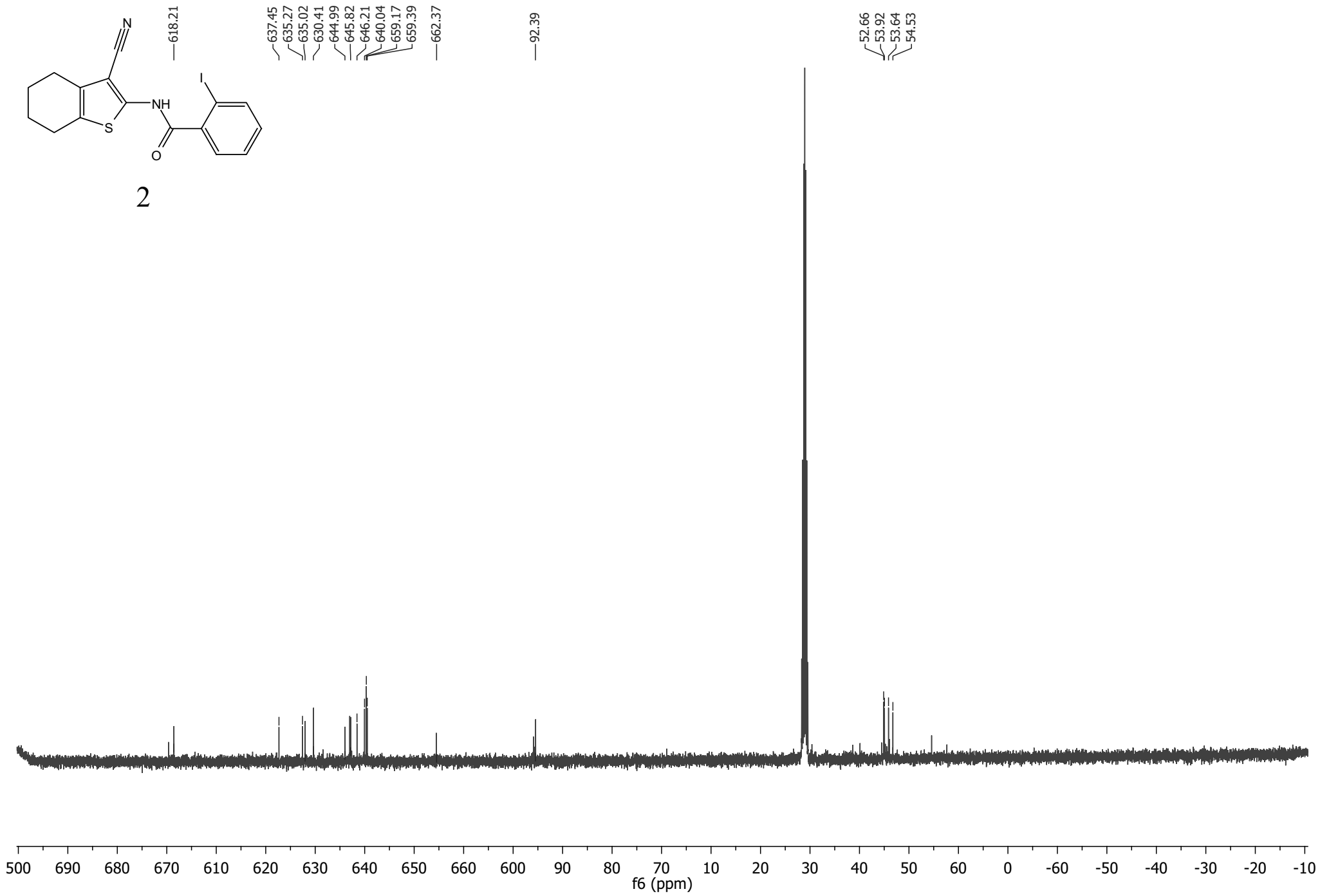


2





2



# 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

165 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)

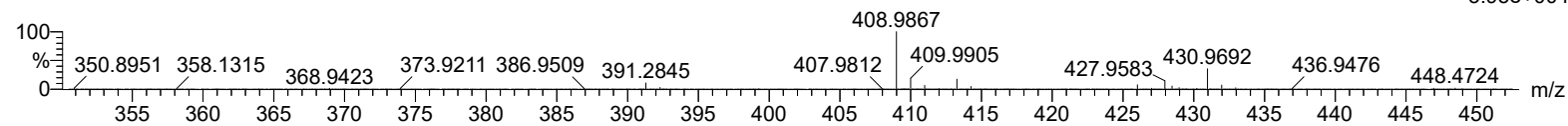
Elements Used:

C: 1-100 H: 1-200 N: 0-6 O: 0-6 S: 1-1 I: 1-1

Salem/Abdelrahman  
T01311922a 7 (0.255) Cm (5:11)

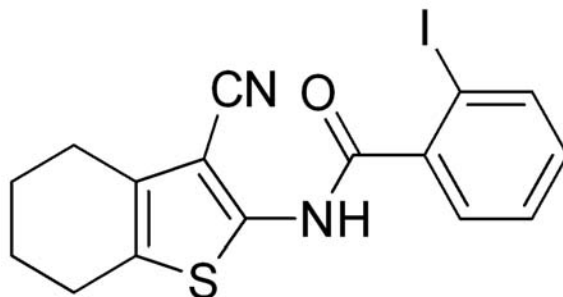
Sample #20

1: TOF MS ES+  
3.95e+004



Minimum: -5.0  
Maximum: 5.0 15.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
408.9867	408.9872	-0.5	-1.2	10.5	650.9	0.0	C16 H14 N2 O S I
	408.9831	3.6	8.8	6.5	662.9	12.1	C11 H14 N4 O3 S I



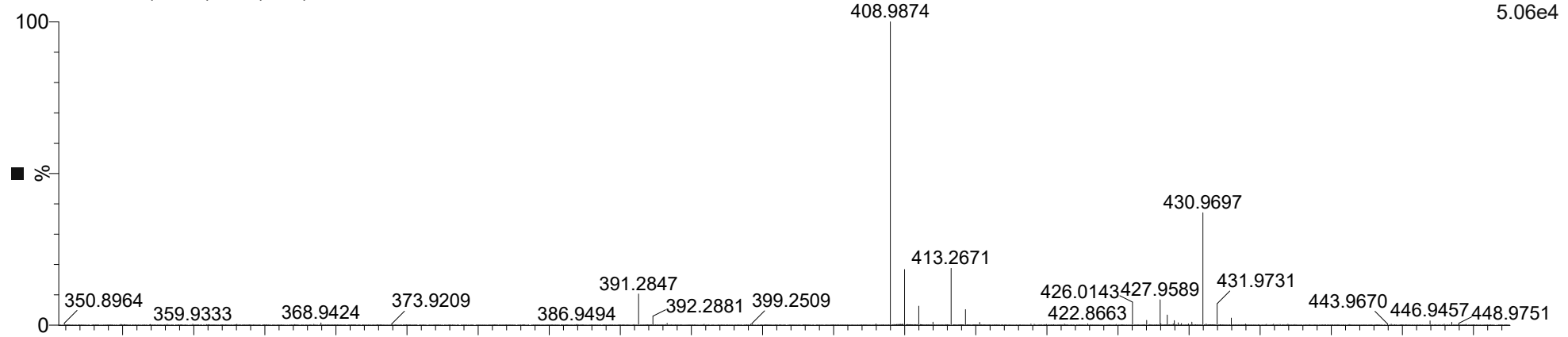
Chemical Formula:



Salem/Abdelrahman

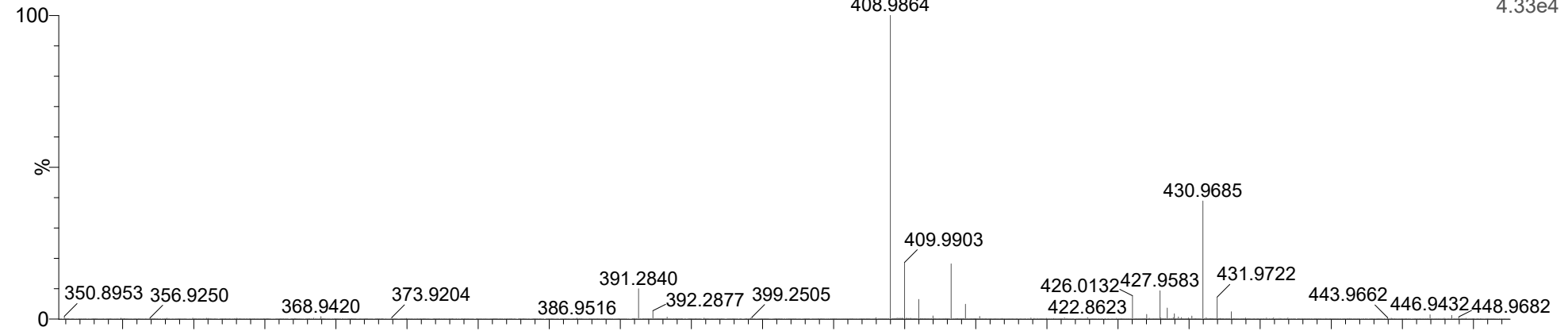
T01311924a 6 (0.222) Cm (5:12)

1: TOF MS ES+  
5.06e4



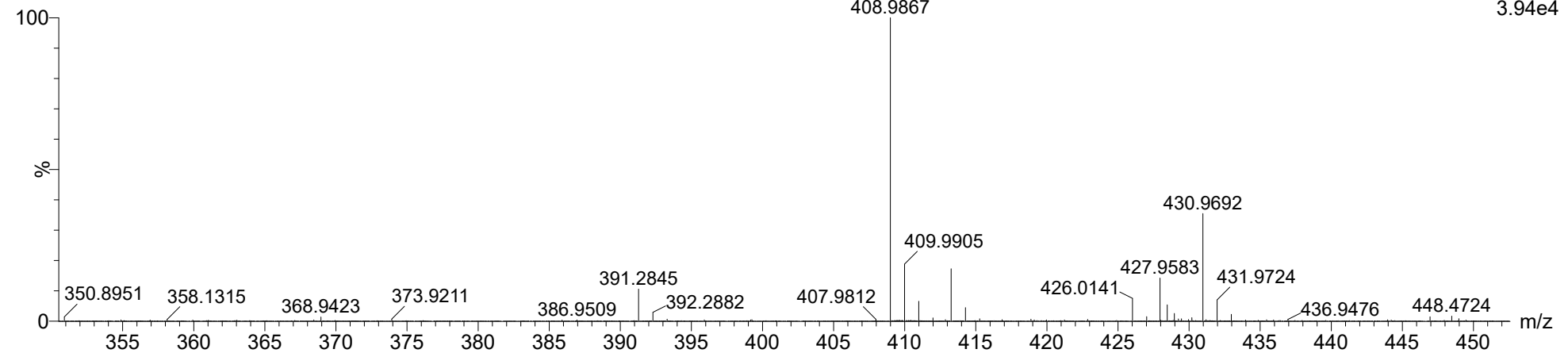
T01311923a 6 (0.221) Cm (5:11)

1: TOF MS ES+  
4.33e4

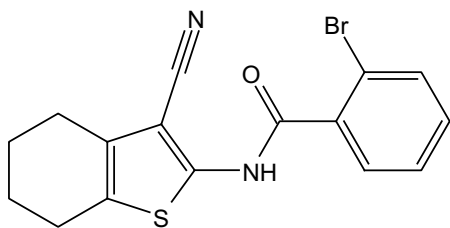


T01311922a 7 (0.255) Cm (5:11)

1: TOF MS ES+  
3.94e4



—12.29



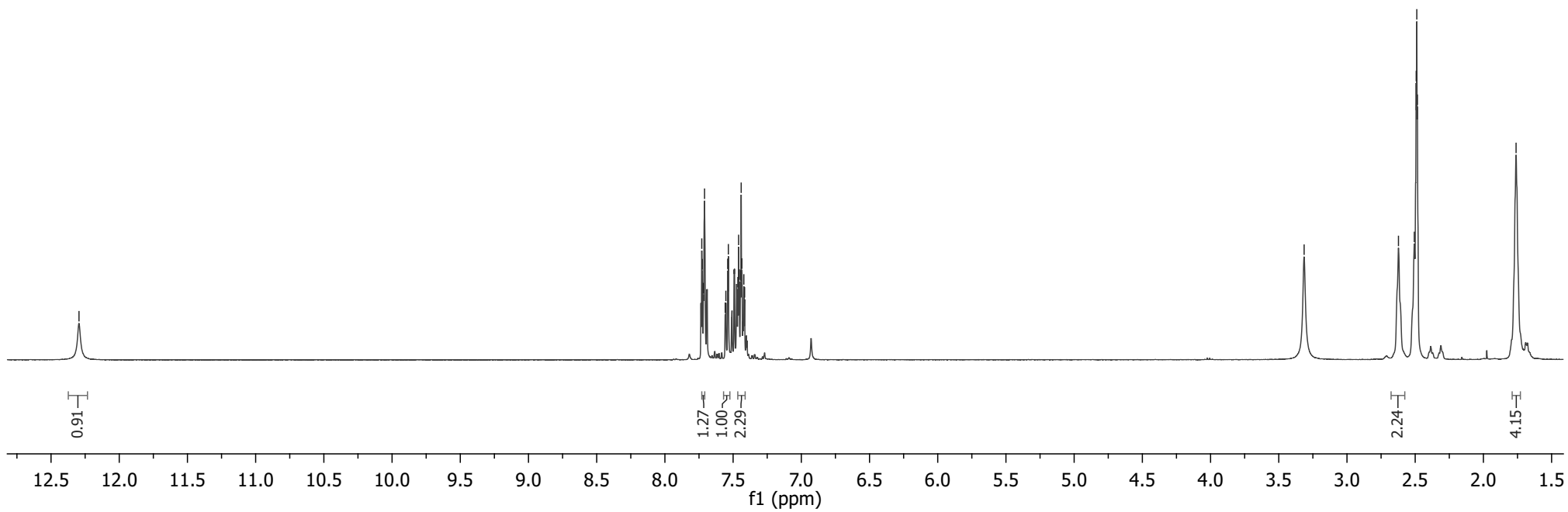
3

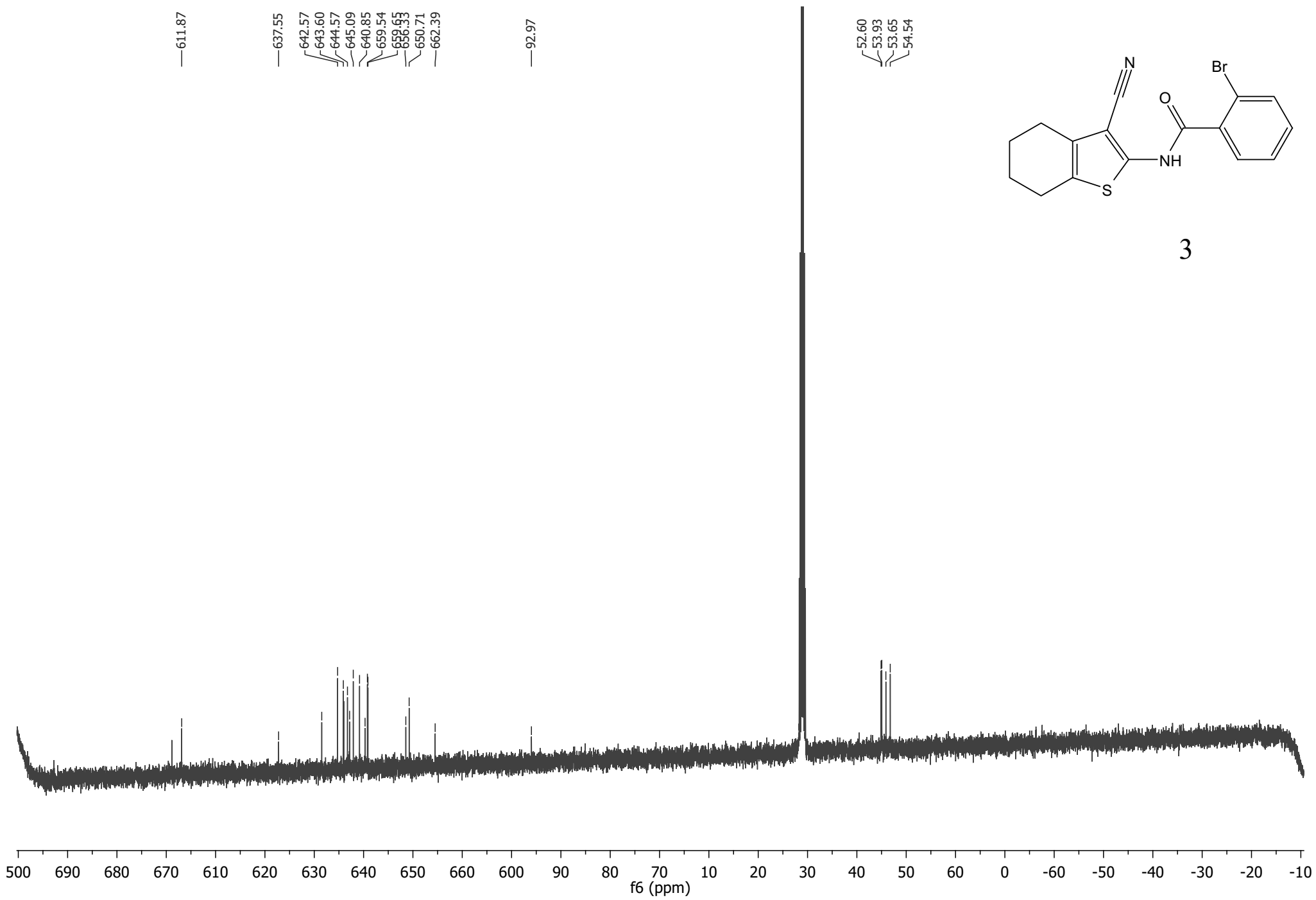
7.73  
7.73  
7.72  
7.71  
7.56  
7.55  
7.54  
7.53  
7.47  
7.46  
7.46  
7.45  
7.44  
7.44  
7.42  
7.42

—3.31

2.62  
2.51  
2.49  
2.48

—1.76





# 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 5 results within limits (all results (up to 1000) for each mass)

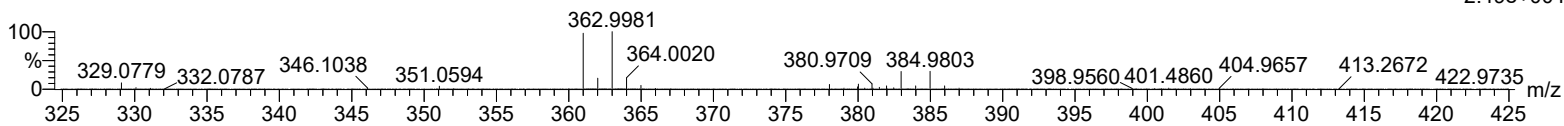
Elements Used:

C: 1-100 H: 1-200 N: 0-6 O: 0-6 S: 1-1 Br: 0-1

Salem/Abdelrahman  
T01311910a 8 (0.289) Cm (8:15)

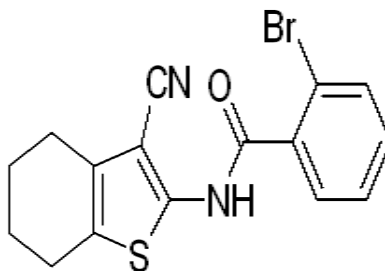
Sample #17

1: TOF MS ES+  
2.49e+004

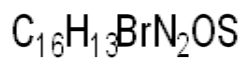


Minimum: -5.0  
Maximum: 5.0 15.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
361.0001	361.0010	-0.9	-2.5	10.5	682.0	0.0	C16 H14 N2 O S Br
	360.9991	1.0	2.8	13.5	716.0	34.0	C12 H5 N6 O6 S
	360.9970	3.1	8.6	6.5	699.4	17.4	C11 H14 N4 O3 S Br
	361.0032	-3.1	-8.6	17.5	716.6	34.6	C17 H5 N4 O4 S
	360.9959	4.2	11.6	21.5	717.7	35.7	C23 H5 O3 S



Chemical Formula:

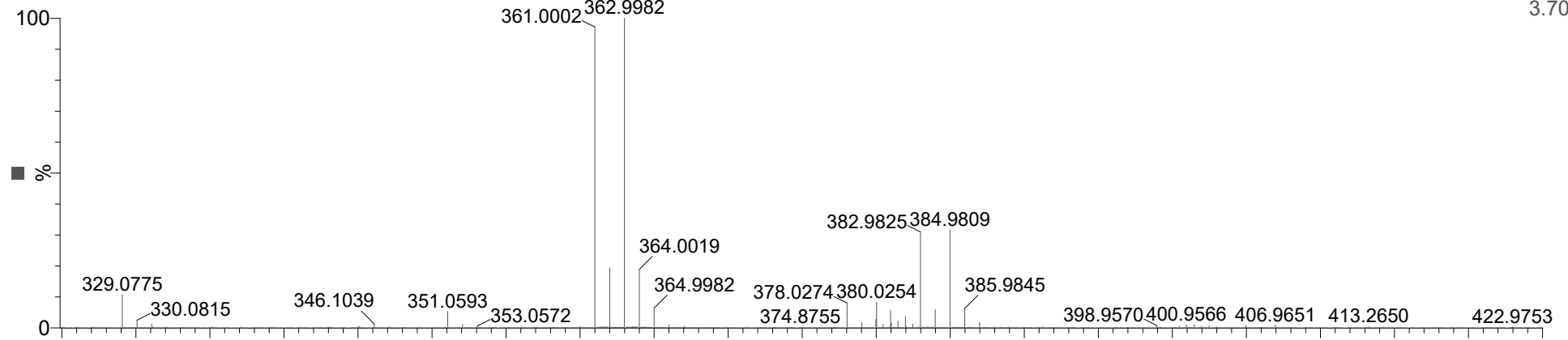


3

Salem/Abdelrahman

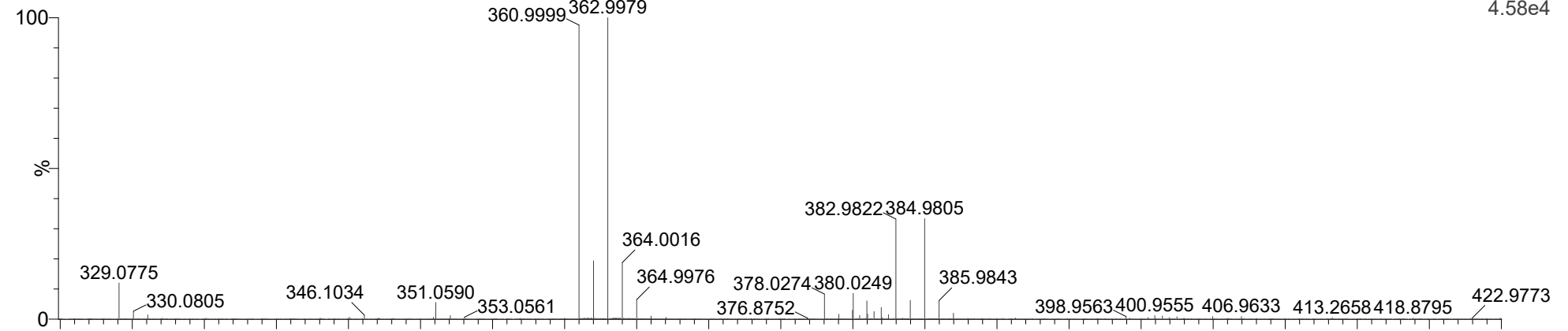
T01311912a 8 (0.289) Cm (7:16)

1: TOF MS ES+  
3.70e4



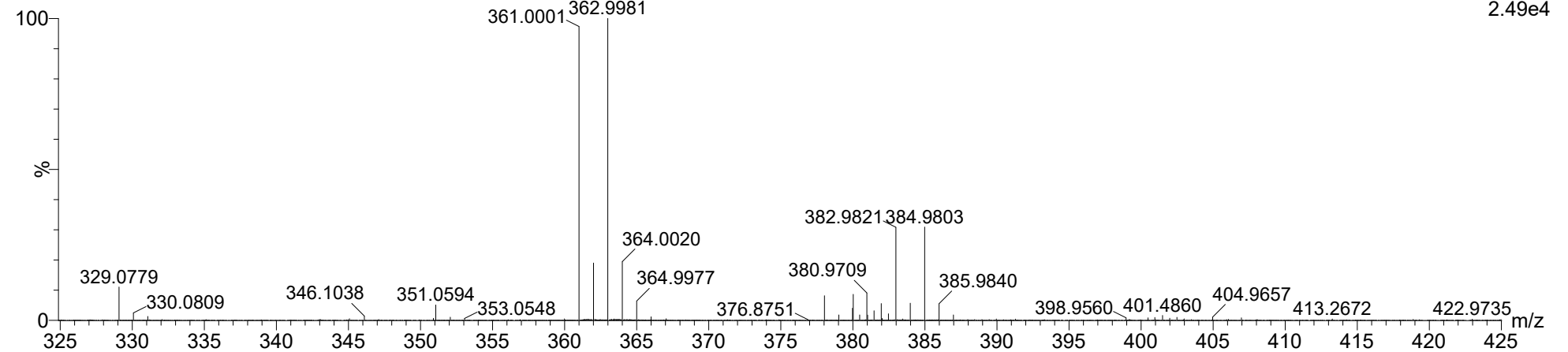
T01311911a 7 (0.255) Cm (5:15)

1: TOF MS ES+  
4.58e4

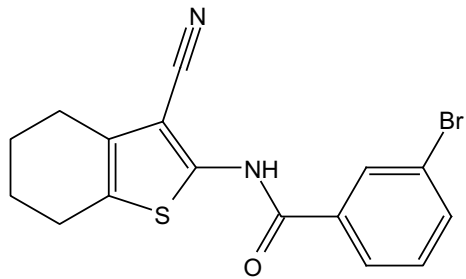


T01311910a 8 (0.289) Cm (8:15)

1: TOF MS ES+  
2.49e4





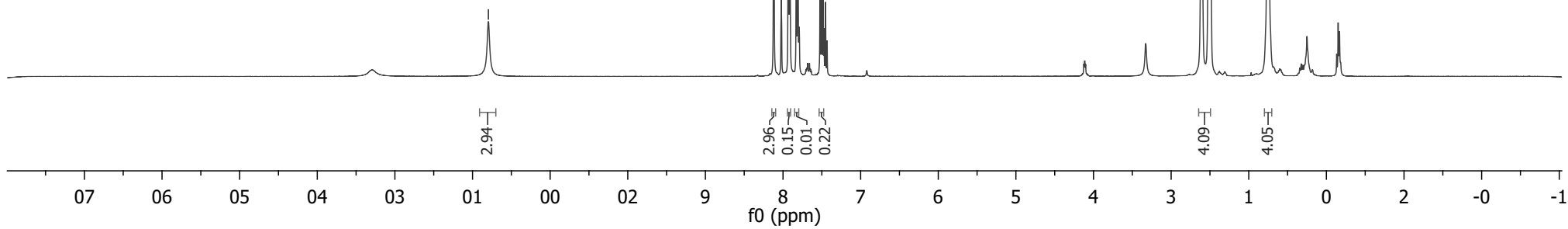
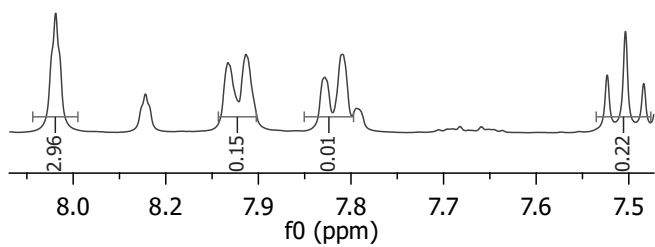
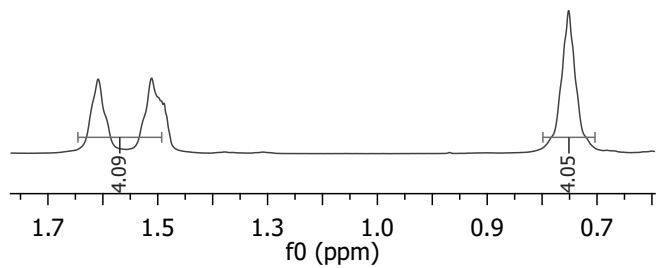


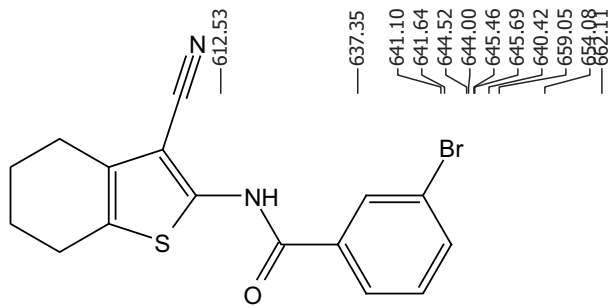
4

—00.82

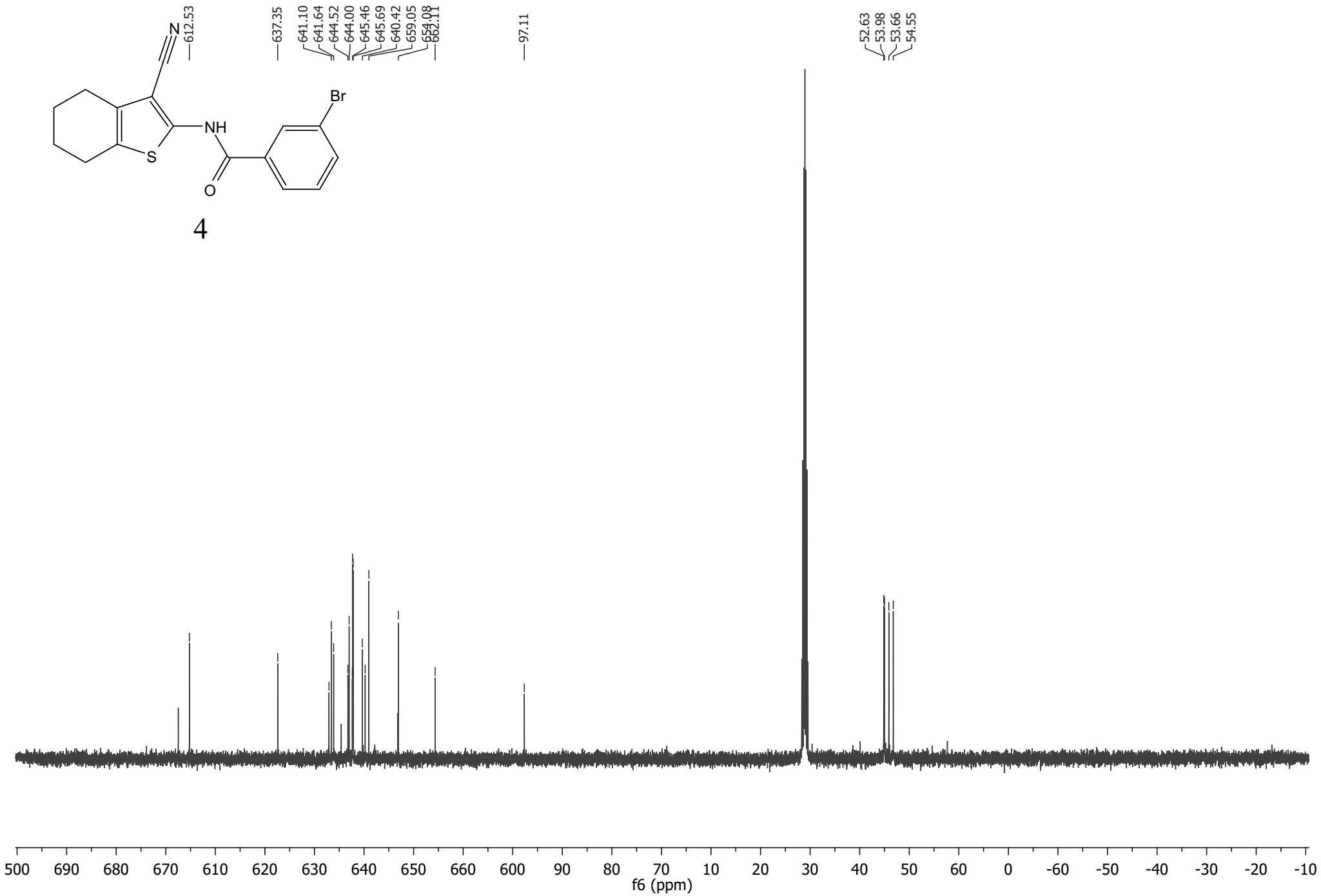
8.01  
7.93  
7.90  
7.83  
7.80  
7.80  
7.51  
7.52  
7.48

1.60  
1.50  
1.49  
1.49  
—0.75





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

384 formula(e) evaluated with 5 results within limits (all results (up to 1000) for each mass)

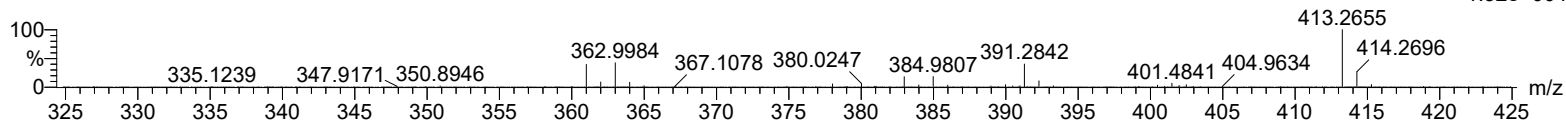
Elements Used:

C: 1-100 H: 1-200 N: 0-6 O: 0-6 S: 1-1 Br: 0-1

Salem/Abdelrahman  
T01311916a 6 (0.222) Cm (5:12)

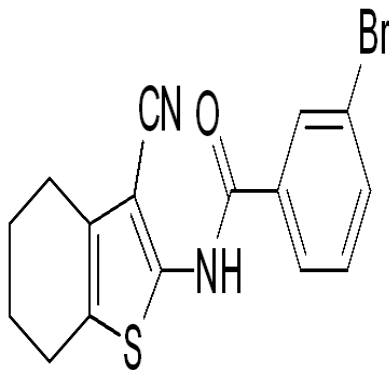
Sample #18

1: TOF MS ES+  
1.32e+004



Minimum: -5.0  
Maximum: 5.0 15.0 100.0

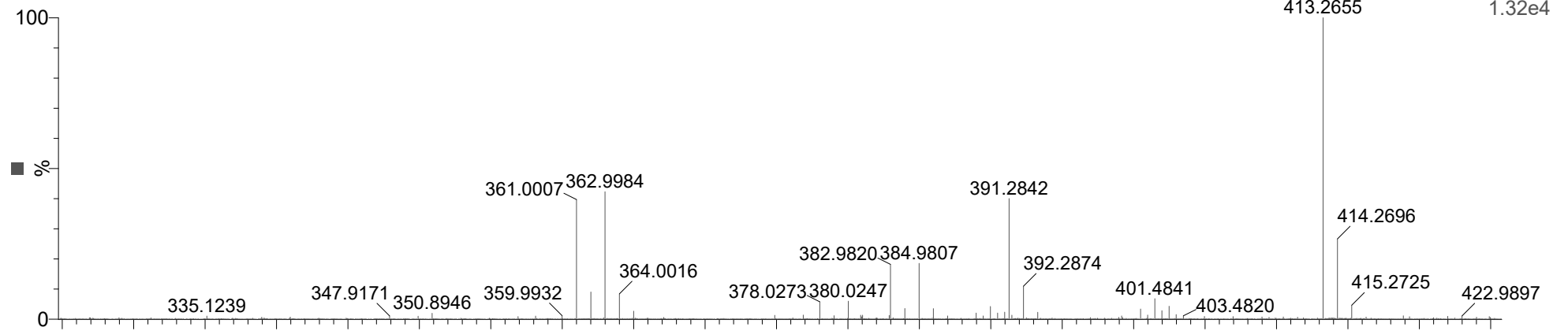
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
361.0006	361.0010	-0.4	-1.1	10.5	475.2	0.0	C16 H14 N2 O S Br
	360.9991	1.5	4.2	13.5	498.6	23.4	C12 H5 N6 O6 S
	361.0032	-2.6	-7.2	17.5	499.6	24.4	C17 H5 N4 O4 S
	360.9970	3.6	10.0	6.5	482.9	7.7	C11 H14 N4 O3 S Br
	360.9959	4.7	13.0	21.5	500.8	25.6	C23 H5 O3 S



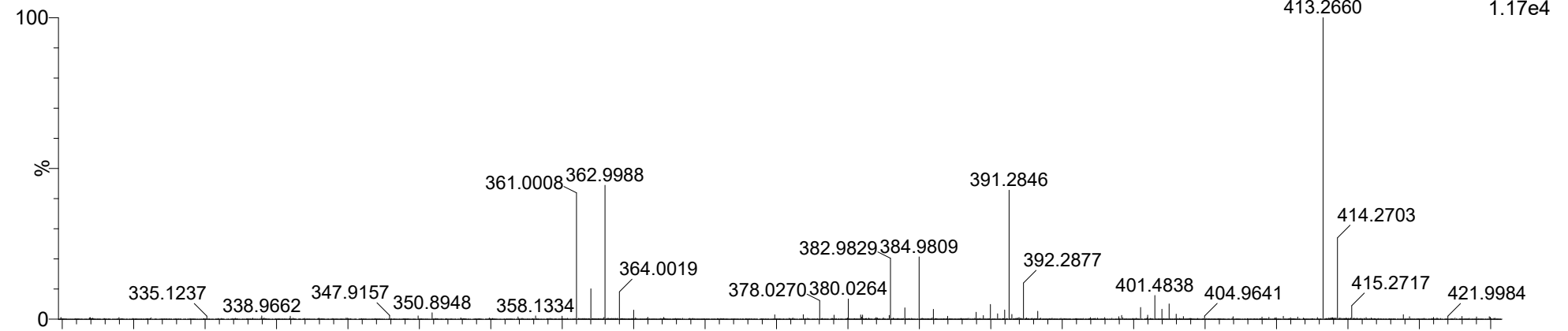
Chemical Formula: C<sub>16</sub>H<sub>13</sub>BrN<sub>2</sub>OS

Salem/Abdelrahman

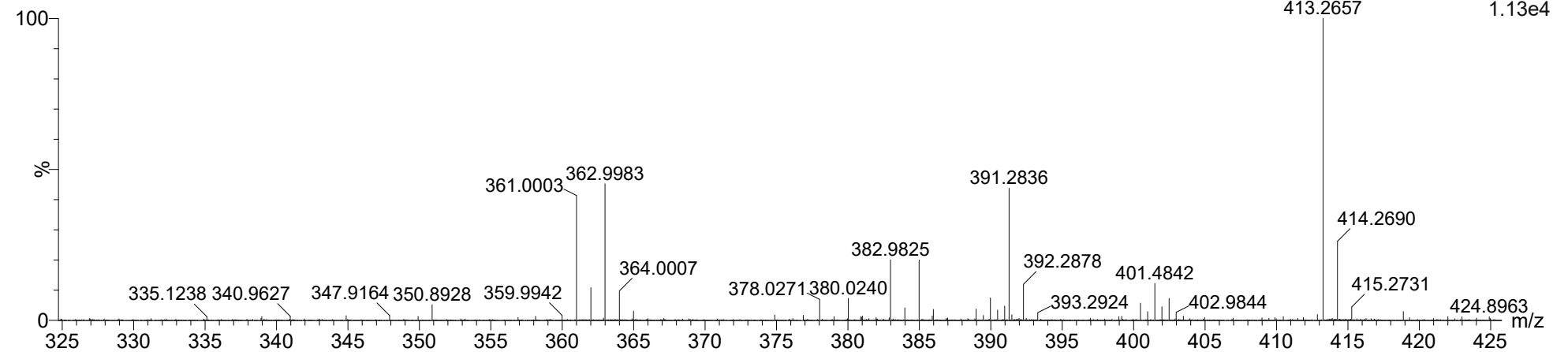
T01311916a 6 (0.222) Cm (5:12)

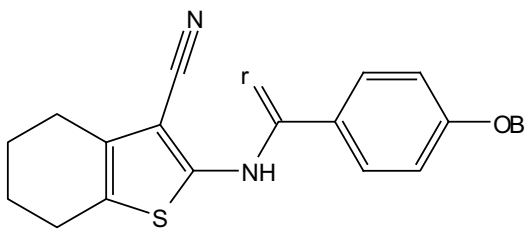


T01311915a 6 (0.222) Cm (5:12)

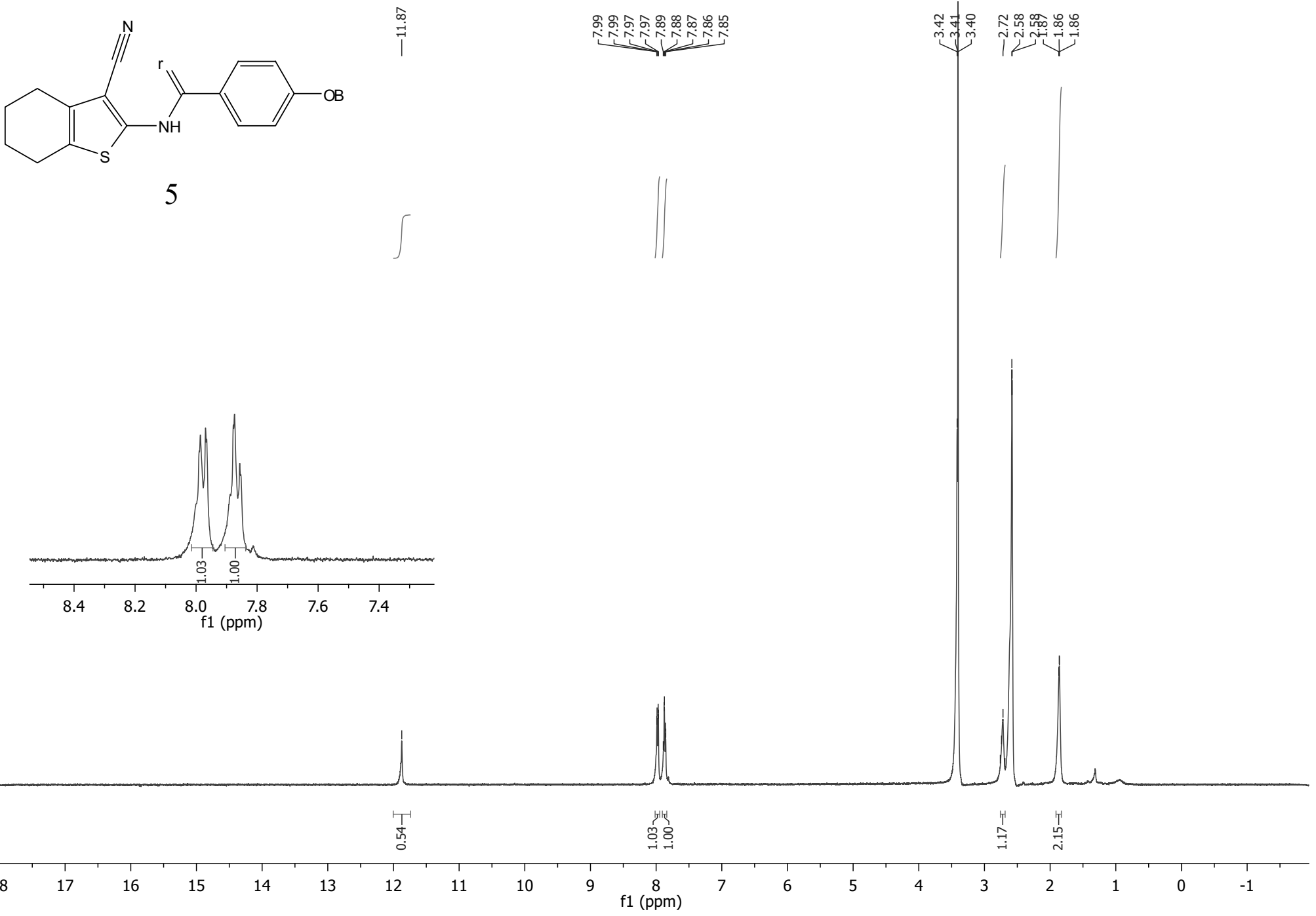


T01311914a 6 (0.221) Cm (4:12)





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

384 formula(e) evaluated with 4 results within limits (all results (up to 1000) for each mass)

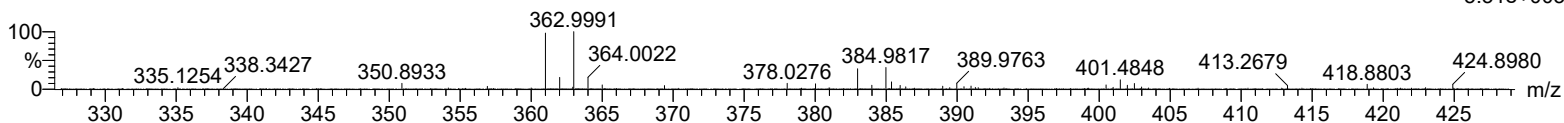
Elements Used:

C: 1-100 H: 1-200 N: 0-6 O: 0-6 S: 1-1 Br: 0-1

Salem/Abdelrahman  
T01311920a 6 (0.222) Cm (5:11)

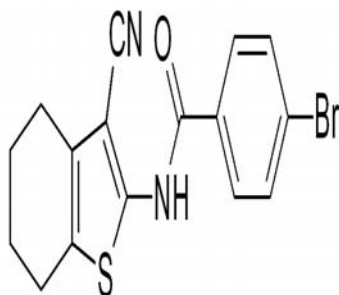
Sample #19

1: TOF MS ES+  
5.31e+003



Minimum: -5.0  
Maximum: 5.0 15.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
361.0012	361.0010	0.2	0.6	10.5	478.1	0.0	C16 H14 N2 O S Br
	361.0032	-2.0	-5.5	17.5	503.1	25.1	C17 H5 N4 O4 S
	360.9991	2.1	5.8	13.5	501.8	23.8	C12 H5 N6 O6 S
	360.9970	4.2	11.6	6.5	489.0	11.0	C11 H14 N4 O3 S Br



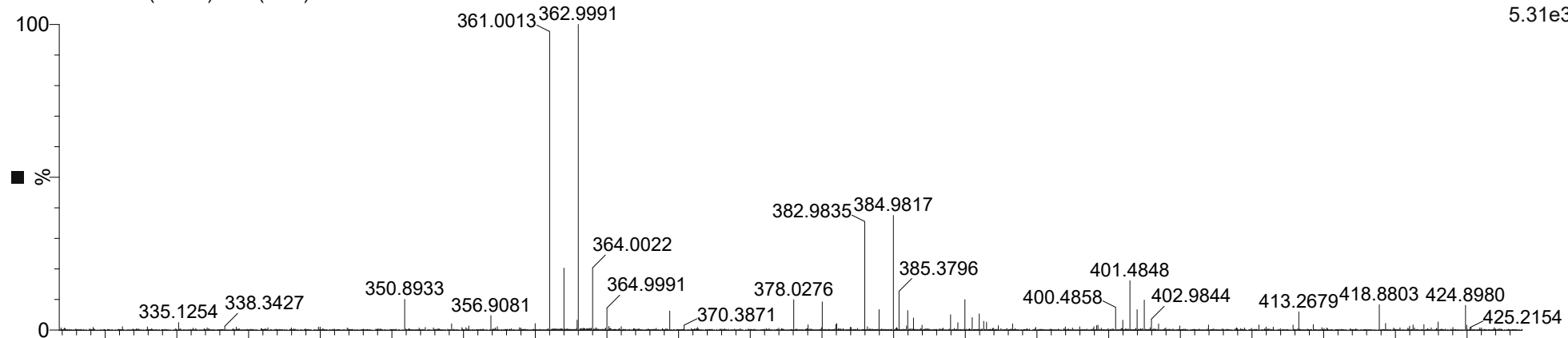
Chemical Formula: C<sub>16</sub>H<sub>13</sub>BrN<sub>2</sub>OS

5

Salem/Abdelrahman

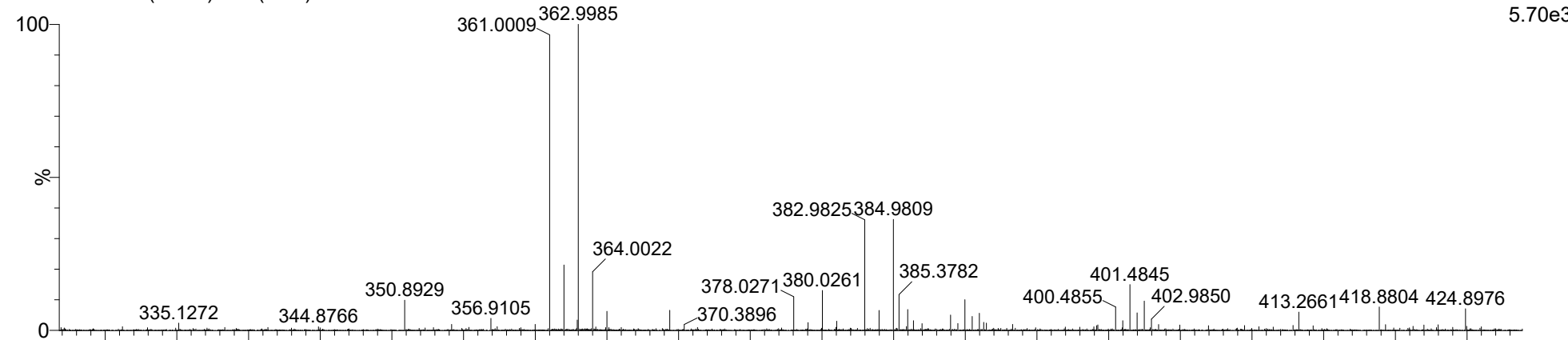
T01311920a 6 (0.222) Cm (5:11)

1: TOF MS ES+  
5.31e3



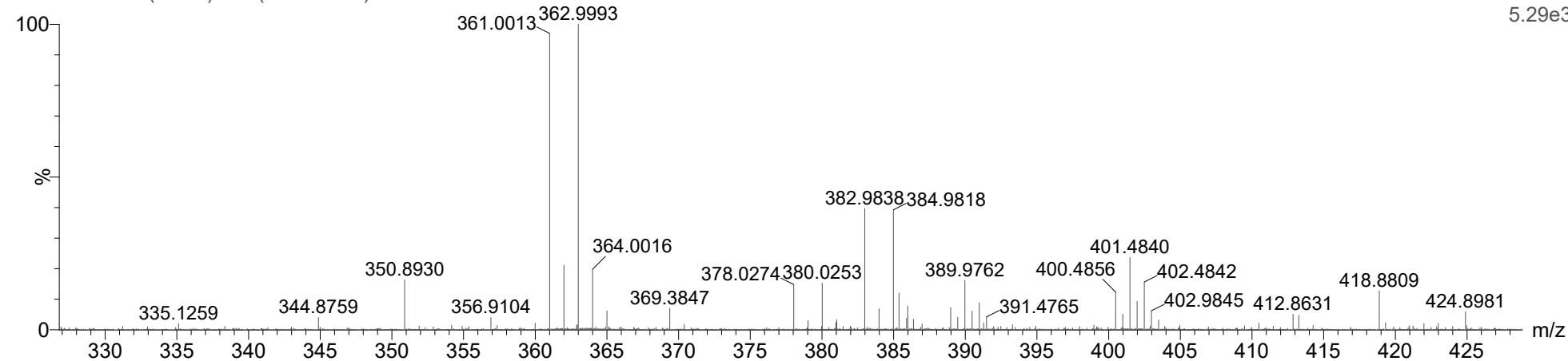
T01311919a 6 (0.222) Cm (5:12)

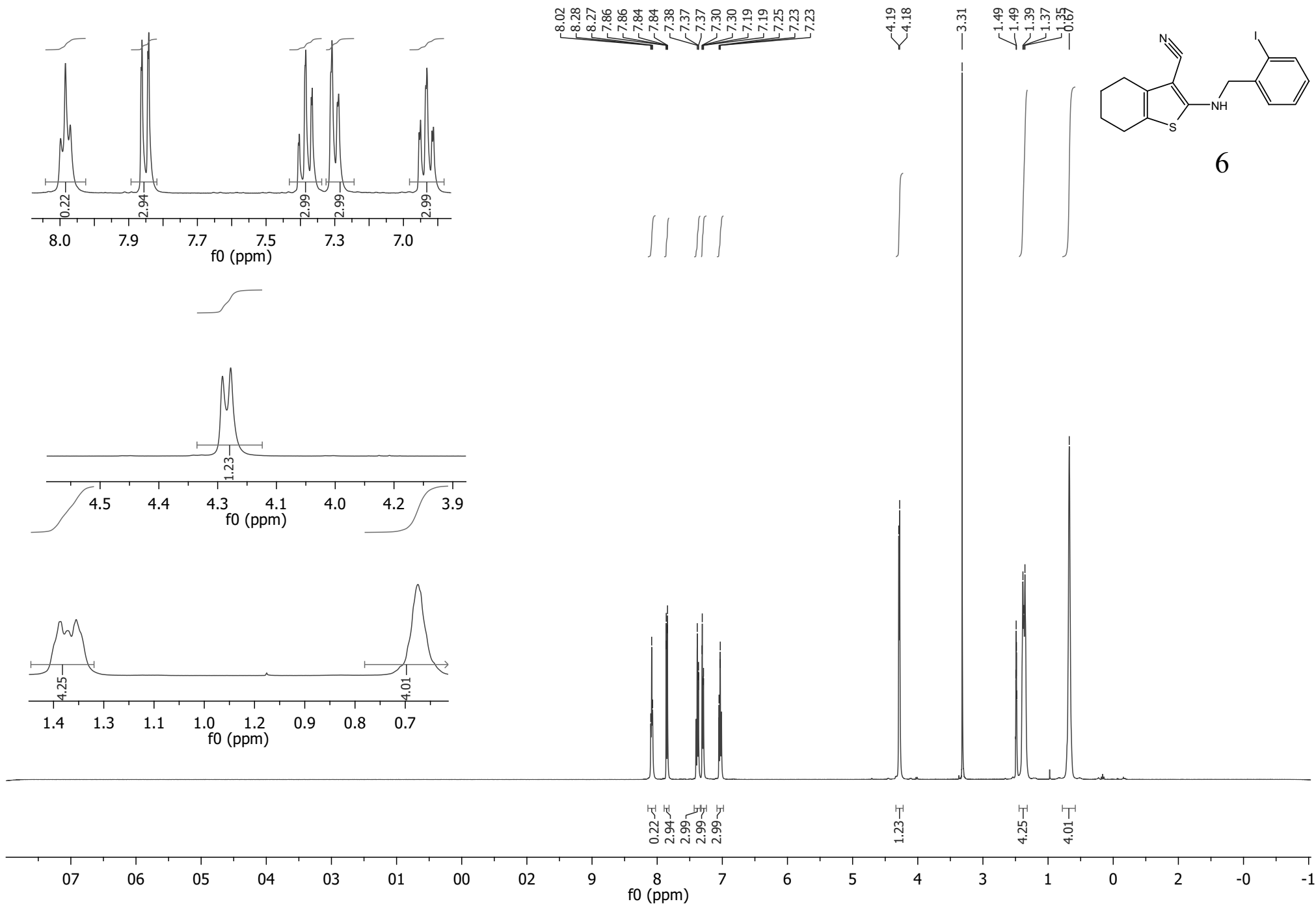
1: TOF MS ES+  
5.70e3



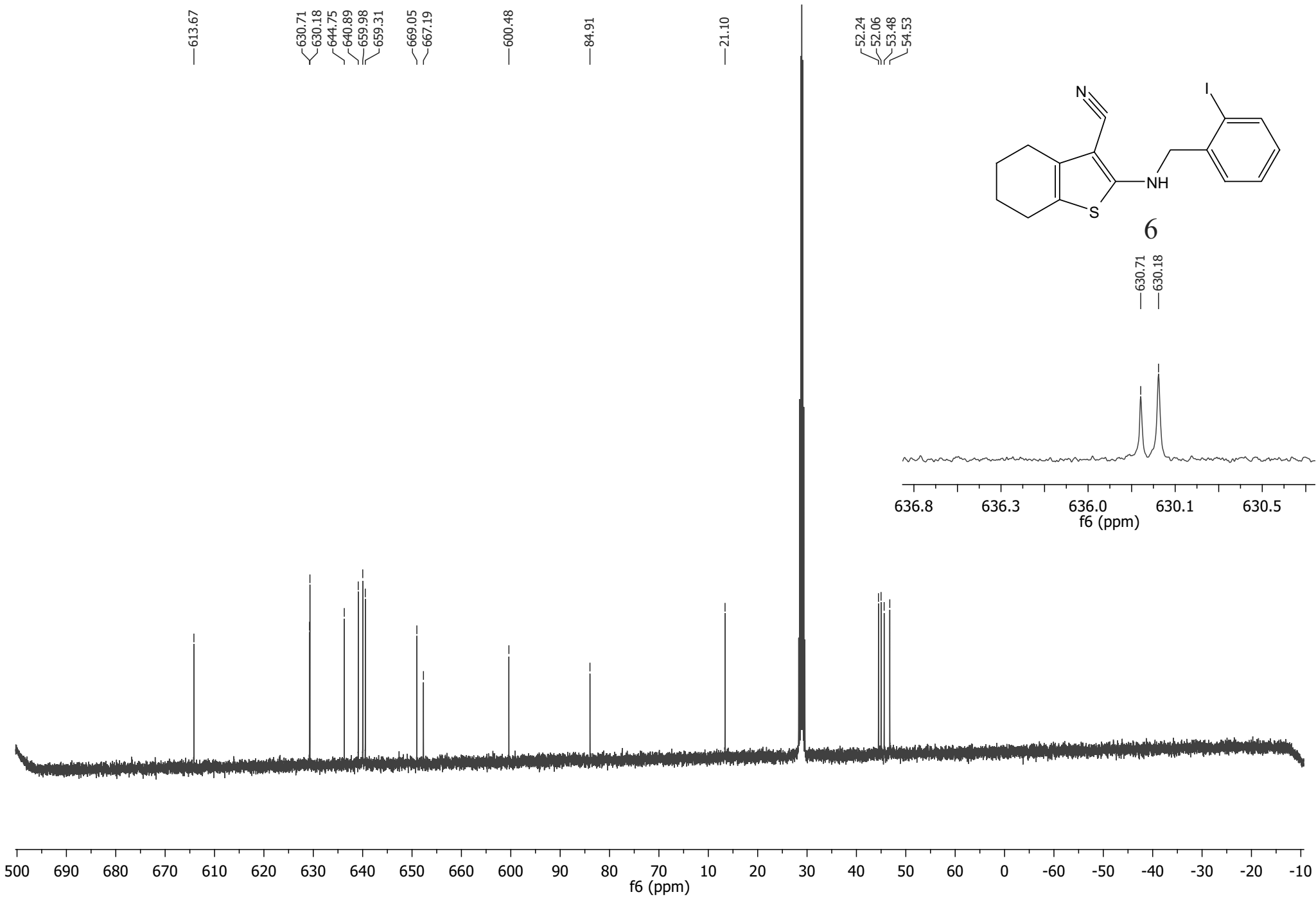
T01311918a 6 (0.222) Cm (5:13-20:26)

1: TOF MS ES+  
5.29e3









# 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

203 formula(e) evaluated with 3 results within limits (all results (up to 1000) for each mass)

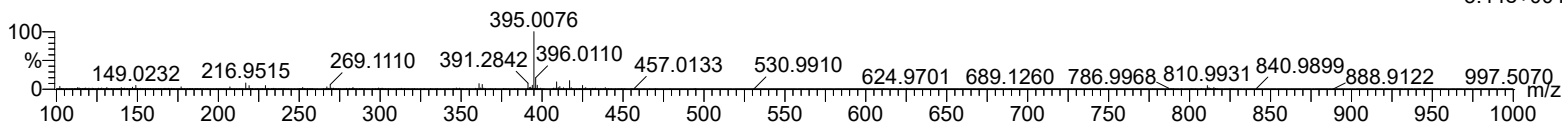
Elements Used:

C: 1-100 H: 1-200 N: 0-6 O: 0-10 S: 1-1 I: 1-1

Salem/Abdelrahman  
T01281950a 6 (0.221) Cm (6:24)

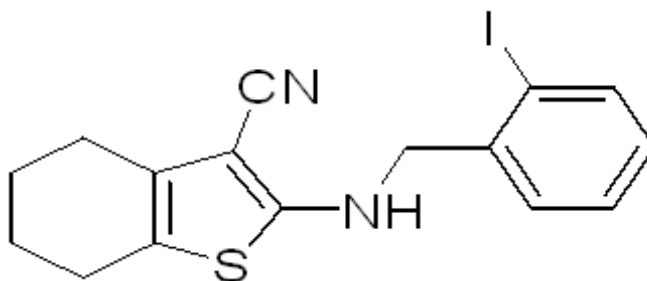
Sample #13

1: TOF MS ES+  
3.44e+004



Minimum: -5.0  
Maximum: 5.0 15.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
395.0077	395.0079	-0.2	-0.5	9.5	667.8	0.0	C16 H16 N2 S I
	395.0097	-2.0	-5.1	-3.5	683.6	15.8	C4 H20 N4 O7 S I
	395.0039	3.8	9.6	5.5	678.6	10.8	C11 H16 N4 O2 S I

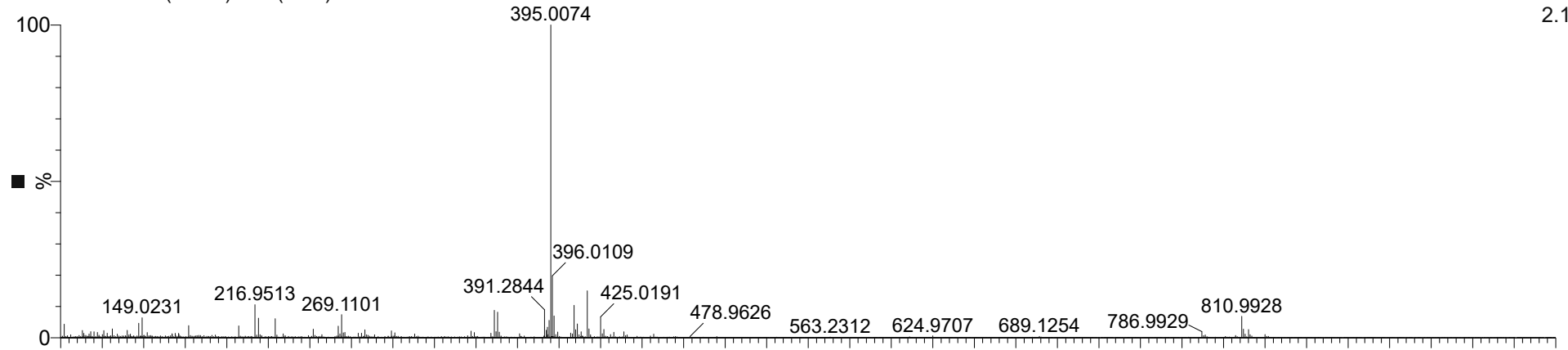


6

Salem/Abdelrahman

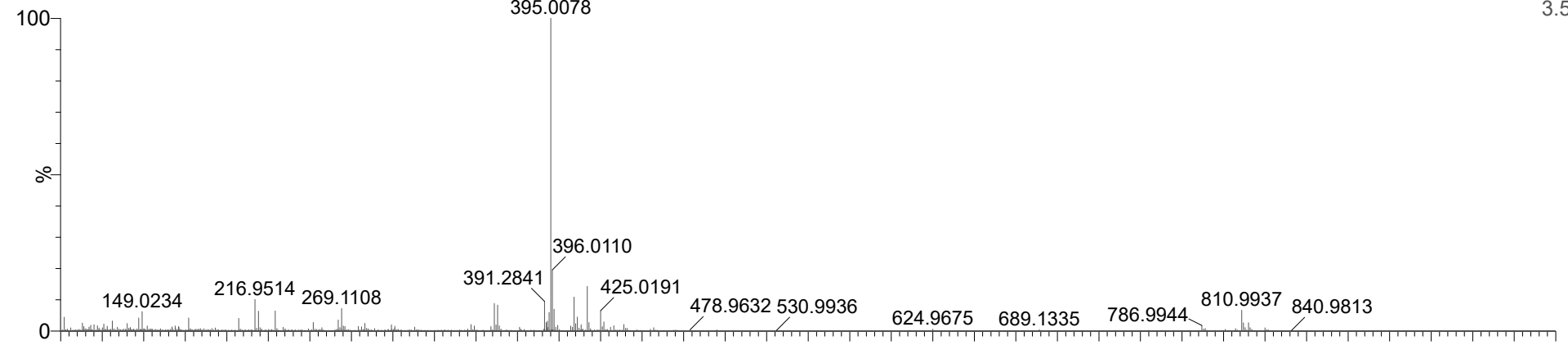
T01281952a 15 (0.534) Cm (4:15)

1: TOF MS ES+  
2.17e4



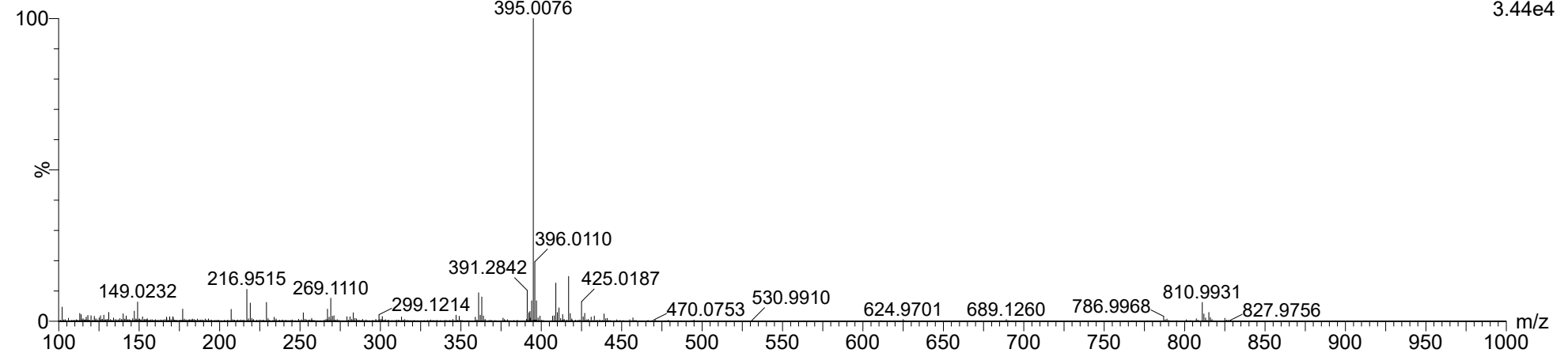
T01281951a 22 (0.789) Cm (7:26)

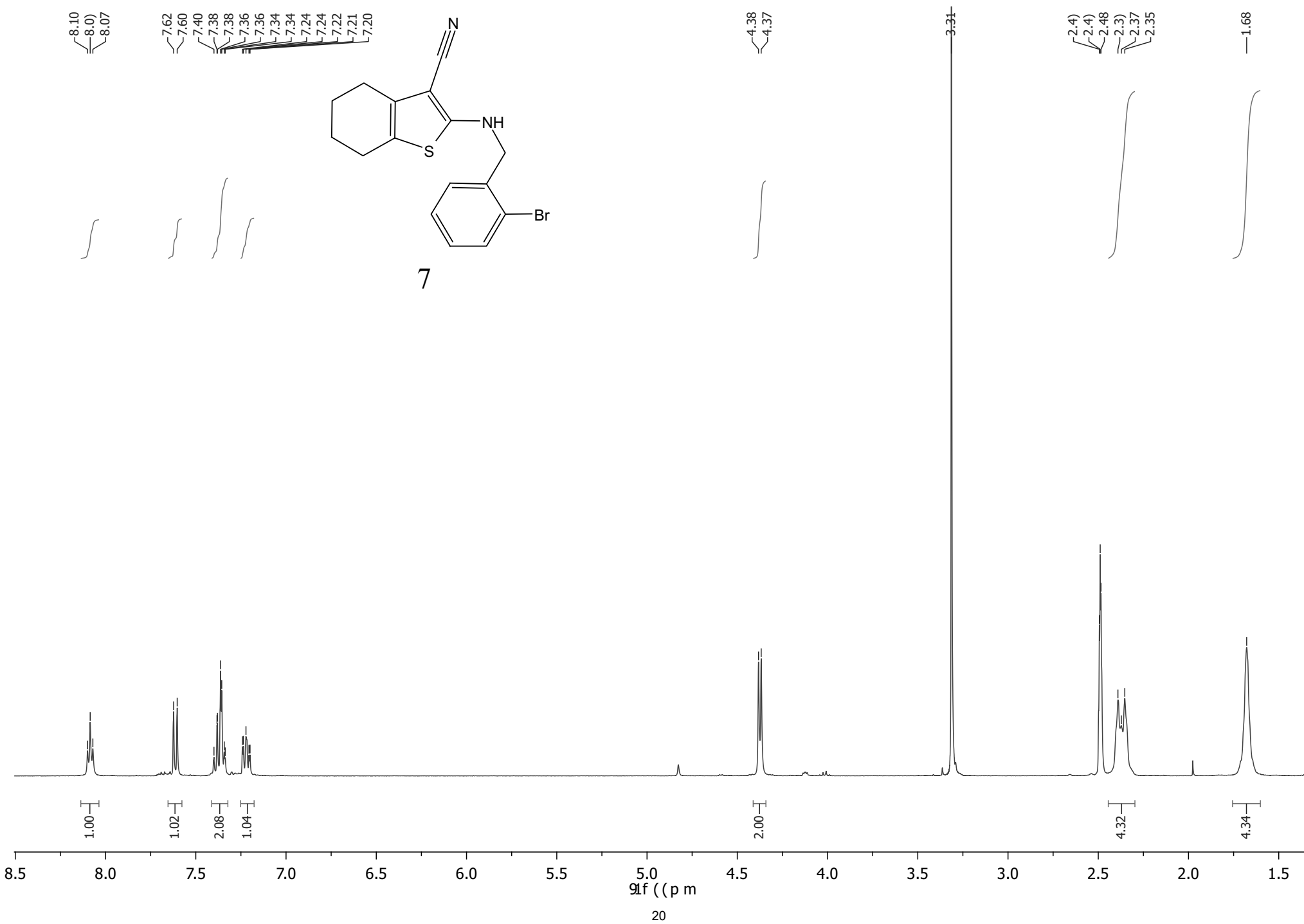
1: TOF MS ES+  
3.53e4

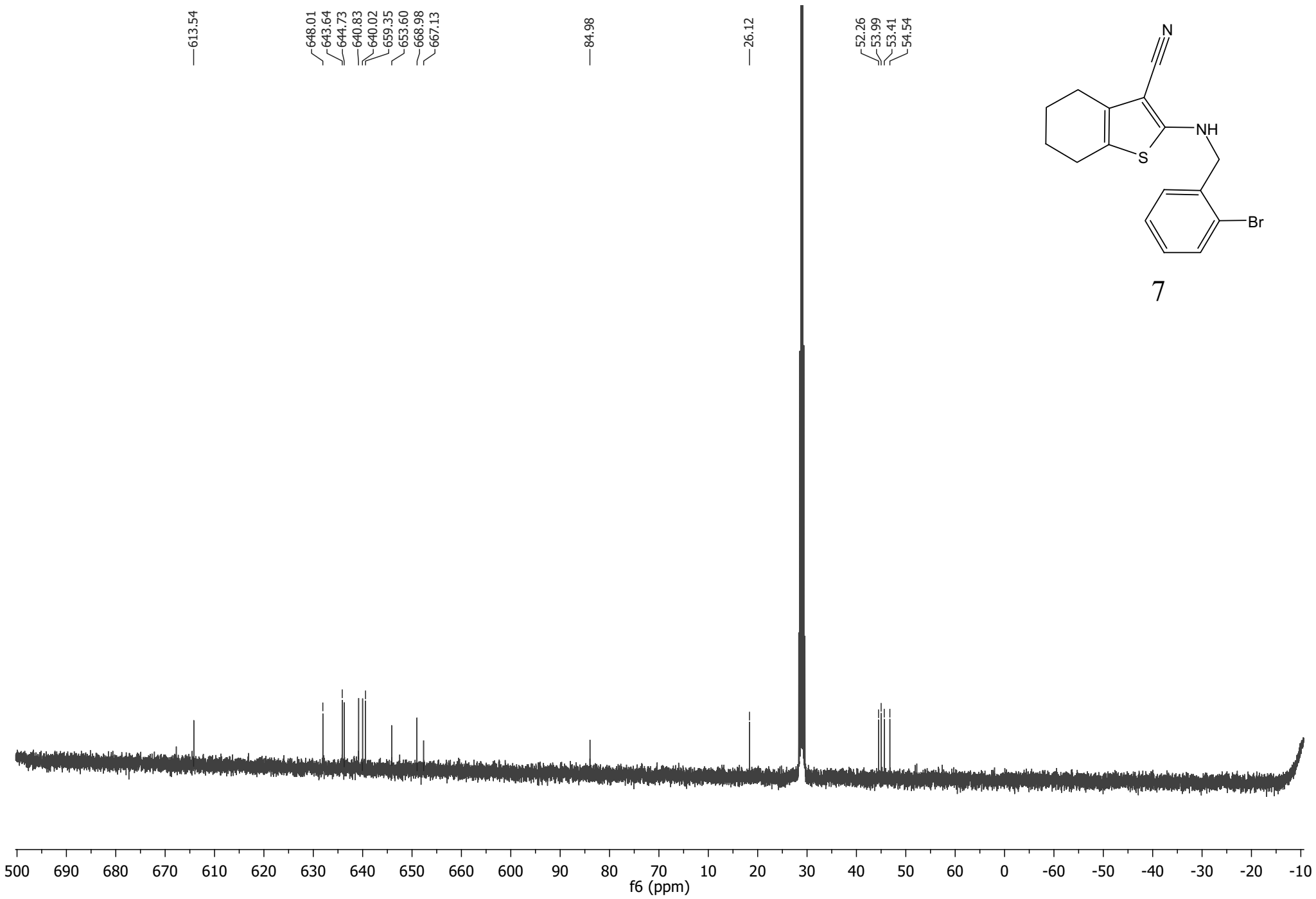


T01281950a 6 (0.221) Cm (6:24)

1: TOF MS ES+  
3.44e4







# 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

506 formula(e) evaluated with 10 results within limits (all results (up to 1000) for each mass)

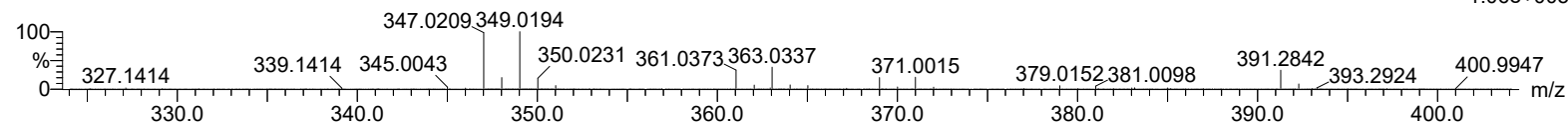
Elements Used:

C: 1-100 H: 1-200 N: 0-6 O: 0-10 S: 1-1 Br: 0-1

Salem/Abdelrahman  
T01281942a 25 (0.890) Cm (5:25)

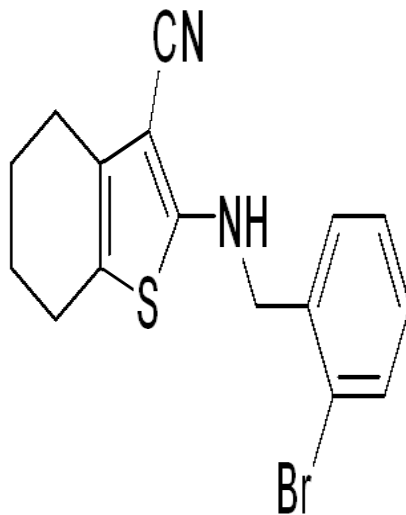
Sample #11

1: TOF MS ES+  
1.06e+005



Minimum: -5.0  
Maximum: 5.0 15.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
347.0209	347.0218	-0.9	-2.6	9.5	979.3	0.0	C16 H16 N2 S Br
	347.0199	1.0	2.9	12.5	1007.6	28.3	C12 H7 N6 O5 S
	347.0225	-1.6	-4.6	11.5	1008.3	29.0	C16 H11 O7 S
	347.0185	2.4	6.9	7.5	1007.5	28.3	C11 H11 N2 O9 S
	347.0236	-2.7	-7.8	-3.5	997.9	18.6	C4 H20 N4 O7 S Br
	347.0239	-3.0	-8.6	16.5	1008.2	28.9	C17 H7 N4 O3 S
	347.0177	3.2	9.2	5.5	991.1	11.8	C11 H16 N4 O2 S Br
	347.0167	4.2	12.1	20.5	1009.2	29.9	C23 H7 O2 S
	347.0164	4.5	13.0	0.5	992.4	13.1	C10 H20 O6 S Br
	347.0257	-4.8	-13.8	3.5	1008.2	28.9	C5 H11 N6 O10 S

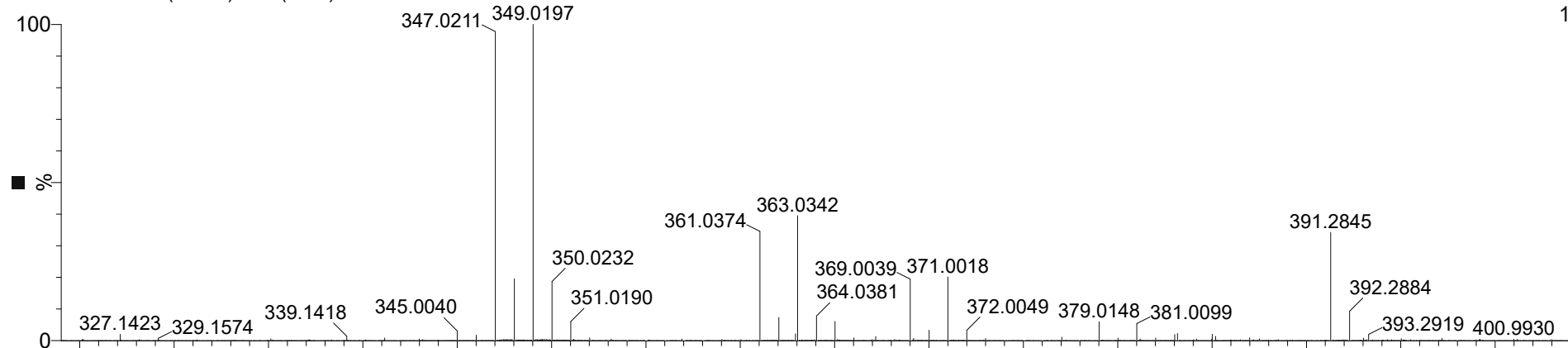


7

Salem/Abdelrahman

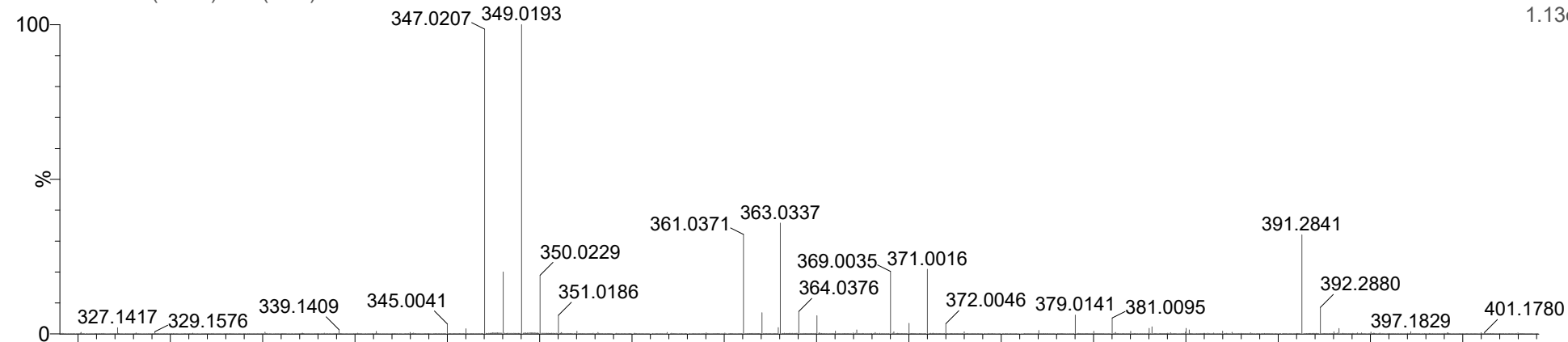
T01281944a 12 (0.433) Cm (6:26)

1: TOF MS ES+  
1.16e5



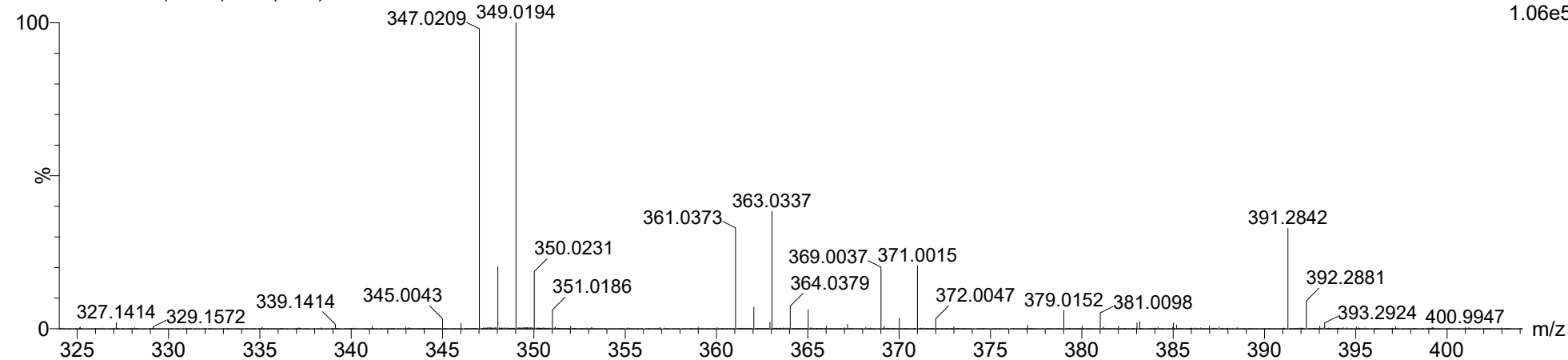
T01281943a 7 (0.255) Cm (4:24)

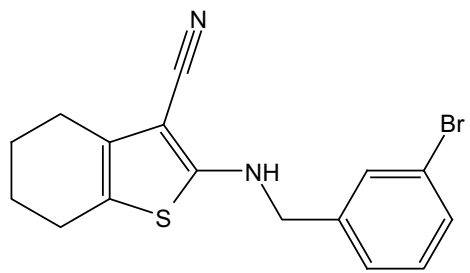
1: TOF MS ES+  
1.13e5



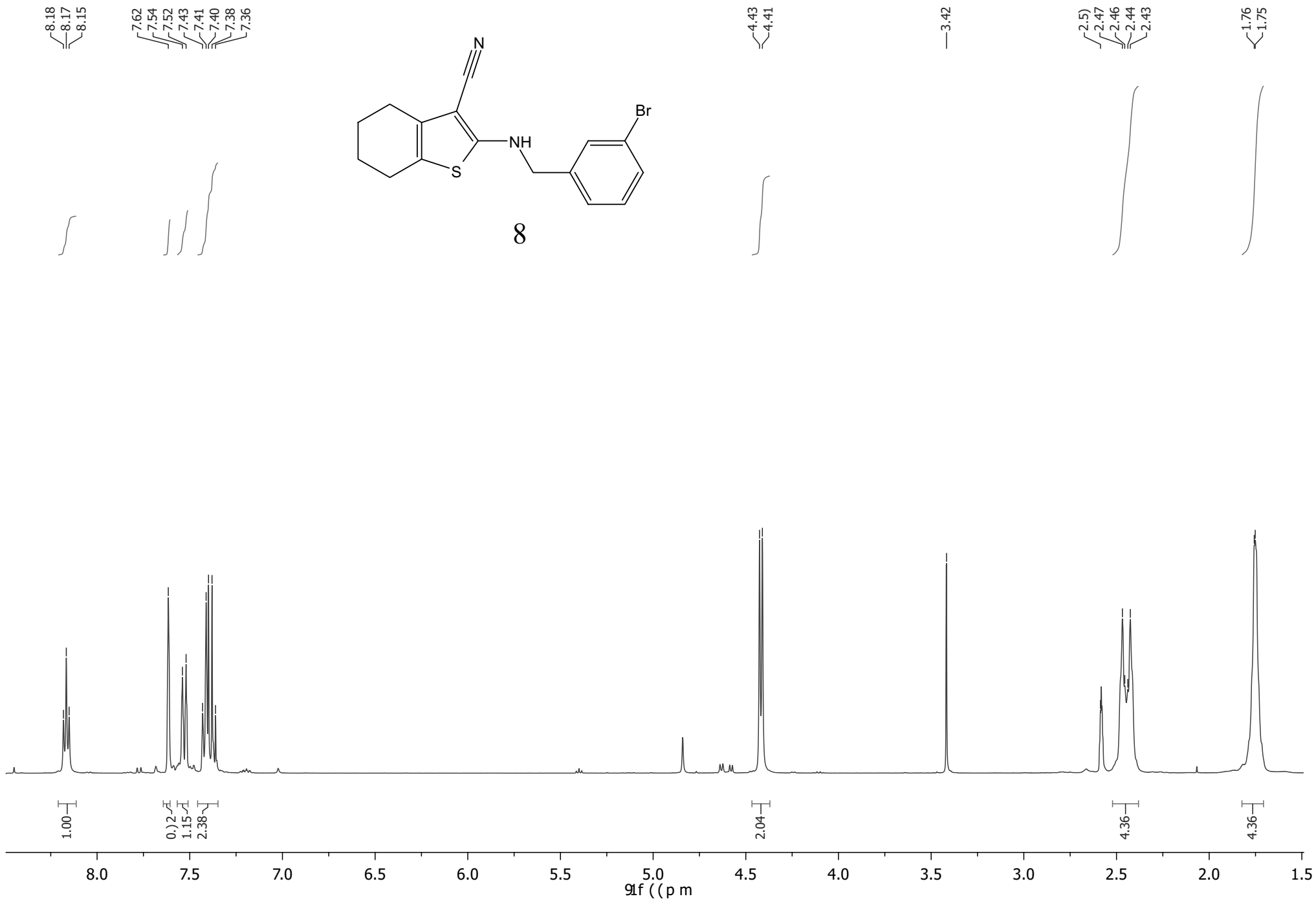
T01281942a 25 (0.890) Cm (5:25)

1: TOF MS ES+  
1.06e5

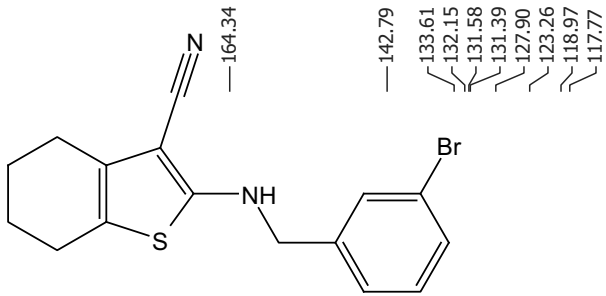




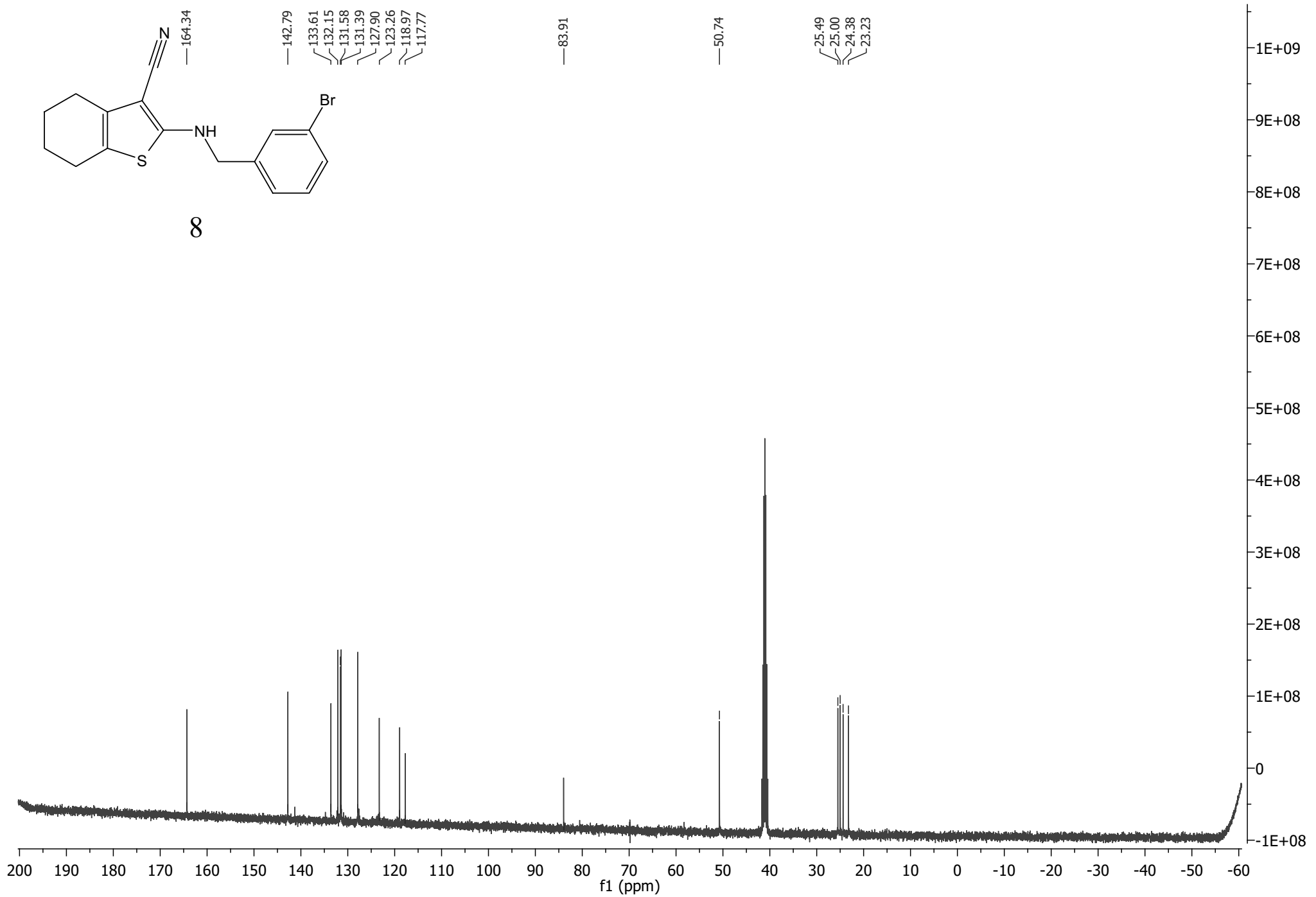
8







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

506 formula(e) evaluated with 10 results within limits (all results (up to 1000) for each mass)

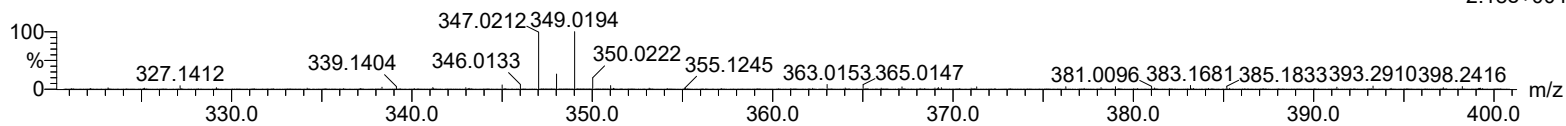
Elements Used:

C: 1-100 H: 1-200 N: 0-6 O: 0-10 S: 1-1 Br: 0-1

Salem/Abdelrahman  
T01281932a 15 (0.534) Cm (6:25)

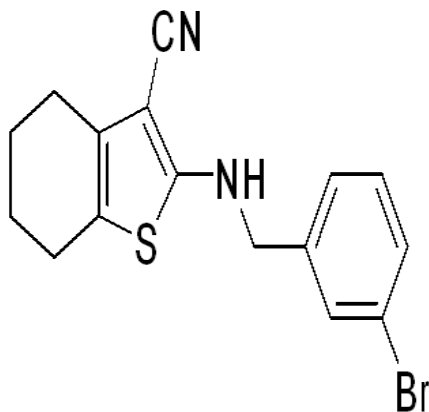
Sample #8

1: TOF MS ES+  
2.18e+004



Minimum: -5.0  
Maximum: 5.0 15.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
347.0212	347.0218	-0.6	-1.7	9.5	769.0	0.0	C16 H16 N2 S Br
347.0199		1.3	3.7	12.5	782.0	13.0	C12 H7 N6 O5 S
347.0225		-1.3	-3.7	11.5	783.0	14.0	C16 H11 O7 S
347.0236		-2.4	-6.9	-3.5	775.5	6.5	C4 H20 N4 O7 S Br
347.0185		2.7	7.8	7.5	782.3	13.3	C11 H11 N2 O9 S
347.0239		-2.7	-7.8	16.5	782.7	13.7	C17 H7 N4 O3 S
347.0177		3.5	10.1	5.5	772.5	3.5	C11 H16 N4 O2 S Br
347.0257		-4.5	-13.0	3.5	781.9	12.9	C5 H11 N6 O10 S
347.0167		4.5	13.0	20.5	783.5	14.5	C23 H7 O2 S
347.0164		4.8	13.8	0.5	774.6	5.6	C10 H20 O6 S Br

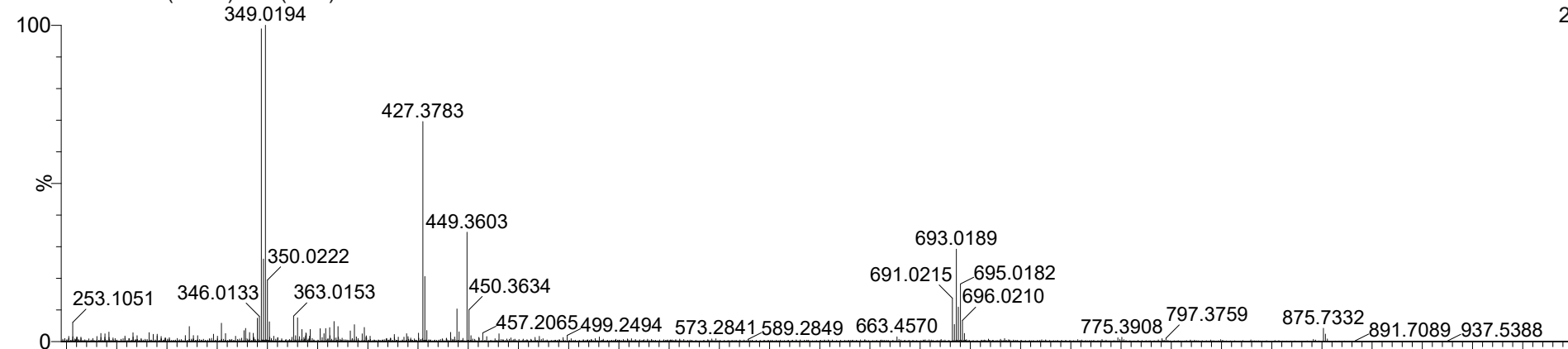


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Salem/Abdelrahman

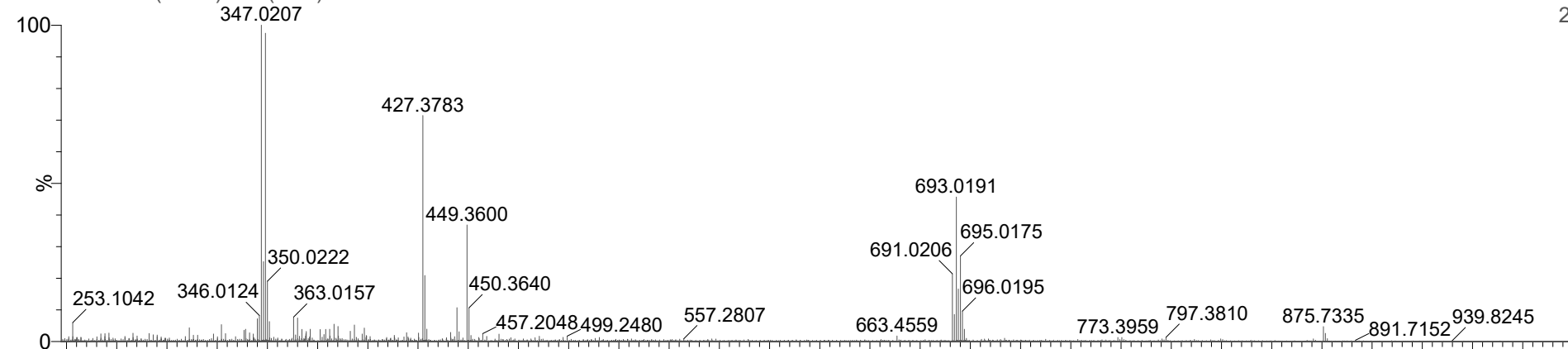
T01281932a 15 (0.534) Cm (6:25)

1: TOF MS ES+  
2.18e4



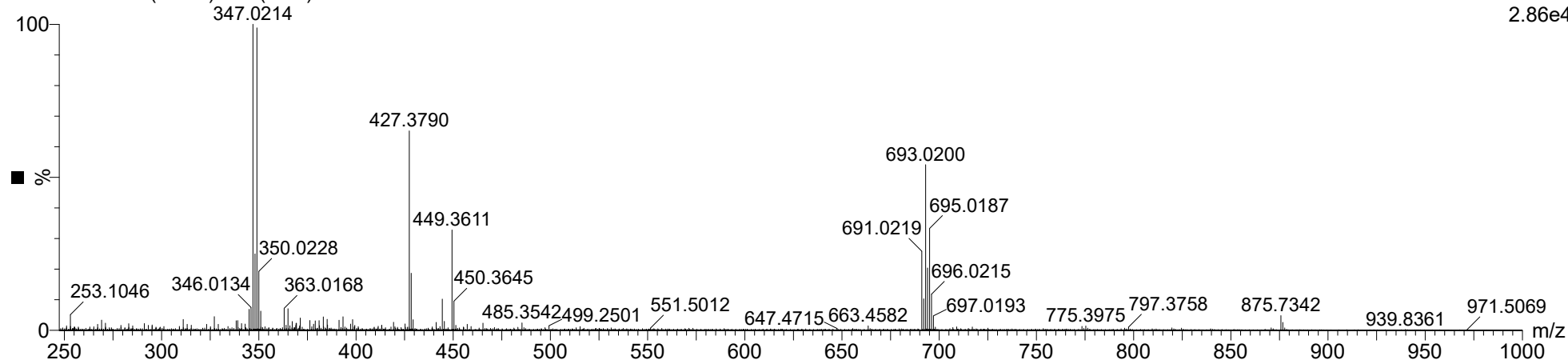
T01281931a 7 (0.255) Cm (5:23)

1: TOF MS ES+  
2.29e4



T01281930a 5 (0.178) Cm (5:24)

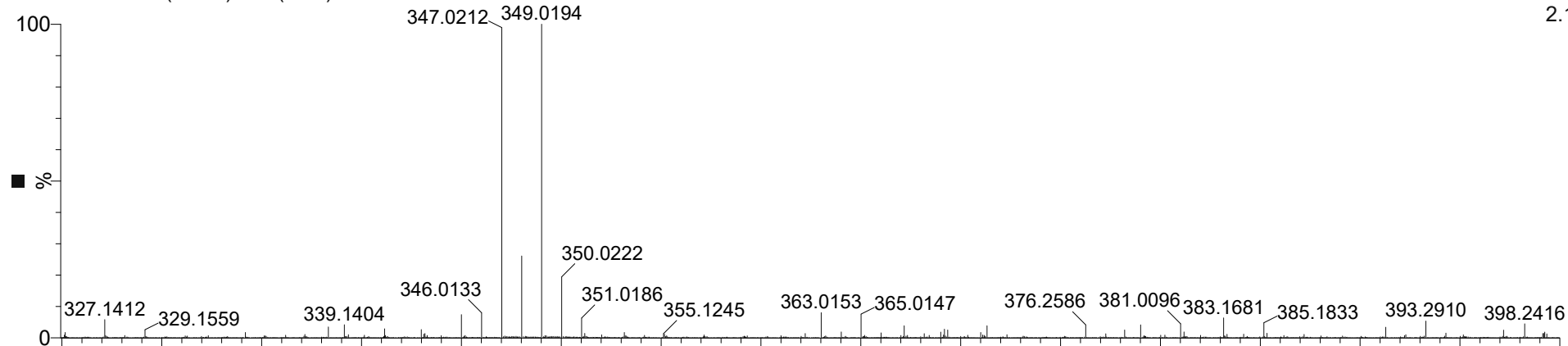
1: TOF MS ES+  
2.86e4



Salem/Abdelrahman

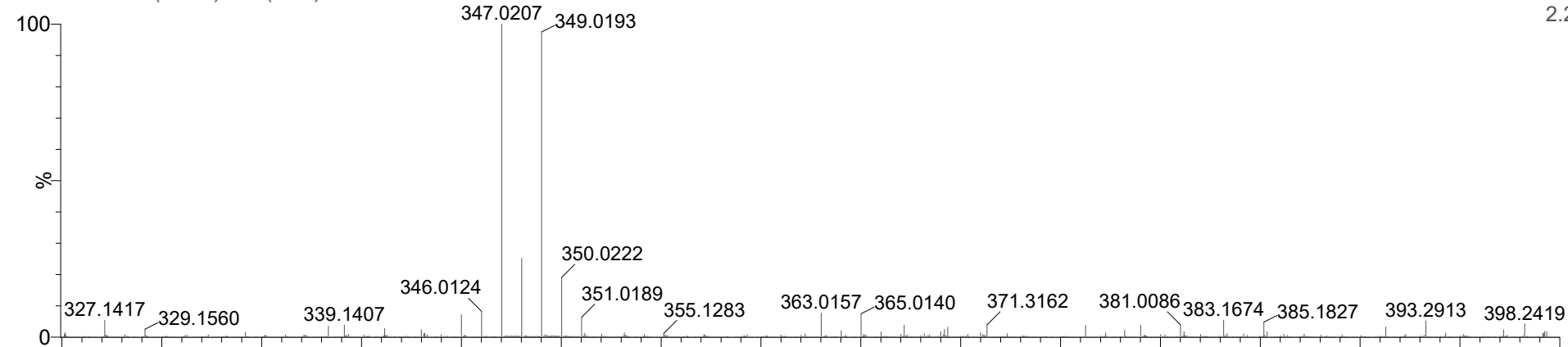
T01281932a 15 (0.534) Cm (6:25)

1: TOF MS ES+  
2.18e4



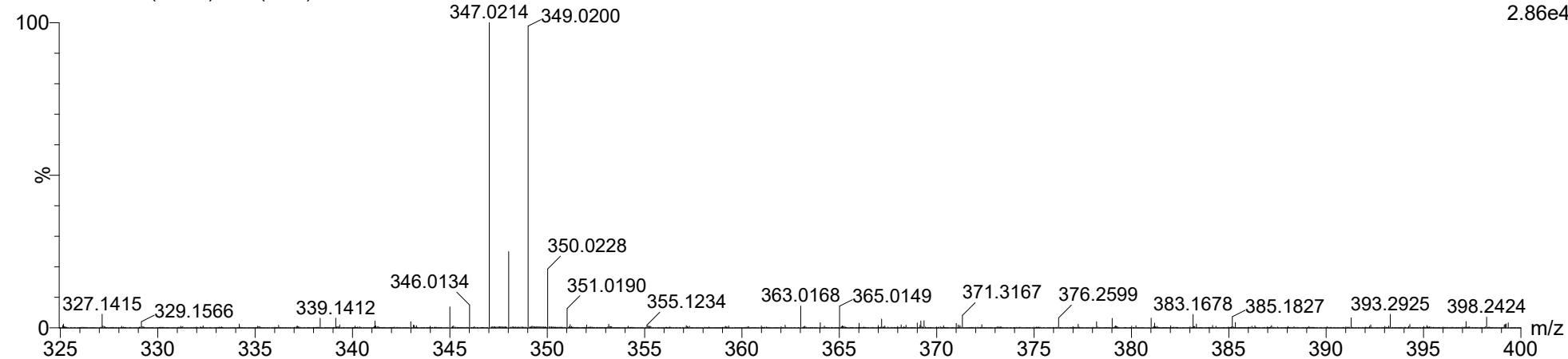
T01281931a 7 (0.255) Cm (5:23)

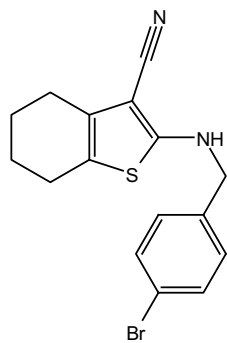
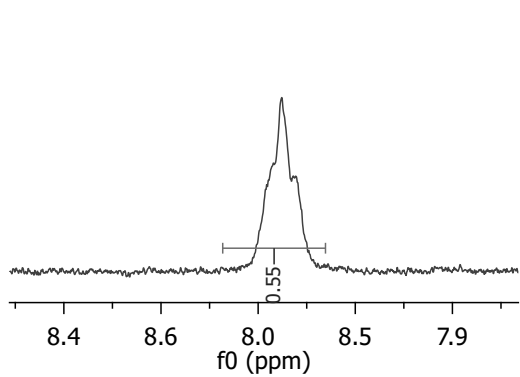
1: TOF MS ES+  
2.29e4



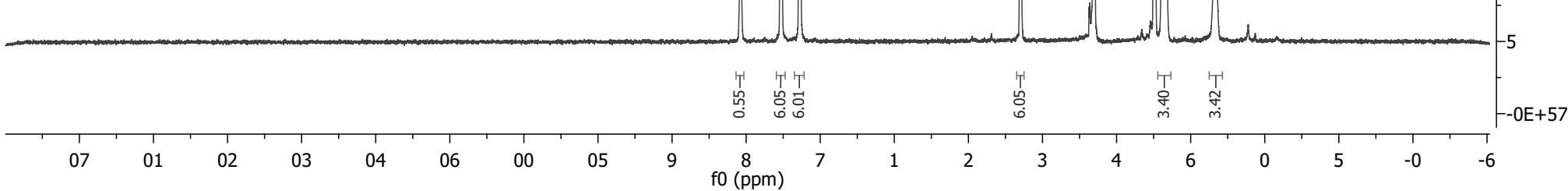
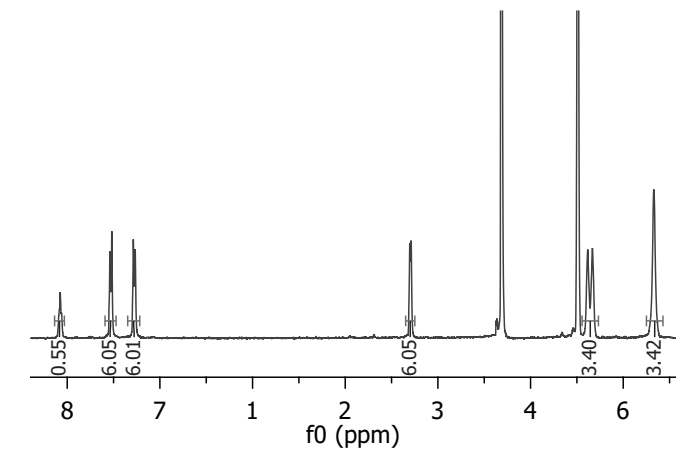
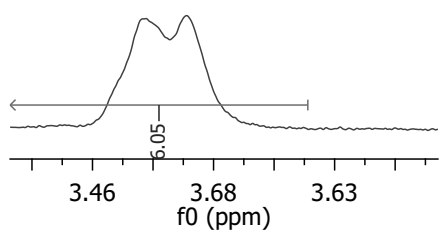
T01281930a 5 (0.178) Cm (5:24)

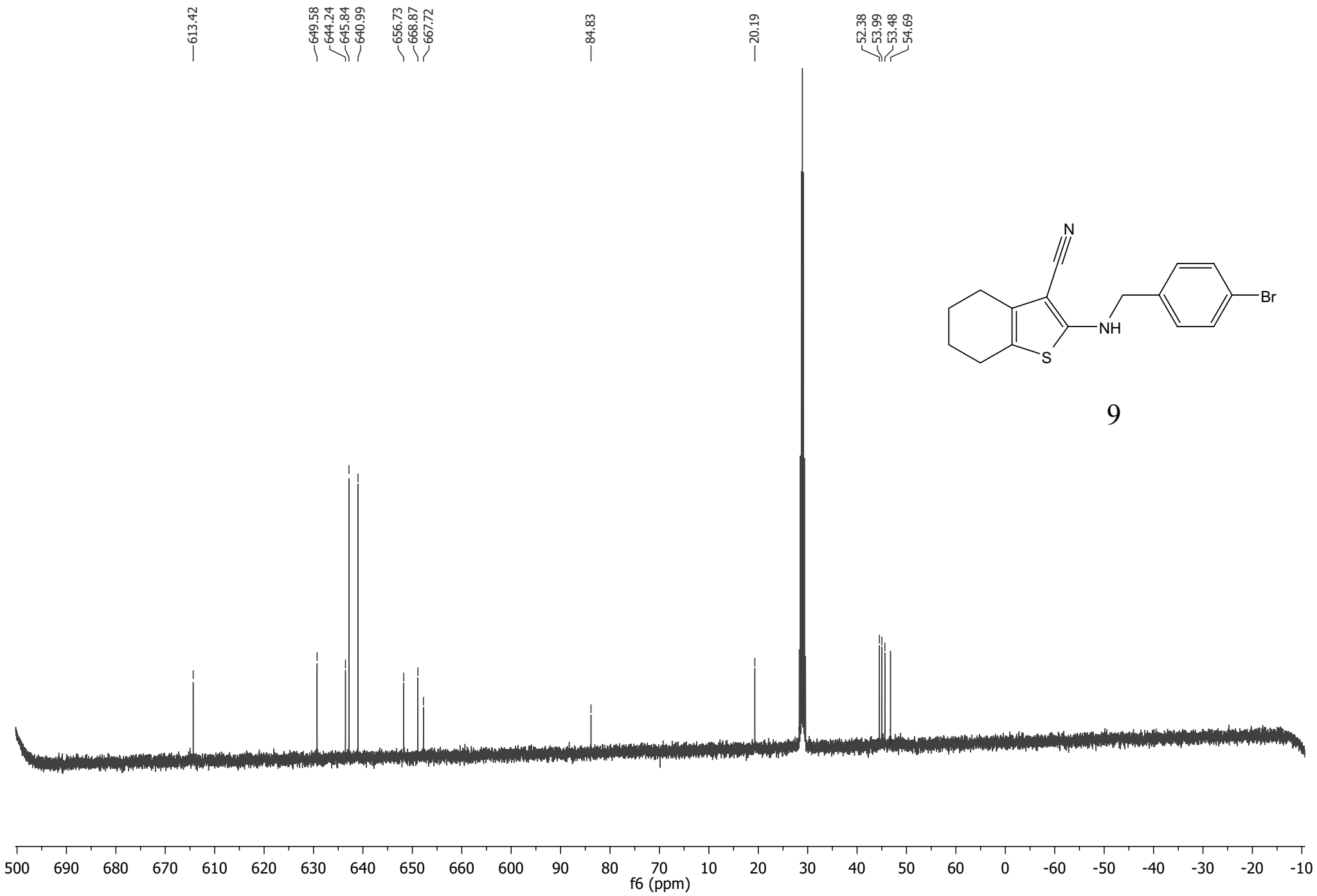
1: TOF MS ES+  
2.86e4





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# 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

506 formula(e) evaluated with 9 results within limits (all results (up to 1000) for each mass)

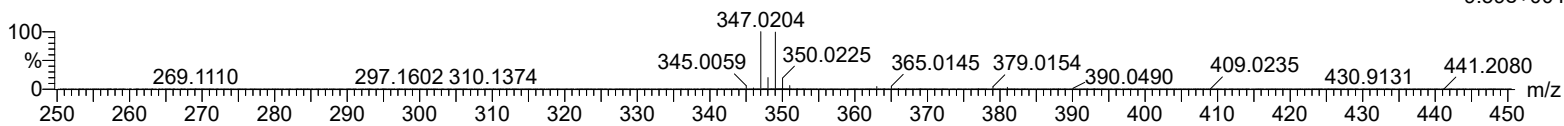
Elements Used:

C: 1-100 H: 1-200 N: 0-6 O: 0-10 S: 1-1 Br: 0-1

Salem/Abdelrahman  
T01281928b 20 (0.712) Cm (4:23)

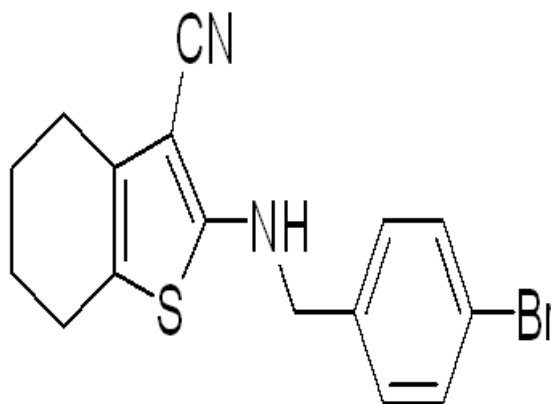
Sample #7

1: TOF MS ES+  
9.59e+004



Minimum: -5.0  
Maximum: 5.0 15.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
347.0203	347.0199	0.4	1.2	12.5	964.1	23.7	C12 H7 N6 O5 S
	347.0218	-1.5	-4.3	9.5	940.4	0.0	C16 H16 N2 S Br
	347.0185	1.8	5.2	7.5	964.0	23.6	C11 H11 N2 O9 S
	347.0225	-2.2	-6.3	11.5	964.9	24.5	C16 H11 O7 S
	347.0177	2.6	7.5	5.5	950.4	10.0	C11 H16 N4 O2 S Br
	347.0236	-3.3	-9.5	-3.5	956.5	16.1	C4 H20 N4 O7 S Br
	347.0167	3.6	10.4	20.5	966.0	25.6	C23 H7 O2 S
	347.0239	-3.6	-10.4	16.5	964.9	24.5	C17 H7 N4 O3 S
	347.0164	3.9	11.2	0.5	951.8	11.4	C10 H20 O6 S Br

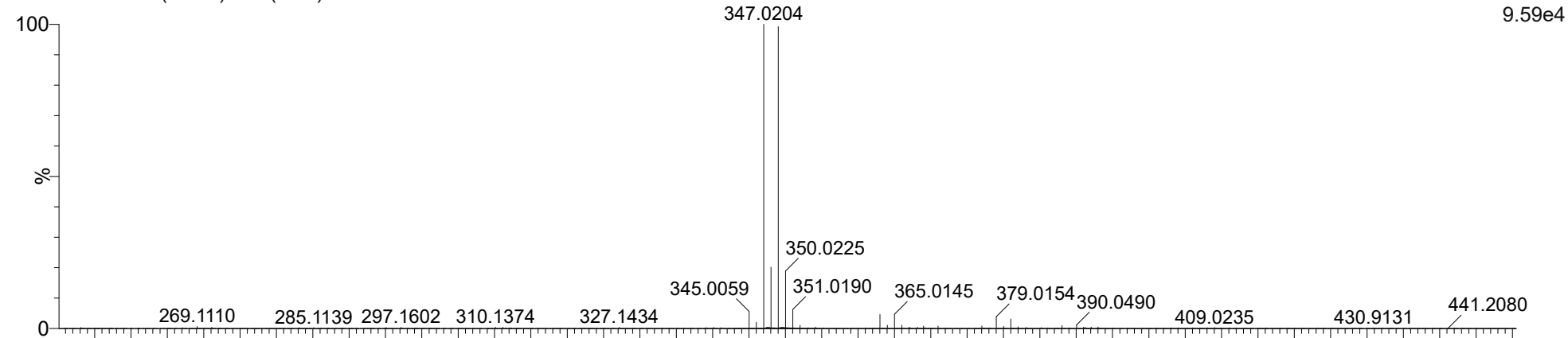


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Salem/Abdelrahman

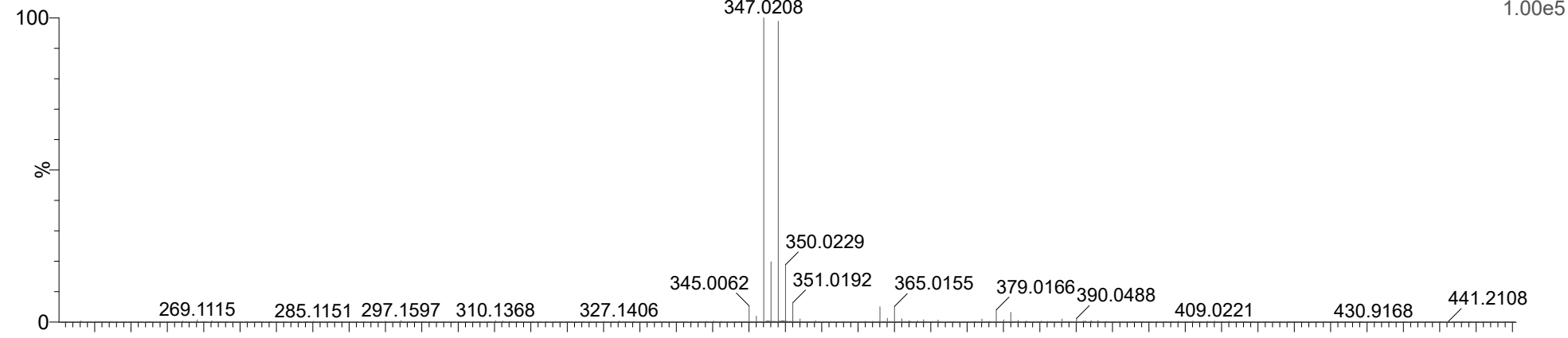
T01281928b 20 (0.712) Cm (4:23)

1: TOF MS ES+  
9.59e4



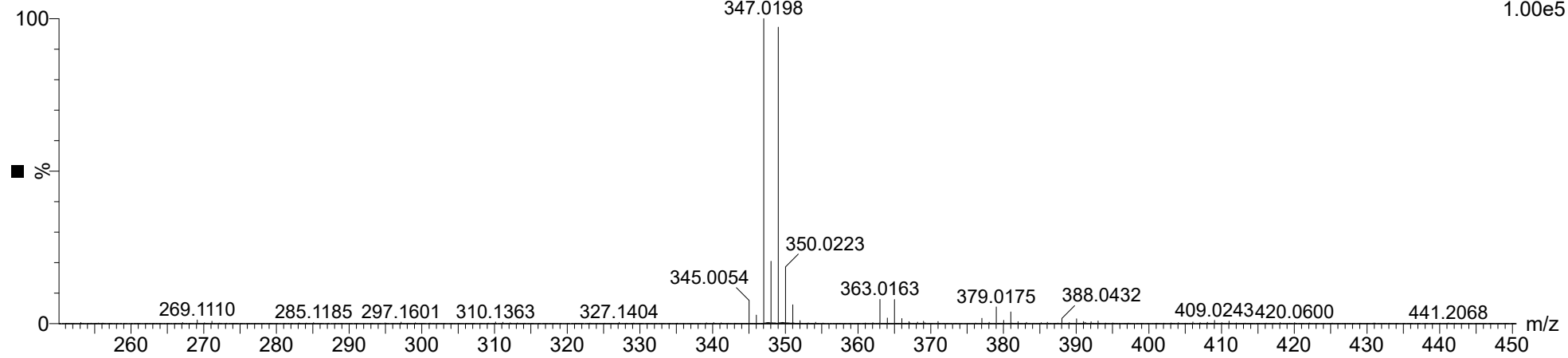
T01281927b 23 (0.823) Cm (3:26)

1: TOF MS ES+  
1.00e5

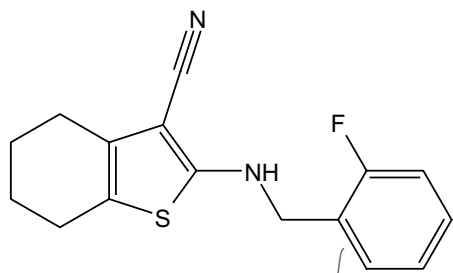


T01281926b 10 (0.356) Cm (5:26)

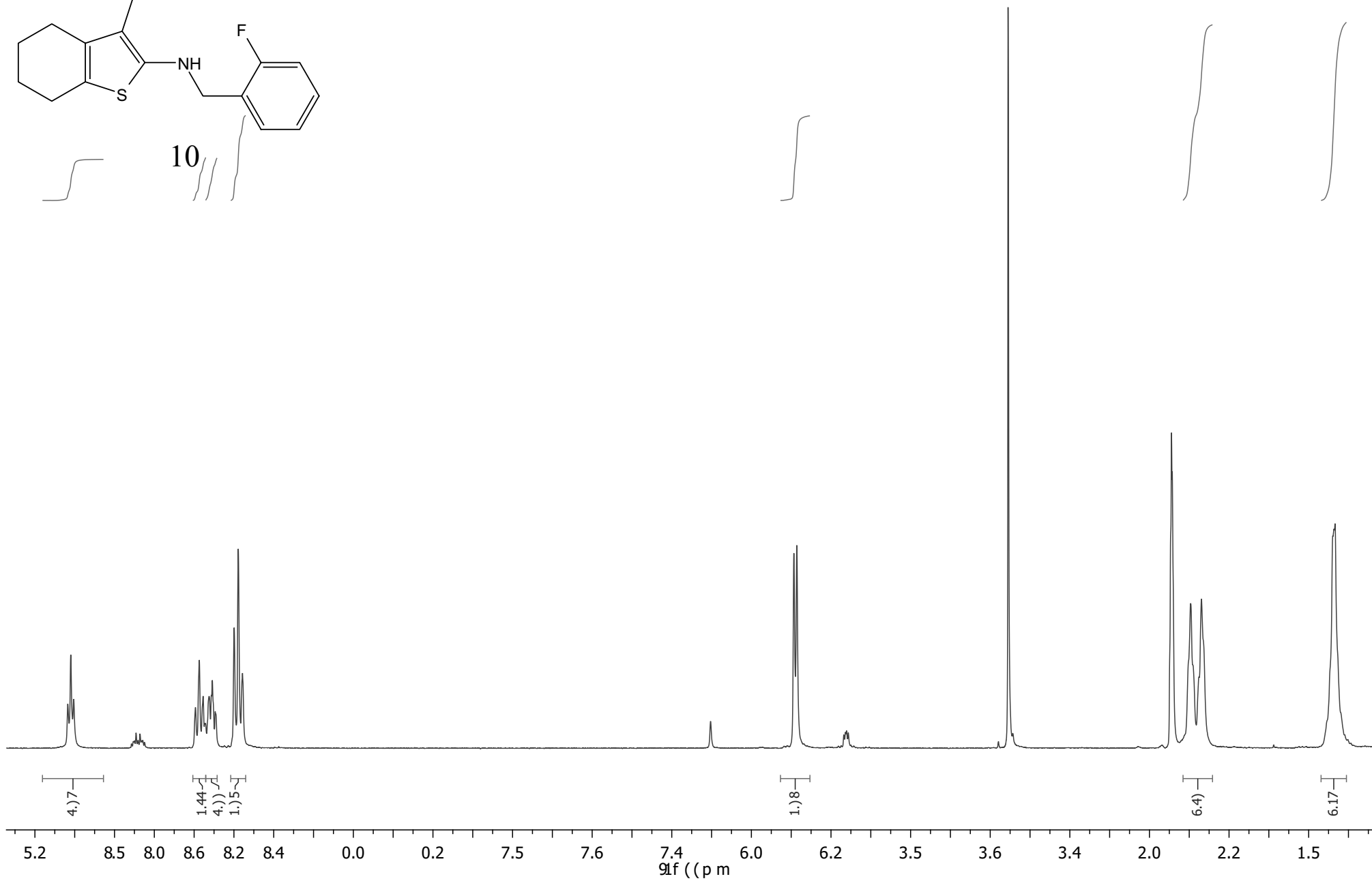
1: TOF MS ES+  
1.00e5

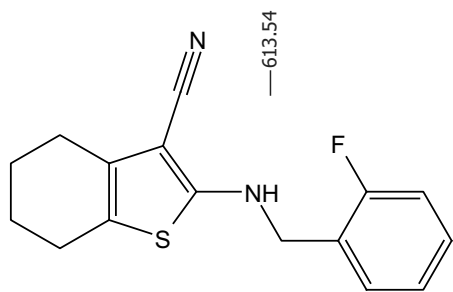




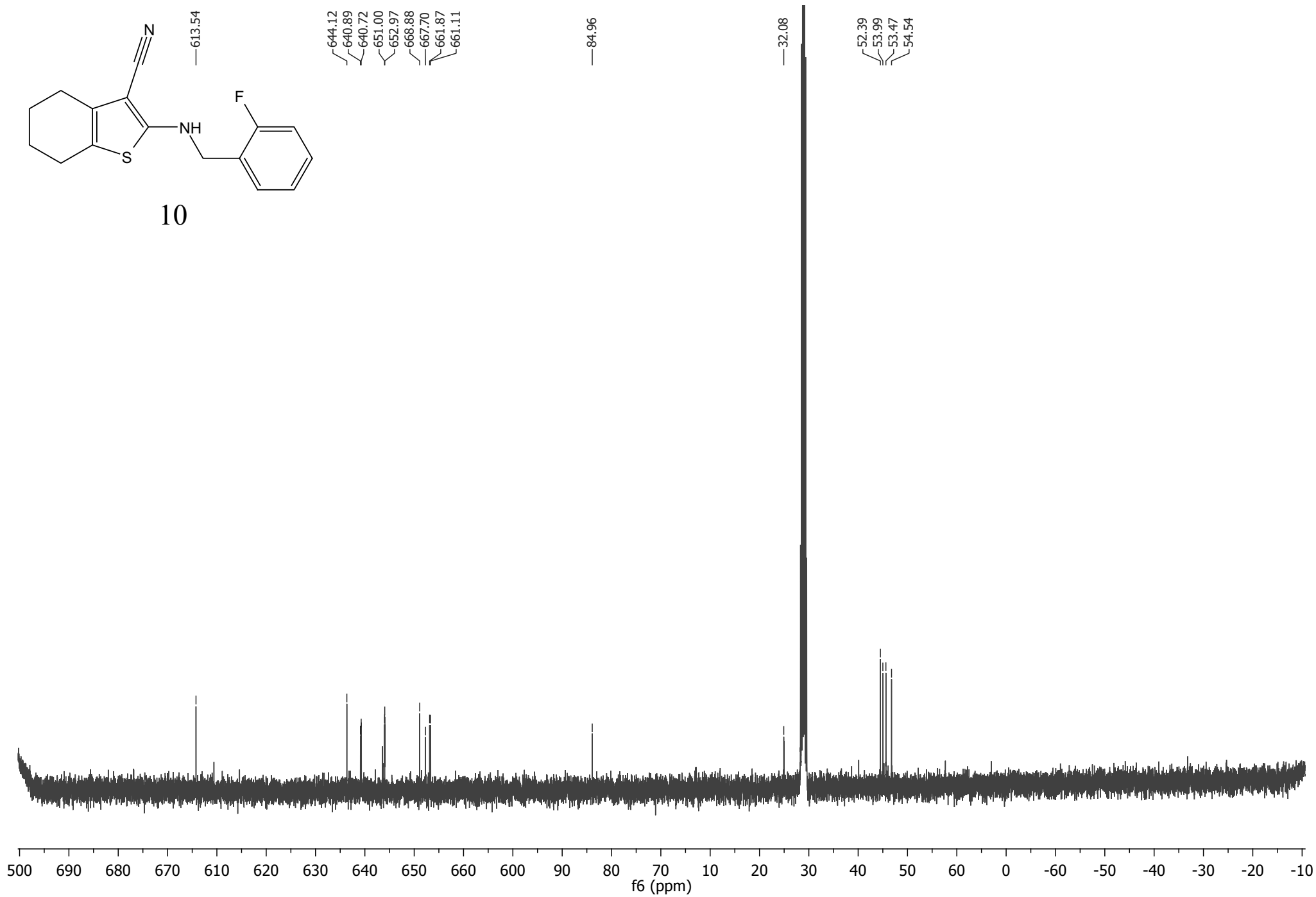


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# Elemental Composition Report

## 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

444 formula(e) evaluated with 8 results within limits (all results (up to 1000) for each mass)

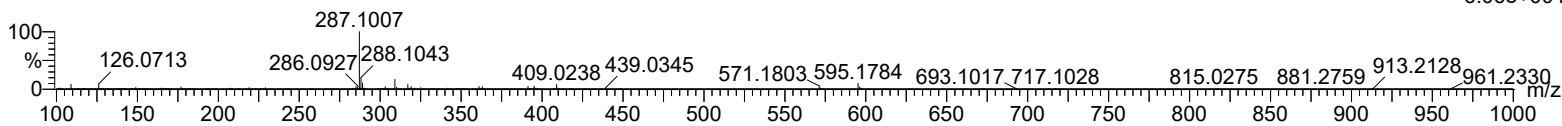
Elements Used:

C: 1-100 H: 1-200 N: 0-6 O: 0-10 S: 1-1 F: 0-1

Salem/Abdelrahman  
T01281955a 9 (0.322) Cm (9:23)

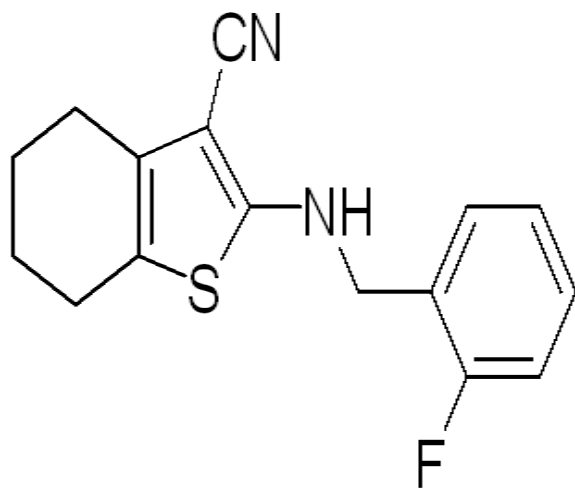
Sample #14

1: TOF MS ES+  
6.06e+004



Minimum: -5.0  
Maximum: 5.0 15.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
287.1007	287.1012	-0.5	-1.7	-4.5	857.6	4.4	C6 H23 O10 S
	287.1018	-1.1	-3.8	9.5	854.0	0.8	C16 H16 N2 S F
	287.1025	-1.8	-6.3	0.5	857.0	3.8	C7 H19 N4 O6 S
	287.0985	2.2	7.7	-3.5	858.8	5.6	C2 H19 N6 O8 S
	287.0978	2.9	10.1	5.5	855.6	2.4	C11 H16 N4 O2 S F
	287.1037	-3.0	-10.4	-3.5	858.3	5.1	C4 H20 N4 O7 S F
	287.0967	4.0	13.9	9.5	854.3	1.1	C14 H15 N4 O S
	287.0965	4.2	14.6	0.5	855.9	2.7	C10 H20 O6 S F

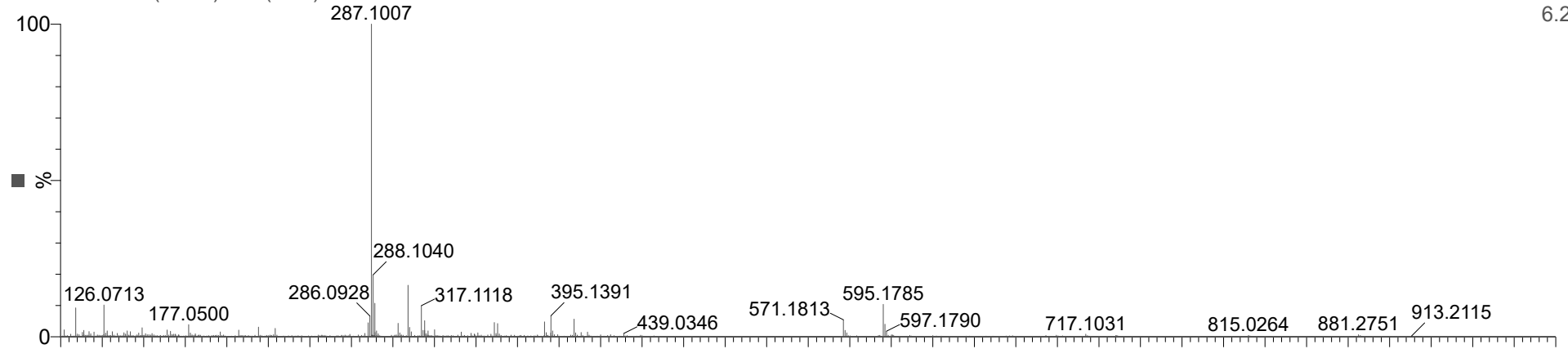


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Salem/Abdelrahman

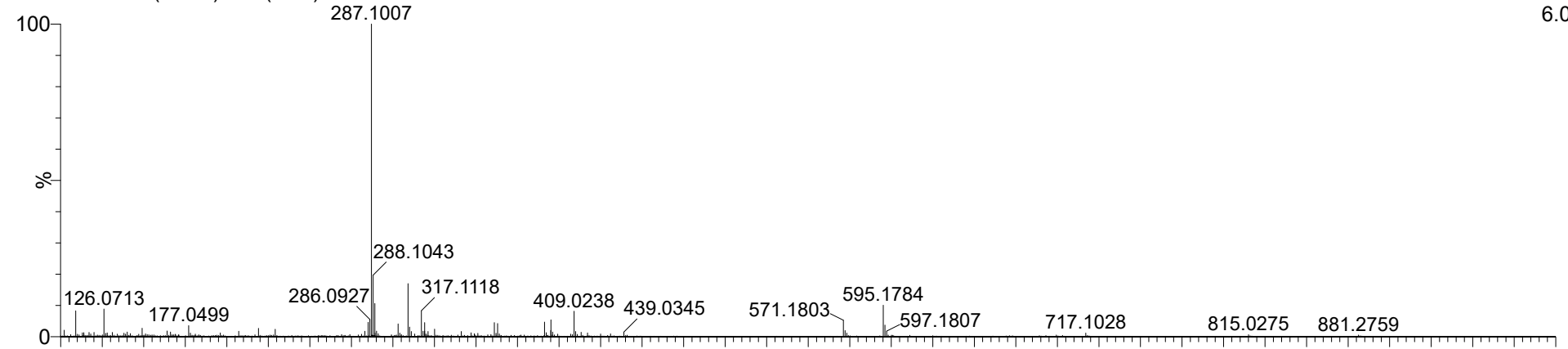
T01281956a 6 (0.221) Cm (6:22)

1: TOF MS ES+  
6.24e4



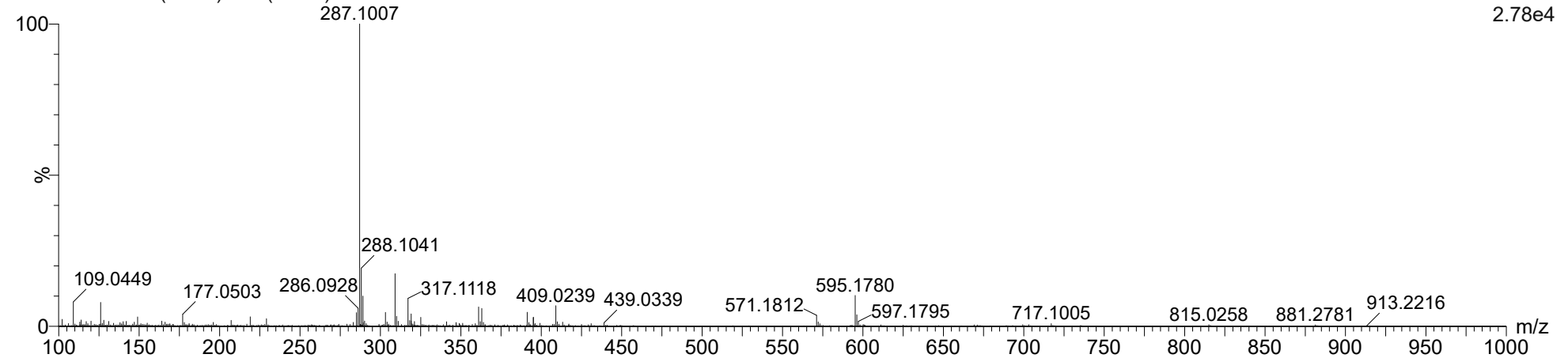
T01281955a 9 (0.322) Cm (9:23)

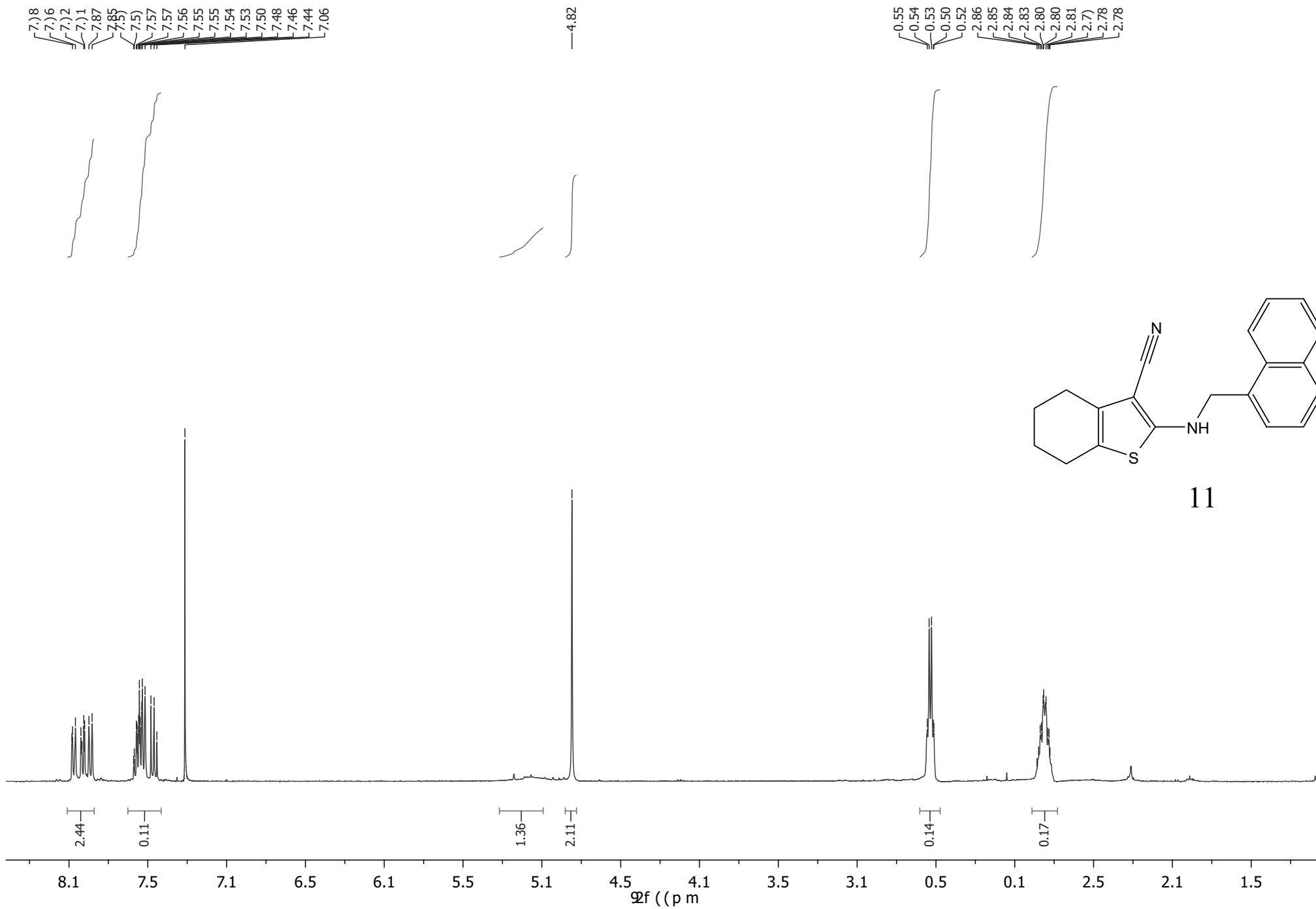
1: TOF MS ES+  
6.06e4



T01281954a 17 (0.611) Cm (10:17)

1: TOF MS ES+  
2.78e4

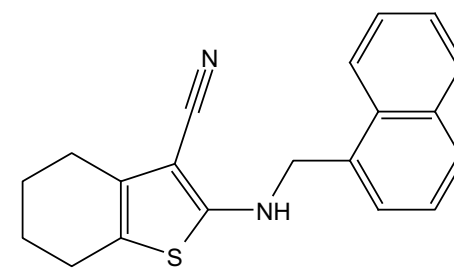




7.8  
7.6  
7.2  
7.1  
7.87  
7.85  
7.5  
7.57  
7.57  
7.56  
7.55  
7.54  
7.53  
7.50  
7.48  
7.46  
7.44  
7.06

4.82

0.55  
0.54  
0.53  
0.50  
0.52  
2.86  
2.85  
2.84  
2.83  
2.80  
2.81  
2.7  
2.78  
2.78



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

793 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

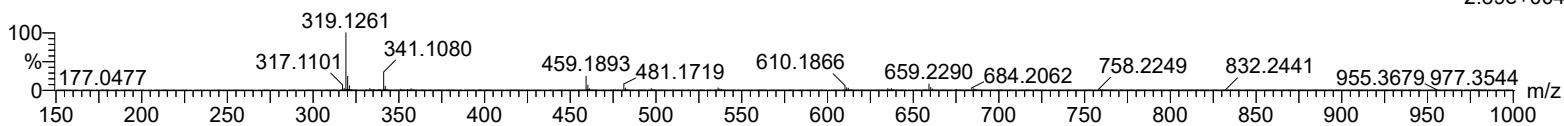
Salem/Abdelrahman

Sample #37

T03251902a 10 (0.356) Cm (9:12-19:27)

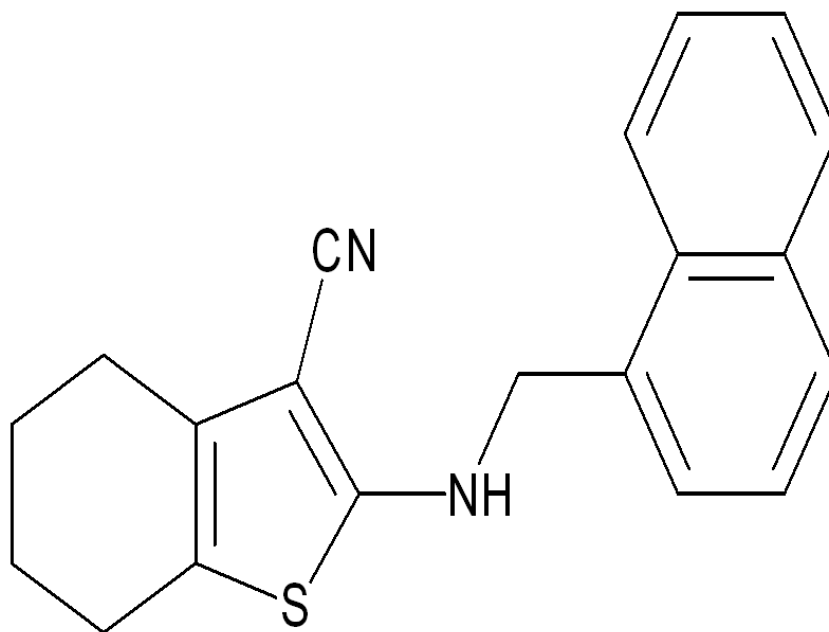
1: TOF MS ES+

2.39e+004



Minimum: -5.0  
Maximum: 5.0 15.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
319.1260	319.1262	-0.2	-0.6	3.5	707.7	16.9	C12 H23 N4 O2 S2
	319.1254	0.6	1.9	4.5	713.9	23.2	C11 H19 N4 O7
	319.1269	-0.9	-2.8	12.5	690.8	0.0	C20 H19 N2 S
	319.1249	1.1	3.4	-1.5	708.8	18.0	C11 H27 O6 S2
	319.1240	2.0	6.3	-0.5	714.4	23.6	C10 H23 O11
	319.1235	2.5	7.8	17.5	712.9	22.2	C23 H15 N2
	319.1287	-2.7	-8.5	-0.5	707.2	16.4	C8 H23 N4 O7 S
	319.1229	3.1	9.7	8.5	701.0	10.2	C15 H19 N4 O2 S
	319.1294	-3.4	-10.7	8.5	713.0	22.3	C16 H19 N2 O5
	319.1303	-4.3	-13.5	7.5	705.7	14.9	C17 H23 N2 S2
	319.1215	4.5	14.1	3.5	703.4	12.7	C14 H23 O6 S

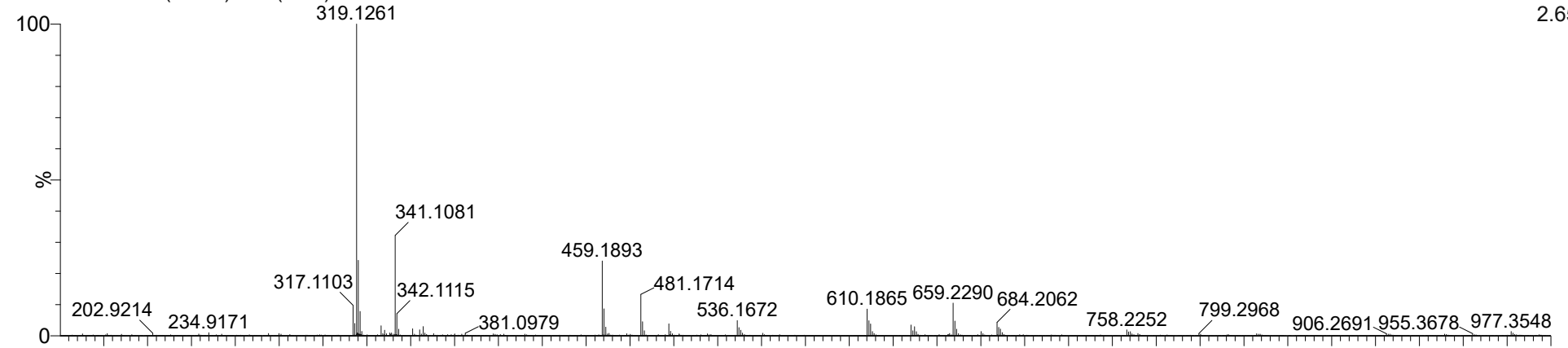


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Salem/Abdelrahman

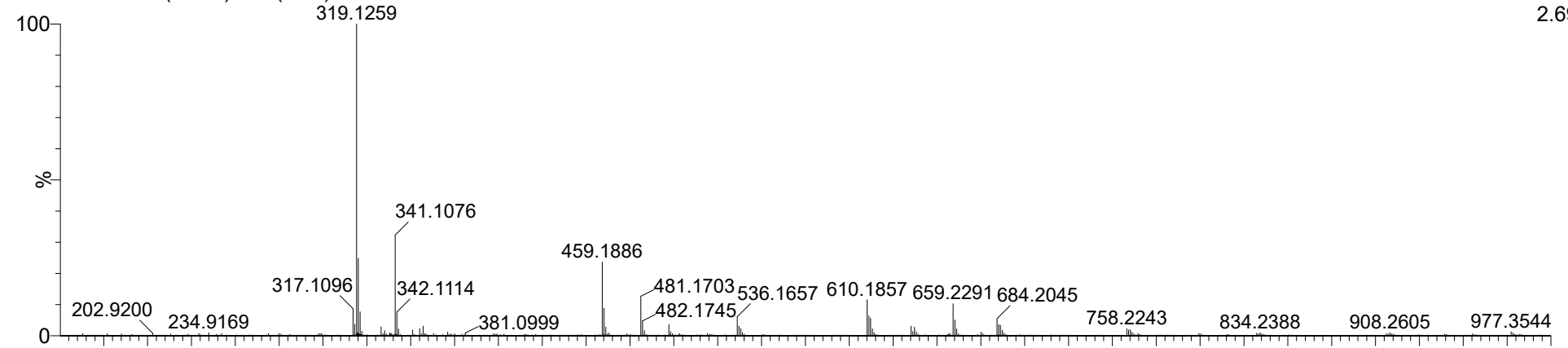
T03251902a 10 (0.356) Cm (8:12)

1: TOF MS ES+  
2.65e4



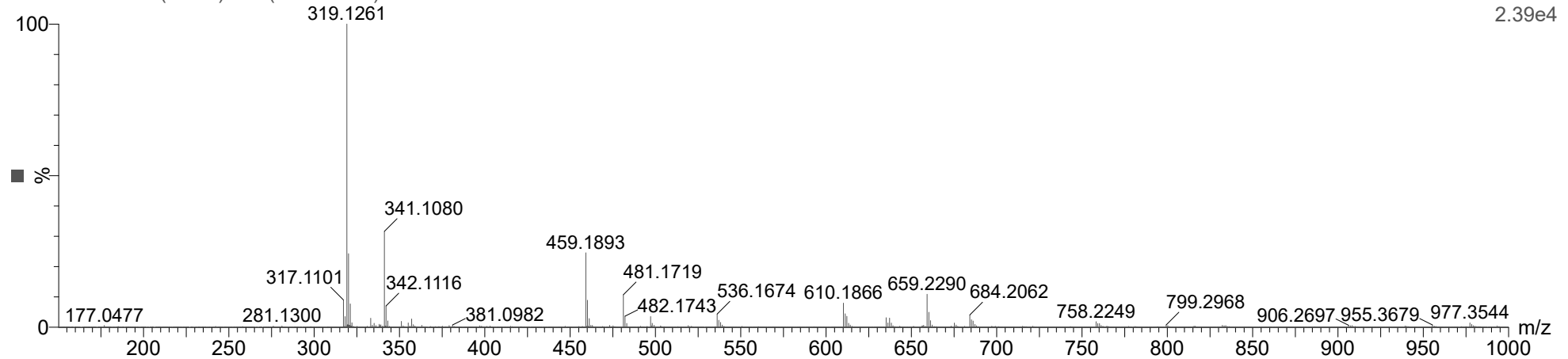
T03251904a 10 (0.356) Cm (8:12)

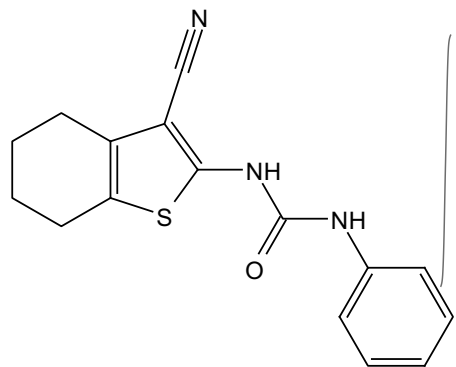
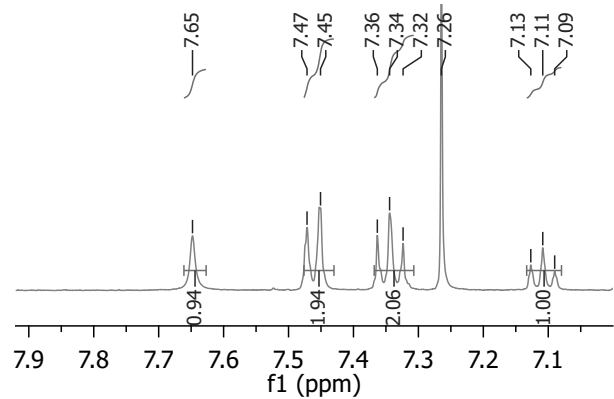
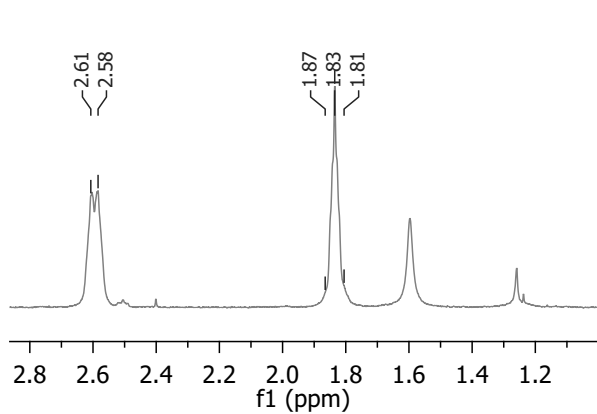
1: TOF MS ES+  
2.69e4



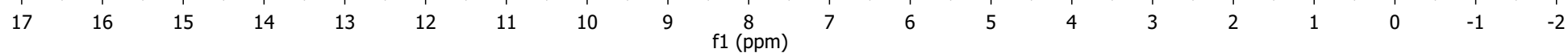
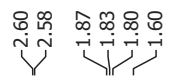
T03251902a 10 (0.356) Cm (9:12-19:27)

1: TOF MS ES+  
2.39e4

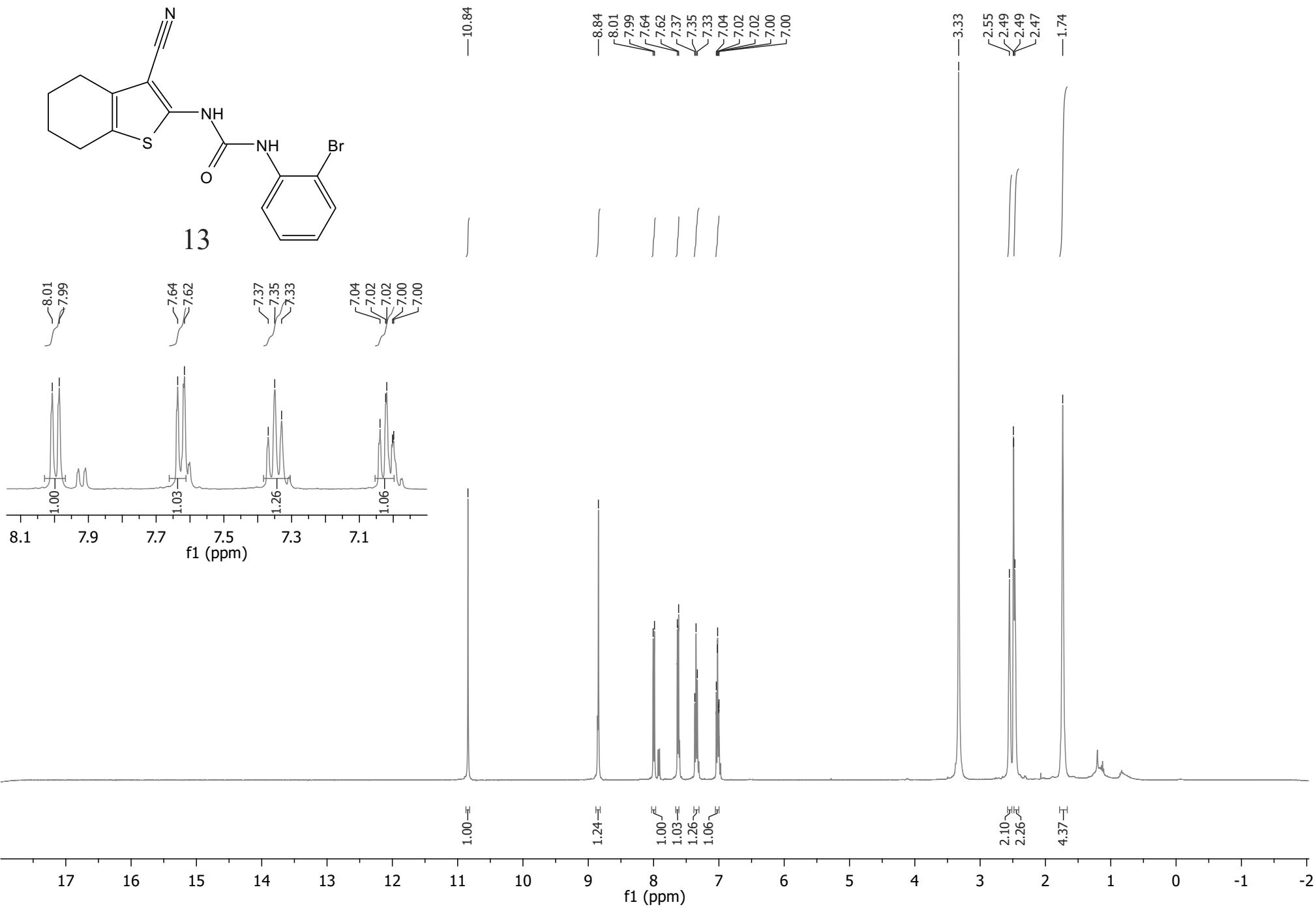
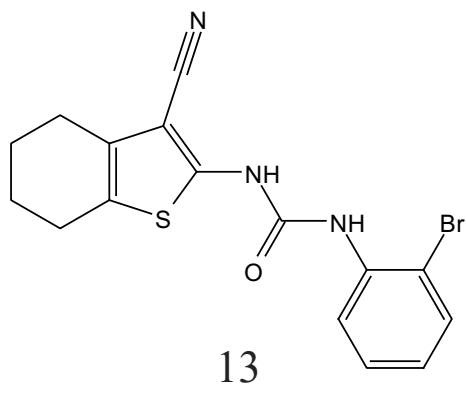




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# Elemental Composition Report

## 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

913 formula(e) evaluated with 9 results within limits (all results (up to 1000) for each mass)

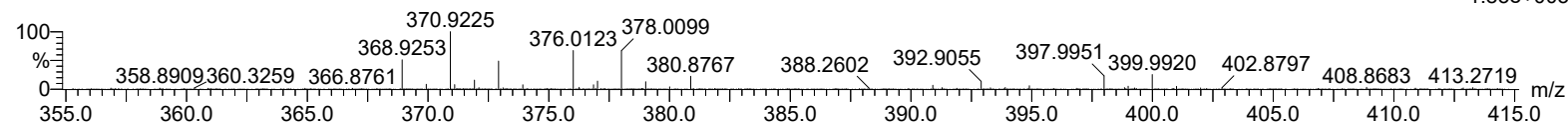
Elements Used:

C: 1-100 H: 1-200 N: 0-5 O: 0-5 S: 0-2 Br: 0-1

Salem/Abdelrahman  
T03041934 10 (0.356) Cm (6:10)

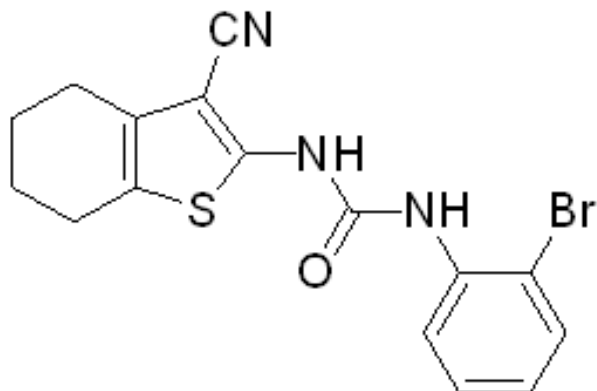
Sample #35

1: TOF MS ES+  
1.83e+003



Minimum: -5.0  
Maximum: 5.0 15.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
376.0123	376.0119	0.4	1.1	10.5	297.4	0.0	C16 H15 N3 O S Br
	376.0113	1.0	2.7	1.5	306.5	9.0	C8 H19 N5 O3 S2 Br
	376.0107	1.6	4.3	22.5	326.8	29.3	C20 H2 N5 O4
	376.0141	-1.8	-4.8	17.5	320.3	22.9	C17 H6 N5 O4 S
	376.0102	2.1	5.6	16.5	316.0	18.5	C20 H10 N O3 S2
	376.0147	-2.4	-6.4	26.5	327.4	30.0	C25 H2 N3 O2
	376.0153	-3.0	-8.0	5.5	305.2	7.8	C13 H19 N3 O S2 Br
	376.0085	3.8	10.1	15.5	309.4	11.9	C19 H11 N3 O Br
	376.0079	4.4	11.7	6.5	305.2	7.8	C11 H15 N5 O3 S Br

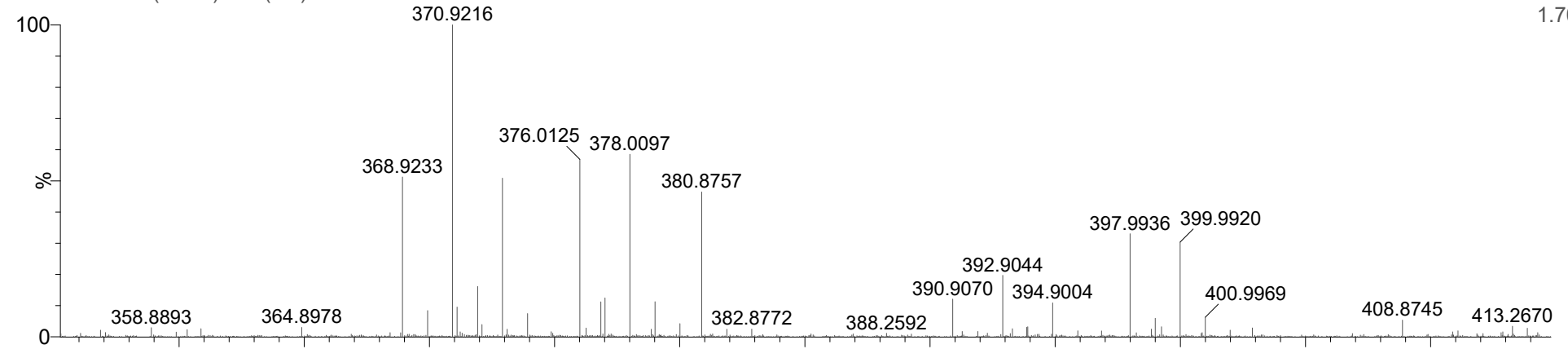


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Salem/Abdelrahman

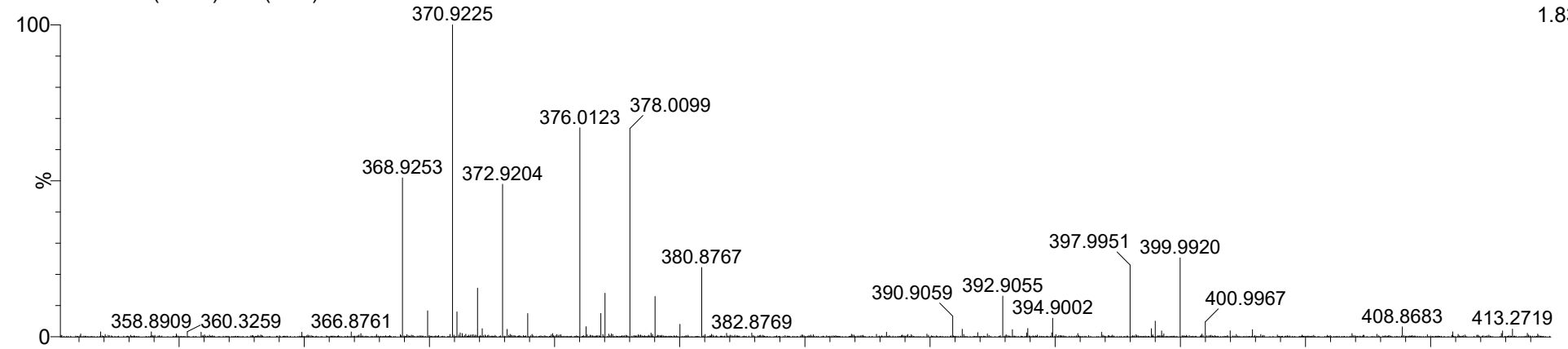
T03041935a 7 (0.255) Cm (5:8)

1: TOF MS ES+  
1.70e3



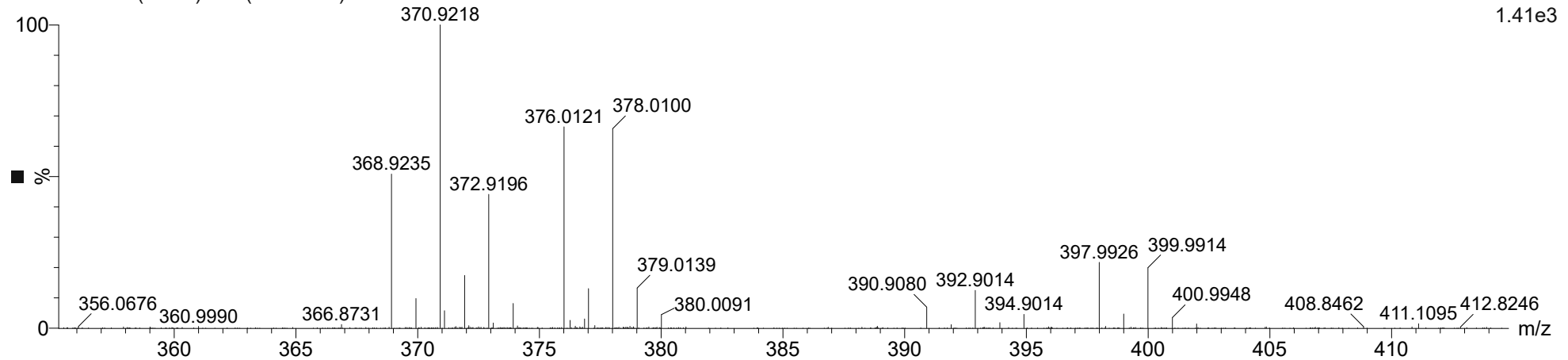
T03041934 10 (0.356) Cm (6:10)

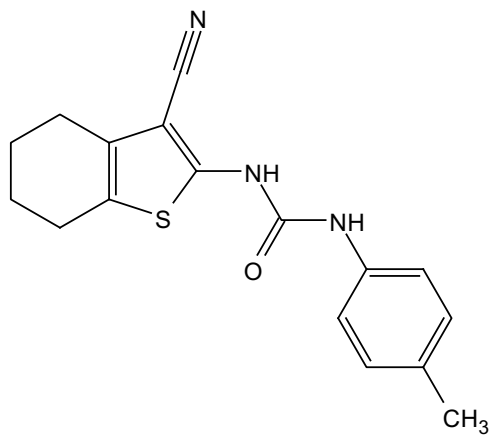
1: TOF MS ES+  
1.83e3



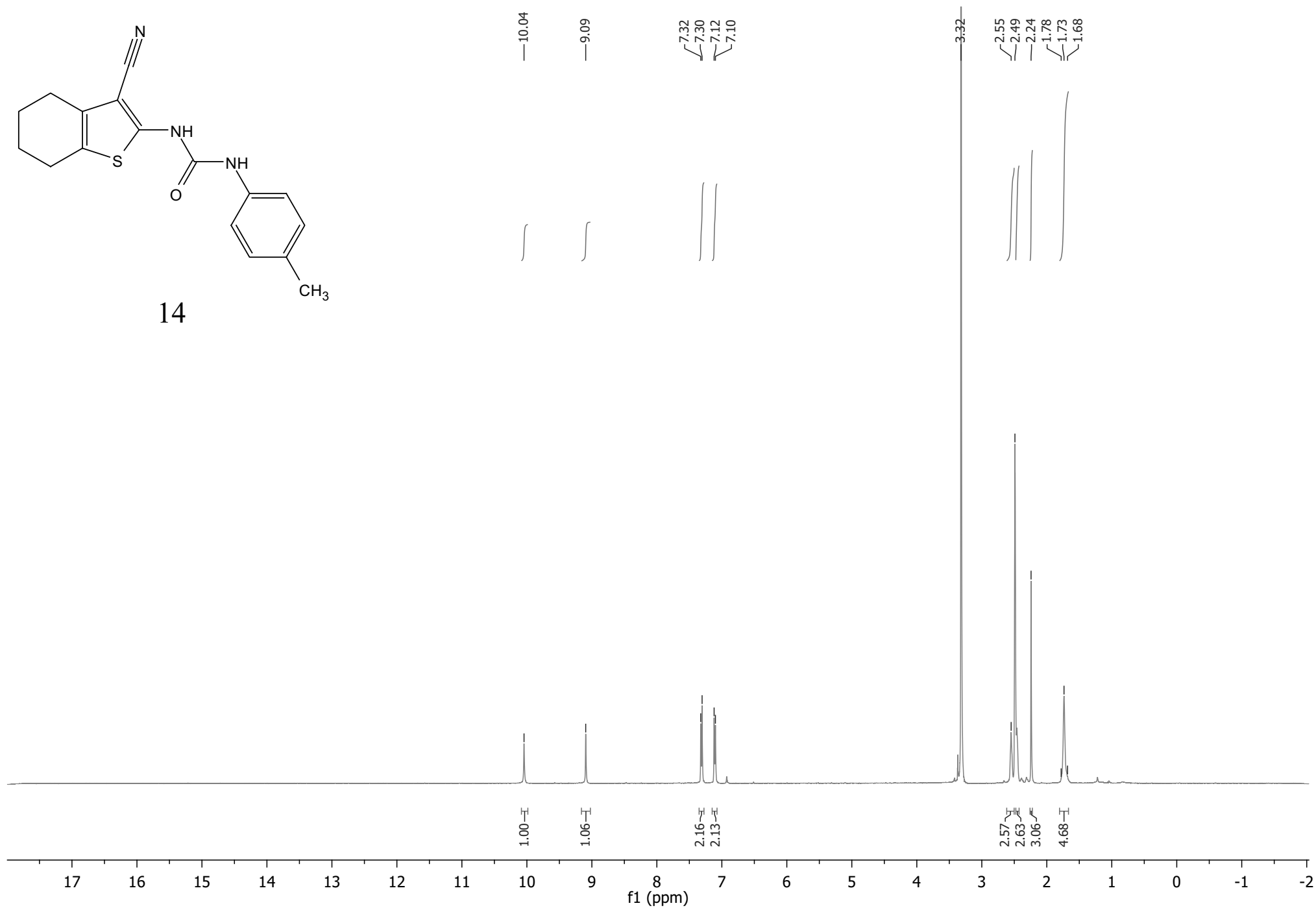
T03041933 8 (0.289) Cm (6:8-15:23)

1: TOF MS ES+  
1.41e3





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

322 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)

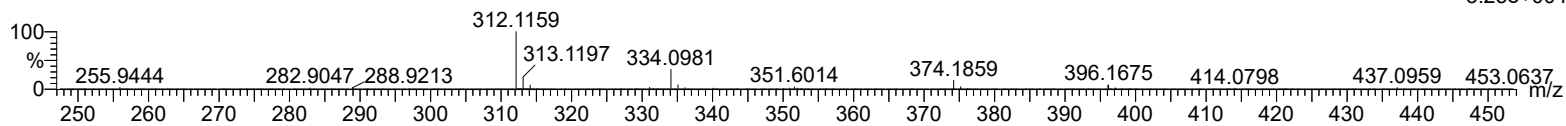
Elements Used:

C: 1-100 H: 1-200 N: 0-6 O: 0-6 S: 1-1 Br: 0-1

Salem/Abdelrahman  
T01311958 6 (0.222) Cm (4:18)

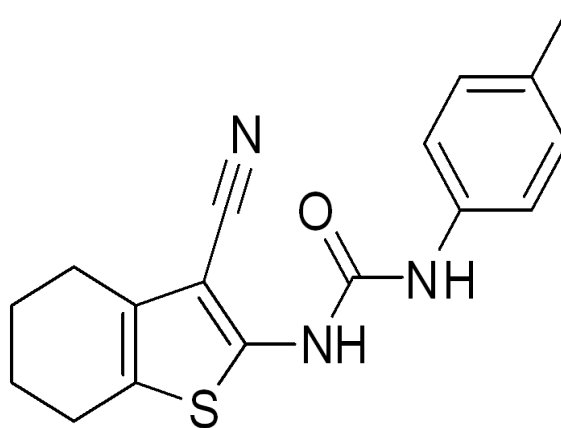
Sample #29

1: TOF MS ES+  
3.25e+004



Minimum: -5.0  
Maximum: 5.0 15.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
312.1160	312.1171	-1.1	-3.5	10.5	663.2	0.0	C17 H18 N3 O S
	312.1130	3.0	9.6	6.5	678.2	15.0	C12 H18 N5 O3 S

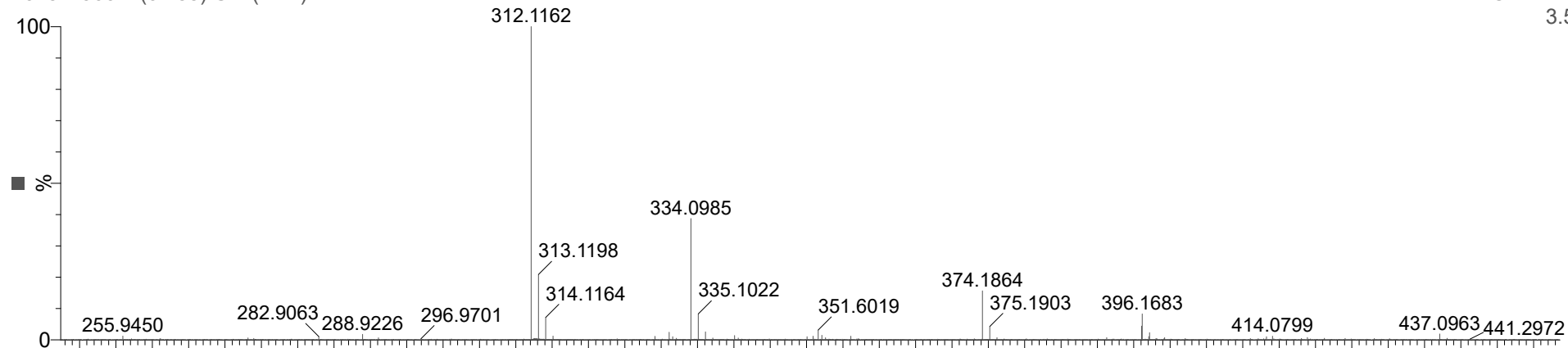


Chemical Formula: C<sub>17</sub>H<sub>17</sub>N<sub>3</sub>OS

Salem/Abdelrahman

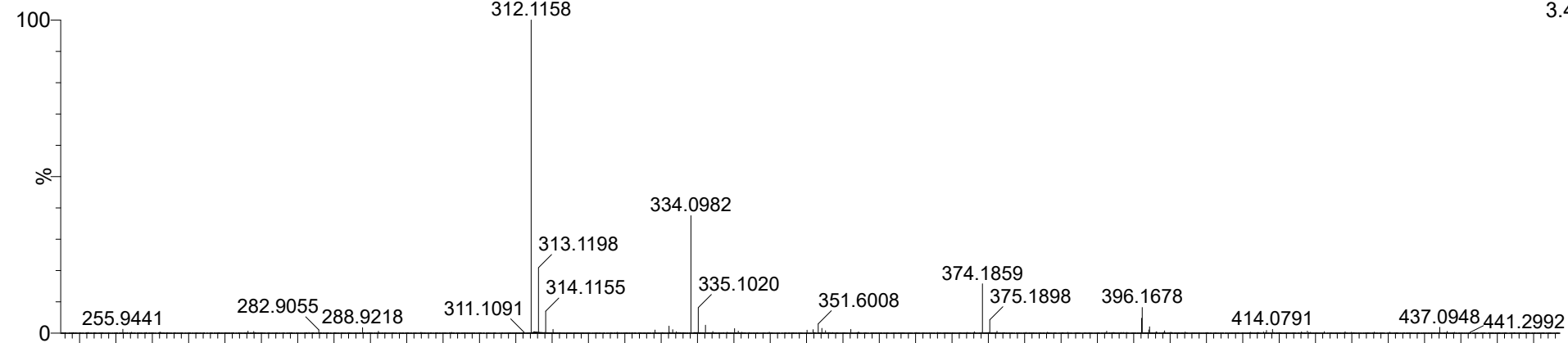
T01311960 7 (0.255) Cm (4:17)

1: TOF MS ES+  
3.55e4



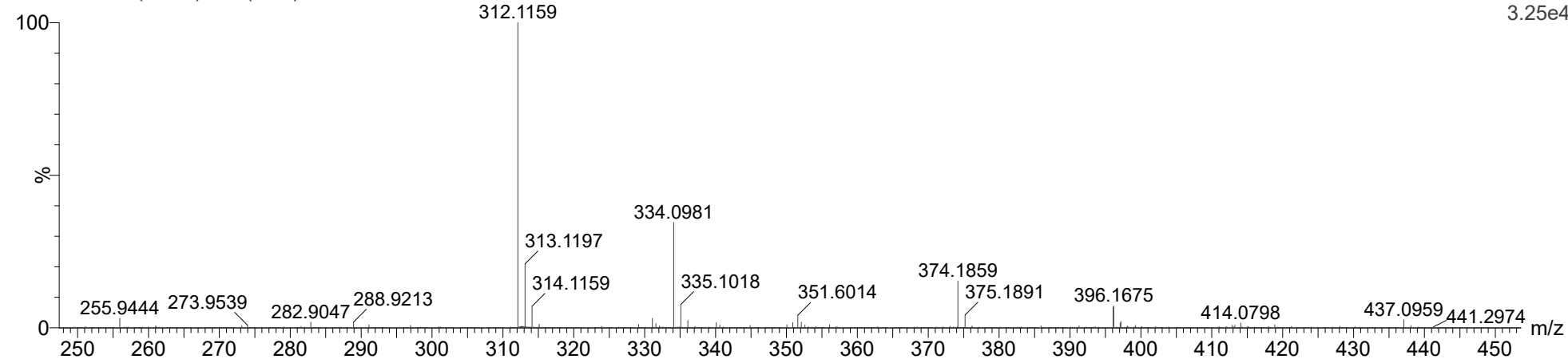
T01311959 7 (0.255) Cm (4:15)

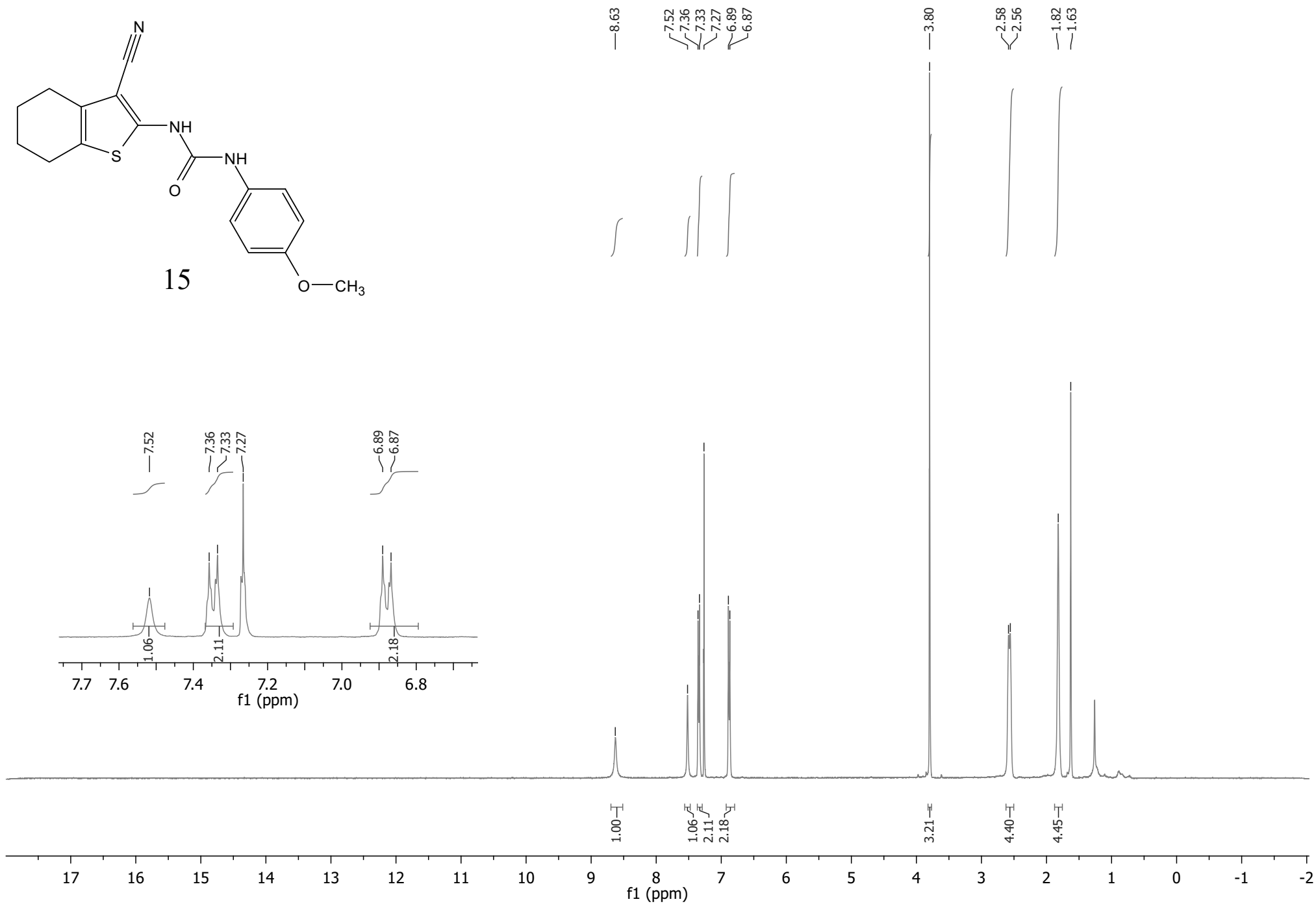
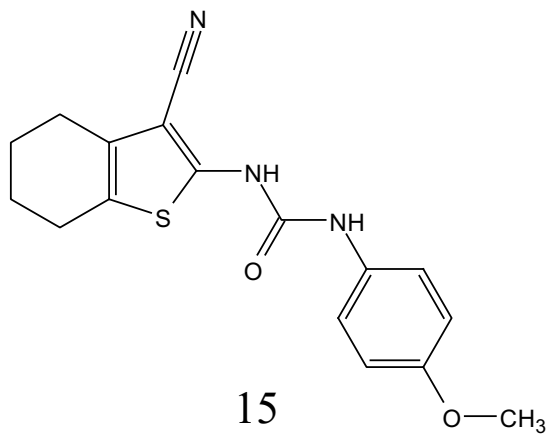
1: TOF MS ES+  
3.43e4



T01311958 6 (0.222) Cm (4:18)

1: TOF MS ES+  
3.25e4





# 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

444 formula(e) evaluated with 7 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 1-100 H: 1-200 N: 0-5 O: 0-5 S: 0-2

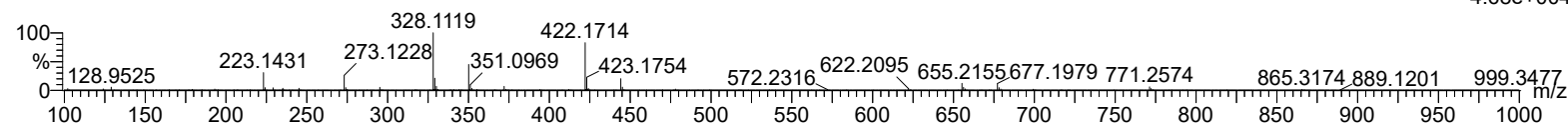
Salem/Abdelrahman

Sample #36

T03041939 7 (0.255) Cm (6:10)

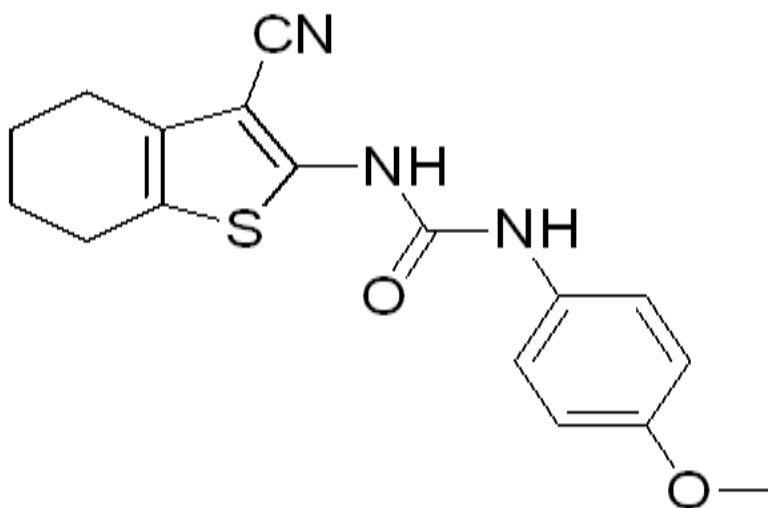
1: TOF MS ES+

4.68e+004



Minimum: -5.0  
Maximum: 5.0 15.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
328.1118	328.1120	-0.2	-0.6	10.5	702.7	0.0	C17 H18 N3 O2 S
	328.1113	0.5	1.5	1.5	716.4	13.7	C9 H22 N5 O4 S2
	328.1126	-0.8	-2.4	19.5	726.5	23.9	C25 H14 N
	328.1086	3.2	9.8	15.5	725.2	22.5	C20 H14 N3 O2
	328.1153	-3.5	-10.7	5.5	714.5	11.8	C14 H22 N3 O2 S2
	328.1080	3.8	11.6	6.5	712.5	9.8	C12 H18 N5 O4 S
	328.1160	-4.2	-12.8	14.5	714.9	12.2	C22 H18 N S



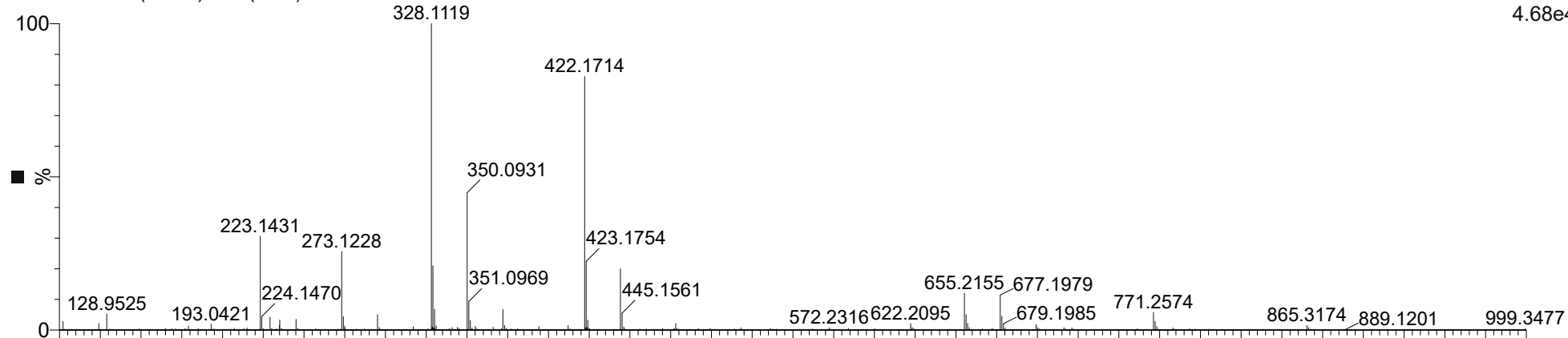
15



Salem/Abdelrahman

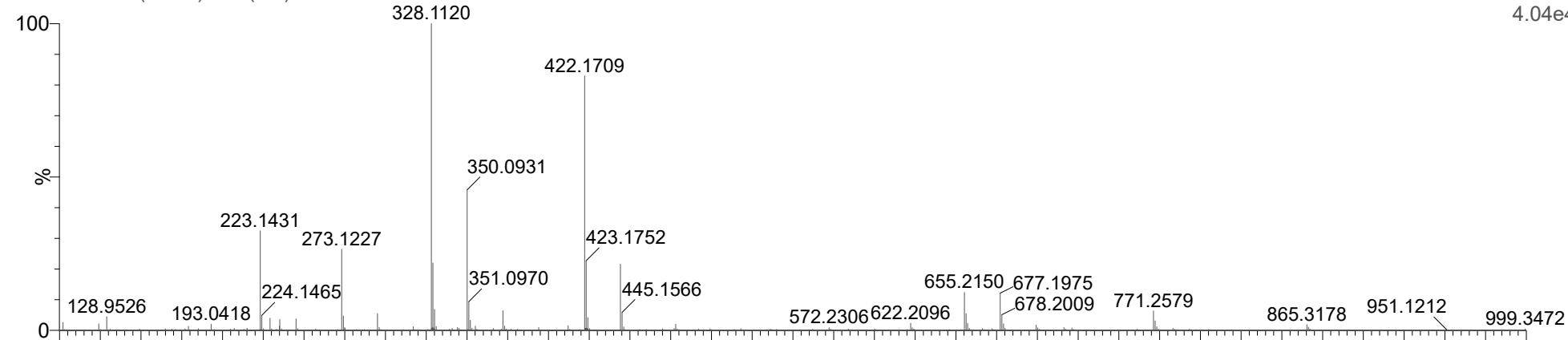
T03041939 7 (0.255) Cm (6:10)

1: TOF MS ES+  
4.68e4



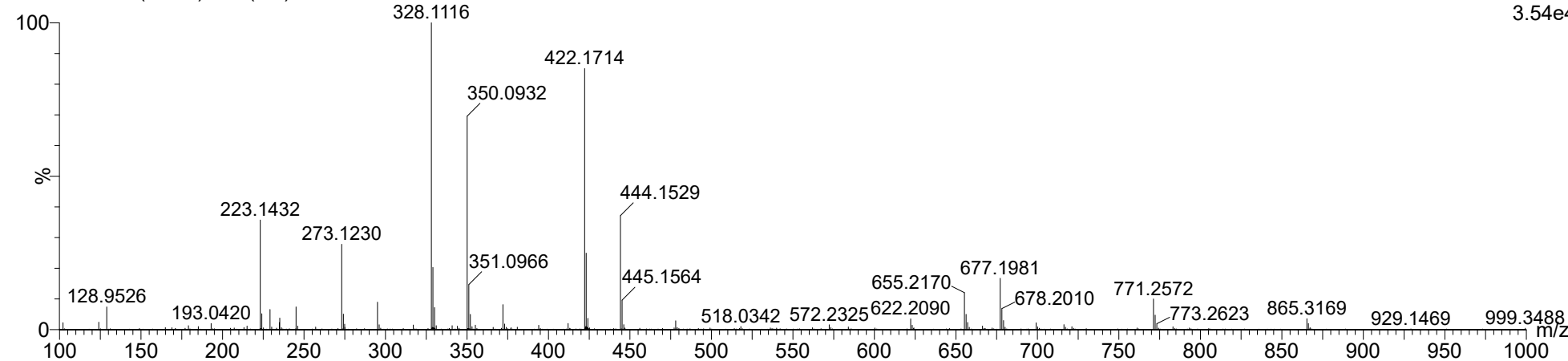
T03041938 7 (0.255) Cm (6:9)

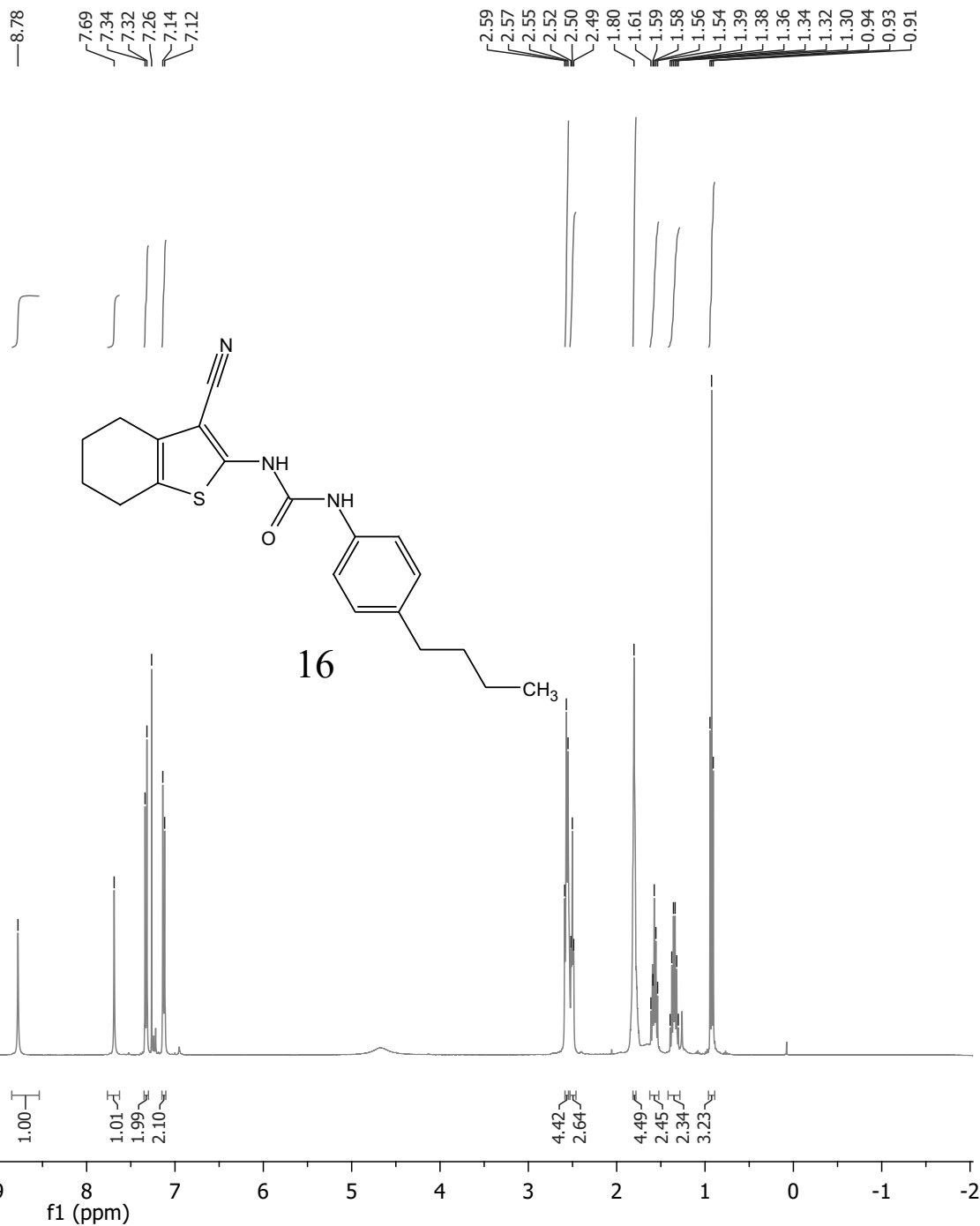
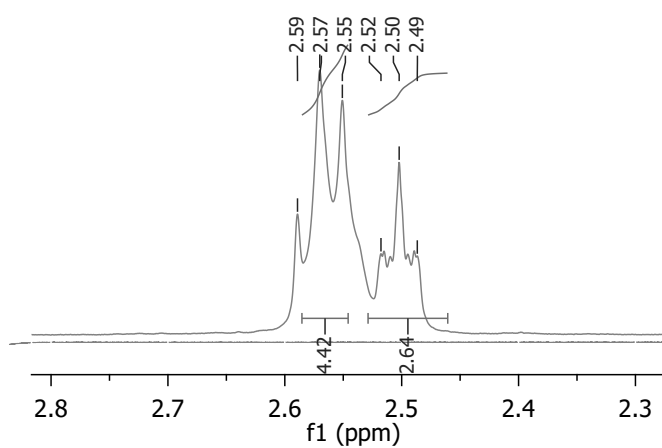
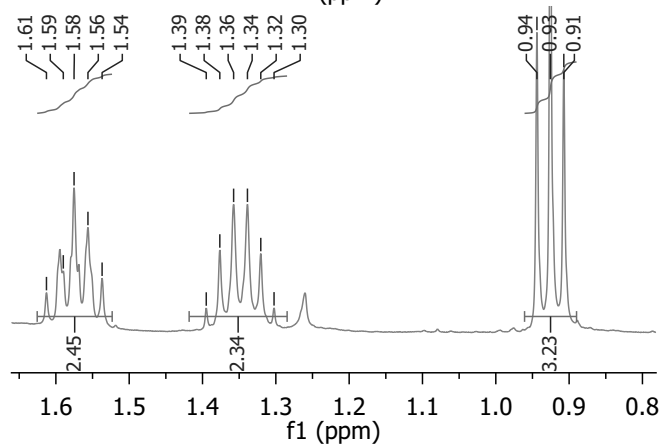
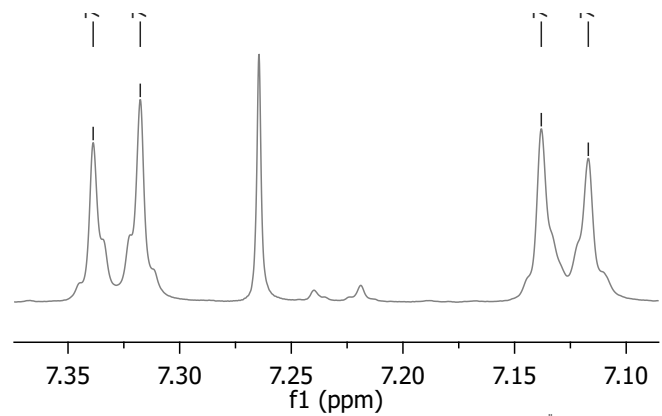
1: TOF MS ES+  
4.04e4

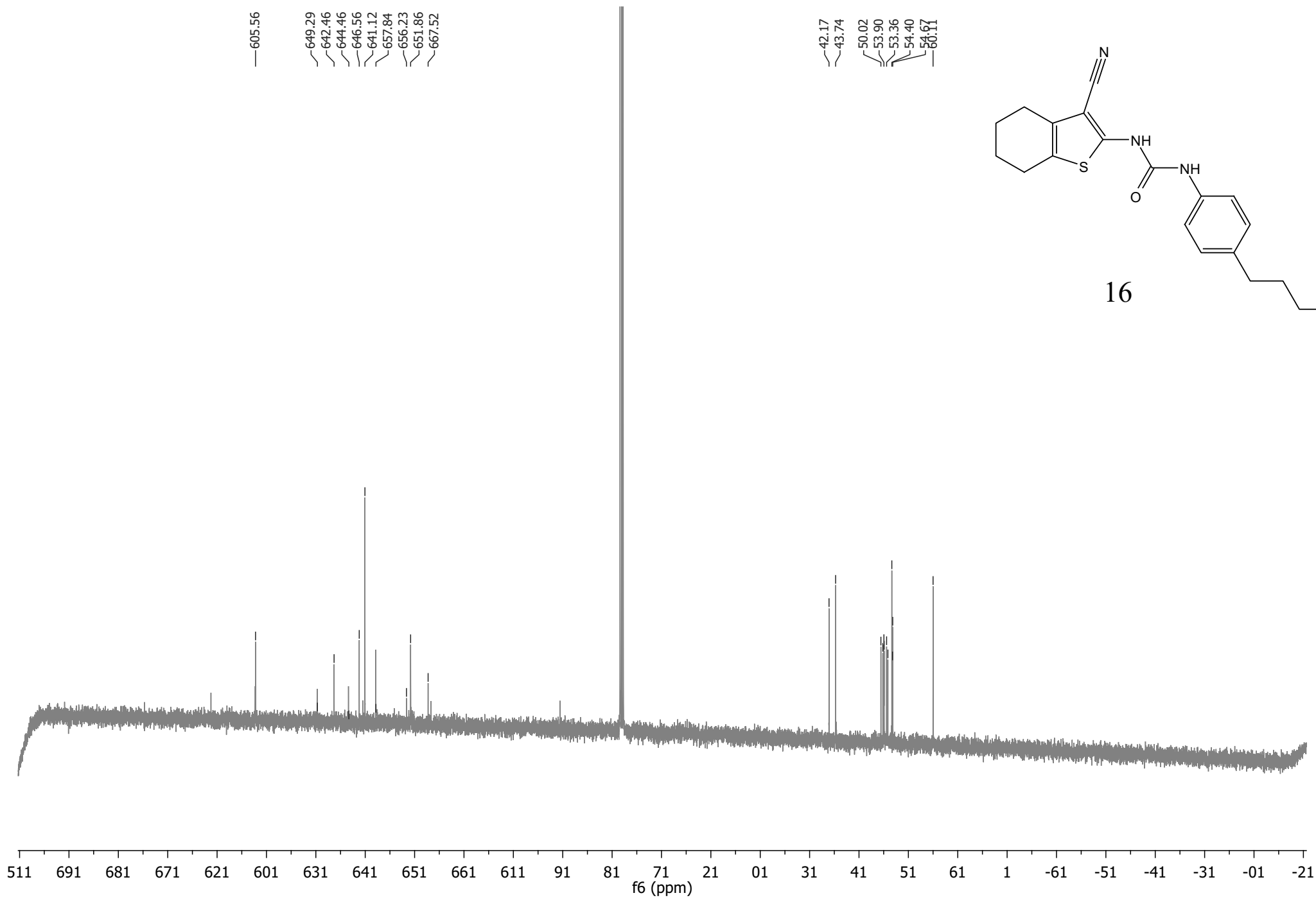


T03041937 7 (0.255) Cm (6:9)

1: TOF MS ES+  
3.54e4







# 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

372 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)

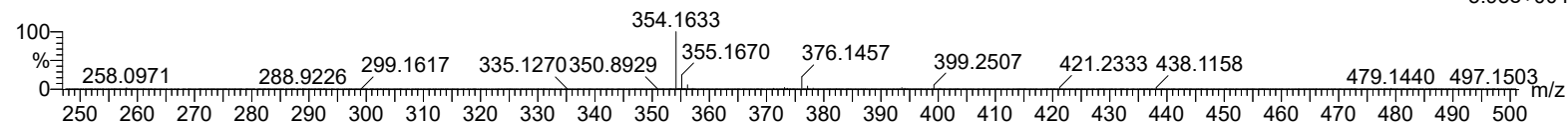
Elements Used:

C: 1-100 H: 1-200 N: 0-6 O: 0-6 S: 1-1 Br: 0-1

Salem/Abdelrahman  
T01311956 7 (0.255) Cm (4:15)

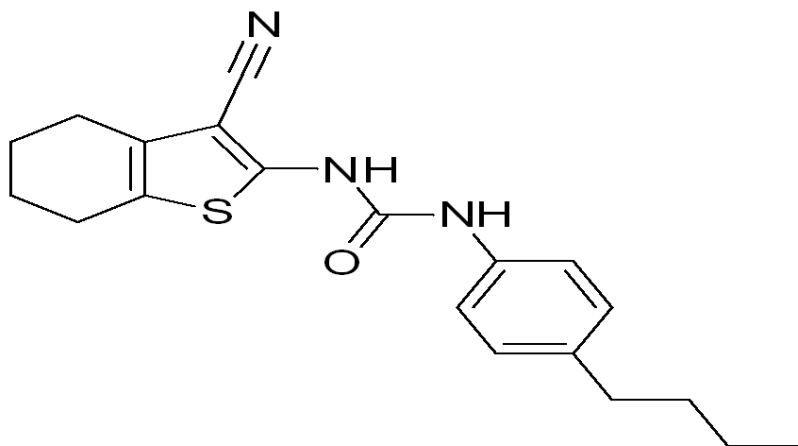
Sample #28

1: TOF MS ES+  
5.95e+004



Minimum: -5.0  
Maximum: 5.0 15.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
354.1632	354.1640	-0.8	-2.3	10.5	751.8	0.0	C20 H24 N3 O S
	354.1600	3.2	9.0	6.5	769.9	18.1	C15 H24 N5 O3 S



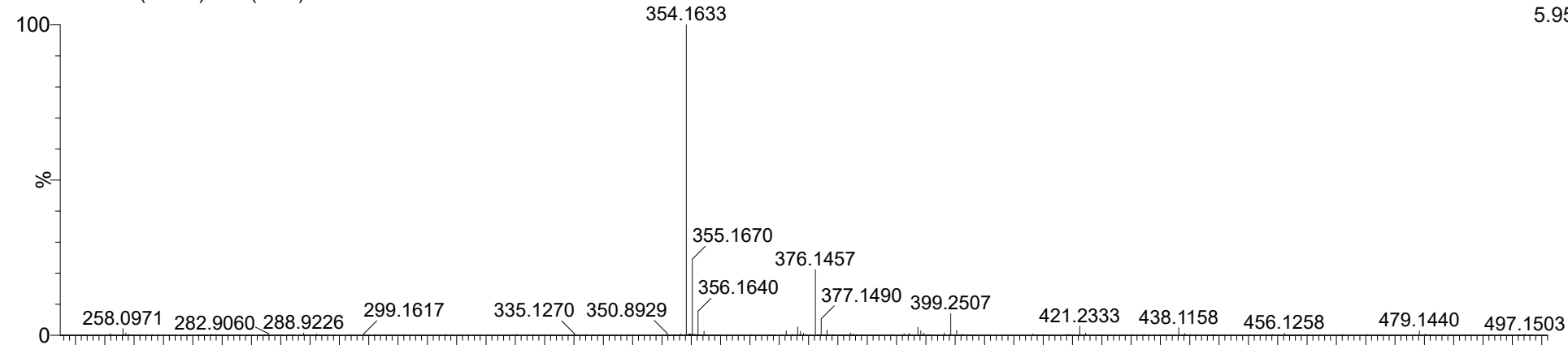
Chemical Formula: C<sub>20</sub>H<sub>23</sub>N<sub>3</sub>OS

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Salem/Abdelrahman

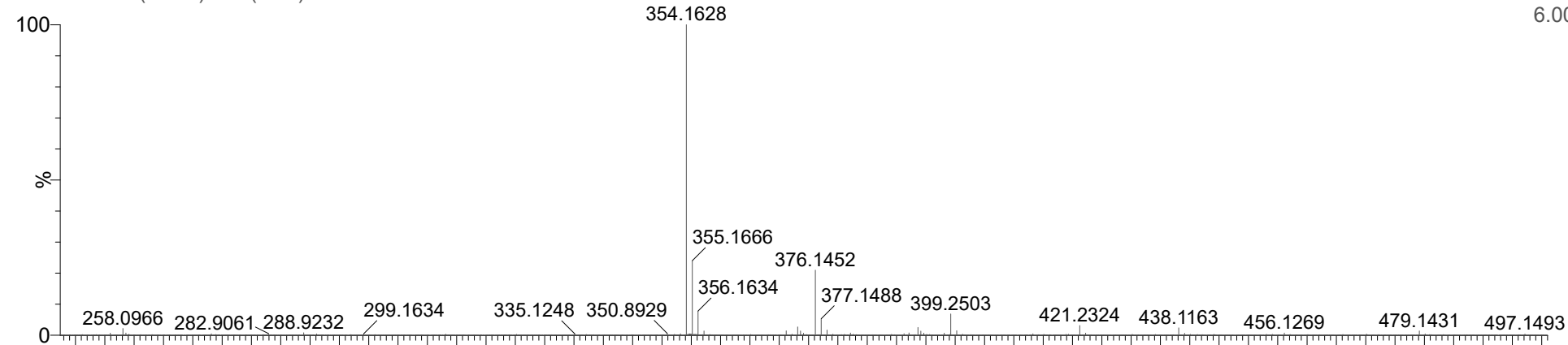
T01311956 7 (0.255) Cm (4:15)

1: TOF MS ES+  
5.95e4



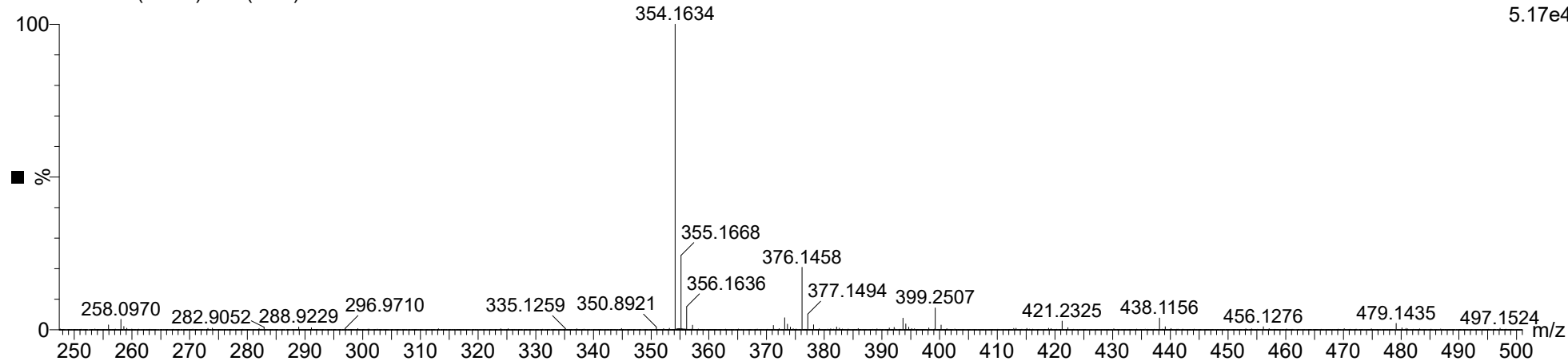
T01311955 6 (0.222) Cm (4:17)

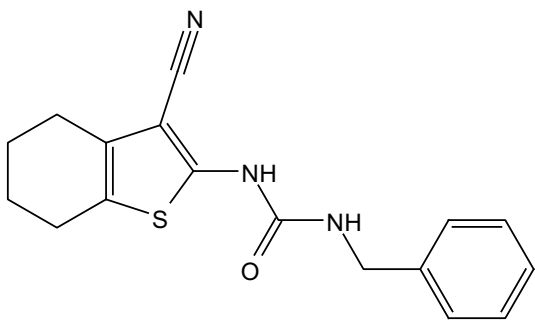
1: TOF MS ES+  
6.00e4



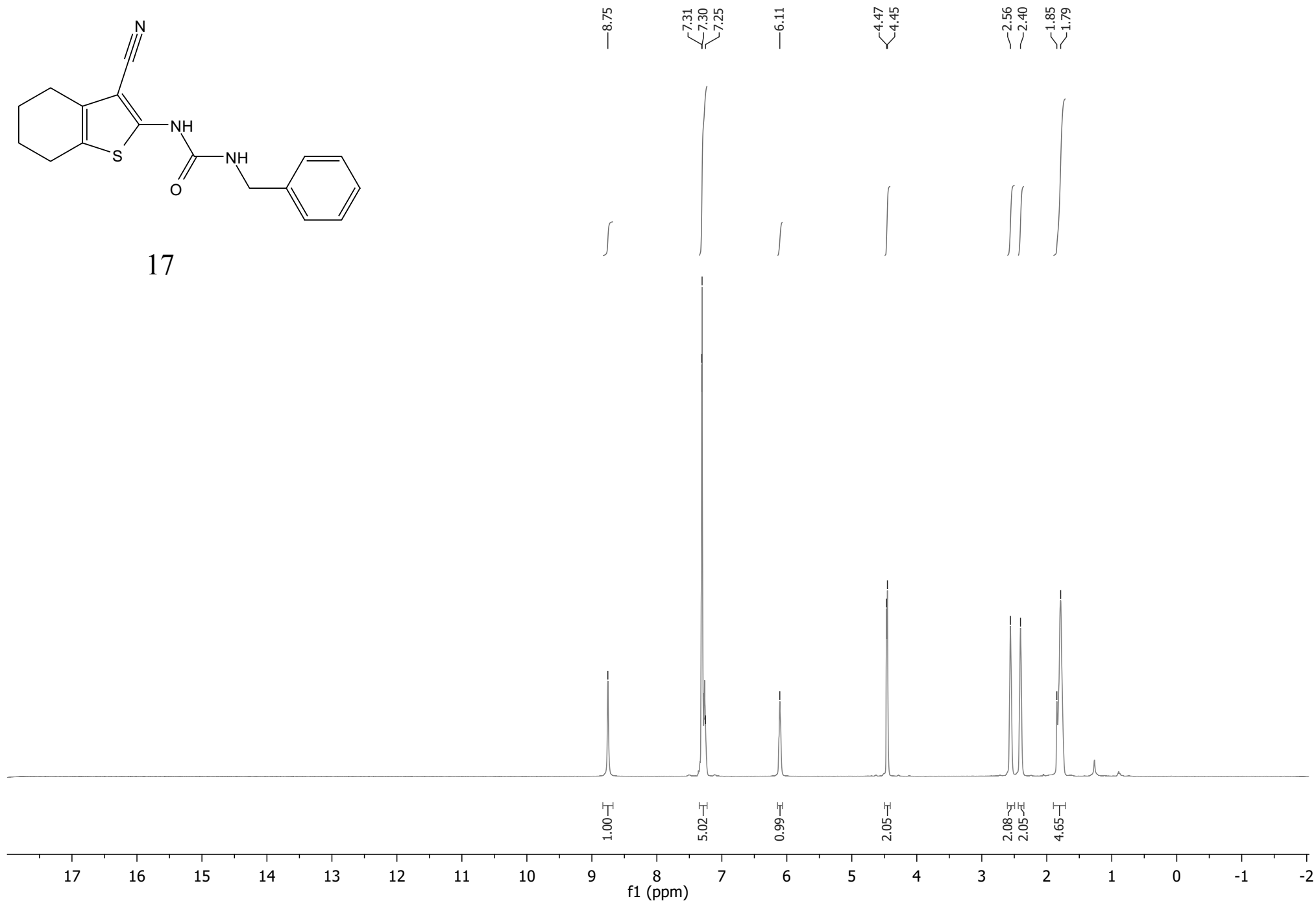
T01311954 7 (0.255) Cm (4:15)

1: TOF MS ES+  
5.17e4





17



603.78  
605.72

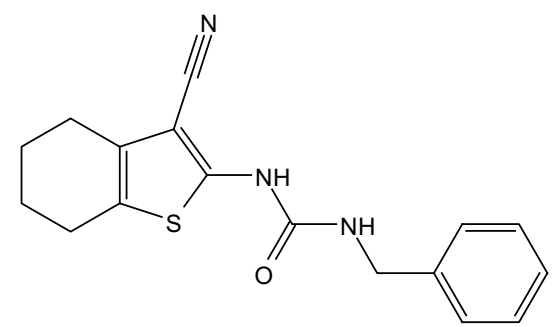
649.41  
646.63  
659.71  
658.01  
658.33  
657.55

667.67

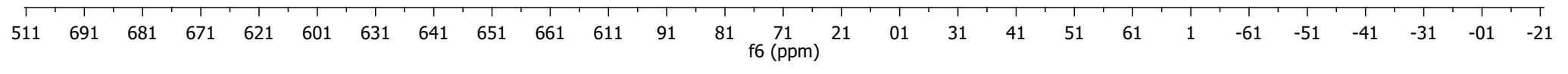
91.65

30.45

53.90  
53.91  
53.56  
54.56



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

322 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)

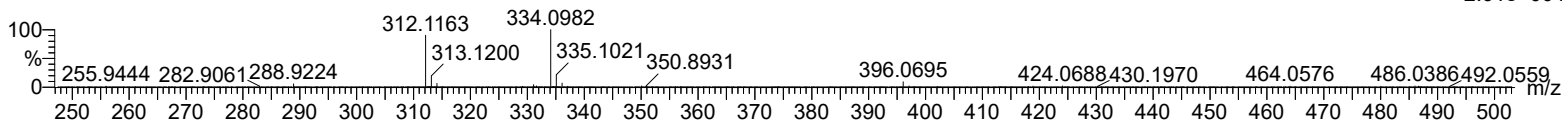
Elements Used:

C: 1-100 H: 1-200 N: 0-6 O: 0-6 S: 1-1 Br: 0-1

Salem/Abdelrahman  
T01311967a 7 (0.255) Cm (4:12)

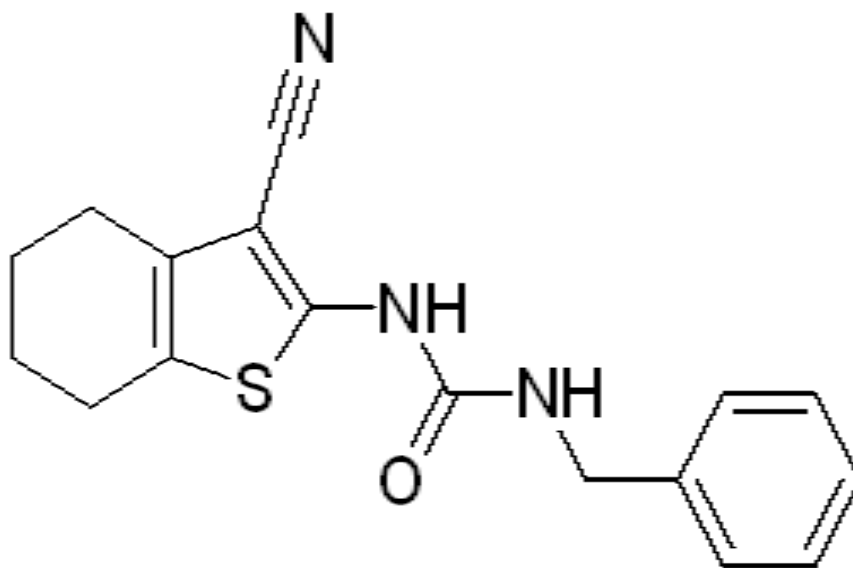
Sample #31

1: TOF MS ES+  
2.61e+004



Minimum: -5.0  
Maximum: 5.0 15.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
312.1163	312.1171	-0.8	-2.6	10.5	605.8	0.0	C17 H18 N3 O S
	312.1130	3.3	10.6	6.5	620.1	14.3	C12 H18 N5 O3 S



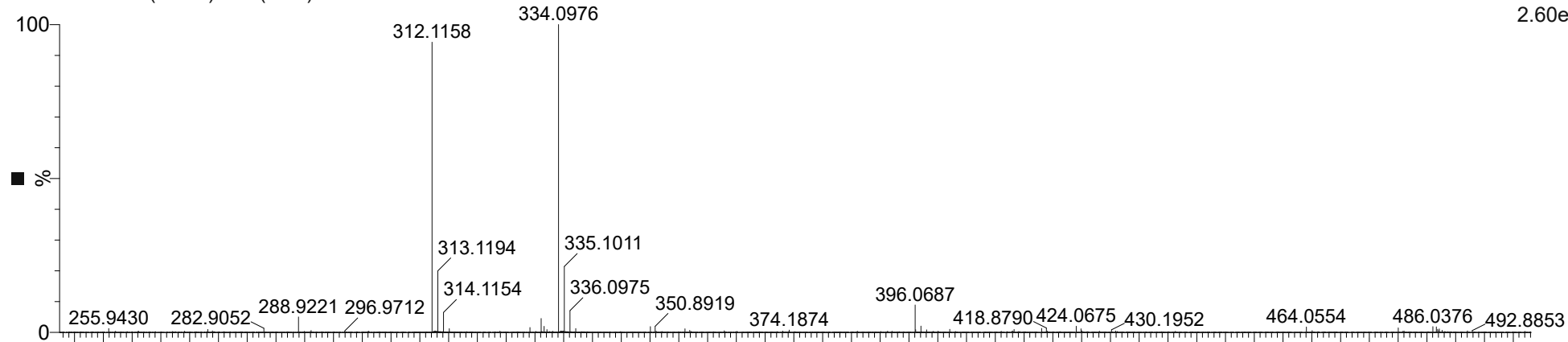
Chemical Formula: C<sub>17</sub>H<sub>17</sub>N<sub>3</sub>OS



Salem/Abdelrahman

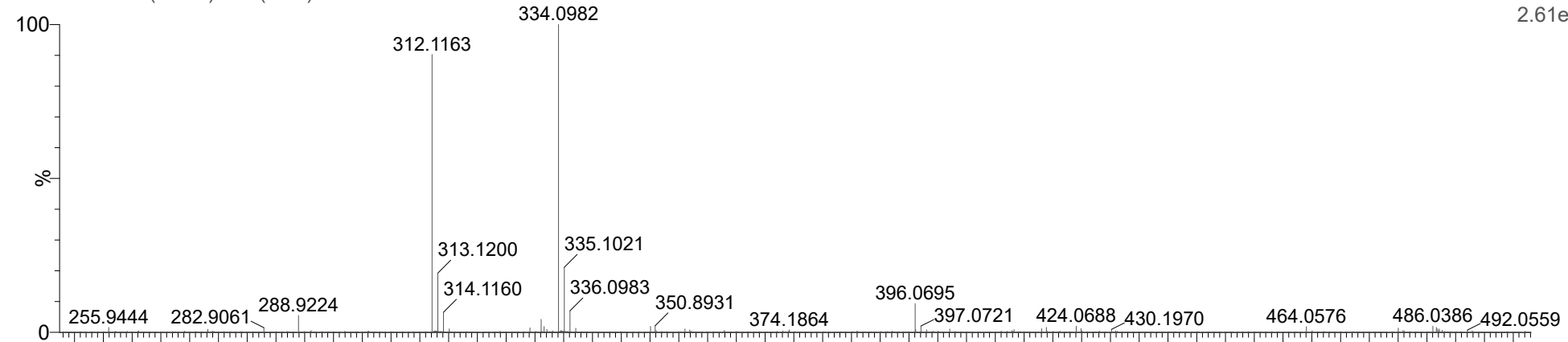
T01311968a 7 (0.255) Cm (4:12)

1: TOF MS ES+  
2.60e4



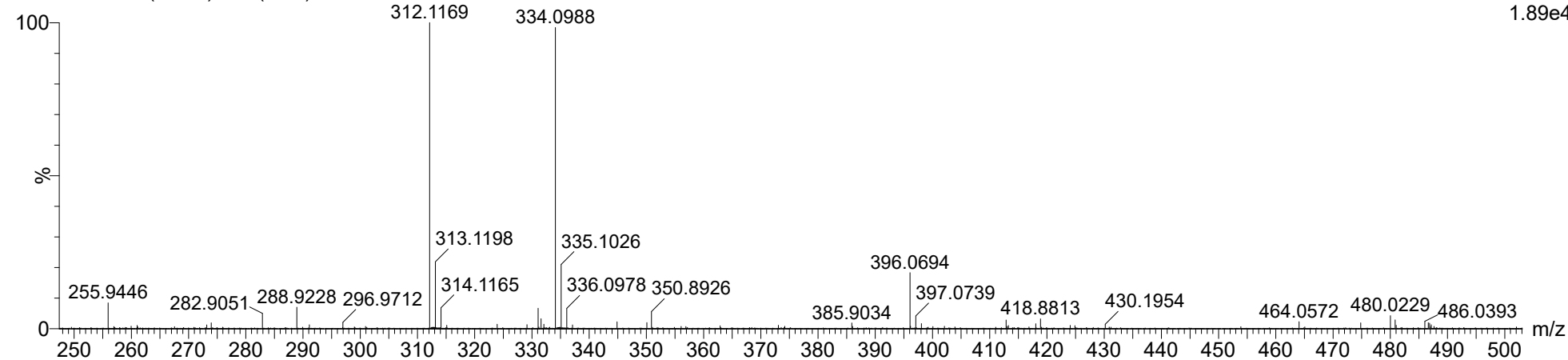
T01311967a 7 (0.255) Cm (4:12)

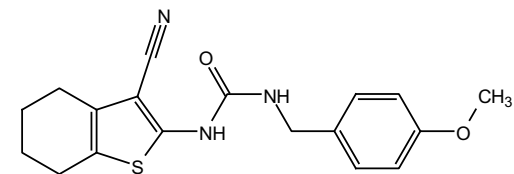
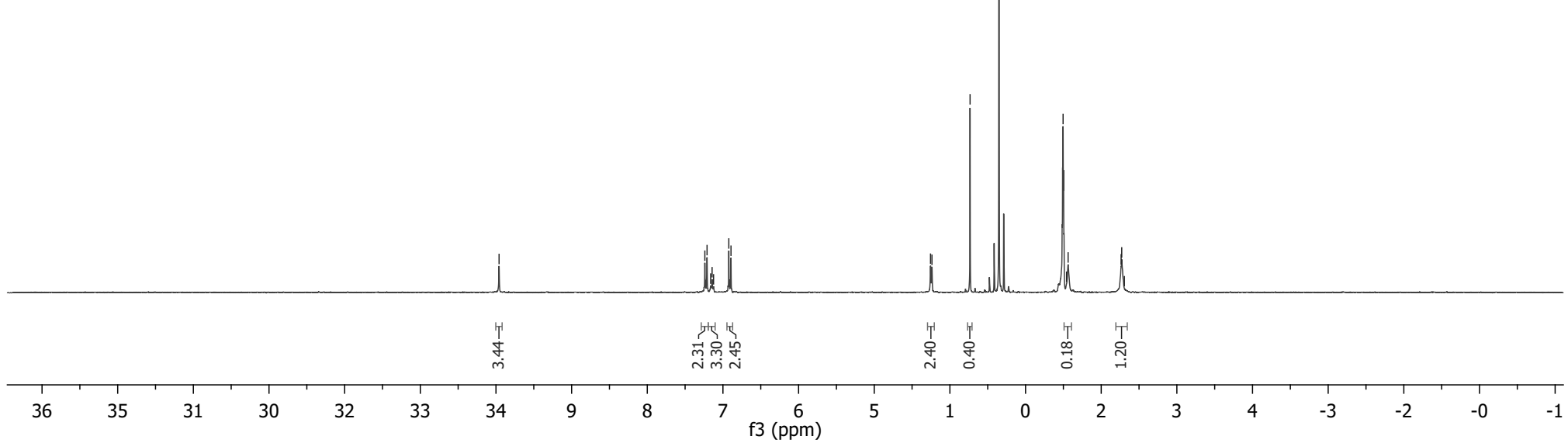
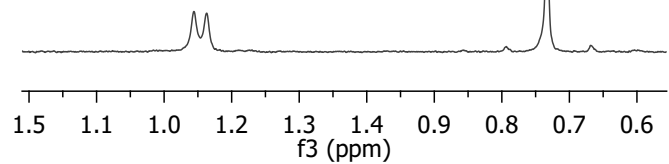
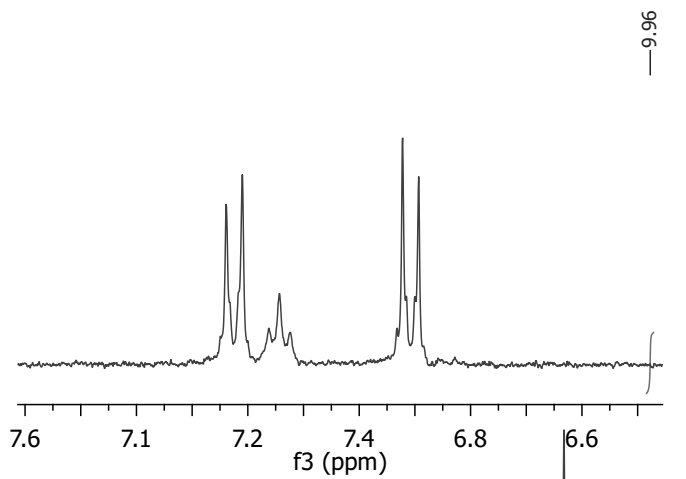
1: TOF MS ES+  
2.61e4



T01311966a 6 (0.222) Cm (4:12)

1: TOF MS ES+  
1.89e4





18

# Elemental Composition Report

## Single Mass Analysis

Tolerance = 3.0 mDa / DBE: min = -5.0, max = 150.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions

399 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)

Elements Used:

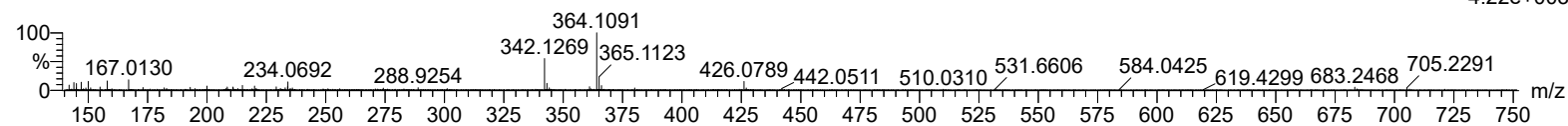
C: 1-100 H: 1-200 N: 0-4 O: 0-10 S: 1-2

Salem/Abdelrahman

#45

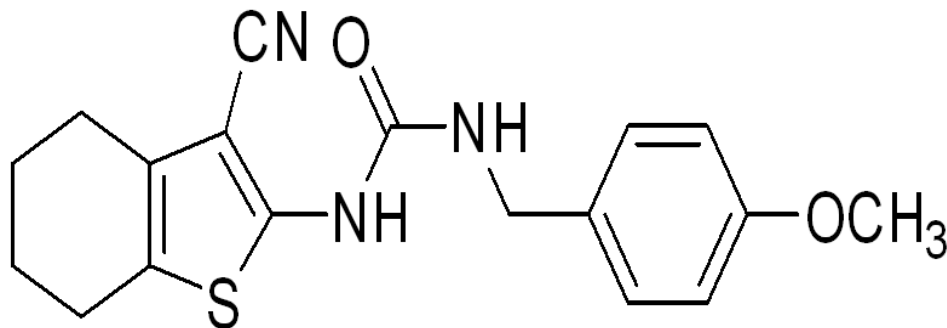
1: TOF MS ES+  
4.22e+003

T05301915 6 (0.222) Cm (4:6)



Minimum: -5.0  
Maximum: 3.0 15.0 150.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
342.1269	342.1276	-0.7	-2.0	10.5	453.0	0.0	C18 H20 N3 O2 S
	342.1256	1.3	3.8	-3.5	463.0	10.0	C9 H28 N O8 S2

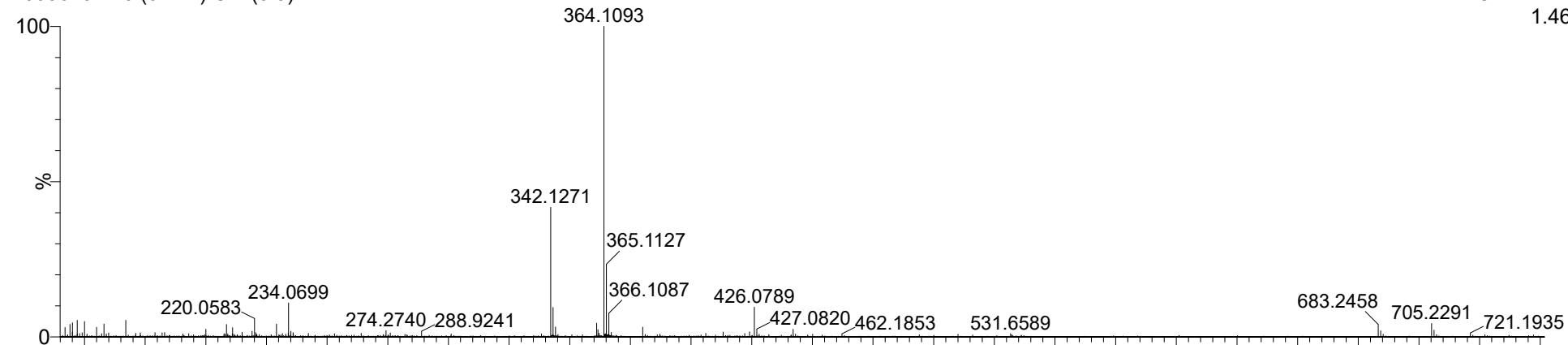


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Salem/Abdelrahman

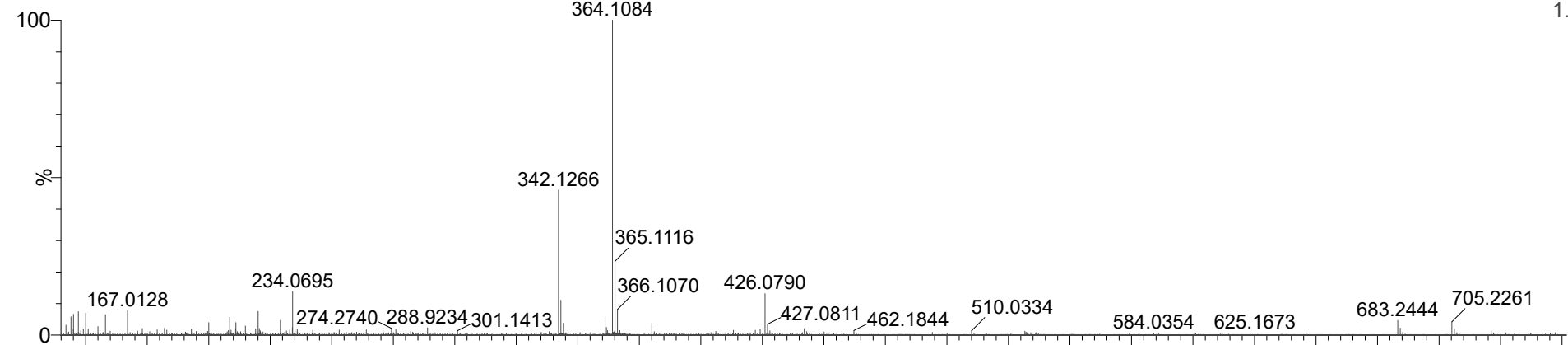
T05301917 6 (0.222) Cm (5:9)

1: TOF MS ES+  
1.46e4



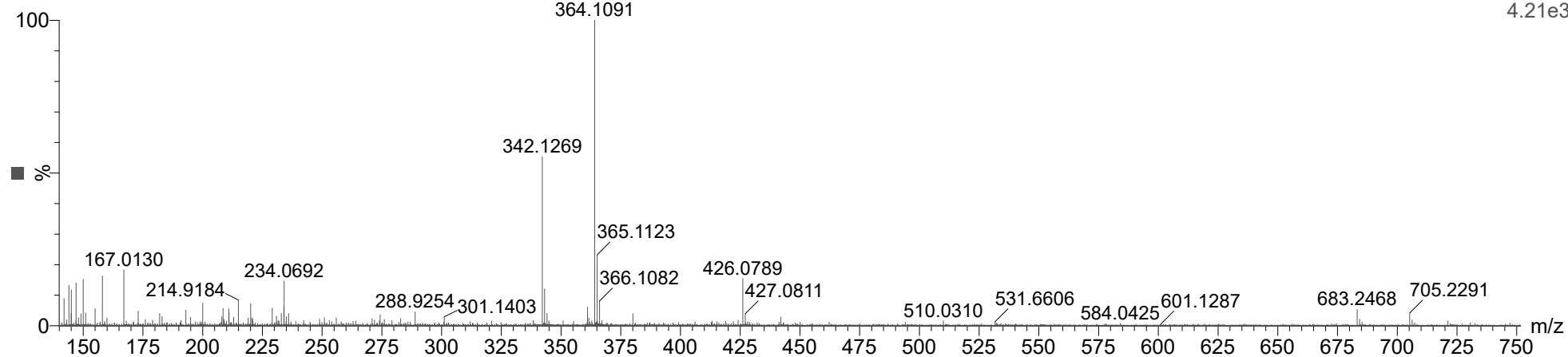
T05301916 6 (0.222) Cm (6:9)

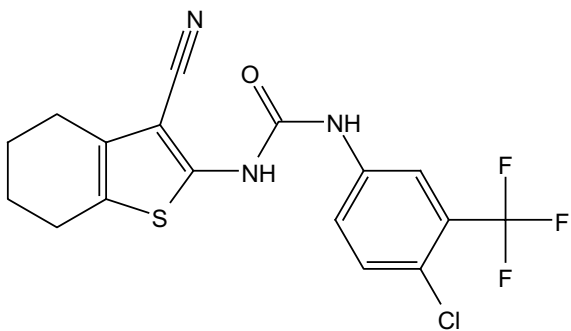
1: TOF MS ES+  
1.07e4



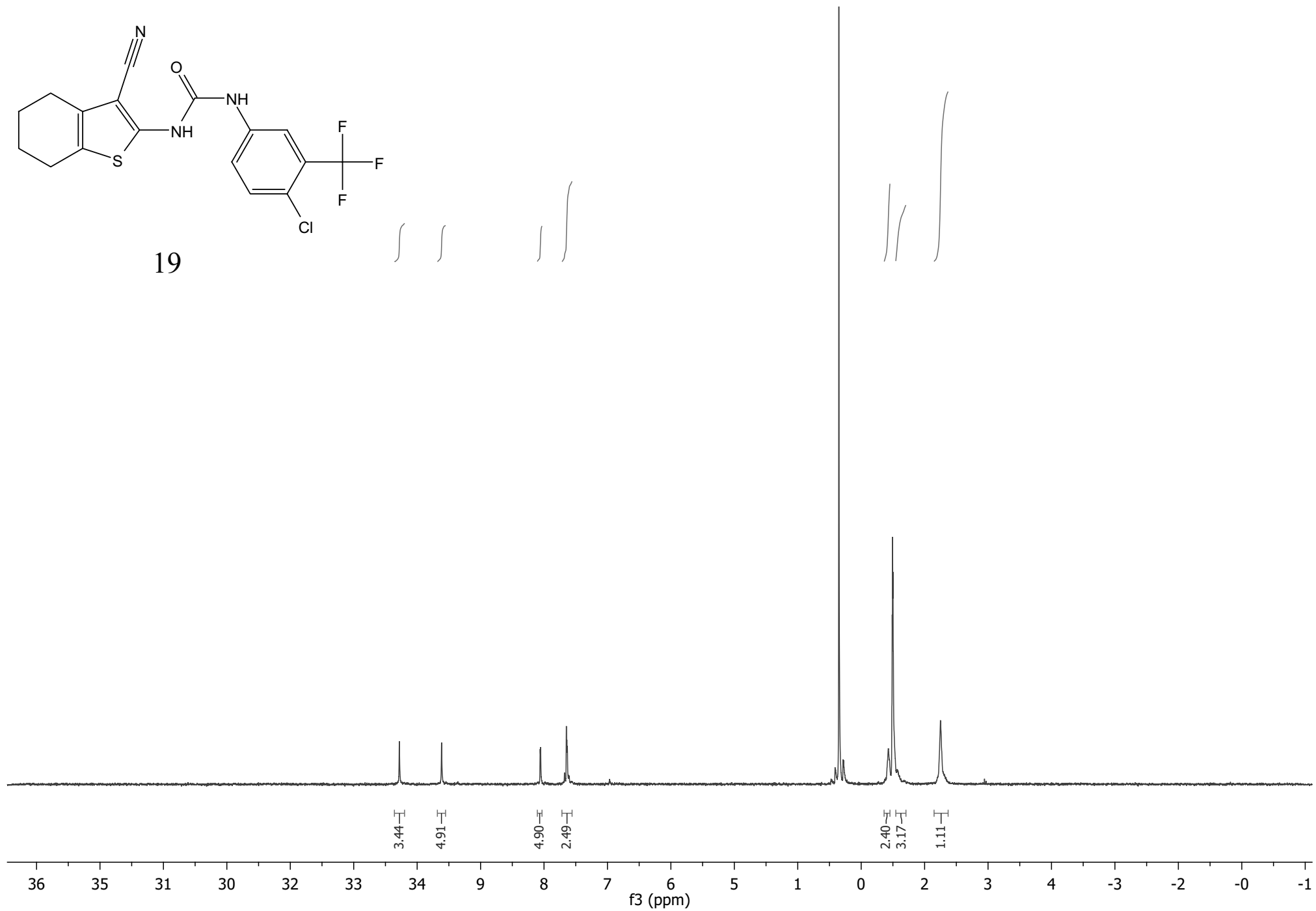
T05301915 6 (0.222) Cm (4:6)

1: TOF MS ES+  
4.21e3





19



# Elemental Composition Report

## Single Mass Analysis

Tolerance = 3.0 mDa / DBE: min = -5.0, max = 150.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions

1518 formula(e) evaluated with 8 results within limits (all results (up to 1000) for each mass)

Elements Used:

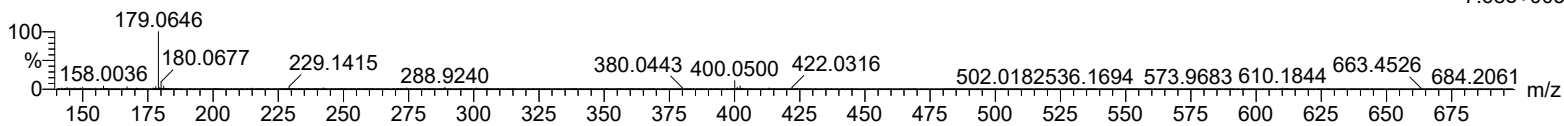
C: 1-100 H: 1-200 N: 0-4 O: 0-10 S: 1-2 Cl: 1-1 F: 0-3

Salem/Abdelrahman

#44

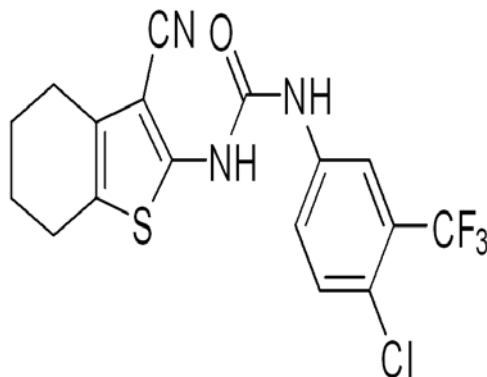
T05301912 6 (0.222) Cm (6:7)

1: TOF MS ES+  
7.68e+003



Minimum: -5.0  
Maximum: 3.0 15.0 150.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
400.0501	400.0503	-0.2	-0.5	-0.5	353.8	6.5	C10 H23 N O9 S2 Cl
	400.0498	0.3	0.7	10.5	347.4	0.2	C17 H14 N3 O S Cl F3
	400.0514	-1.3	-3.2	-4.5	356.2	9.0	C7 H24 N O10 S2 Cl F
	400.0487	1.4	3.5	14.5	349.8	2.6	C20 H13 N3 S Cl F2
	400.0521	-2.0	-5.0	9.5	351.0	3.8	C17 H17 N3 S2 Cl F2
	400.0480	2.1	5.2	0.5	355.2	8.0	C10 H20 N O10 S Cl F
	400.0523	-2.2	-5.5	13.5	350.3	3.0	C19 H15 N3 O3 S Cl
	400.0478	2.3	5.7	-3.5	356.6	9.3	C8 H22 N O7 S2 Cl F3

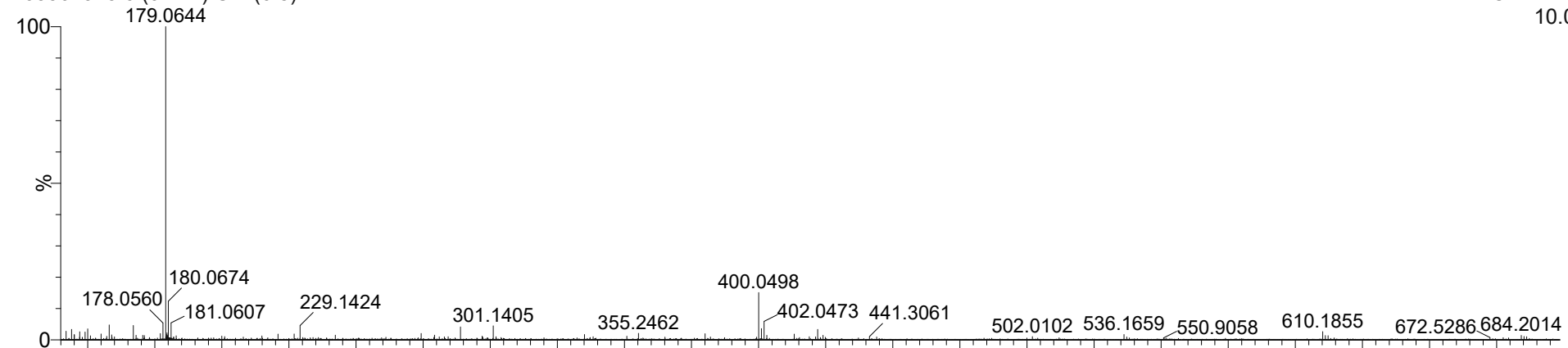


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Salem/Abdelrahman

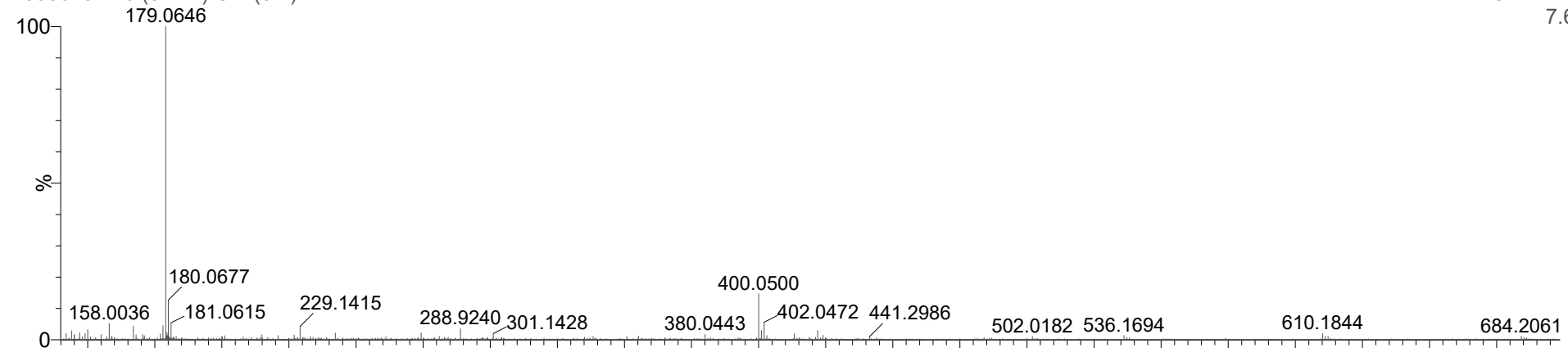
T05301913 6 (0.222) Cm (6:8)

1: TOF MS ES+  
10.00e3



T05301912 6 (0.222) Cm (6:7)

1: TOF MS ES+  
7.68e3



T05301911 6 (0.222) Cm (6:8)

1: TOF MS ES+  
1.22e4

