

Supporting Information

Data File: C:\LabSolutions\Data\Analz\data\SO-1_52.lcd

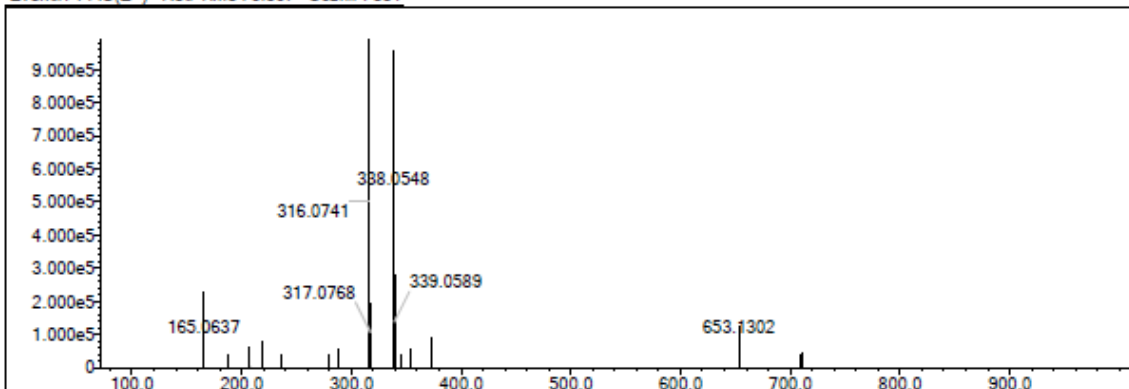
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	8	20	O	2	1	6	Cl	1	0	2	I	3	0	0	H
C	4	12	25	F	1	0	0	Br	1	0	1					
N	3	3	6	S	2	1	3	Ru	2	0	0					

Error Margin (ppm): 10
 HC Ratio: unlimited
 Max Isotopes: 3
 MSn Iso RI (%): 10.00

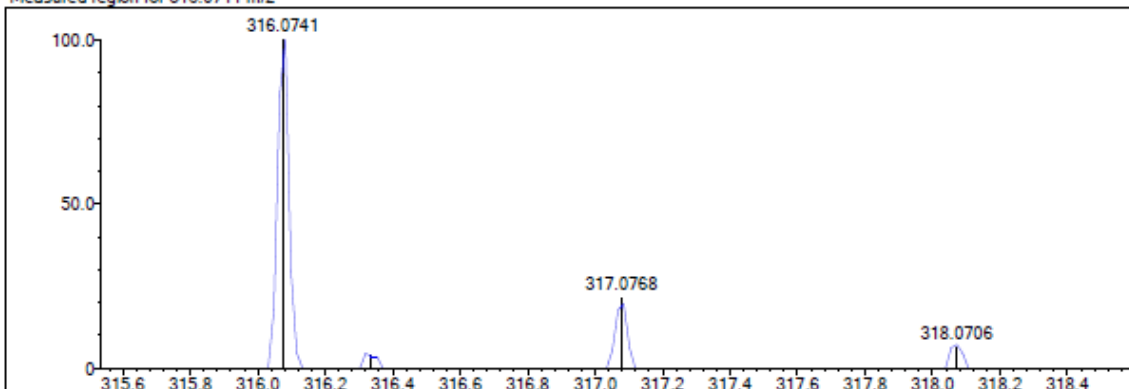
DBE Range: 0.0 - 15.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

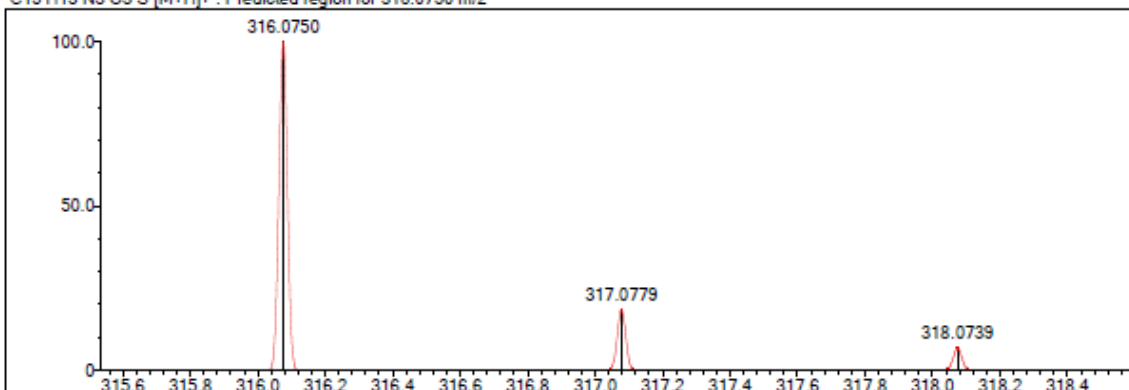
Event#: 1 MS(E+) Ret. Time : 5.867 Scan#: 881



Measured region for 316.0741 m/z



C15 H13 N3 O3 S [M+H]⁺ : Predicted region for 316.0750 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	76.70	C15 H13 N3 O3 S	[M+H] ⁺	316.0741	316.0750	-0.9	-2.85	80.42	11.0

Figure 1. Compound 3a Mass spectrum

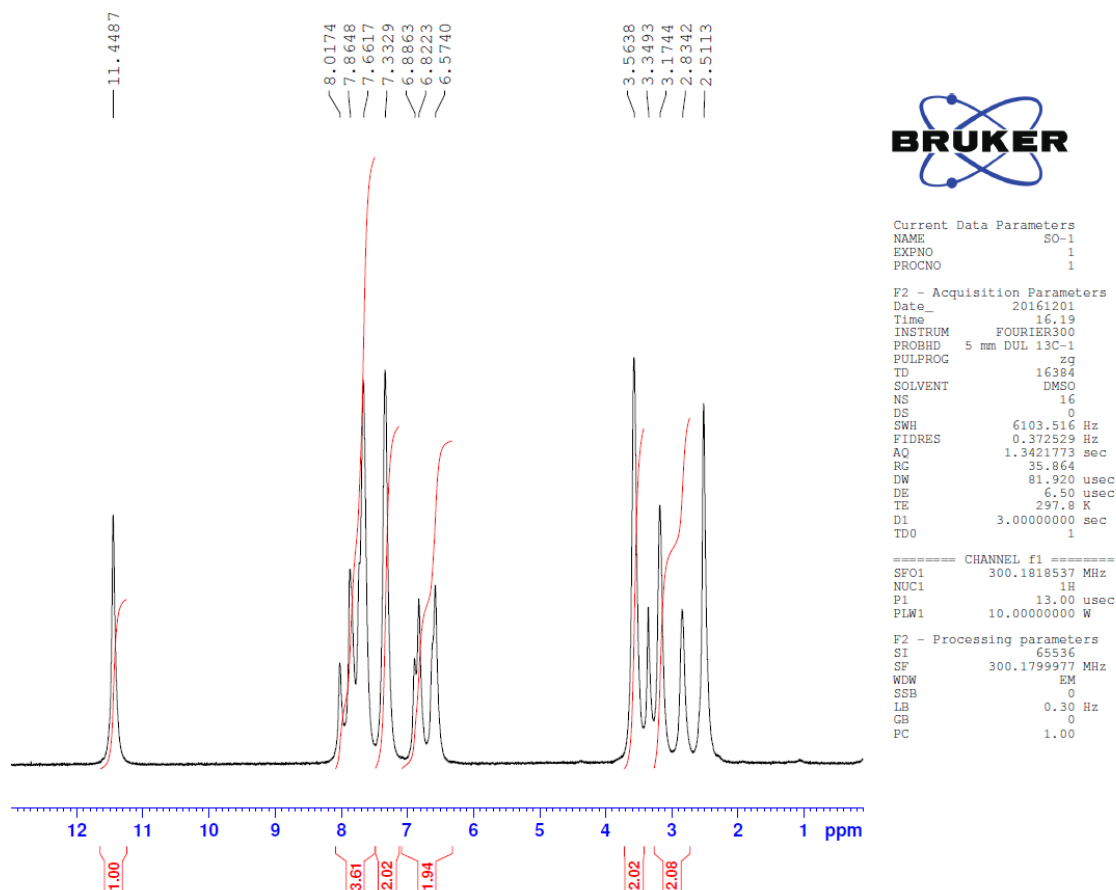


Figure 2. Compound 3a ^1H NMR spectrum

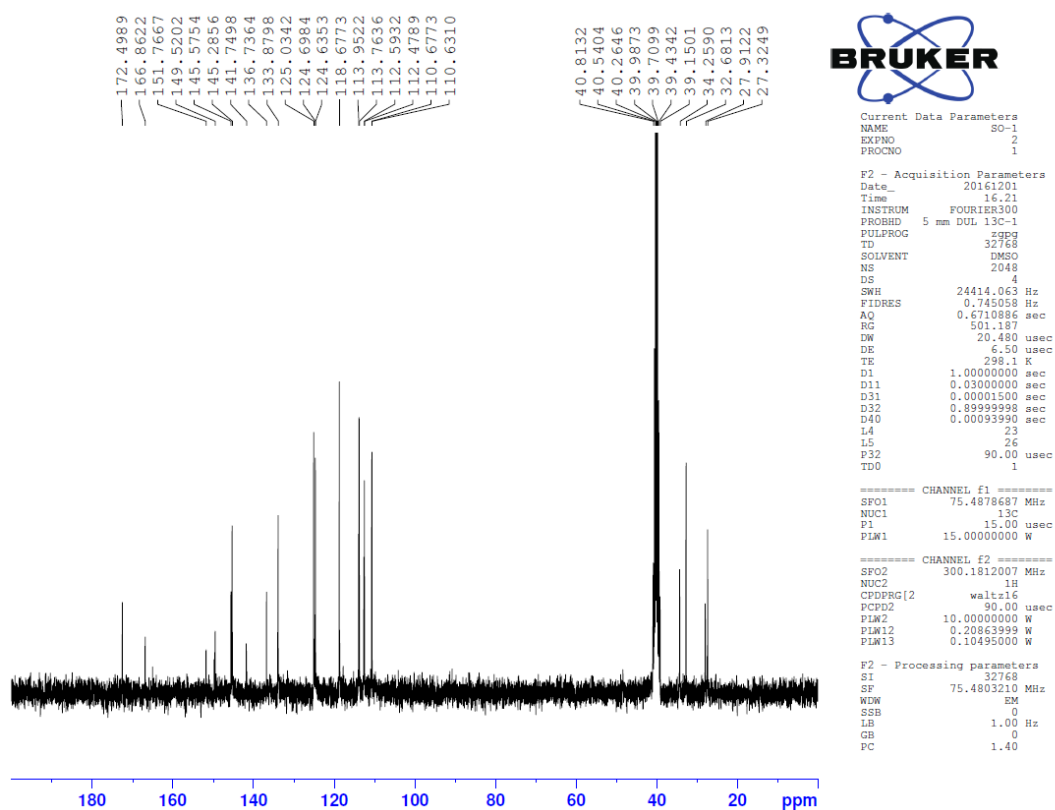


Figure 3. Compound 3a ^{13}C NMR spectrum

Data File: C:\LabSolutions\Data\Analz\lderya\SO-2_53.lcd

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	8	20	O	2	1	6	Cl	1	0	0	I	3	0	0	H
C	4	12	25	F	1	0	0	Br	1	0	1					
N	3	3	6	S	2	1	3	Ru	2	0	0					

Error Margin (ppm): 10

HC Ratio: unlimited

Max Isotopes: 3

MSn Iso RI (%): 10.00

DBE Range: 0.0 - 15.0

Apply N Rule: yes

Isotope RI (%): 1.00

MSn Logic Mode: AND

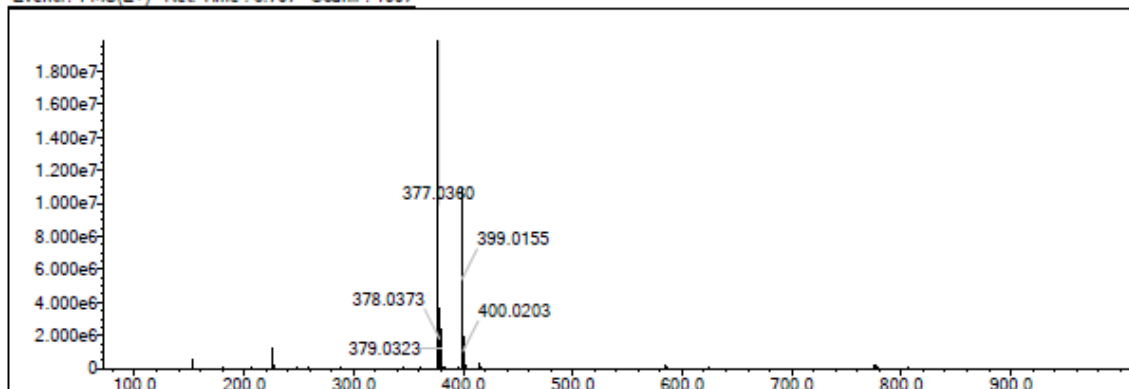
Electron Ions: both

Use MSn Info: no

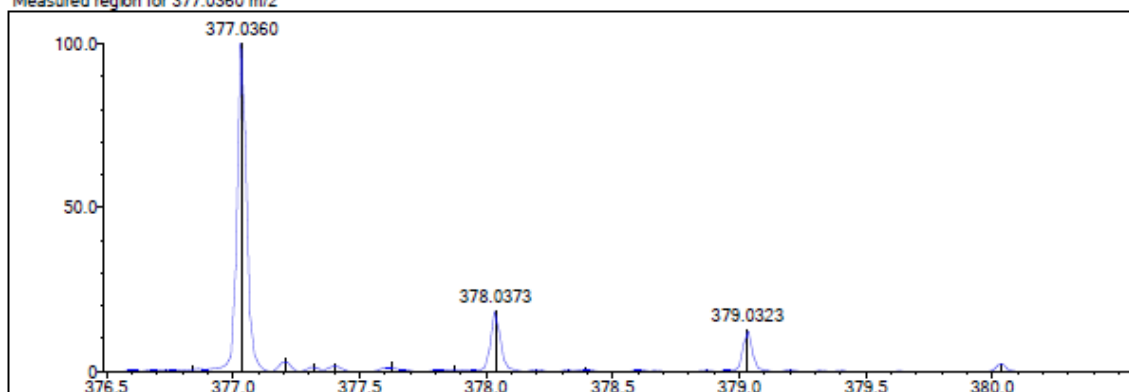
Isotope Res: 10000

Max Results: 500

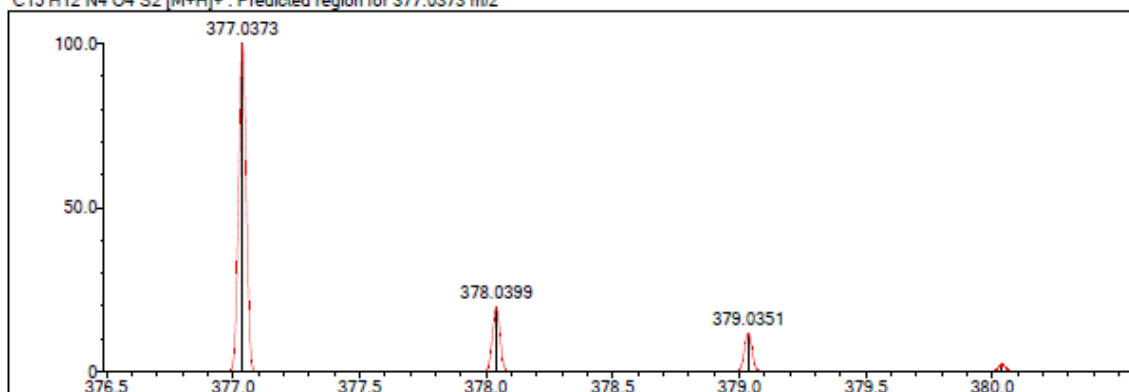
Event#: 1 MS(E+) Ret. Time : 6.707 Scan#: 1007



Measured region for 377.0360 m/z



C15 H12 N4 O4 S2 [M+H]⁺ : Predicted region for 377.0373 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	71.04	C15 H12 N4 O4 S2	[M+H] ⁺	377.0360	377.0373	-1.3	-3.45	75.68	12.0

Figure 4. Compound 3b Mass spectrum

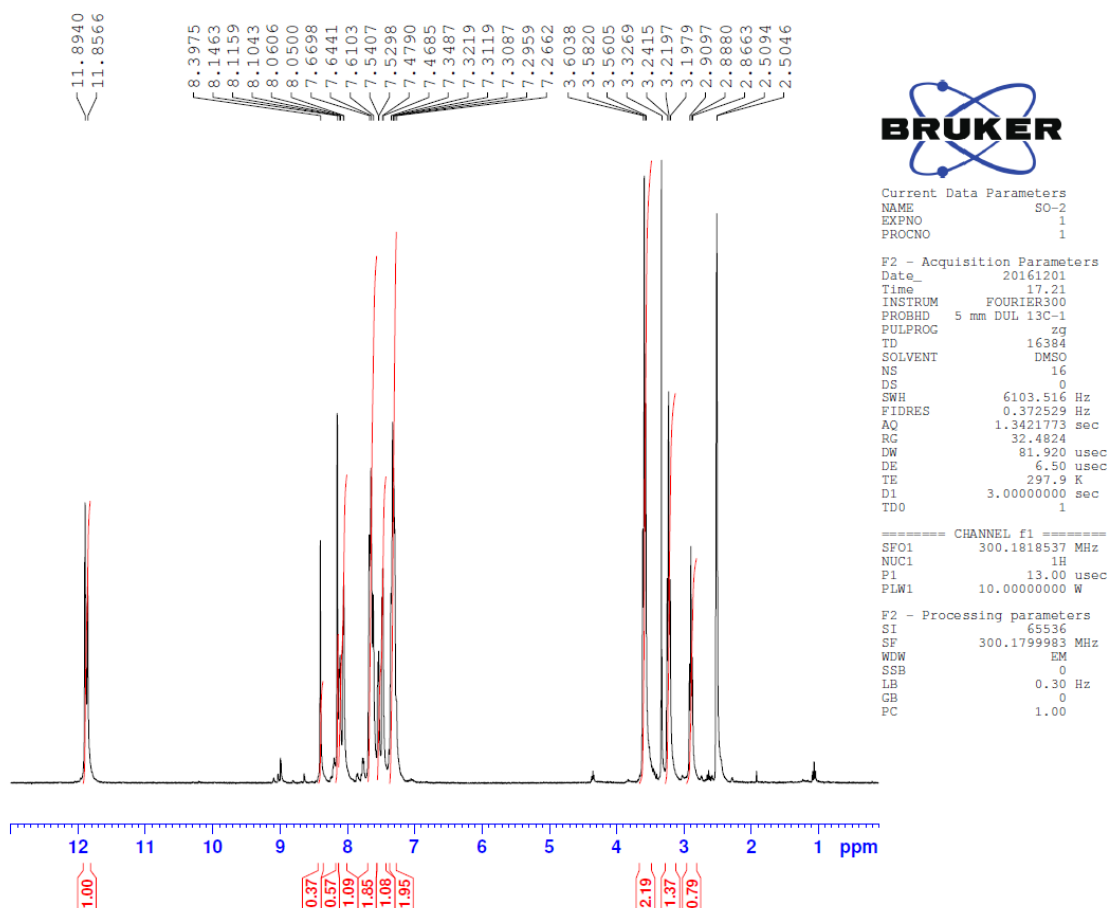


Figure 5. Compound 3b ^1H NMR spectrum

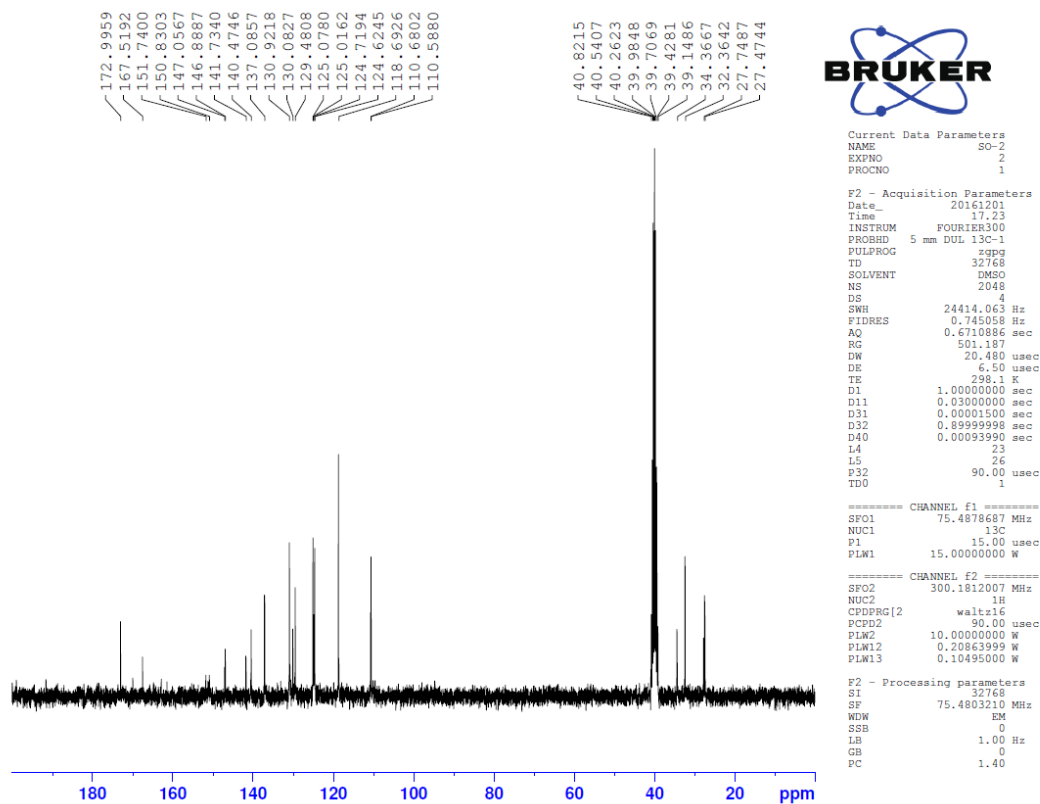


Figure 6. Compound 3b ^{13}C NMR spectrum

Data File: C:\LabSolutions\Data\Analiz\deriv\SO-3_54.lod

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	8	20	O	2	1	6	Cl	1	0	0	I	3	0	0	H
C	4	15	25	F	1	0	0	Br	1	0	1					
N	3	3	6	S	2	1	3	Ru	2	0	0					

Error Margin (ppm): 10

HC Ratio: unlimited

Max Isotopes: 3

MSn Iso RI (%): 10.00

DBE Range: 0.0 - 15.0

Apply N Rule: yes

Isotope RI (%): 1.00

MSn Logic Mode: AND

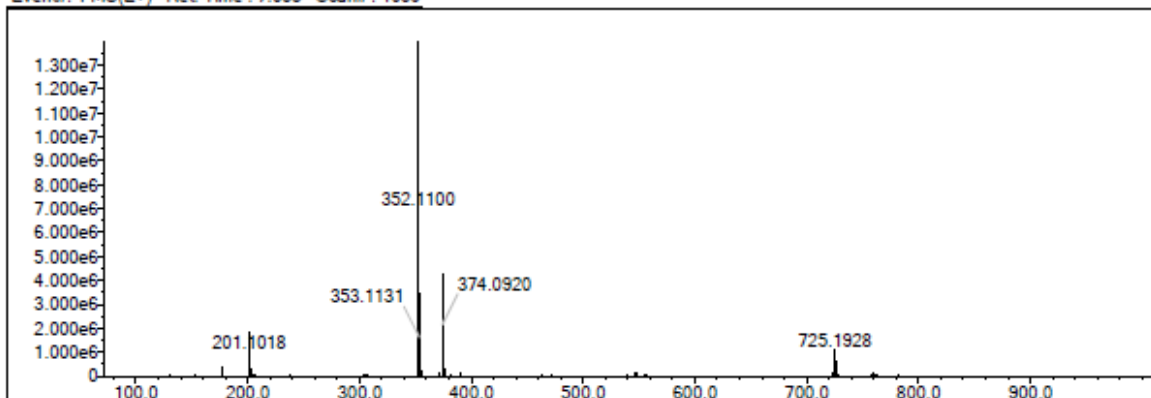
Electron Ions: both

Use MSn Info: no

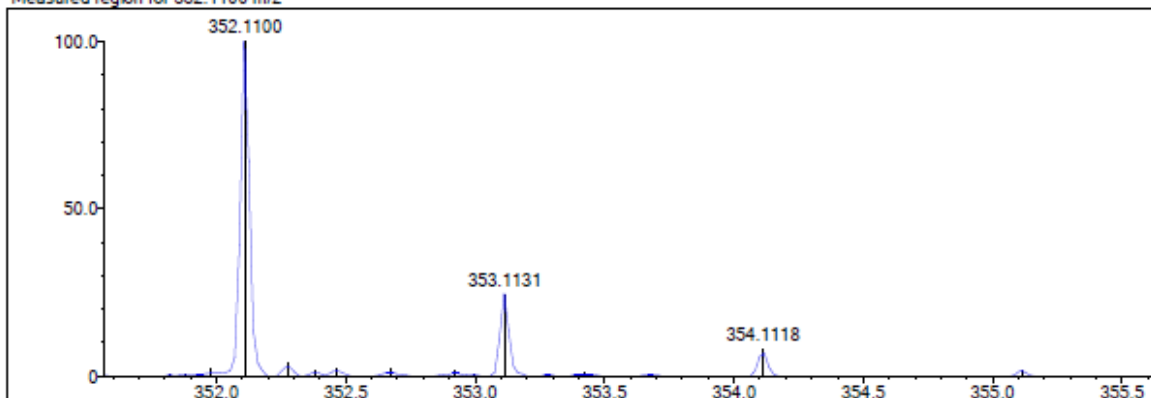
Isotope Res: 10000

Max Results: 500

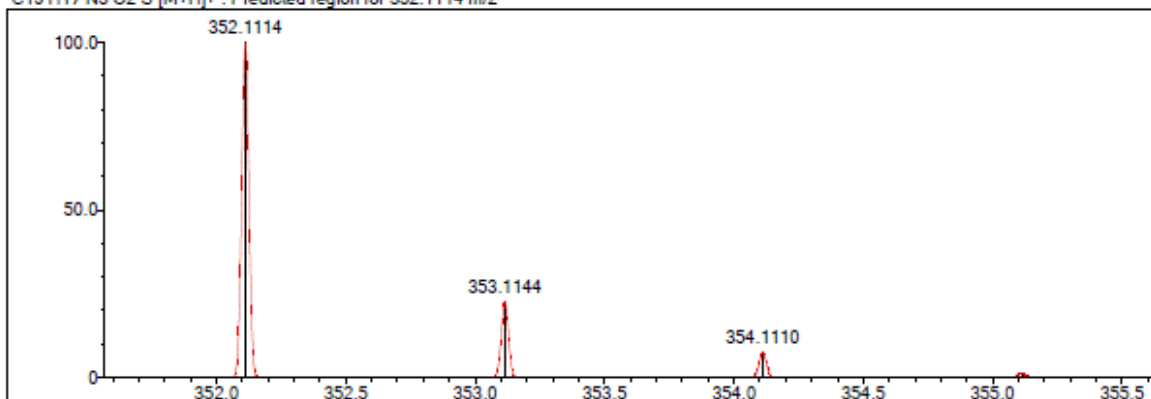
Event#: 1 MS(E+) Ret. Time : 7.053 Scan#: 1059



Measured region for 352.1100 m/z



C19 H17 N3 O2 S [M+H]⁺ : Predicted region for 352.1114 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	74.45	C19 H17 N3 O2 S	[M+H] ⁺	352.1100	352.1114	-1.4	-3.98	80.44	13.0

Figure 7. Compound 3c Mass spectrum

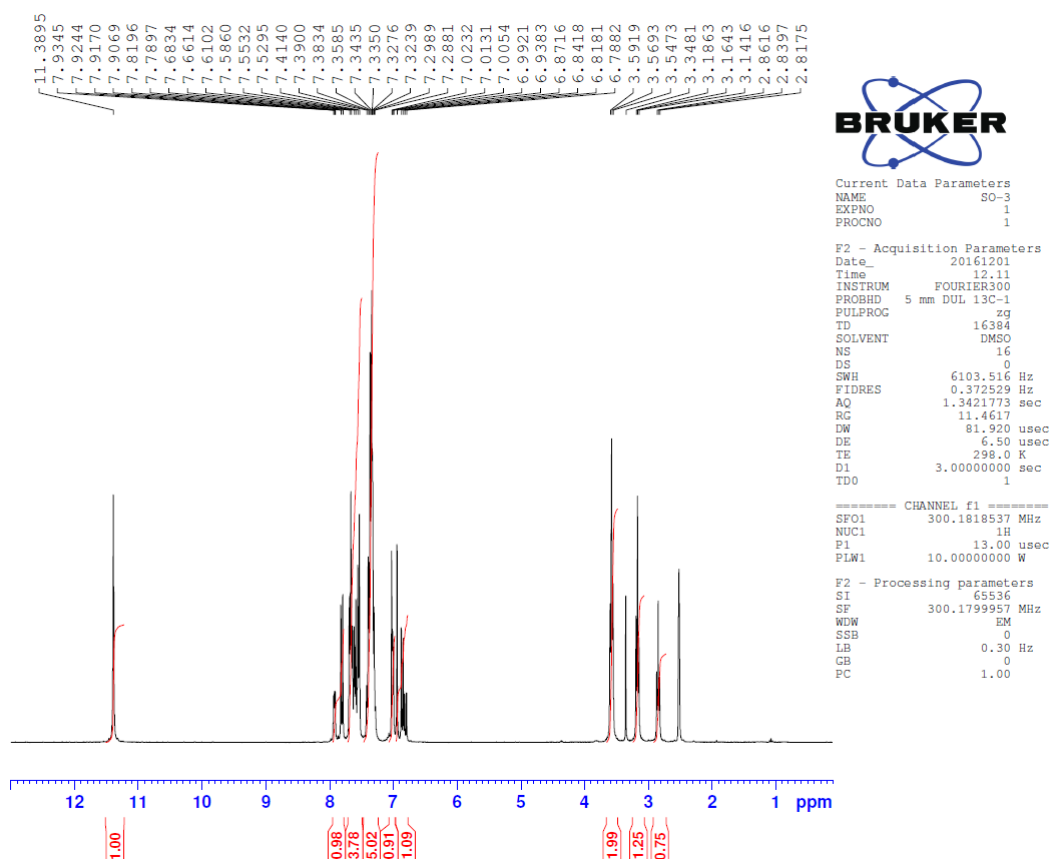


Figure 8. Compound 3c ^1H NMR spectrum

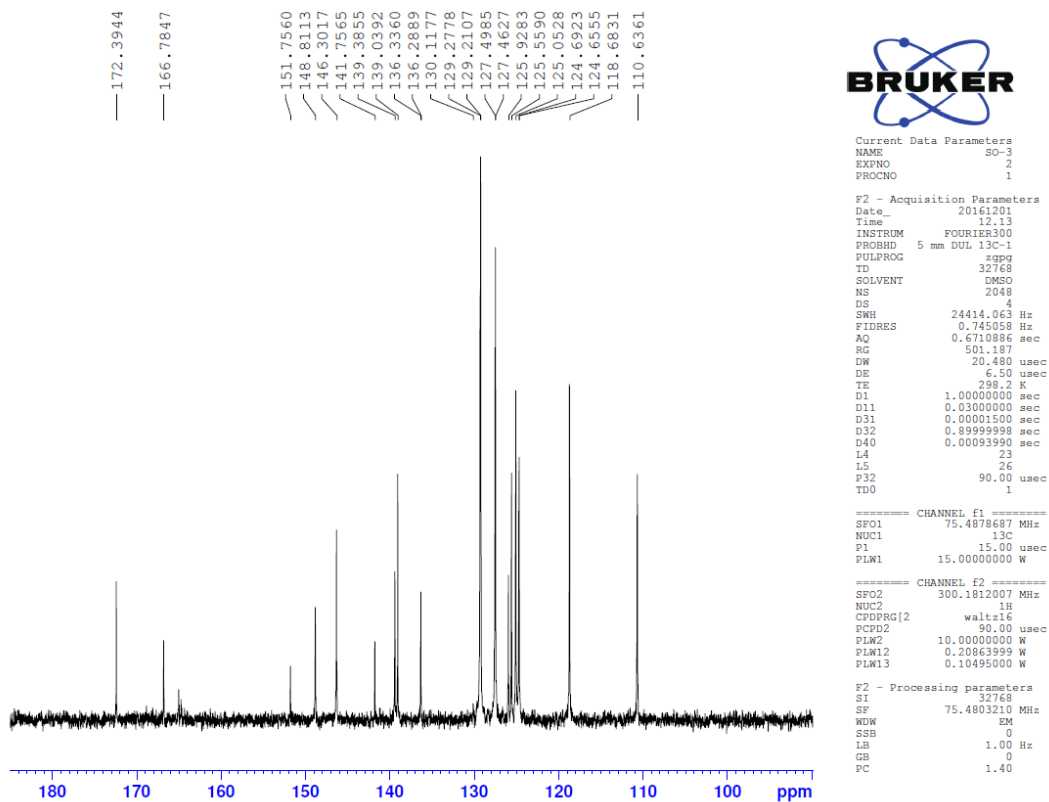


Figure 9. Compound 3c ^{13}C NMR spectrum

Data File: C:\LabSolutions\Data\Analz\Idea\SO-4_55.lod

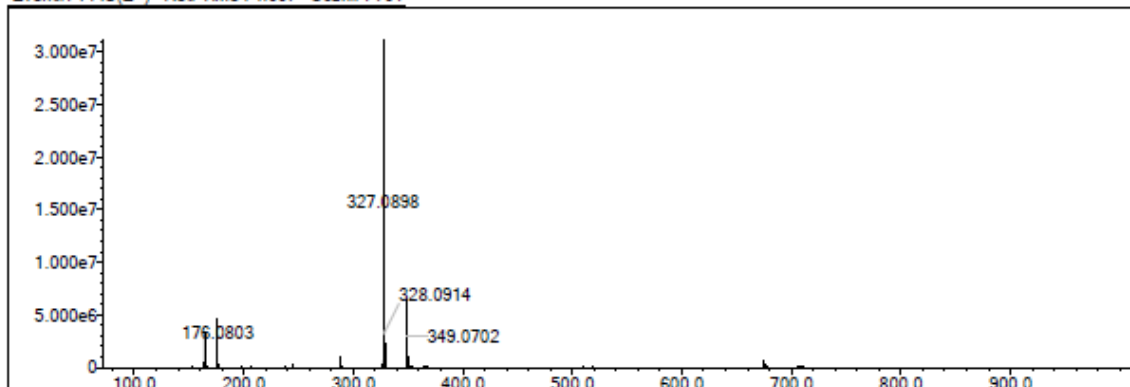
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	8	20	O	2	1	6	Cl	1	0	0	I	3	0	0	H
C	4	15	25	F	1	0	0	Br	1	0	1					
N	3	3	6	S	2	1	3	Ru	2	0	0					

Error Margin (ppm): 10
 HC Ratio: unlimited
 Max Isotopes: 3
 MSn Iso RI (%): 10.00

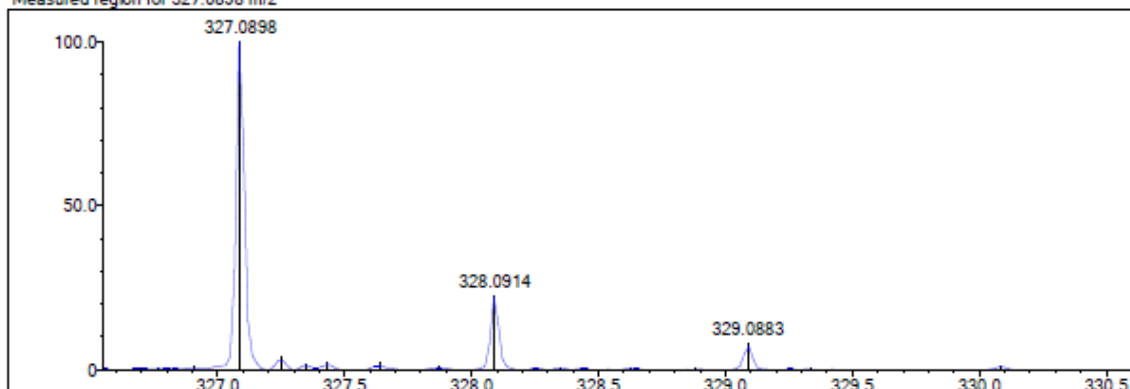
DBE Range: 0.0 - 15.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

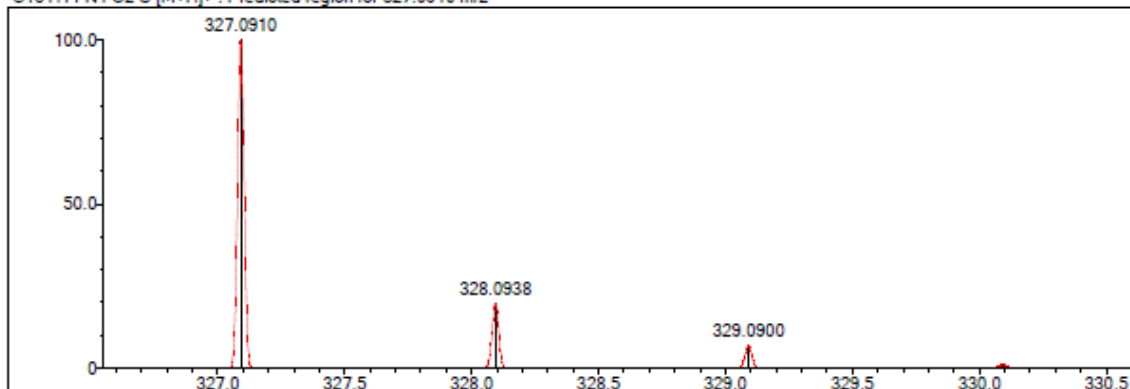
Event#: 1 MS(E+) Ret. Time : 4.667 Scan#: 701



Measured region for 327.0898 m/z



C16 H14 N4 O2 S [M+H]⁺ : Predicted region for 327.0910 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	51.74	C16 H14 N4 O2 S	[M+H] ⁺	327.0898	327.0910	-1.2	-3.67	55.45	12.0

Figure 10. Compound 3d Mass spectrum

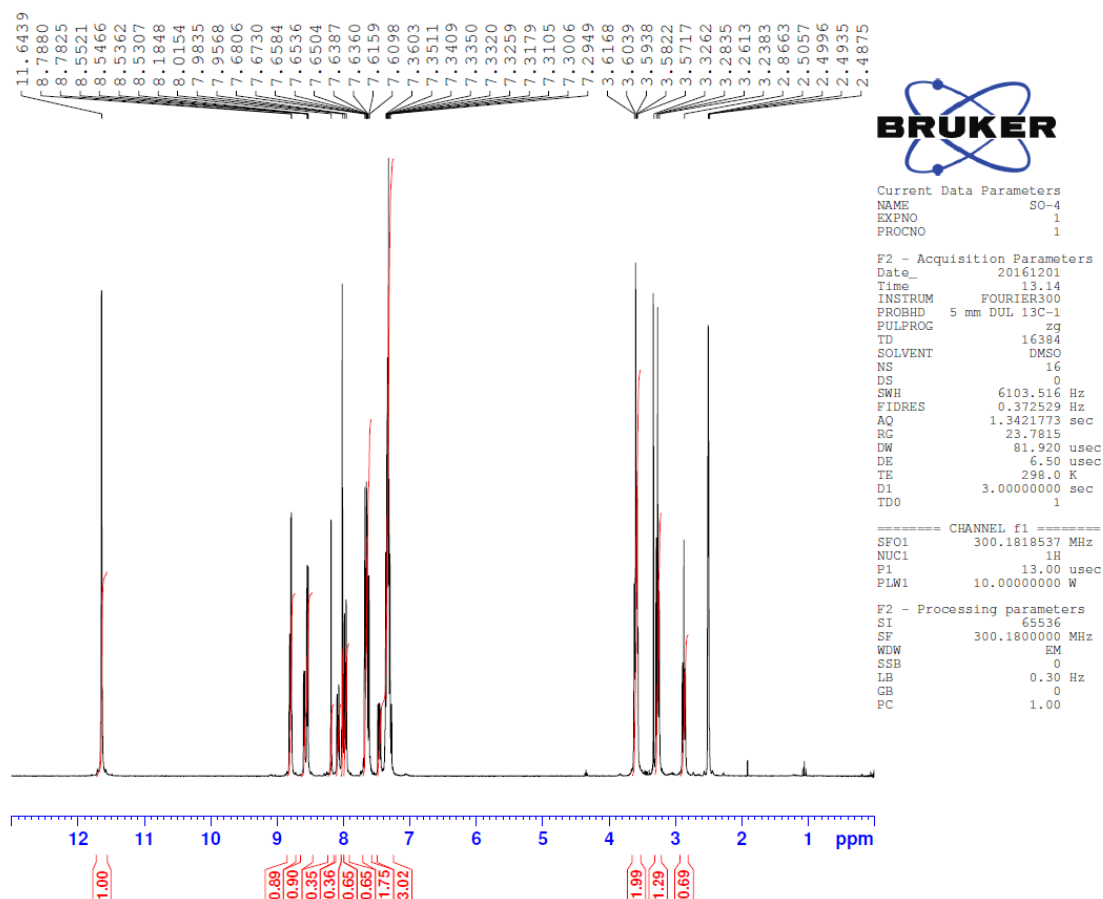


Figure 11. Compound 3d ^1H NMR spectrum

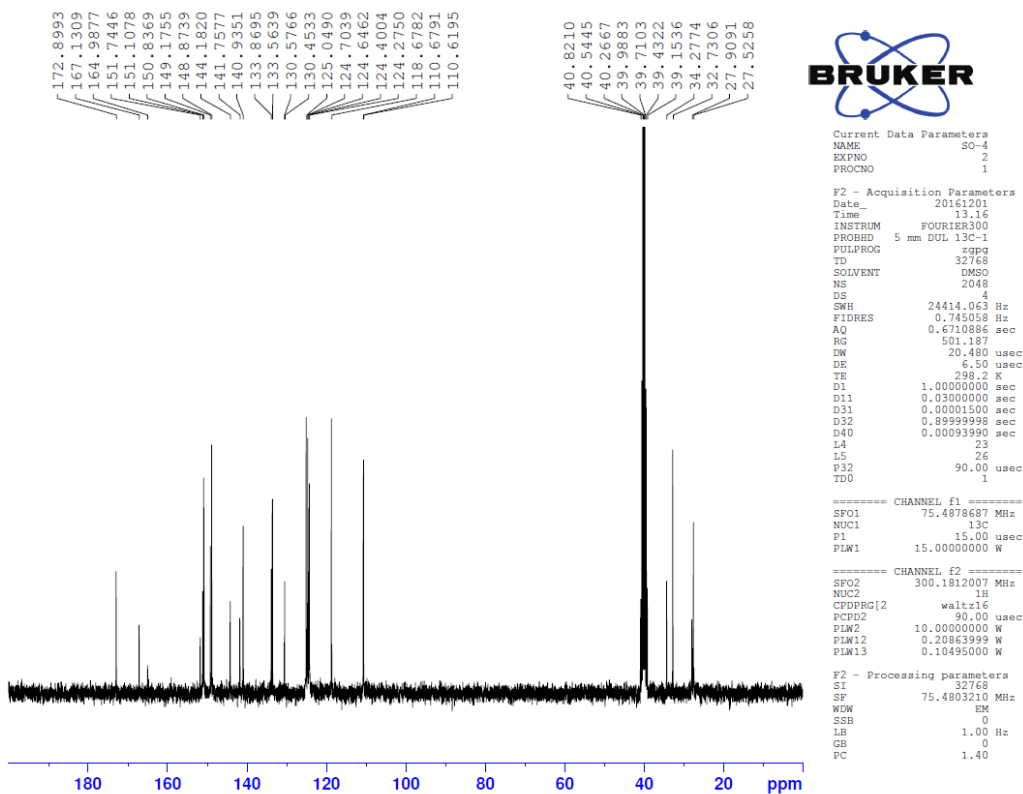


Figure 12. Compound 3d ^{13}C NMR spectrum

Data File: C:\LabSolutions\Data\Analz\Idea\ISO-5_56.lod

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	8	20	O	2	1	6	Cl	1	0	0	I	3	0	0	H
C	4	15	25	F	1	0	0	Br	1	0	1					
N	3	3	6	S	2	1	3	Ru	2	0	0					

Error Margin (ppm): 10

HC Ratio: unlimited

Max Isotopes: 3

MSn Iso RI (%): 10.00

DBE Range: 0.0 - 15.0

Apply N Rule: yes

Isotope RI (%): 1.00

MSn Logic Mode: AND

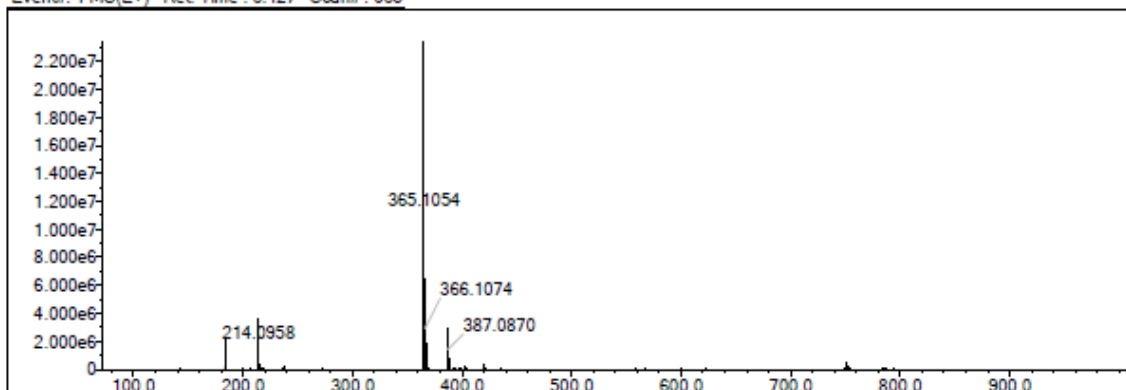
Electron Ions: both

Use MSn Info: no

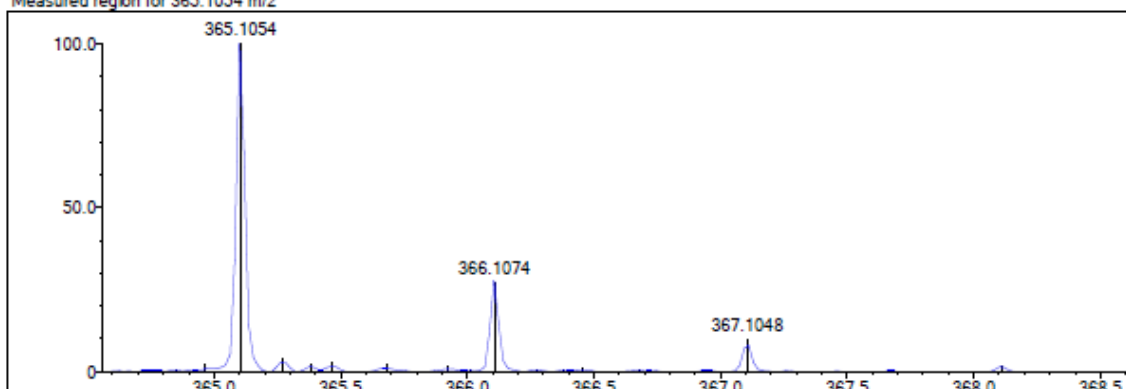
Isotope Res: 10000

Max Results: 500

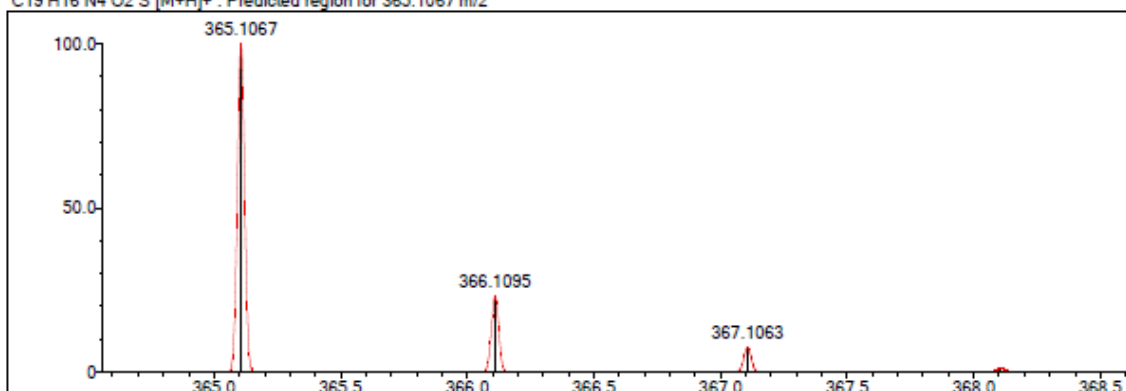
Event#: 1 MS(E+) Ret. Time : 6.427 Scan#: 965



Measured region for 365.1054 m/z



C19 H16 N4 O2 S [M+H]⁺ : Predicted region for 365.1067 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	70.96	C19 H16 N4 O2 S	[M+H] ⁺	365.1054	365.1067	-1.3	-3.56	75.81	14.0

Figure 13. Compound 3e Mass spectrum

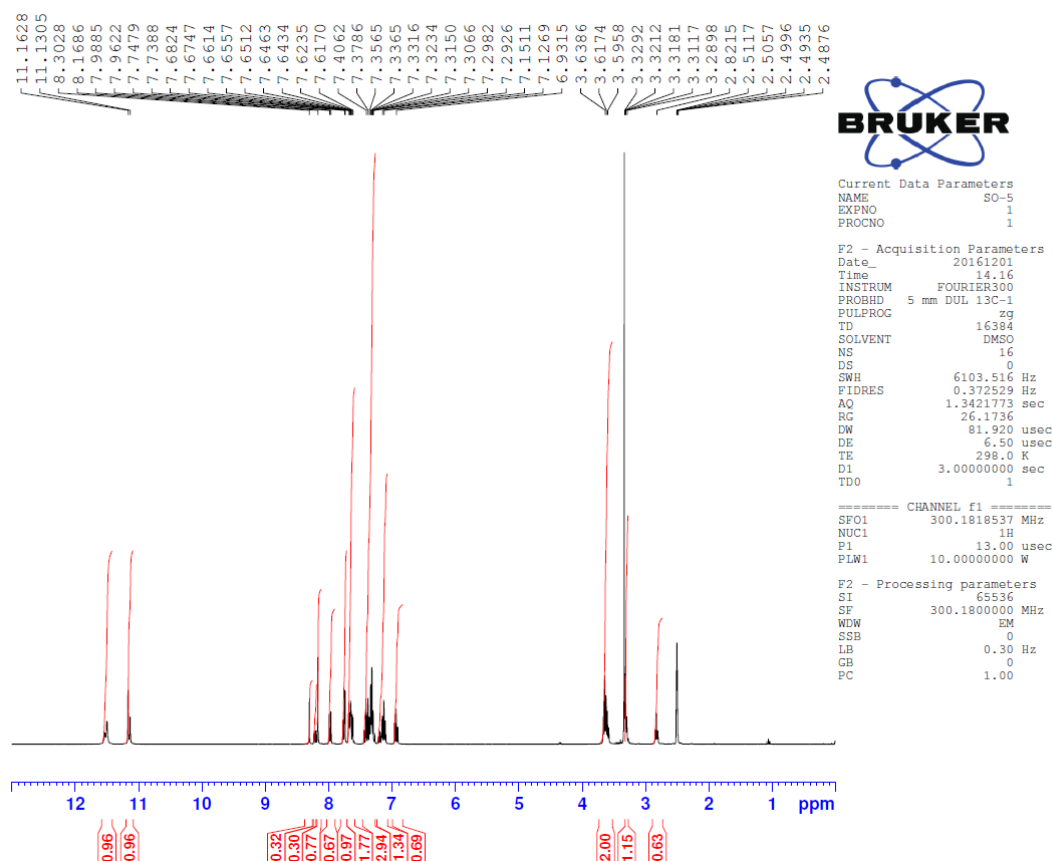


Figure 14. Compound 3e ^1H NMR spectrum

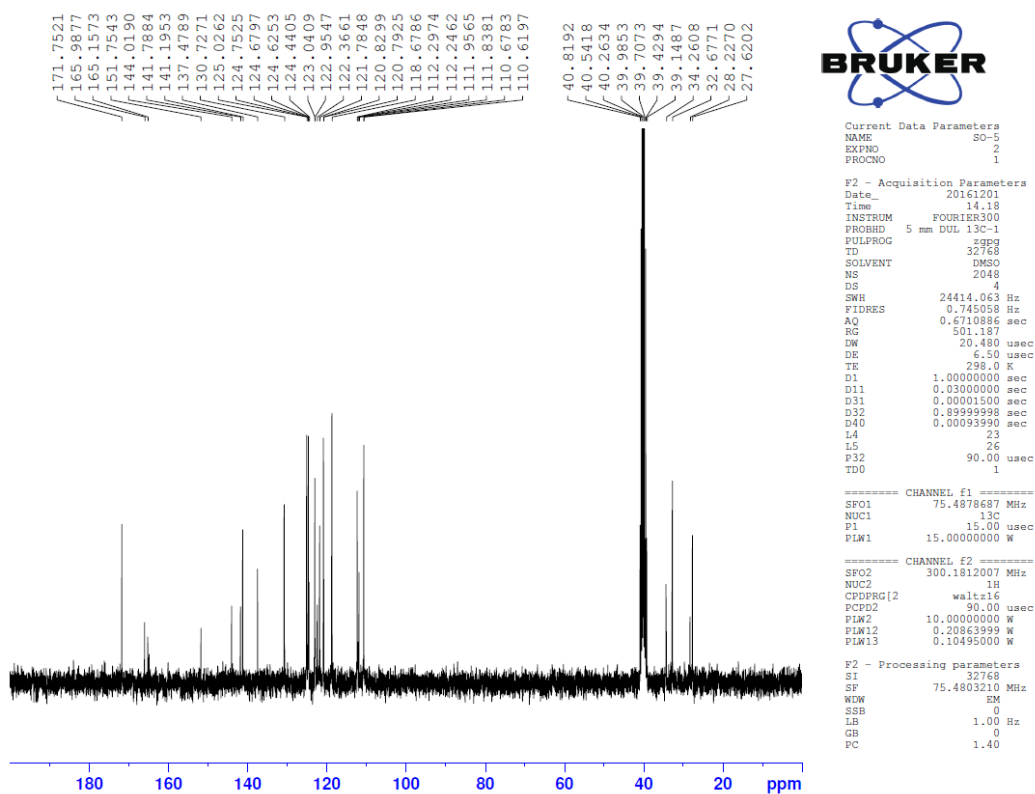


Figure 15. Compound 3e ^{13}C NMR spectrum

Data File: C:\LabSolutions\Data\Analiz\derya\NO-1_46.lod

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	9	20	O	2	1	6	Cl	1	0	2	I	3	0	0	H
C	4	18	25	F	1	0	1	Br	1	0	1					
N	3	3	6	S	2	2	2	Ru	2	0	0					

Error Margin (ppm): 5

HC Ratio: unlimited

Max Isotopes: 3

MSn Iso RI (%): 10.00

DBE Range: 12.0 - 15.0

Apply N Rule: yes

Isotope RI (%): 1.00

MSn Logic Mode: AND

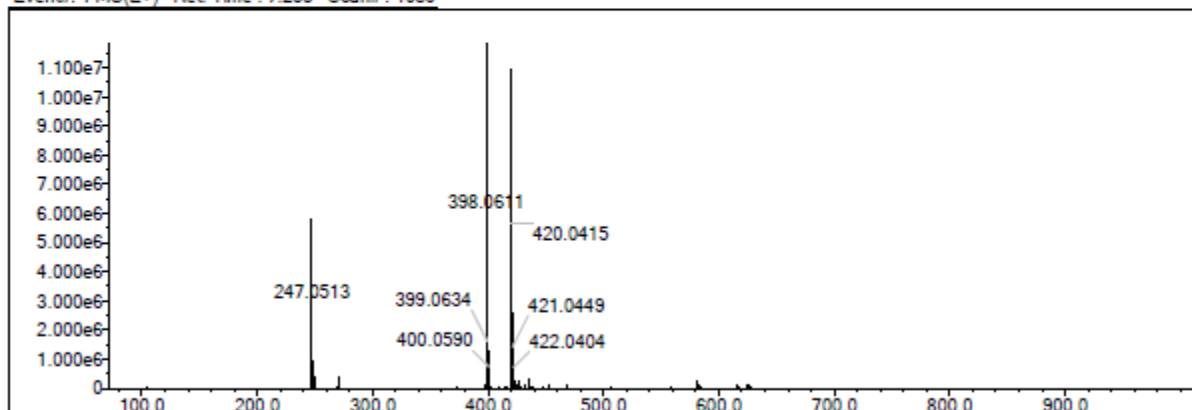
Electron Ions: both

Use MSn Info: no

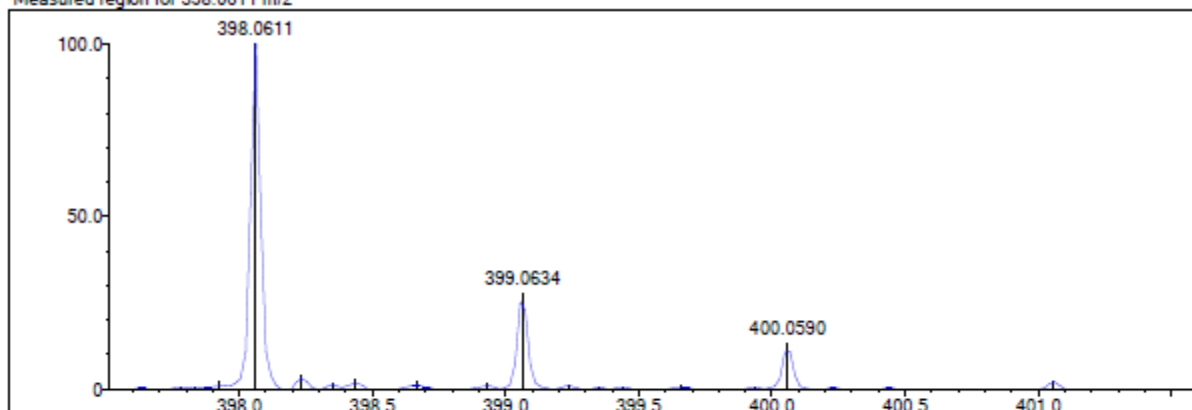
Isotope Res: 10000

Max Results: 500

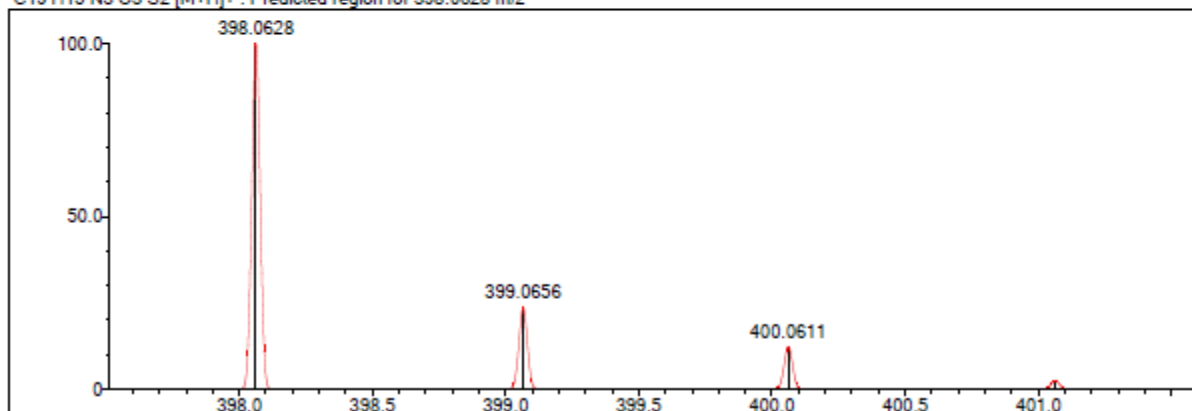
Event#: 1 MS(E+) Ret. Time : 7.253 Scan#: 1089



Measured region for 398.0611 m/z



C19 H15 N3 O3 S2 [M+H]⁺: Predicted region for 398.0628 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	86.48	C19 H15 N3 O3 S2	[M+H] ⁺	398.0611	398.0628	-1.7	-4.27	94.18	14.0

Figure 16. Compound 5a Mass spectrum

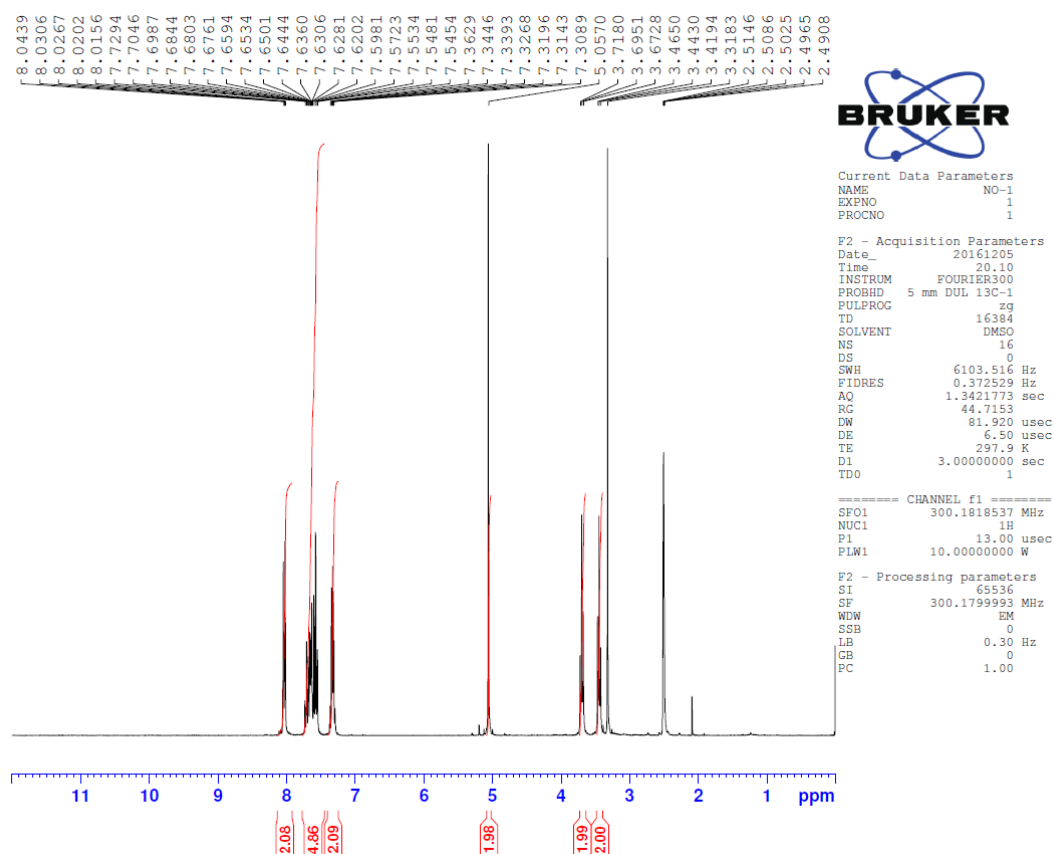


Figure 17. Compound 5a ^1H NMR spectrum

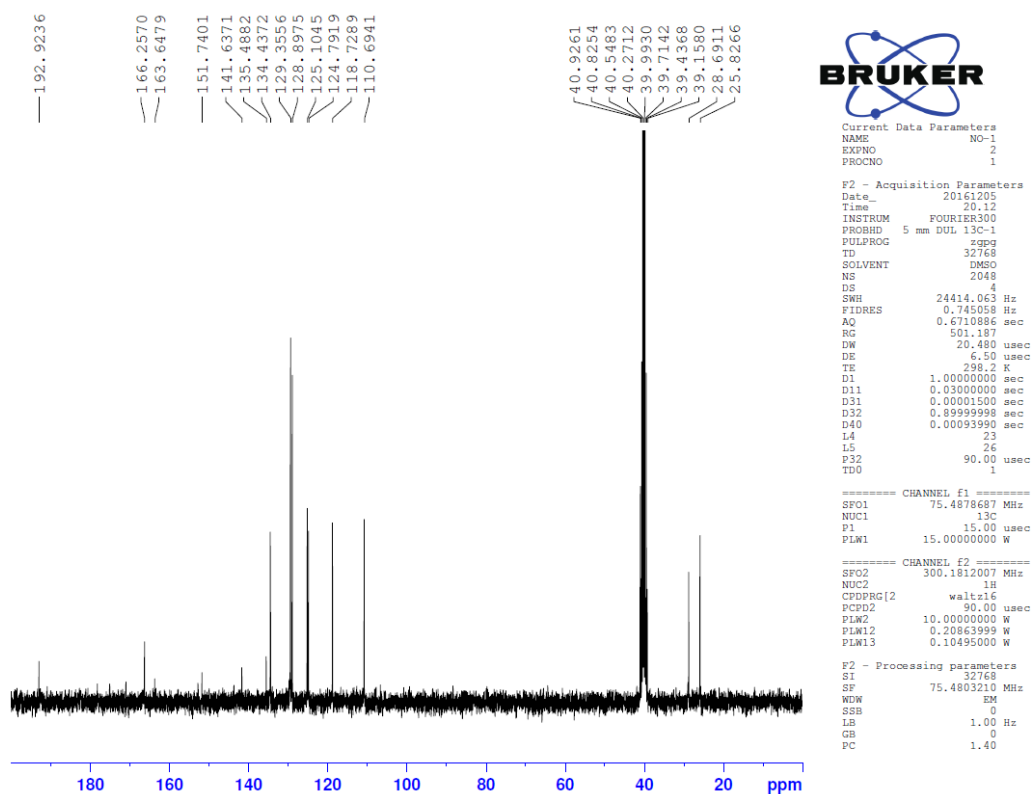


Figure 18. Compound 5a ^{13}C NMR spectrum

Data File: C:\LabSolutions\Data\Analiz\data\NO-2_47.lcd

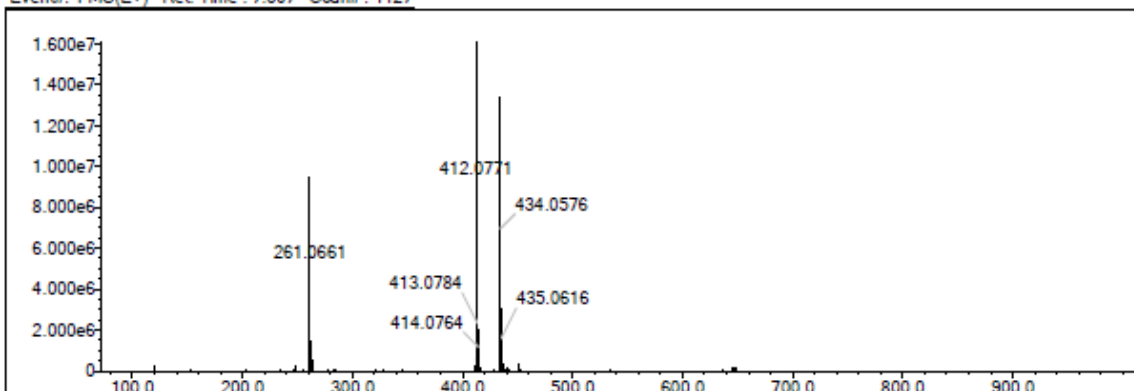
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	9	20	O	2	1	6	Cl	1	0	2	I	3	0	0	H
C	4	18	25	F	1	0	1	Br	1	0	1					
N	3	3	6	S	2	2	2	Ru	2	0	0					

Error Margin (ppm): 5
 HC Ratio: unlimited
 Max Isotopes: 3
 MSn Iso RI (%): 10.00

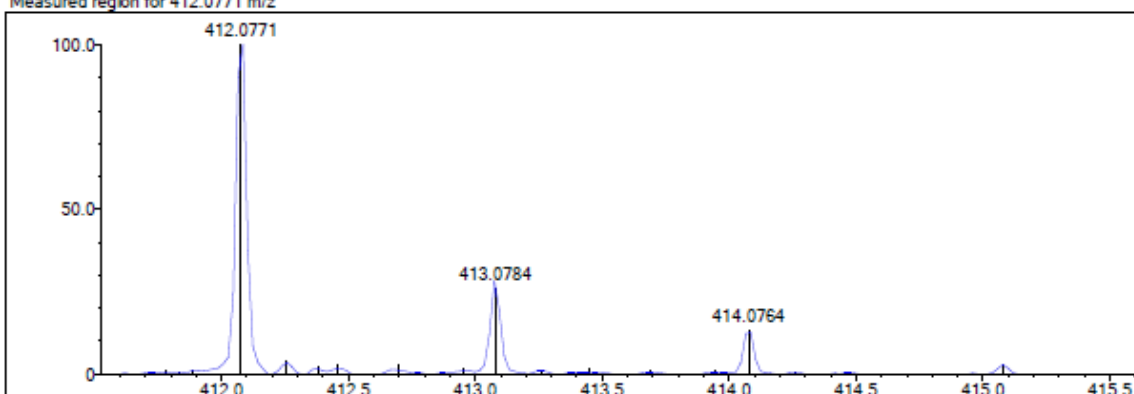
DBE Range: 12.0 - 15.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

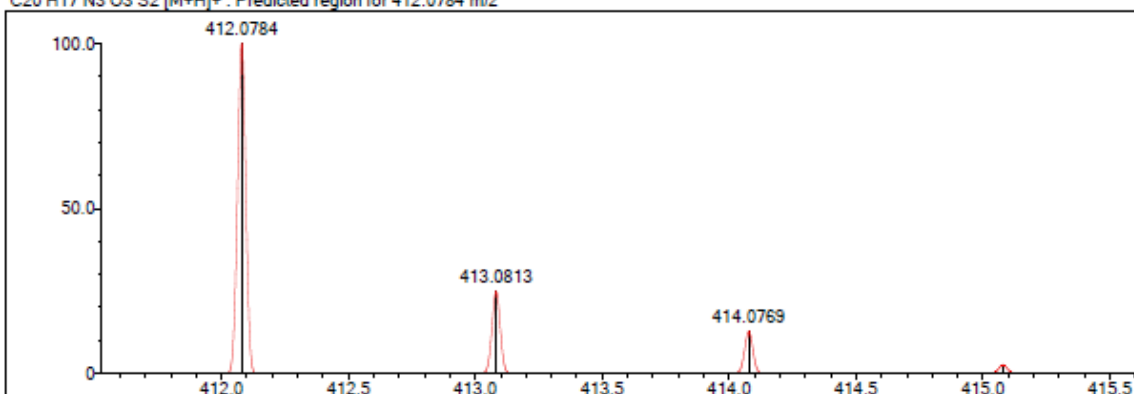
Event#: 1 MS(E+) Ret. Time : 7.507 Scan#: 1127



Measured region for 412.0771 m/z



C20 H17 N3 O3 S2 [M+H]⁺ : Predicted region for 412.0784 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	94.63	C20 H17 N3 O3 S2	[M+H] ⁺	412.0771	412.0784	-1.3	-3.15	100.00	14.0

Figure 19. Compound 5b Mass spectrum

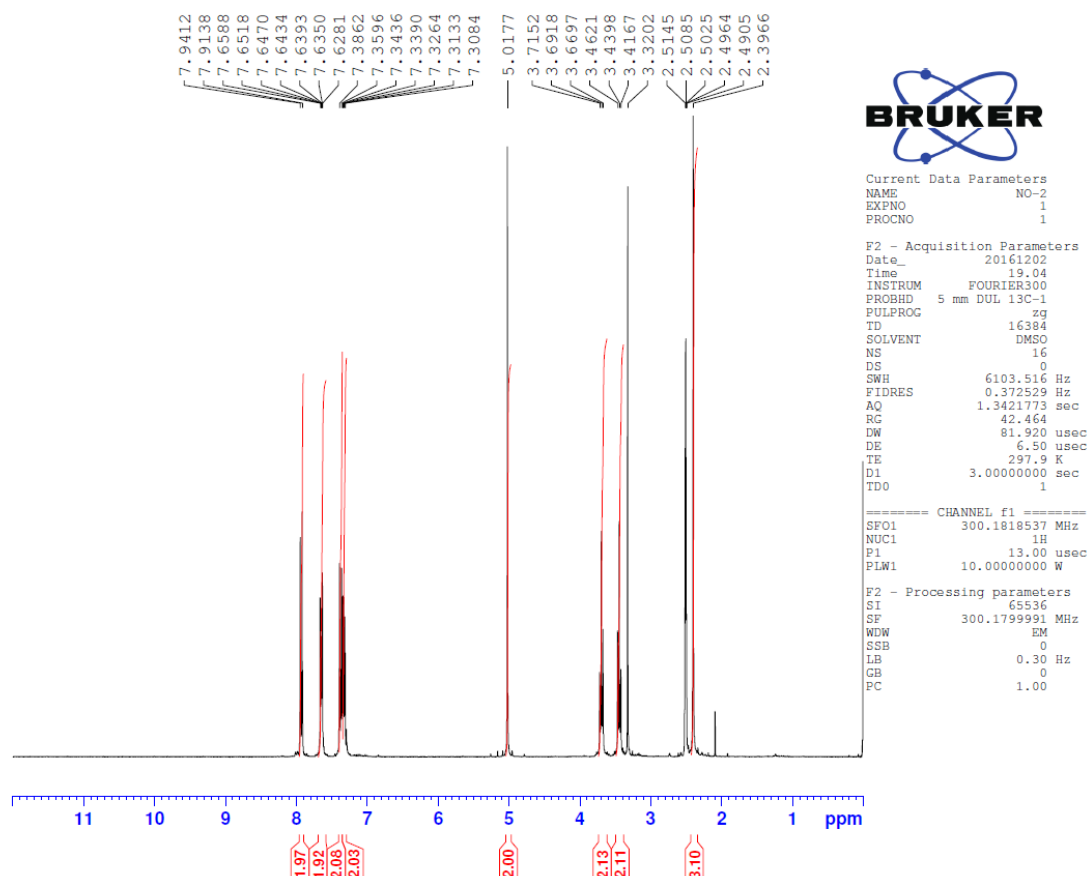


Figure 20. Compound 5b ^1H NMR spectrum

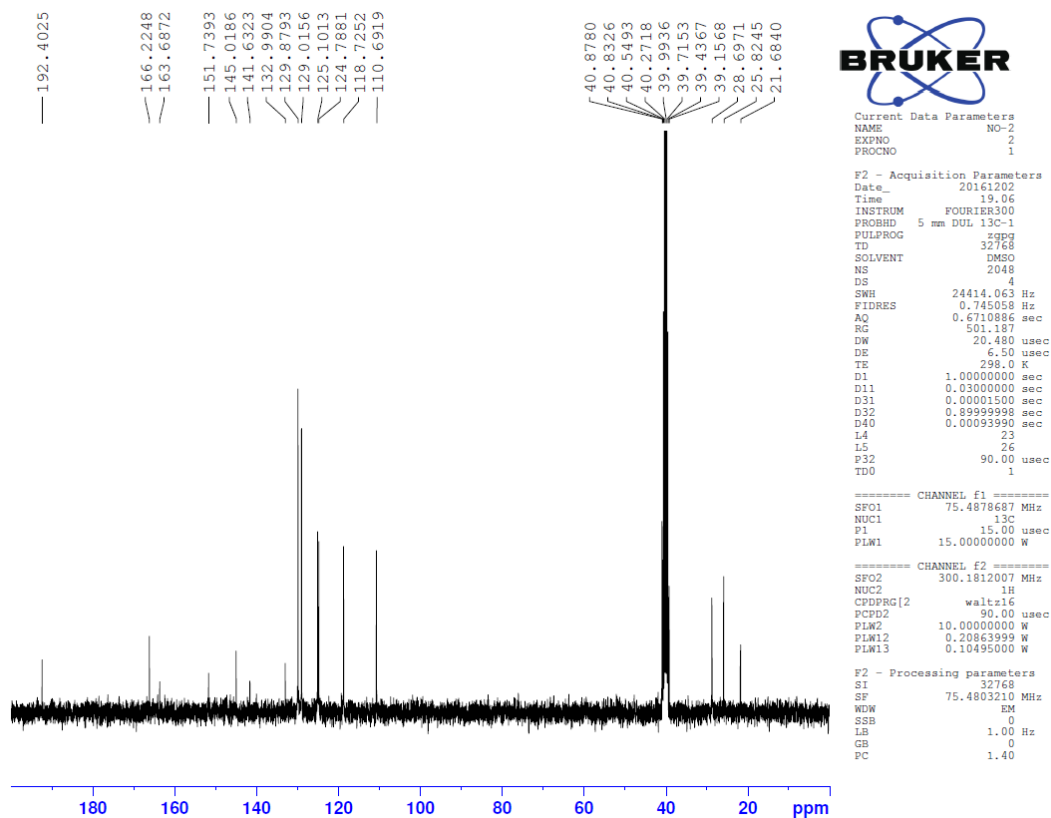


Figure 21. Compound 5b ^{13}C NMR spectrum

Data File: C:\LabSolutions\Data\Analiz\denya\NO-3_48.lod

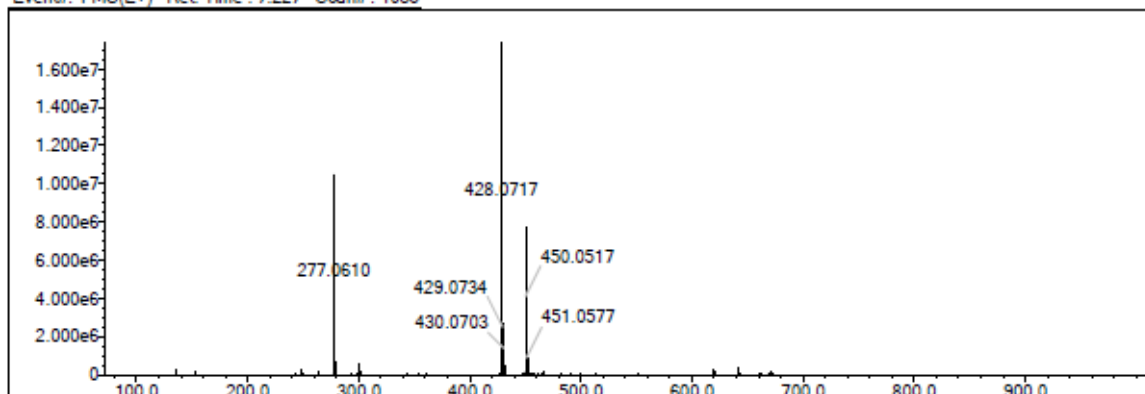
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct	
H	1	9	20	O	2	1	6	Cl	1	0	2		1	3	0	0	H
C	4	18	25	F	1	0	1	Br	1	0	1						
N	3	3	6	S	2	2	2	Ru	2	0	0						

Error Margin (ppm): 10
 HC Ratio: unlimited
 Max Isotopes: 3
 MSn Iso RI (%): 10.00

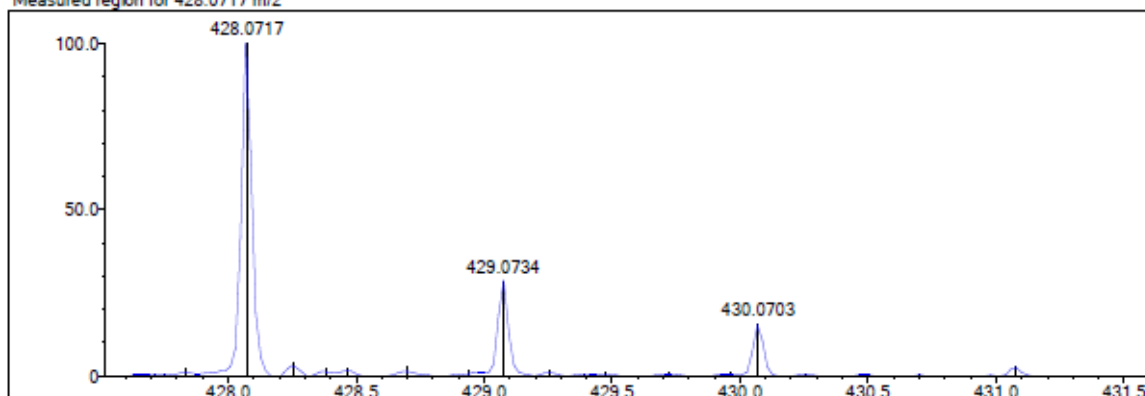
DBE Range: 12.0 - 15.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

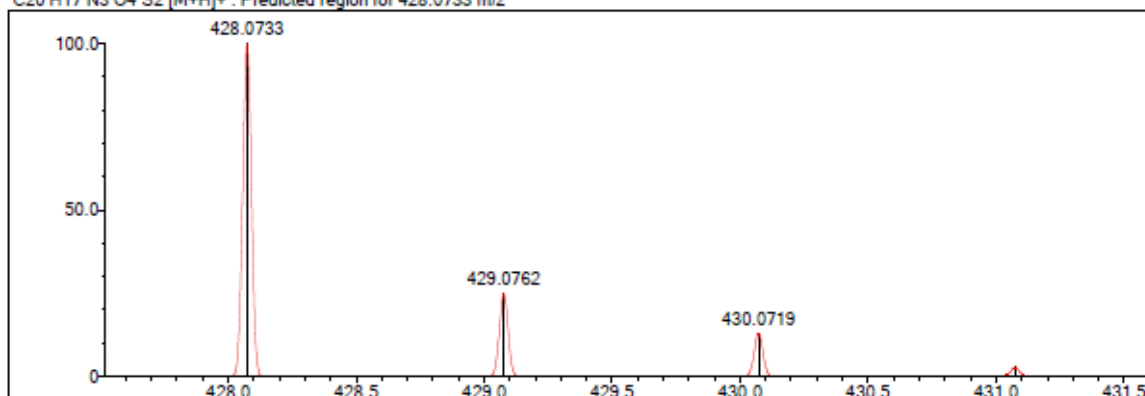
Event#: 1 MS(E+) Ret. Time : 7.227 Scan#: 1085



Measured region for 428.0717 m/z



C20 H17 N3 O4 S2 [M+H]⁺ : Predicted region for 428.0733 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	74.27	C20 H17 N3 O4 S2	[M+H] ⁺	428.0717	428.0733	-1.6	-3.74	79.73	14.0

Figure 22. Compound 5c Mass spectrum

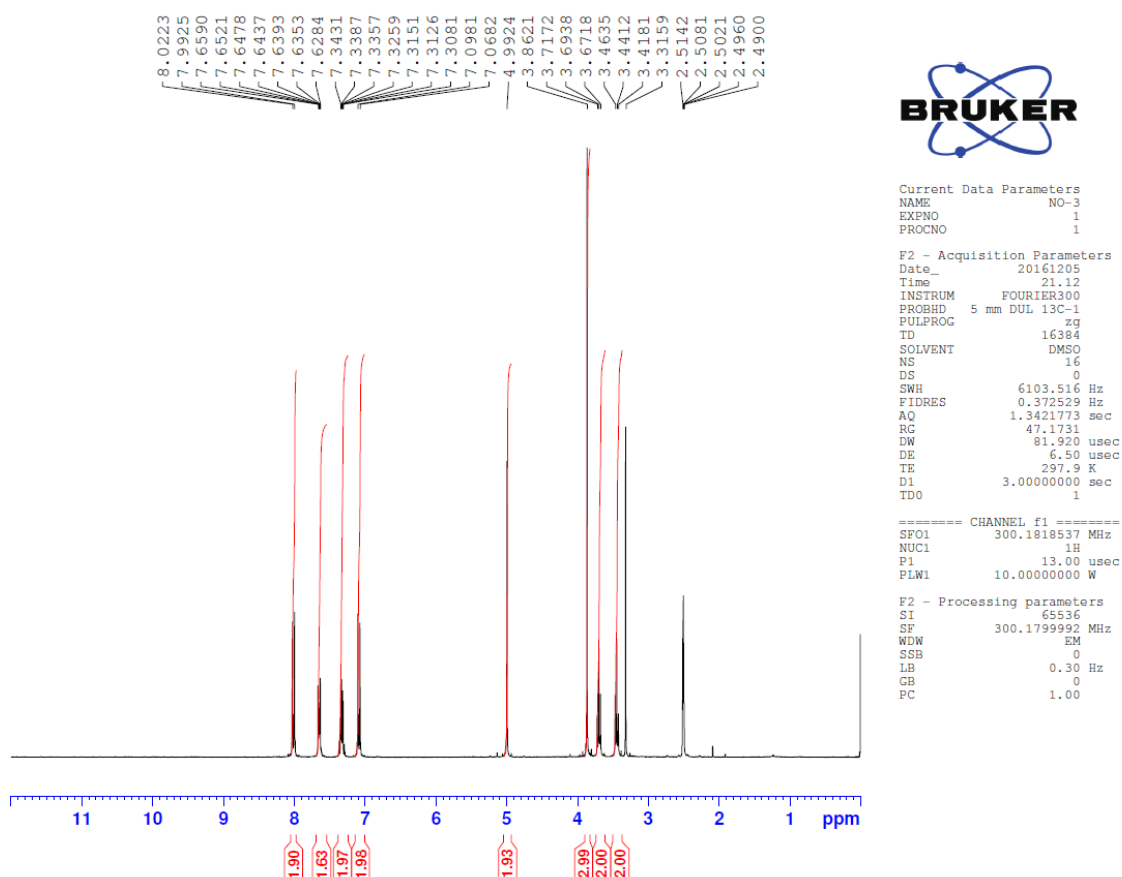


Figure 23. Compound 5c ^1H NMR spectrum

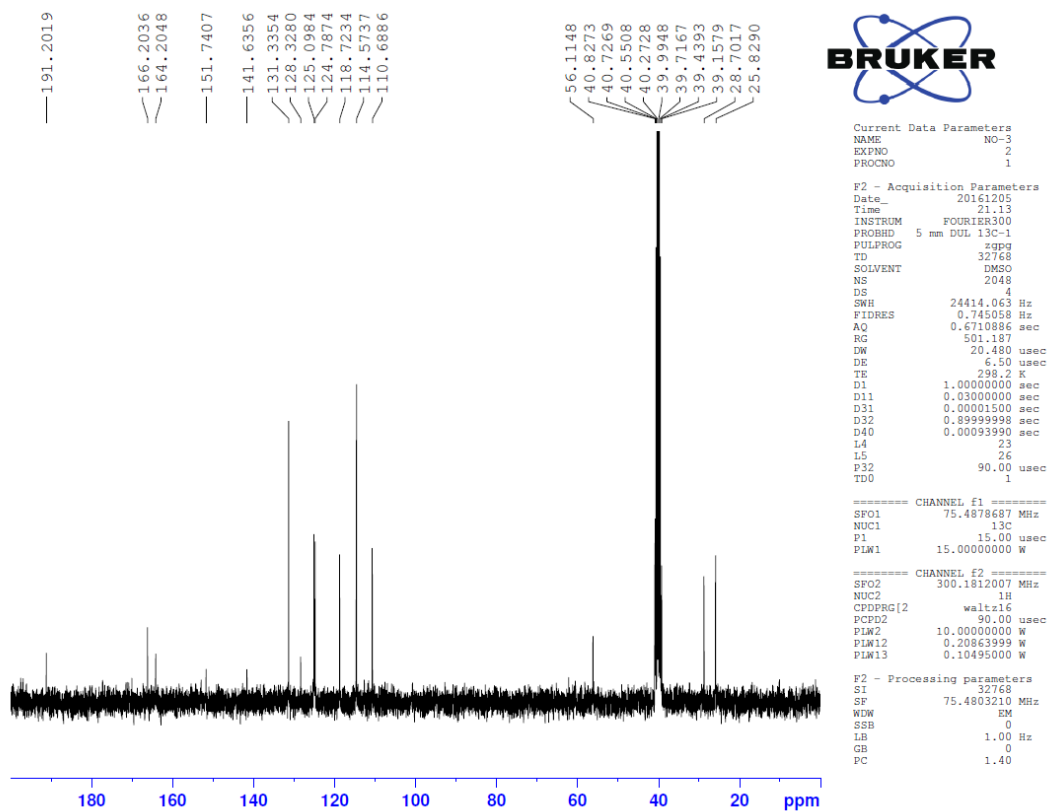


Figure 24. Compound 5c ^{13}C NMR spectrum

Data File: C:\LabSolutions\Data\Analiz\denya\NO-4_49 lod

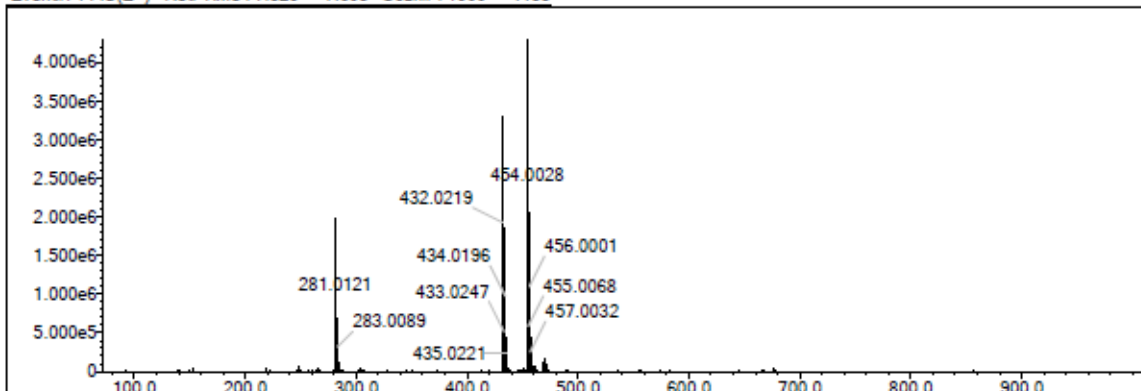
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	9	20	O	2	1	6	Cl	1	0	2	I	3	0	0	H
C	4	18	25	F	1	0	1	Br	1	0	1					
N	3	3	6	S	2	2	2	Ru	2	0	0					

Error Margin (ppm): 10
 HC Ratio: unlimited
 Max Isotopes: 3
 MSn Iso RI (%): 10.00

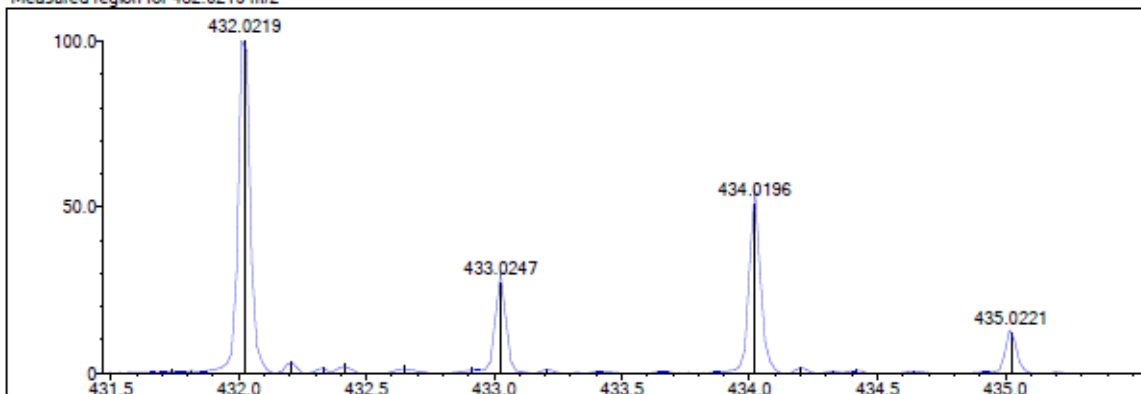
DBE Range: 12.0 - 15.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

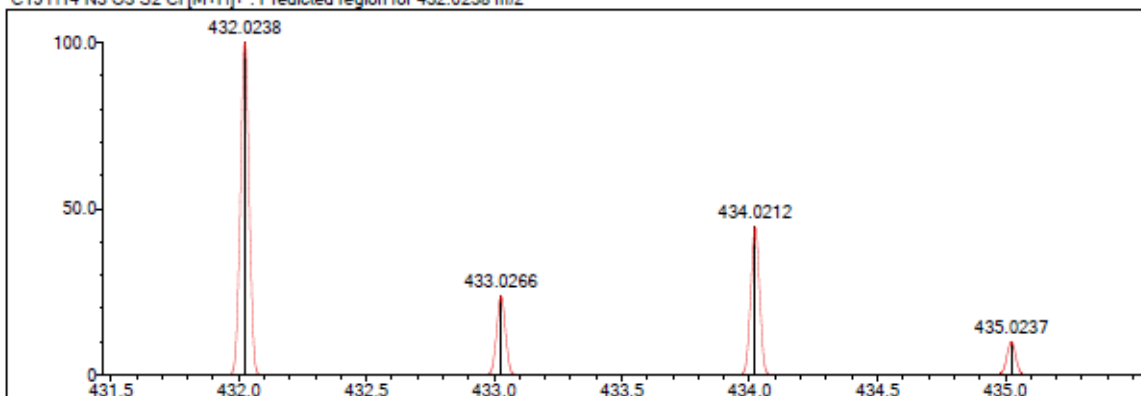
Event#: 1 MS(E+) Ret. Time : 7.320 -> 7.693 Scan#: 1099 -> 1155



Measured region for 432.0219 m/z



C19 H14 N3 O3 S2 Cl [M+H]⁺ : Predicted region for 432.0238 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	70.20	C19 H14 N3 O3 S2 Cl	[M+H] ⁺	432.0219	432.0238	-1.9	-4.40	76.73	14.0

Figure 25. Compound 5d Mass spectrum

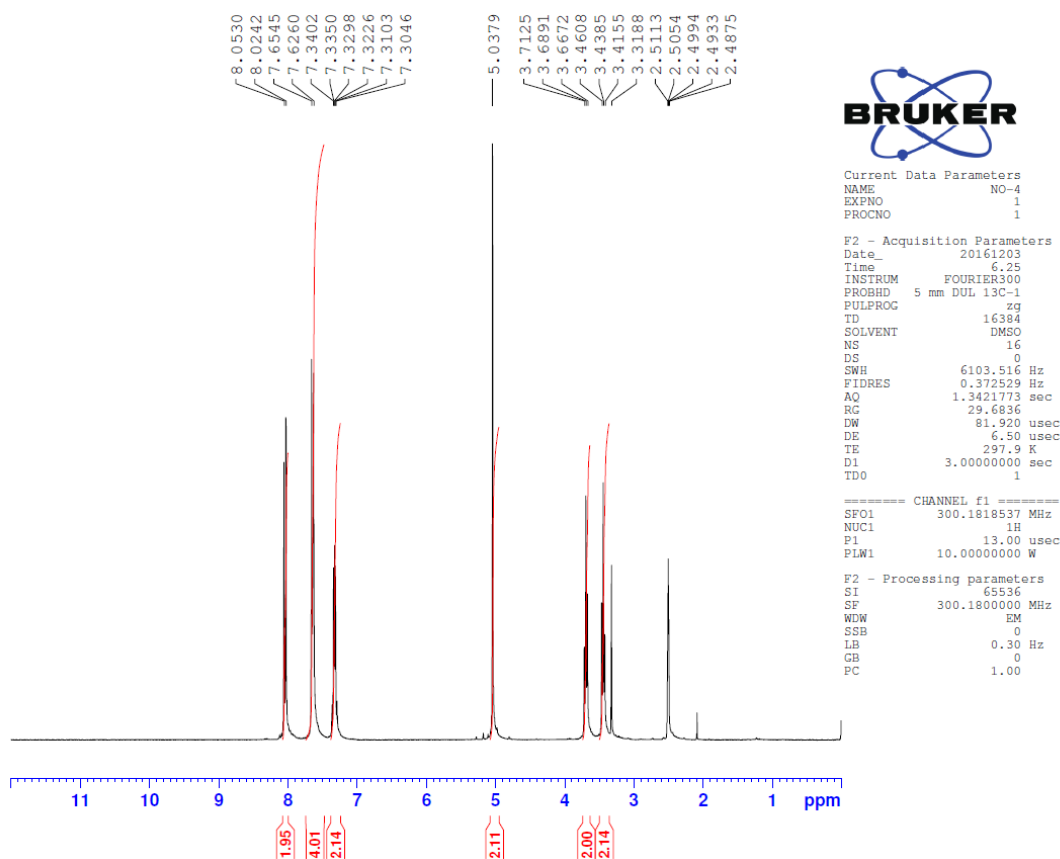


Figure 26. Compound 5d ^1H NMR spectrum

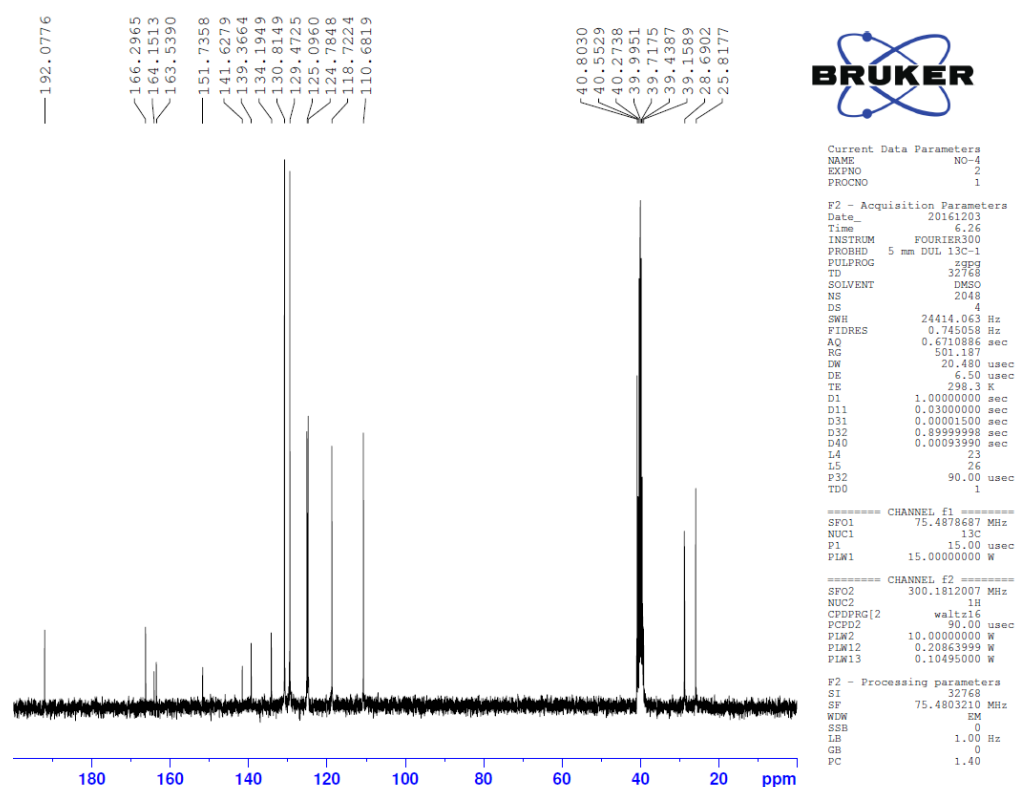


Figure 27. Compound 5d ^{13}C NMR spectrum

Data File: C:\LabSolutions\Data\Analiz\derya\NO-5_50.lod

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	9	20	O	2	1	6	Cl	1	0	2	I	3	0	0	H
C	4	18	25	F	1	0	1	Br	1	0	1					
N	3	3	6	S	2	2	2	Ru	2	0	0					

Error Margin (ppm): 10

HC Ratio: unlimited

Max Isotopes: 3

MSn Iso RI (%): 10.00

DBE Range: 12.0 - 15.0

Apply N Rule: yes

Isotope RI (%): 1.00

MSn Logic Mode: AND

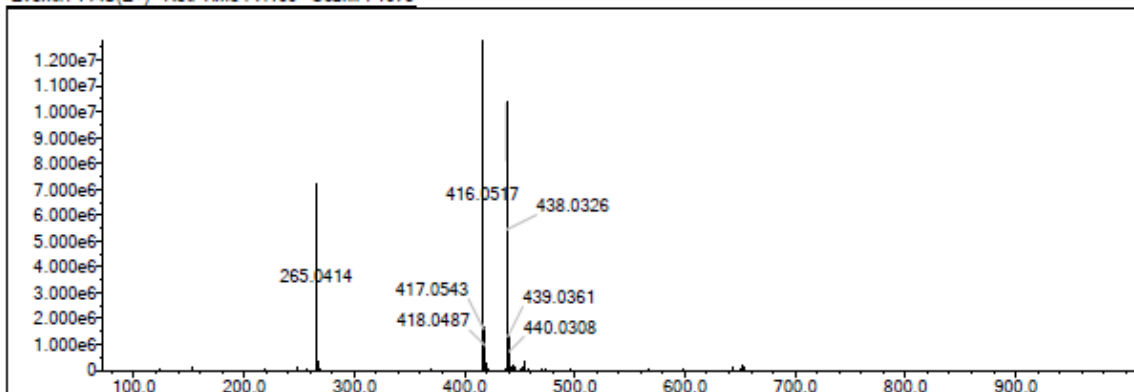
Electron Ions: both

Use MSn Info: no

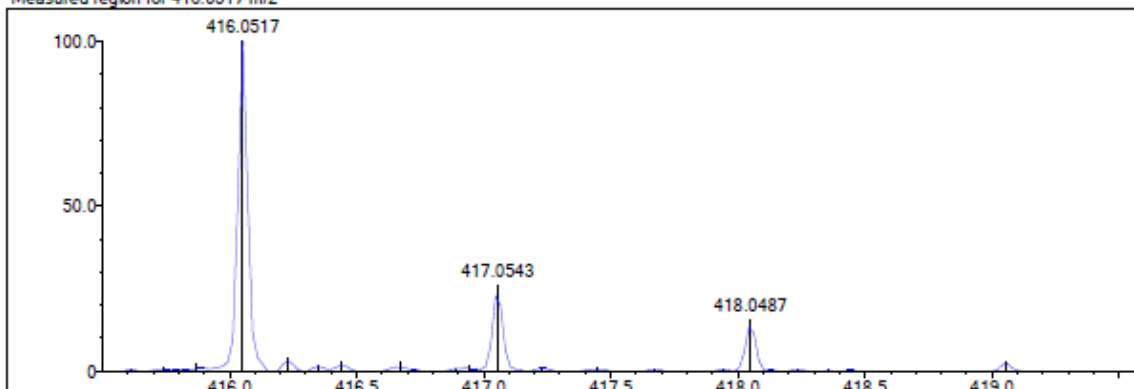
Isotope Res: 10000

Max Results: 500

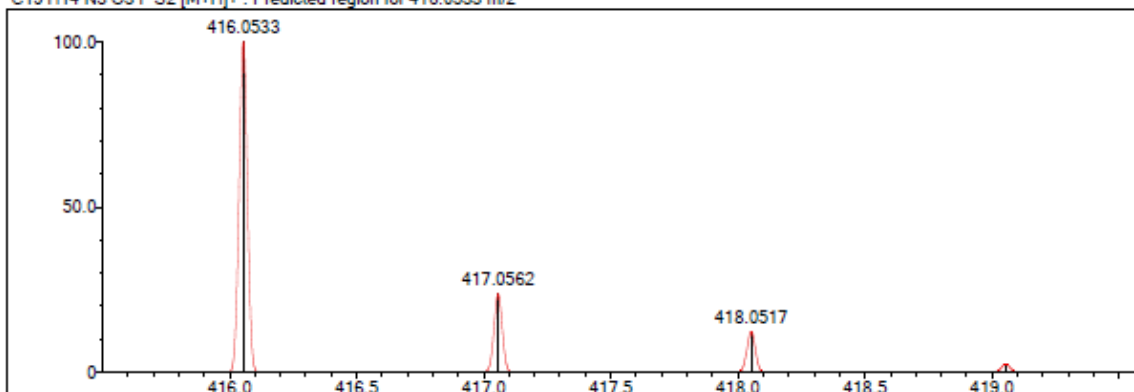
Event#: 1 MS(E+) Ret. Time : 7.160 Scan#: 1075



Measured region for 416.0517 m/z



C19 H14 N3 O3 F S2 [M+H]⁺ : Predicted region for 416.0533 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	88.45	C19 H14 N3 O3 F S2	[M+H] ⁺	416.0517	416.0533	-1.6	-3.85	95.23	14.0

Figure 28. Compound 5e Mass spectrum

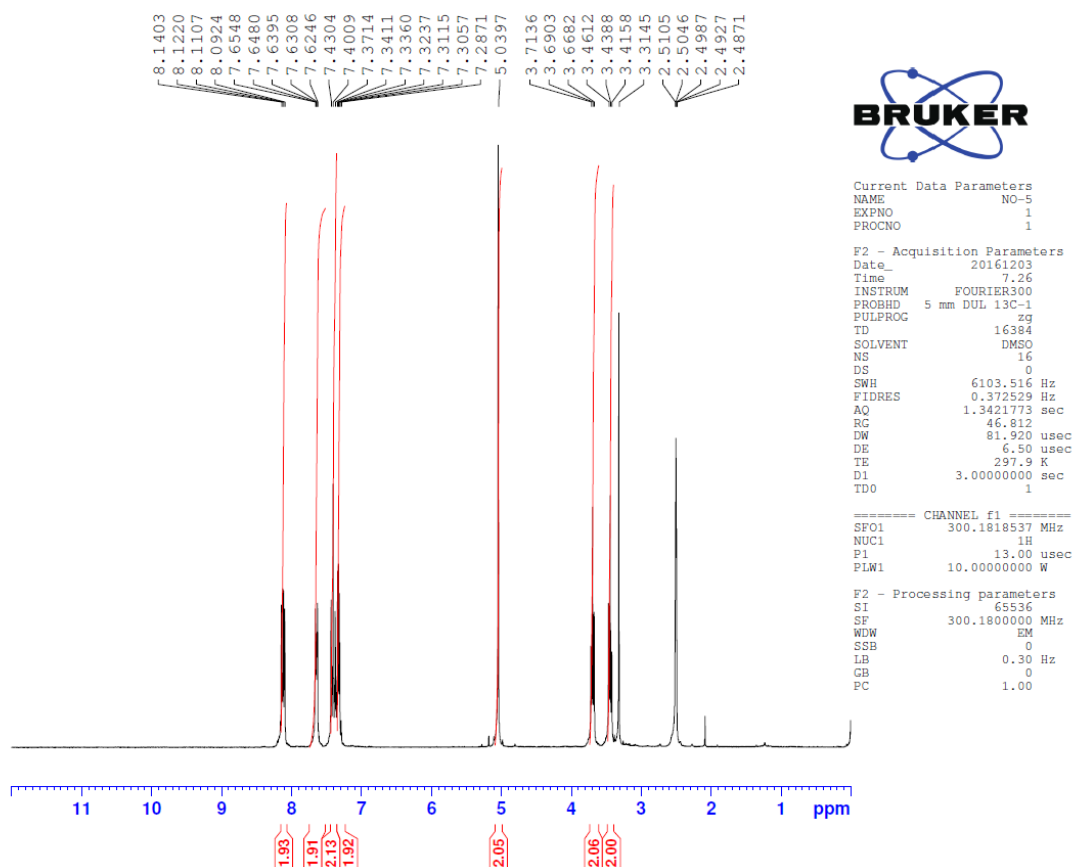


Figure 29. Compound 5e ^1H NMR spectrum

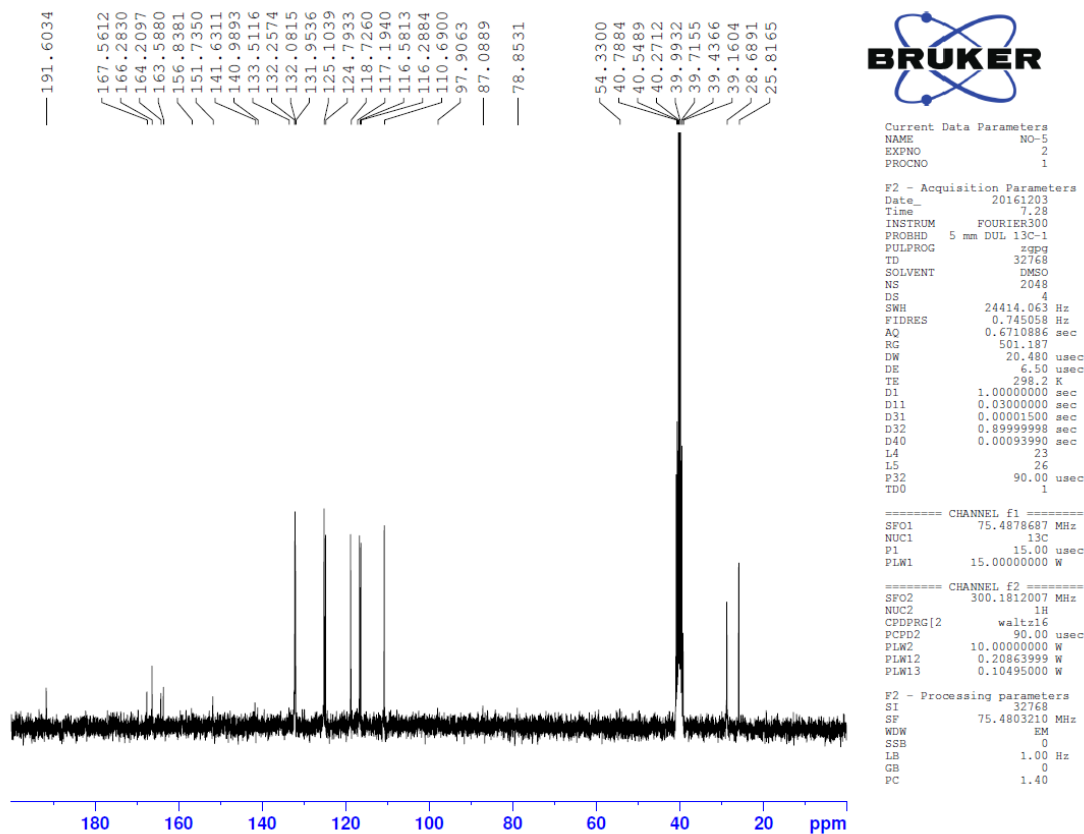


Figure 30. Compound 5e ^{13}C NMR spectrum

Data File: C:\LabSolutions\Data\Analiz\denya\NO-6_51.lod

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	9	20	O	2	1	6	Cl	1	0	2	I	3	0	0	H
C	4	18	25	F	1	0	1	Br	1	0	1					
N	3	3	6	S	2	2	2	Ru	2	0	0					

Error Margin (ppm): 10

HC Ratio: unlimited

Max Isotopes: 3

MSn Iso RI (%): 10.00

DBE Range: 12.0 - 15.0

Apply N Rule: yes

Isotope RI (%): 1.00

MSn Logic Mode: AND

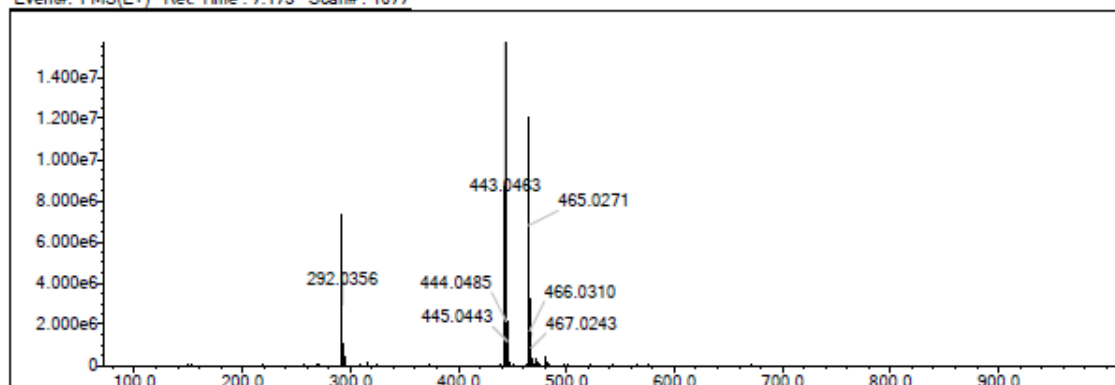
Electron Ions: both

Use MSn Info: no

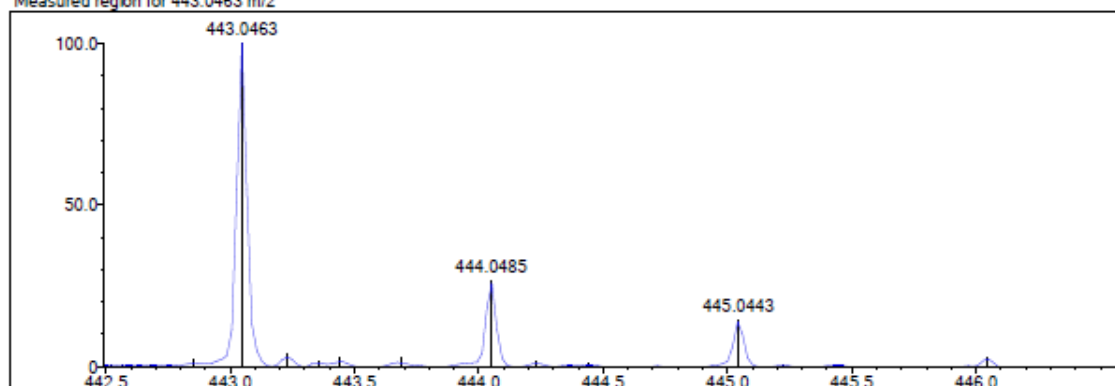
Isotope Res: 10000

Max Results: 500

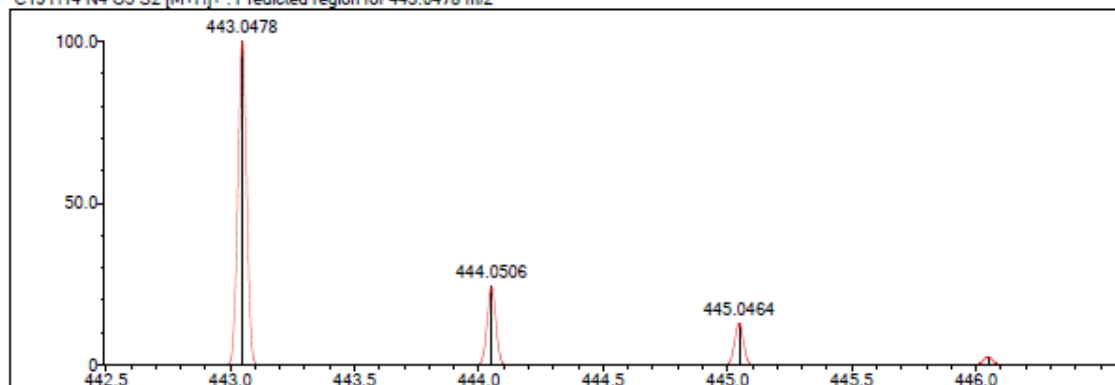
Event#: 1 MS(E+) Ret. Time : 7.173 Scan#: 1077



Measured region for 443.0463 m/z



C19 H14 N4 O5 S2 [M+H]⁺ : Predicted region for 443.0478 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	93.14	C19 H14 N4 O5 S2	[M+H] ⁺	443.0463	443.0478	-1.5	-3.39	99.06	15.0

Figure 31. Compound 5f Mass spectrum

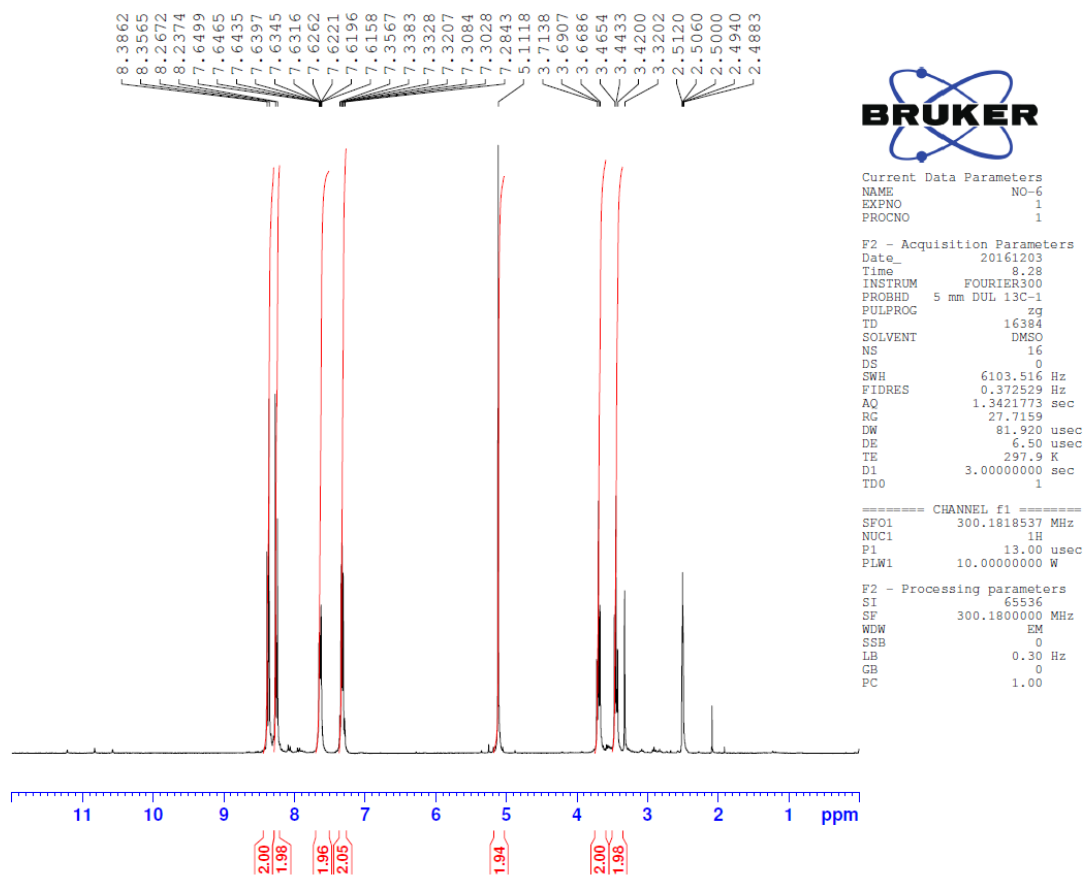


Figure 32. Compound 5f ^1H NMR spectrum

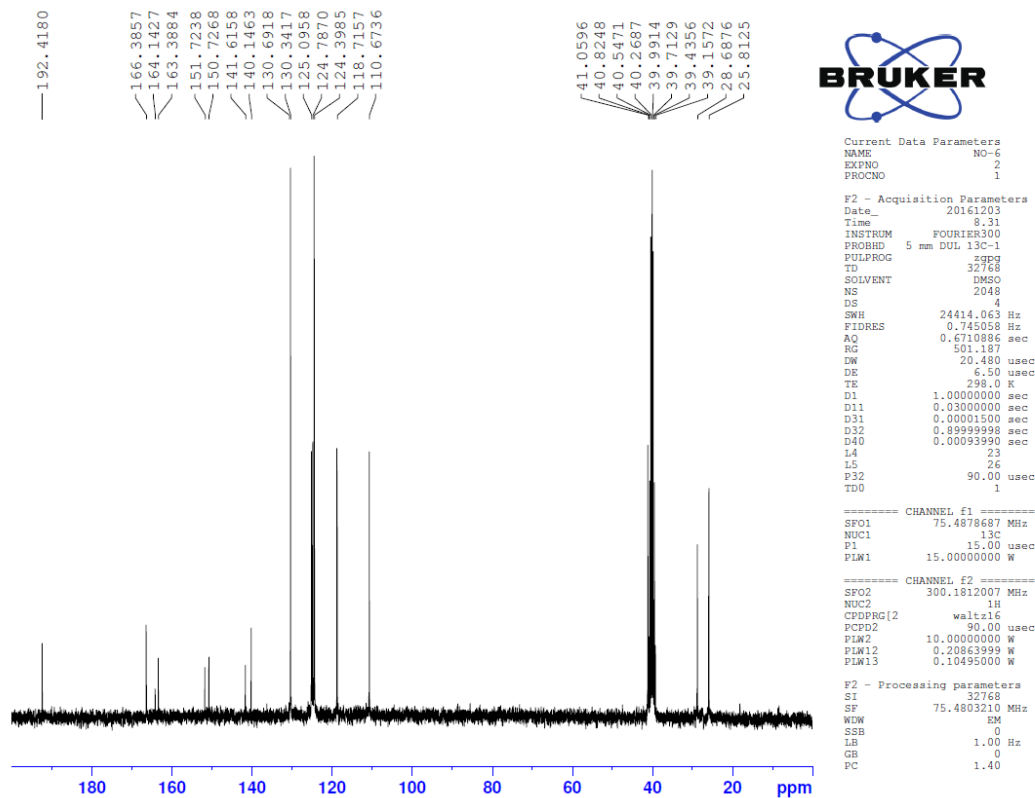


Figure 33. Compound 5f ^{13}C NMR spectrum