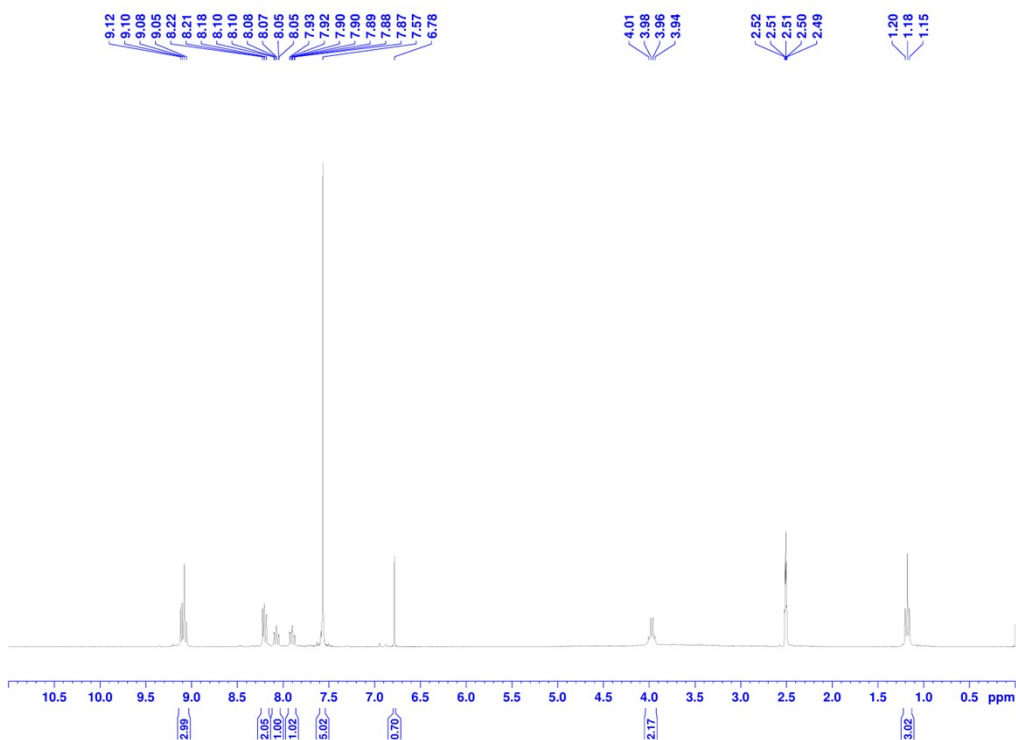


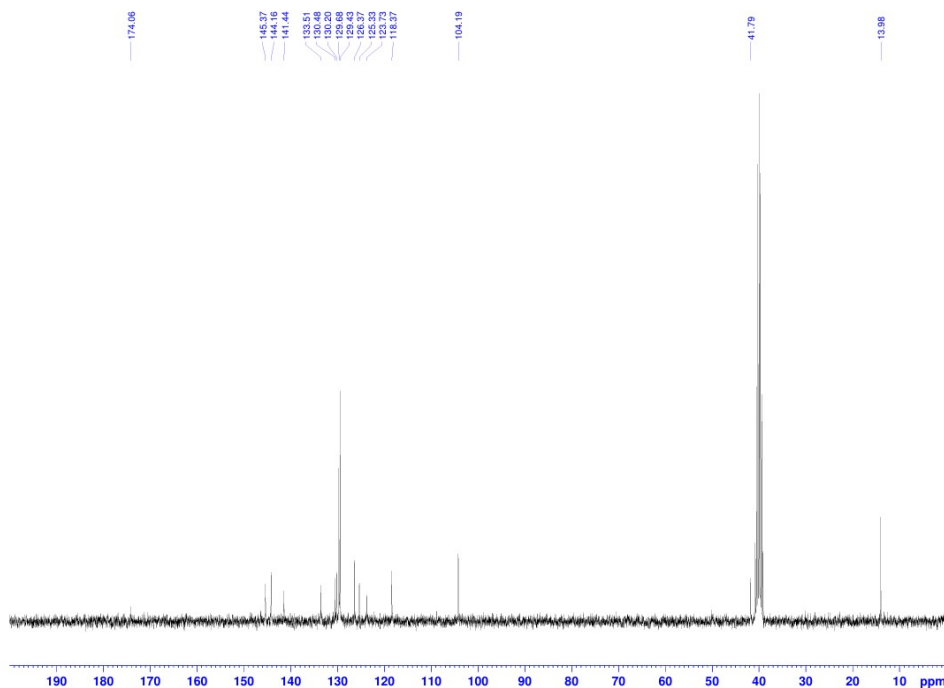
SUPPORTING INFORMATION

Quinoline/Thiazole Compounds as Selective Acetylcholinesterase Inhibitors: Synthesis and Biological Assessment



Current Data Parameters U
 NAME
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 2025
 Time 1
 INSTRUM FOURIE
 PROBHD 5 mm DUL 13C-1H/
 PULPROG
 TD 1
 SOLVENT
 NS
 DS
 SWH 6103
 FIDRES 0.37
 AQ 1.342
 RG 40.
 DW 81
 DE
 TE 2
 D1 3.0000
 TDO
 ===== CHANNEL f1 =====
 SFO1 300.181
 NUC1
 P1 1
 PLW1 10.0000
 F2 - Processing parameters
 S1 5
 SF 300.179
 WDW
 SSB
 LB
 GB
 PC

Spectra 1. ¹H-NMR spectra of compound 3a



Current Data Parameters
 NAME UMB-1
 EXPNO 11
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20250106
 Time 11.25
 INSTRUM FOURIER300
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 32768
 SOLVENT DMSO
 NS 2048
 DS 4
 SWH 24414.062 Hz
 FIDRES 0.745058 Hz
 AQ 0.6710886 sec
 RG 501.187
 DW 20.480 usec
 DE 6.50 usec
 TE 294.2 K
 D1 1.00000000 sec
 D11 0.00000000 sec
 D31 0.00001500 sec
 D32 0.89999998 sec
 D40 0.00093990 sec
 L4 23
 L5 26
 P32 90.00 usec
 TDO 1
 ===== CHANNEL f1 =====
 SFO1 75.4878687 MHz
 NUC1 13C
 P1 15.00 usec
 PLW1 15.00000000 W
 ===== CHANNEL f2 =====
 SFO2 300.1812007 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 10.00000000 W
 PLW12 0.20860000 W
 PLW13 0.10430000 W
 F2 - Processing parameters
 S1 32768
 SF 75.4803210 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Spectra 2. ¹³C-NMR spectra of compound 3a

Data File: C:\LabSolutions\Data\Analiz\Derya\UMB-1_31.lcd

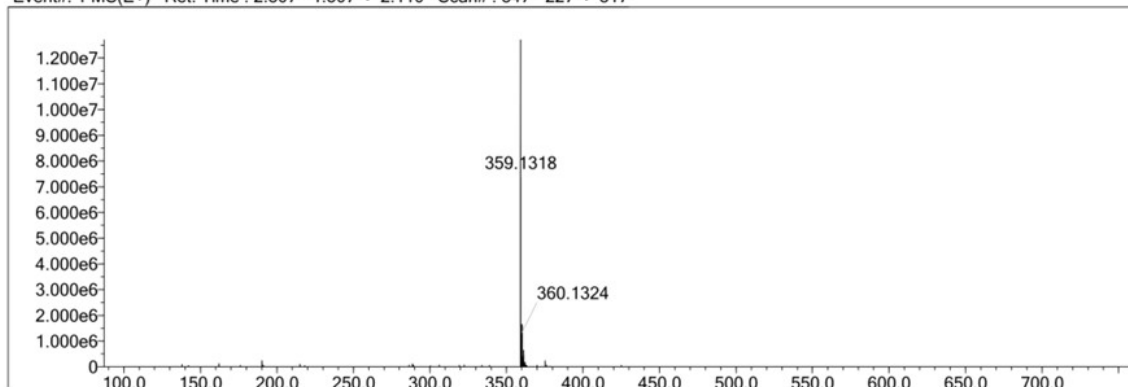
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	5	35	O	2	0	0	S	2	0	4	Ru	2	0	0	H
C	4	9	35	F	1	0	0	Cl	1	0	0	Pd	2	0	0	
N	3	0	4	P	3	0	0	Br	1	0	0	I	3	0	0	

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

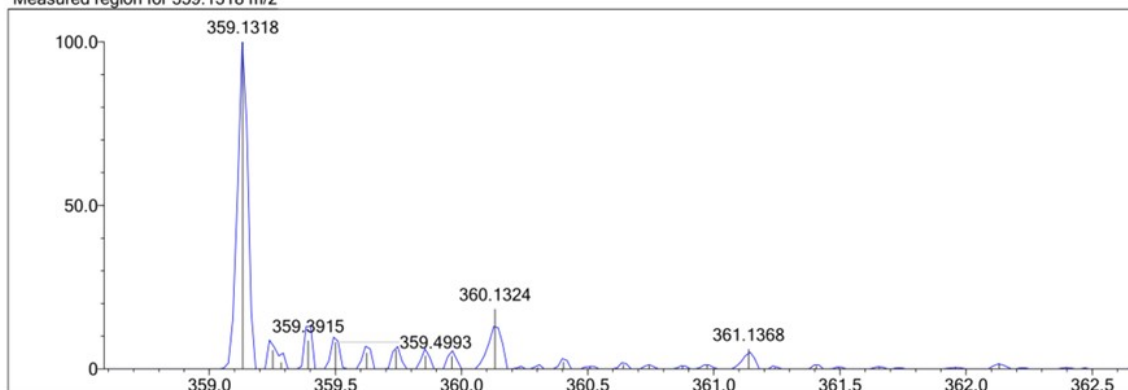
DBE Range: 0.0 - 20.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: yes
 Isotope Res: 9000
 Max Results: 50

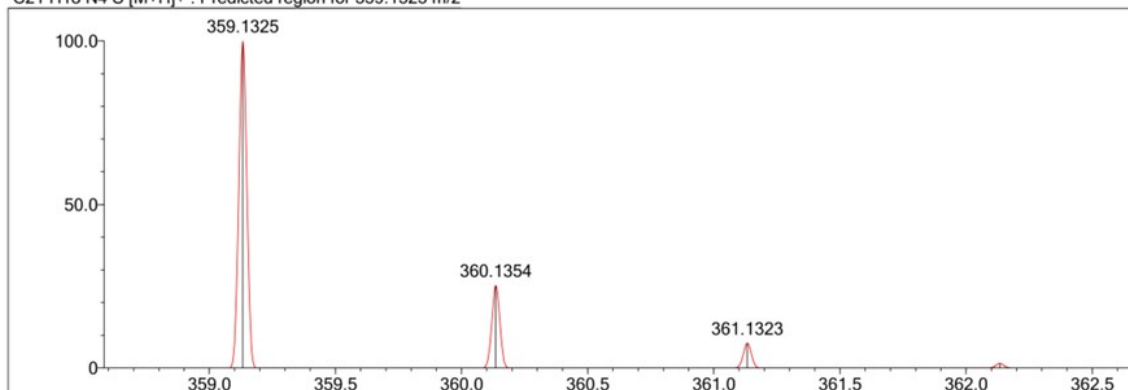
Event#: 1 MS(E+) Ret. Time : 2.307 - 1.507 -> 2.110 Scan# : 347 - 227 -> 317



Measured region for 359.1318 m/z

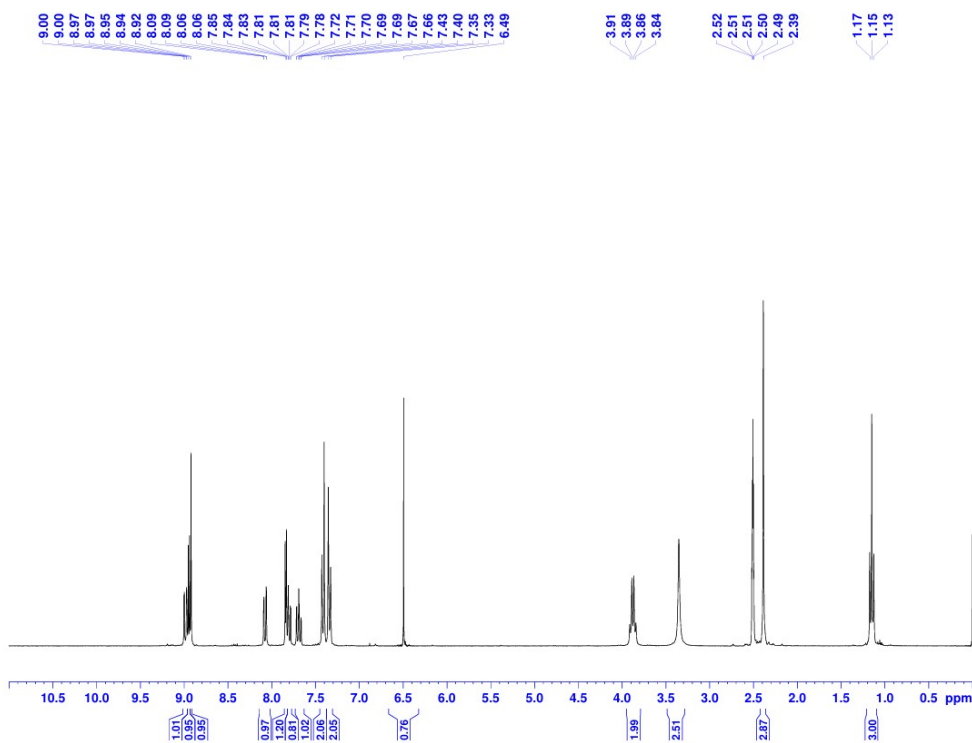


C21 H18 N4 S [M+H]⁺ : Predicted region for 359.1325 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	61.17	C21 H18 N4 S	[M+H] ⁺	359.1318	359.1325	-0.7	-1.95	62.65	15.0

Spectra 3. HRMS spectra of compound 3a

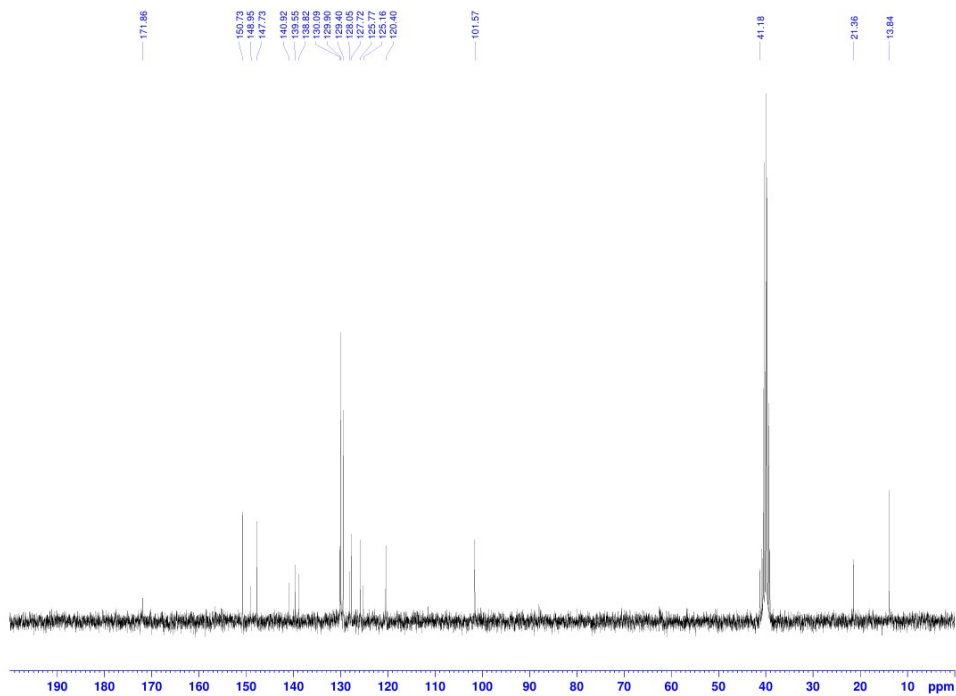


Current Data Parameters
 NAME UMB-2
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20241227
 Time 13.04
 INSTRUM FOURIER300
 PROBHD 5 mm DUL 13C-1
 PULPROG zg
 TD 16384
 SOLVENT DMSO
 NS 16
 DS 0
 SWH 6103.516 Hz
 FIDRES 0.372629 Hz
 AQ 1.3421773 sec
 RG 35707
 DW 81.920 usec
 DE 6.50 usec
 TE 294.1 K
 D1 3.0000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 300.1818537 MHz
 NUC1 1H
 P1 13.00 usec
 PLW1 10.0000000 W
 F2 - Processing parameters
 SI 6556
 SF 300.1799977 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Spectra 4. ¹H-NMR spectra of compound 3b



Current Data Parameters
 NAME UMB-2
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20241227
 Time 13.06
 INSTRUM FOURIER300
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg
 TD 32768
 SOLVENT DMSO
 NS 870
 DS 4
 SWH 24414.062 Hz
 FIDRES 0.745058 Hz
 AQ 0.6710886 sec
 RG 501.187
 DW 20.480 usec
 DE 6.50 usec
 TE 294.2 K
 D1 1.0000000 sec
 D11 0.0300000 sec
 D31 0.0000150 sec
 D32 0.8999999 sec
 D40 0.0009399 sec
 L4 23
 L5 26
 P32 90.00 usec
 TD0 1

===== CHANNEL f1 =====
 SFO1 75.4878687 MHz
 NUC1 13C
 P1 15.00 usec
 PLW1 15.0000000 W

===== CHANNEL f2 =====
 SFO2 300.1812007 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 10.0000000 W
 PLW12 0.2086399 W
 PLW13 0.1049500 W

F2 - Processing parameters
 SI 32768
 SF 75.4803210 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Spectra 5. ¹³C-NMR spectra of compound 3b

Data File: C:\LabSolutions\Data\Analiz\Derya\UMB-2_22.lcd

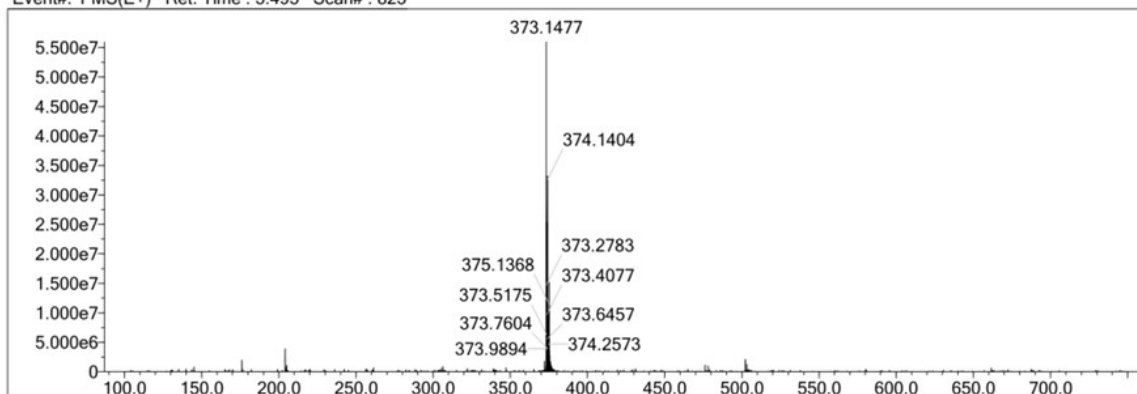
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	5	35	O	2	0	4	S	2	0	2	Ru	2	0	0	H
C	4	9	35	F	1	0	0	Cl	1	0	0	Pd	2	0	0	
N	3	4	8	P	3	0	0	Br	1	0	0	I	3	0	0	

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

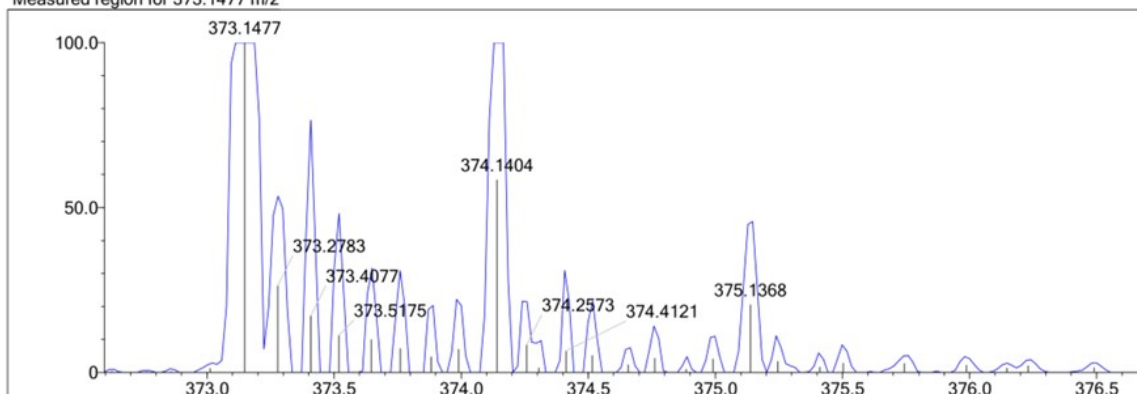
DBE Range: 8.0 - 30.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: yes
 Isotope Res: 9000
 Max Results: 50

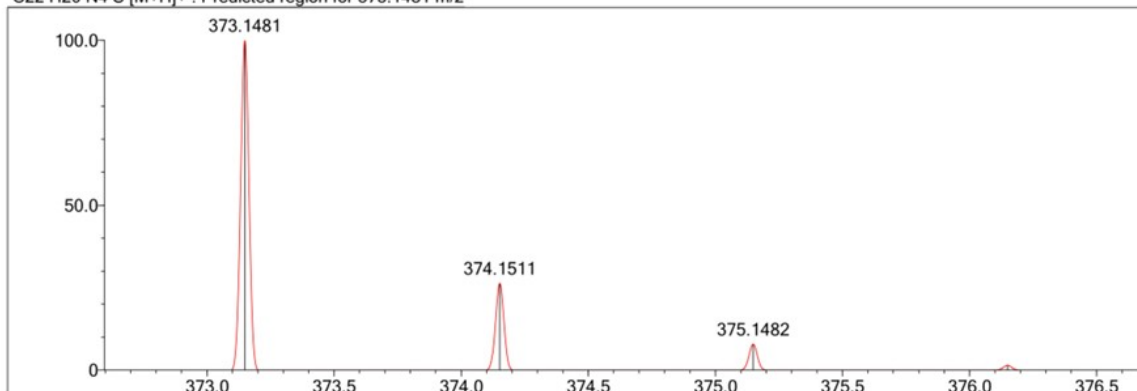
Event#: 1 MS(E+) Ret. Time : 5.493 Scan#: 825



Measured region for 373.1477 m/z

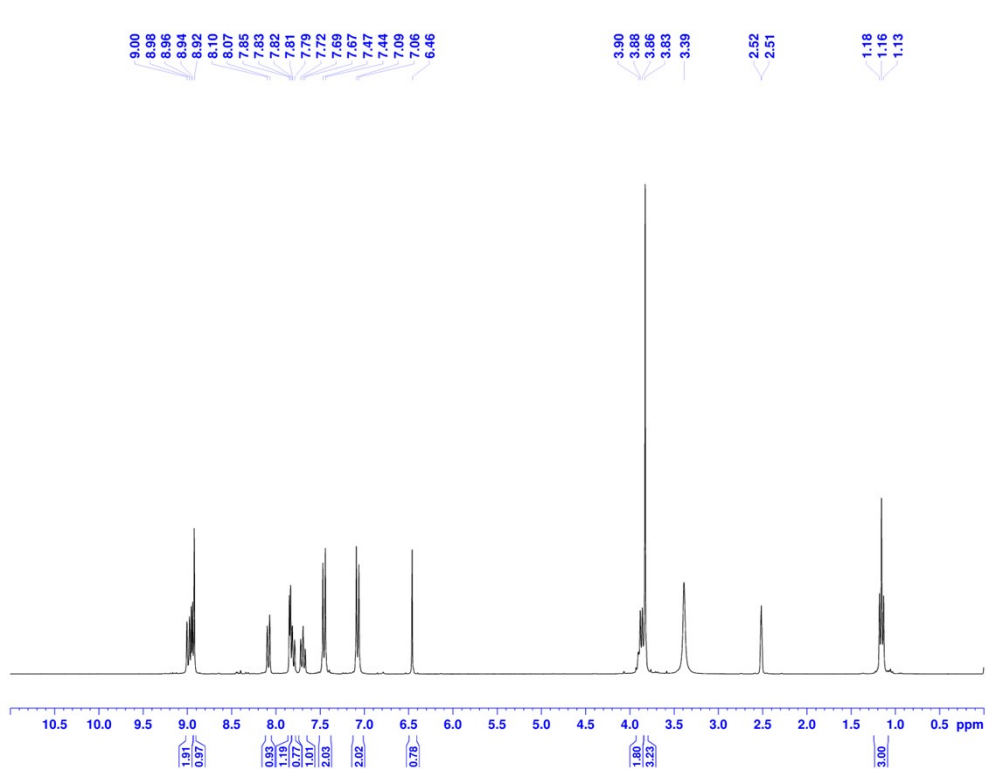


C22 H20 N4 S [M+H]+ : Predicted region for 373.1481 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	26.28	C22 H20 N4 S	[M+H]+	373.1477	373.1481	-0.4	-1.07	26.32	15.0

Spectra 6. HRMS spectra of compound 3b



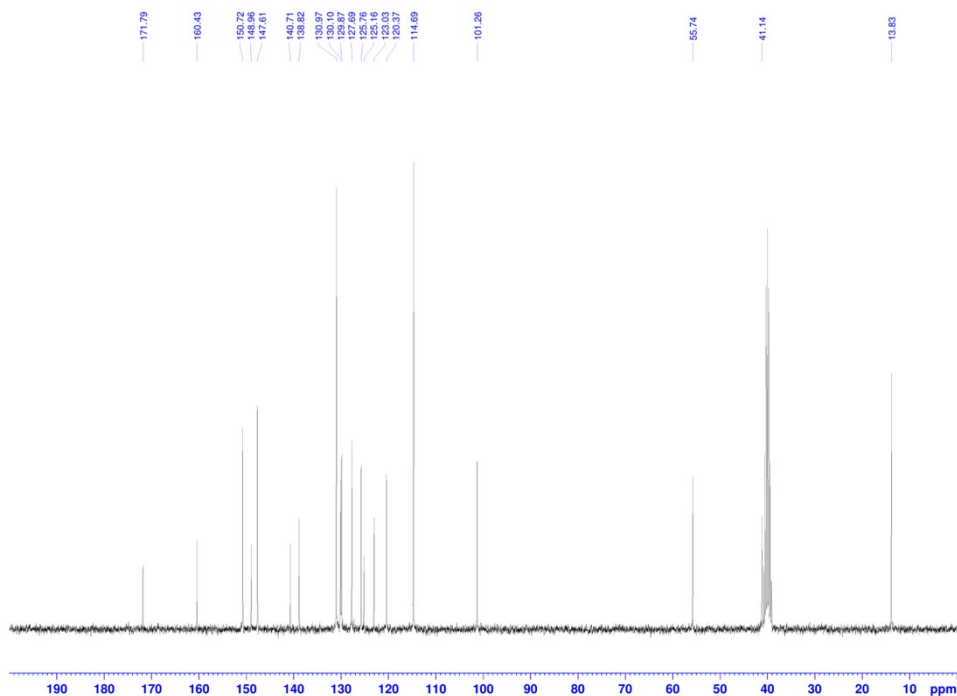
Current Data Parameters
 NAME UMB-3
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20250102
 Time 11:14
 INSTRUM FOURIER300
 PROBHD 5 mm DUL 13C-1
 PULPROG zg
 TD 16384
 SOLVENT DMSO
 NS 16
 DS 0
 SWH 6103.516 Hz
 FIDRES 0.372529 Hz
 AQ 1.3421773 sec
 RG 15.976
 DW 81.520 usec
 DE 6.50 usec
 TE 293.8 K
 D1 3.00000000 sec
 TD0

===== CHANNEL f1 =====
 SFO1 300.1818537 MHz
 NUC1 1H
 P1 13.00 usec
 PLW1 10.00000000 W

F2 - Processing parameters
 SI 65536
 SF 300.1799849 MHz
 WDW EM
 SSB 0
 LB 0.0 Hz
 GB 0
 PC 1.00

Spectra 7. ¹H-NMR spectra of compound 3c



Current Data Parameters
 NAME UMB-3
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20250102
 Time 11:15
 INSTRUM FOURIER300
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg
 TD 32768
 SOLVENT DMSO
 NS 2048
 DS 4
 SWH 24414.062 Hz
 FIDRES 0.745058 Hz
 AQ 0.6710886 sec
 RG 501.187
 DW 20.480 usec
 DE 6.50 usec
 TE 293.7 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 D31 0.00001500 sec
 D32 0.89999998 sec
 D40 0.00033990 sec
 L4 23
 L5 26
 P32 90.00 usec
 TD0 1

===== CHANNEL f1 =====
 SFO1 75.4878687 MHz
 NUC1 13C
 P1 15.00 usec
 PLW1 15.00000000 W

===== CHANNEL f2 =====
 SFO2 300.1812007 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 10.00000000 W
 PLW12 0.20863990 W
 PLW13 0.10495000 W

F2 - Processing parameters
 SI 32768
 SF 75.4803210 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Spectra 8. ¹³C-NMR spectra of compound 3c

Data File: C:\LabSolutions\Data\Analiz\Derya\UMB-3_23.lcd

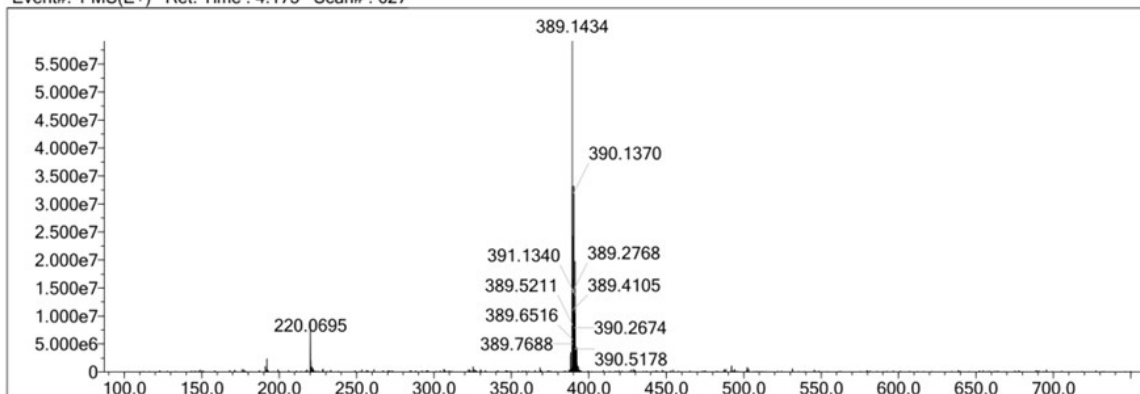
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	5	35	O	2	0	4	S	2	0	2	Ru	2	0	0	H
C	4	9	35	F	1	0	0	Cl	1	0	0	Pd	2	0	0	
N	3	4	8	P	3	0	0	Br	1	0	0	I	3	0	0	

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

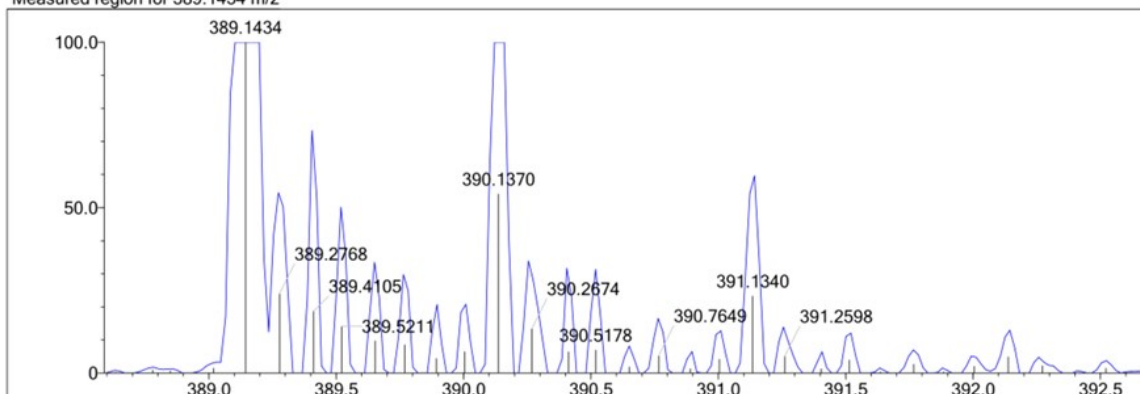
DBE Range: 8.0 - 30.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: yes
 Isotope Res: 9000
 Max Results: 50

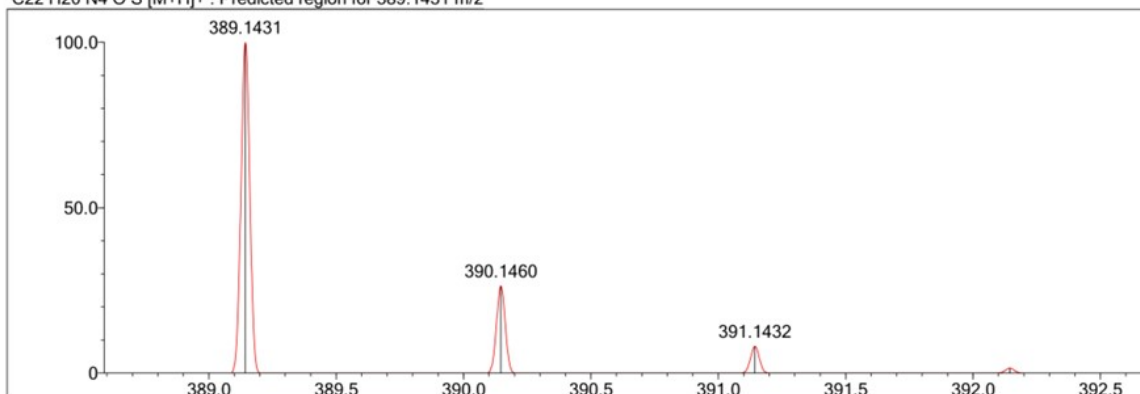
Event#: 1 MS(E+) Ret. Time : 4.173 Scan#: 627



Measured region for 389.1434 m/z

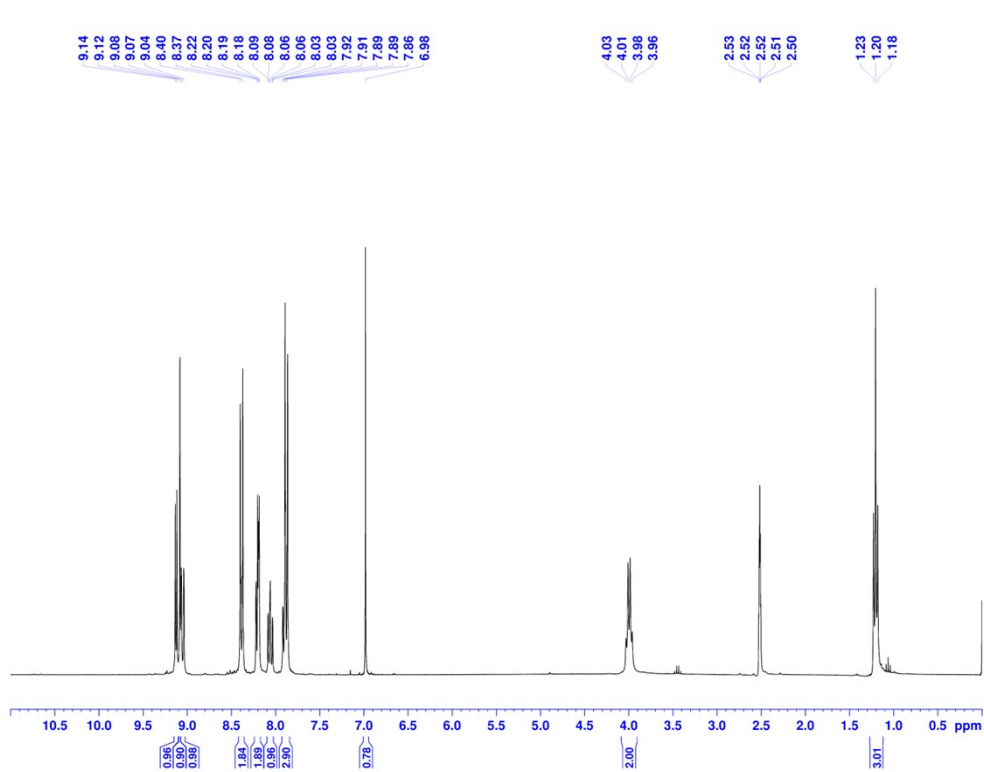


C22 H20 N4 O S [M+H]⁺ : Predicted region for 389.1431 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	28.35	C22 H20 N4 O S	[M+H] ⁺	389.1434	389.1431	0.3	0.77	28.35	15.0

Spectra 9. HRMS spectra of compound 3c



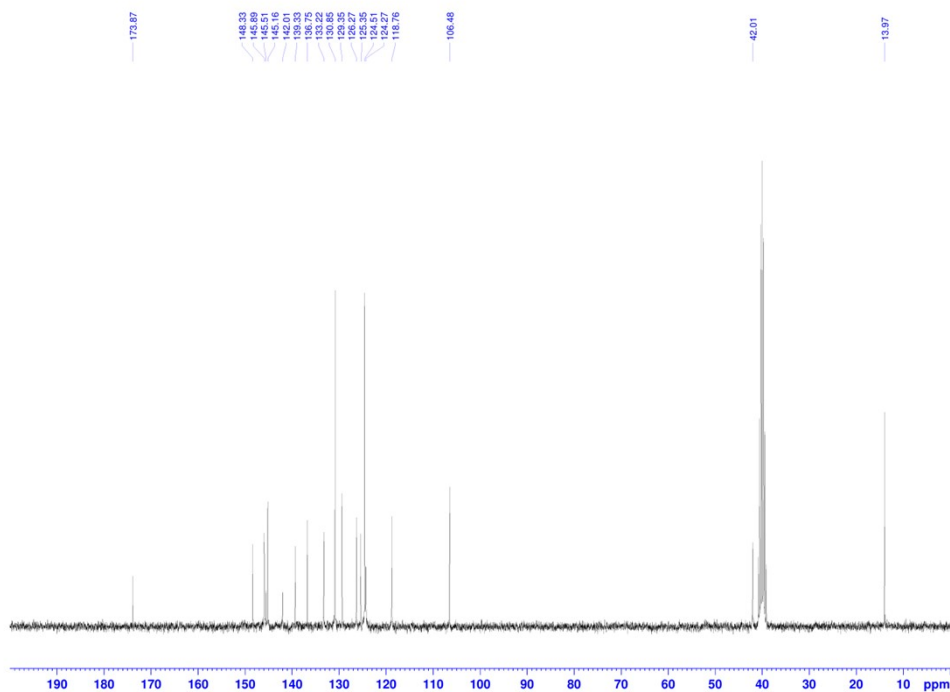
Current Data Parameters
 NAME UMB-4
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20241228
 Time 11.44
 INSTRUM FOURIER300
 PROBHD 5 mm DUL 13C-1
 PULPROG zg
 TD 16384
 SOLVENT DMSO
 NS 16
 DS 0
 SWH 6103.516 Hz
 FIDRES 0.372529 Hz
 AQ 1.3421773 sec
 RG 21.3366
 DW 81.920 usec
 DE 6.50 usec
 TE 294.1 K
 D1 3.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 300.1818537 MHz
 NUC1 1H
 P1 15.00 usec
 PLW1 10.00000000 W

F2 - Processing parameters
 SI 65536
 SF 300.1799948 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Spectra 10. ¹H-NMR spectra of compound 3d



Current Data Parameters
 NAME UMB-4
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20241228
 Time 11.46
 INSTRUM FOURIER300
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg
 TD 32768
 SOLVENT DMSO
 NS 2048
 DS 1
 SWH 24414.062 Hz
 FIDRES 0.745058 Hz
 AQ 0.6710886 sec
 RG 501.187
 DW 20.480 usec
 DE 6.50 usec
 TE 294.1 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 D31 0.00001500 sec
 D32 0.89999998 sec
 D40 0.00093990 sec
 L4 23
 L5 26
 P32 90.00 usec
 TD0 1

===== CHANNEL f1 =====
 SFO1 75.4878687 MHz
 NUC1 13C
 P1 15.00 usec
 PLW1 15.00000000 W

===== CHANNEL f2 =====
 SFO2 300.1812007 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 10.00000000 W
 PLW12 0.20863999 W
 PLW13 0.10495000 W

F2 - Processing parameters
 SI 32768
 SF 75.4803210 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Spectra 11. ¹³C-NMR spectra of compound 3d

Data File: C:\LabSolutions\Data\Analiz\Derya\UMB-4_24.lcd

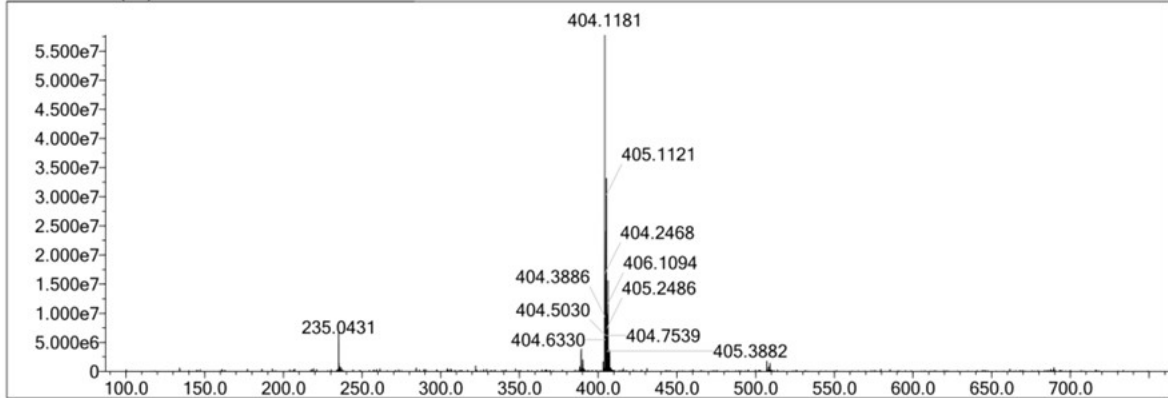
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H	1	5	35	O	2	0	4	S	2	0	2	Ru	2	0	0	H
C	4	9	35	F	1	0	0	Cl	1	0	0	Pd	2	0	0	
N	3	4	8	P	3	0	0	Br	1	0	0	I	3	0	0	

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

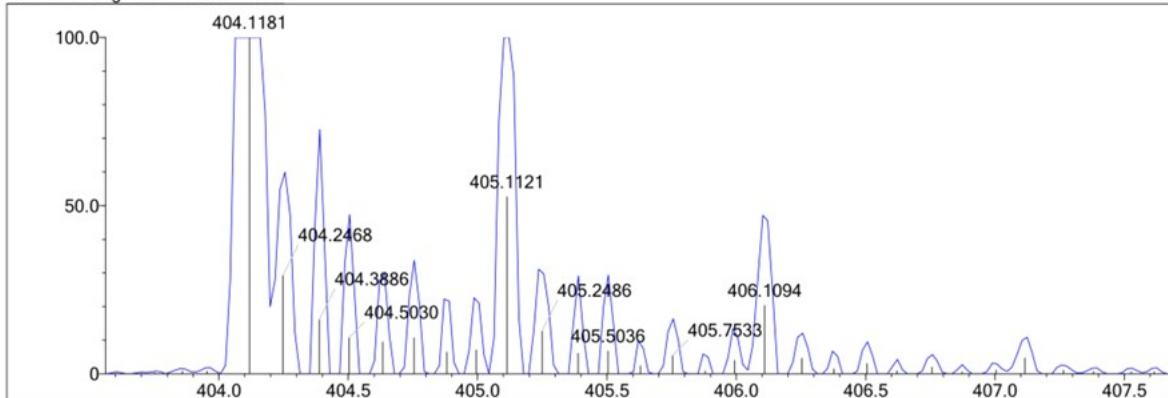
DBE Range: 8.0 - 30.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: yes
 Isotope Res: 9000
 Max Results: 50

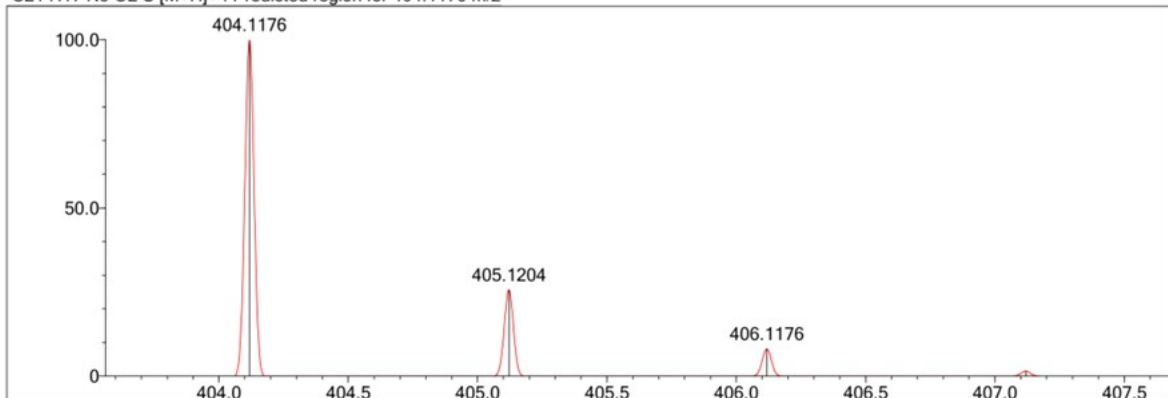
Event#: 1 MS(E+) Ret. Time : 4.280 Scan#: 643



Measured region for 404.1181 m/z

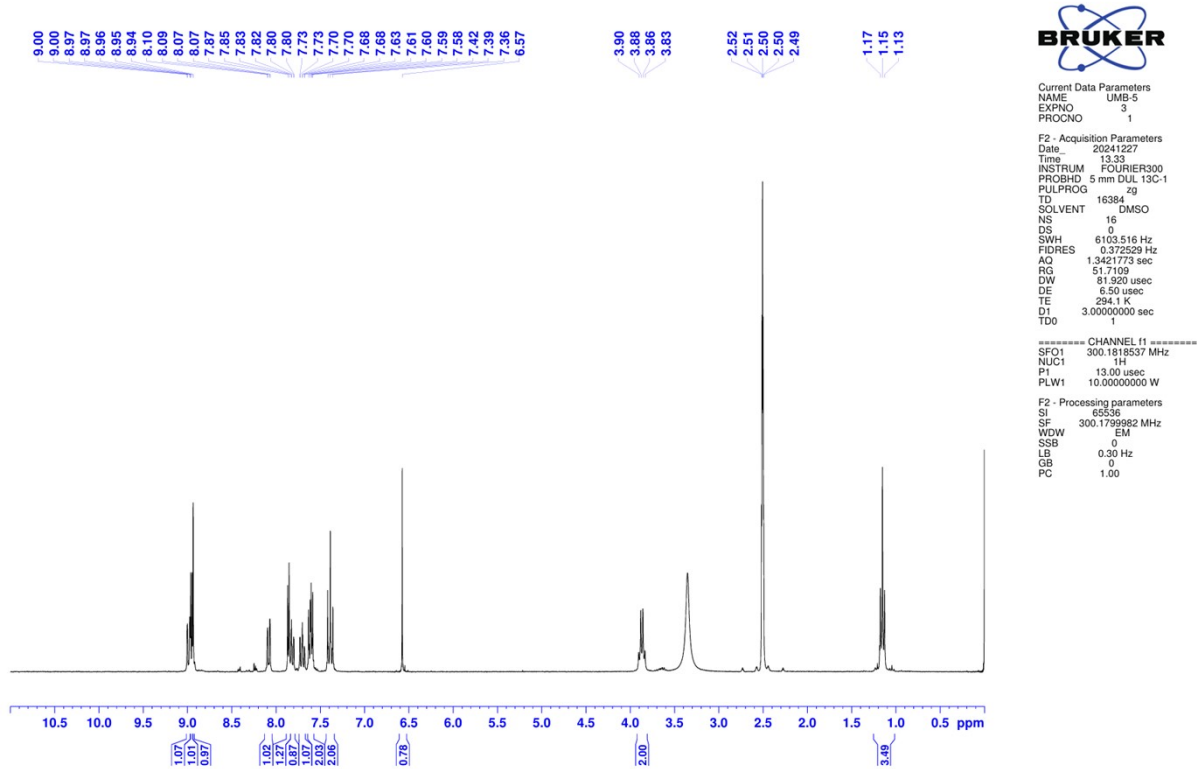


C21 H17 N5 O2 S [M+H]+ : Predicted region for 404.1176 m/z

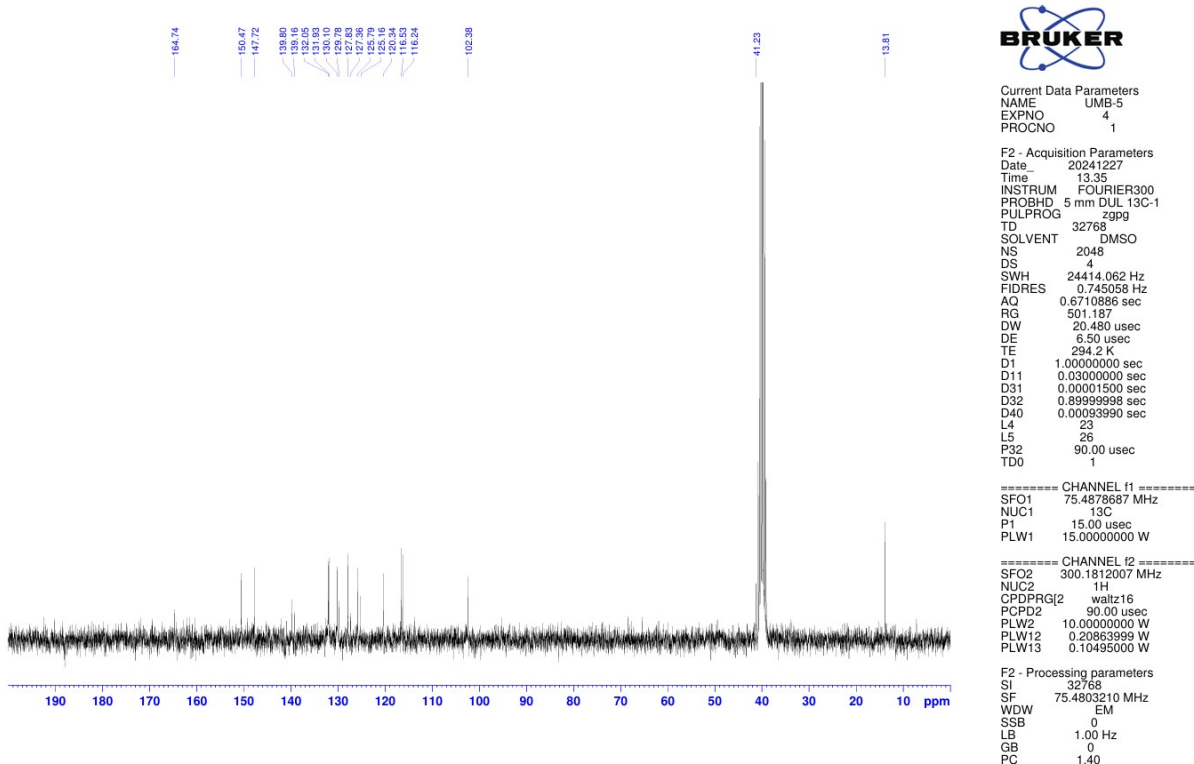


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	29.78	C21 H17 N5 O2 S	[M+H] ⁺	404.1181	404.1176	0.5	1.24	29.96	16.0

Spectra 12. HRMS spectra of compound 3d



Spectra 13. ¹H-NMR spectra of compound 3e



Spectra 14. ¹³C-NMR spectra of compound 3e

Data File: C:\LabSolutions\Data\Analiz\Derya\UMB-5_25.lcd

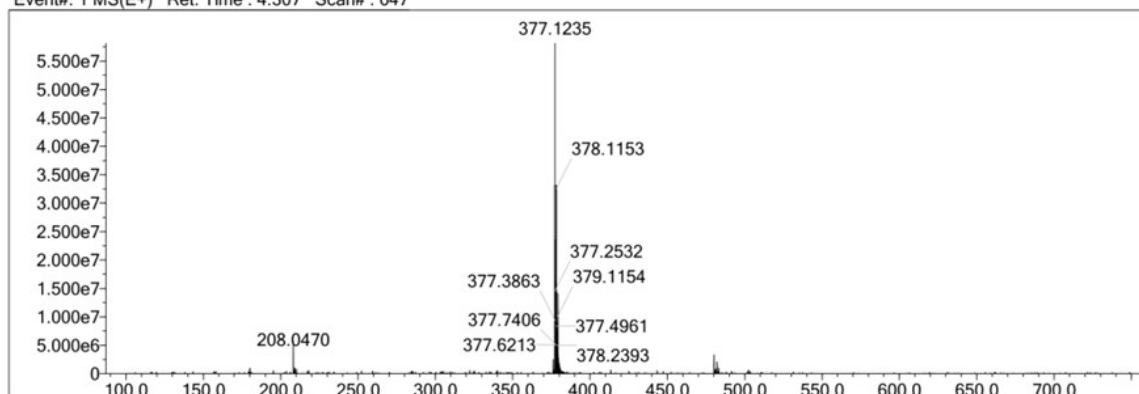
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	5	35	O	2	0	3	S	2	0	2	Ru	2	0	0	H
C	4	9	35	F	1	0	1	Cl	1	0	0	Pd	2	0	0	
N	3	4	8	P	3	0	0	Br	1	0	0	I	3	0	0	

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

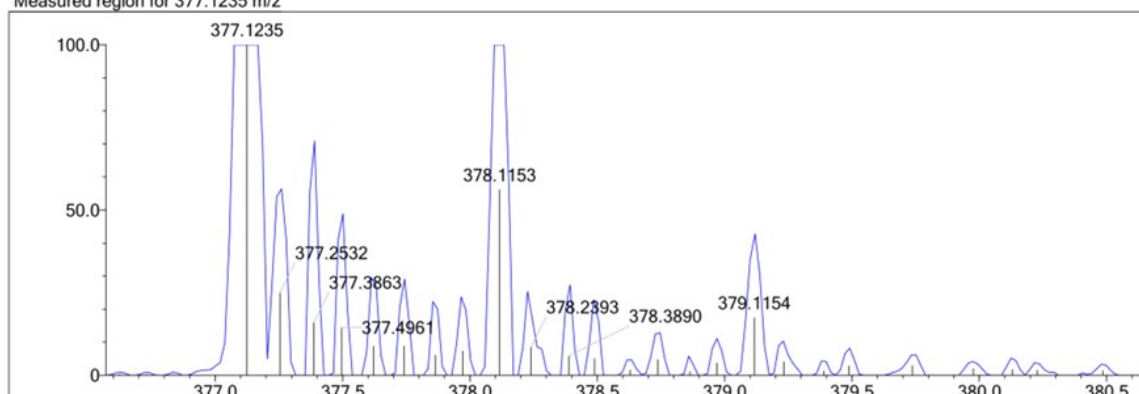
DBE Range: 8.0 - 30.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: yes
 Isotope Res: 9000
 Max Results: 50

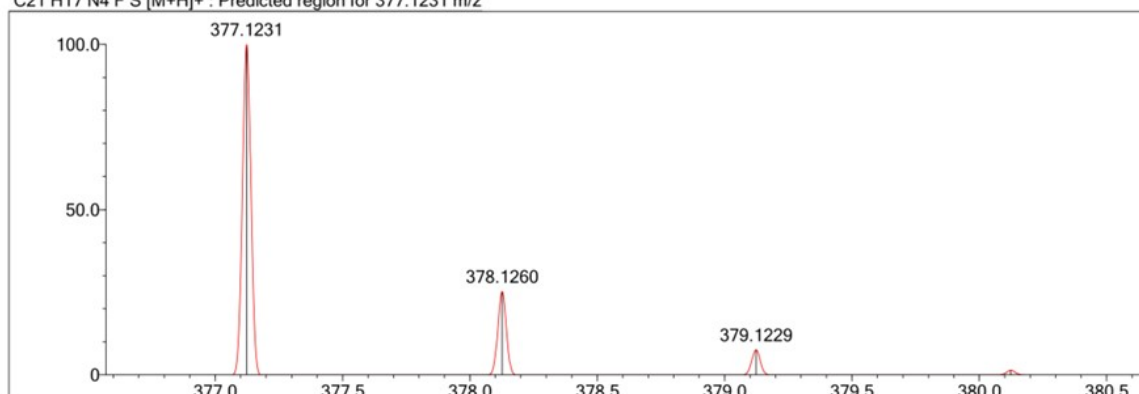
Event#: 1 MS(E+) Ret. Time : 4.307 Scan#: 647



Measured region for 377.1235 m/z

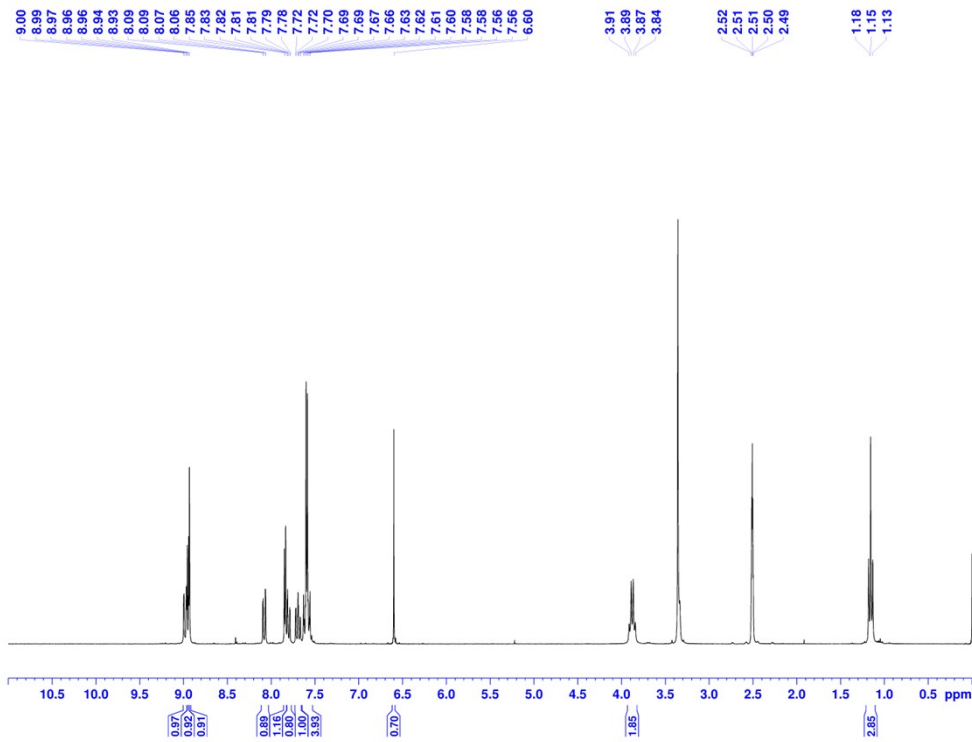


C21 H17 N4 F S [M+H]⁺ : Predicted region for 377.1231 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	26.07	C21 H17 N4 F S	[M+H] ⁺	377.1235	377.1231	0.4	1.06	26.11	15.0

Spectra 15. HRMS spectra of compound 3e



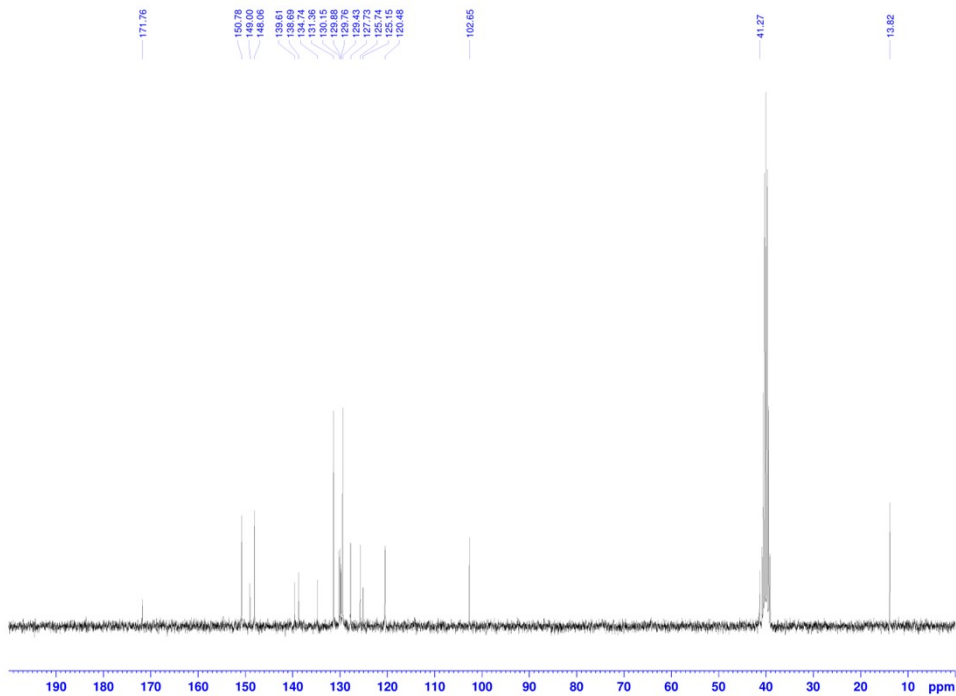
Current Data Parameters
 NAME UMB-6.2
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20241227
 Time 9.51
 INSTRUM FOURIER300
 PROBHD 5 mm DUL 13C-1
 PULPROG zg
 TD 16384
 SOLVENT DMSO
 NS 16
 DS 0
 SWH 6103.516 Hz
 FIDRES 0.372529 Hz
 AQ 1.3421773 sec
 RG 39.3552
 DW 81.920 usec
 DE 6.50 usec
 TE 294.1 K
 D1 3.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 300.1818537 MHz
 NUC1 1H
 P1 13.00 usec
 PLW1 10.00000000 W

F2 - Processing parameters
 SI 65536
 SF 300.1789975 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Spectra 16. ^1H -NMR spectra of compound 3f



Current Data Parameters
 NAME UMB-6.2
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20241227
 Time 9.53
 INSTRUM FOURIER300
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg
 TD 32768
 SOLVENT DMSO
 NS 2048
 DS 4
 SWH 24414.062 Hz
 FIDRES 0.745059 Hz
 AQ 0.6710886 sec
 RG 501.187
 DW 20.480 usec
 DE 6.50 usec
 TE 294.2 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 D31 0.00015000 sec
 D32 0.89999999 sec
 D40 0.00093990 sec
 L4 23
 L5 26
 P32 90.00 usec
 TD0 1

===== CHANNEL f1 =====
 SFO1 75.4878687 MHz
 NUC1 13C
 P1 15.00 usec
 PLW1 15.00000000 W

===== CHANNEL f2 =====
 SFO2 300.1812007 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 10.00000000 W
 PLW12 0.20863999 W
 PLW13 0.10495000 W

F2 - Processing parameters
 SI 32768
 SF 75.4803210 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Spectra 17. ^{13}C -NMR spectra of compound 3f

Data File: C:\LabSolutions\Data\Analiz\Derya\UMB-6.2_86.lcd

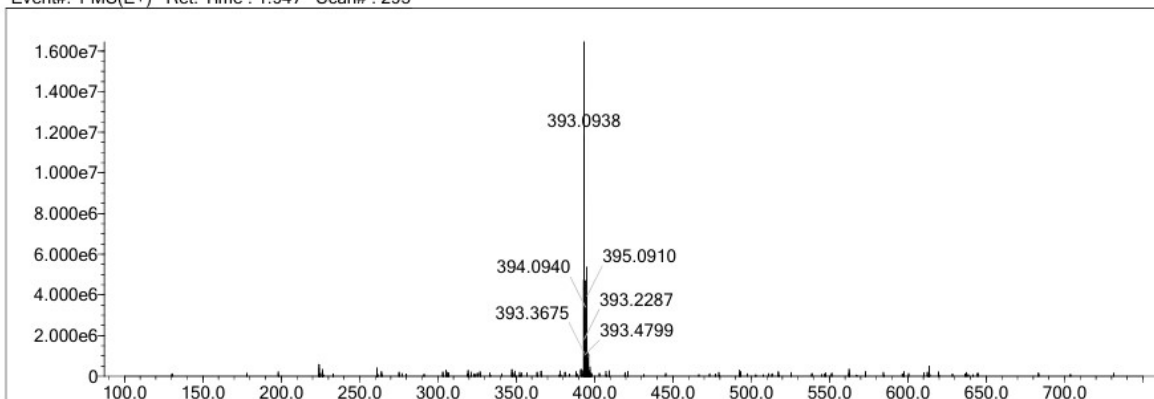
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	15	30	O	2	0	0	S	2	1	1	Ru	2	0	0	H
C	4	12	37	F	1	0	0	Cl	1	0	1	Pd	2	0	0	
N	3	1	6	P	3	0	0	Br	1	0	0	I	3	0	0	

Error Margin (ppm): 10
 HC Ratio: unlimited
 Max Isotopes: 5
 MSn Iso RI (%): 10.00

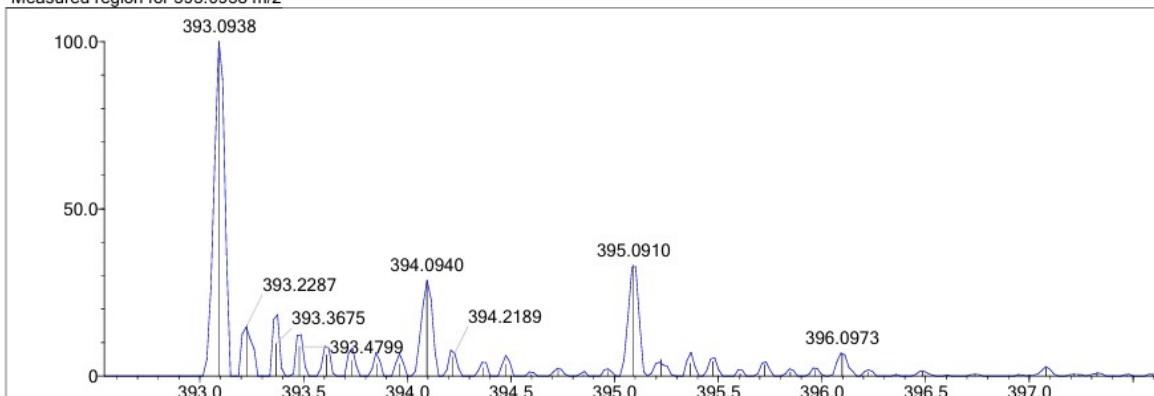
DBE Range: 5.0 - 20.0
 Apply N Rule: no
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: yes
 Isotope Res: 9000
 Max Results: 50

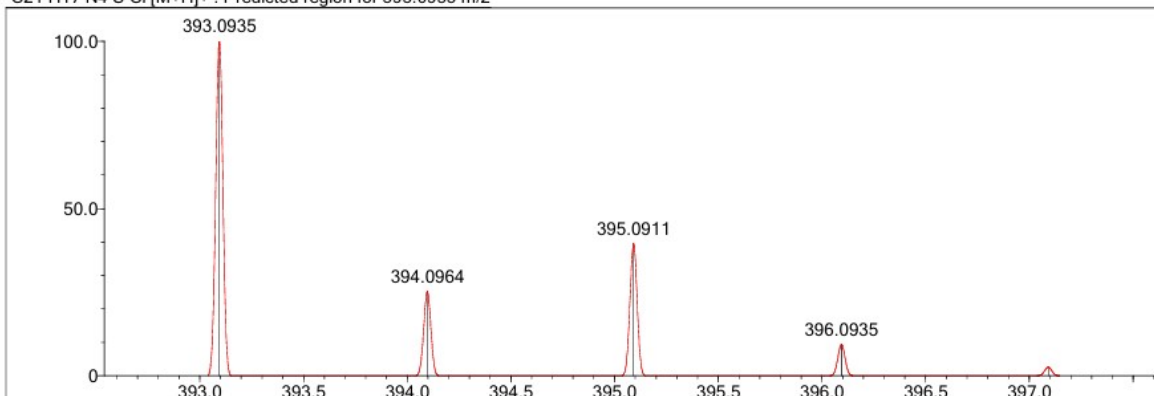
Event#: 1 MS(E+) Ret. Time : 1.947 Scan#: 293



Measured region for 393.0938 m/z

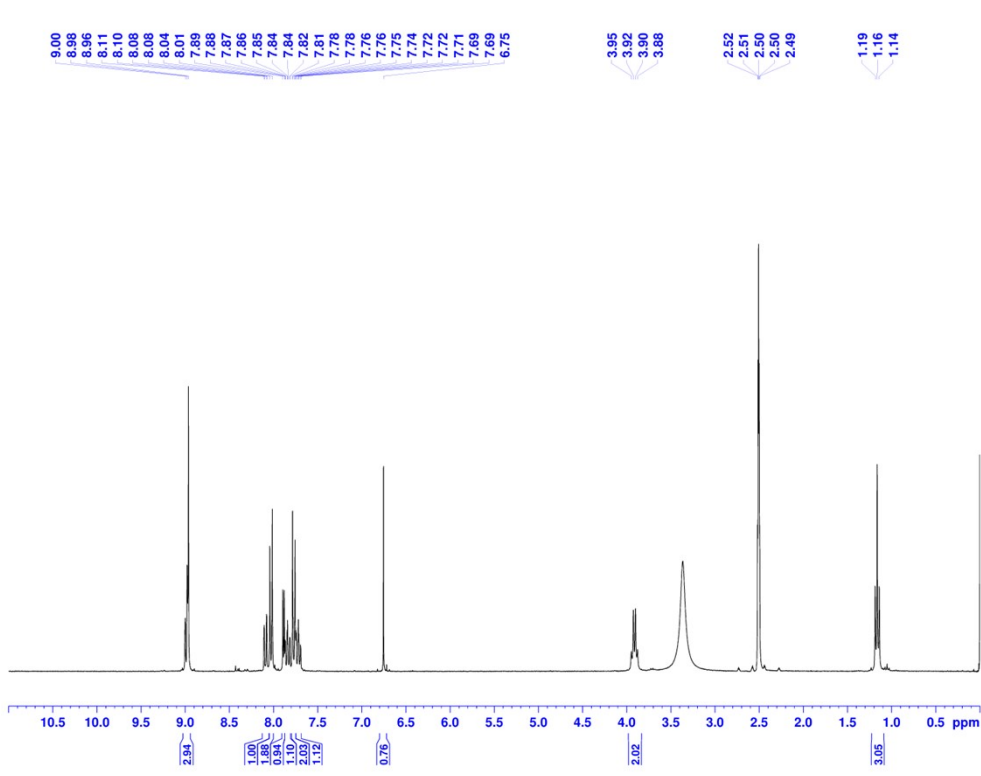


C21 H17 N4 S Cl [M+H]⁺ : Predicted region for 393.0935 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	68.18	C21 H17 N4 S Cl	[M+H] ⁺	393.0938	393.0935	0.3	0.76	68.18	15.0

Spectra 18. HRMS spectra of compound 3f



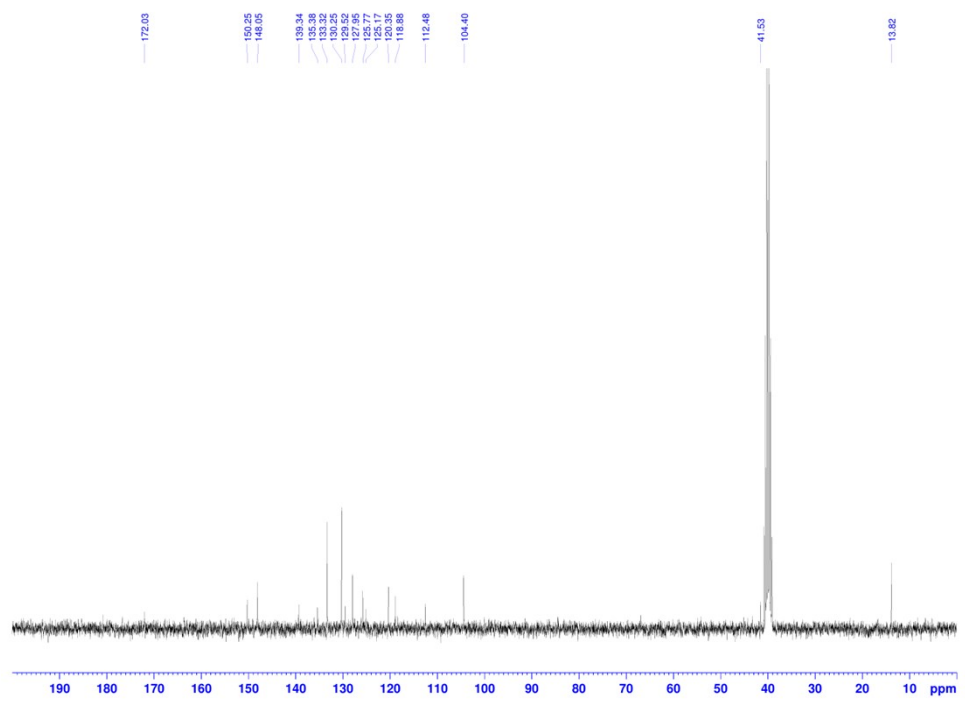
Current Data Parameters
 NAME UMB-8
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20241227
 Time 10.53
 INSTRUM FOURIER300
 PROBHD 5 mm DUL 13C-1
 PULPROG zg
 TD 16384
 SOLVENT DMSO
 NS 16
 DS 0
 SWH 6103.516 Hz
 FIDRES 0.372529 Hz
 AQ 1.3421773 sec
 RG 47.3558
 DW 61.920 usec
 DE 6.50 usec
 TE 294.1 K
 D1 3.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 300.1818537 MHz
 NUC1 1H
 P1 13.00 usec
 PLW1 10.00000000 W

F2 - Processing parameters
 SI 65536
 SF 300.1799981 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Spectra 19. ¹H-NMR spectra of compound 3g



Current Data Parameters
 NAME UMB-8
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20241227
 Time 10.55
 INSTRUM FOURIER300
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg
 TD 32768
 SOLVENT DMSO
 NS 2048
 DS 4
 SWH 24414.062 Hz
 FIDRES 0.745058 Hz
 AQ 0.6710886 sec
 RG 501.187
 DW 20.480 usec
 DE 6.50 usec
 TE 294.2 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 D31 0.00001500 sec
 D32 0.89999998 sec
 D40 0.00093990 sec
 L4 23
 L5 26
 P32 90.00 usec
 TD0 1

===== CHANNEL f1 =====
 SFO1 75.4878687 MHz
 NUC1 13C
 P1 15.00 usec
 PLW1 15.00000000 W

===== CHANNEL f2 =====
 SFO2 300.1812007 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 10.00000000 W
 PLW12 0.20863999 W
 PLW13 0.10495000 W

F2 - Processing parameters
 SI 32768
 SF 75.4803210 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Spectra 20. ¹³C-NMR spectra of compound 3g

Data File: C:\LabSolutions\Data\Analiz\Derya\UMB-8_27.lcd

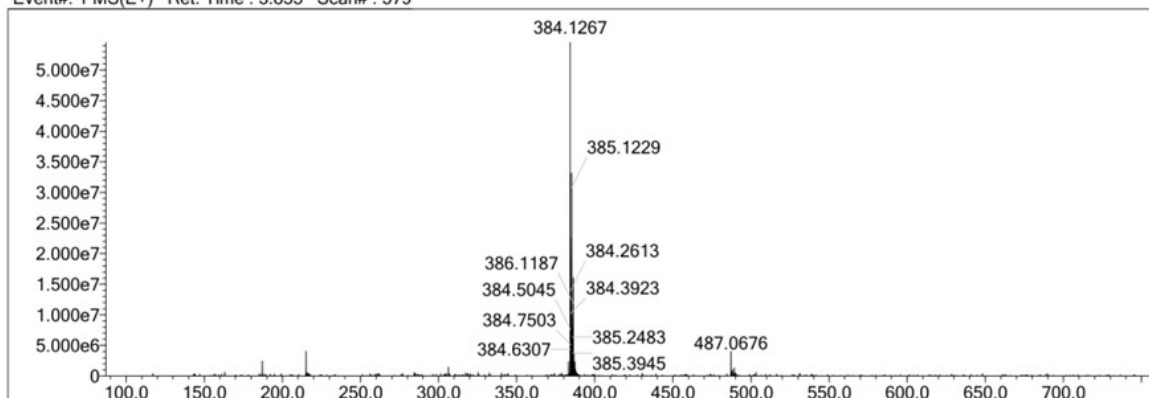
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	5	35	O	2	0	0	S	2	0	2	Ru	2	0	0	H
C	4	9	35	F	1	0	1	Cl	1	0	0	Pd	2	0	0	
N	3	4	8	P	3	0	0	Br	1	0	0	I	3	0	0	

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

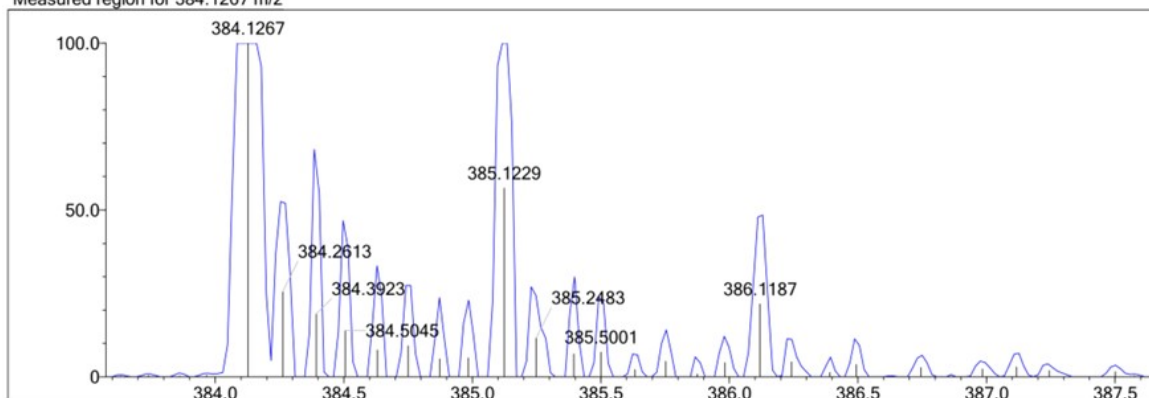
DBE Range: 8.0 - 30.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: yes
 Isotope Res: 9000
 Max Results: 50

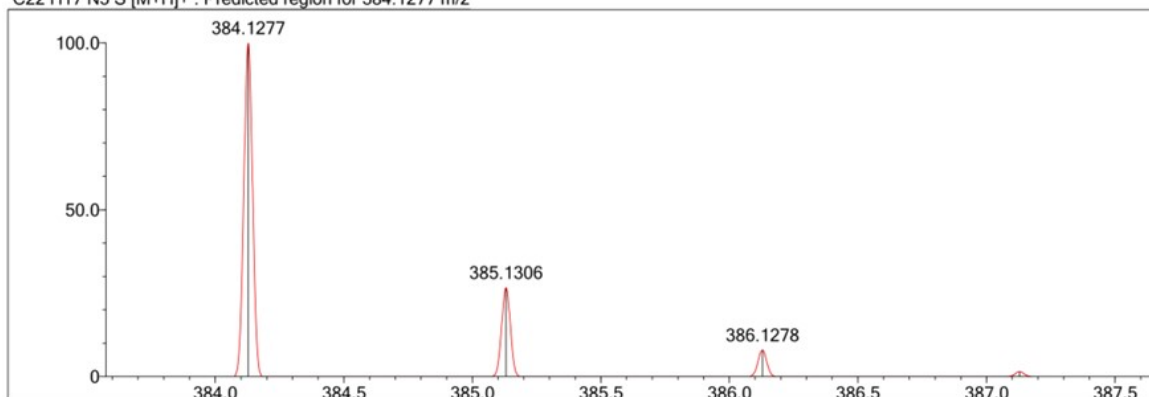
Event#: 1 MS(E+) Ret. Time : 3.853 Scan#: 579



Measured region for 384.1267 m/z

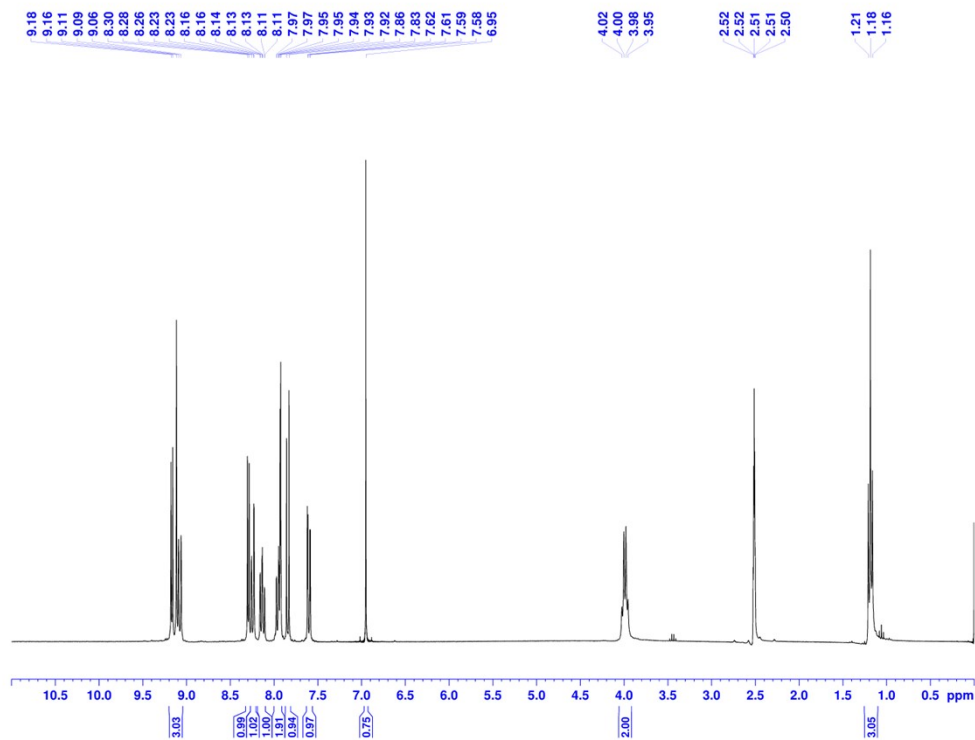


C22 H17 N5 S [M+H]⁺ : Predicted region for 384.1277 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	21.72	C22 H17 N5 S	[M+H] ⁺	384.1267	384.1277	-1.0	-2.60	22.62	17.0

Spectra 21. HRMS spectra of compound 3g

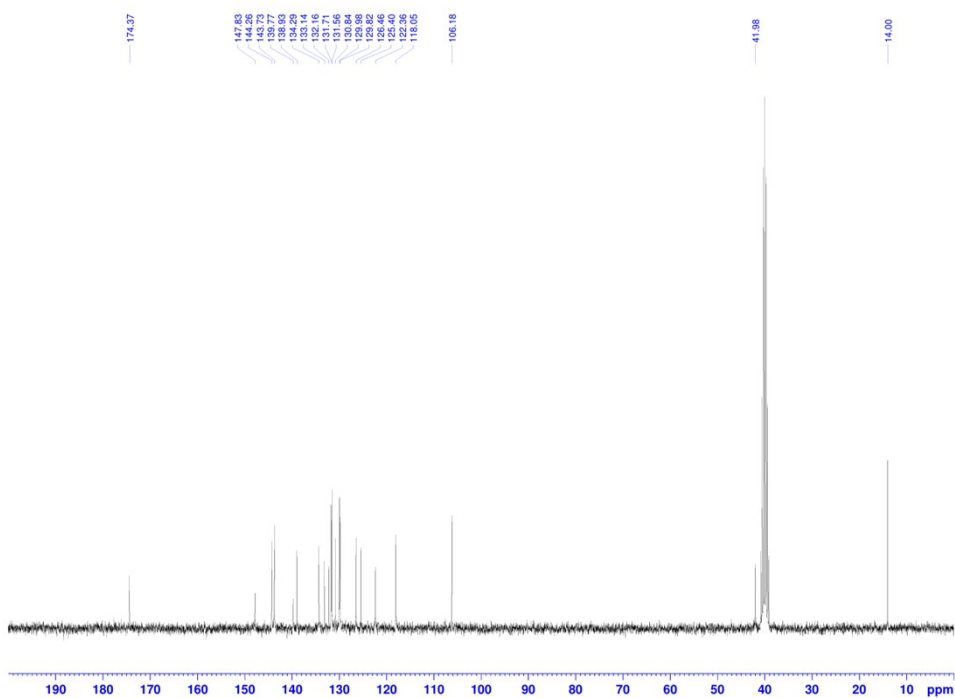


Current Data Parameters
 NAME UMB-10
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20241227
 Time 18:39
 INSTRUM FOURIER300
 PROBHD 5 mm DUL 13C-1
 PULPROG zg
 TD 16384
 SOLVENT DMSO
 NS 16
 DS 0
 SWH 6103.516 Hz
 FIDRES 0.372529 Hz
 AQ 1.3421773 sec
 RG 29.7739
 DW 81.920 usec
 DE 6.50 usec
 TE 294.2 K
 D1 3.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 300.1818537 MHz
 NUC1 1H
 P1 13.00 usec
 PLW1 10.00000000 W
 F2 - Processing parameters
 SI 65536
 SF 300.179868 MHz
 WDW EM
 SSB 0
 LB 0.0 Hz
 GB 0
 PC 1.00

Spectra 22. ¹H-NMR spectra of compound 3h



Current Data Parameters
 NAME UMB-10
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20241227
 Time 18:41
 INSTRUM FOURIER300
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg
 TD 32768
 SOLVENT DMSO
 NS 2048
 DS 4
 SWH 24414.062 Hz
 FIDRES 0.745058 Hz
 AQ 0.6710886 sec
 RG 501.187
 DW 20.480 usec
 DE 6.50 usec
 TE 294.2 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 D31 0.00001500 sec
 D32 0.89999998 sec
 D40 0.00003990 sec
 L4 23
 L5 26
 P32 90.00 usec
 TD0 1

===== CHANNEL f1 =====
 SFO1 75.4878687 MHz
 NUC1 13C
 P1 15.00 usec
 PLW1 15.00000000 W
 ===== CHANNEL f2 =====
 SFO2 300.1812007 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 10.00000000 W
 PLW12 0.20853998 W
 PLW13 0.10495000 W

F2 - Processing parameters
 SI 32768
 SF 75.4803210 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Spectra 23. ¹³C-NMR spectra of compound 3h

Data File: C:\LabSolutions\Data\Analiz\Derya\UMB-10_29.lcd

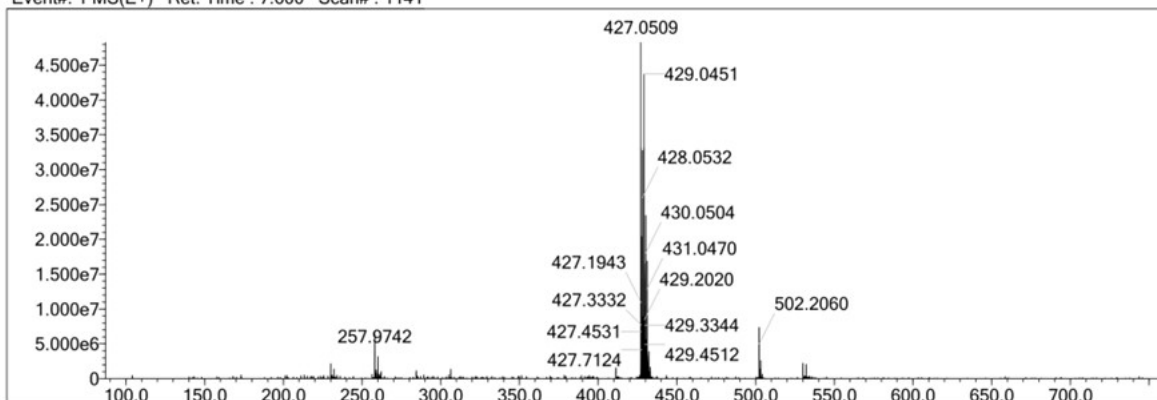
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	5	35	O	2	0	0	S	2	0	2	Ru	2	0	0	H
C	4	9	35	F	1	0	0	Cl	1	0	2	Pd	2	0	0	
N	3	4	8	P	3	0	0	Br	1	0	0	I	3	0	0	

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

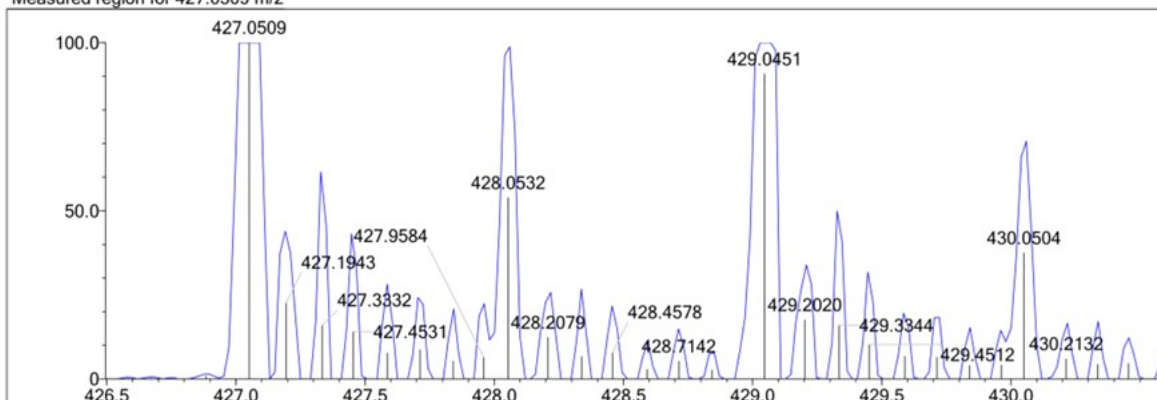
DBE Range: 8.0 - 19.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: yes
 Isotope Res: 9000
 Max Results: 50

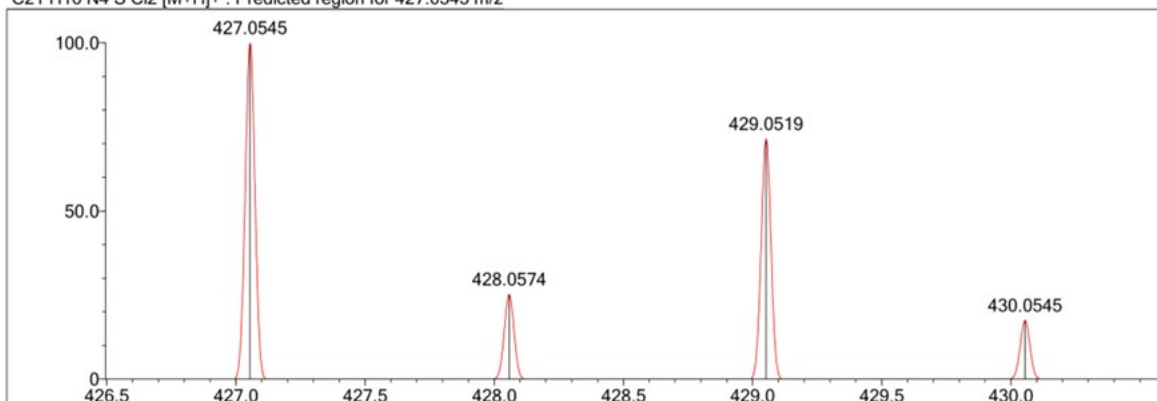
Event#: 1 MS(E+) Ret. Time : 7.600 Scan#: 1141



Measured region for 427.0509 m/z

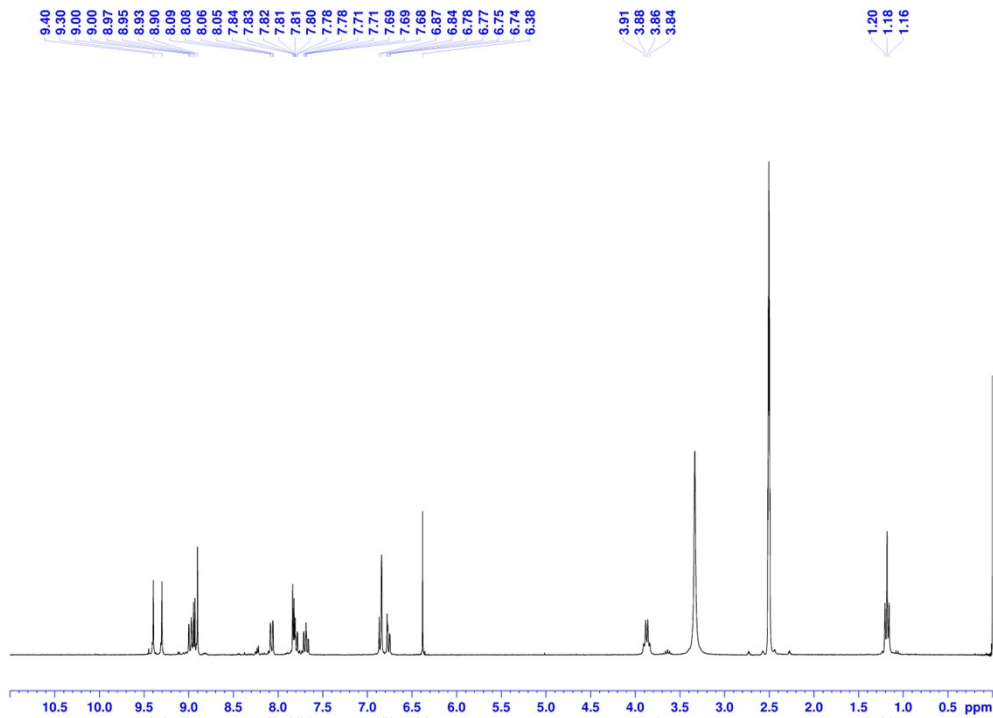


C21 H16 N4 S Cl2 [M+H]⁺ : Predicted region for 427.0545 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	20.23	C21 H16 N4 S Cl2	[M+H] ⁺	427.0509	427.0545	-3.6	-8.43	36.31	15.0

Spectra 24. HRMS spectra of compound 3h



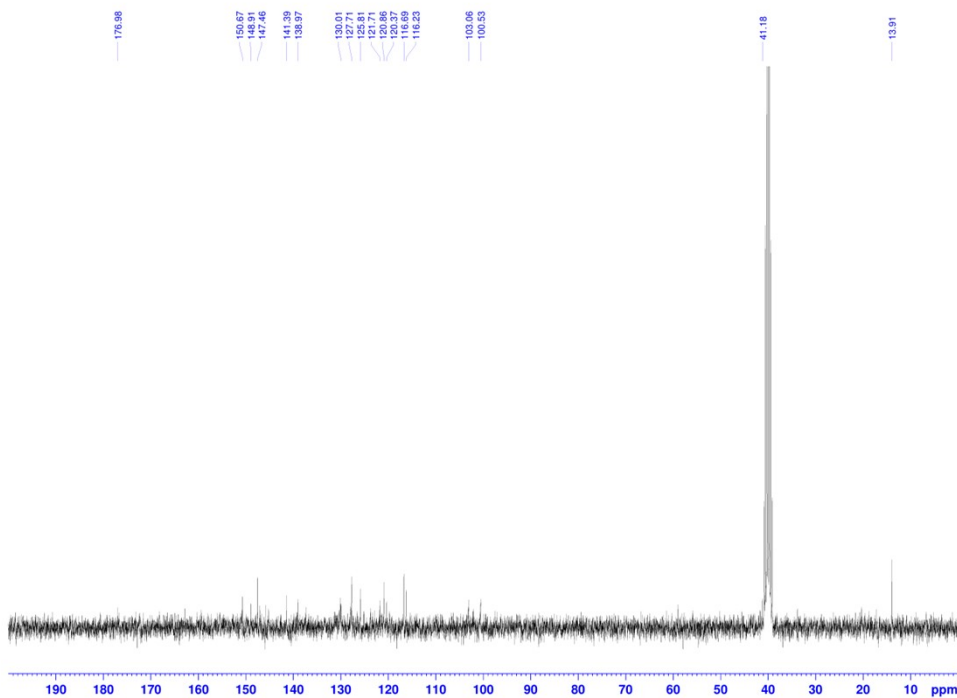
Current Data Parameters
 NAME: UMB-11-Mayys
 EXPNO: 3
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20250515
 Time: 11.17
 INSTRUM: FOURIER300
 PROBHD: 5 mm DUL 13C-1
 PULPROG: zg
 TD: 16384
 SOLVENT: DMSO
 NS: 16
 DS: 0
 SWH: 6103.516 Hz
 FIDRES: 0.372529 Hz
 AQ: 1.3421773 sec
 RG: 59.8758
 DW: 81.920 usec
 DE: 6.50 usec
 TE: 297.0 K
 D1: 3.00000000 sec
 TDO: 1

===== CHANNEL f1 =====
 SFO1: 300.1818337 MHz
 NUC1: 1H
 P1: 13.00 usec
 PLW1: 10.00000000 W

F2 - Processing parameters
 SI: 6536
 SF: 300.1799991 MHz
 WDW: EM
 SSB: 0
 LB: 0.30 Hz
 GB: 0
 PC: 1.00

Spectra 25. ¹H-NMR spectra of compound 3i



Current Data Parameters
 NAME: UMB-11-Mayys
 EXPNO: 4
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20250515
 Time: 11.19
 INSTRUM: FOURIER300
 PROBHD: 5 mm DUL 13C-1
 PULPROG: zgpg
 TD: 32768
 SOLVENT: DMSO
 NS: 2048
 DS: 4
 SWH: 24414.062 Hz
 FIDRES: 0.745058 Hz
 AQ: 0.6710886 sec
 RG: 501.187
 DW: 20.480 usec
 DE: 6.50 usec
 TE: 296.9 K
 D1: 1.00000000 sec
 D11: 0.03000000 sec
 D31: 0.00015000 sec
 D32: 0.89999998 sec
 D40: 0.00093990 sec
 L4: 23
 L5: 26
 P32: 90.00 usec
 TDO: 1

===== CHANNEL f1 =====
 SFO1: 75.4878687 MHz
 NUC1: 13C
 P1: 15.00 usec
 PLW1: 15.00000000 W

===== CHANNEL f2 =====
 SFO2: 300.1812007 MHz
 NUC2: 1H
 CPDPRG2: waltz16
 PCPD2: 90.00 usec
 PLW2: 10.00000000 W
 PLW12: 0.20863999 W
 PLW13: 0.10495000 W

F2 - Processing parameters
 SI: 32768
 SF: 75.4803210 MHz
 WDW: EM
 SSB: 0
 LB: 1.00 Hz
 GB: 0
 PC: 1.40

Spectra 26. ¹³C-NMR spectra of compound 3i

Data File: C:\LabSolutions\Data\Analiz\Derya\UMB-11_30.lcd

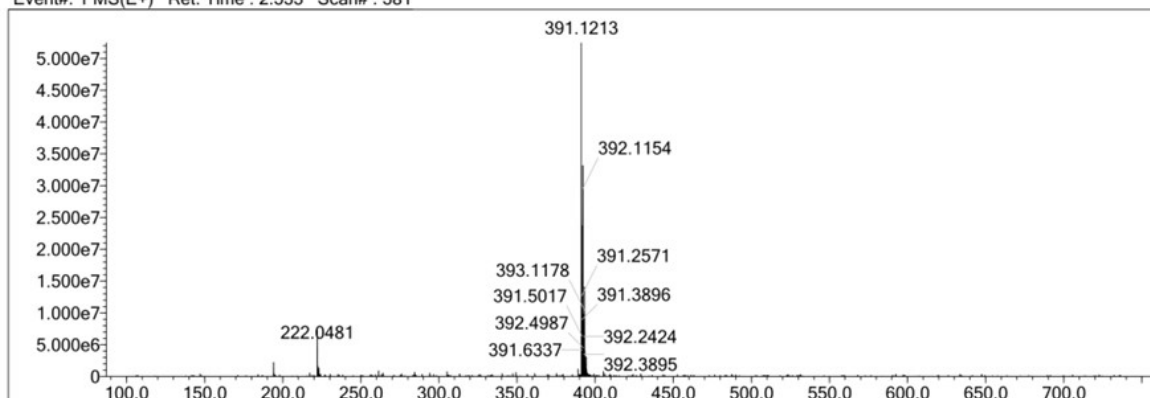
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	5	35	O	2	2	2	S	2	0	2	Ru	2	0	0	H
C	4	9	35	F	1	0	0	Cl	1	0	2	Pd	2	0	0	
N	3	4	8	P	3	0	0	Br	1	0	0	I	3	0	0	

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

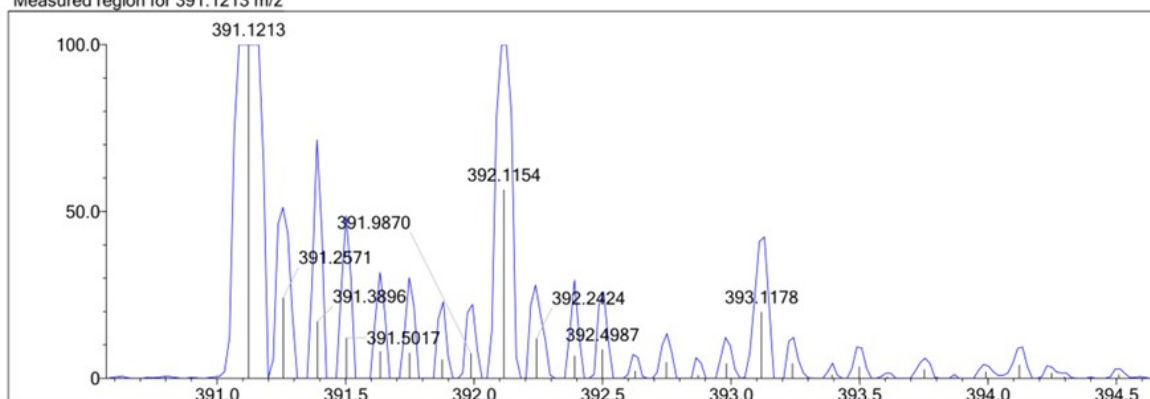
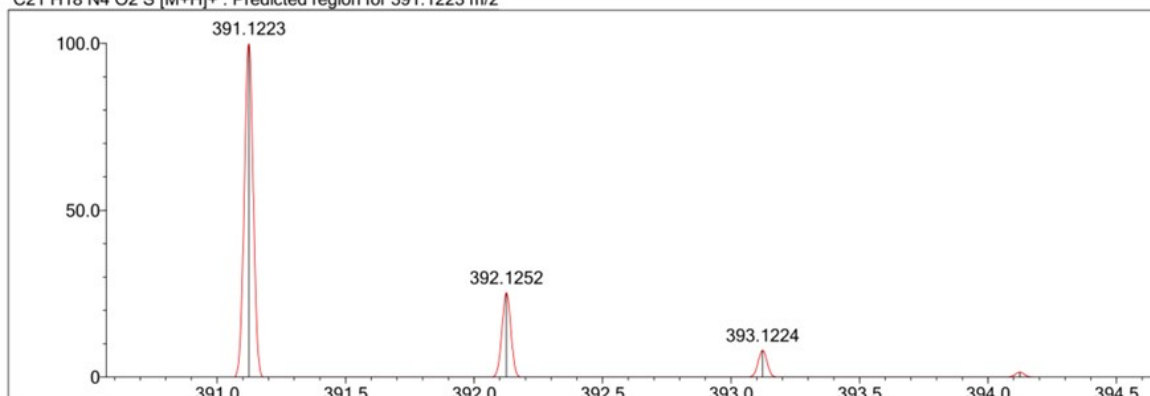
DBE Range: 8.0 - 19.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: yes
 Isotope Res: 9000
 Max Results: 50

Event#: 1 MS(E+) Ret. Time : 2.533 Scan#: 381

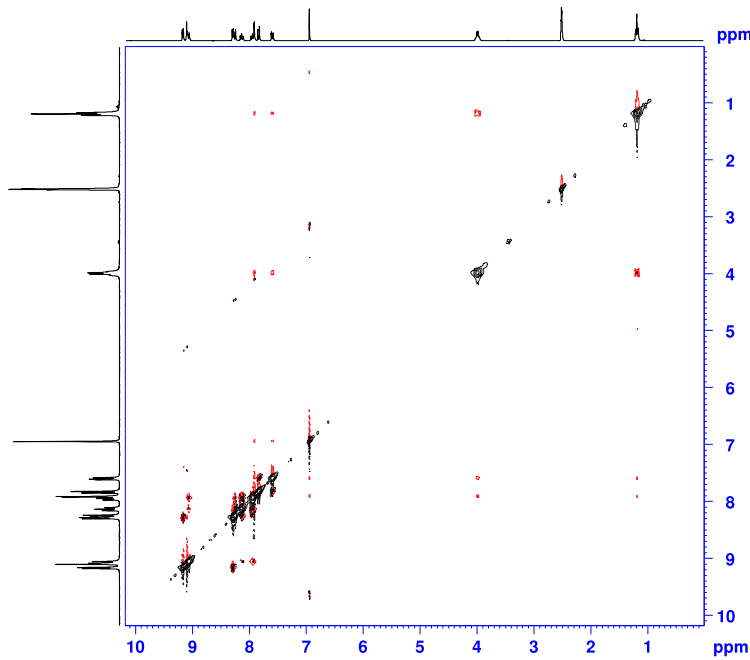


Measured region for 391.1213 m/z

C21 H18 N4 O2 S [M+H]⁺ : Predicted region for 391.1223 m/z

Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	30.03	C21 H18 N4 O2 S	[M+H] ⁺	391.1213	391.1223	-1.0	-2.56	31.25	15.0

Spectra 27. HRMS spectra of compound 3i



```
Current Data Parameters
NAME      UMB-10
EXFNO    22
PROCNO    1

F2 - Acquisition Parameters
Date_     20250218
Time      23.14
INSTRUM   FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG   noesyph
TD         2048
SOLVENT   DMSO
NS         64
DS         4
SWH        3051.758 Hz
FIDRES    1.490116 Hz
AQ         0.3355443 sec
RG         39.767
DE         163.840 usec
TE         299.9 K
D0         0.00014725 sec
D1         1.97304797 sec
D8         0.20000001 sec
D33        0.00016380 sec
INO        0.00032760 sec

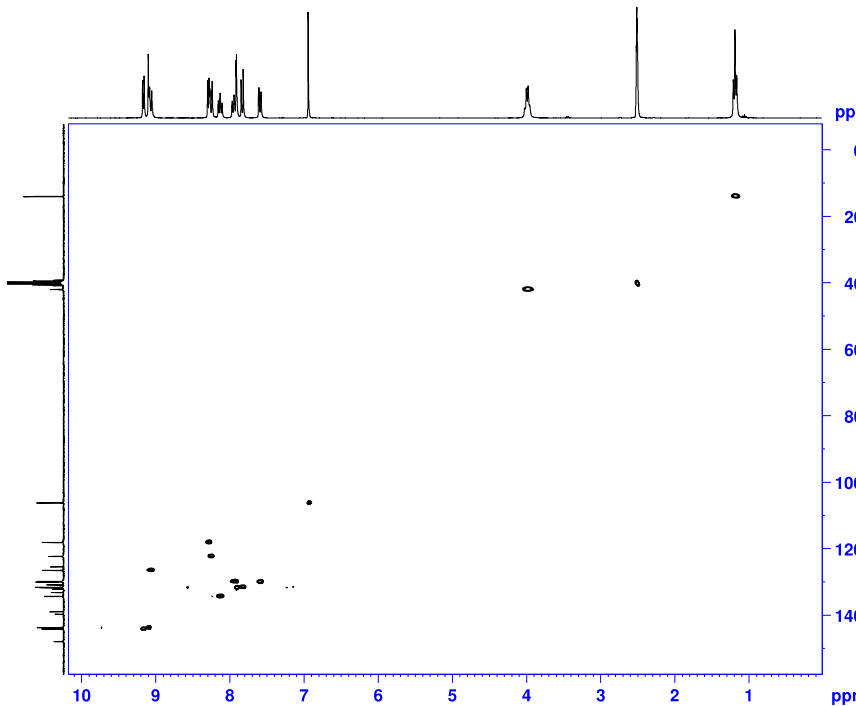
===== CHANNEL f1 =====
SF01      300.1815269 MHz
NUC1      1H
P1         13.00 usec
PLW1      10.00000000 W

F1 - Acquisition parameters
TD         256
SF01      300.1815 MHz
FIDRES    11.923941 Hz
SW        10.183 ppm
FMODE     TPPI

F2 - Processing parameters
SI         1024
SF         300.1799969 MHz
WDW        QSINE
SSB        2
LB         0 Hz
GB         0
FC         1.00

F1 - Processing parameters
SI         1024
MC2        TPPI
SF         300.1799969 MHz
WDW        QSINE
SSB        2
LB         0 Hz
GB         0
```

Spectra 28. NOESY spectra of compound 3i



```
Current Data Parameters
NAME      UMB-10
EXFNO    21
PROCNO    1

F2 - Acquisition Parameters
Date_     20250218
Time      23.14
INSTRUM   FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG   hsqcph3
TD         2048
SOLVENT   DMSO
NS         64
DS         4
SWH        3051.758 Hz
FIDRES    1.490116 Hz
AQ         0.3355443 sec
RG         39.767
DE         163.840 usec
TE         299.9 K
D0         0.00014725 sec
D1         1.97304797 sec
D8         0.20000001 sec
D33        0.00016380 sec
INO        0.00032760 sec

===== CHANNEL f1 =====
SF01      300.1815269 MHz
NUC1      1H
P1         13.00 usec
PLW1      10.00000000 W

===== CHANNEL f2 =====
SF02      125.7603500 MHz
NUC2      13C
P2         13.00 usec
PLW2      10.00000000 W

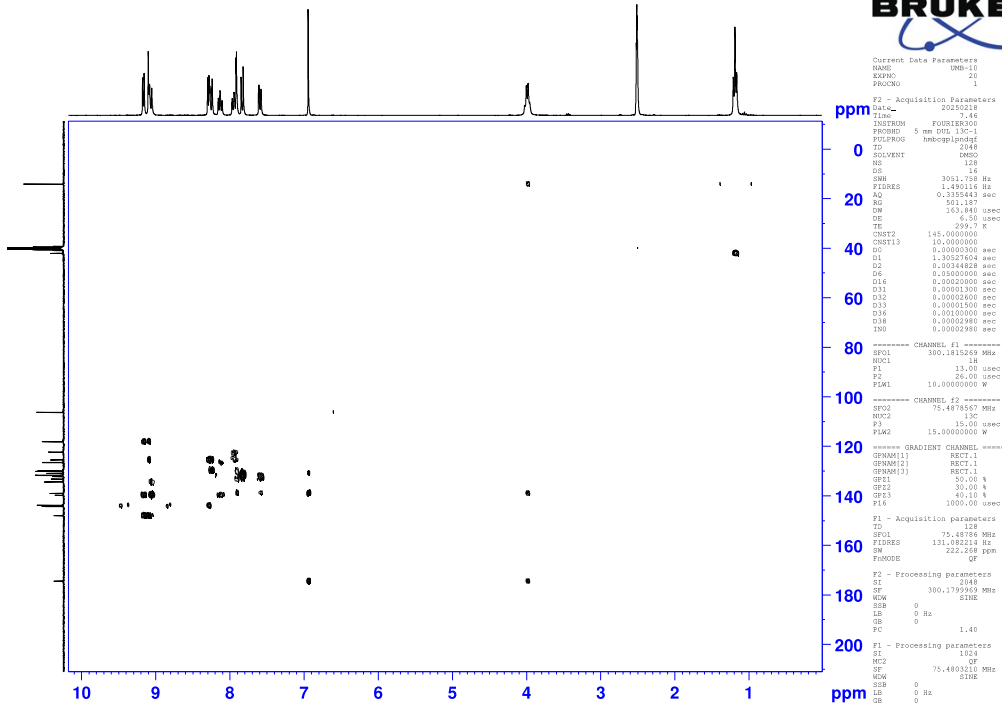
===== GRADIENT CHANNEL =====
GRNAM[1]  GR11
GRNAM[2]  GR12
GRNAM[3]  GR13
GR11      80.00 u
GR12      20.14 u
GR13      1000.00 usec

F1 - Acquisition parameters
TD         256
SF01      300.1815 MHz
FIDRES    11.923941 Hz
SW        10.183 ppm
FMODE     TPPI

F2 - Processing parameters
SI         1024
SF         300.1799969 MHz
WDW        QSINE
SSB        2
LB         0 Hz
GB         0
FC         1.00

F1 - Processing parameters
SI         1024
MC2        TPPI
SF         300.1799969 MHz
WDW        QSINE
SSB        2
LB         0 Hz
GB         0
```

Spectra 29. HSQC spectra of compound 3i



Spectra 30. HMBC spectra of compound 3i