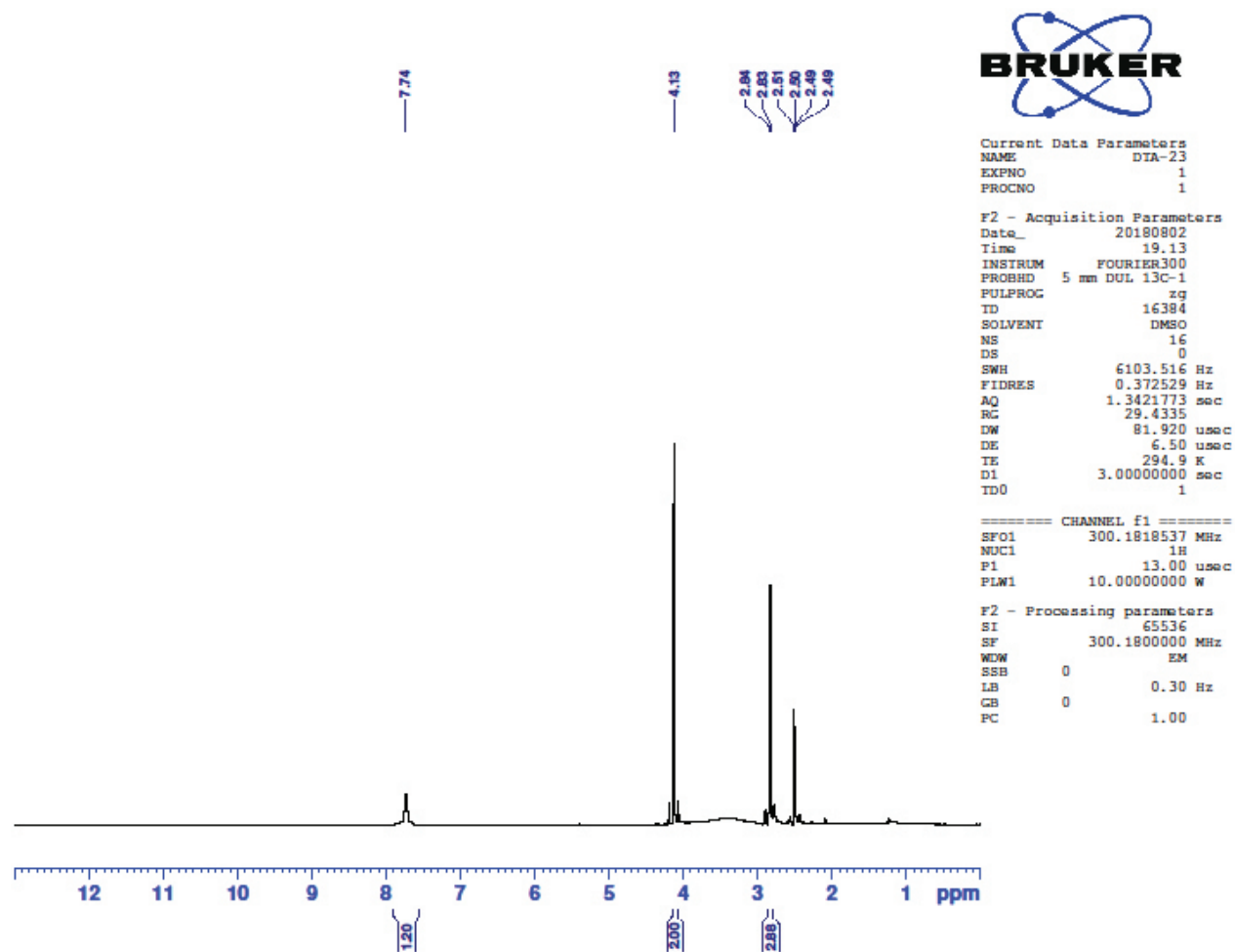
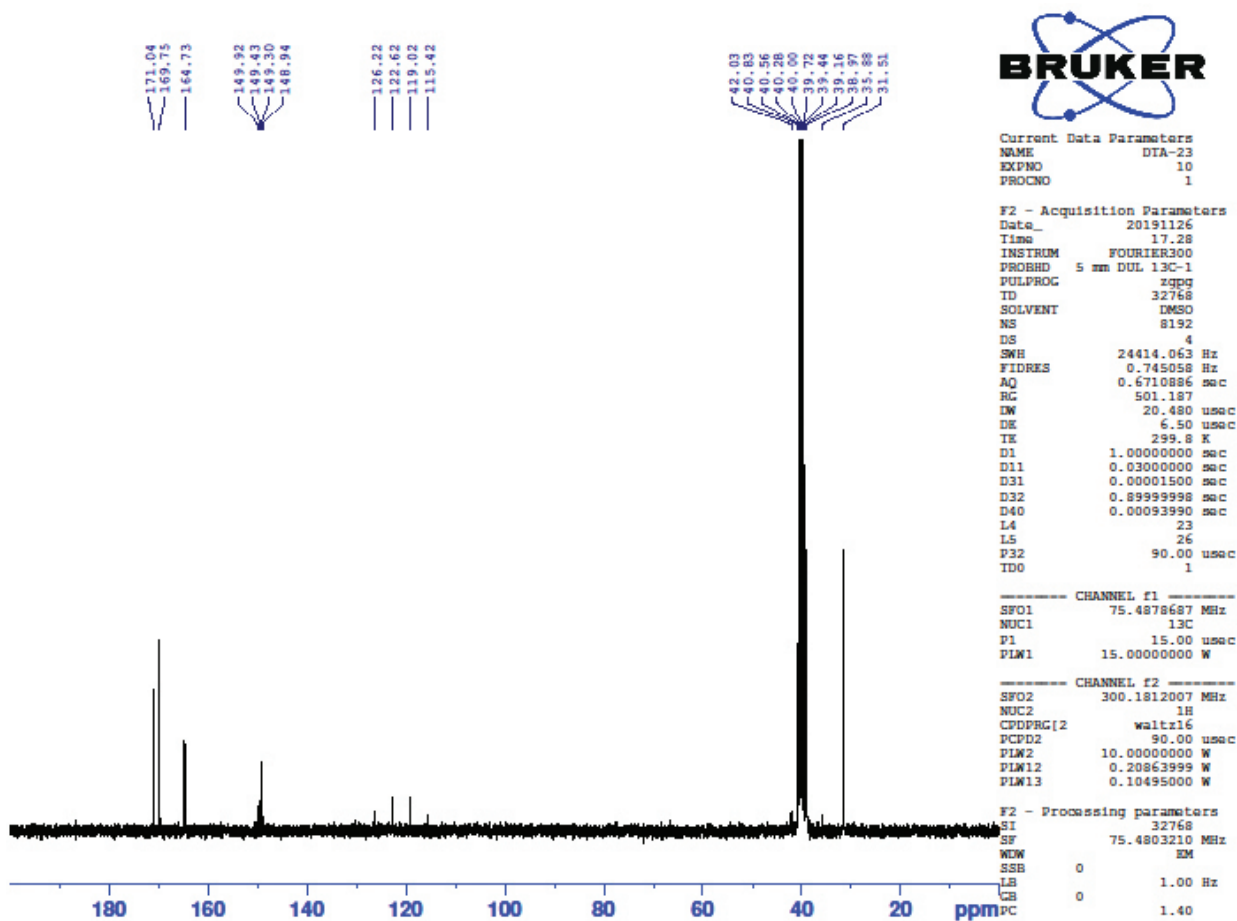


Supporting Information

Spectrum 1. ^1H -NMR spectrum of compound 4a.

Spectrum 2. ¹³C-NMR spectrum of compound 4a.

Formula Predictor Report - dta-23_1.lcd

Page 1 of 1

Data File: C:\LabSolutions\Data\Analz\deriv\dta-23_1.lcd

Elmt	Val	Min	Max	Elmt	Val	Min	Max	Elmt	Val	Min	Max	Elmt	Val	Min	Max	Use Adduct
H	1	6	15	O	2	0	6	S	2	3	3	Ru	2	0	0	H
C	4	8	15	F	1	3	3	Cl	1	0	0	Pd	2	0	0	
N	3	0	6	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: 5.0 - 20.0

Apply N Rule: yes

Isotope RI (%): 1.00

MSn Logic Mode: AND

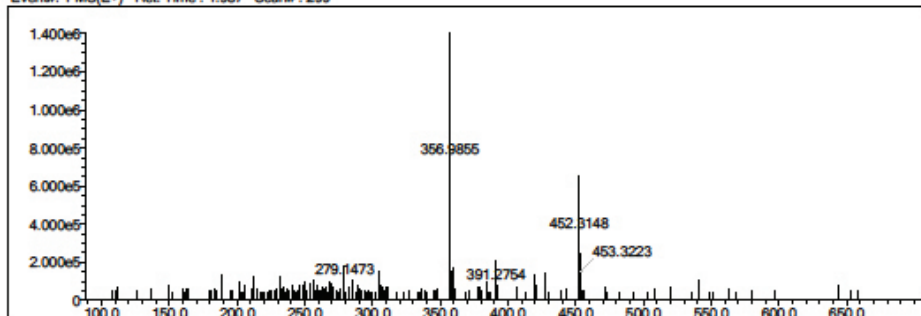
Electron Ions: both

Use MSn Info: yes

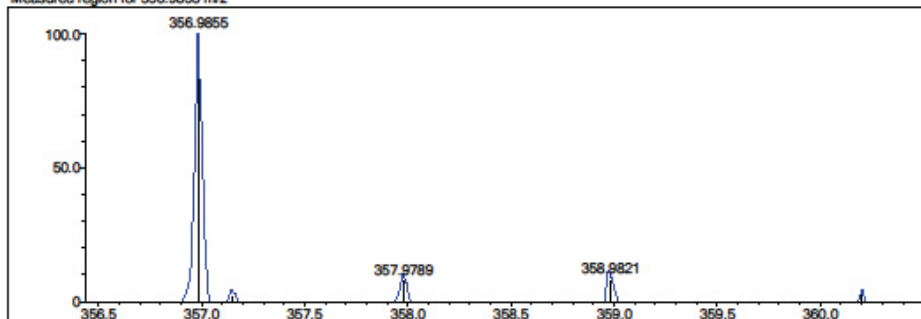
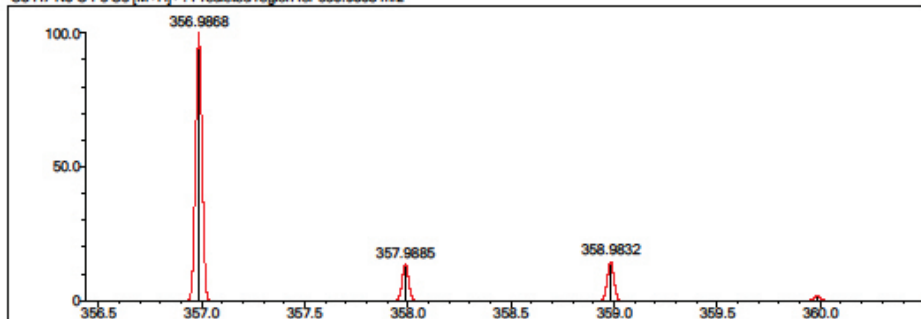
Isotope Res: 9000

Max Results: 100

Event#: 1 MS(E+) Ret. Time: 1.987 Scan#: 299

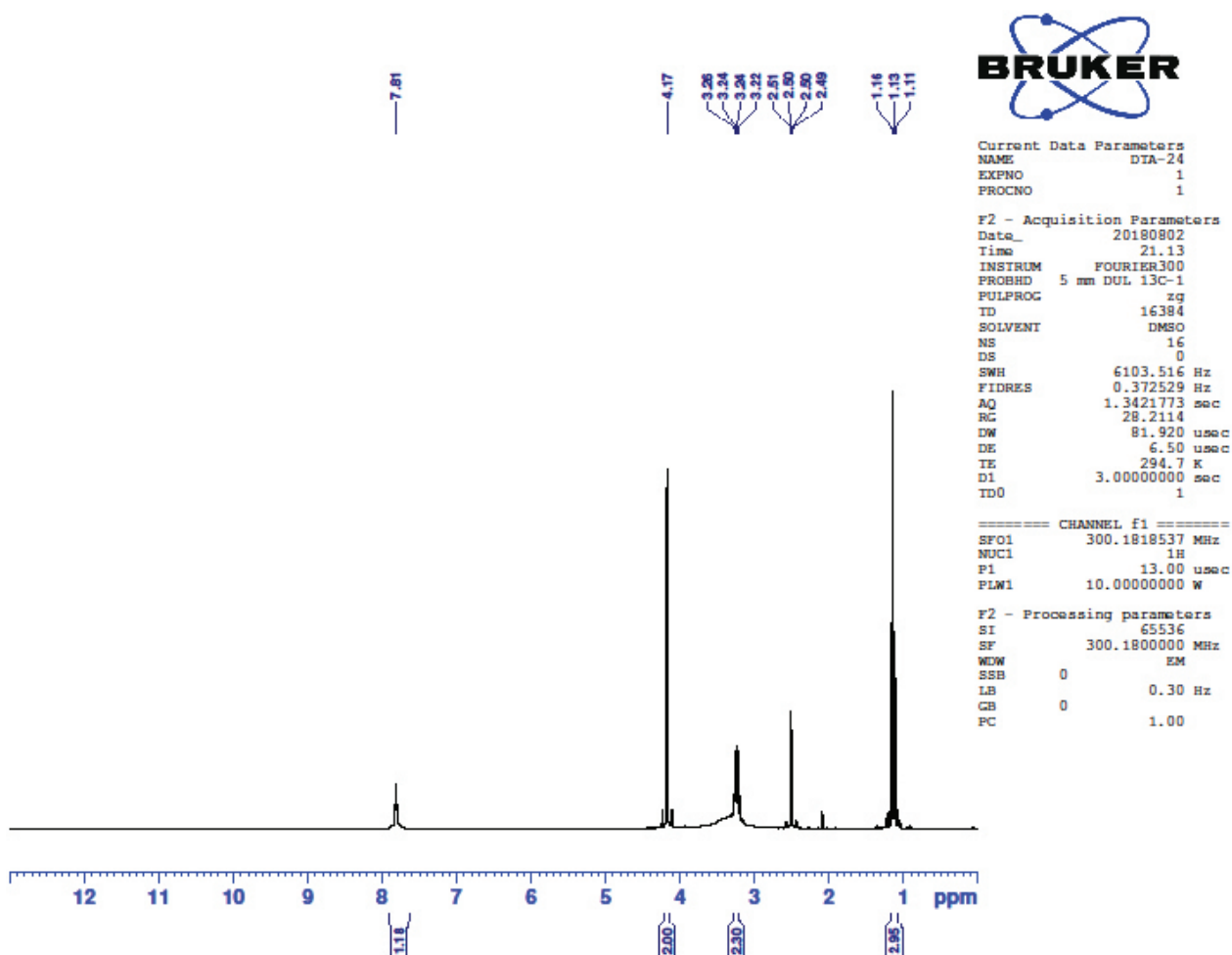


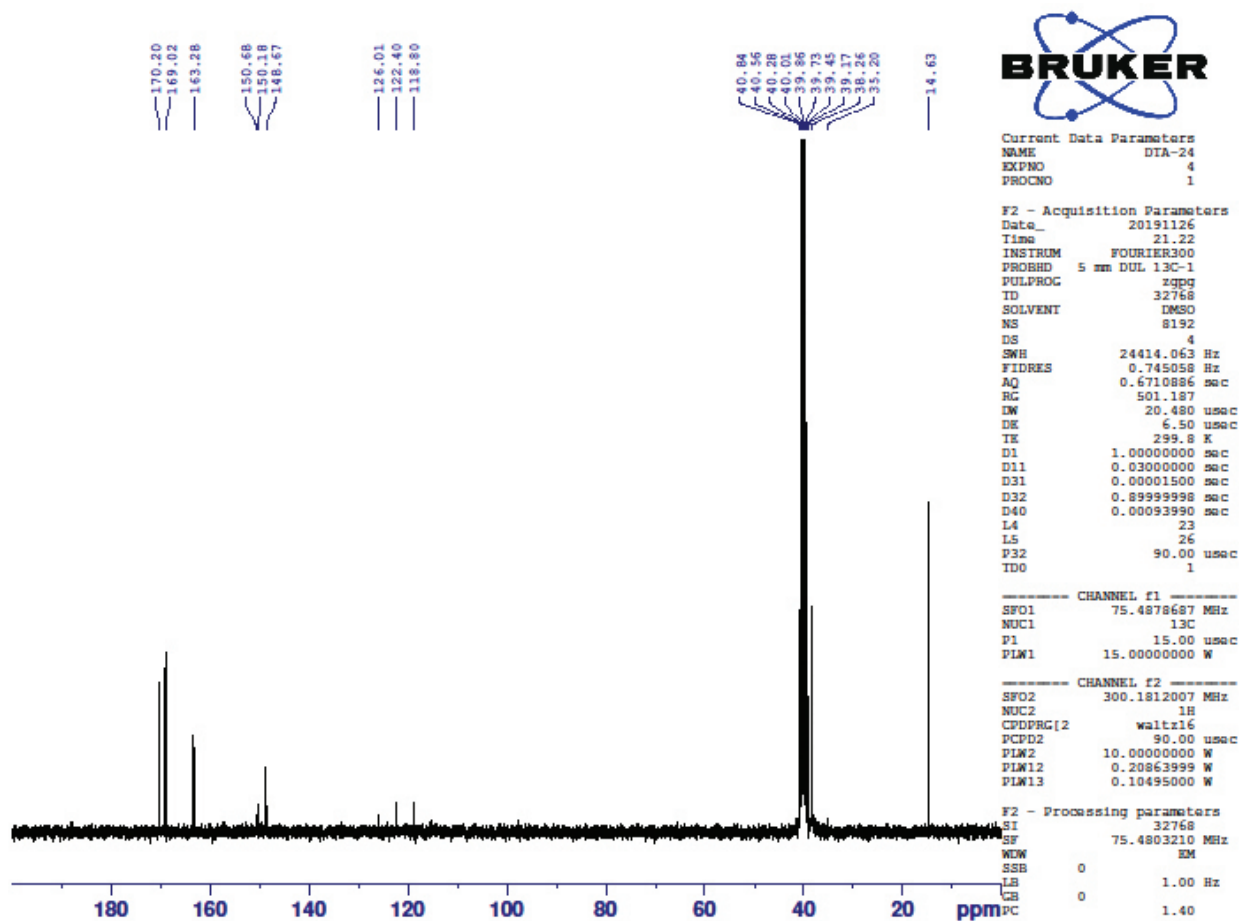
Measured region for 356.9855 m/z

C8 H7 N6 O F3 S3 [M+H]⁺: Predicted region for 356.9868 m/z

Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	36.66	C8 H7 N6 O F3 S3	[M+H] ⁺	356.9855	356.9868	-1.3	-3.64	39.26	7.0

Spectrum 3. HRMS spectrum of compound 4a.

Spectrum 4. ^1H -NMR spectrum of compound **4b**.

Spectrum 5. ^{13}C -NMR spectrum of compound 4b.

Formula Predictor Report - dta-24_2.lcd

Page 1 of 1

Data File: C:\LabSolutions\Data\Analysis\dery\dta-24_2.lcd

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

Error Margin (ppm): 6

HC Ratio: unlimited

Max Isotopes: 3

MSn Iso RI (%): 10.00

DBE Range: 5.0 - 20.0

Apply N Rule: yes

Isotope RI (%): 1.00

MSn Logic Mode: AND

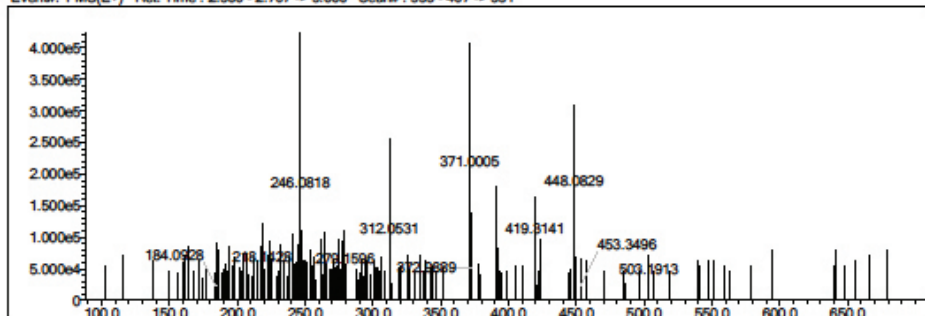
Electron Ions: both

Use MSn Info: yes

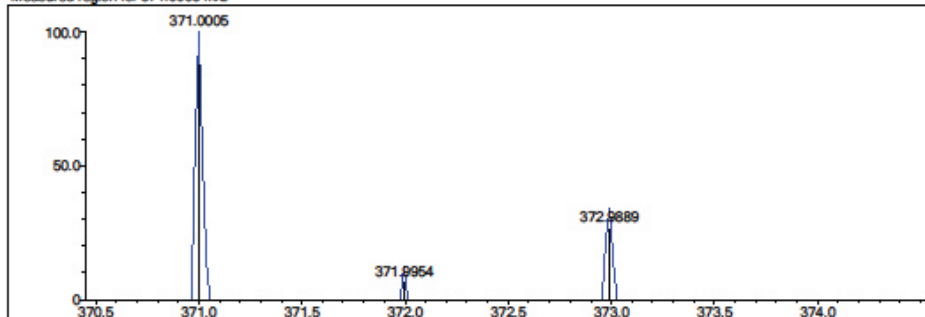
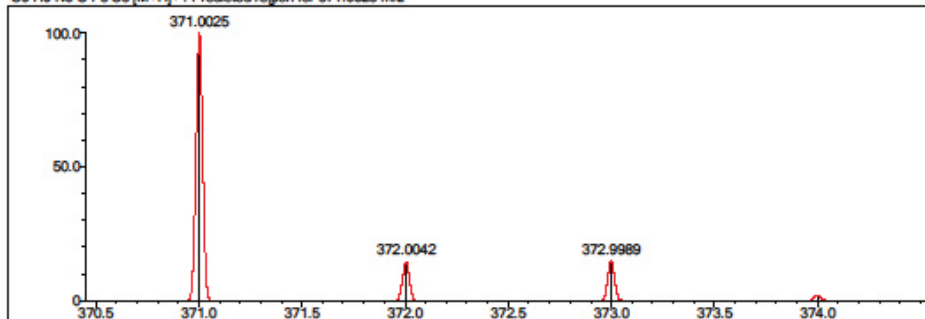
Isotope Res: 9000

Max Results: 100

Event#: 1 MS(E+) Ret. Time : 2.360 - 2.707 -> 3.666 Scan#: 355 - 407 -> 551

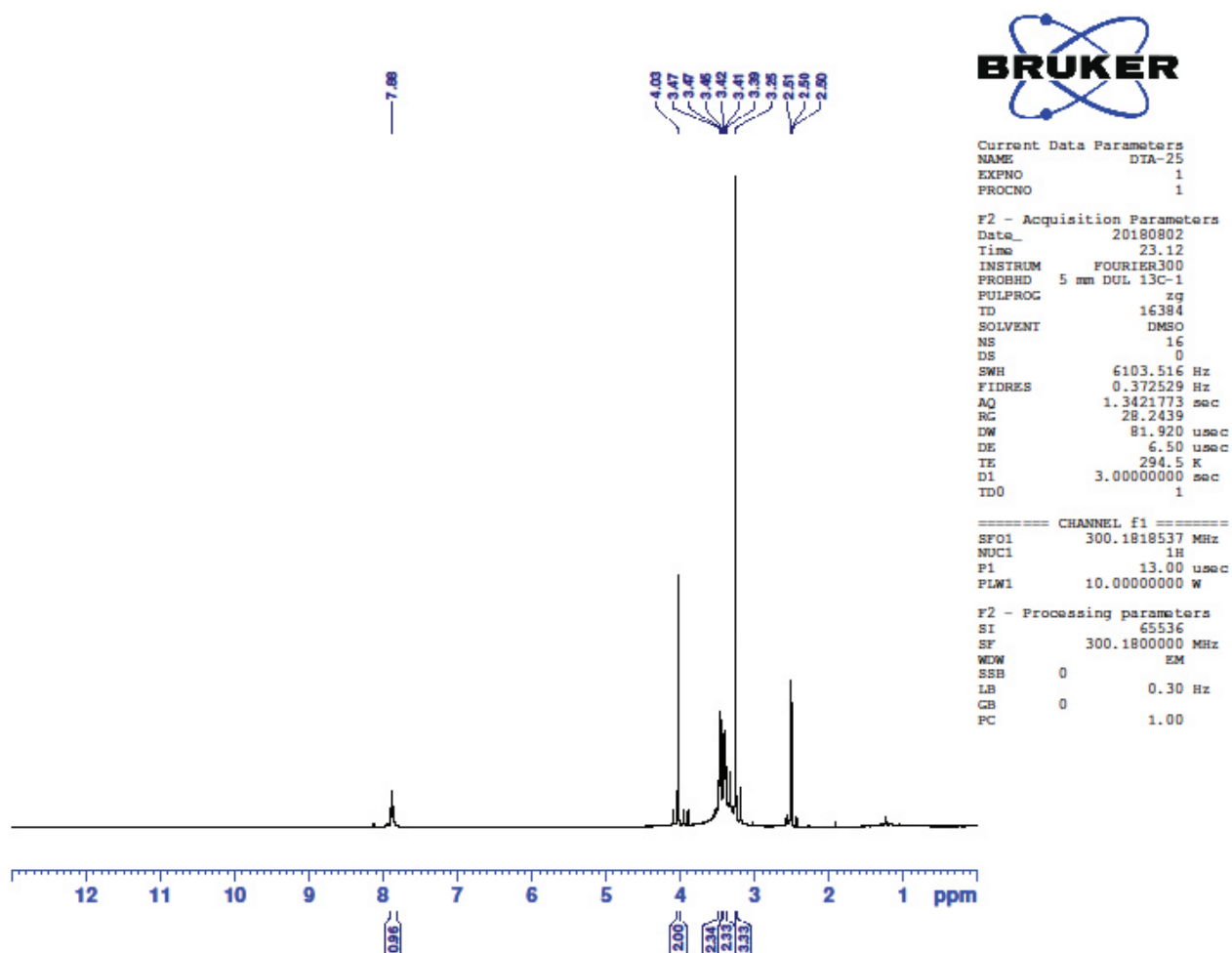


Measured region for 371.0005 m/z

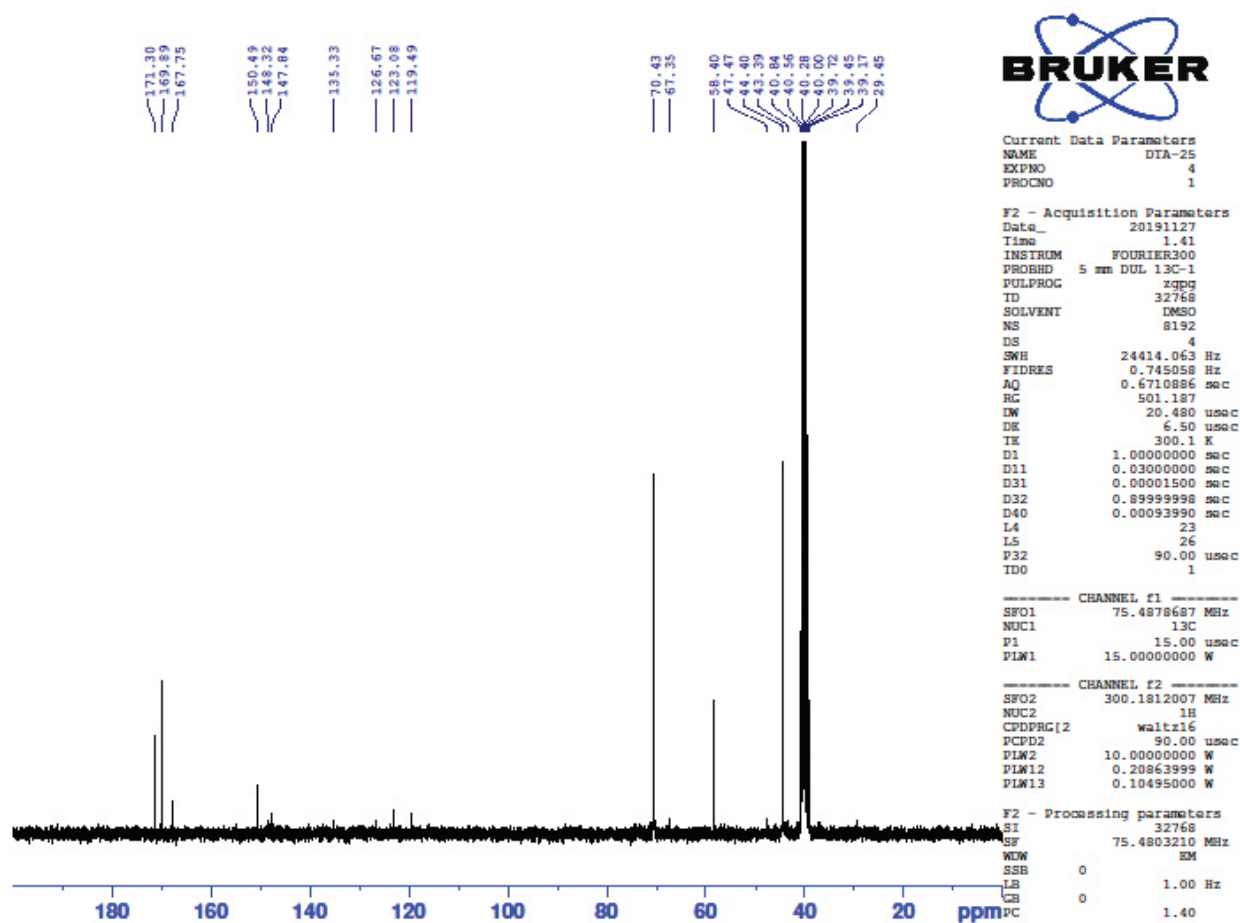
C9 H9 N6 O F3 S3 [M+H]⁺ : Predicted region for 371.0025 m/z

Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	29.48	C9 H9 N6 O F3 S3	[M+H] ⁺	371.0005	371.0025	-2.0	-5.39	34.24	7.0

Spectrum 6. HRMS spectrum of compound 4b.



Spectrum 7. ^1H -NMR spectrum of compound **4c**.

Spectrum 8. ¹³C-NMR spectrum of compound 4c.

Formula Predictor Report - dts-25_3.lcd

Page 1 of 1

Data File: C:\LabSolutions\Data\Analz\deriv\dt-25_3.lcd

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

Error Margin (ppm): 6

DBE Range: 5.0 - 20.0

Electron Ions: both

HC Ratio: unlimited

Apply N Rule: yes

Use MSn Info: yes

Max Isotopes: 3

Isotope RI (%): 1.00

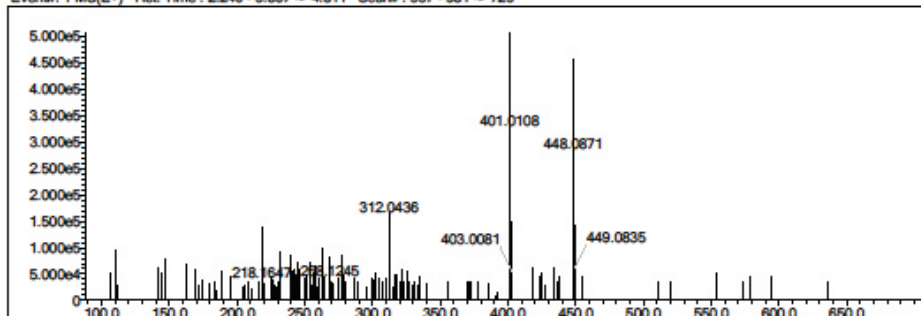
Isotope Res: 9000

MSn Iso RI (%): 10.00

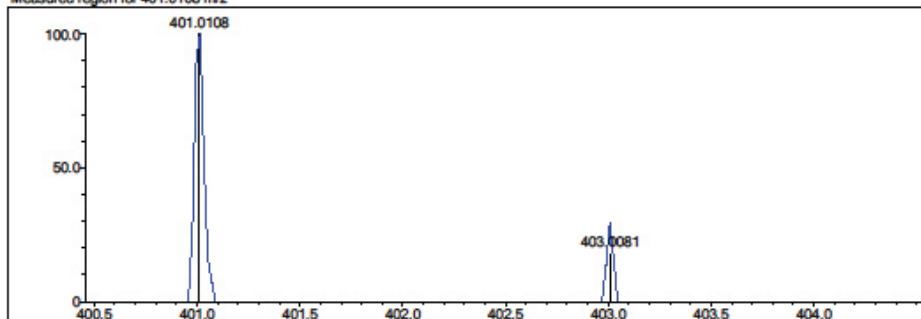
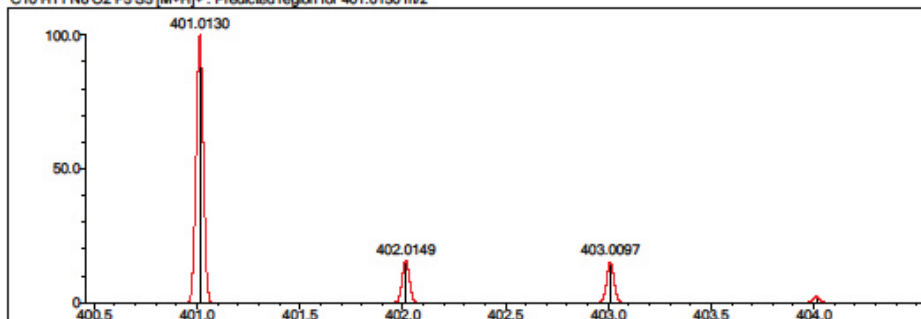
MSn Logic Mode: AND

Max Results: 100

Event#: 1 MS(E+) Ret. Time : 2.240 - 3.867 -> 4.811 Scan#: 337 - 581 -> 723

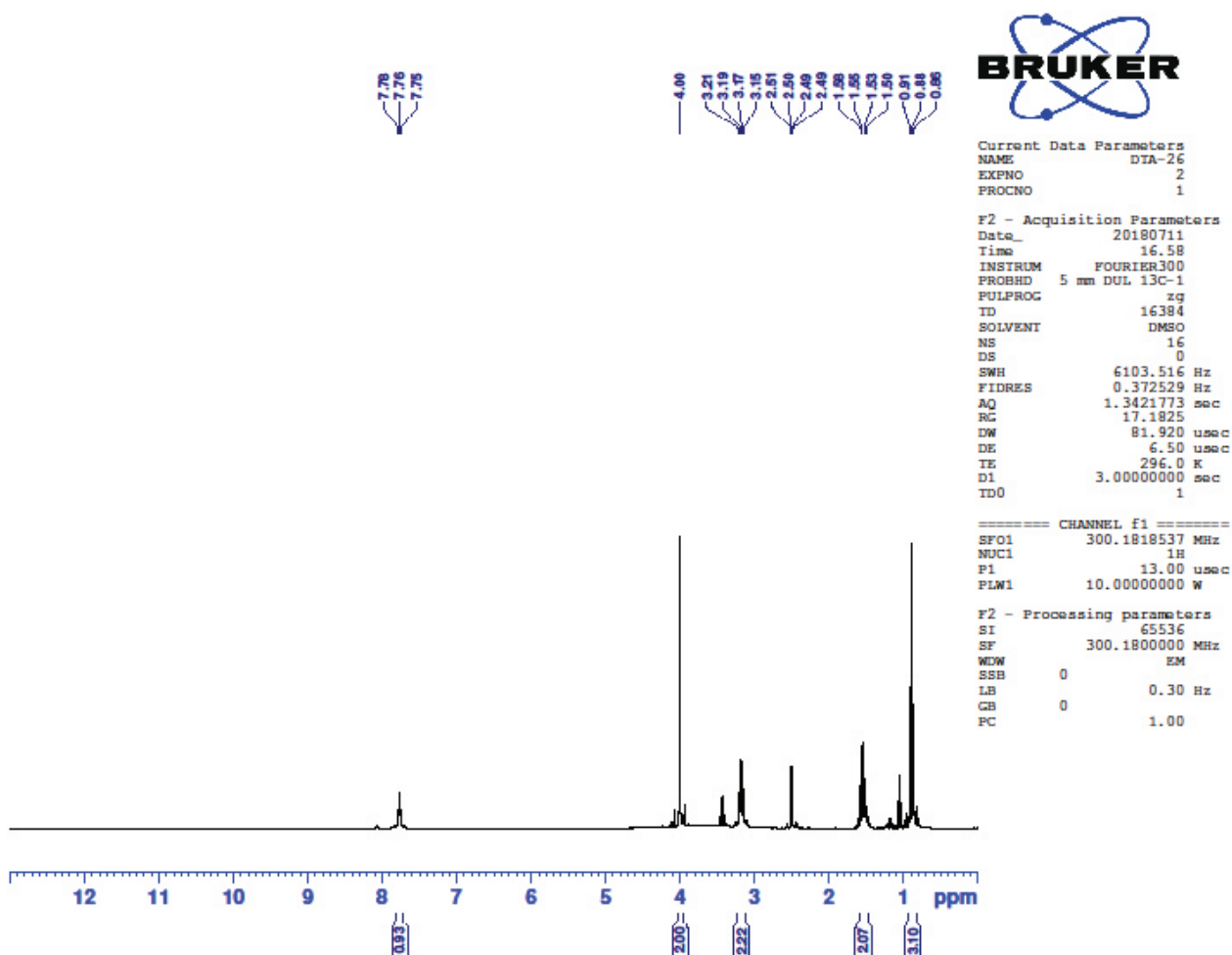


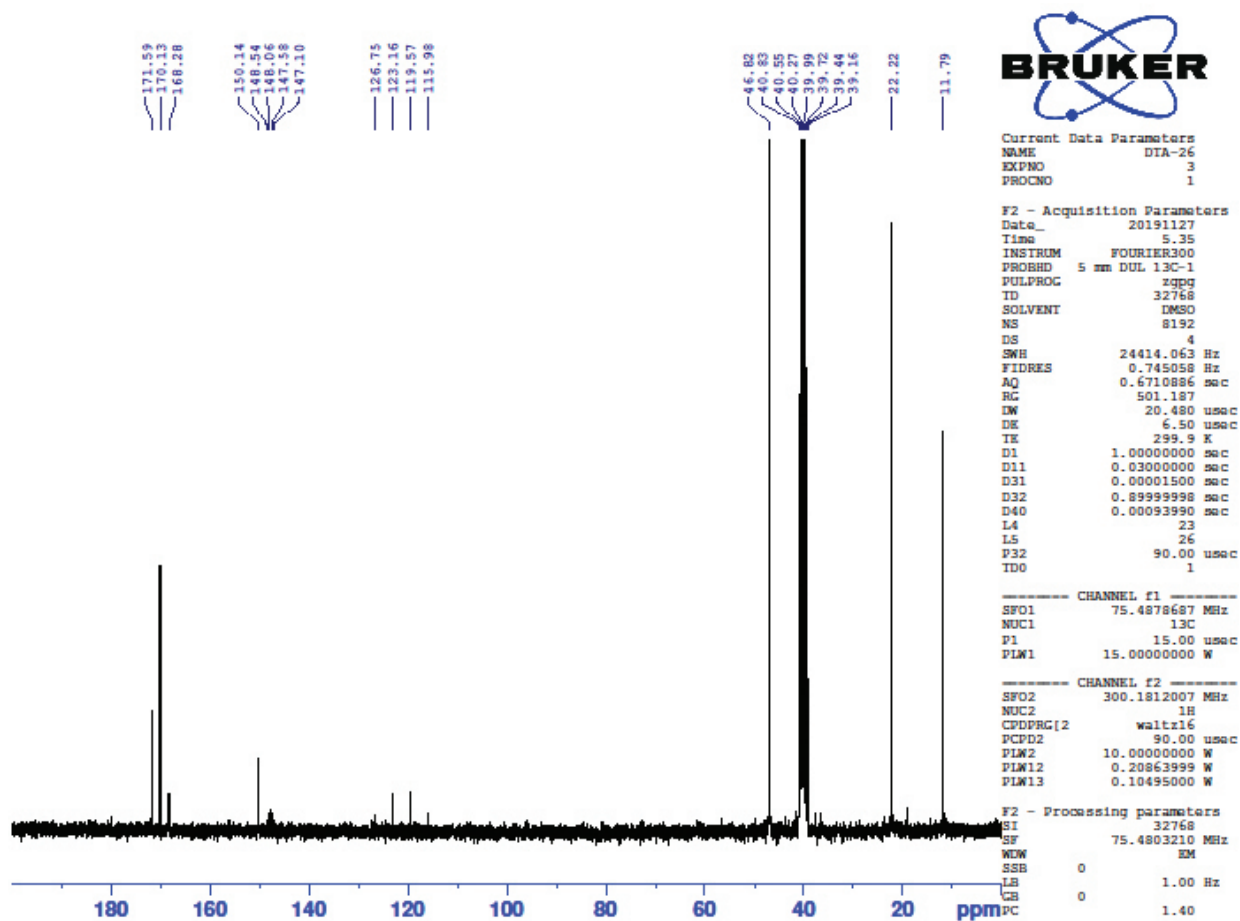
Measured region for 401.0108 m/z

C10 H11 N6 O2 F3 S3 [M+H]⁺ : Predicted region for 401.0130 m/z

Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	52.37	C10 H11 N6 O2 F3 S3	[M+H] ⁺	401.0108	401.0130	-2.2	-5.48	61.53	7.0

Spectrum 9. HRMS spectrum of compound 4c.

Spectrum 10. ^1H -NMR spectrum of compound 4d.

Spectrum 11. ^{13}C -NMR spectrum of compound 4d.

Formula Predictor Report - dta-26_4.lcd

Page 1 of 1

Data File: C:\LabSolutions\Data\Analysis\dery\dta-26_4.lcd

Elmt	Val	Min	Max	Elmt	Val	Min	Max	Elmt	Val	Min	Max	Elmt	Val	Min	Max	Use Adduct
H	1	6	15	O	2	0	6	S	2	3	3	Ru	2	0	0	H
C	4	8	15	F	1	3	3	Cl	1	0	0	Pd	2	0	0	
N	3	0	6	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: 5.0 - 20.0

Apply N Rule: yes

Isotope RI (%): 1.00

MSn Logic Mode: AND

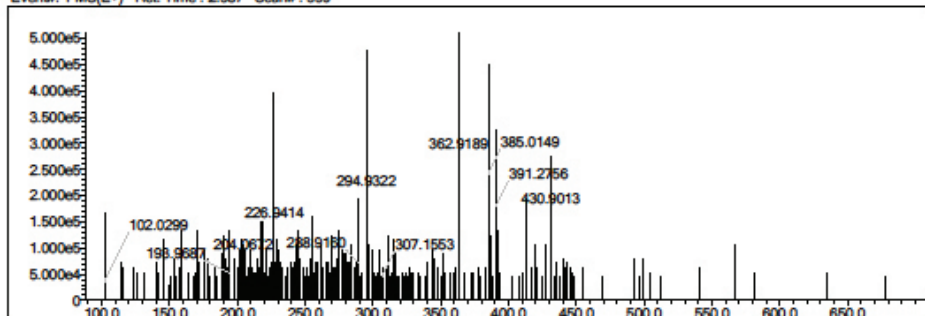
Electron Ions: both

Use MSn Info: yes

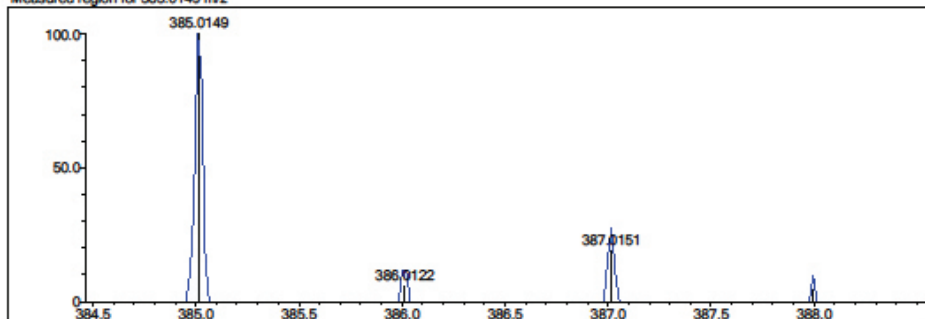
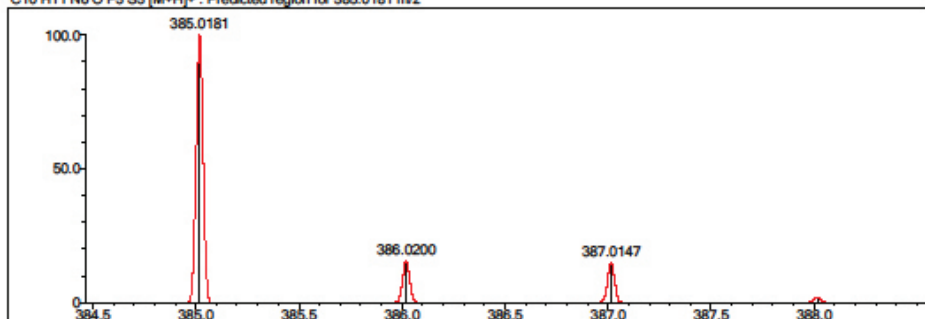
Isotope Res: 9000

Max Results: 100

Event#: 1 MS(E+) Ret. Time : 2.387 Scan#: 359

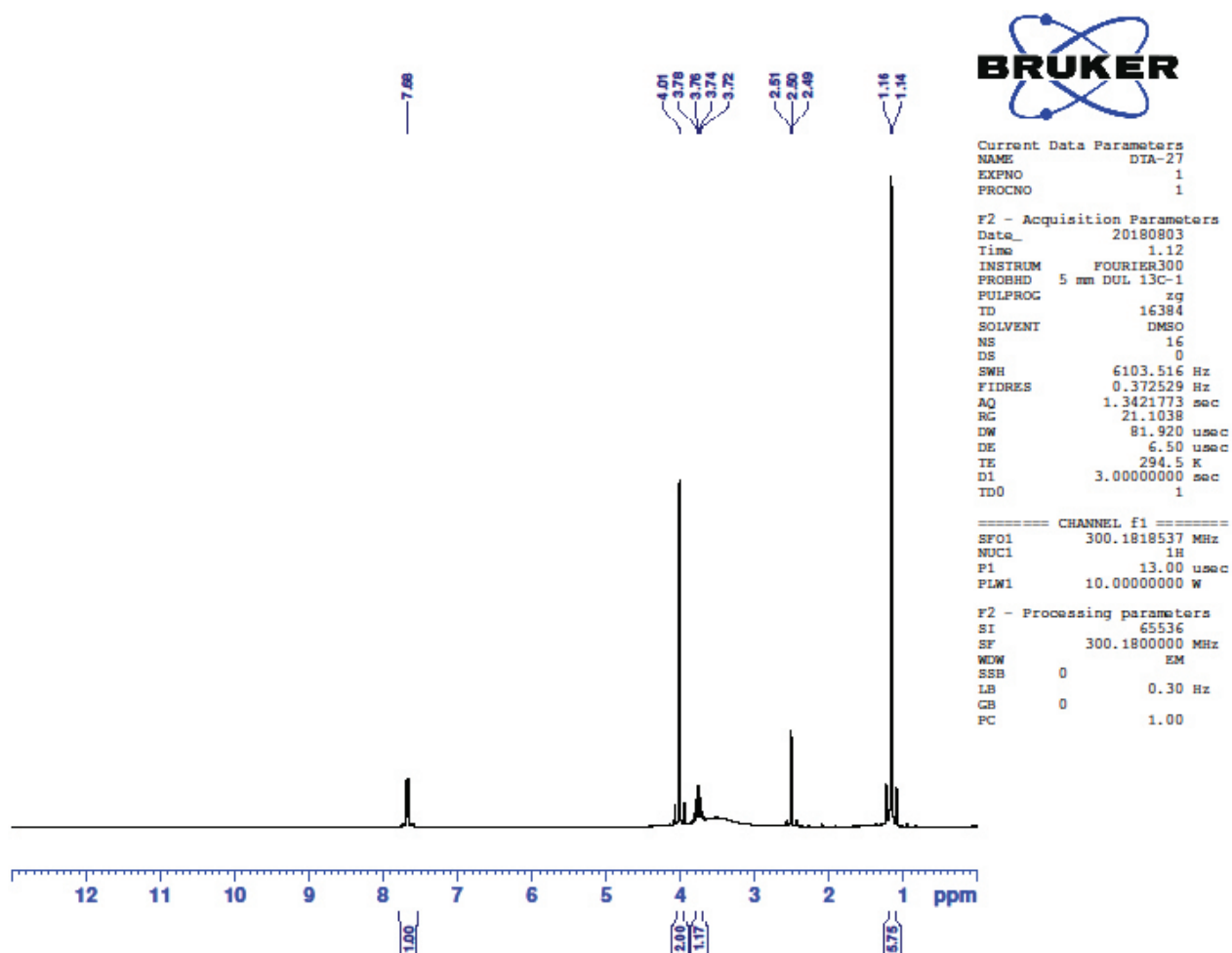


Measured region for 385.0149 m/z

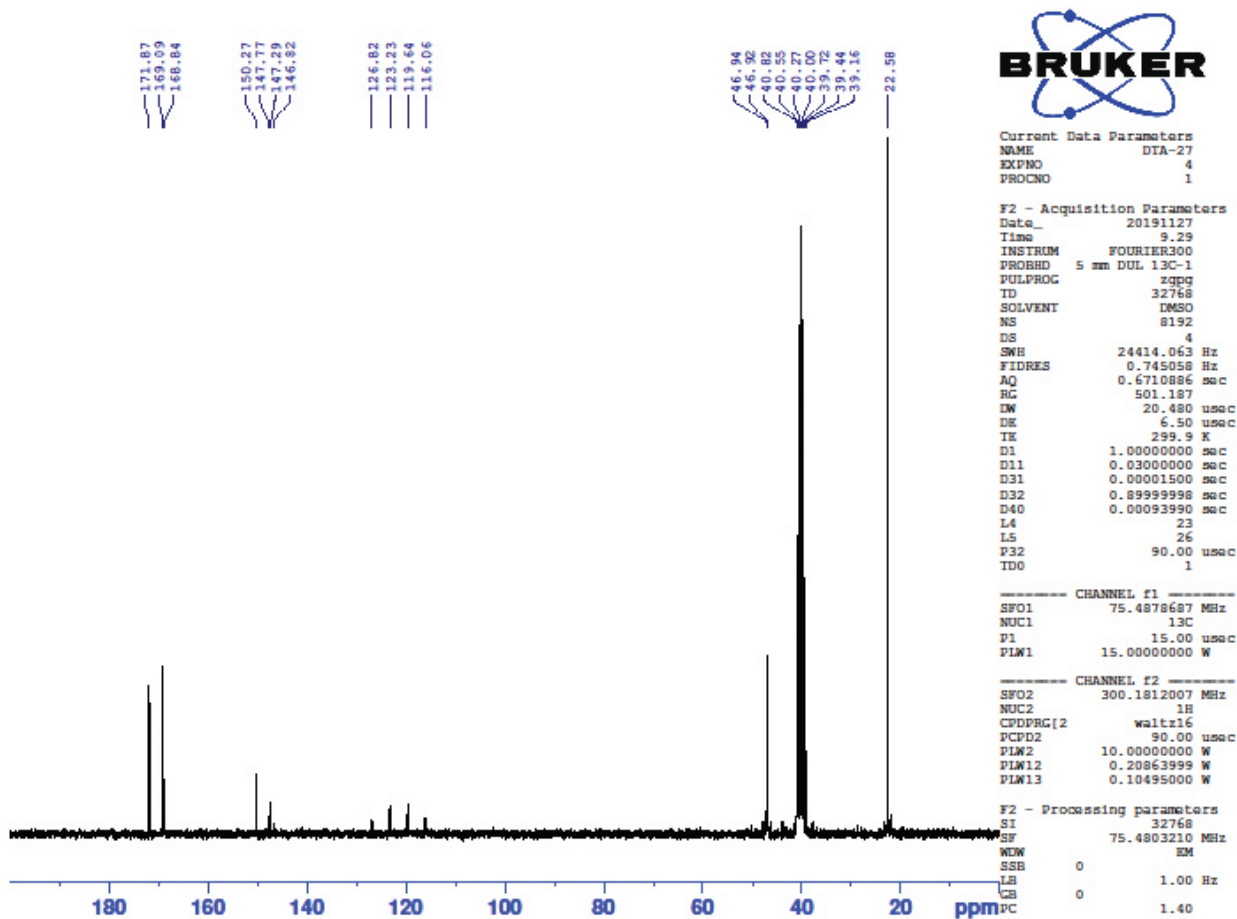
C10 H11 N6 O F3 S3 [M+H]⁺ : Predicted region for 385.0181 m/z

Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	25.49	C10 H11 N6 O F3 S3	[M+H] ⁺	385.0149	385.0181	-3.2	-8.31	44.81	7.0

Spectrum 12. HRMS spectrum of compound 4d.



Spectrum 13. ^1H -NMR spectrum of compound 4e.

Spectrum 14. ^{13}C -NMR spectrum of compound 4e.

Formula Predictor Report - dts-27_5.lcd

Page 1 of 1

Data File: C:\LabSolutions\Data\Analz\deriv\dts-27_5.lcd

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

Error Margin (ppm): 10

DBE Range: 5.0 - 20.0

Electron Ions: both

HC Ratio: unlimited

Apply N Rule: yes

Use MSn Info: yes

Max Isotopes: 3

Isotope RI (%): 1.00

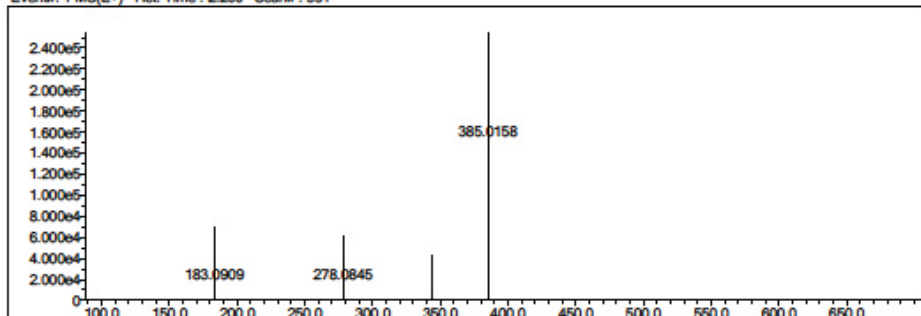
Isotope Res: 9000

MSn Iso RI (%): 10.00

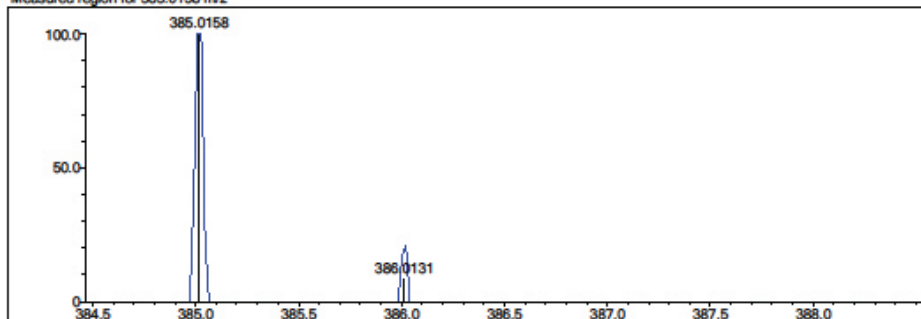
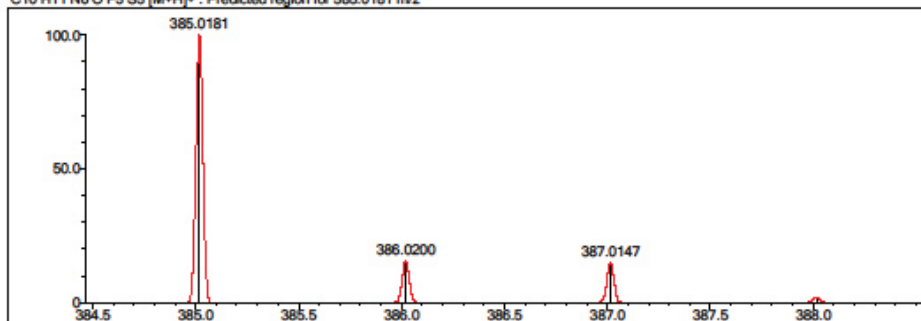
MSn Logic Mode: AND

Max Results: 100

Event#: 1 MS(E+) Ret. Time : 2.200 Scan#: 331

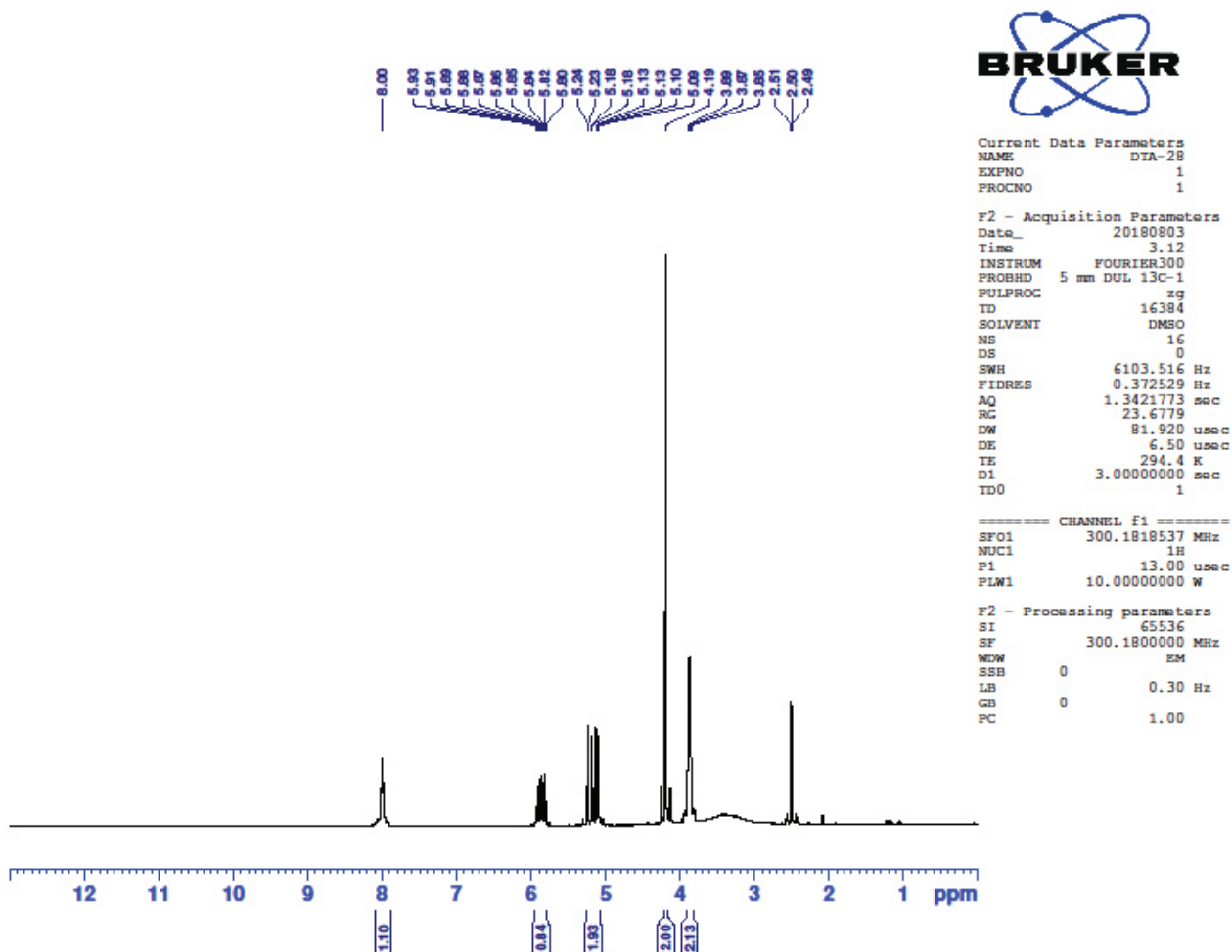


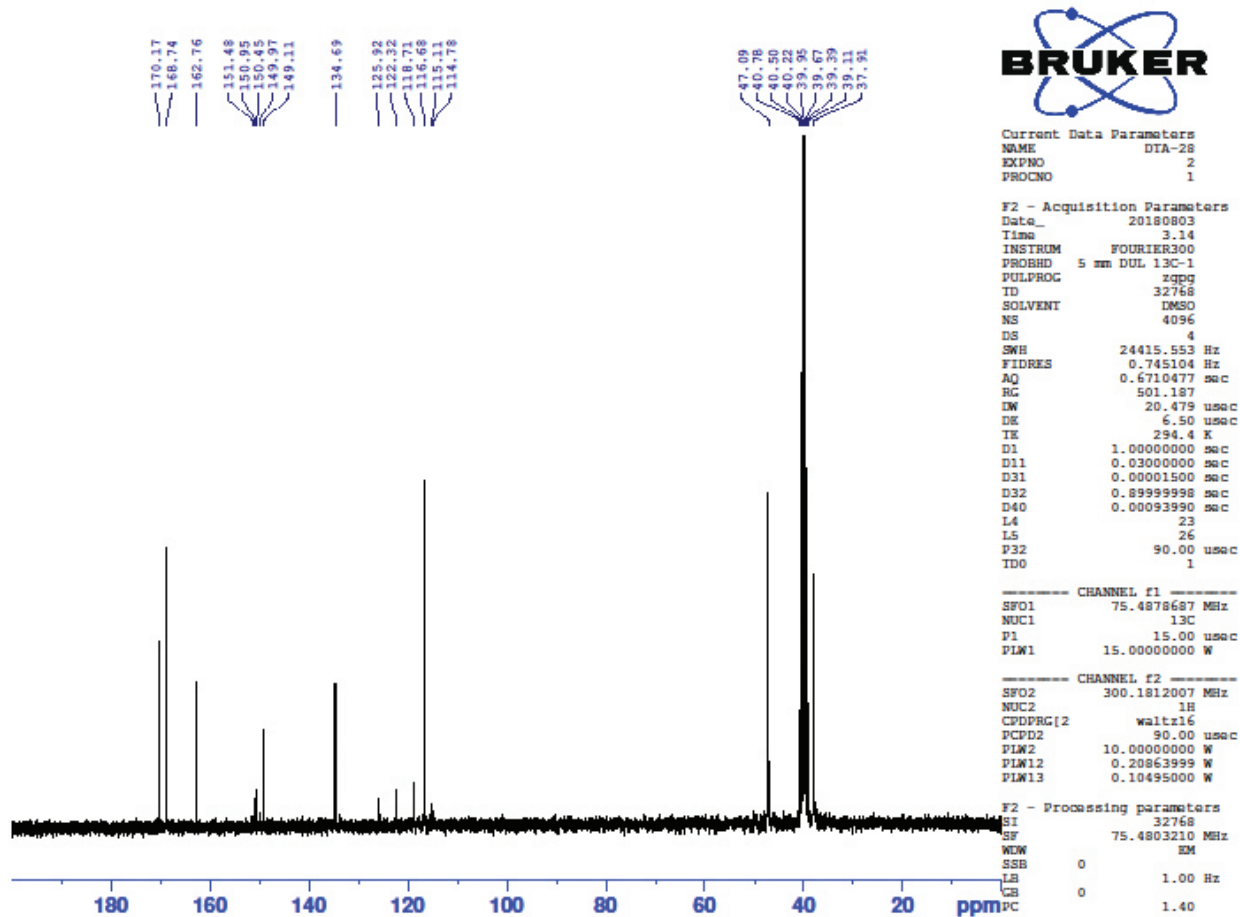
Measured region for 385.0158 m/z

C10 H11 N6 O F3 S3 [M+H]⁺ : Predicted region for 385.0181 m/z

Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	0.00	C10 H11 N6 O F3 S3	[M+H] ⁺	385.0158	385.0181	-2.3	-5.97	0.00	7.0

Spectrum 15. HRMS spectrum of compound 4e.

Spectrum 16. ^1H -NMR spectrum of compound 4f.

Spectrum 17. ^{13}C -NMR spectrum of compound 4f.

Formula Predictor Report - dta-28_6.lcd

Page 1 of 1

Data File: C:\LabSolutions\Data\Analysis\derya\dta-28_6.lcd

Elmt	Val	Min	Max	Elmt	Val	Min	Max	Elmt	Val	Min	Max	Elmt	Val	Min	Max	Use Adduct
H	1	6	15	O	2	0	6	S	2	3	3	Ru	2	0	0	H
C	4	8	15	F	1	3	3	Cl	1	0	0	Pd	2	0	0	
N	3	0	6	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: 5.0 - 20.0

Apply N Rule: yes

Isotope RI (%): 1.00

MSn Logic Mode: AND

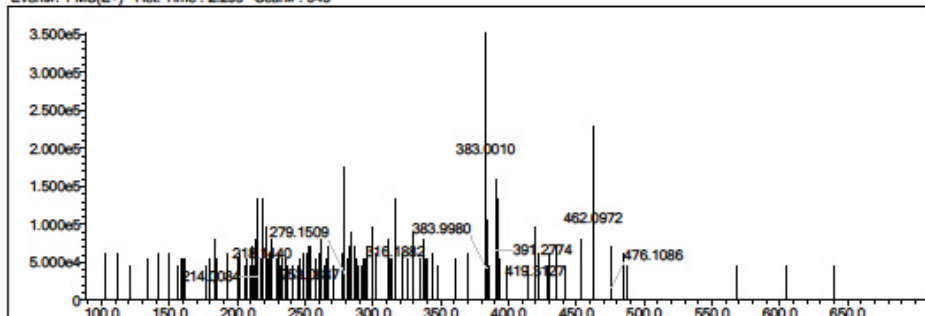
Electron Ions: both

Use MSn Info: yes

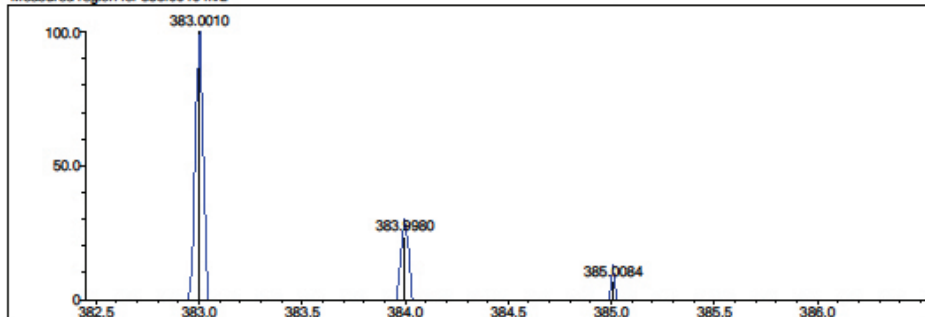
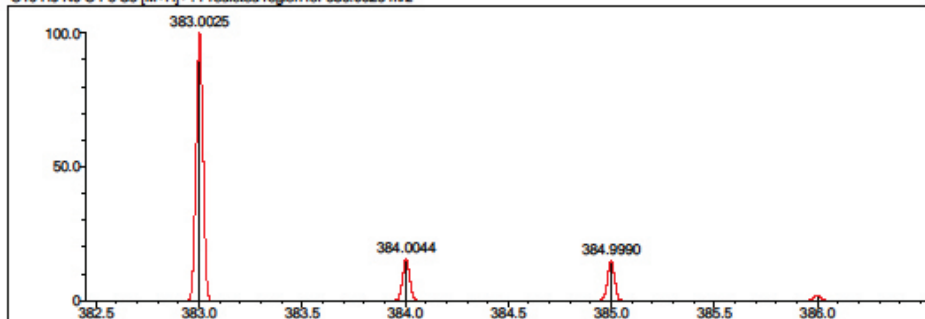
Isotope Res: 9000

Max Results: 100

Event#: 1 MS(E+) Ret. Time : 2.293 Scan#: 345

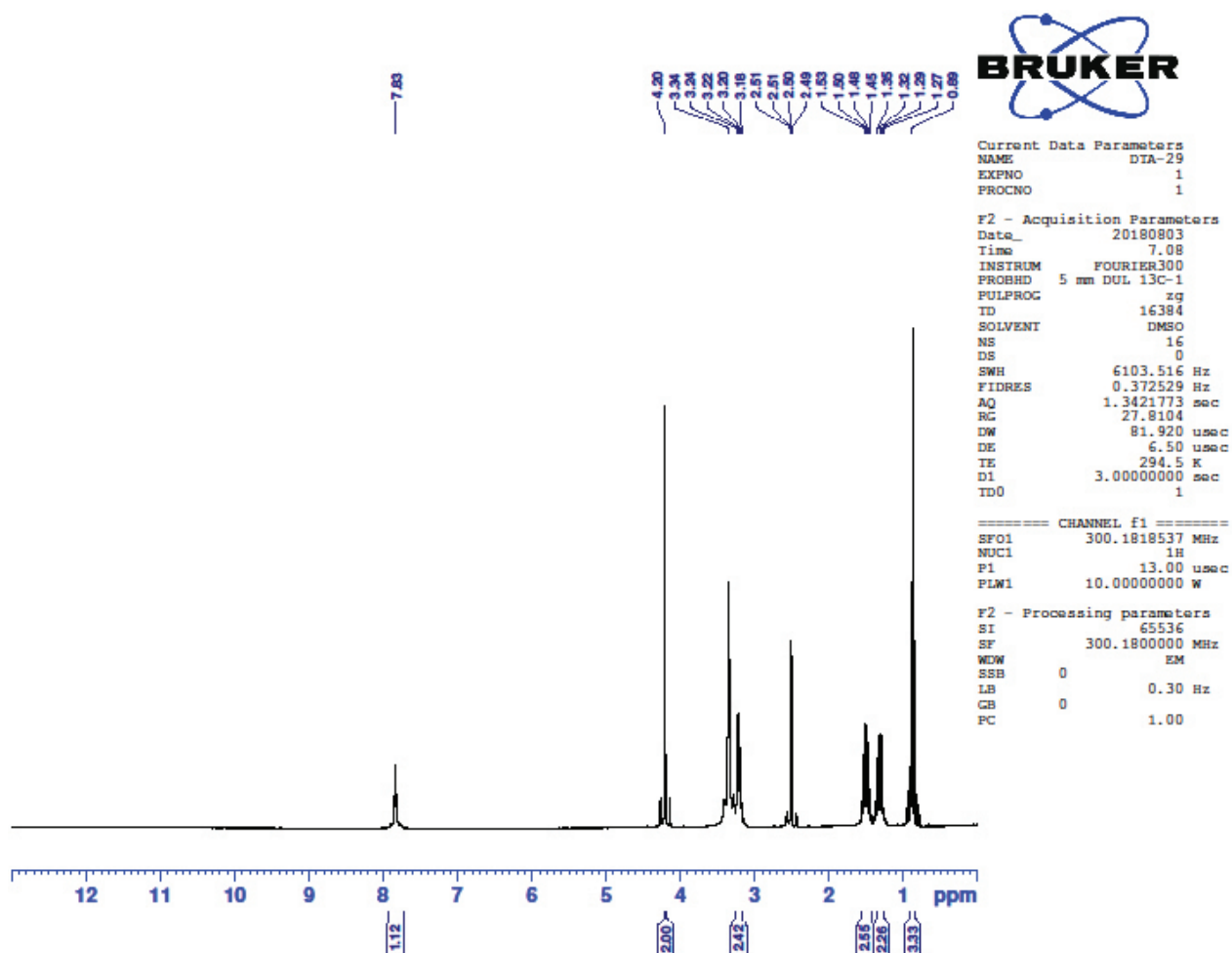


Measured region for 383.0010 m/z

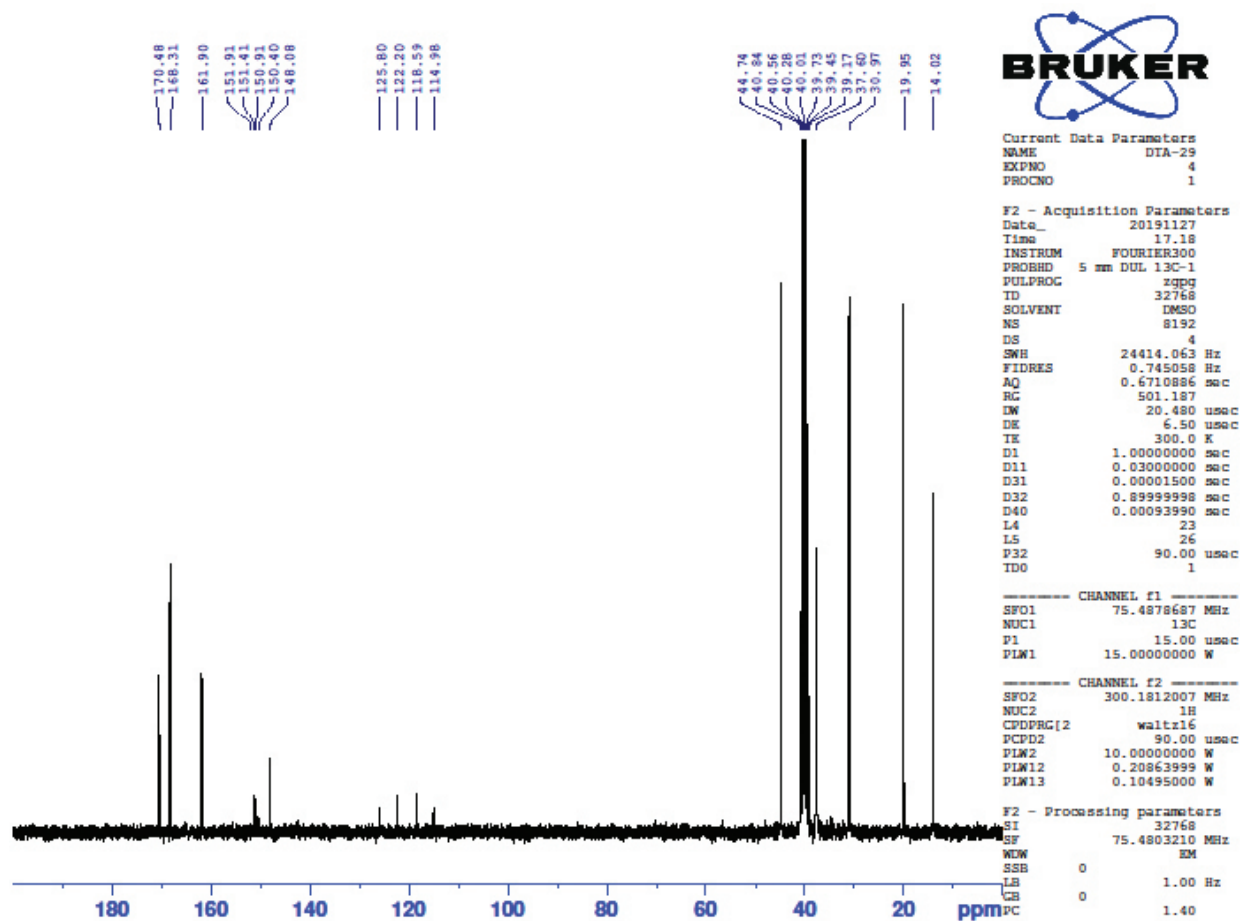
C10 H9 N6 O F3 S3 [M+H]⁺ : Predicted region for 383.0025 m/z

Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	35.40	C10 H9 N6 O F3 S3	[M+H] ⁺	383.0010	383.0025	-1.5	-3.92	38.18	8.0

Spectrum 18. HRMS spectrum of compound 4f.



Spectrum 19. ^1H -NMR spectrum of compound **4g**.

Spectrum 20. ¹³C-NMR spectrum of compound 4g.

Formula Predictor Report - dts-29_7.lcdPage 1 of 1

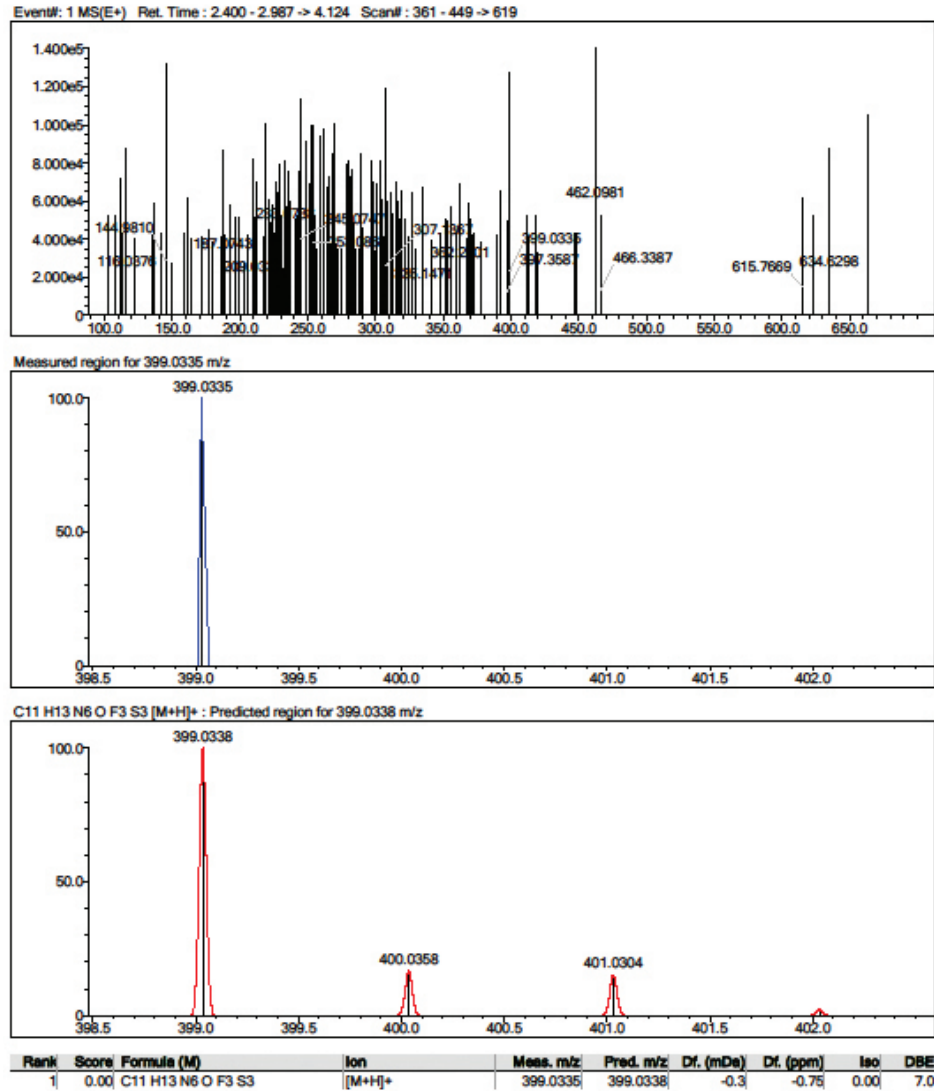
Data File: C:\LabSolutions\Data\Analz\deriv\dts-29_7.lcd

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

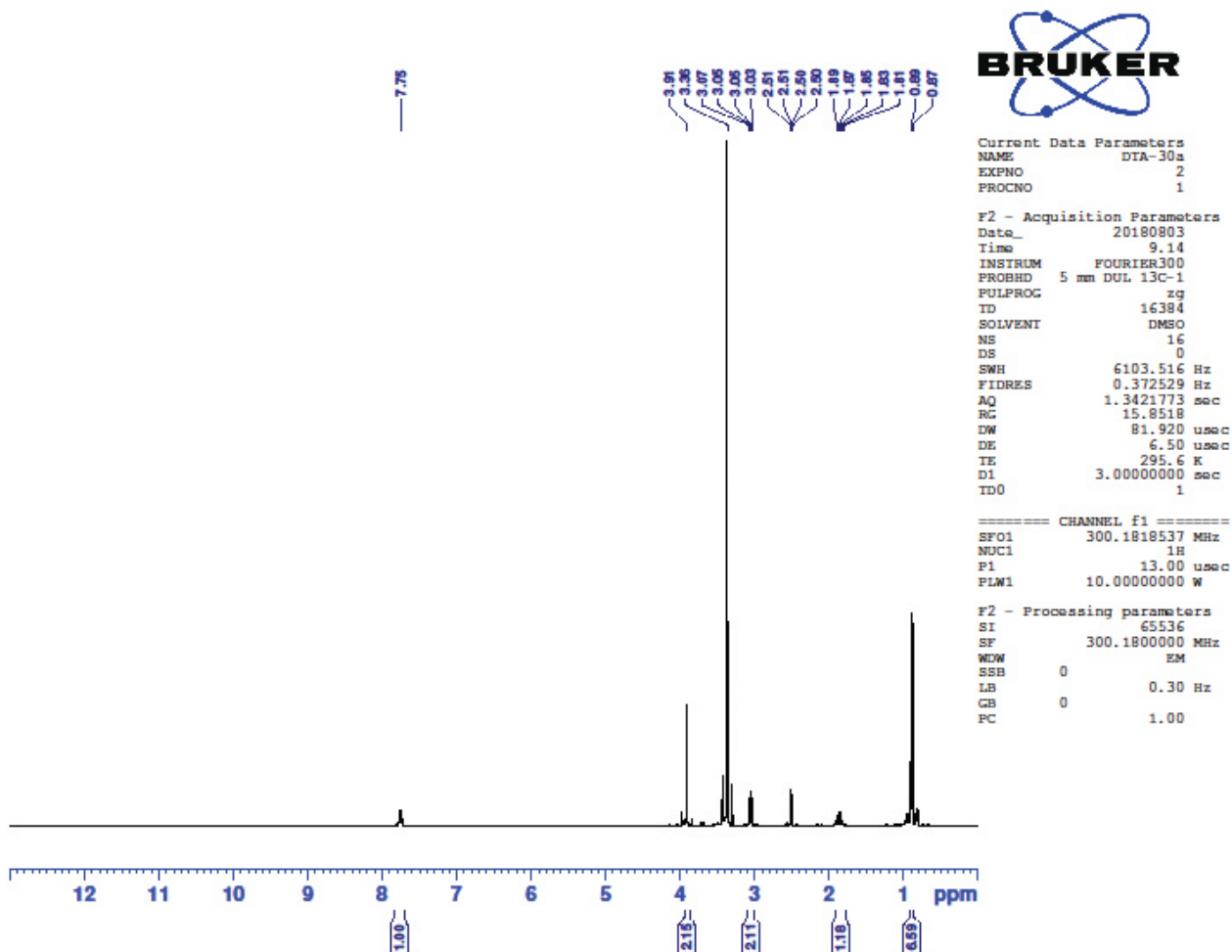
Error Margin (ppm): 25
HC Ratio: unlimited
Max Isotopes: 3
MSn Iso RI (%): 10.00

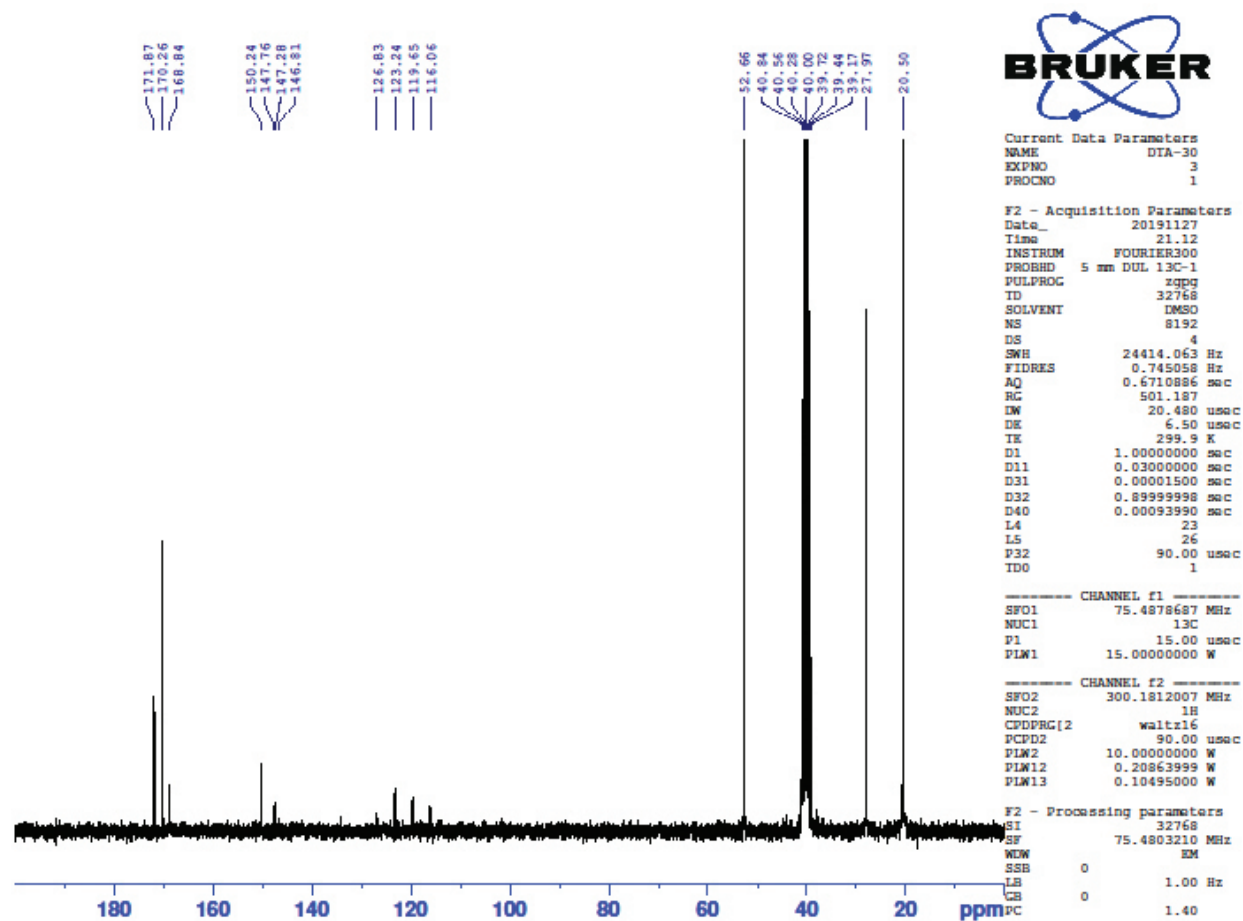
DBE Range: 5.0 - 20.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

Electron Ions: both
Use MSn Info: yes
Isotope Res: 9000
Max Results: 100



Spectrum 21. HRMS spectrum of compound 4g.

Spectrum 22. ¹H-NMR spectrum of compound 4h.

Spectrum 23. ^{13}C -NMR spectrum of compound 4h.

Formula Predictor Report - dta-30_8.lcd

Page 1 of 1

Data File: C:\LabSolutions\Data\Analysis\deriv\tda-30_8.lcd

Elmt	Val	Min	Max	Elmt	Val	Min	Max	Elmt	Val	Min	Max	Elmt	Val	Min	Max	Use Adduct
H	1	6	15	O	2	0	6	S	2	3	3	Ru	2	0	0	H
C	4	8	15	F	1	3	3	Cl	1	0	0	Pd	2	0	0	
N	3	0	6	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: 5.0 - 20.0

Apply N Rule: yes

Isotope RI (%): 1.00

MSn Logic Mode: AND

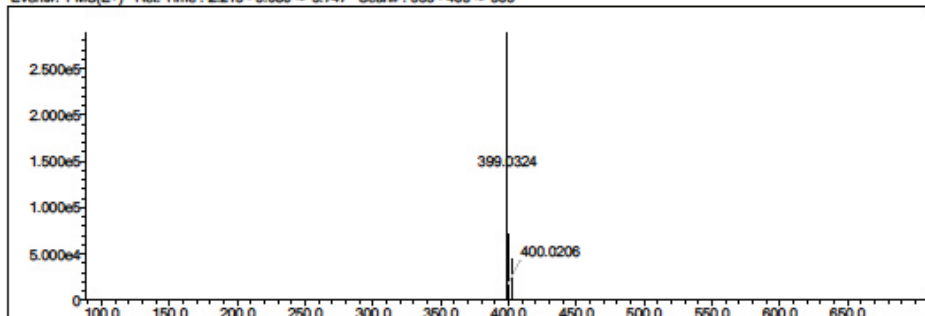
Electron Ions: both

Use MSn Info: yes

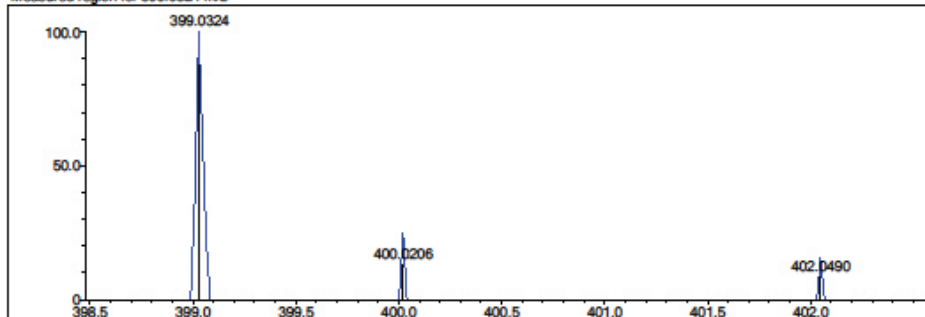
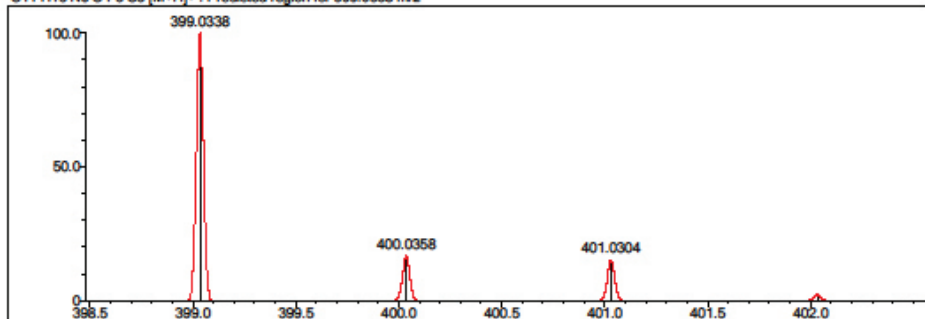
Isotope Res: 9000

Max Results: 100

Event#: 1 MS(E+) Ret. Time : 2.213 - 3.060 -> 3.747 Scan#: 333 - 463 -> 563



Measured region for 399.0324 m/z

C11 H13 N6 O F3 S3 [M+H]⁺ : Predicted region for 399.0338 m/z

Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	24.99	C11 H13 N6 O F3 S3	[M+H] ⁺	399.0324	399.0338	-1.4	-3.51	26.67	7.0

Spectrum 24. HRMS spectrum of compound 4h.

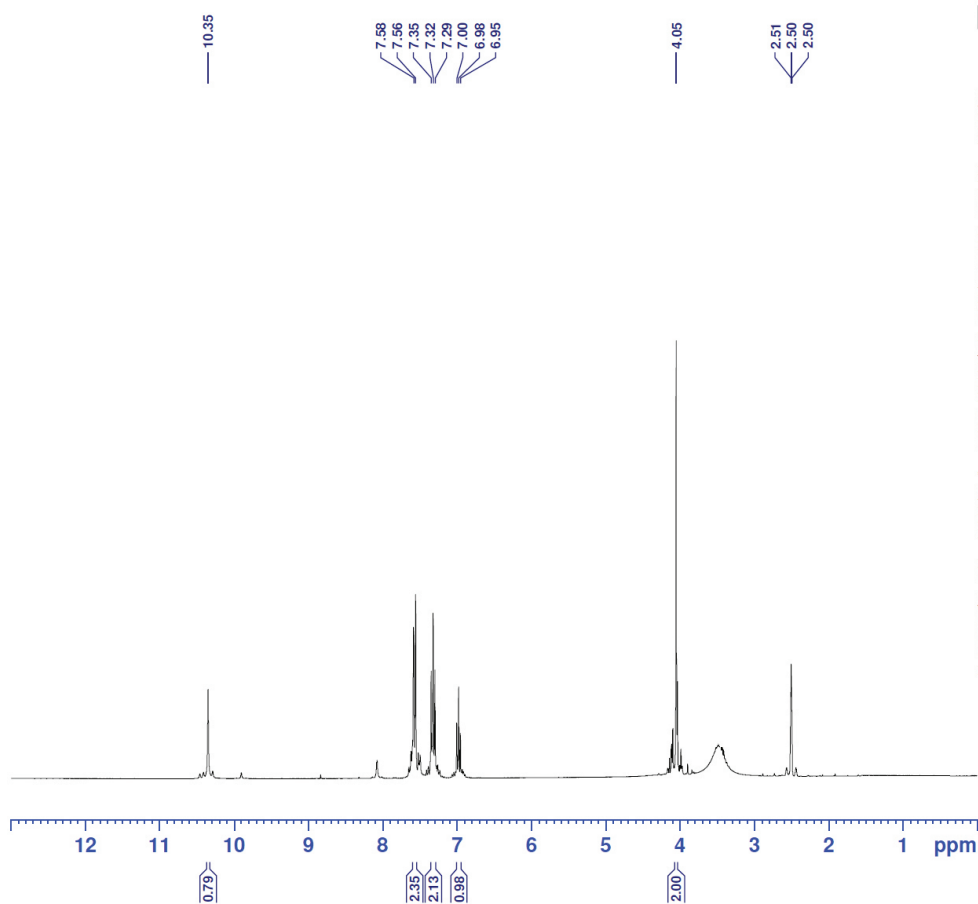


Current Data Parameters
NAME DTA-32
EXPNO 3
PROCNO 1

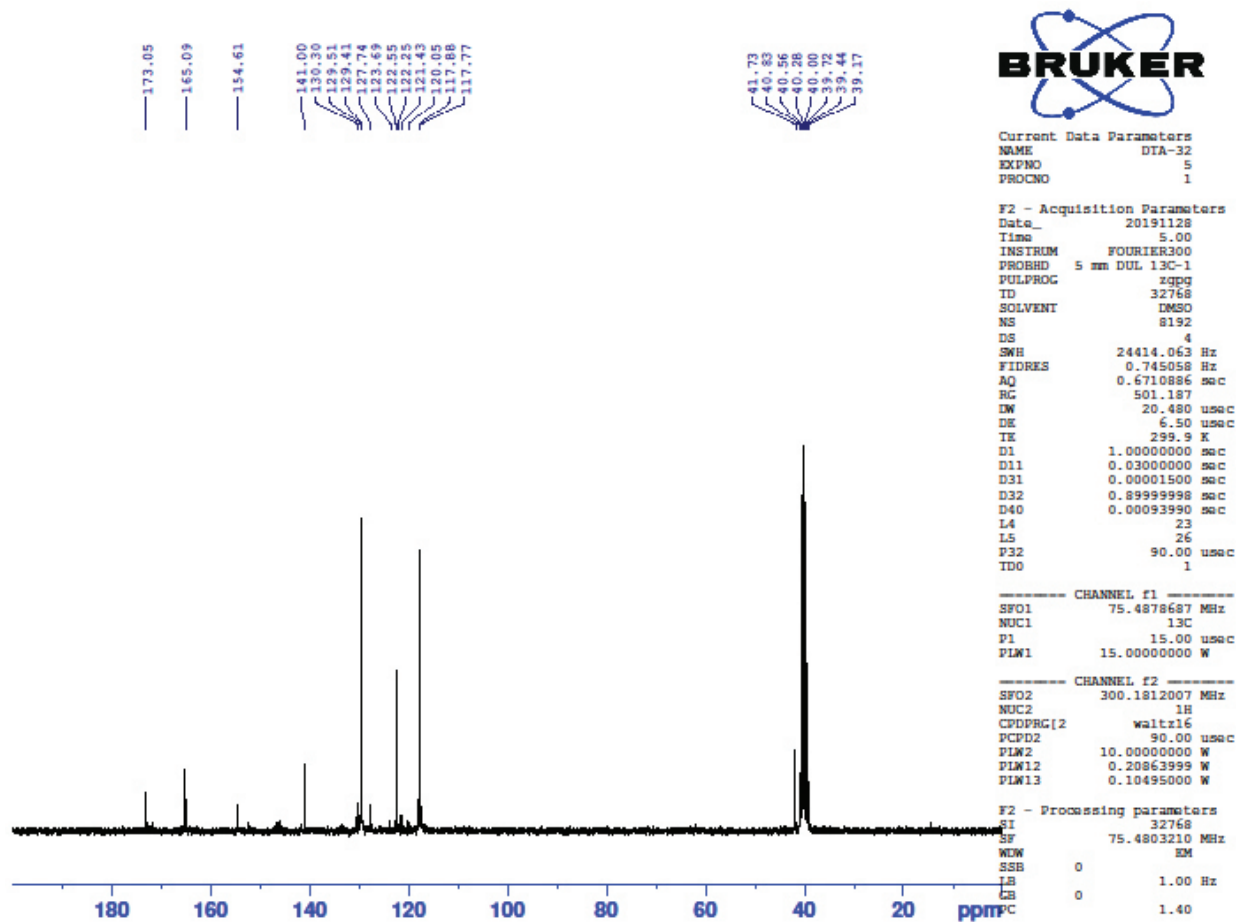
F2 - Acquisition Parameters
Date_ 20190618
Time 11.26
INSTRUM FOURIER300
PROBHD 5 mm DUL 13C-1
PULPROG zg
TD 16384
SOLVENT DMSO
NS 16
DS 0
SWH 6103.516 Hz
FIDRES 0.372529 Hz
AQ 1.3421773 sec
RG 23.5866
DW 81.920 usec
DE 6.50 usec
TE 296.4 K
D1 3.00000000 sec
TD0 1

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

F2 - Processing parameters
SI 65536
SF 300.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Spectrum 25. ^1H -NMR spectrum of compound **4i**.

Spectrum 26. ^{13}C -NMR spectrum of compound 4i.

Formula Predictor Report - dta-32_10.lcd

Page 1 of 1

Data File: C:\LabSolutions\Data\Analz\deriv\dta-32_10.lcd

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

Error Margin (ppm): 5

DBE Range: 7.0 - 20.0

Electron Ions: both

HC Ratio: unlimited

Apply N Rule: yes

Use MSn Info: yes

Max Isotopes: 3

Isotope RI (%): 1.00

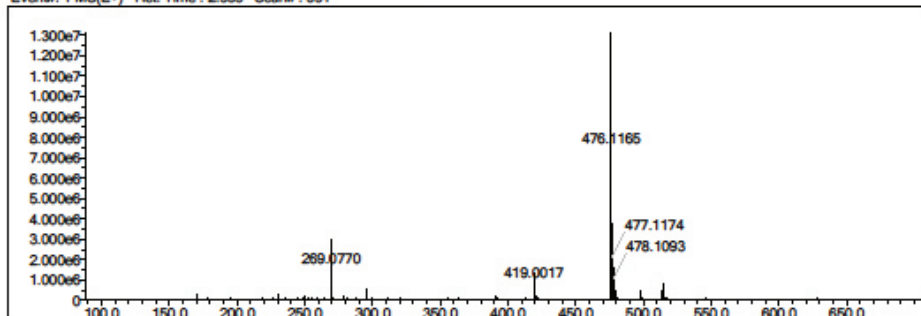
Isotope Res: 9000

MSn Iso RI (%): 10.00

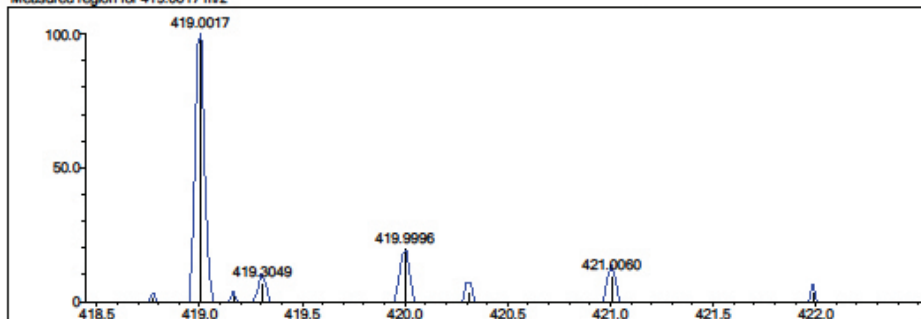
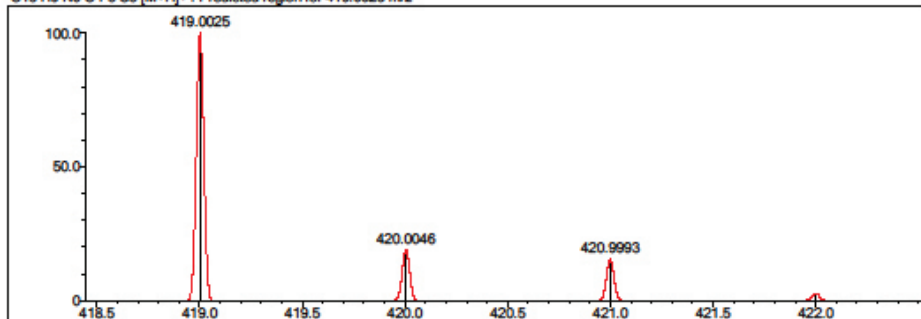
MSn Logic Mode: AND

Max Results: 100

Event#: 1 MS(E+) Ret. Time : 2.333 Scan#: 351

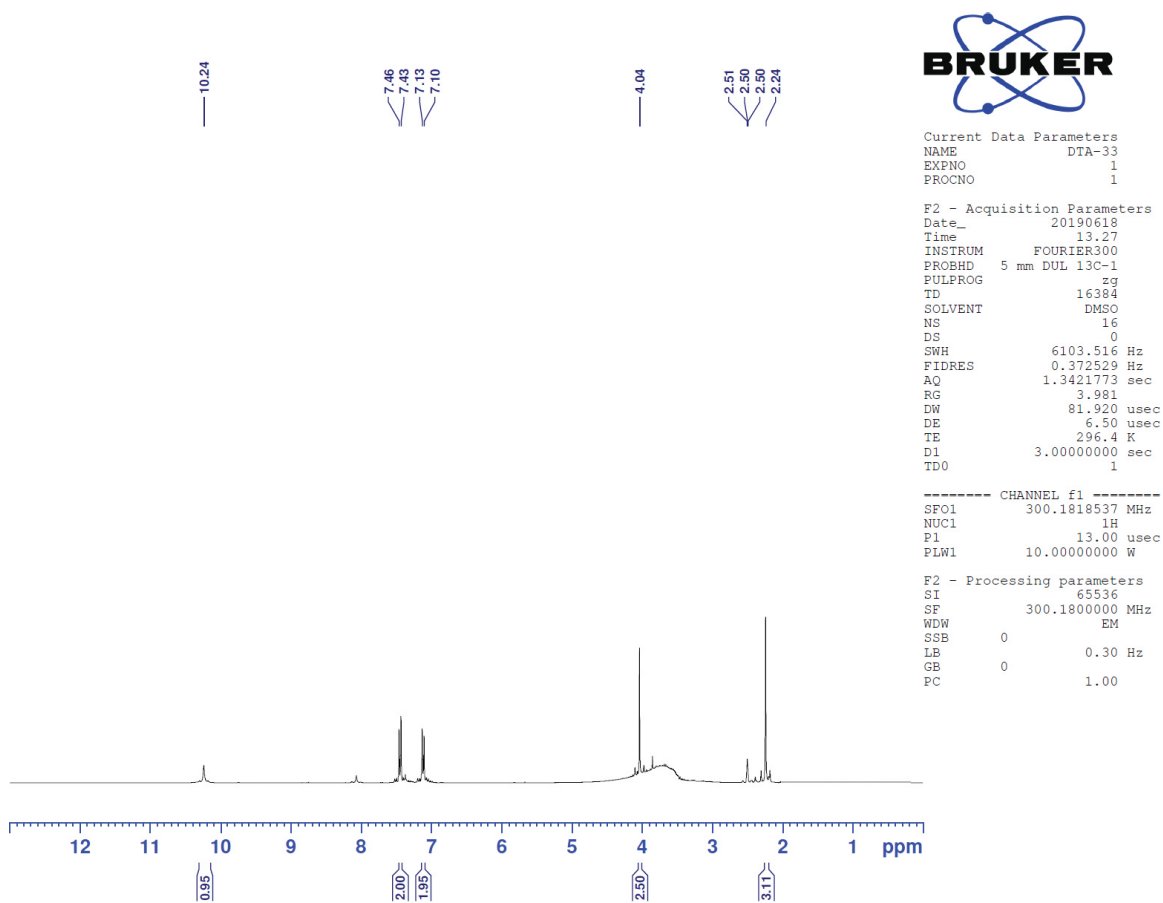


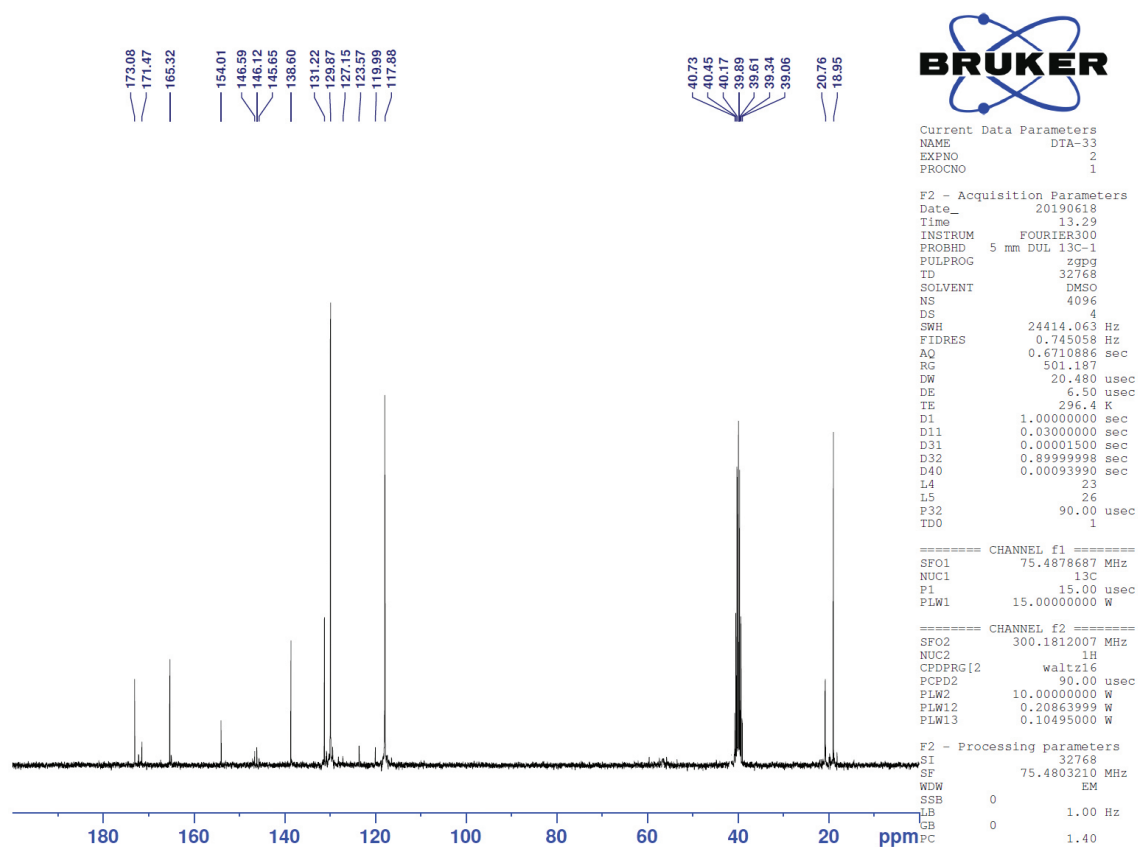
Measured region for 419.0017 m/z

C13 H9 N6 O F3 S3 [M+H]⁺ : Predicted region for 419.0025 m/z

Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	69.38	C13 H9 N6 O F3 S3	[M+H] ⁺	419.0017	419.0025	-0.8	-1.91	71.00	11.0

Spectrum 27. HRMS spectrum of compound 4i.

Spectrum 28. ¹H-NMR spectrum of compound 4j.

Spectrum 29. ¹³C-NMR spectrum of compound 4j.

Formula Predictor Report - dta-33_11.lcd

Page 1 of 1

Data File: C:\LabSolutions\Data\Analysis\dery\dta-33_11.lcd

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

Error Margin (ppm): 15

HC Ratio: unlimited

Max Isotopes: 3

MSn Iso RI (%): 10.00

DBE Range: 7.0 - 12.0

Apply N Rule: yes

Isotope RI (%): 1.00

MSn Logic Mode: AND

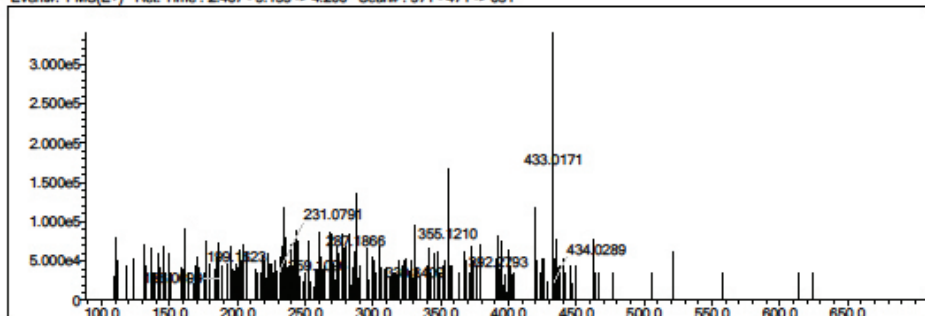
Electron Ions: both

Use MSn Info: yes

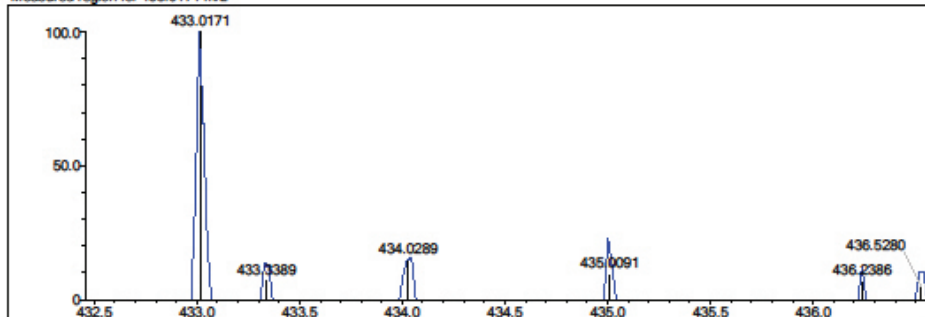
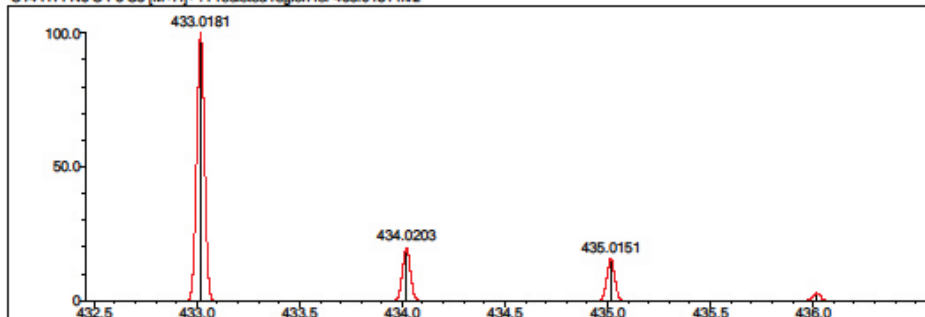
Isotope Res: 9000

Max Results: 100

Event#: 1 MS(E+) Ret. Time : 2.467 - 3.133 -> 4.206 Scan#: 371 - 471 -> 631



Measured region for 433.0171 m/z

C14 H11 N6 O F3 S3 [M+H]⁺ : Predicted region for 433.0181 m/z

Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	37.27	C14 H11 N6 O F3 S3	[M+H] ⁺	433.0171	433.0181	-1.0	-2.31	38.54	11.0

Spectrum 30. HRMS spectrum of compound 4j.