

SUPPLEMENTARY DATA

Novel Substituted Oxadiazole - Piperazine Derivatives as Potential MAO Inhibitors: Design, Synthesis, *In Vitro* and *In Silico* Studies

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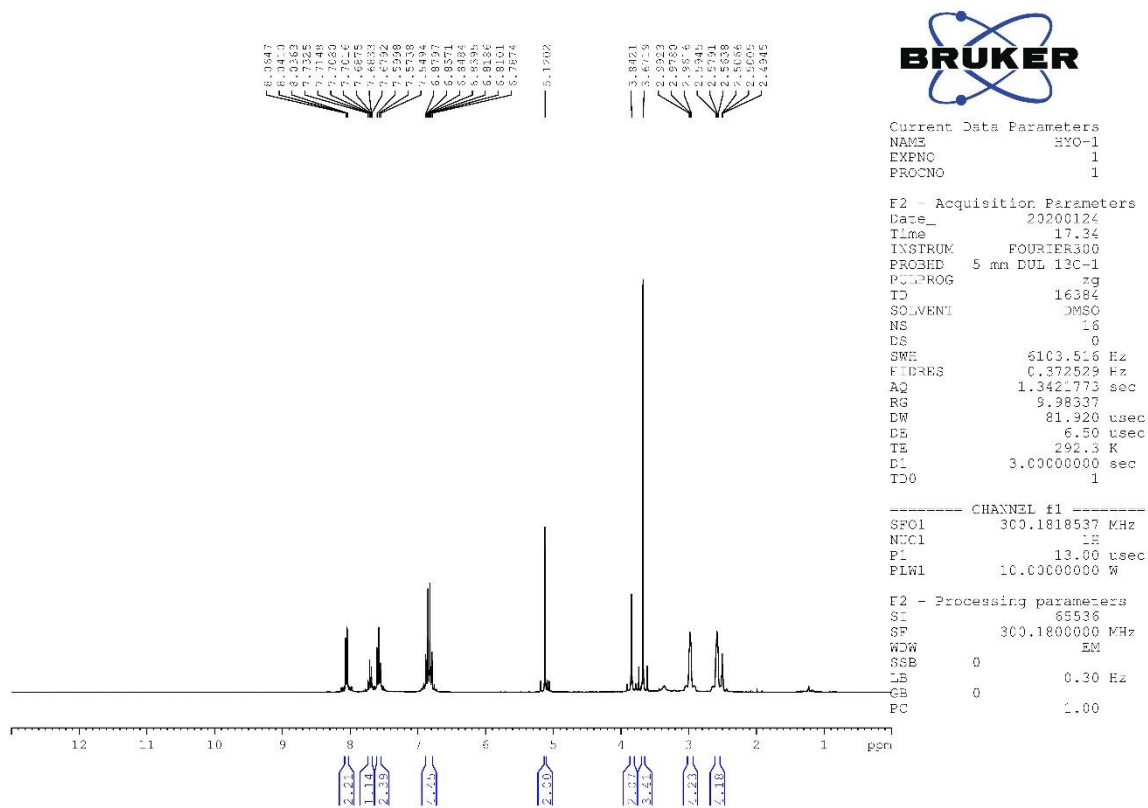
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Data 1. ¹H-NMR spectrum of compound 4a



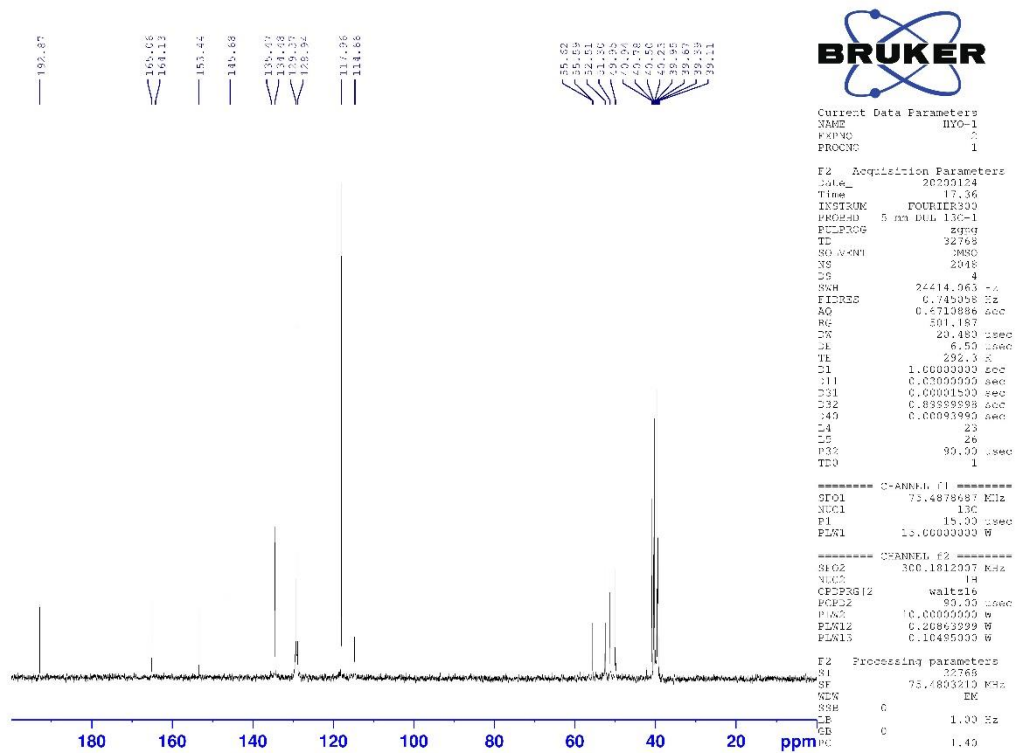
Current Data Parameters
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 EXPGN: 1
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20200124
 Time: 17.34
 INSTRUM: FOURIER300
 PROBED: 5 mm DUL 13C-1
 PULPROG: zg
 TD: 16384
 SOLVENT: DMSO
 NS: 16
 DS: 0
 SWE: 6103.516 Hz
 FIDRES: 0.372529 Hz
 AQ: 1.3421773 sec
 RG: 9.38337
 DW: 81.920 usec
 DE: 6.50 usec
 TE: 292.3 K
 D1: 3.0000000 sec
 TD0: 1

----- CHANNEL f1 -----
 SFO1: 300.1818537 MHz
 NUCL1: 1H
 PL: 13.00 usec
 PLW1: 10.0000000 W

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

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



Data 3. HRMS spectrum of compound 4a

Formula Predictor Report - HYD-1_43.lcd

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Data File: C:\LabSolutions\Data\Analiz\deryal\HYD-1_43.lcd

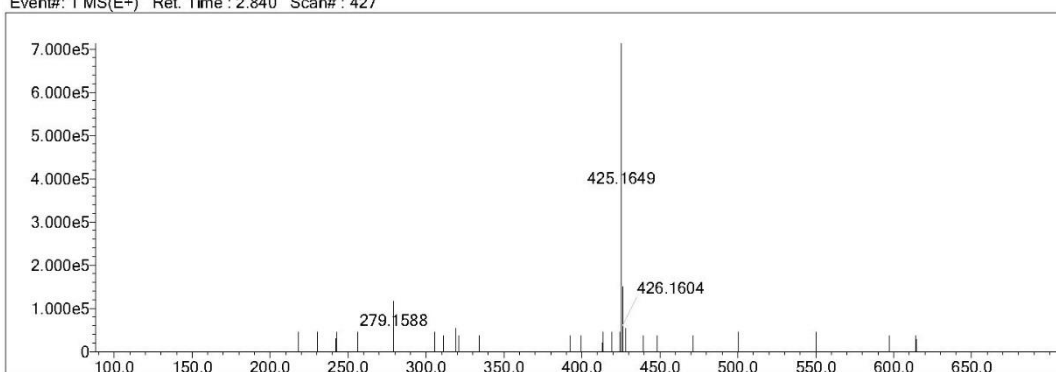
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C	4	5	35	F	1	0	0	Cl	1	0	0	Pd	2	0	0	
N	3	0	6	P	3	0	0	Br	1	0	0	I	3	0	0	

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

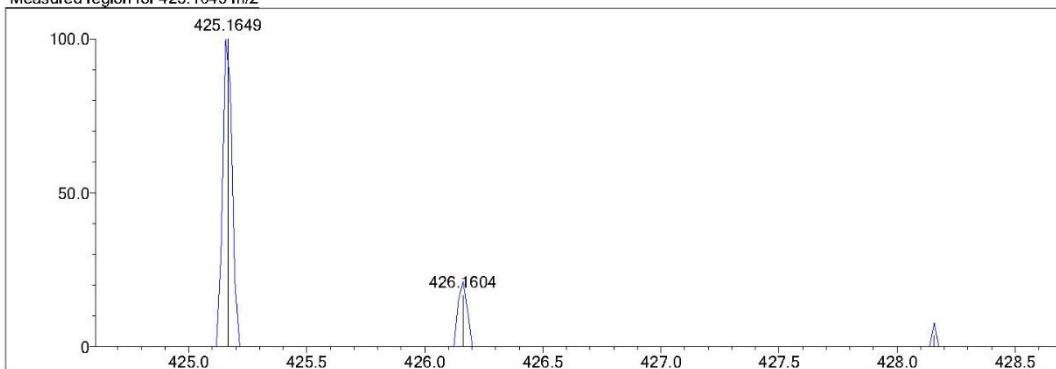
DBE Range: 5.0 - 20.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: yes
 Isotope Res: 9000
 Max Results: 150

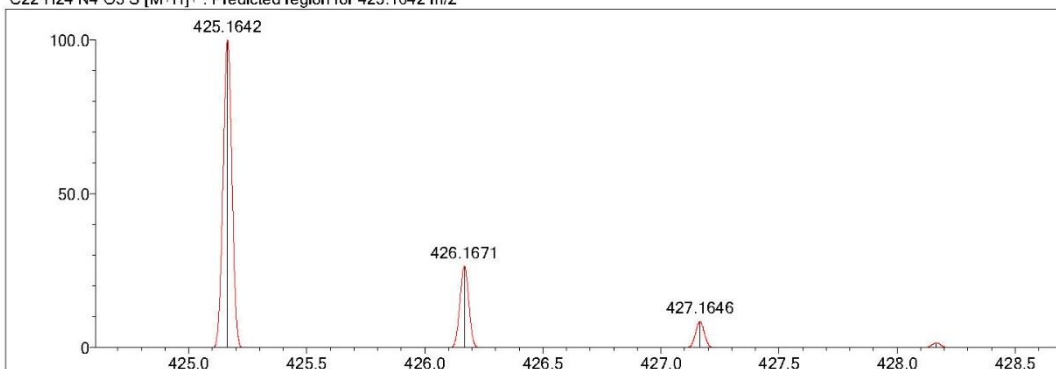
Event#: 1 MS(E+) Ret. Time : 2.840 Scan# : 427



Measured region for 425.1649 m/z

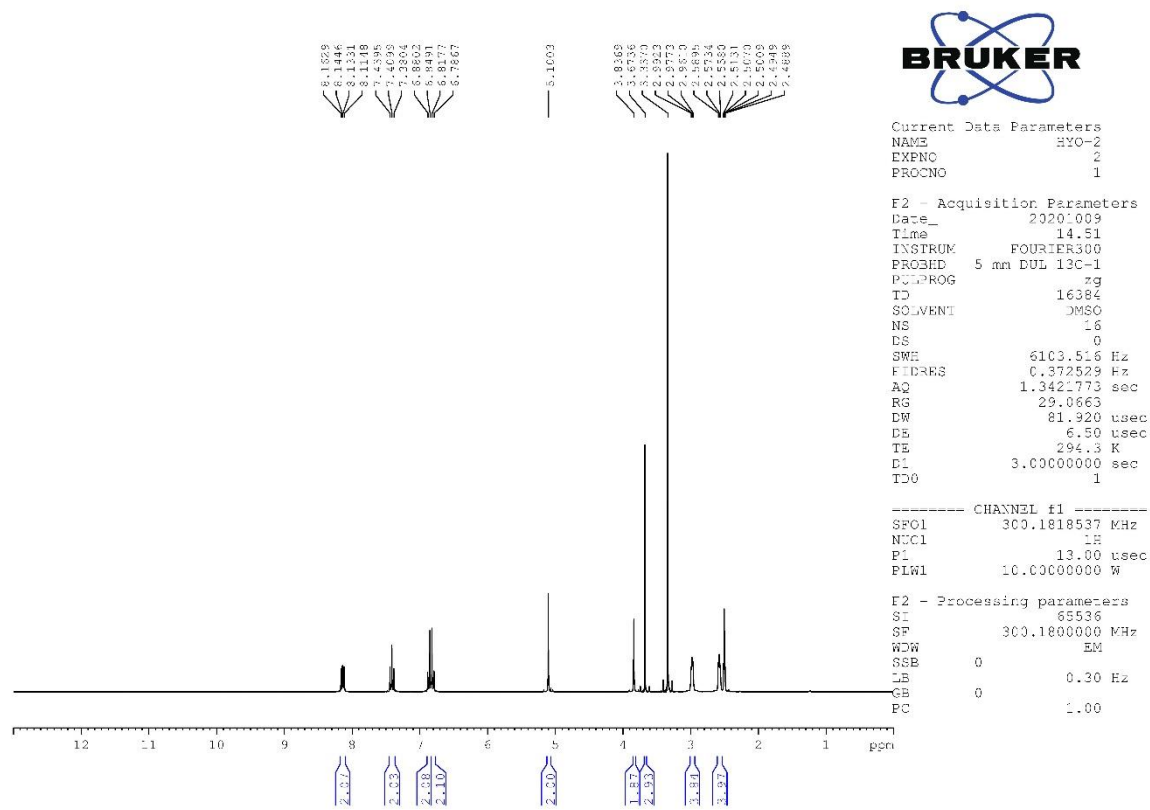


C22 H24 N4 O3 S [M+H]+ : Predicted region for 425.1642 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	53.01	C22 H24 N4 O3 S	[M+H]+	425.1649	425.1642	0.7	1.65	53.89	13.0

Data 4. ¹H-NMR spectrum of compound 4b



Data 6. HRMS spectrum of compound 4b

Formula Predictor Report - HYD-2_44.lcd

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Data File: C:\LabSolutions\Data\Analyze\deriv\HYD-2_44.lcd

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	5	40	O	2	0	3	S	2	1	1	Ru	2	0	0	H
C	4	5	35	F	1	1	1	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

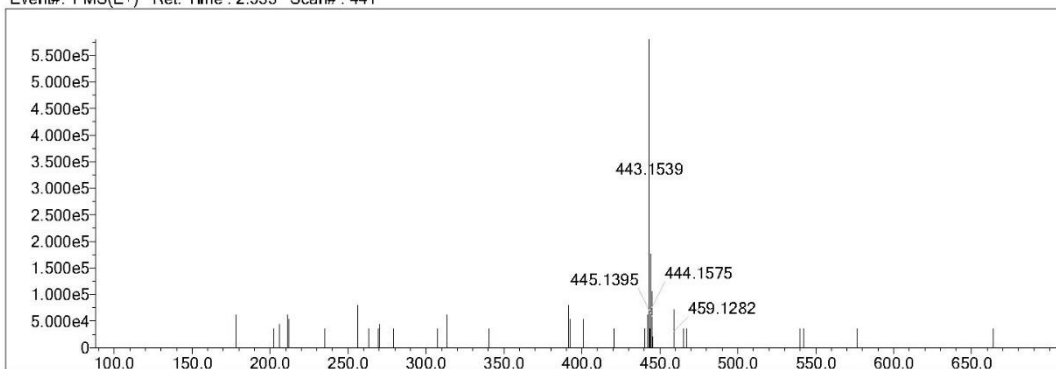
Electron Ions: both

Use MSn Info: yes

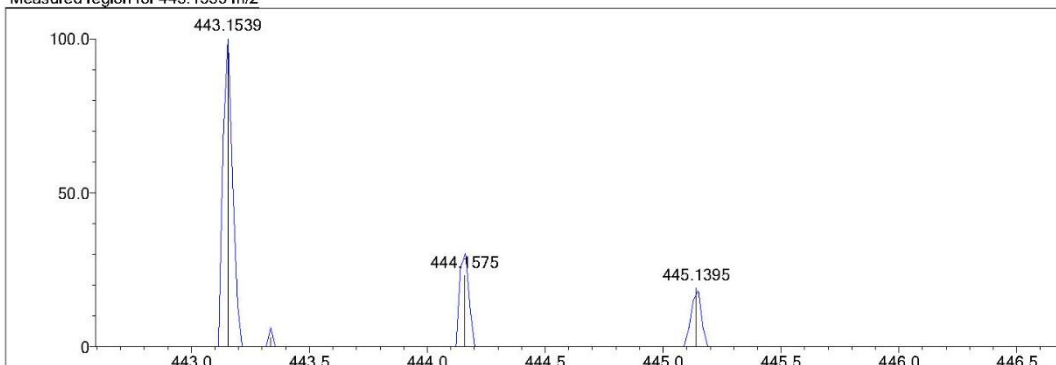
Isotope Res: 9000

Max Results: 150

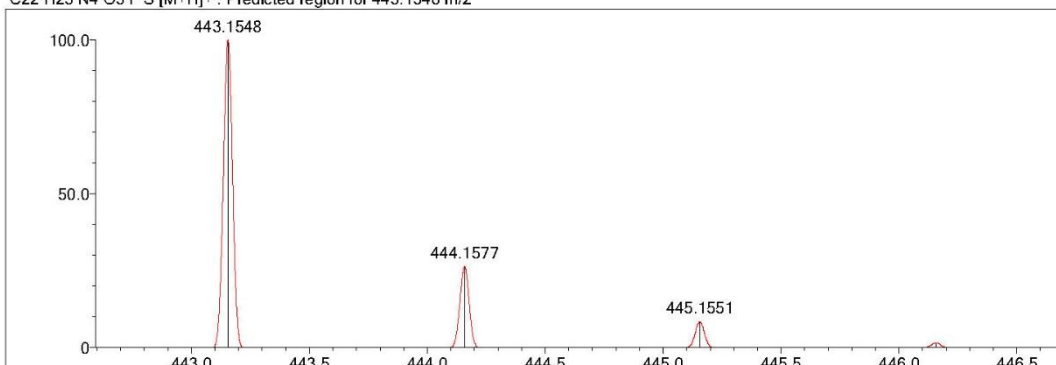
Event#: 1 MS(E+) Ret. Time : 2.933 Scan# : 441



Measured region for 443.1539 m/z

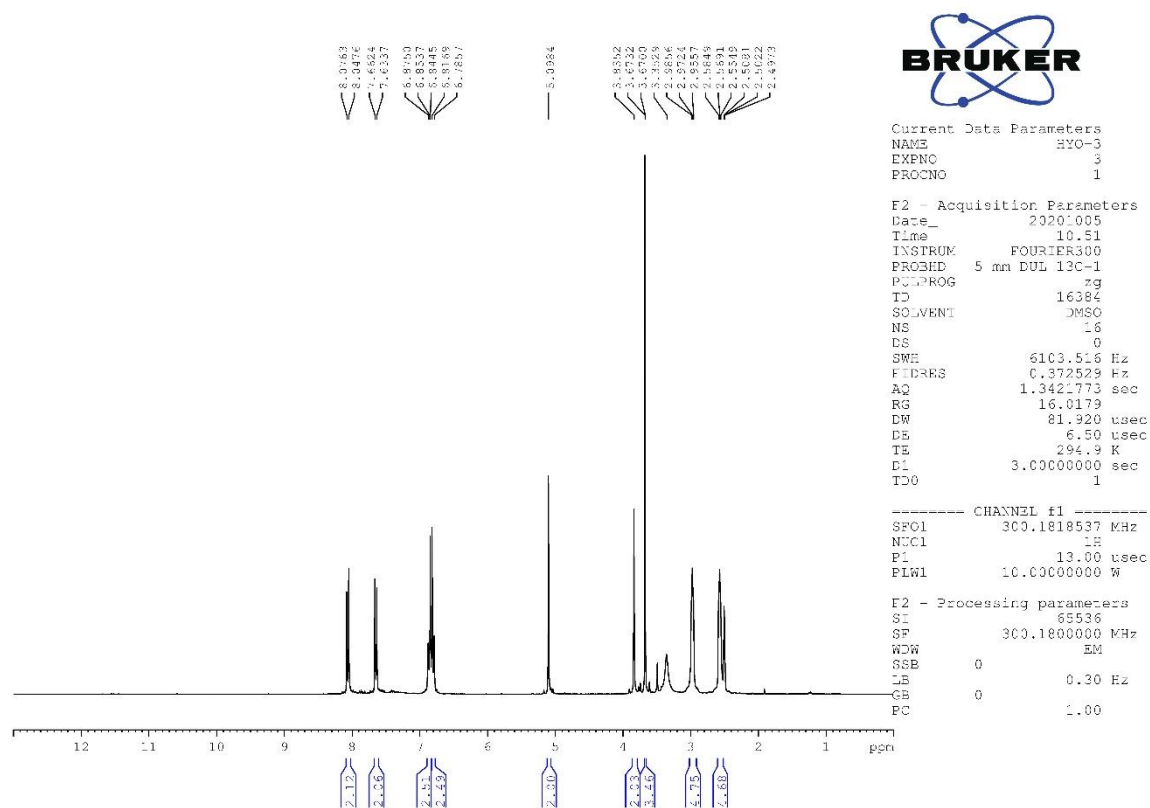


C22 H23 N4 O3 F S [M+H]⁺ : Predicted region for 443.1548 m/z

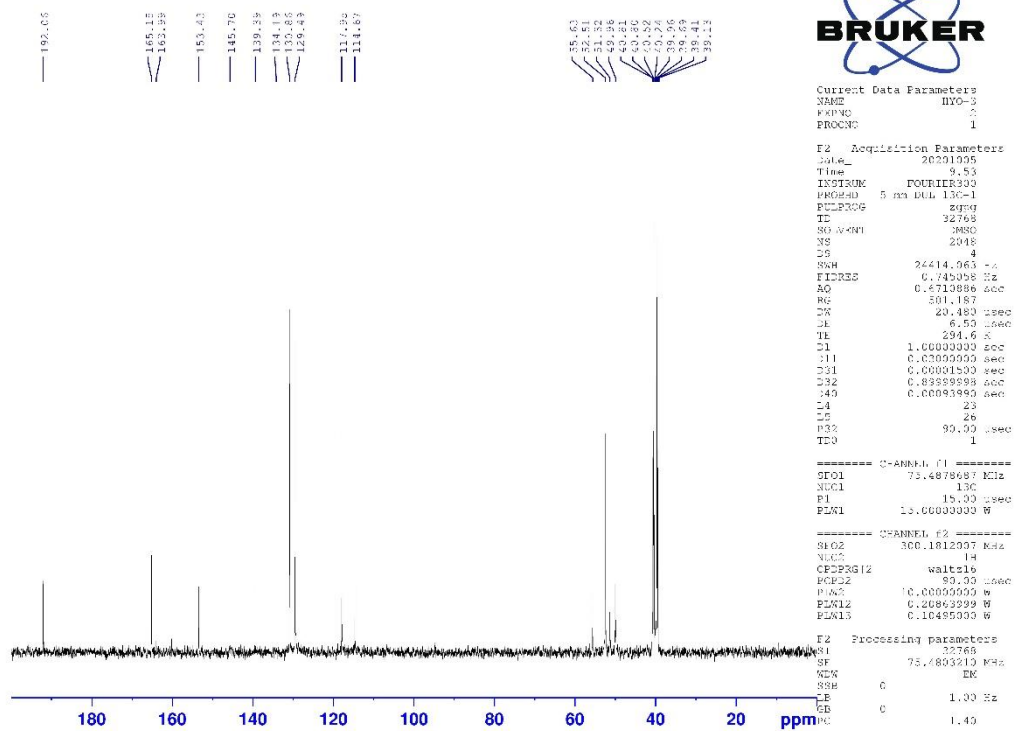


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	52.68	C ₂₂ H ₂₃ N ₄ O ₃ F S	[M+H] ⁺	443.1539	443.1548	-0.9	-2.03	54.08	13.0

Data 7. ¹H-NMR spectrum of compound 4c



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



Data 9. HRMS spectrum of compound 4c

Formula Predictor Report - HYD-3_45.lcd

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Data File: C:\LabSolutions\Data\Analyze\deriv\HYD-3_45.lcd

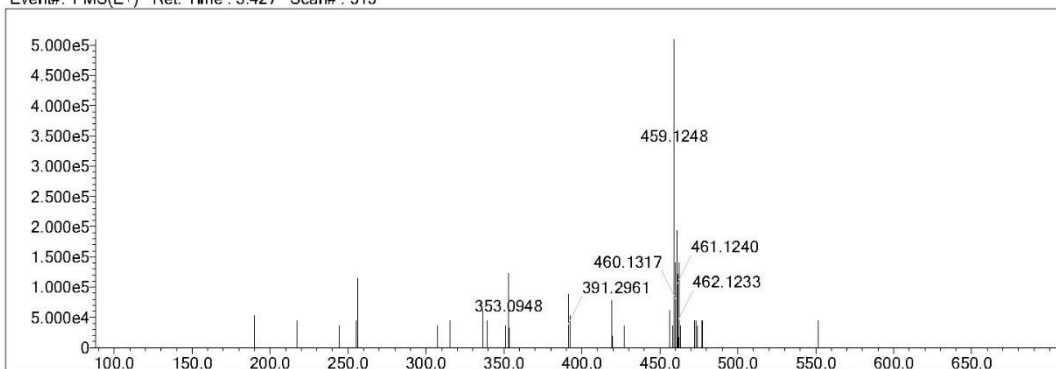
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	5	40	O	2	0	3	S	2	1	1	Ru	2	0	0	H
C	4	5	35	F	1	0	0	Cl	1	1	1	Pd	2	0	0	
N	3	0	6	P	3	0	0	Br	1	0	0	I	3	0	0	

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

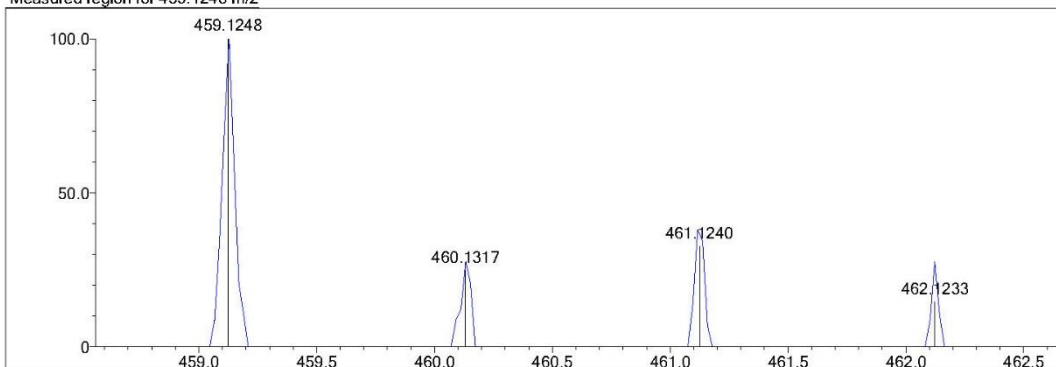
DBE Range: 5.0 - 20.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: yes
 Isotope Res: 9000
 Max Results: 150

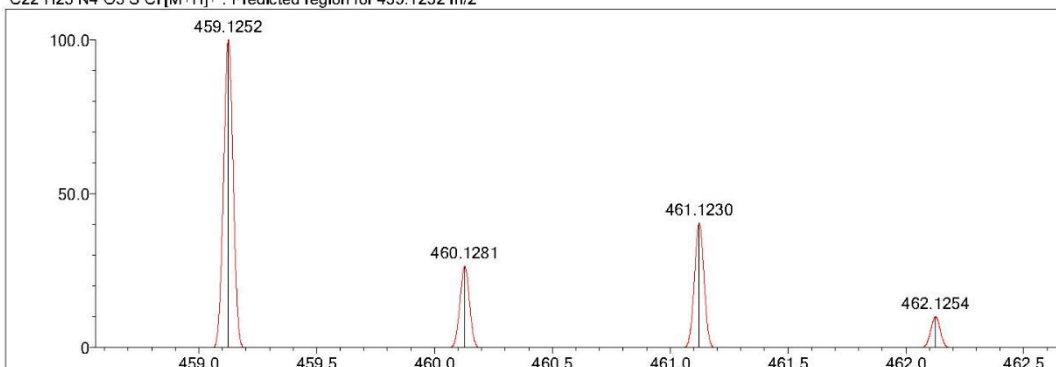
Event#: 1 MS(E+) Ret. Time : 3.427 Scan# : 515



Measured region for 459.1248 m/z

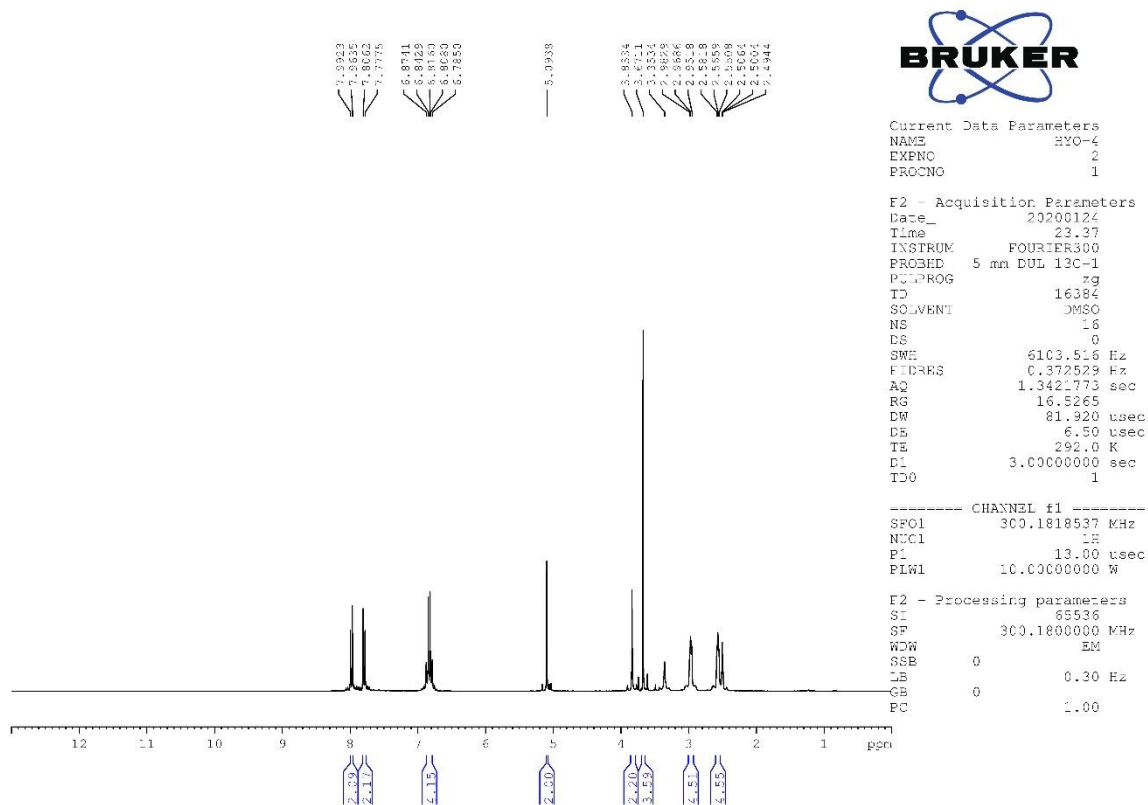


C22 H23 N4 O3 S Cl [M+H]⁺ : Predicted region for 459.1252 m/z

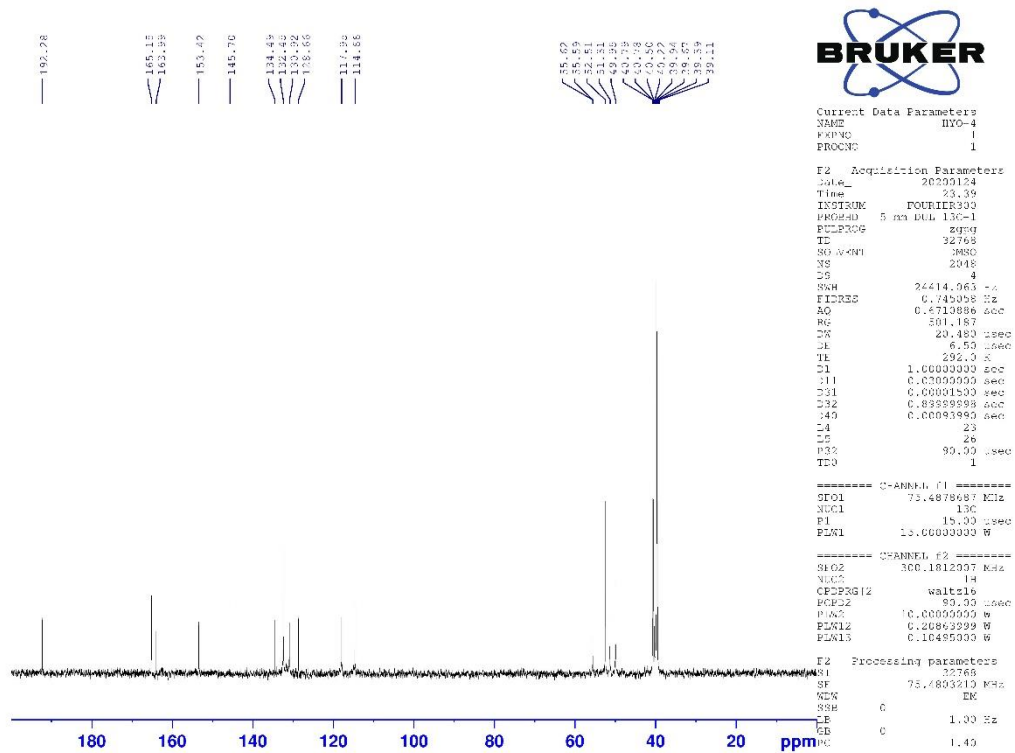


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	48.32	C22 H23 N4 O3 S Cl	[M+H] ⁺	459.1248	459.1252	-0.4	-0.87	48.32	13.0

Data 10. ¹H-NMR spectrum of compound 4d



Data 11. ¹³C-NMR spectrum of compound 4d



Data 12. HRMS spectrum of compound 4d

Formula Predictor Report - HYD-4_46.lcd

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Data File: C:\LabSolutions\Data\Analyze\deriva\HYD-4_46.lcd

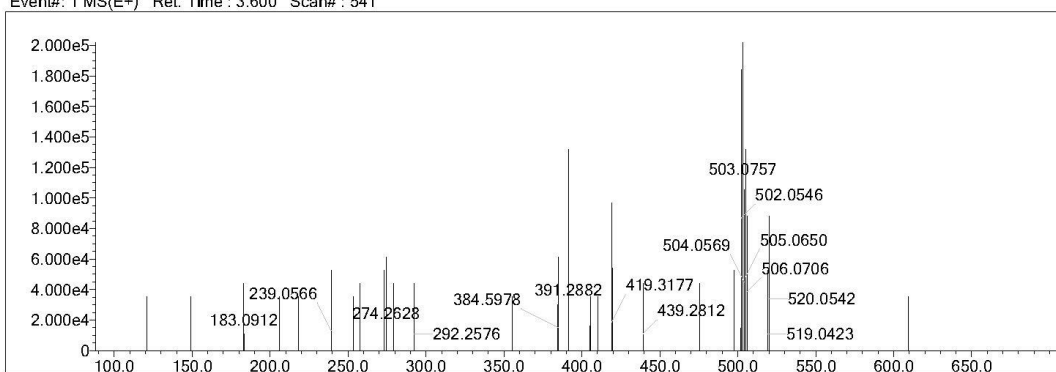
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H	1	5	40	O	2	0	3	S	2	1	1	Ru	2	0	0	H
C	4	5	35	F	1	0	0	Cl	1	0	0	Pd	2	0	0	
N	3	0	6	P	3	0	0	Br	1	1	1	I	3	0	0	

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

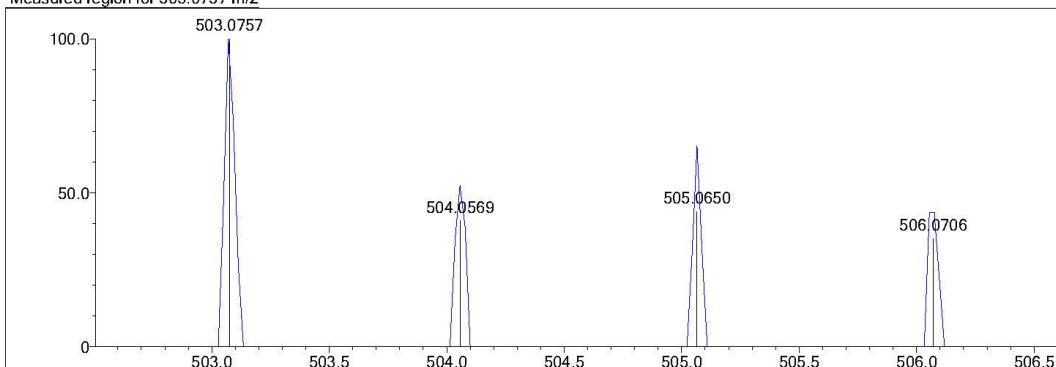
DBE Range: 5.0 - 20.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: yes
 Isotope Res: 9000
 Max Results: 150

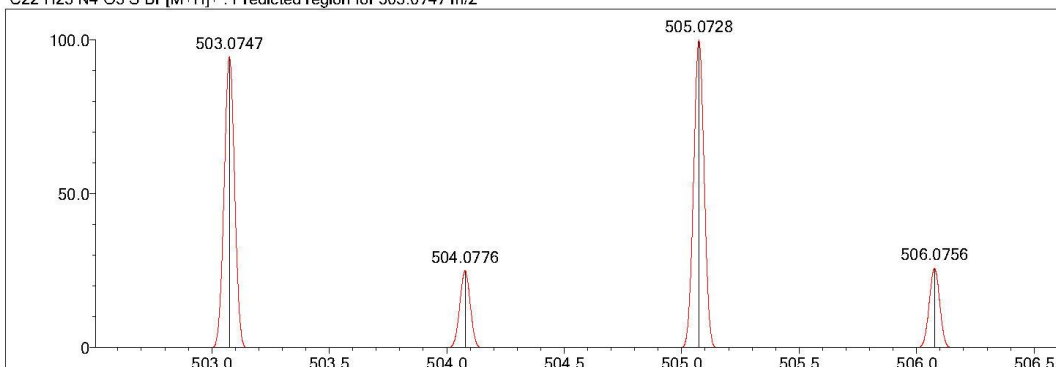
Event#: 1 MS(E+) Ret. Time : 3.600 Scan# : 541



Measured region for 503.0757 m/z

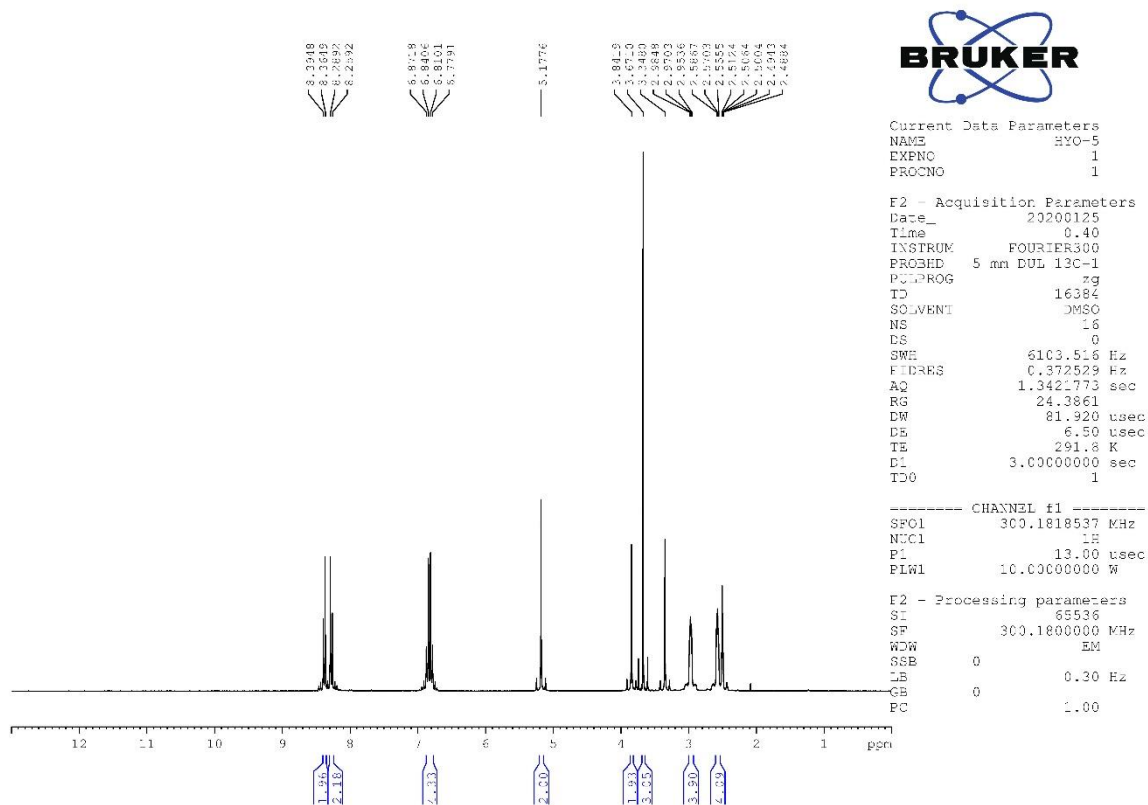


C22 H23 N4 O3 S Br [M+H]⁺ : Predicted region for 503.0747 m/z

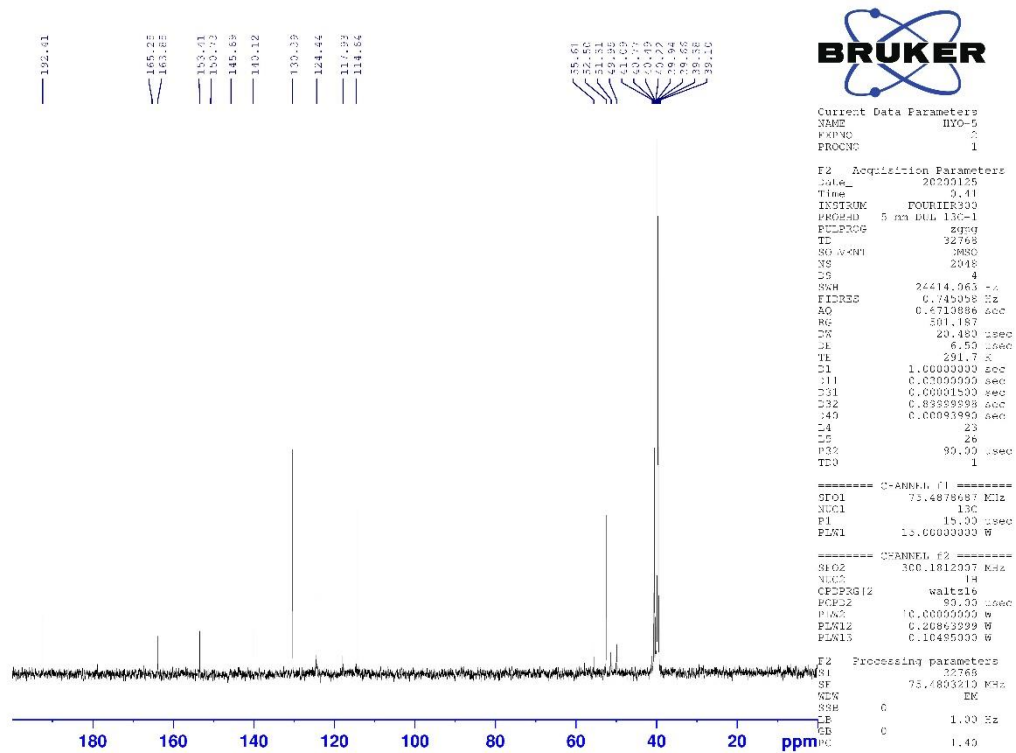


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDs)	Df. (ppm)	Iso	DBE
1	16.77	C22 H23 N4 O3 S Br	[M+H] ⁺	503.0757	503.0747	1.0	1.99	17.20	13.0

Data 13. ¹H-NMR spectrum of compound 4e



Data 14. ¹³C-NMR spectrum of compound 4e



Data 15. HRMS spectrum of compound 4e

Formula Predictor Report - HYD-5_47.lcd

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Data File: C:\LabSolutions\Data\Analyze\deriv\HYD-5_47.lcd

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	5	40	O	2	0	5	S	2	1	1	Ru	2	0	0	H
C	4	5	35	F	1	0	0	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

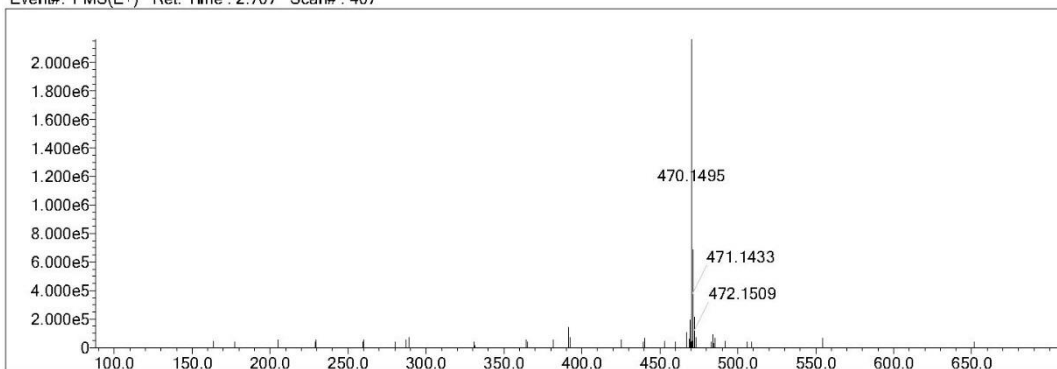
Electron Ions: both

Use MSn Info: yes

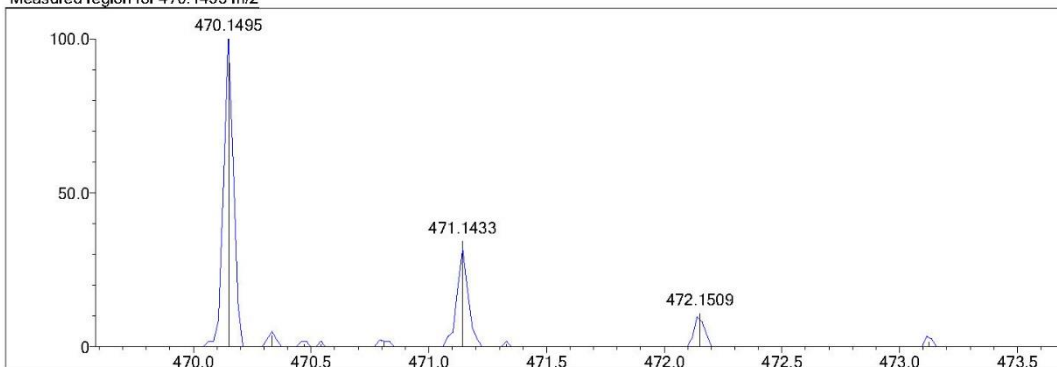
Isotope Res: 9000

Max Results: 150

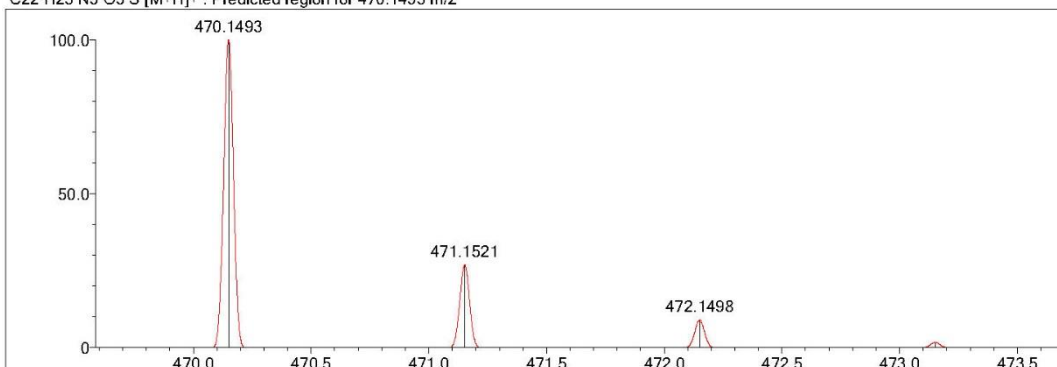
Event#: 1 MS(E+) Ret. Time : 2.707 Scan# : 407



Measured region for 470.1495 m/z



C22 H23 N5 O5 S [M+H]⁺ : Predicted region for 470.1493 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	61.36	C22 H23 N5 O5 S	[M+H] ⁺	470.1495	470.1493	0.2	0.43	61.36	14.0