

**Novel 1,3,4-thiadiazole compounds as potential MAO-A inhibitors-Design, synthesis, biological evaluation and molecular modelling**

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Address: Bulent Ecevit University, Faculty of Pharmacy, Department of Pharmaceutical Chemistry, 67600, Zonguldak, Turkey.

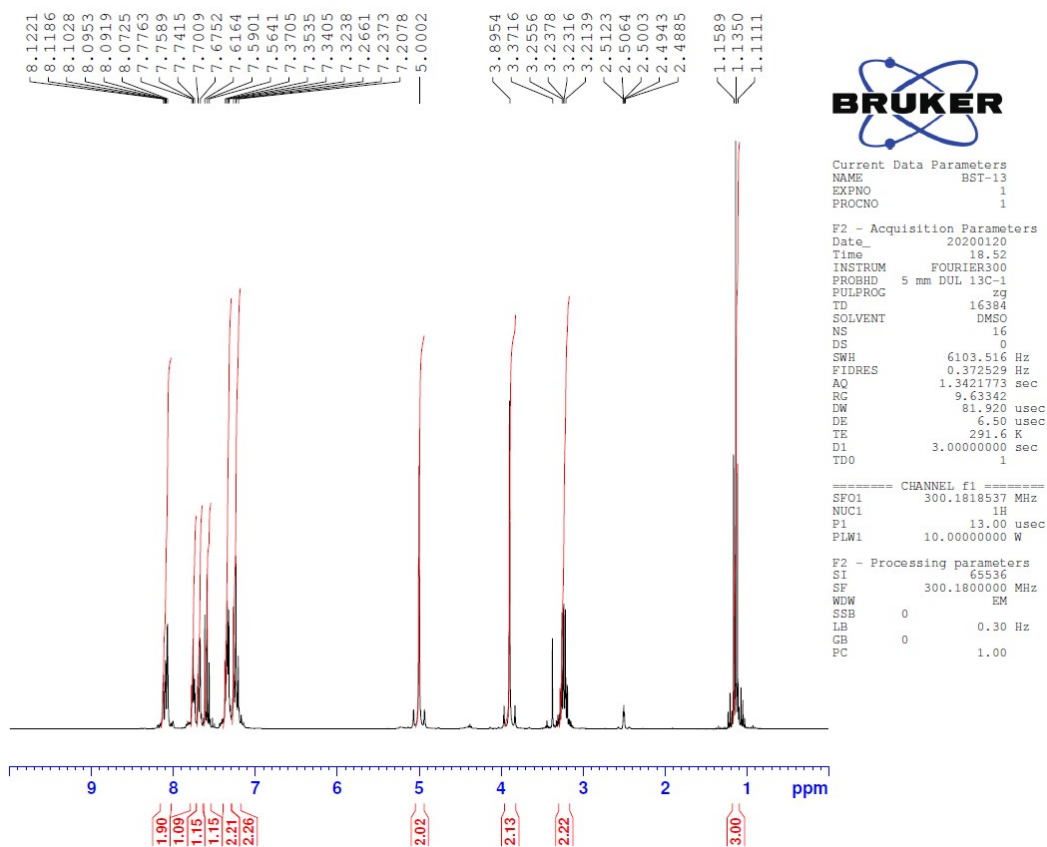


Figure S1. <sup>1</sup>H NMR spectrum of compound 6a.

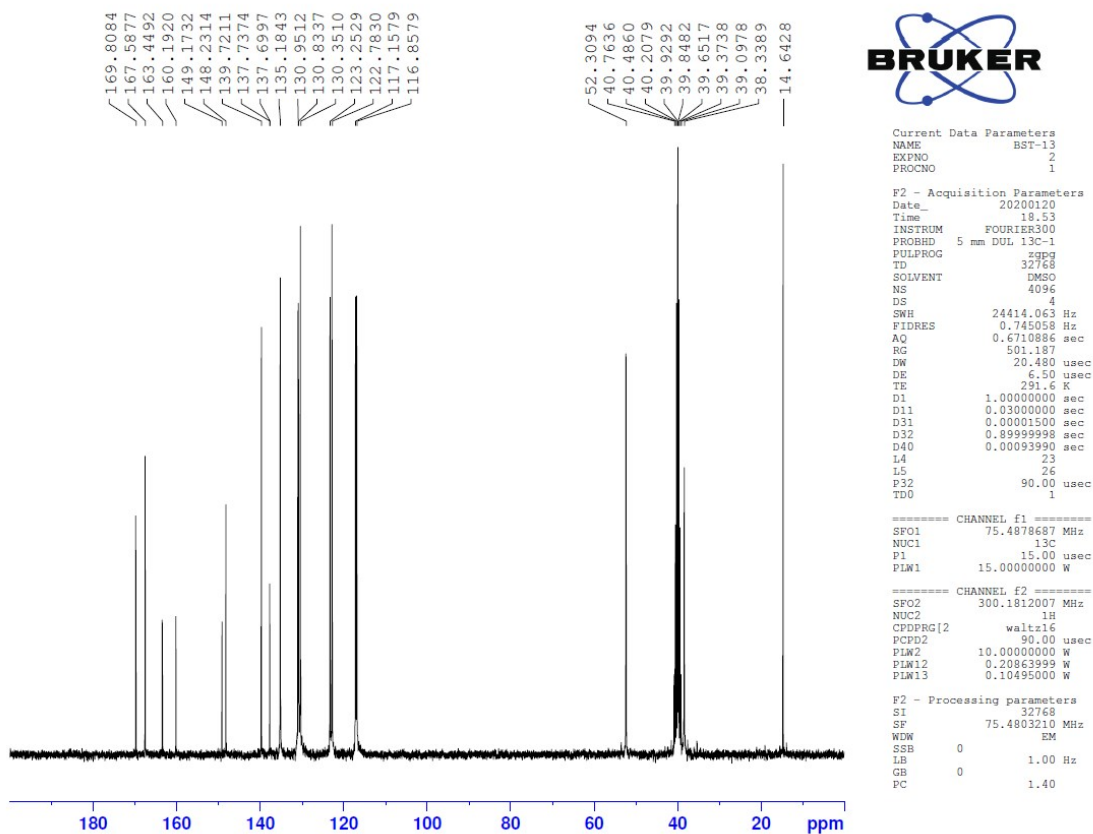


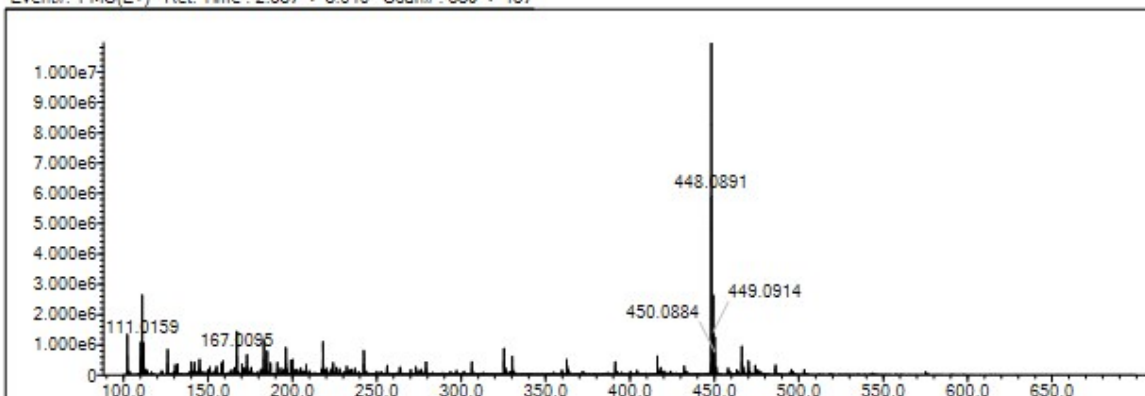
Figure S2. <sup>13</sup>C NMR spectrum of compound 6a.

Data File: C:\LabSolutions\Data\Analiz\uacl\BST-13\_6.lcd

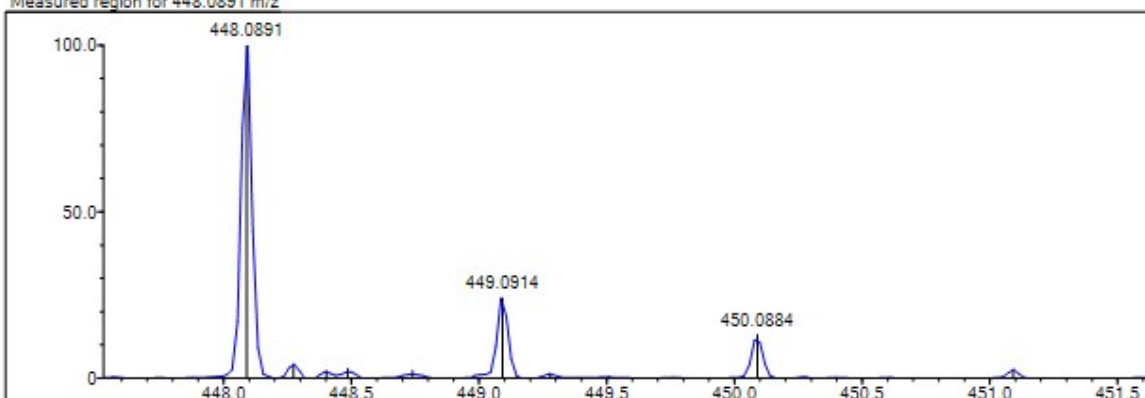
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C	4	8	30	F	1	0	1	Cl	1	0	0	Pd	2	0	0	
N	3	4	5	P	3	0	0	Br	1	0	0	I	3	0	0	

Error Margin (ppm): 5  
 DBE Range: 7.0 - 15.0  
 Electron Ions: both  
 HC Ratio: unlimited  
 Apply N Rule: yes  
 Use MSn Info: yes  
 Max Isotopes: 3  
 Isotope RI (%): 1.00  
 MSn Iso RI (%): 10.00  
 MSn Logic Mode: AND  
 Isotope Res: 9000  
 Max Results: 100

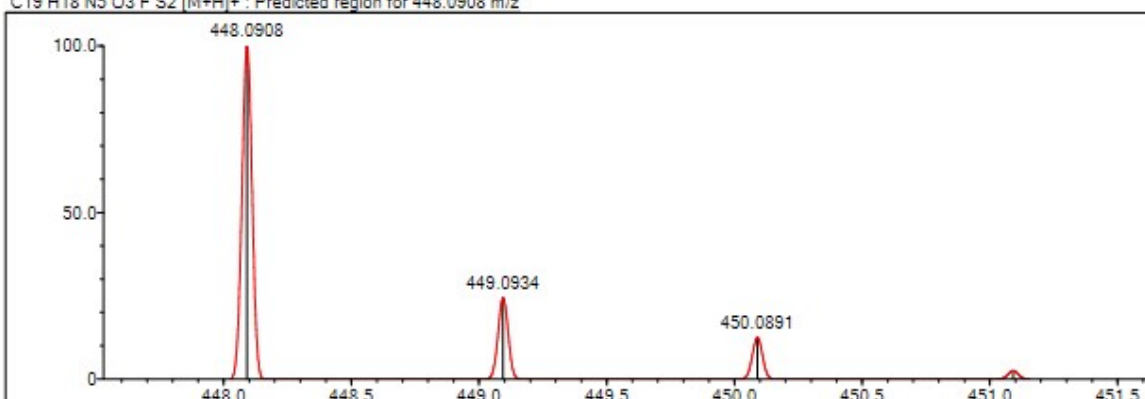
Event#: 1 MS(E+) Ret. Time : 2.587 -> 3.040 Scan#: 389 -> 457



Measured region for 448.0891 m/z



C19 H18 N5 O3 F S2 [M+H]+ : Predicted region for 448.0908 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	92.48	C19 H18 N5 O3 F S2	[M+H] <sup>+</sup>	448.0891	448.0908	-1.7	-3.79	99.42	13.0

Figure S3. Mass spectrum of compound 6a.

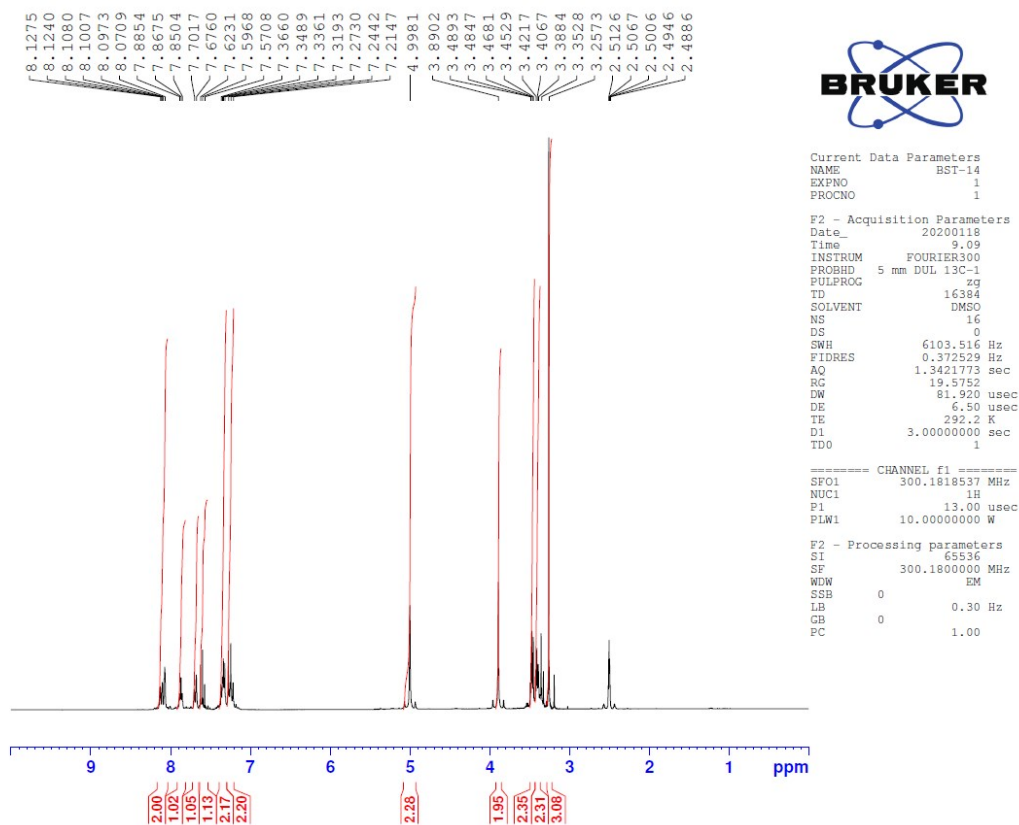


Figure S4.  $^1\text{H}$  NMR spectrum of compound **6b**.

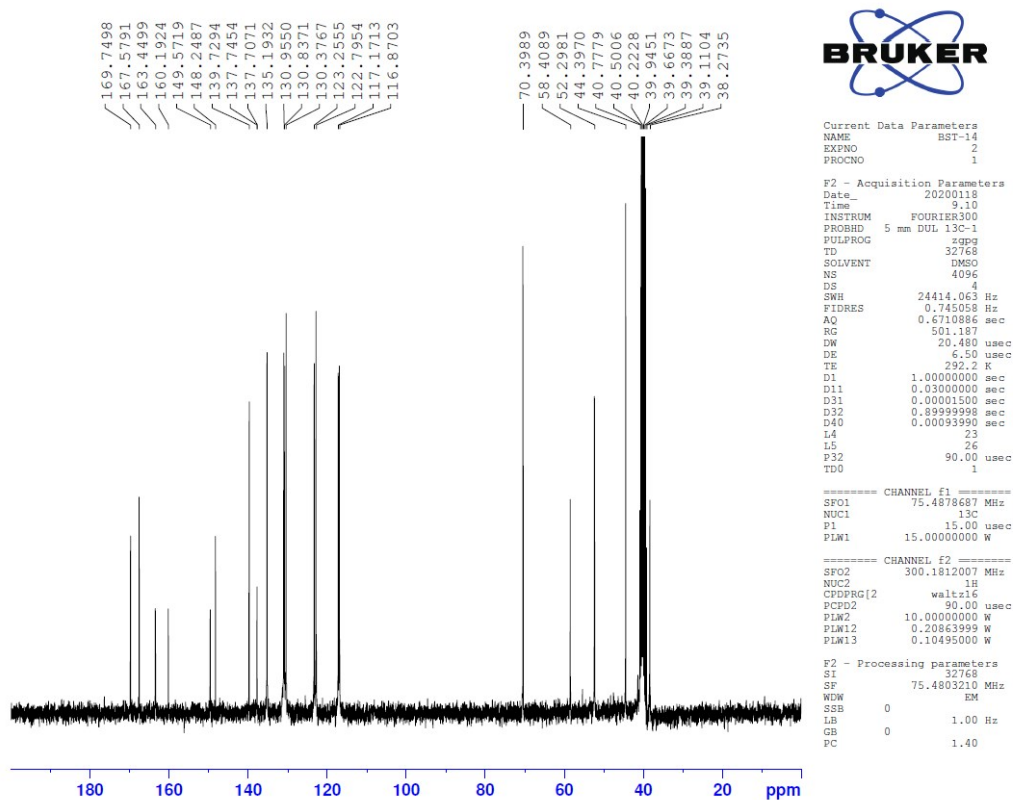


Figure S5.  $^{13}\text{C}$  NMR spectrum of compound **6b**.

Data File: C:\LabSolutions\Data\Analiz\uaoc\BST-14\_7.lcd

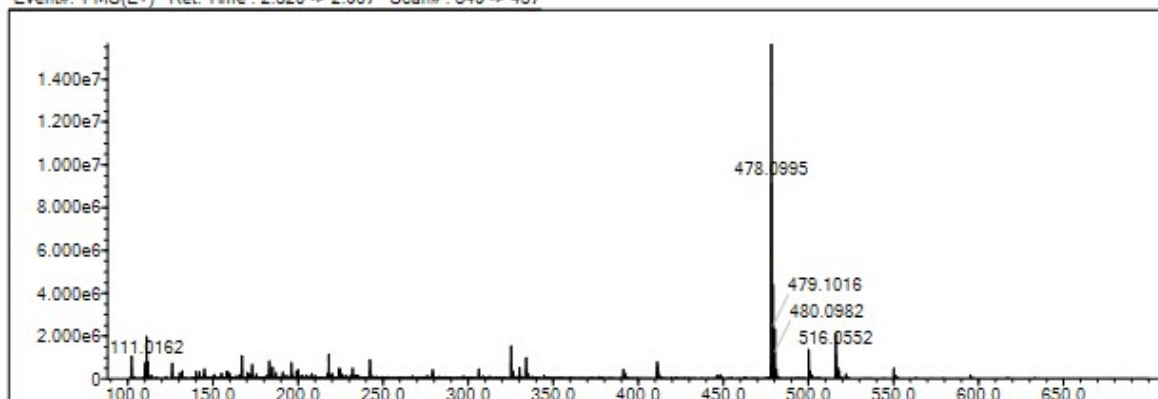
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	6	30	O	2	3	4	S	2	2	3	Ru	2	0	0	H
C	4	8	30	F	1	0	1	Cl	1	0	0	Pd	2	0	0	
N	3	4	5	P	3	0	0	Br	1	0	0	I	3	0	0	

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

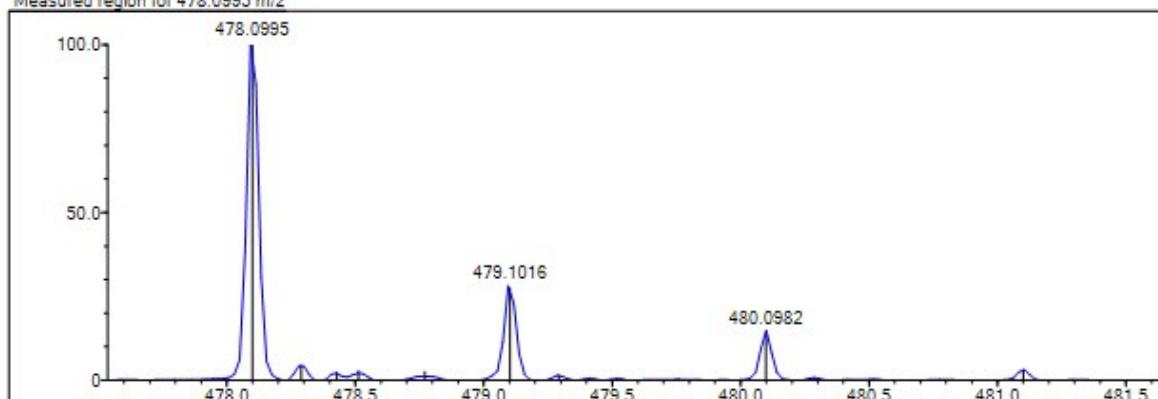
DBE Range: 7.0 - 15.0  
 Apply N Rule: yes  
 Isotope RI (%): 1.00  
 MSn Logic Mode: AND

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

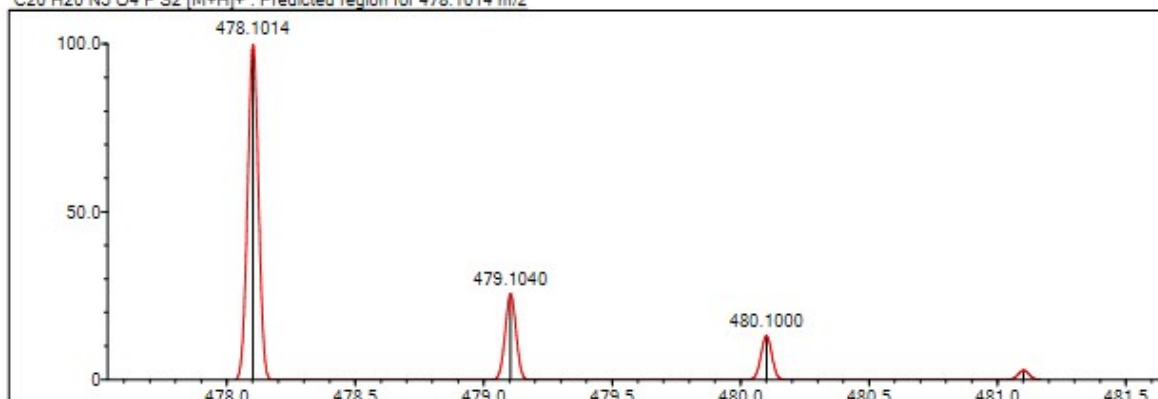
Event#: 1 MS(E+) Ret. Time: 2.320 -> 2.907 Scan#: 349 -> 437



Measured region for 478.0995 m/z



C20 H20 N5 O4 F S2 [M+H]+ : Predicted region for 478.1014 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	85.52	C20 H20 N5 O4 F S2	[M+H]+	478.0995	478.1014	-1.9	-3.97	92.38	13.0

Figure S6. Mass spectrum of compound 6b.

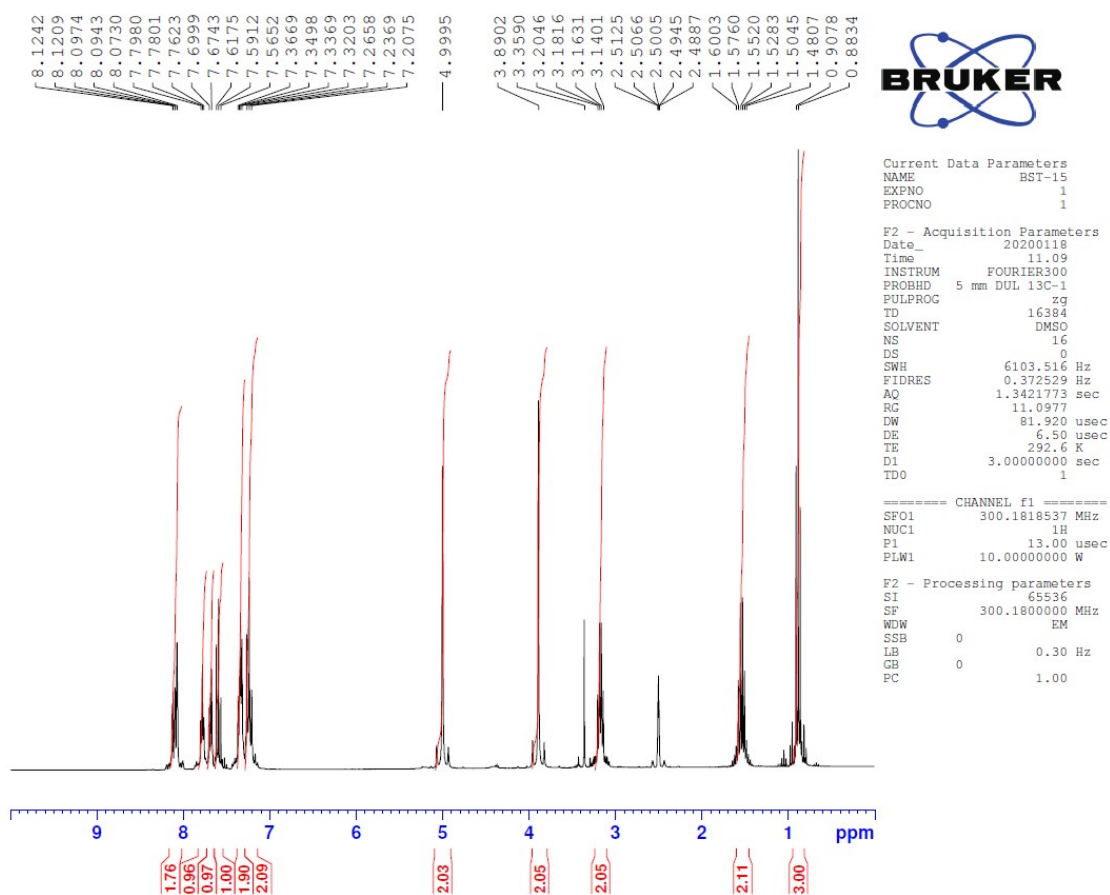


Figure S7. <sup>1</sup>H NMR spectrum of compound 6c.

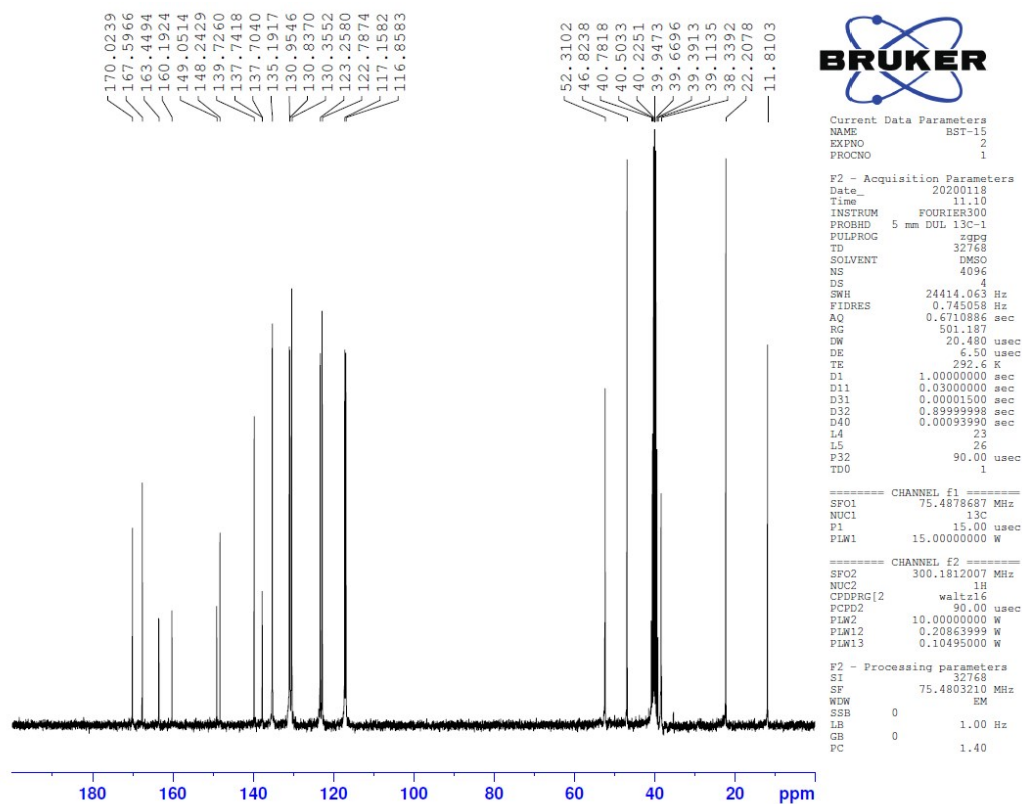


Figure S8. <sup>13</sup>C NMR spectrum of compound 6c.

Data File: C:\LabSolutions\Data\Analiz\luc\BST-15\_8.lcd

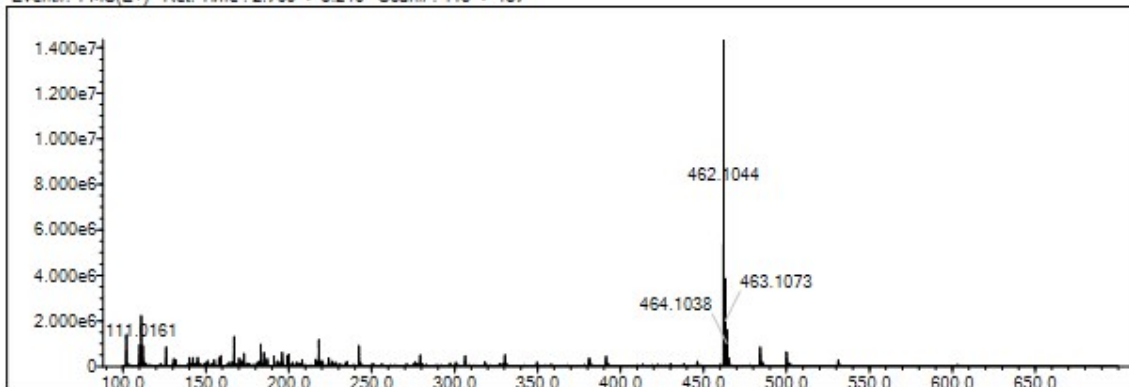
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	6	30	O	2	3	4	S	2	2	3	Ru	2	0	0	H
C	4	8	30	F	1	0	1	Cl	1	0	0	Pd	2	0	0	
N	3	4	5	P	3	0	0	Br	1	0	0	I	3	0	0	

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

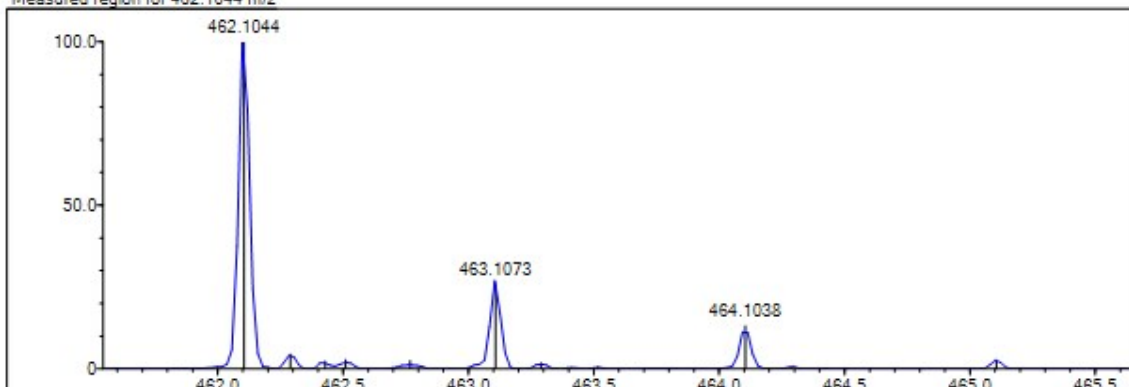
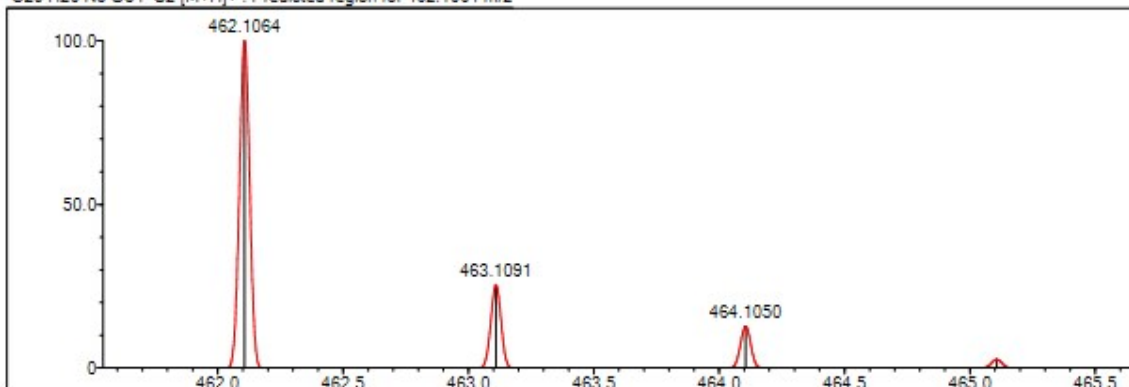
DBE Range: 7.0 - 15.0  
 Apply N Rule: yes  
 Isotope RI (%): 1.00  
 MSn Logic Mode: AND

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

Event#: 1 MS(E+) Ret. Time : 2.760 -&gt; 3.240 Scan#: 415 -&gt; 487



Measured region for 462.1044 m/z

C20 H20 N5 O3 F S2 [M+H]<sup>+</sup> : Predicted region for 462.1064 m/z

Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	75.98	C20 H20 N5 O3 F S2	[M+H] <sup>+</sup>	462.1044	462.1064	-2.0	-4.33	82.88	13.0

Figure S9. Mass spectrum of compound 6c.

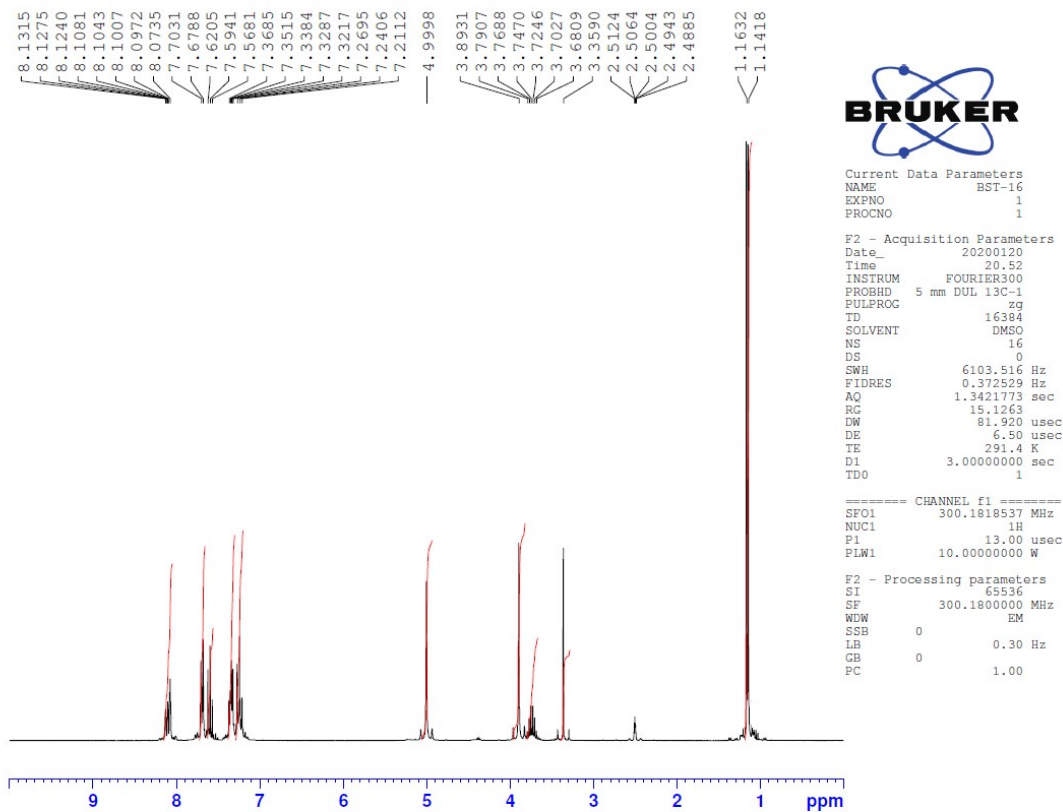


Figure S10. <sup>1</sup>H NMR spectrum of compound 6d.

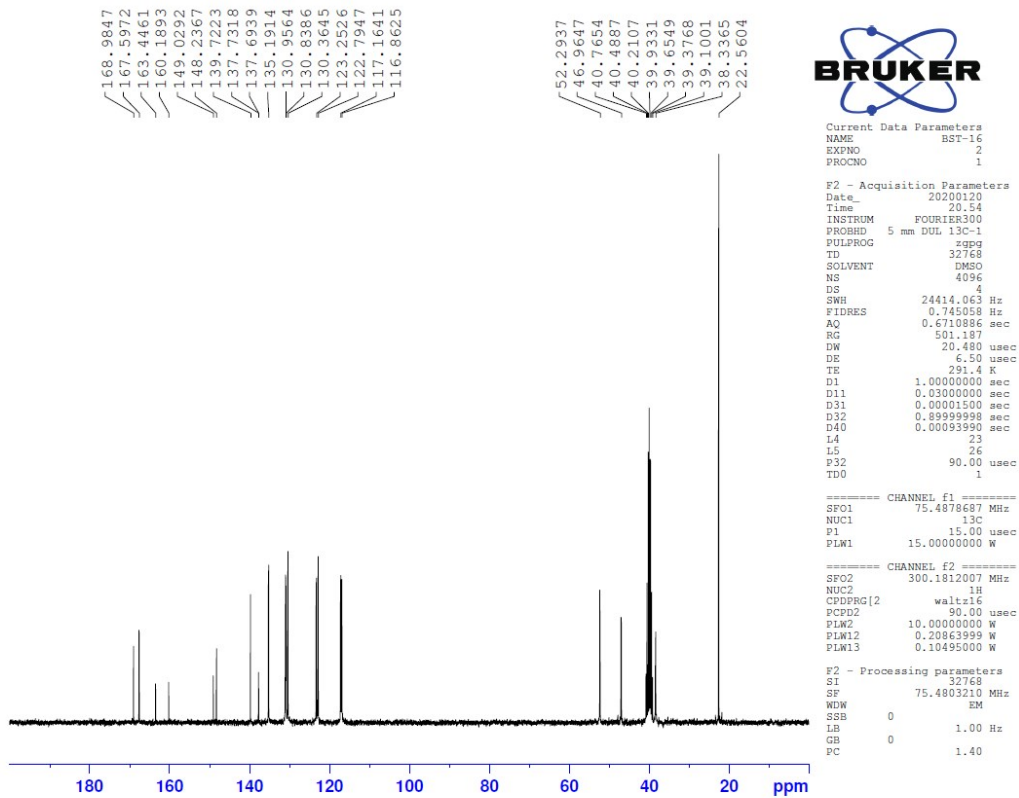


Figure S11. <sup>13</sup>C NMR spectrum of compound 6d.



Data File: C:\LabSolutions\Data\Analiz\luc\BST-16\_9.lcd

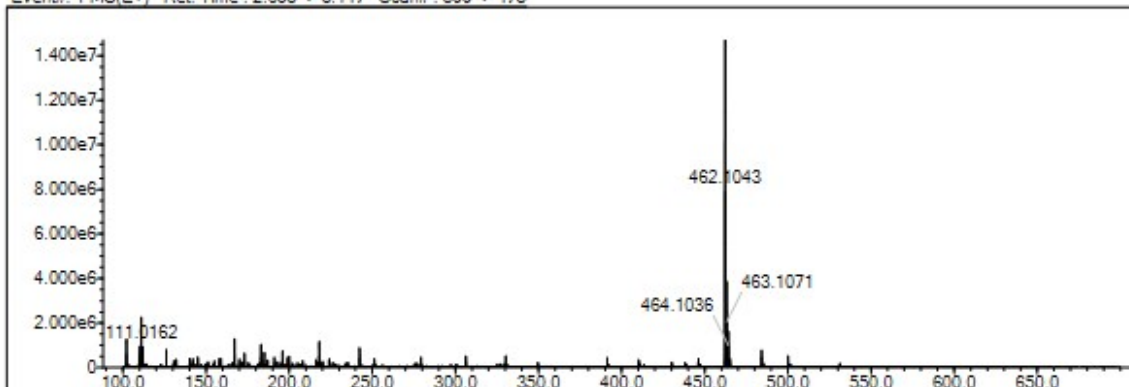
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	6	30	O	2	3	4	S	2	2	3	Ru	2	0	0	H
C	4	8	30	F	1	0	1	Cl	1	0	0	Pd	2	0	0	
N	3	4	5	P	3	0	0	Br	1	0	0	I	3	0	0	

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

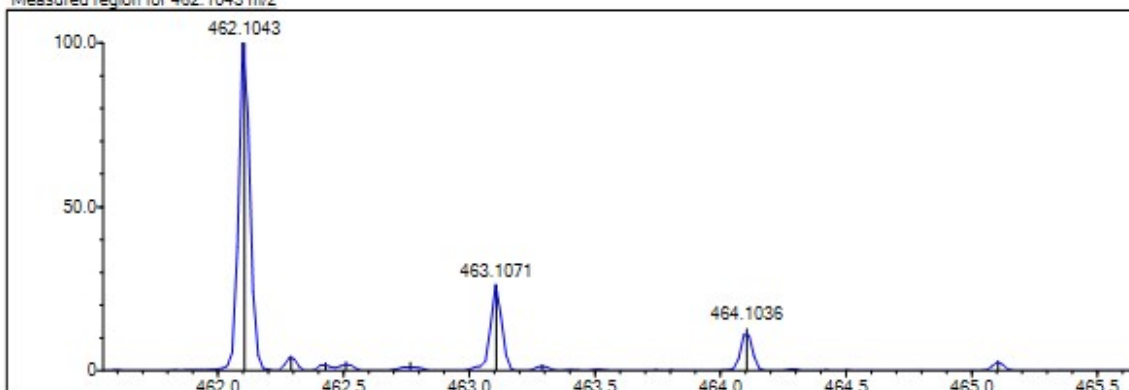
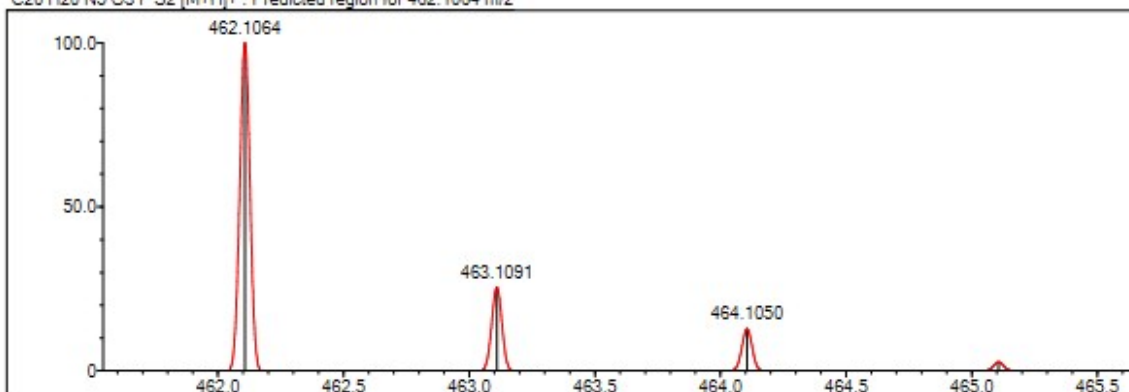
DBE Range: 7.0 - 15.0  
 Apply N Rule: yes  
 Isotope RI (%): 1.00  
 MSn Logic Mode: AND

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

Event#: 1 MS(E+) Ret. Time : 2.653 -&gt; 3.147 Scan#: 399 -&gt; 473



Measured region for 462.1043 m/z

C20 H20 N5 O3 F S2 [M+H]<sup>+</sup> : Predicted region for 462.1064 m/z

Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	74.37	C <sub>20</sub> H <sub>20</sub> N <sub>5</sub> O <sub>3</sub> F S <sub>2</sub>	[M+H] <sup>+</sup>	462.1043	462.1064	-2.1	-4.54	81.59	13.0

Figure S12. Mass spectrum of compound 6d.

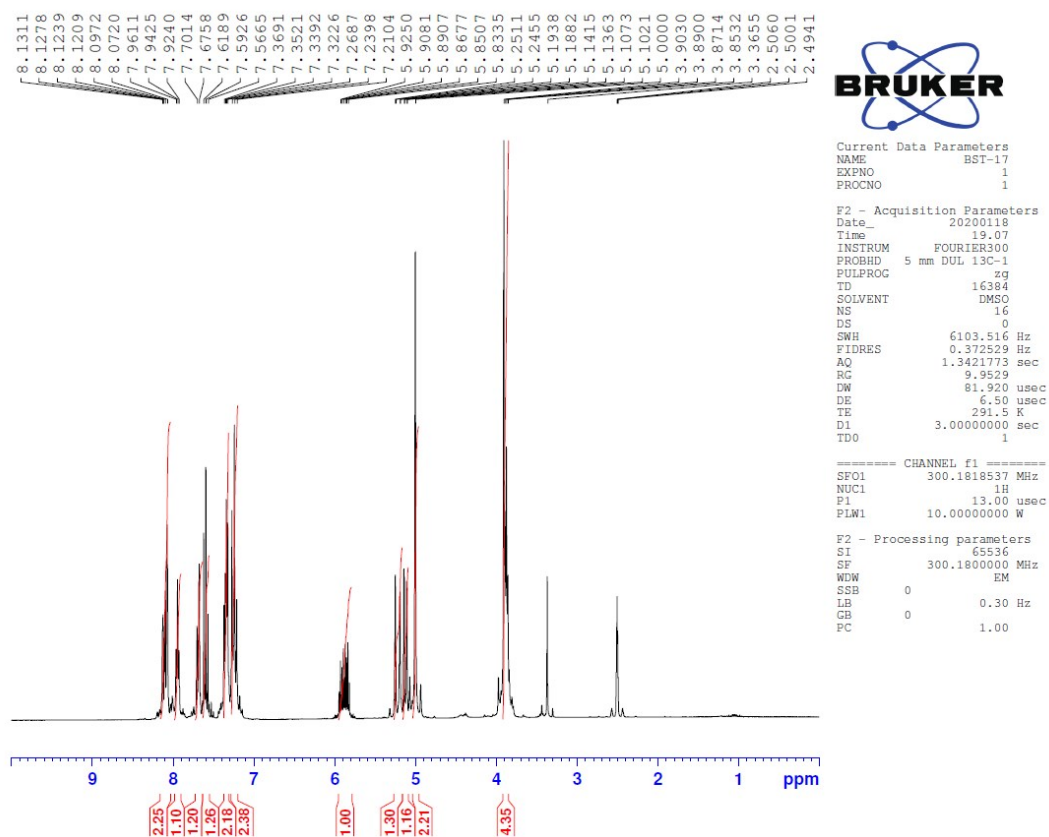


Figure S13. <sup>1</sup>H NMR spectrum of compound 6e.

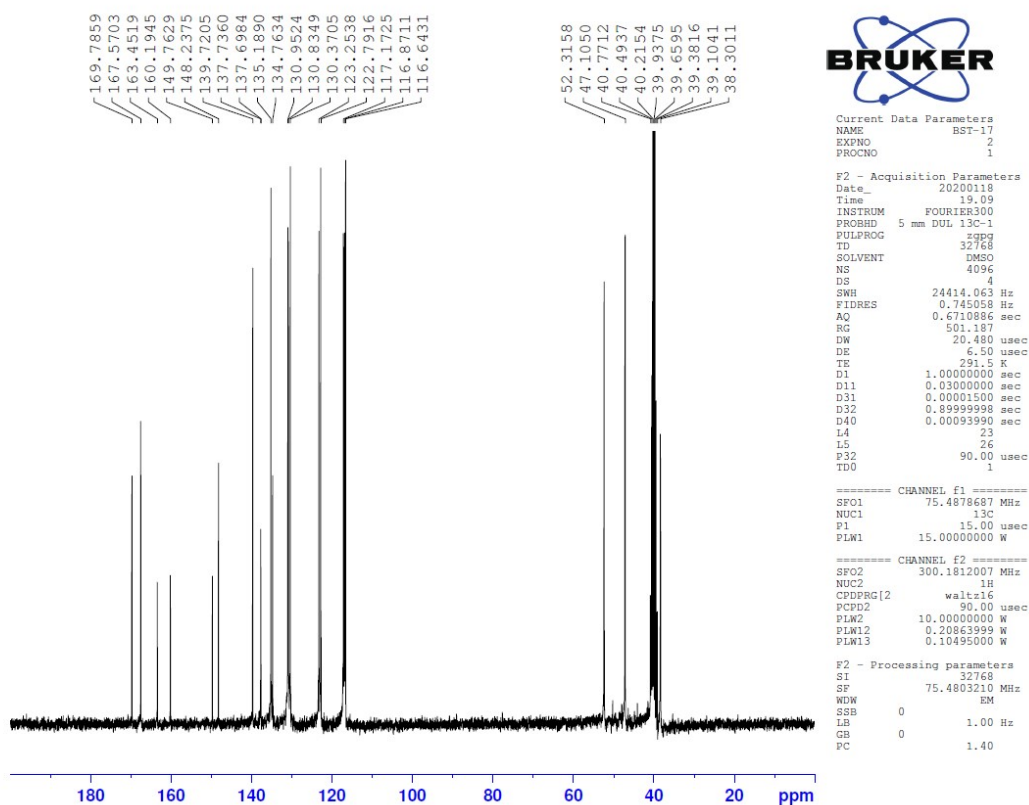


Figure S14. <sup>13</sup>C NMR spectrum of compound 6e.

Data File: C:\LabSolutions\Data\Analiz\uacl\BST-17\_10.lcd

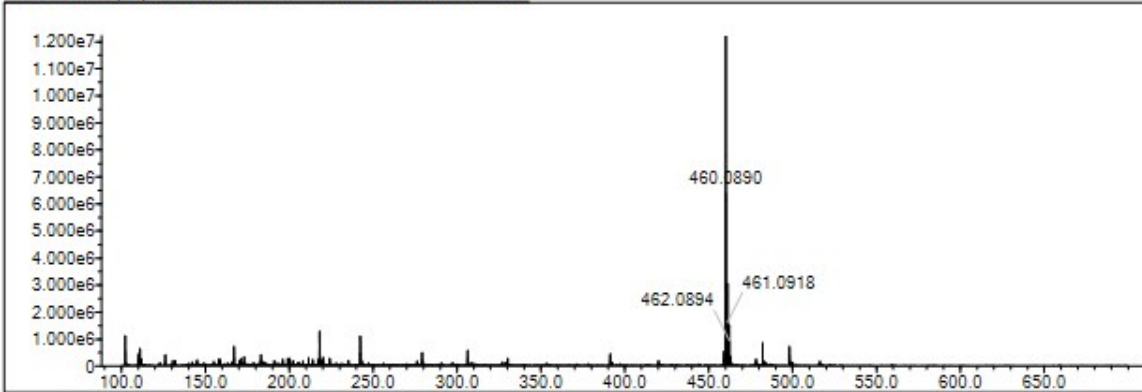
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	6	30	O	2	3	4	S	2	2	3	Ru	2	0	0	H
C	4	8	30	F	1	0	1	Cl	1	0	0	Pd	2	0	0	
N	3	4	5	P	3	0	0	Br	1	0	0	I	3	0	0	

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

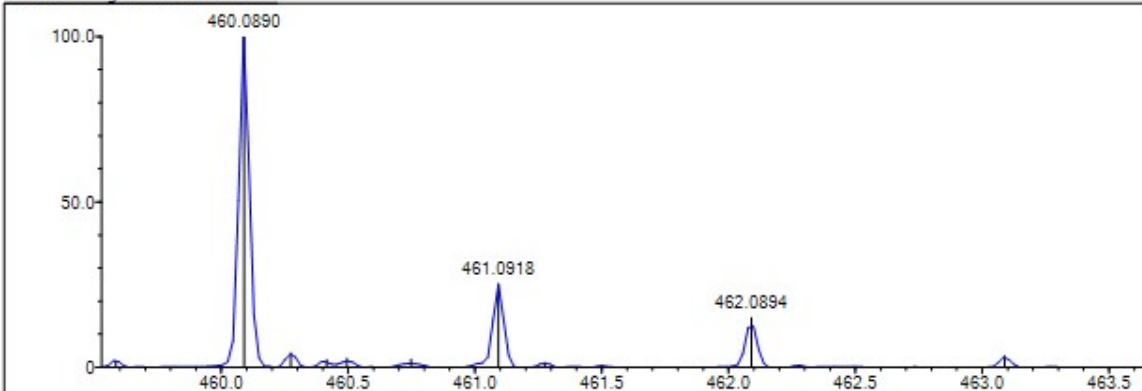
DBE Range: 7.0 - 16.0  
 Apply N Rule: no  
 Isotope RI (%): 1.00  
 MSn Logic Mode: AND

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

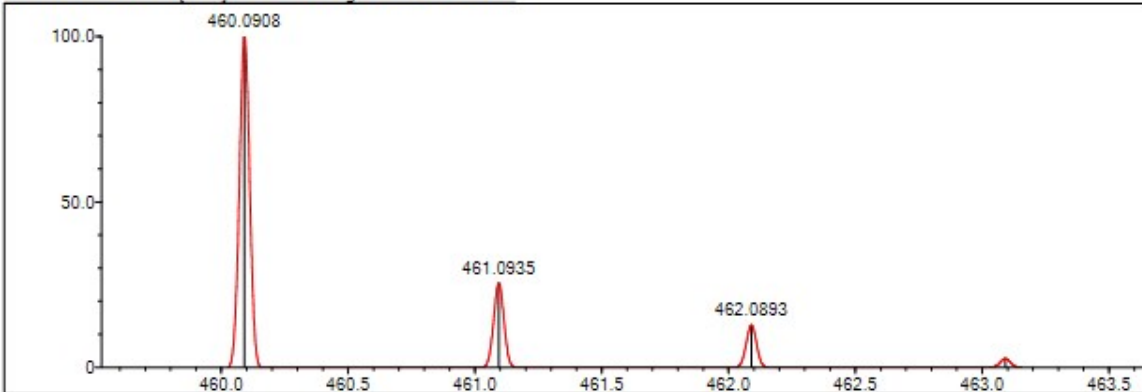
Event#: 1 MS(E+) Ret. Time: 3.507 -> 3.787 Scan#: 527 -> 569



Measured region for 460.0890 m/z



C20 H18 N5 O3 F S2 [M+H]+ : Predicted region for 460.0908 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	81.38	C20 H18 N5 O3 F S2	[M+H]+	460.0890	460.0908	-1.8	-3.91	87.76	14.0

Figure S15. Mass spectrum of compound 6e.

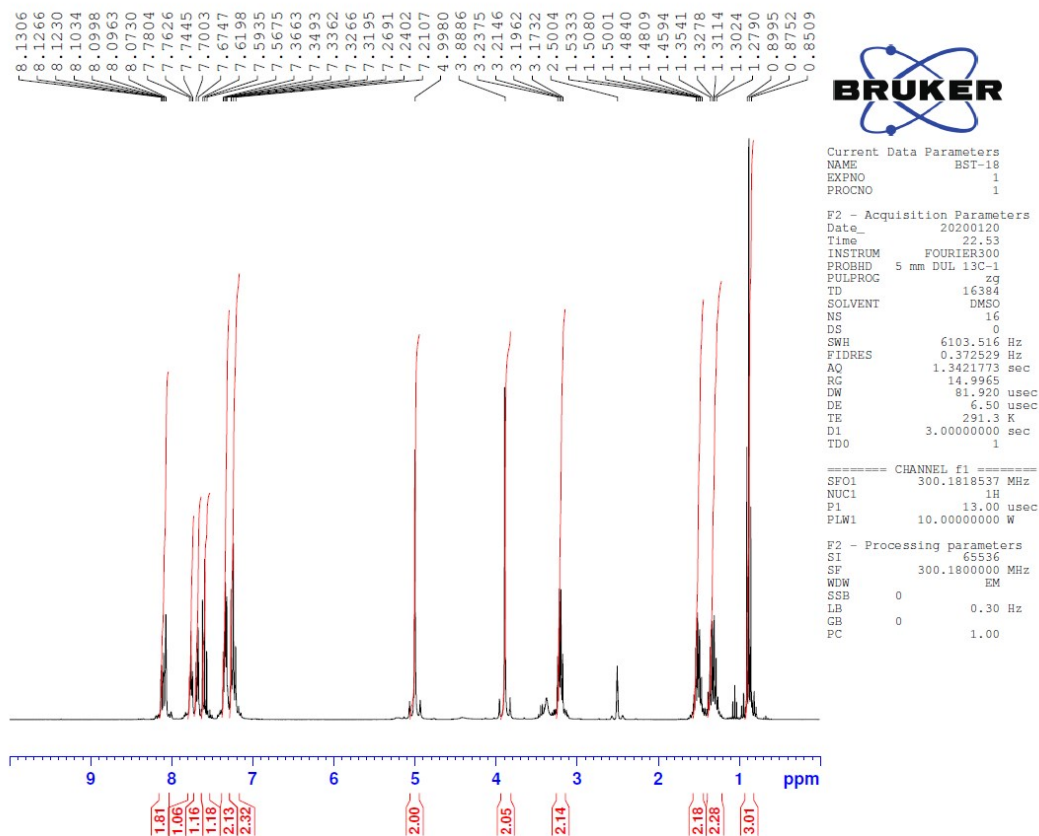


Figure S16. <sup>1</sup>H NMR spectrum of compound **6f**.

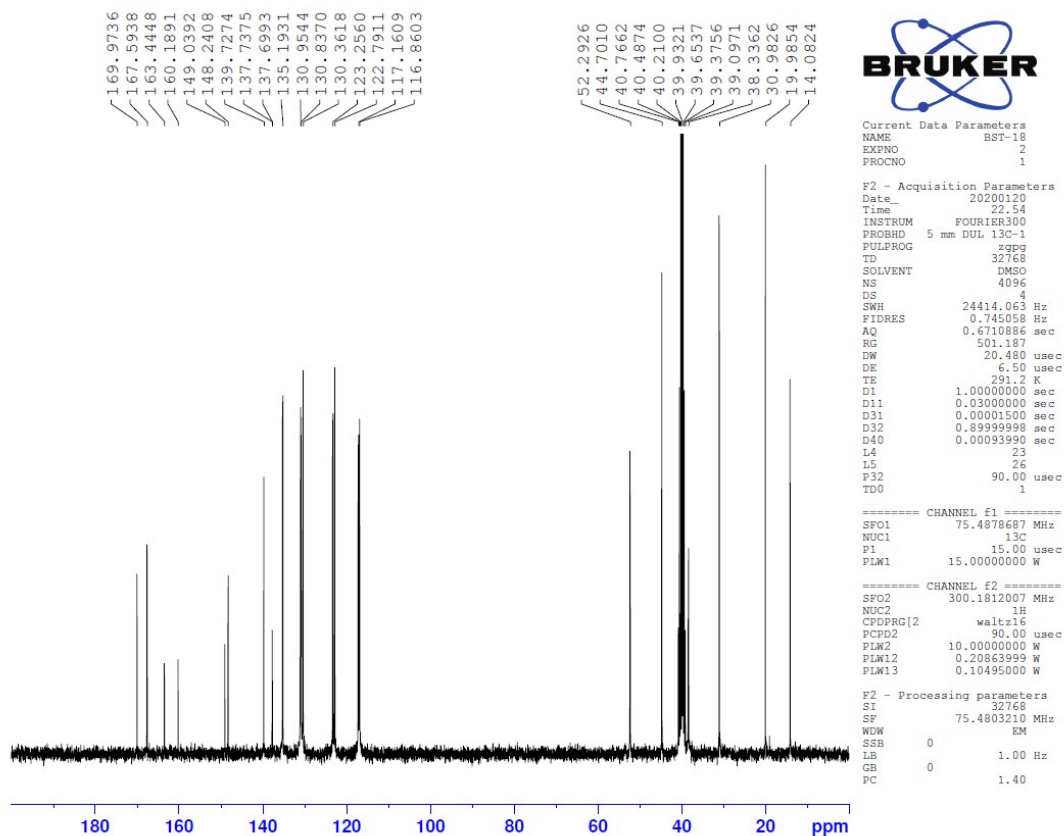


Figure S17. <sup>13</sup>C NMR spectrum of compound **6f**.

Data File: C:\LabSolutions\Data\Analiz\uo\BST-18\_11.lcd

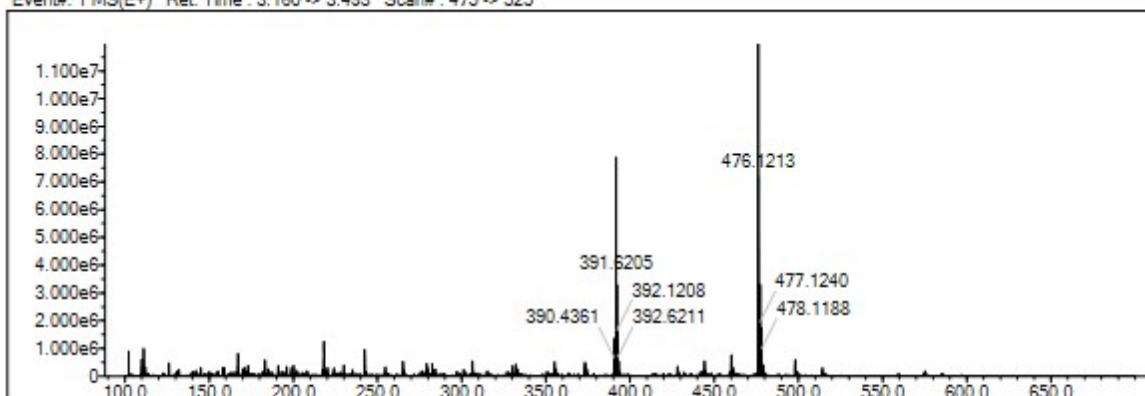
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H	1	6	30	O	2	3	4	S	2	2	3	Ru	2	0	0	H
C	4	8	30	F	1	0	1	Cl	1	0	0	Pd	2	0	0	
N	3	4	5	P	3	0	0	Br	1	0	0	I	3	0	0	

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

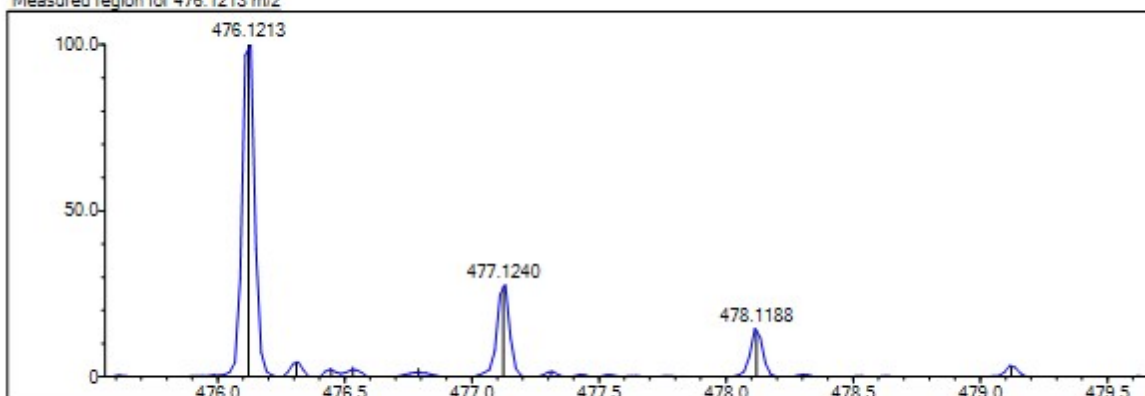
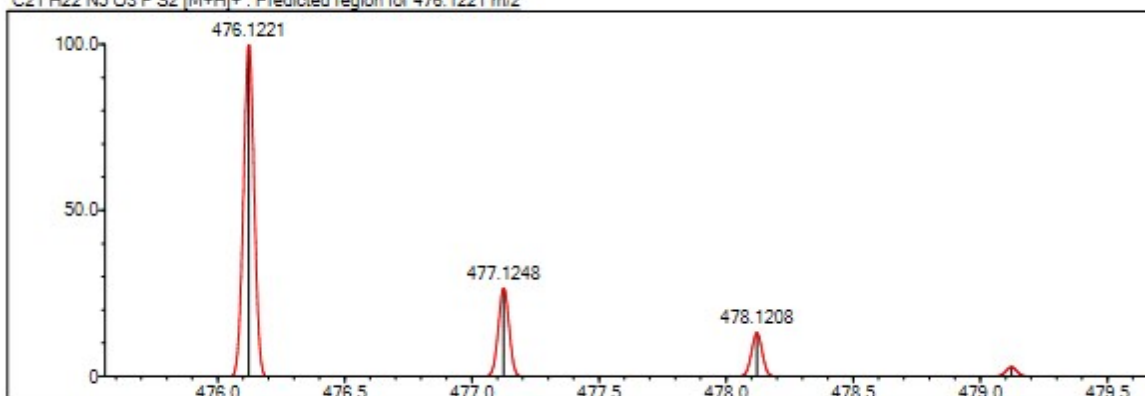
DBE Range: 7.0 - 16.0  
 Apply N Rule: no  
 Isotope RI (%): 1.00  
 MSn Logic Mode: AND

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

Event#: 1 MS(E+) Ret. Time : 3.160 -&gt; 3.493 Scan#: 475 -&gt; 525



Measured region for 476.1213 m/z

C21 H22 N5 O3 F S2 [M+H]<sup>+</sup>: Predicted region for 476.1221 m/z

Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	98.30	C21 H22 N5 O3 F S2	[M+H] <sup>+</sup>	476.1213	476.1221	-0.8	-1.68	100.00	13.0

Figure S18. Mass spectrum of compound 6f.

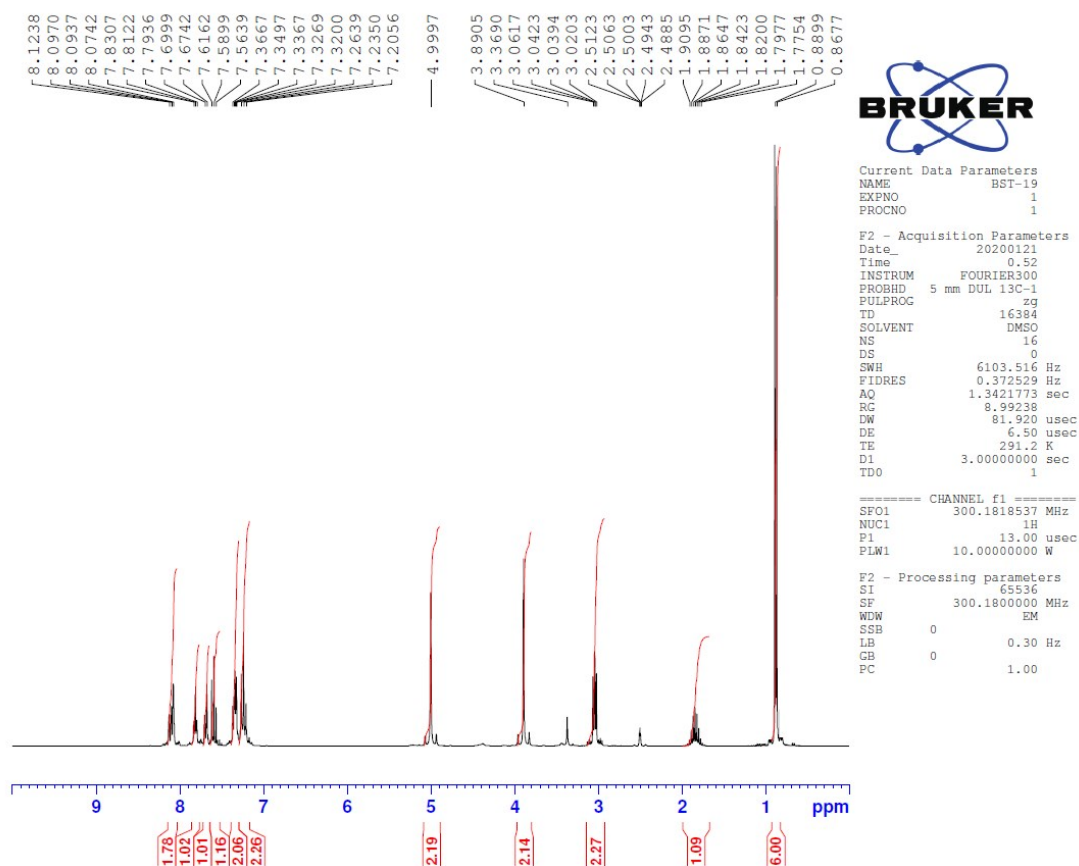


Figure S19.  $^1\text{H}$  NMR spectrum of compound **6g**.

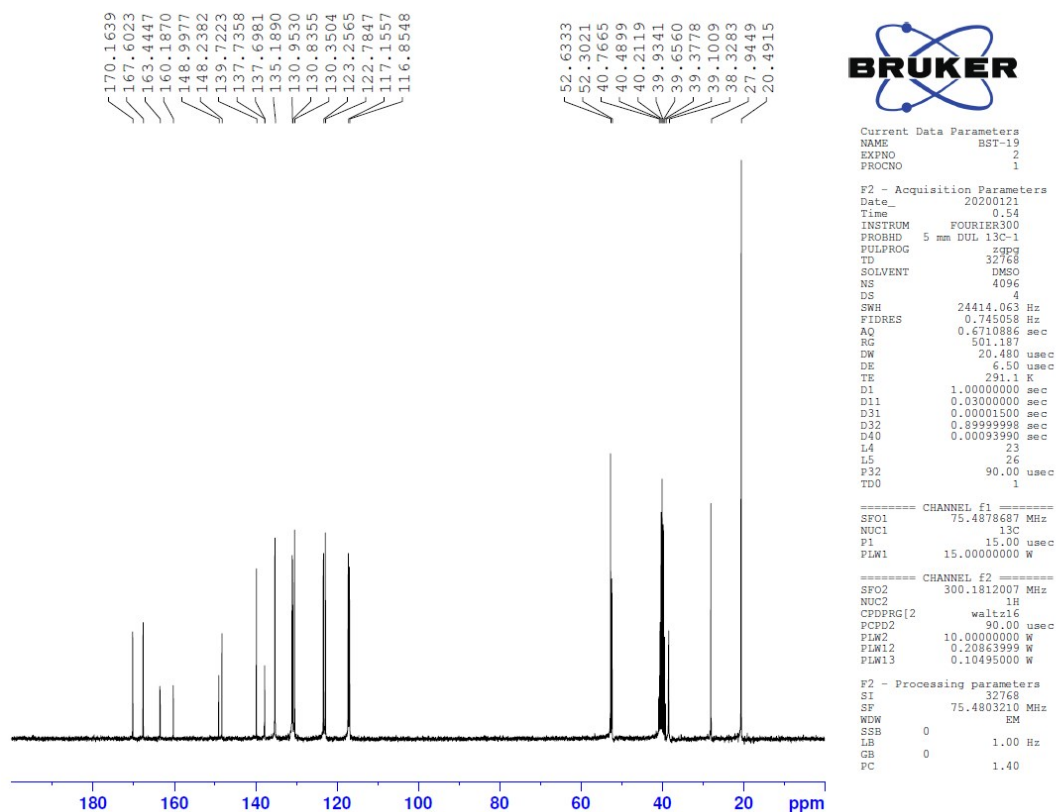


Figure S20.  $^{13}\text{C}$  NMR spectrum of compound **6g**.

Data File: C:\LabSolutions\Data\Analiz\luc\BST-19\_12.lcd

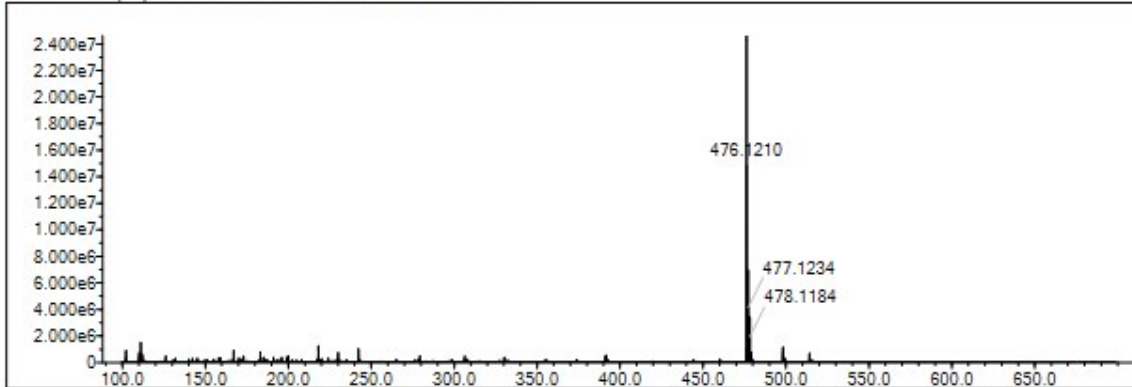
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	6	30	O	2	3	4	S	2	2	3	Ru	2	0	0	H
C	4	8	30	F	1	0	1	Cl	1	0	0	Pd	2	0	0	
N	3	4	5	P	3	0	0	Br	1	0	0	I	3	0	0	

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

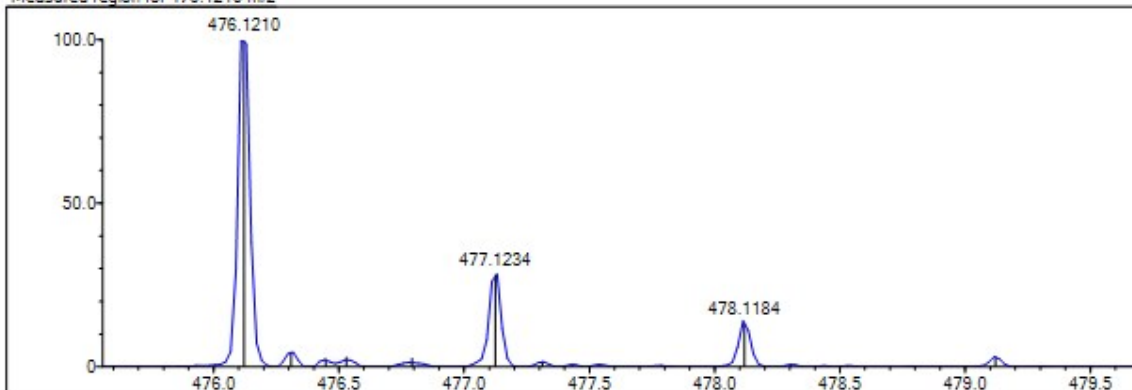
DBE Range: 7.0 - 16.0  
 Apply N Rule: no  
 Isotope RI (%): 1.00  
 MSn Logic Mode: AND

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

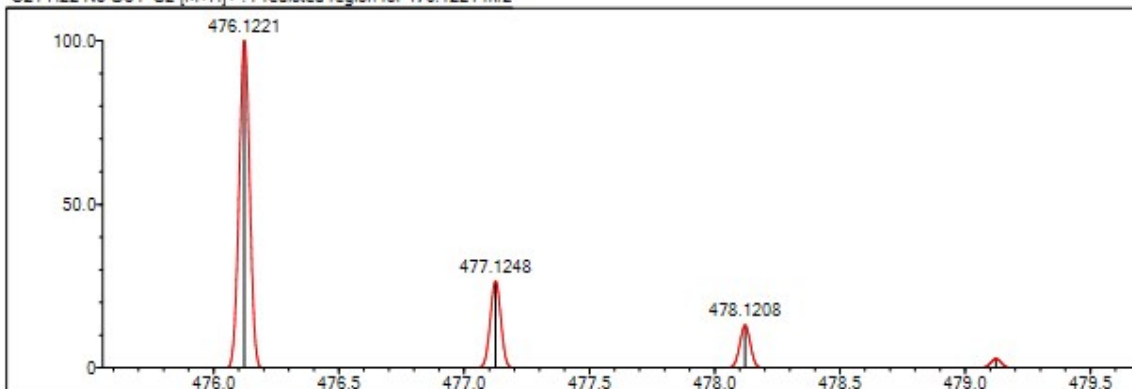
Event#: 1 MS(E+) Ret. Time : 2.933 -> 3.333 Scan#: 441 -> 501



Measured region for 476.1210 m/z



C21 H22 N5 O3 F S2 [M+H]+ : Predicted region for 476.1221 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	96.72	C21 H22 N5 O3 F S2	[M+H] <sup>+</sup>	476.1210	476.1221	-1.1	-2.31	100.00	13.0

Figure S21. Mass spectrum of compound 6g.

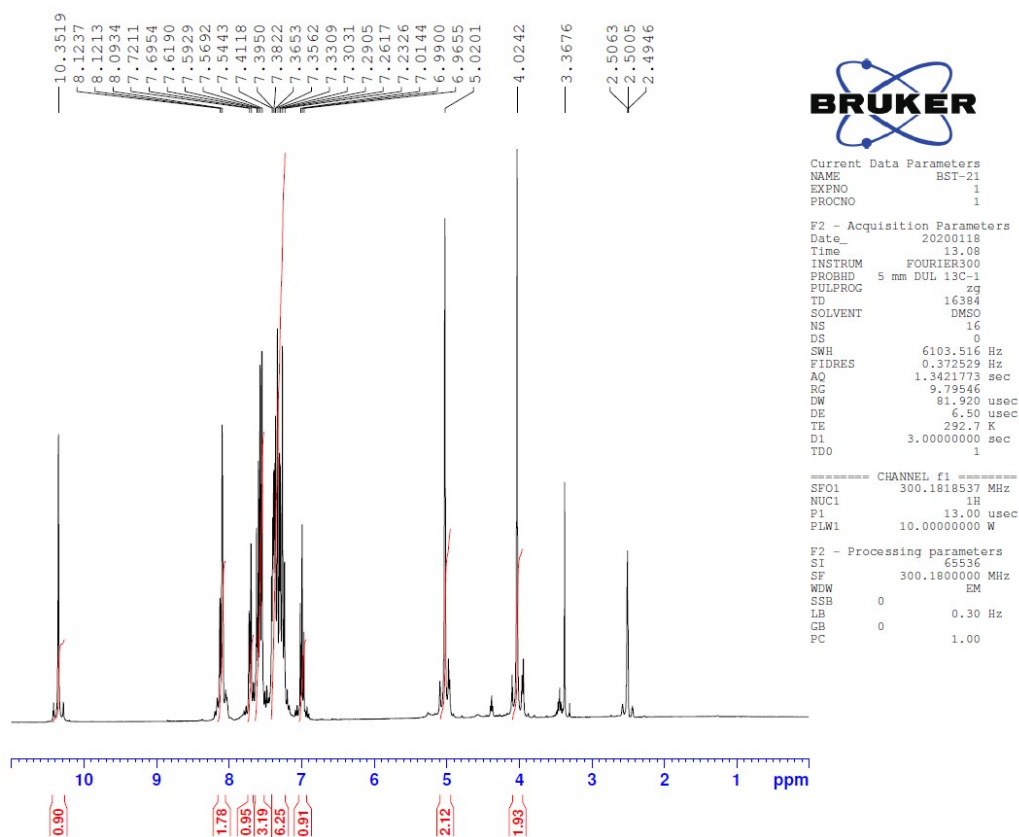


Figure S22. <sup>1</sup>H NMR spectrum of compound 6h.

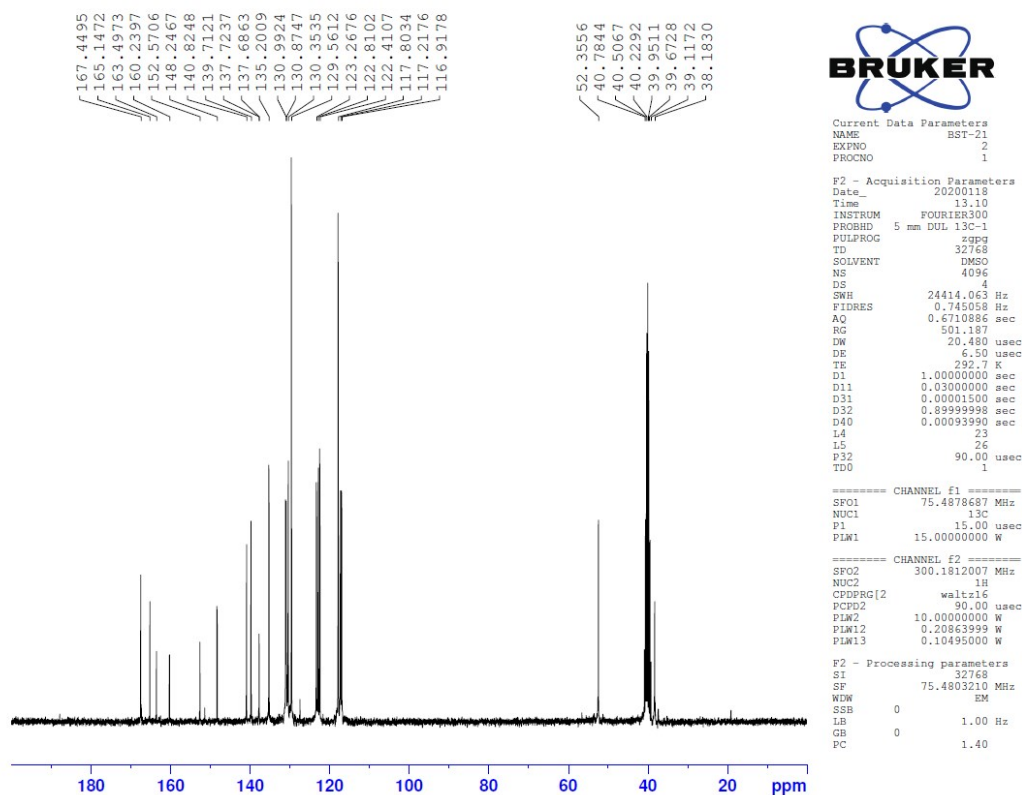


Figure S23. <sup>13</sup>C NMR spectrum of compound 6h.



Data File: C:\LabSolutions\Data\Analiz\usc\BST-21\_13.lcd

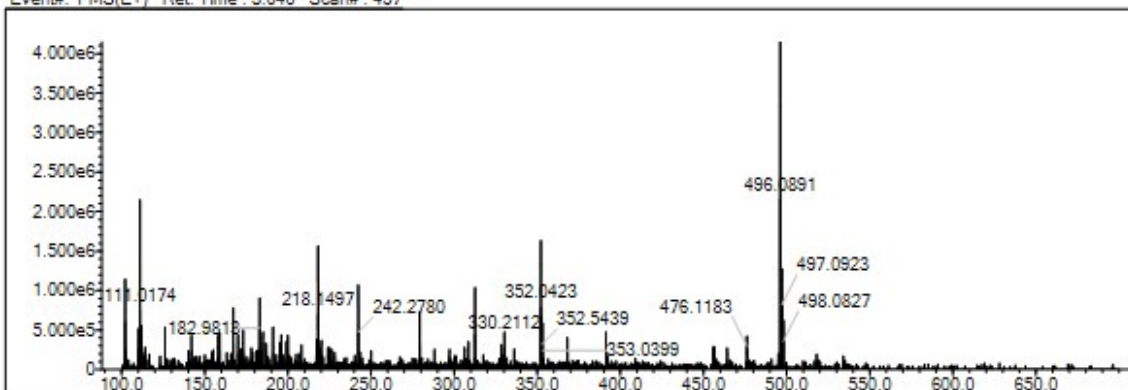
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	6	30	O	2	3	4	S	2	2	3	Ru	2	0	0	H
C	4	8	30	F	1	0	1	Cl	1	0	0	Pd	2	0	0	
N	3	4	5	P	3	0	0	Br	1	0	0	I	3	0	0	

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

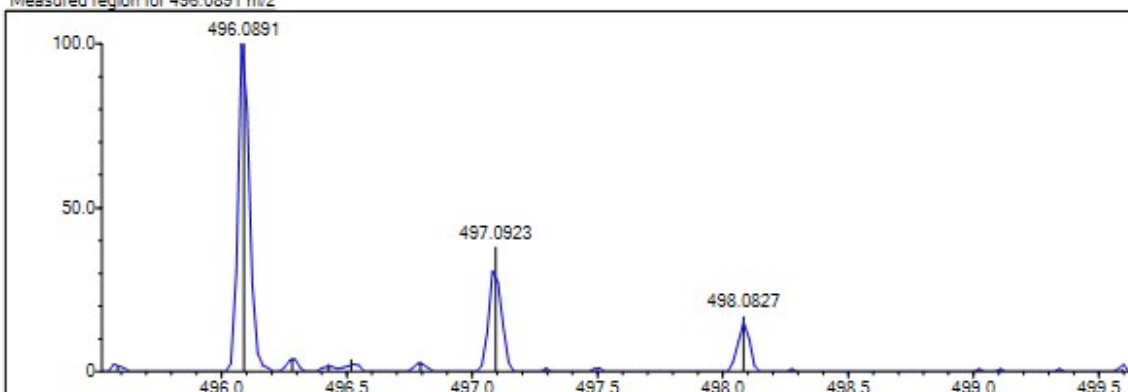
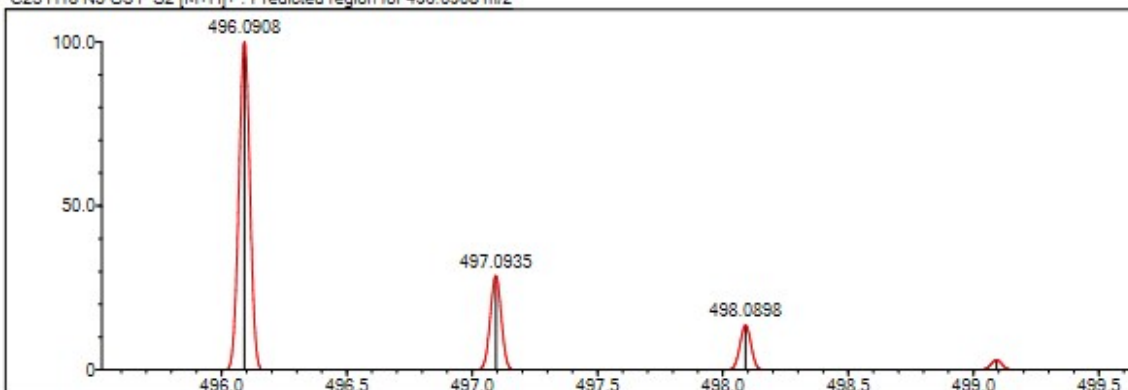
DBE Range: 7.0 - 20.0  
 Apply N Rule: yes  
 Isotope RI (%): 1.00  
 MSn Logic Mode: AND

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

Event#: 1 MS(E+) Ret. Time : 3.040 Scan#: 457



Measured region for 496.0891 m/z

C23 H18 N5 O3 F S2 [M+H]<sup>+</sup> : Predicted region for 496.0908 m/z

Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	48.35	C23 H18 N5 O3 F S2	[M+H] <sup>+</sup>	496.0891	496.0908	-1.7	-3.43	51.48	17.0

Figure S24. Mass spectrum of compound 6h.

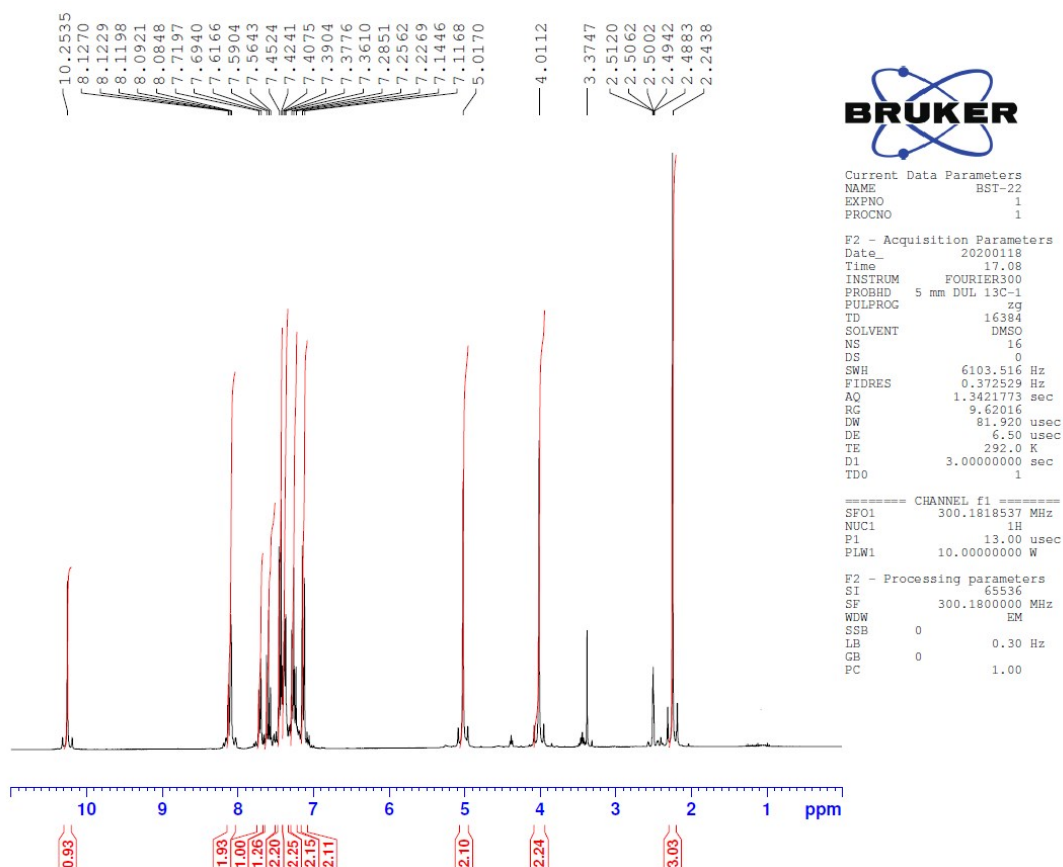


Figure S25. <sup>1</sup>H NMR spectrum of compound **6i**.

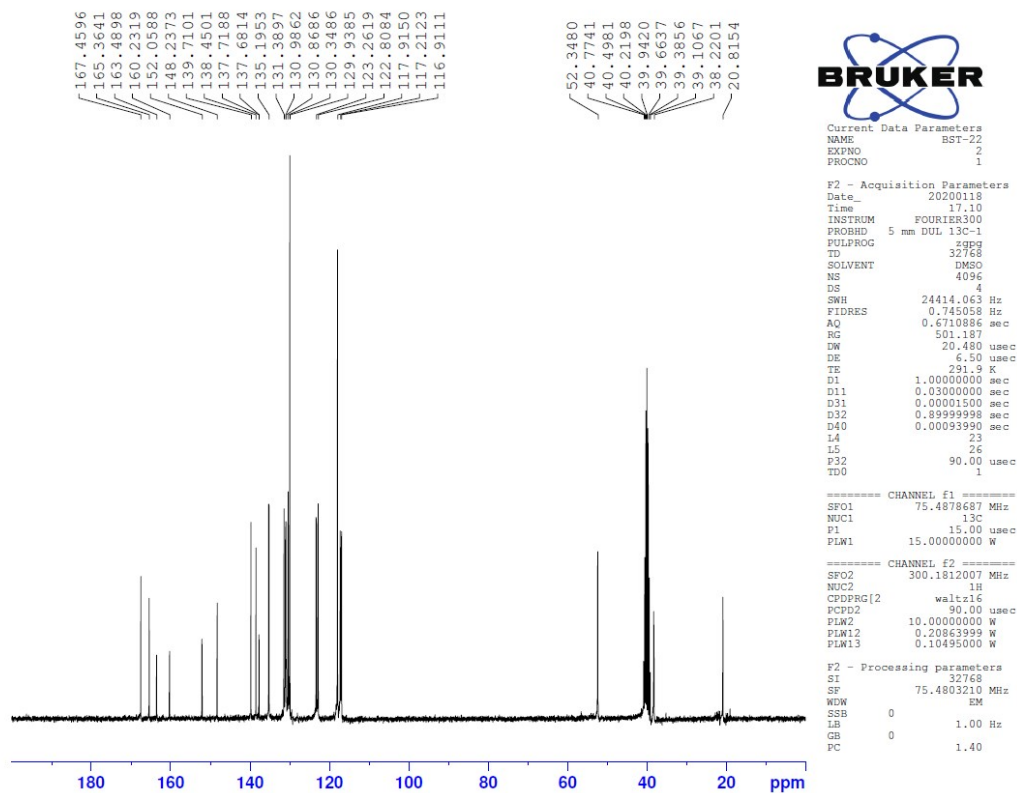


Figure S26. <sup>13</sup>C NMR spectrum of compound **6i**.

Data File: C:\LabSolutions\Data\Analiz\luc\BST-22\_14.lcd

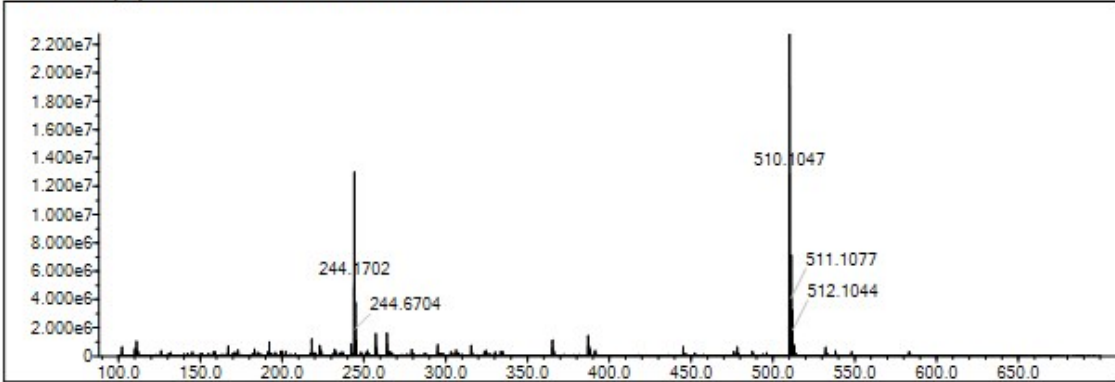
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	6	30	O	2	3	4	S	2	2	3	Ru	2	0	0	H
C	4	8	30	F	1	0	1	Cl	1	0	0	Pd	2	0	0	
N	3	4	5	P	3	0	0	Br	1	0	0	I	3	0	0	

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

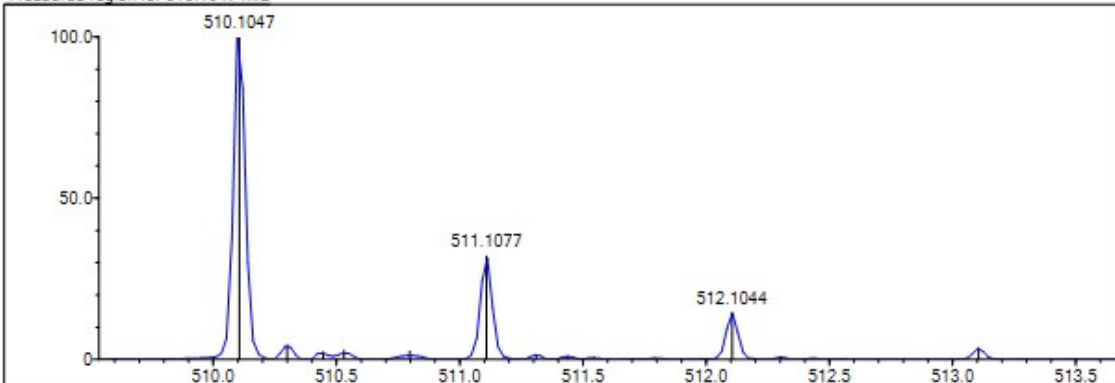
DBE Range: 7.0 - 20.0  
 Apply N Rule: yes  
 Isotope RI (%): 1.00  
 MSn Logic Mode: AND

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

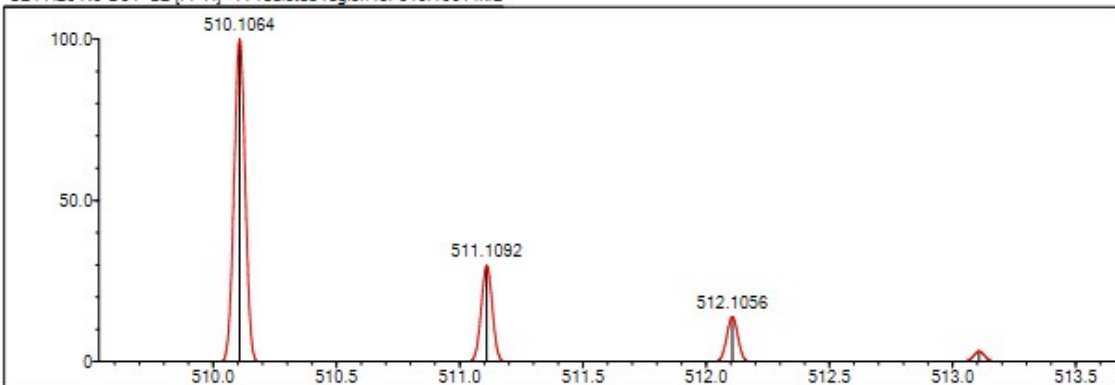
Event#: 1 MS(E+) Ret. Time : 3.080 -> 3.360 Scan#: 463 -> 505



Measured region for 510.1047 m/z



C24 H20 N5 O3 F S2 [M+H]<sup>+</sup> : Predicted region for 510.1064 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	82.62	C24 H20 N5 O3 F S2	[M+H] <sup>+</sup>	510.1047	510.1064	-1.7	-3.33	87.73	17.0

Figure S27. Mass spectrum of compound 6i.