

SUPPORTING INFORMATION

Synthesis of Novel Benzothiazol Derivatives and Investigation of Their Enzyme Inhibitor Effects Against Alzheimer's Disease

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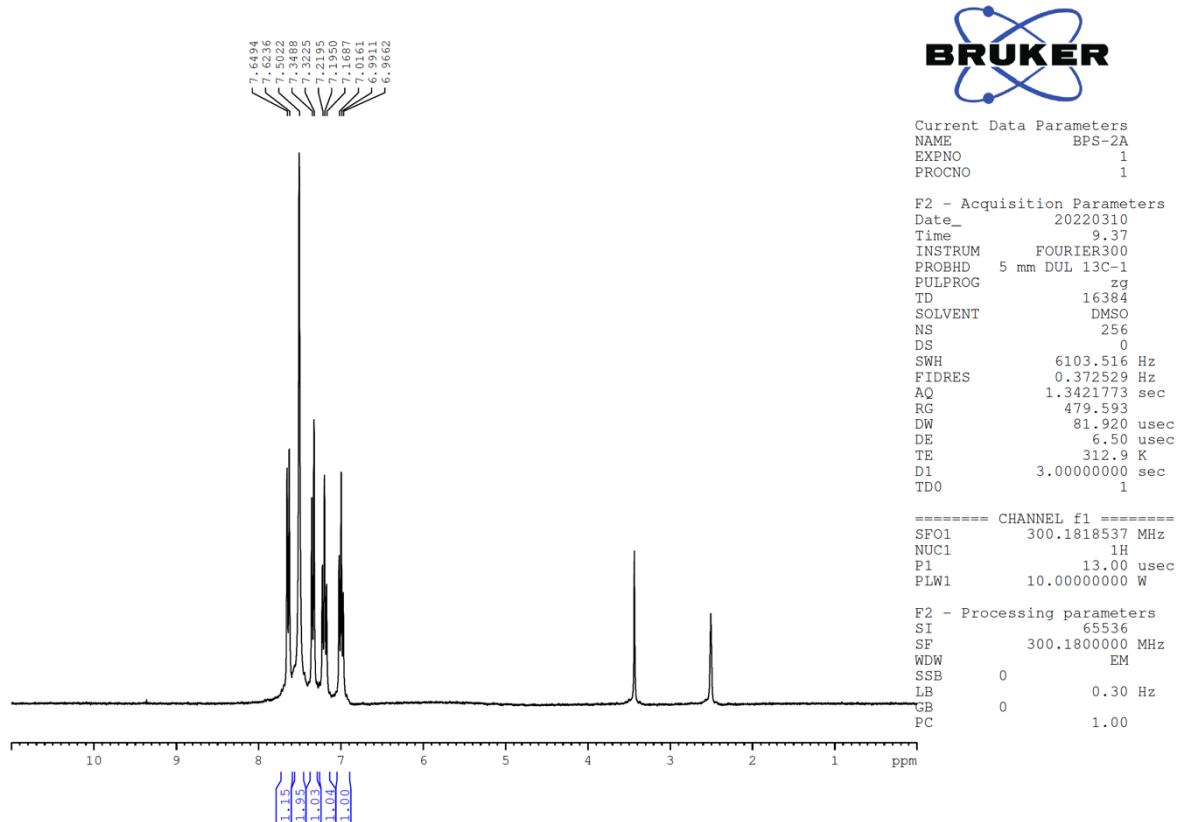


Figure S1. ¹H-NMR spectra of compounds 2a

Data File: C:\LabSolutions\Data\Analiz\deya\BPS-2A_226.lcd

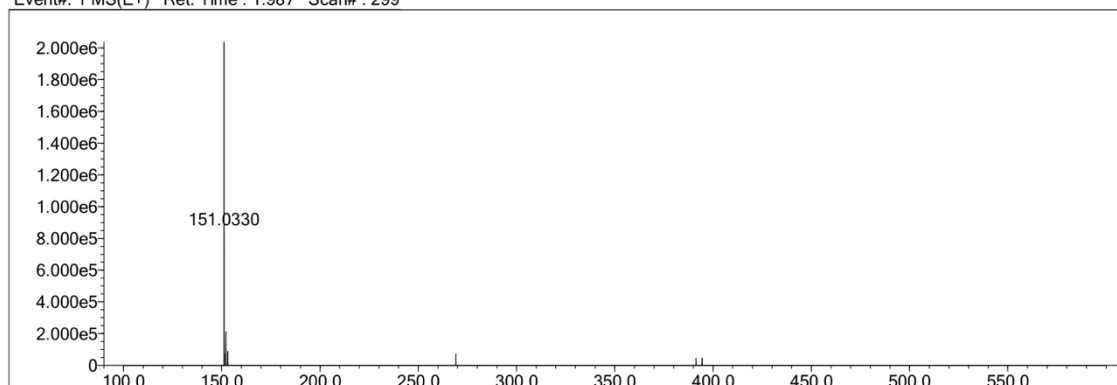
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C	4	5	30	F	1	0	0	Cl	1	0	0	Pd	2	0	0	
N	3	0	5	P	3	0	0	Br	1	0	0	I	3	0	0	

Error Margin (ppm): 15
 HC Ratio: unlimited
 Max Isotopes: 3
 MSn Iso RI (%): 10.00

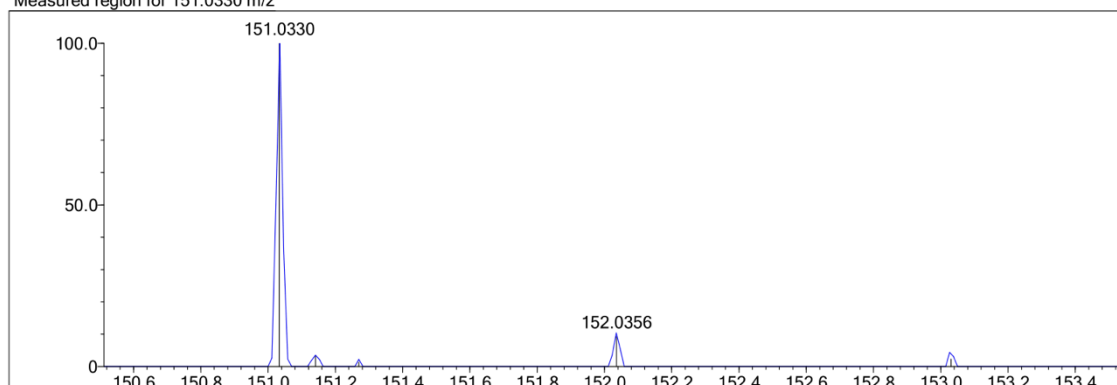
DBE Range: 5.0 - 20.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: yes
 Isotope Res: 9000
 Max Results: 500

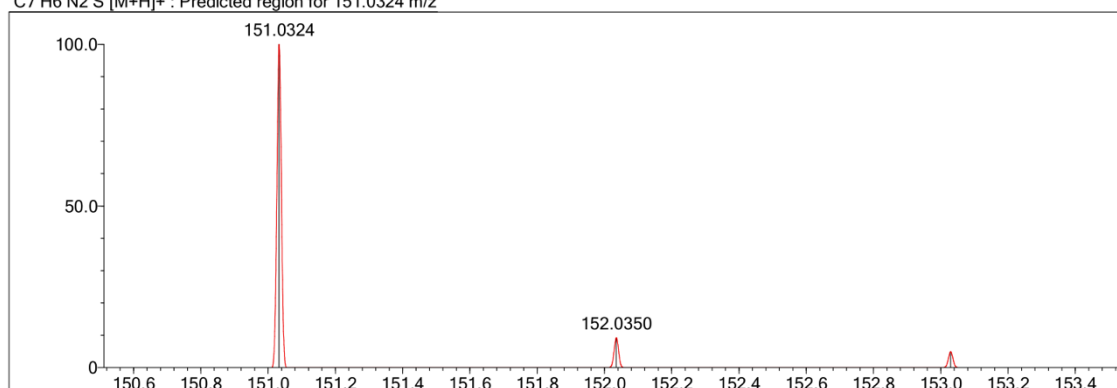
Event#: 1 MS(E+) Ret. Time : 1.987 Scan#: 299



Measured region for 151.0330 m/z



C7 H6 N2 S [M+H]⁺ : Predicted region for 151.0324 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	67.82	C7 H6 N2 S	[M+H] ⁺	151.0330	151.0324	0.6	3.97	73.26	6.0

Figure S2. HRMS spectra of compounds 2a

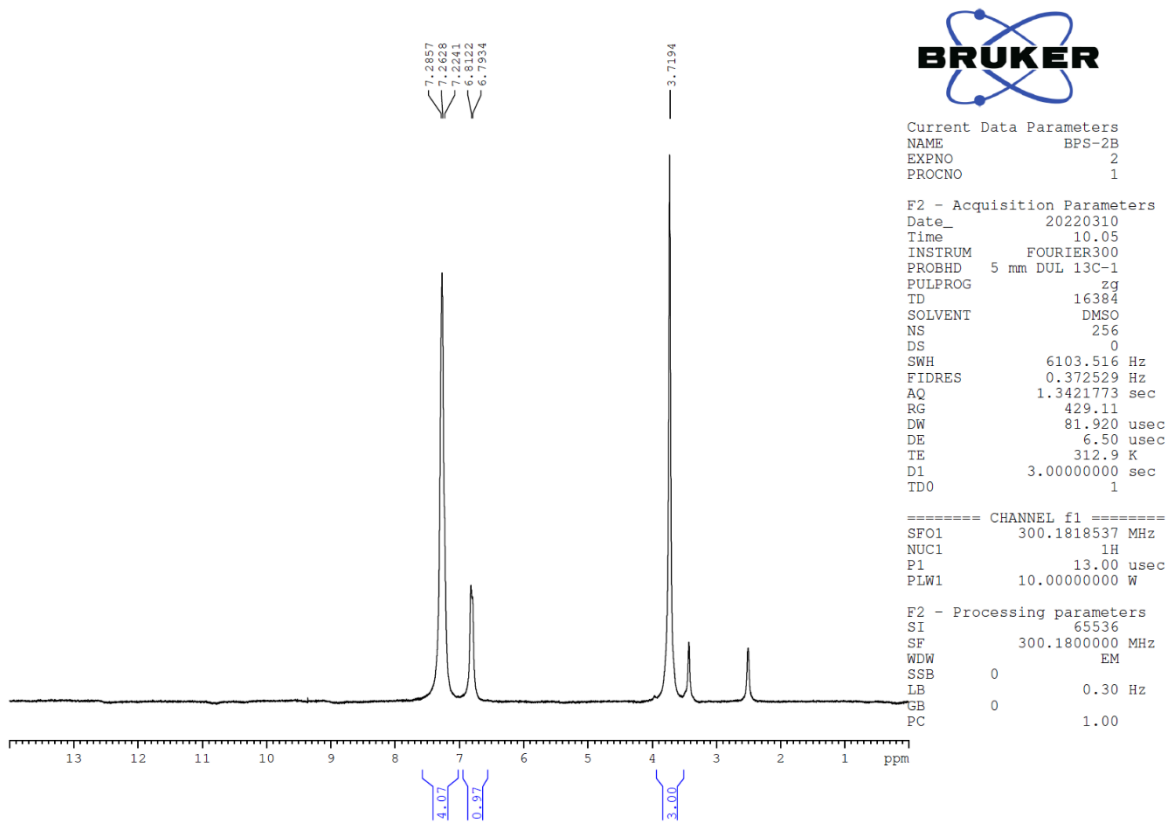


Figure S3. ¹H-NMR spectra of compounds **2b**

Data File: C:\LabSolutions\Data\Analiz\dera\BPS-2B_227.lcd

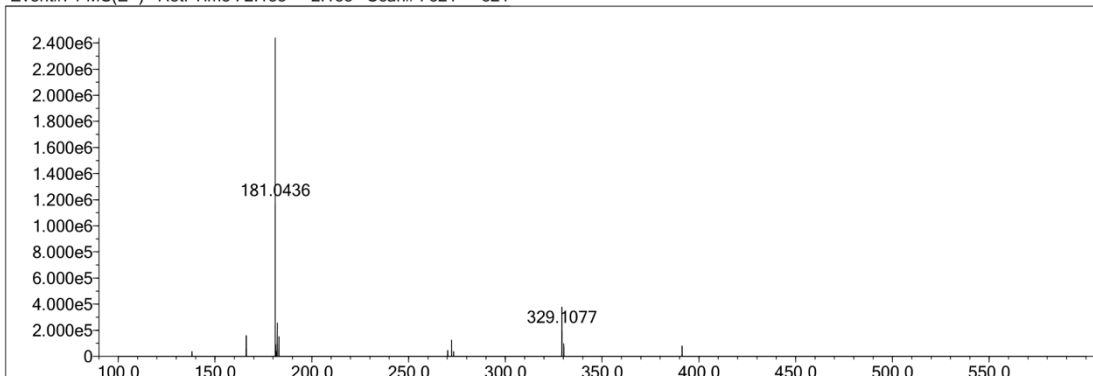
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	5	35	O	2	0	5	S	2	1	1	Ru	2	0	0	H
C	4	5	30	F	1	0	0	Cl	1	0	0	Pd	2	0	0	
N	3	0	5	P	3	0	0	Br	1	0	0	I	3	0	0	

Error Margin (ppm): 15
 HC Ratio: unlimited
 Max Isotopes: 3
 MSn Iso RI (%): 10.00

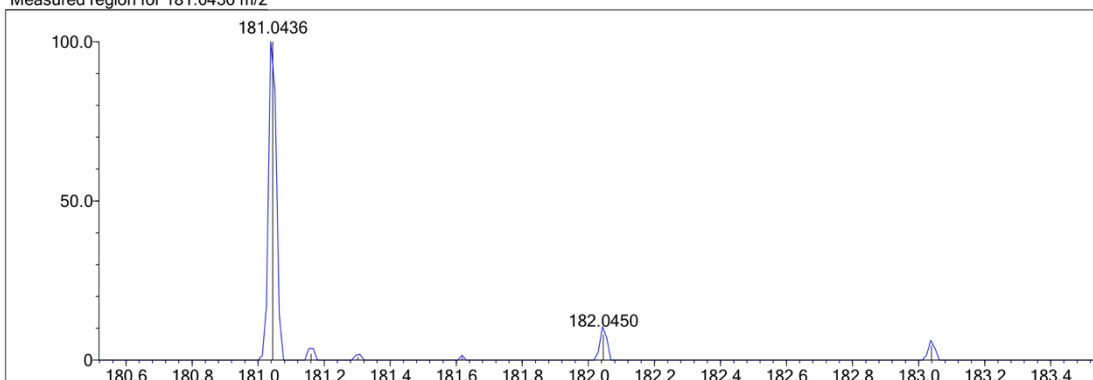
DBE Range: 5.0 - 20.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: yes
 Isotope Res: 9000
 Max Results: 500

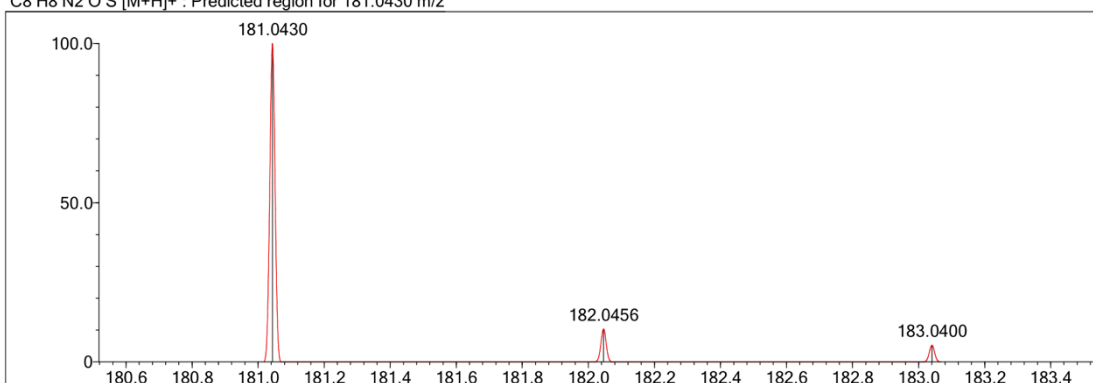
Event#: 1 MS(E+) Ret. Time : 2.133 -> 2.133 Scan# : 321 -> 321



Measured region for 181.0436 m/z



C8 H8 N2 O S [M+H]⁺ : Predicted region for 181.0430 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	79.33	C8 H8 N2 O S	[M+H] ⁺	181.0436	181.0430	0.6	3.31	84.20	6.0

Figure S4. HRMS spectra of compounds 2b

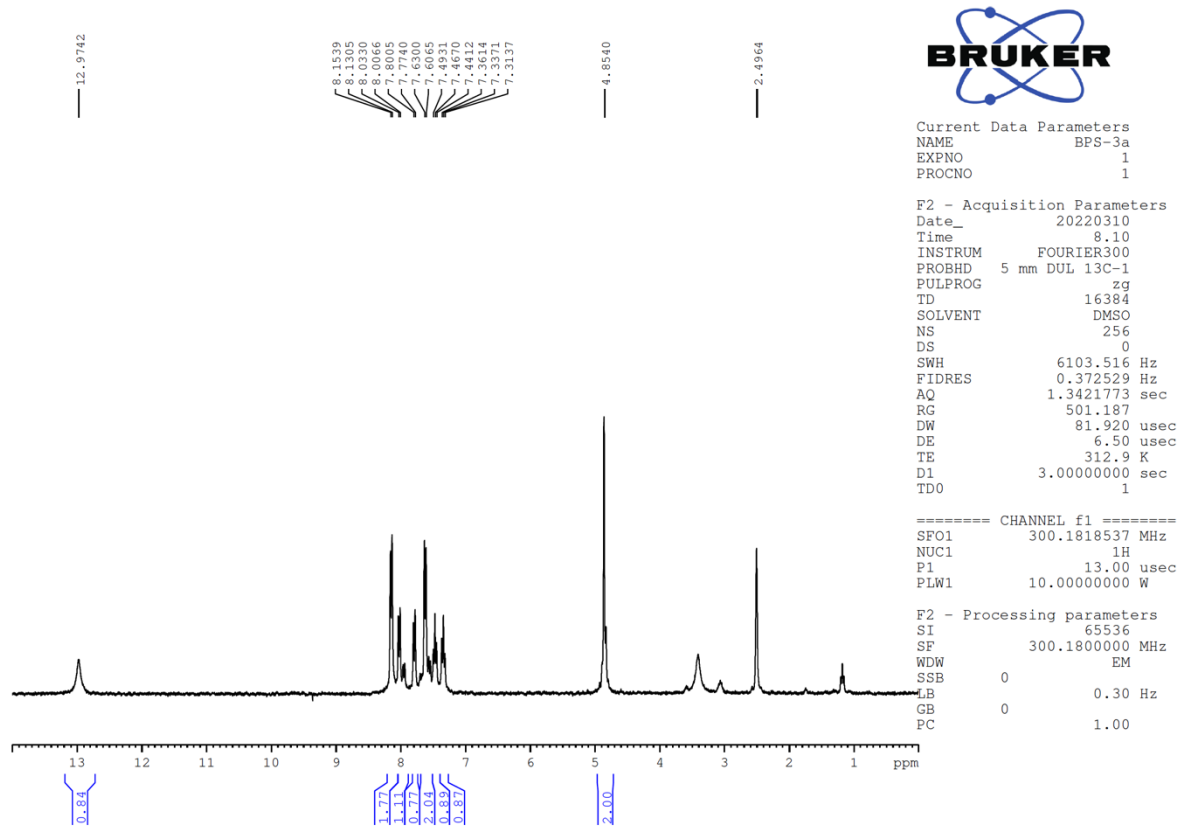


Figure S5. $^1\text{H-NMR}$ spectra of compounds **3a**

Data File: C:\LabSolutions\Data\Analiz\derya\BPS-3A_229.lcd

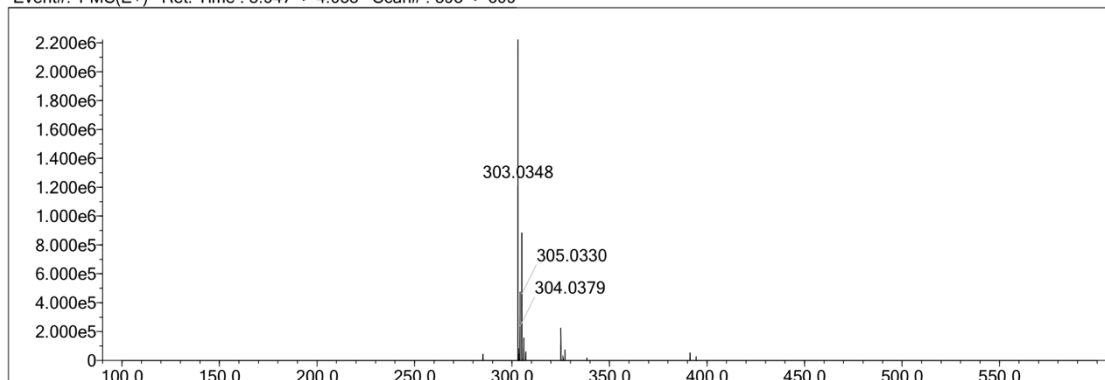
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	5	35	O	2	0	5	S	2	1	1	Ru	2	0	0	H
C	4	5	30	F	1	0	0	Cl	1	0	1	Pd	2	0	0	
N	3	0	5	P	3	0	0	Br	1	0	0	I	3	0	0	

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

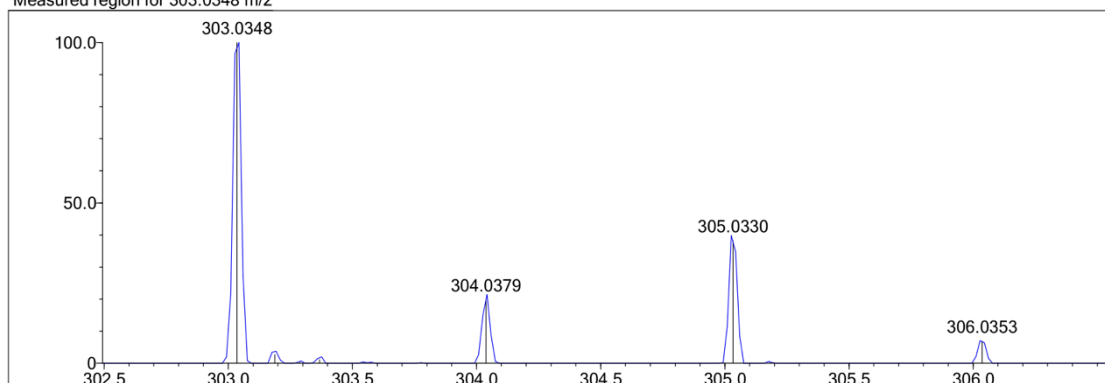
DBE Range: 5.0 - 15.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: yes
 Isotope Res: 9000
 Max Results: 500

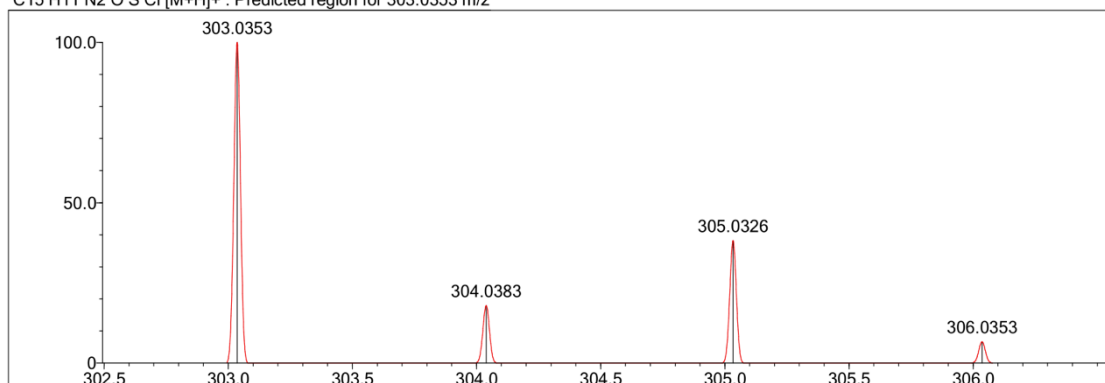
Event#: 1 MS(E+) Ret. Time : 3.947 -> 4.053 Scan#: 593 -> 609



Measured region for 303.0348 m/z



C15 H11 N2 O S Cl [M+H]⁺ : Predicted region for 303.0353 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	98.38	C15 H11 N2 O S Cl	[M+H] ⁺	303.0348	303.0353	-0.5	-1.65	100.00	11.0

Figure S6. HRMS spectra of compounds 3a

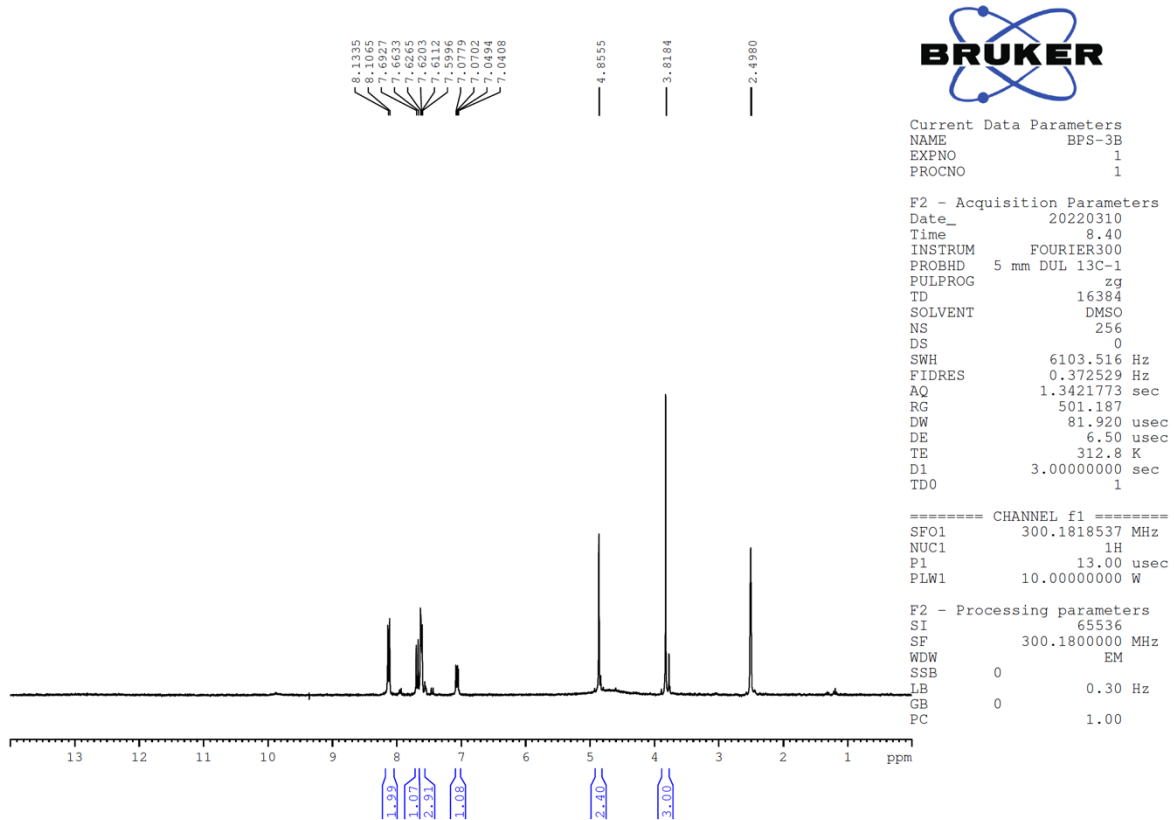


Figure S7. ¹H-NMR spectra of compounds **3b**

Data File: C:\LabSolutions\Data\Analiz\dera\BPS-3B_228.lcd

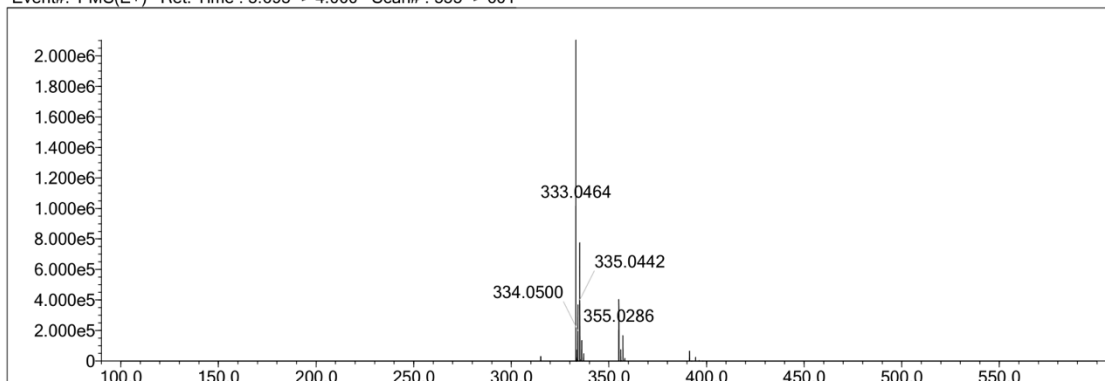
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	5	35	O	2	0	5	S	2	1	1	Ru	2	0	0	H
C	4	5	30	F	1	0	0	Cl	1	0	1	Pd	2	0	0	
N	3	0	5	P	3	0	0	Br	1	0	0	I	3	0	0	

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

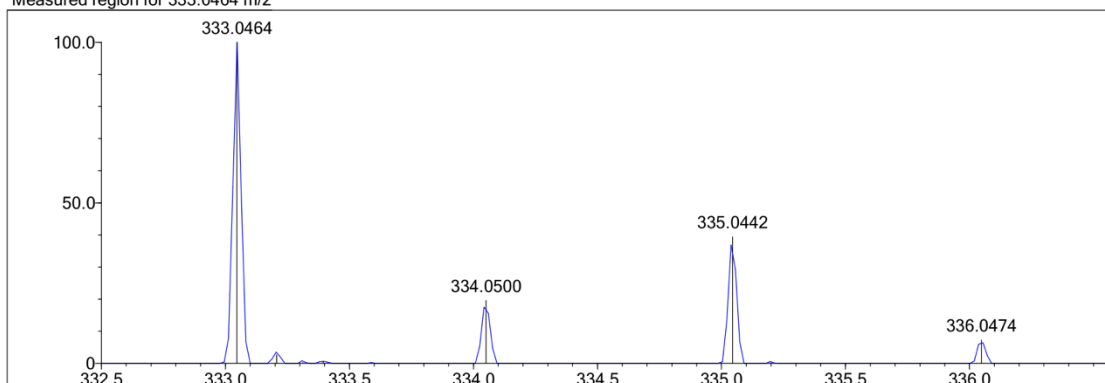
DBE Range: 5.0 - 20.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: yes
 Isotope Res: 9000
 Max Results: 500

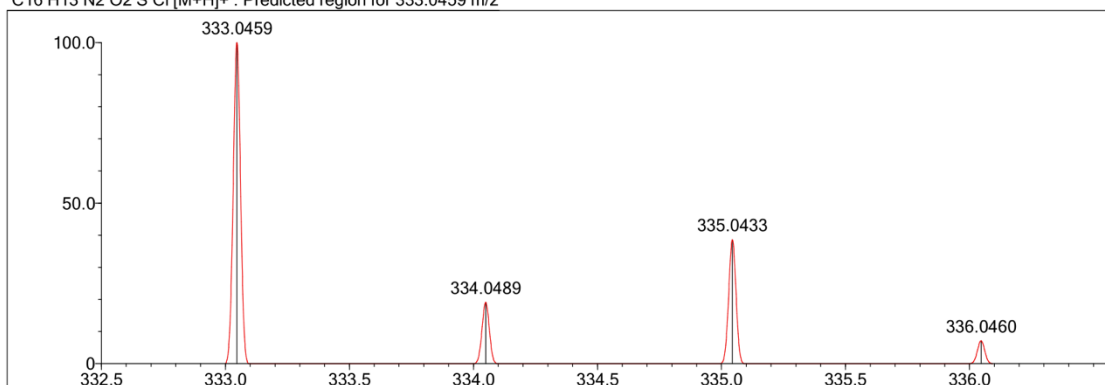
Event#: 1 MS(E+) Ret. Time : 3.693 -> 4.000 Scan#: 555 -> 601



Measured region for 333.0464 m/z



C16 H13 N2 O2 S Cl [M+H]⁺ : Predicted region for 333.0459 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	91.87	C16 H13 N2 O2 S Cl	[M+H] ⁺	333.0464	333.0459	0.5	1.50	93.03	11.0

Figure S8. HRMS spectra of compounds **3b**

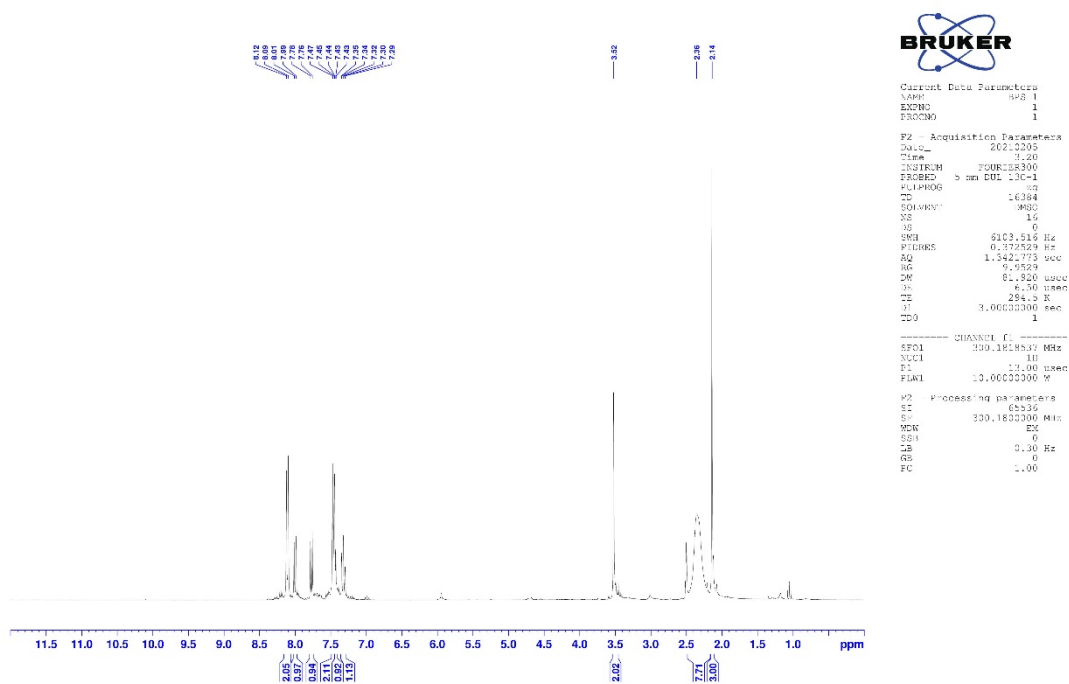


Figure S9. $^1\text{H-NMR}$ spectra of compounds **4a**

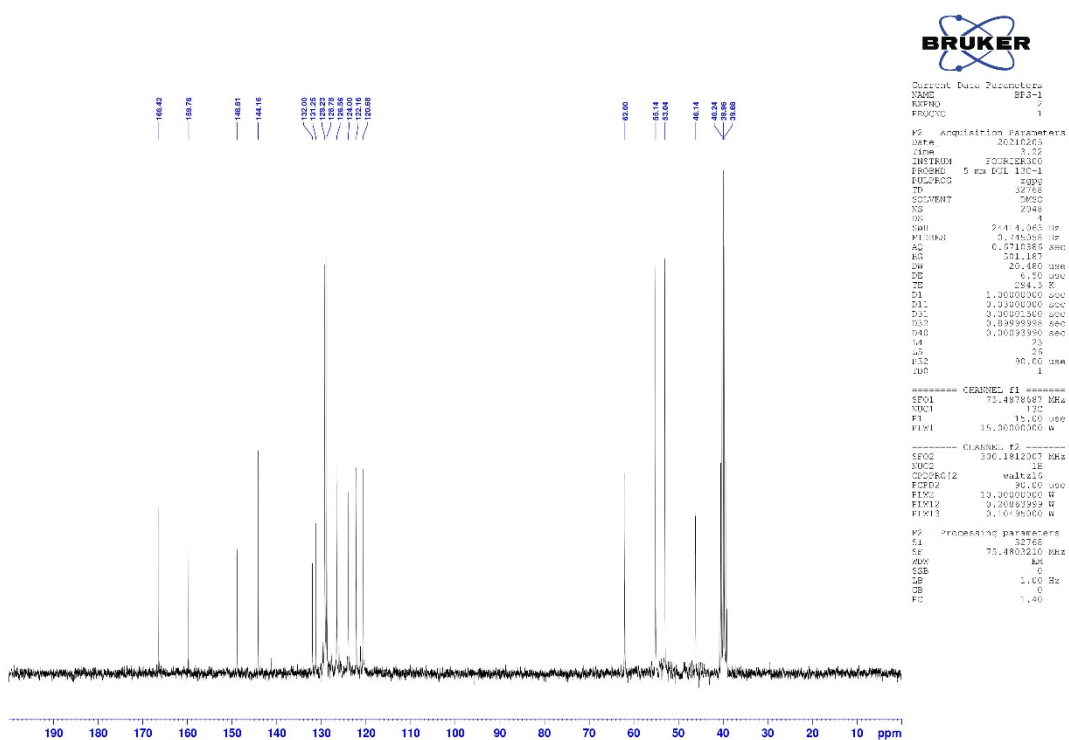


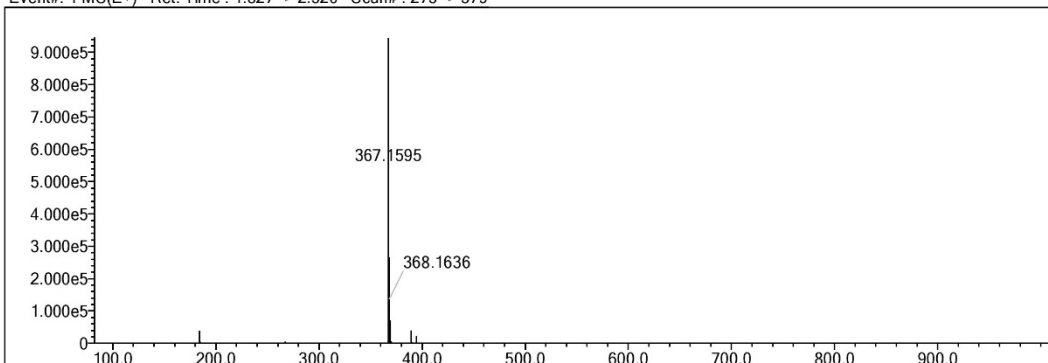
Figure S10. $^{13}\text{C-NMR}$ spectra of compounds **4a**

Data File: C:\LabSolutions\Data\Analiz\dera\BPS-1_158.lcd

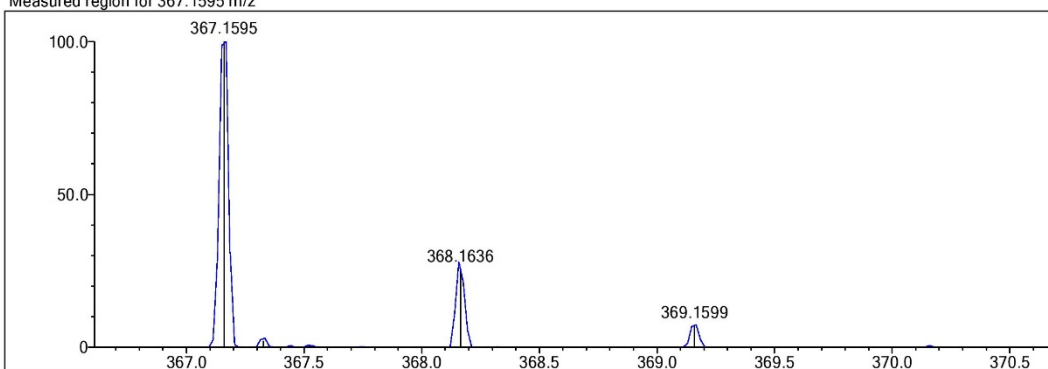
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
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C	4	10	40	F	1	0	0	Cl	1	0	0	Pd	2	0	0	
N	3	0	5	P	3	0	0	Br	1	0	0	I	3	0	0	

Error Margin (ppm): 5
 DBE Range: 5.0 - 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
 Max Results: 150

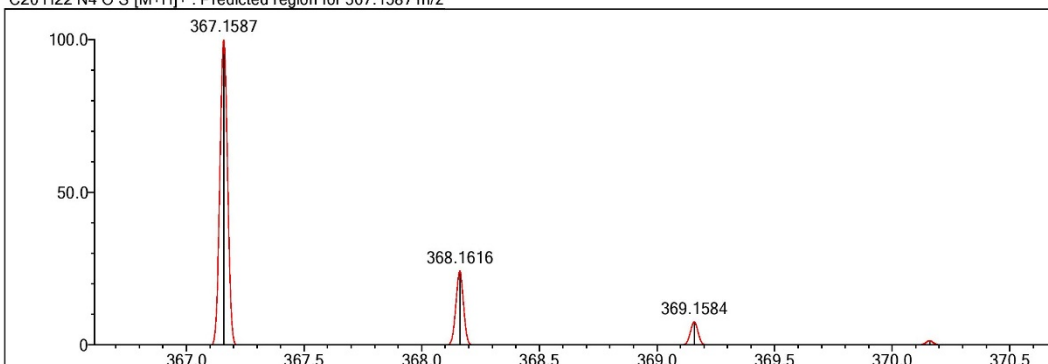
Event#: 1 MS(E+) Ret. Time : 1.827 -> 2.520 Scan# : 275 -> 379



Measured region for 367.1595 m/z



C20 H22 N4 O S [M+H]⁺ : Predicted region for 367.1587 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Is	DBE
1	97.05	C ₂₀ H ₂₂ N ₄ O S	[M+H] ⁺	367.1595	367.1587	0.8	2.18	100.00	12.0

Figure S11. HRMS spectra of compounds 4a

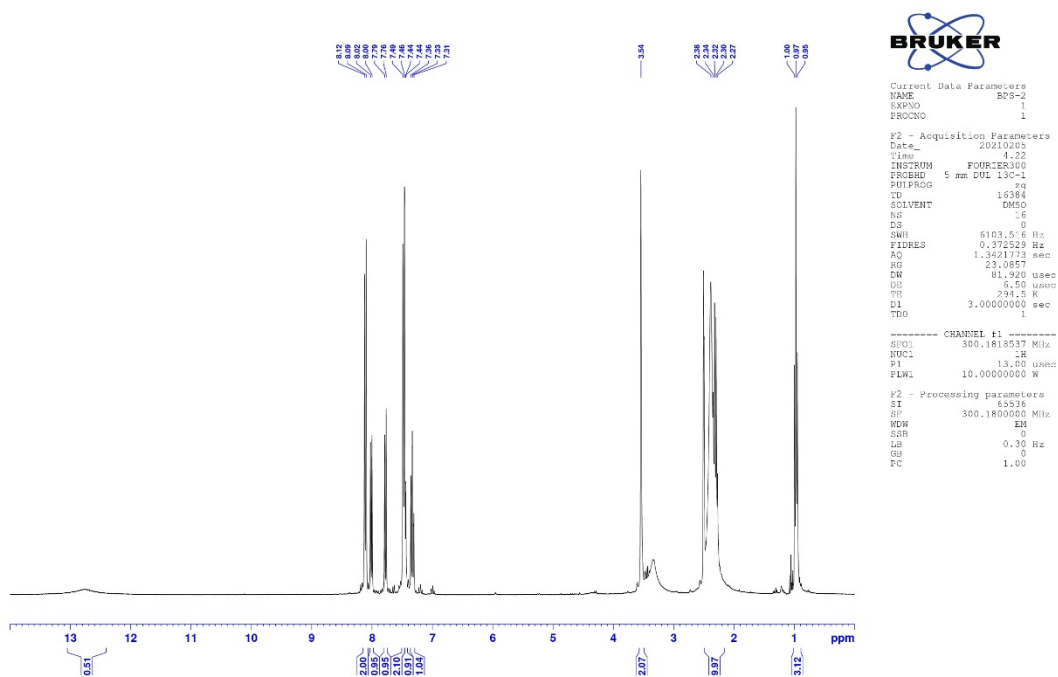


Figure S12. ¹H-NMR spectra of compounds **4b**

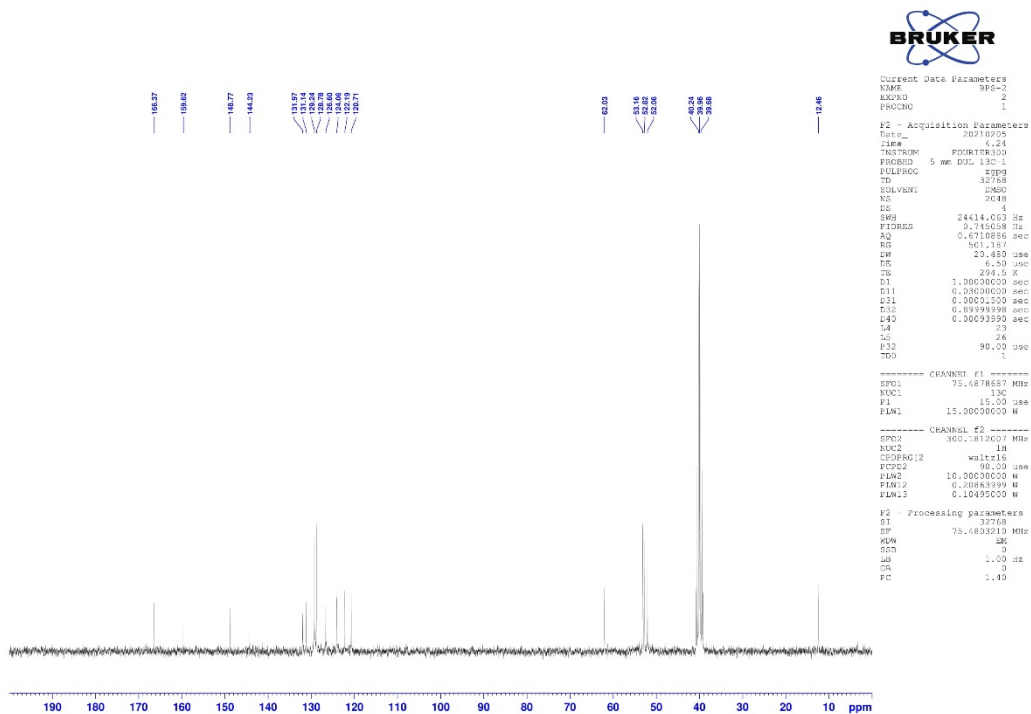


Figure S13. ¹³C-NMR spectra of compounds **4b**

Data File: C:\LabSolutions\Data\Analiz\dera\BPS-2_159.lcd

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C	4	10	40	F	1	0	0	Cl	1	0	0	Pd	2	0	0	
N	3	0	5	P	3	0	0	Br	1	0	0	I	3	0	0	

Error Margin (ppm): 5

DBE Range: 5.0 - 15.0

Electron Ions: both

HC Ratio: unlimited

Apply N Rule: yes

Use MSn Info: yes

Max Isotopes: 3

Isotope RI (%): 1.00

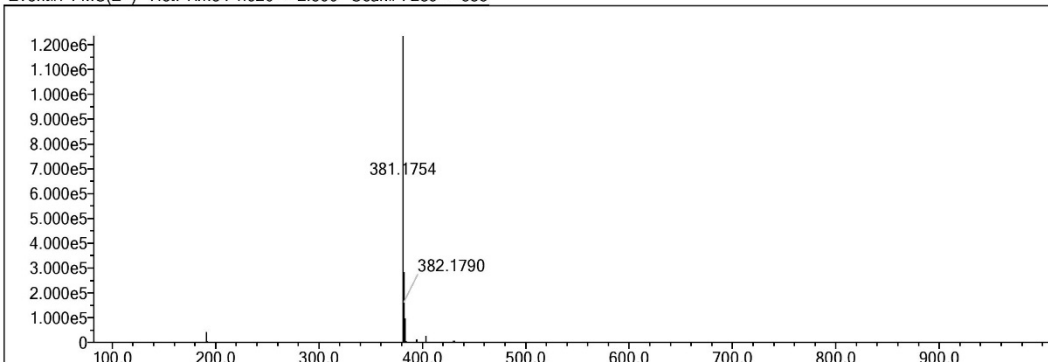
Isotope Res: 9000

MSn Iso RI (%): 10.00

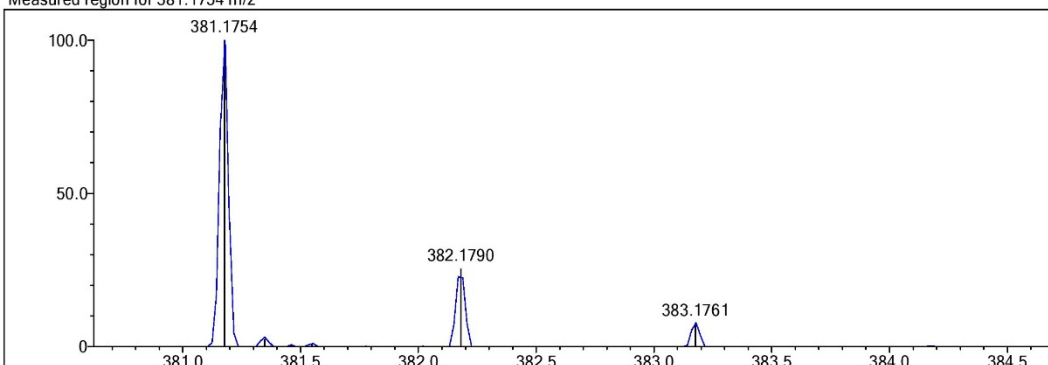
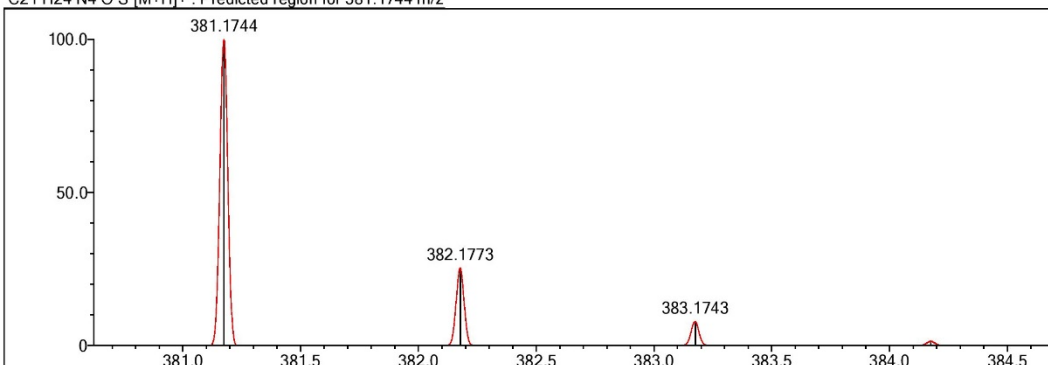
MSn Logic Mode: AND

Max Results: 150

Event#: 1 MS(E+) Ret. Time : 1.920 -> 2.560 Scan#: 289 -> 385



Measured region for 381.1754 m/z

C21 H24 N4 O S [M+H]⁺ : Predicted region for 381.1744 m/z

Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	76.93	C21 H24 N4 O S	[M+H] ⁺	381.1754	381.1744	1.0	2.62	80.18	12.0

Figure S14. HRMS spectra of compounds 4b

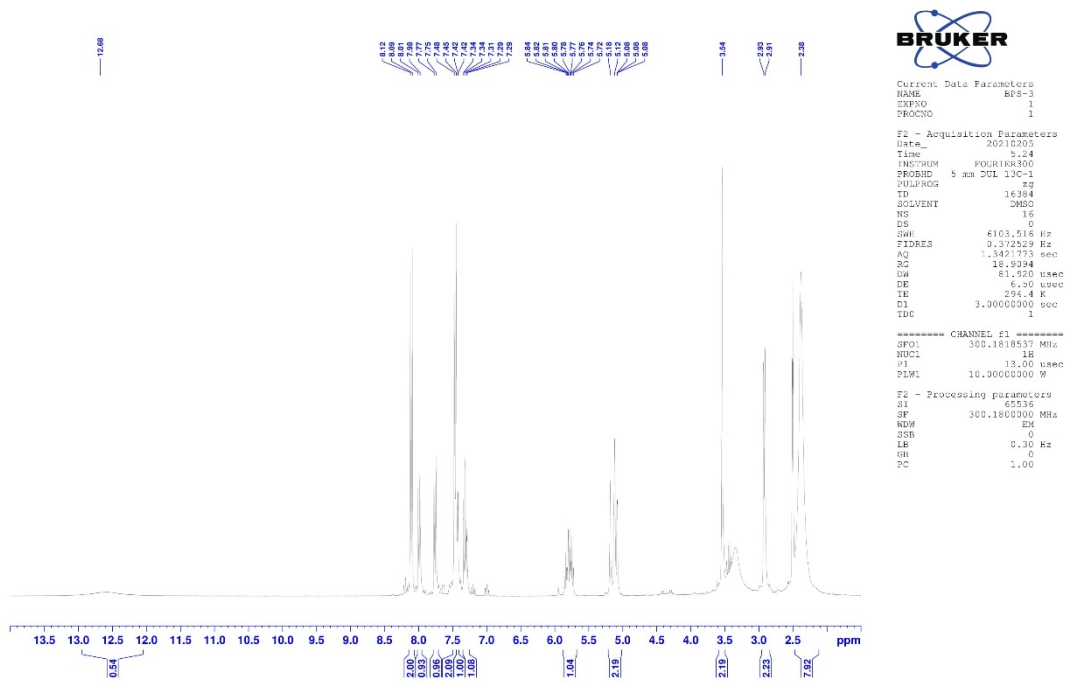


Figure S15. ¹H-NMR spectra of compounds 4c

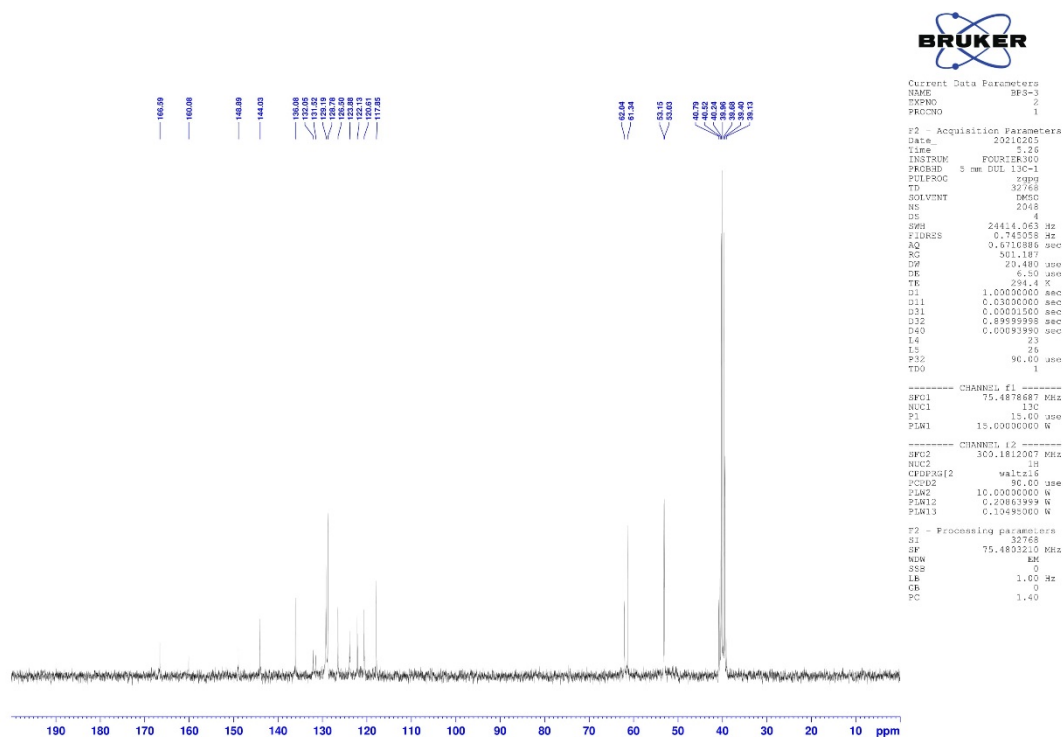


Figure S16. ¹³C-NMR spectra of compounds 4c

Data File: C:\LabSolutions\Data\Analiz\derya\BPS-3_160.lcd

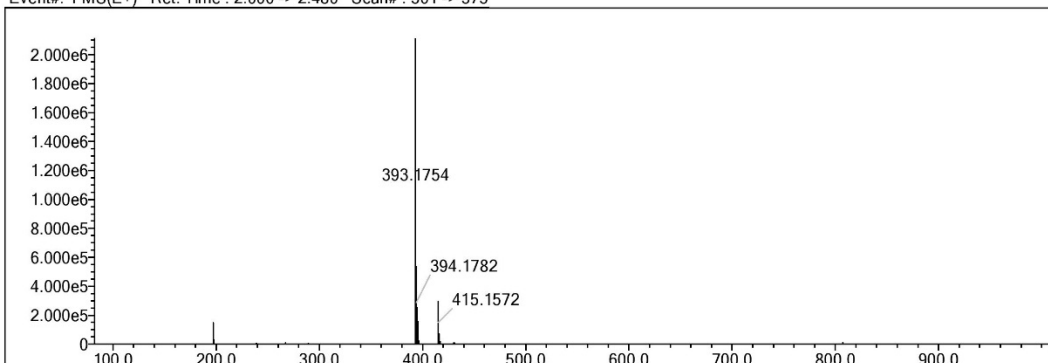
Elmt	Val	Min	Max	Elmt	Val	Min	Max	Elmt	Val	Min	Max	Elmt	Val	Min	Max	Use Adduct
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C	4	10	40	F	1	0	0	Cl	1	0	0	Pd	2	0	0	
N	3	0	5	P	3	0	0	Br	1	0	0	I	3	0	0	

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

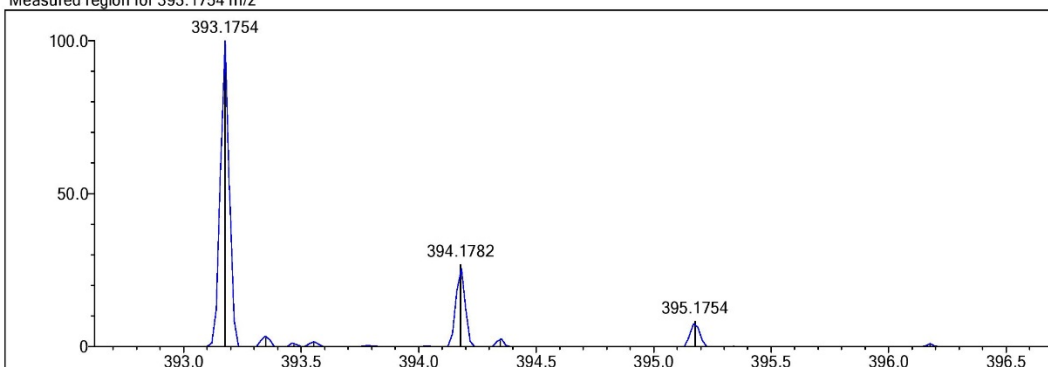
DBE Range: 5.0 - 15.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

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

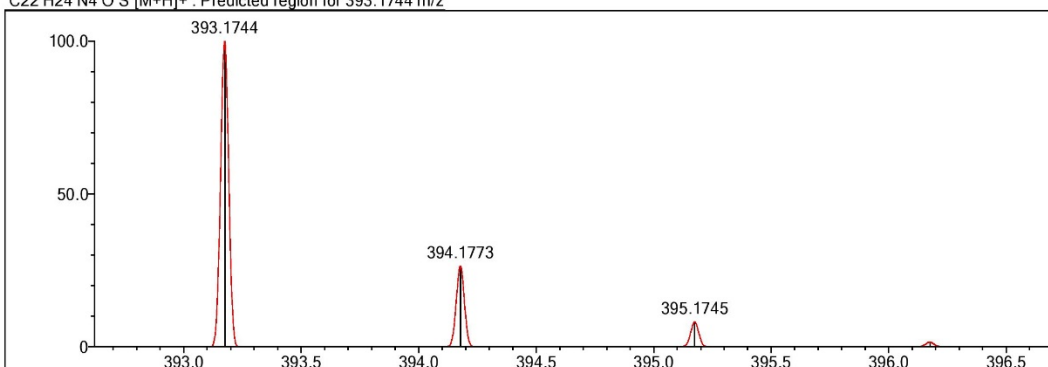
Event#: 1 MS(E+) Ret. Time : 2.000 -> 2.480 Scan# : 301 -> 373



Measured region for 393.1754 m/z



C22 H24 N4 O S [M+H]⁺ : Predicted region for 393.1744 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	89.53	C22 H24 N4 O S	[M+H] ⁺	393.1754	393.1744	1.0	2.54	93.12	13.0

Figure S17. HRMS spectra of compounds 4c

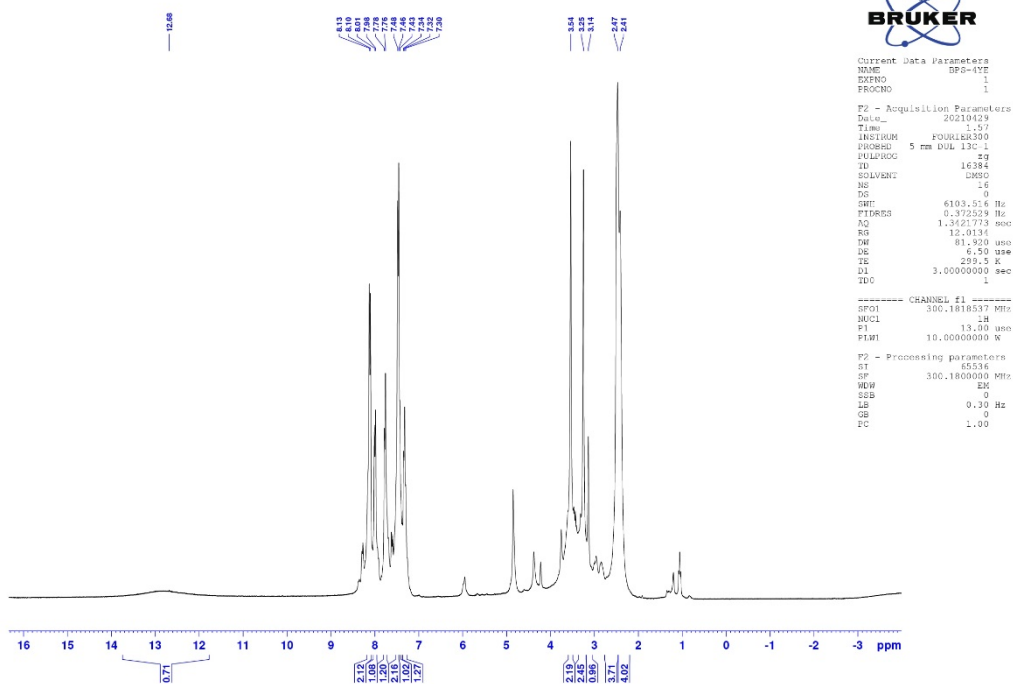


Figure S18. ¹H-NMR spectra of compounds 4d

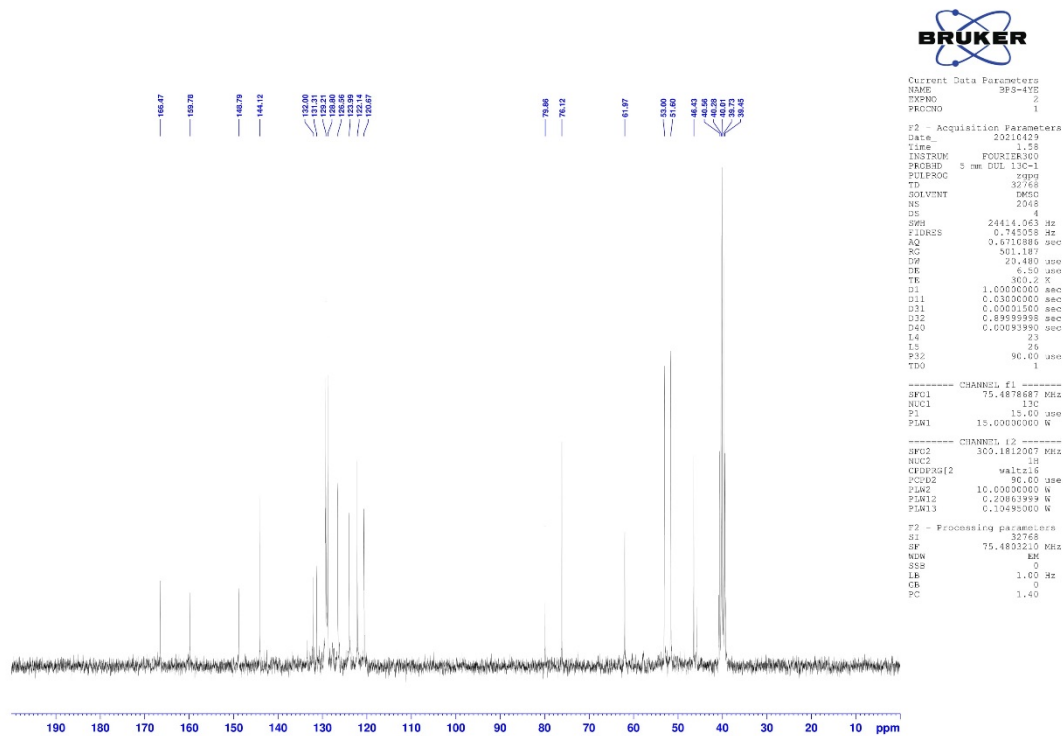


Figure S19. ¹³C-NMR spectra of compounds 4d

Data File: C:\LabSolutions\Data\Analiz\derya\BPS-4_161.lcd

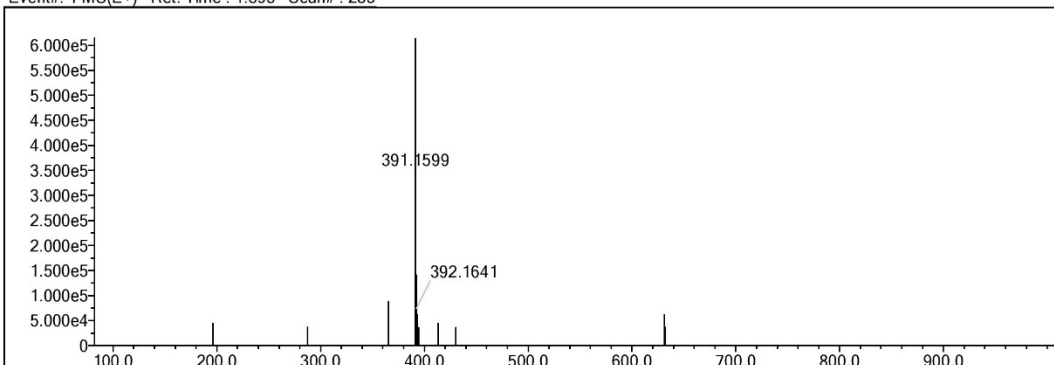
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	10	40	O	2	0	5	S	2	0	2	Ru	2	0	0	H
C	4	10	40	F	1	0	0	Cl	1	0	0	Pd	2	0	0	
N	3	1	5	P	3	0	0	Br	1	0	0	I	3	0	0	

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

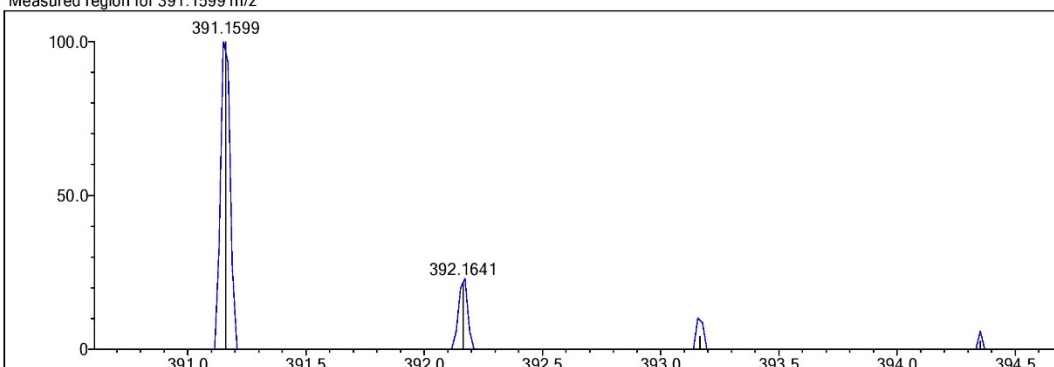
DBE Range: 5.0 - 15.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

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

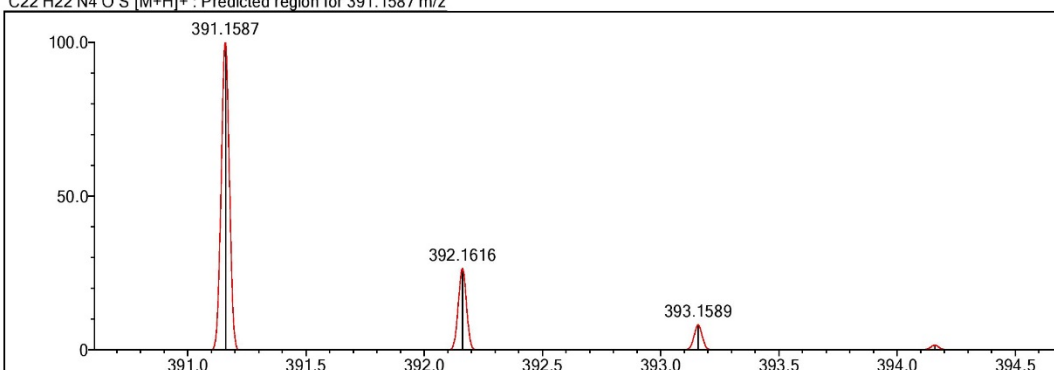
Event#: 1 MS(E+) Ret. Time : 1.893 Scan# : 285



Measured region for 391.1599 m/z



C22H22N4OS [M+H]⁺: Predicted region for 391.1587 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	62.15	C22H22N4OS	[M+H] ⁺	391.1599	391.1587	1.2	3.07	65.54	14.0

Figure S20. HRMS spectra of compounds 4d

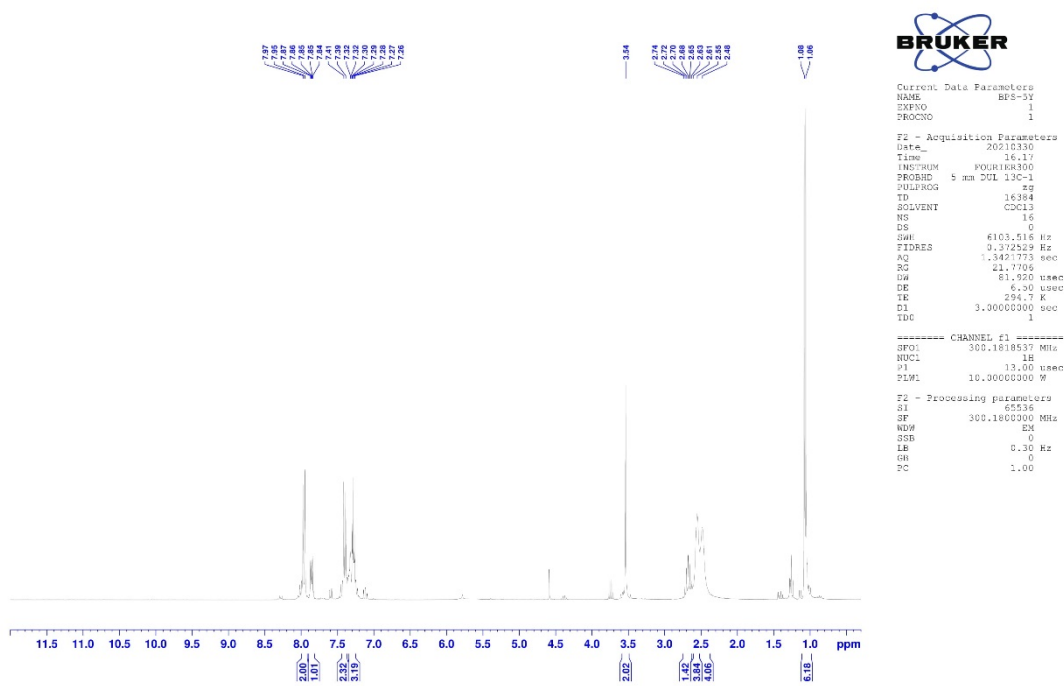


Figure S21. ¹H-NMR spectra of compounds 4e

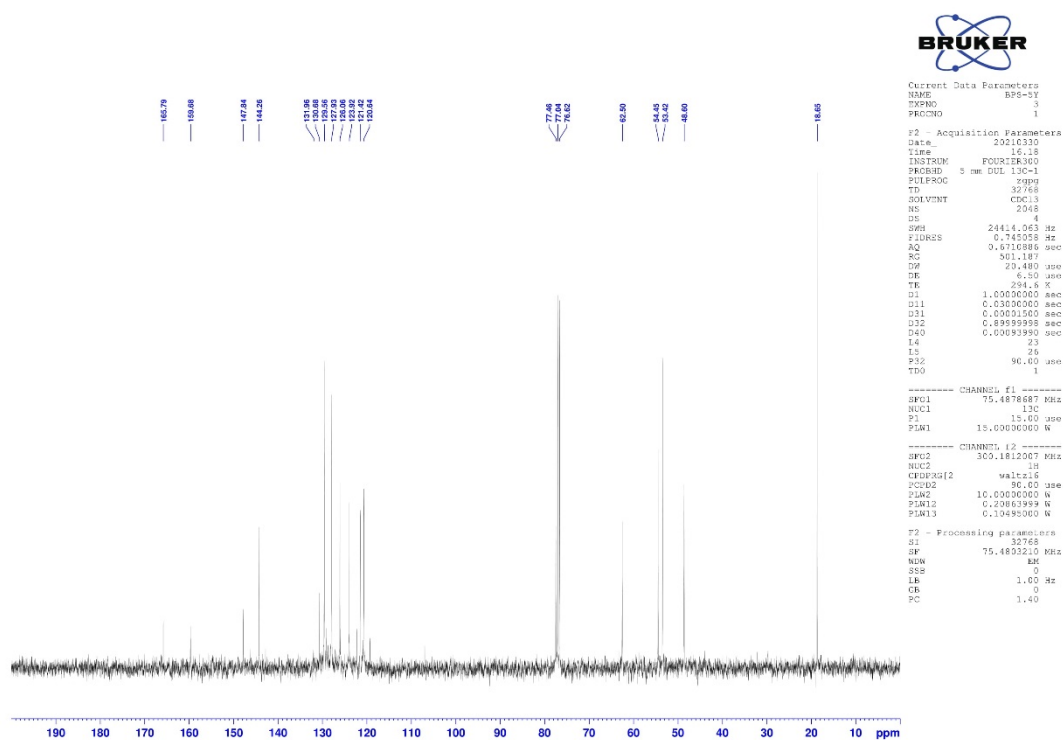


Figure S22. ¹³C-NMR spectra of compounds 4e

Data File: C:\LabSolutions\Data\Analiz\deryal\BPS-5_162.lcd

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	10	40	O	2	0	5	S	2	0	2	Ru	2	0	0	H
C	4	10	40	F	1	0	0	Cl	1	0	0	Pd	2	0	0	
N	3	1	5	P	3	0	0	Br	1	0	0	I	3	0	0	

Error Margin (ppm): 5

DBE Range: 5.0 - 15.0

Electron Ions: both

HC Ratio: unlimited

Apply N Rule: yes

Use MSn Info: yes

Max Isotopes: 3

Isotope RI (%): 1.00

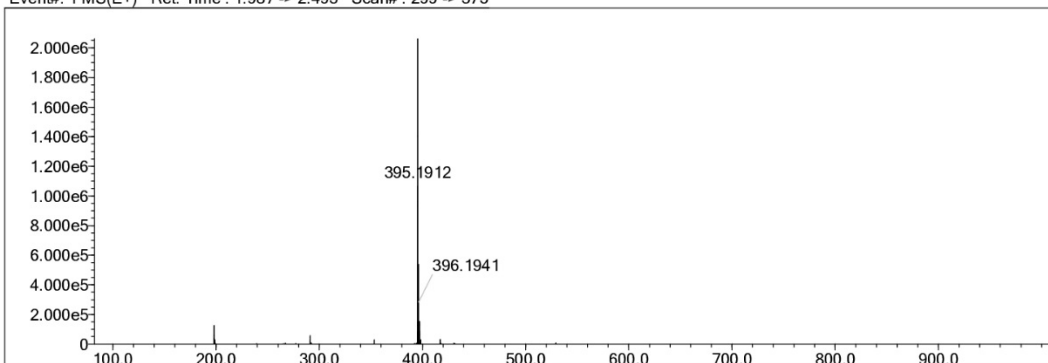
Isotope Res: 9000

MSn Iso RI (%): 10.00

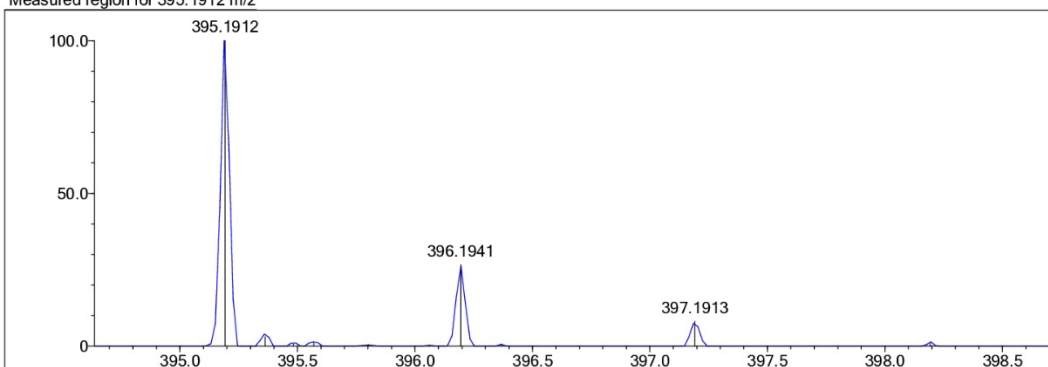
MSn Logic Mode: AND

Max Results: 150

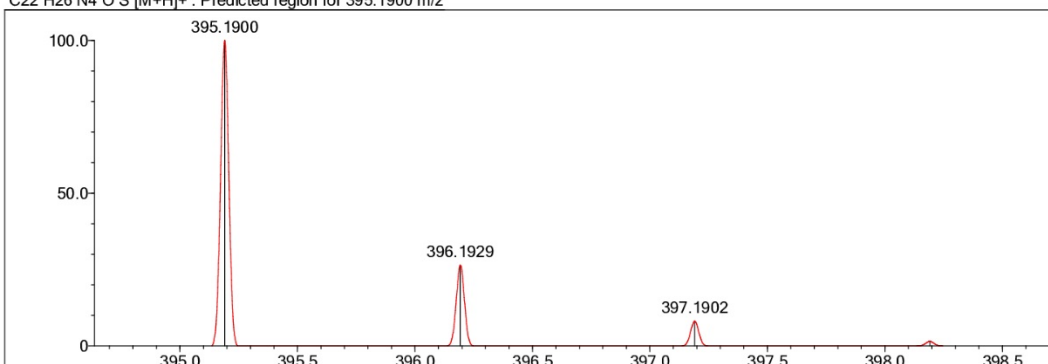
Event#: 1 MS(E+) Ret. Time : 1.987 -> 2.493 Scan# : 299 -> 375



Measured region for 395.1912 m/z



C22 H26 N4 O S [M+H]+ : Predicted region for 395.1900 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	94.90	C22 H26 N4 O S	[M+H]+	395.1912	395.1900	1.2	3.04	100.00	12.0

Figure S23. HRMS spectra of compounds 4e

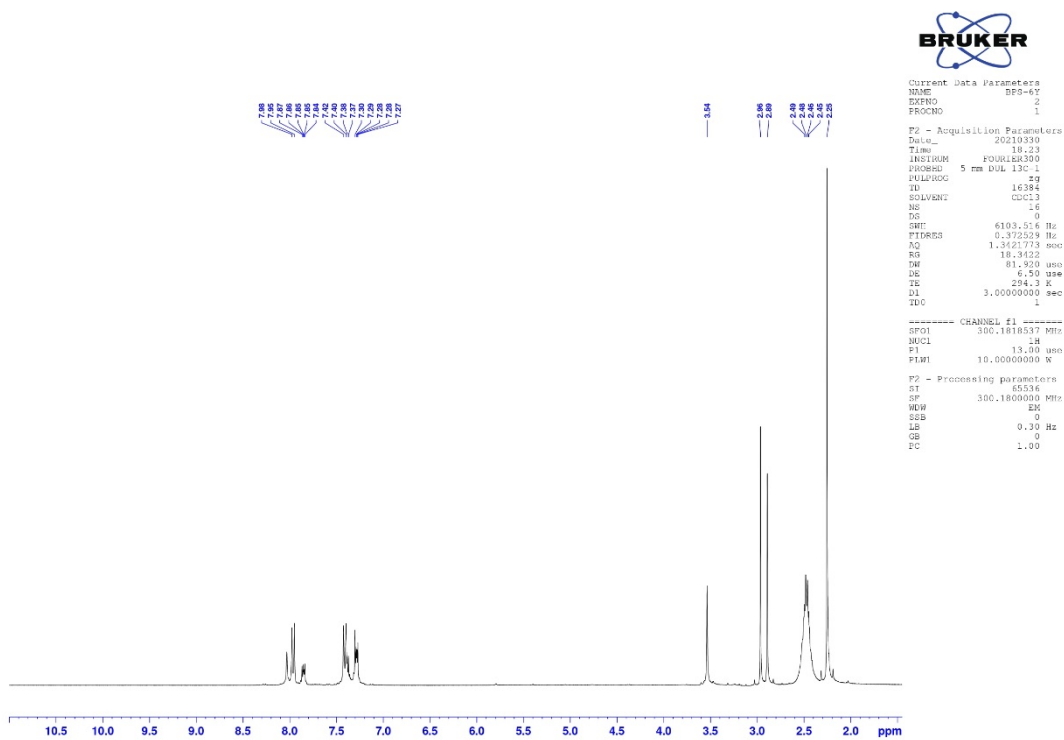


Figure S24. ¹H-NMR spectra of compounds 4f

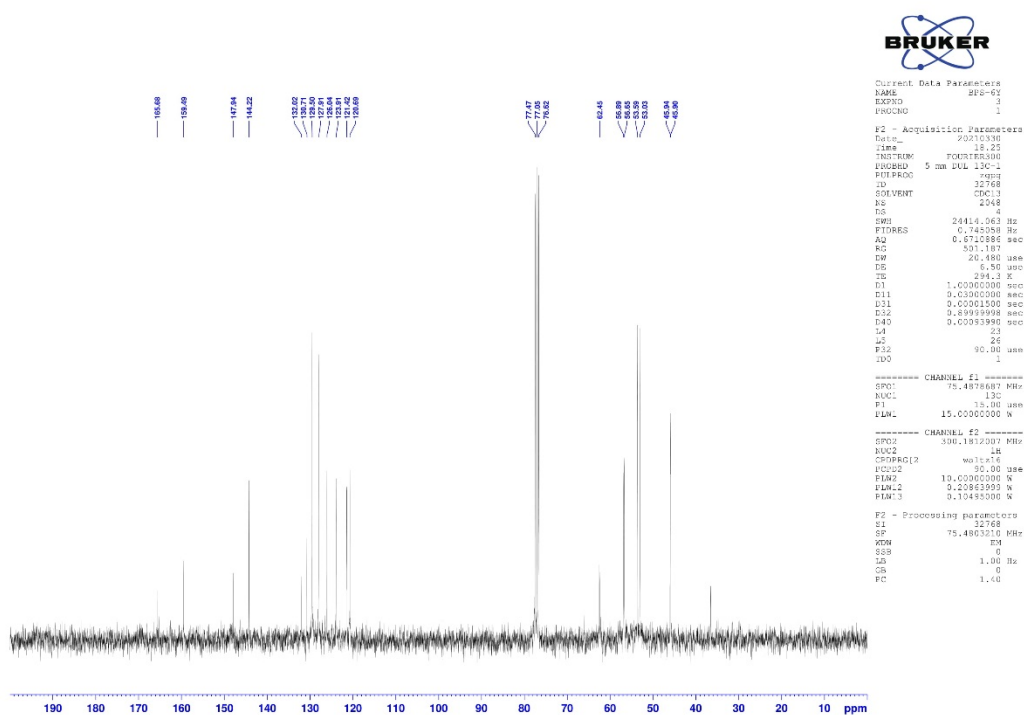


Figure S25. ¹³C-NMR spectra of compounds 4f

Data File: C:\LabSolutions\Data\Analiz\dera\BPS-6_163.lcd

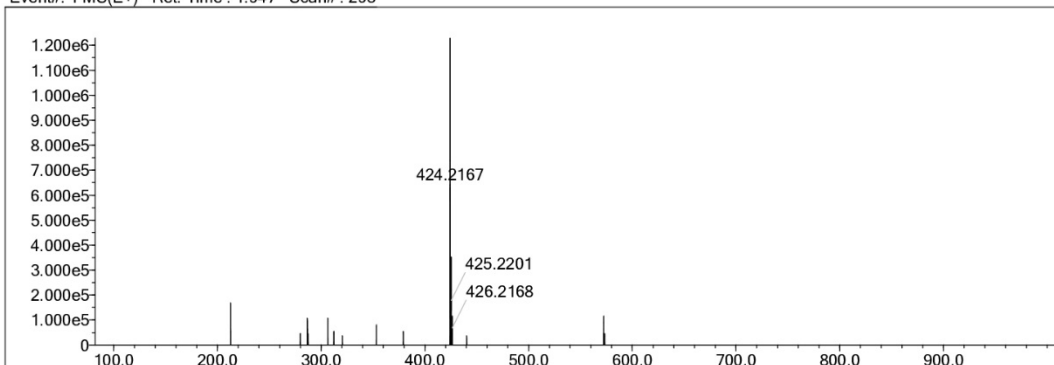
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	10	40	O	2	0	5	S	2	0	2	Ru	2	0	0	H
C	4	10	40	F	1	0	0	Cl	1	0	0	Pd	2	0	0	
N	3	2	5	P	3	0	0	Br	1	0	0	I	3	0	0	

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

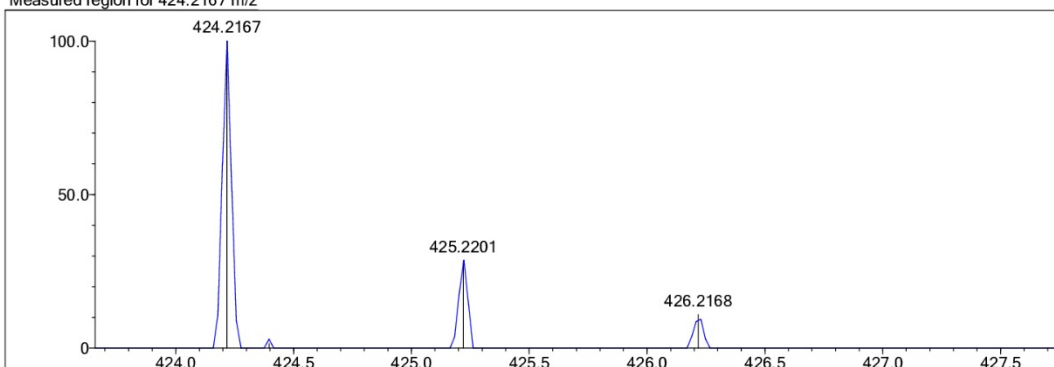
DBE Range: 5.0 - 15.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

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

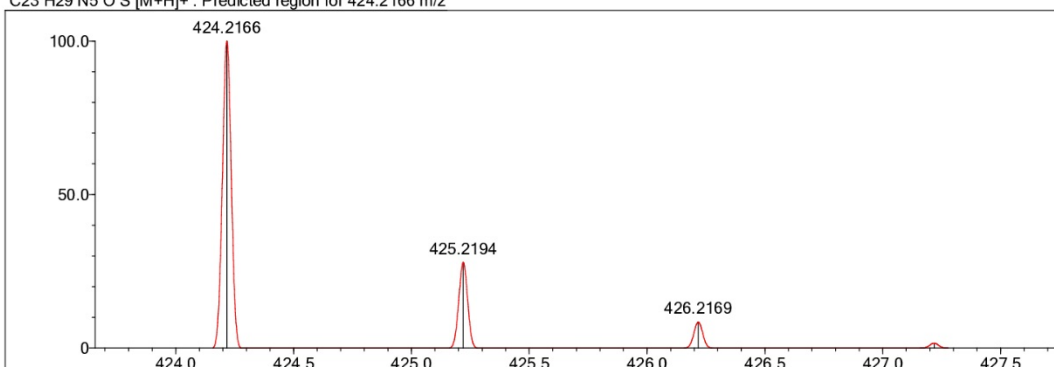
Event#: 1 MS(E+) Ret. Time : 1.947 Scan#: 293



Measured region for 424.2167 m/z



C23 H29 N5 O S [M+H]+ : Predicted region for 424.2166 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	98.87	C23 H29 N5 O S	[M+H]+	424.2167	424.2166	0.1	0.24	98.87	12.0

Figure S26. HRMS spectra of compounds 4f

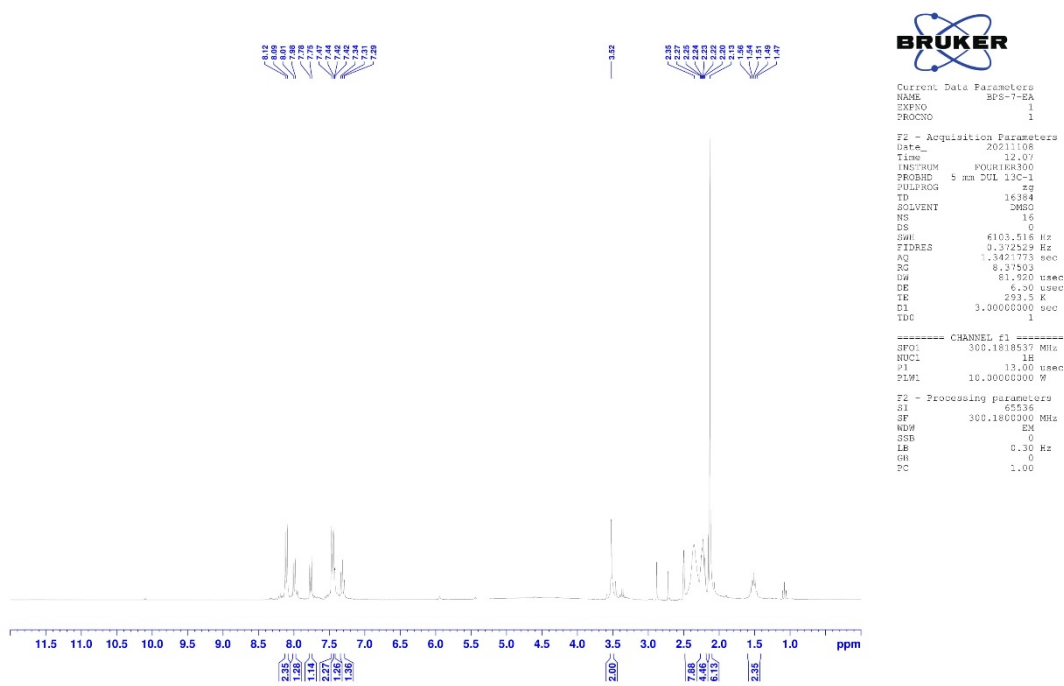


Figure S27. ¹H-NMR spectra of compounds **4g**

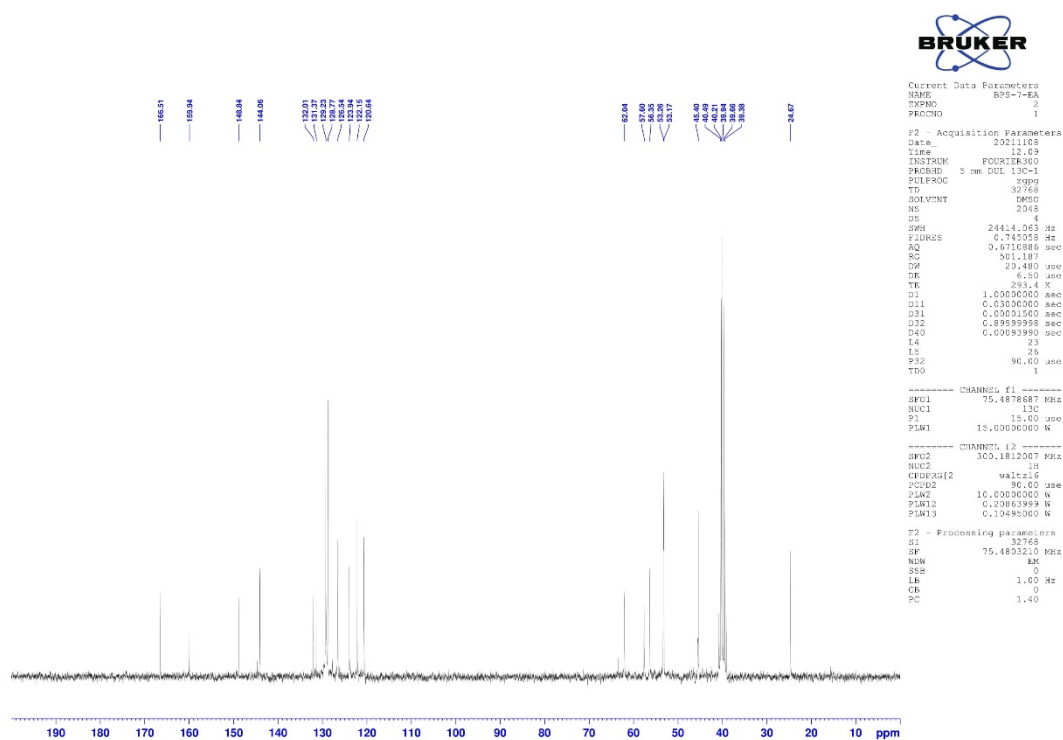


Figure S28. ¹³C-NMR spectra of compounds **4g**

Data File: C:\LabSolutions\Data\Analiz\derya\BPS-7_164.lcd

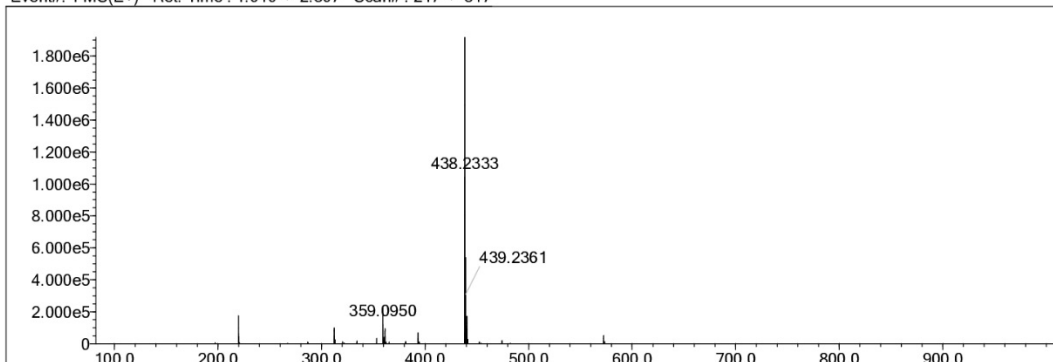
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	10	40	O	2	0	5	S	2	0	2	Ru	2	0	0	H
C	4	10	40	F	1	0	0	Cl	1	0	0	Pd	2	0	0	
N	3	2	5	P	3	0	0	Br	1	0	0	I	3	0	0	

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

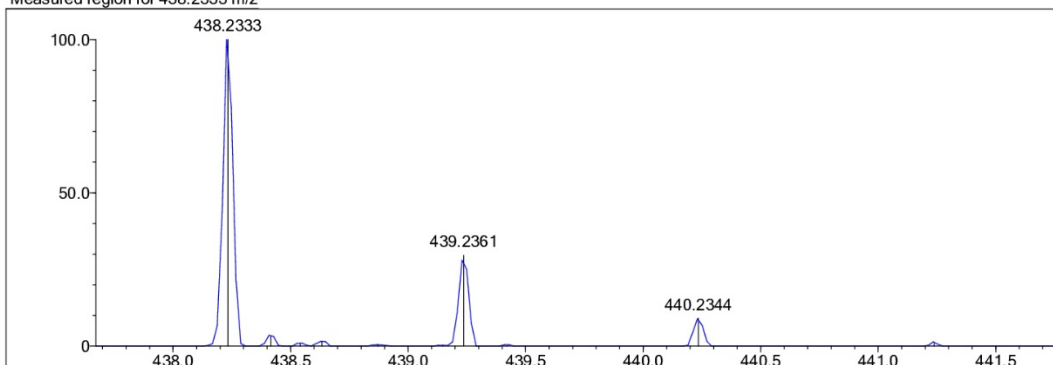
DBE Range: 5.0 - 15.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

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

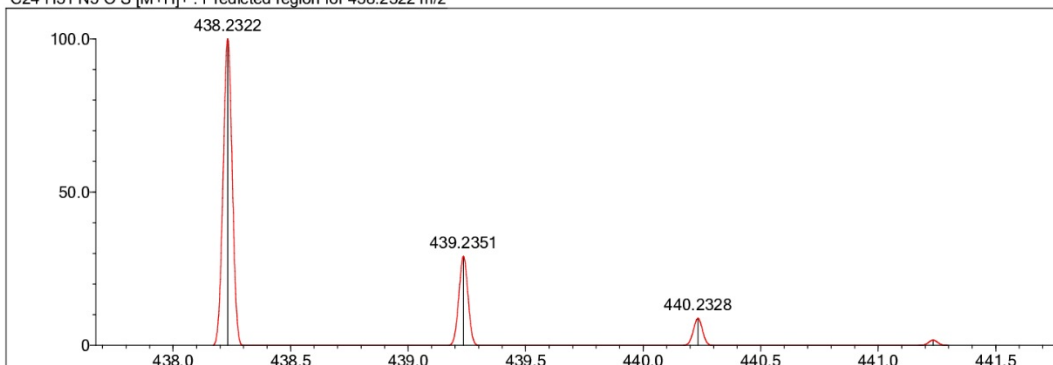
Event#: 1 MS(E+) Ret. Time : 1.640 -> 2.307 Scan#: 247 -> 347



Measured region for 438.2333 m/z



C24 H31 N5 O S [M+H]⁺ : Predicted region for 438.2322 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	91.64	C24 H31 N5 O S	[M+H] ⁺	438.2333	438.2322	1.1	2.51	95.23	12.0

Figure S29. HRMS spectra of compounds 4g

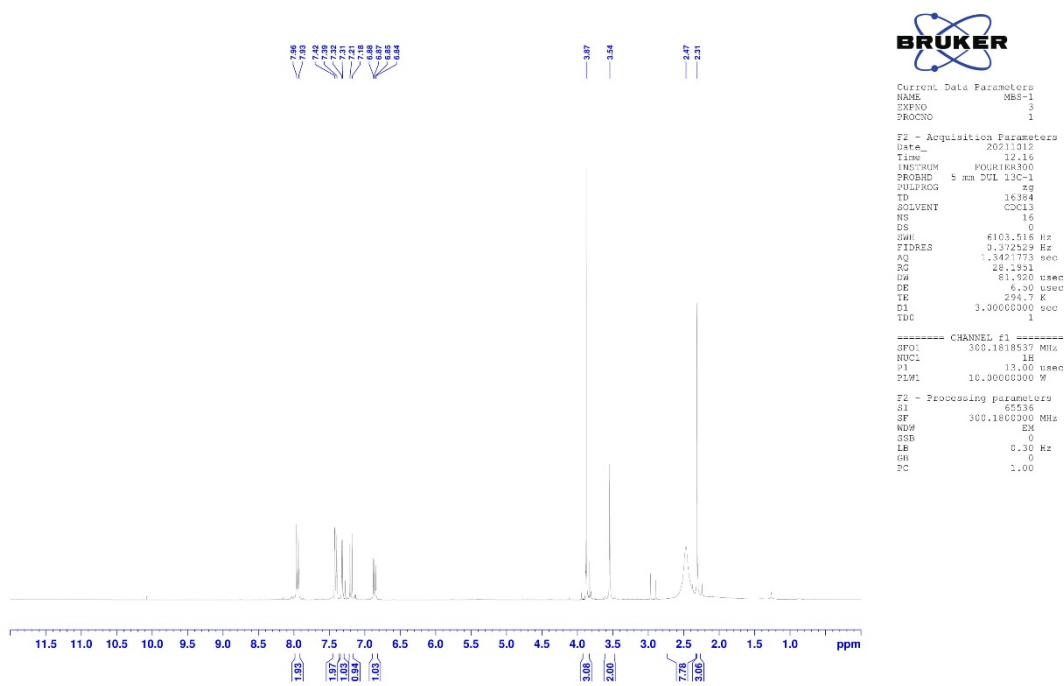


Figure S30. ¹H-NMR spectra of compounds 4h

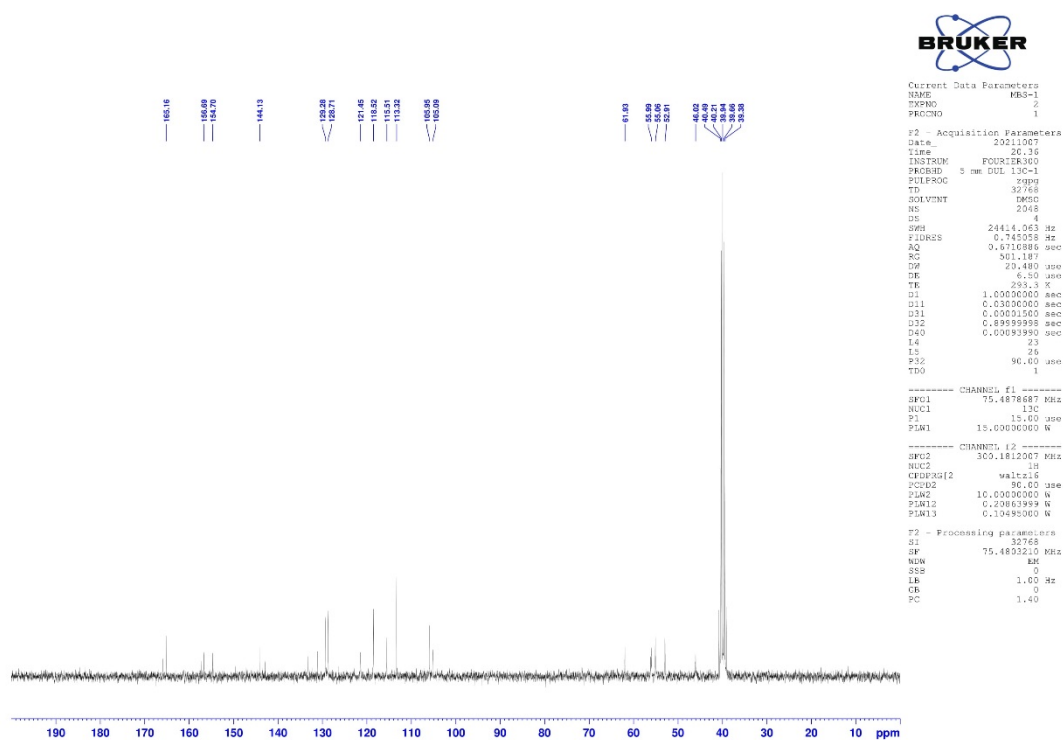


Figure S31. ¹³C-NMR spectra of compounds 4h

Data File: C:\LabSolutions\Data\Analiz\derya\MBS-1_166.lcd

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	10	40	O	2	0	5	S	2	0	1	Ru	2	0	0	H
C	4	10	40	F	1	0	0	Cl	1	0	0	Pd	2	0	0	
N	3	2	5	P	3	0	0	Br	1	0	0	I	3	0	0	

Error Margin (ppm): 5

DBE Range: 5.0 - 15.0

Electron Ions: both

HC Ratio: unlimited

Apply N Rule: yes

Use MSn Info: yes

Max Isotopes: 3

Isotope RI (%): 1.00

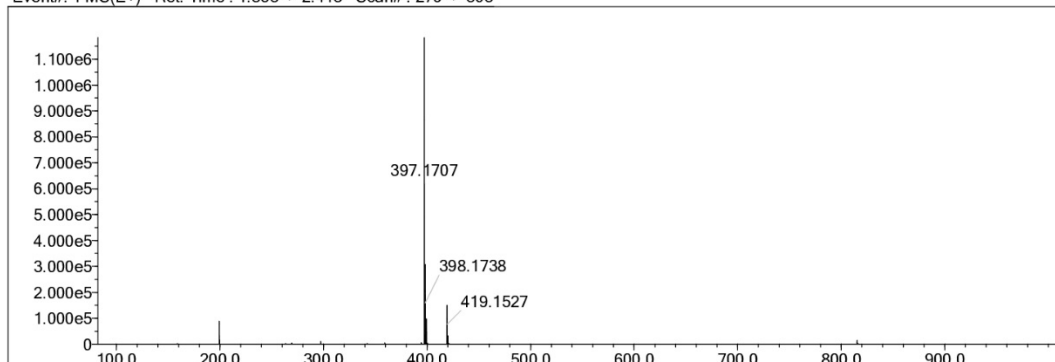
Isotope Res: 9000

MSn Iso RI (%): 10.00

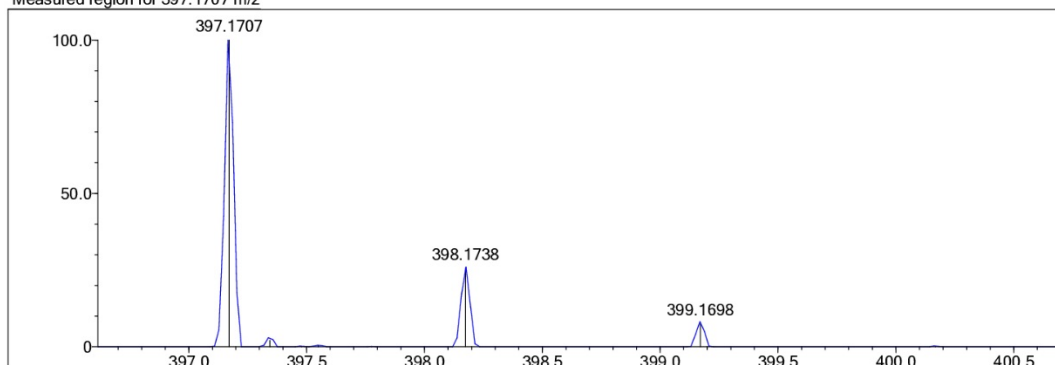
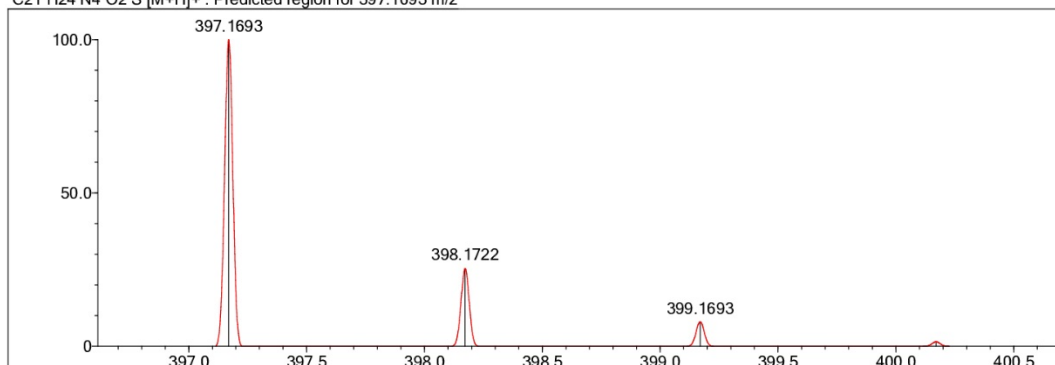
MSn Logic Mode: AND

Max Results: 150

Event#: 1 MS(E+) Ret. Time : 1.853 -> 2.413 Scan#: 279 -> 363



Measured region for 397.1707 m/z

C21 H24 N4 O2 S [M+H]⁺ : Predicted region for 397.1693 m/z

Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	79.91	C21 H24 N4 O2 S	[M+H] ⁺	397.1707	397.1693	1.4	3.52	85.29	12.0

Figure S32. HRMS spectra of compounds 4h

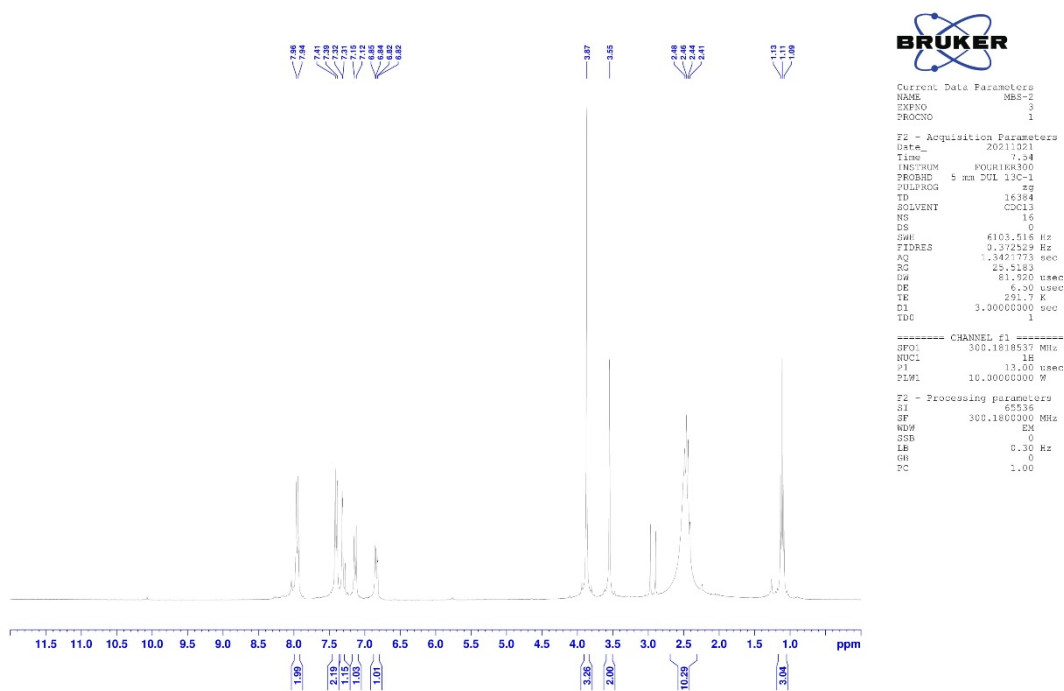


Figure S33. ¹H-NMR spectra of compounds 4i

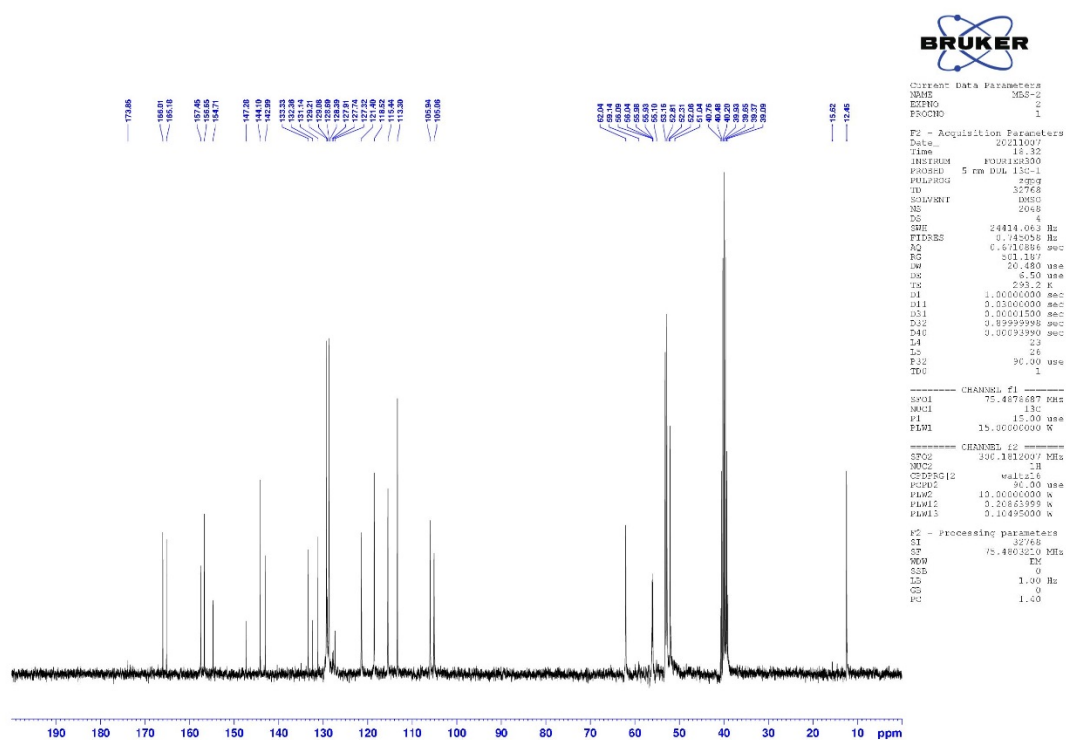


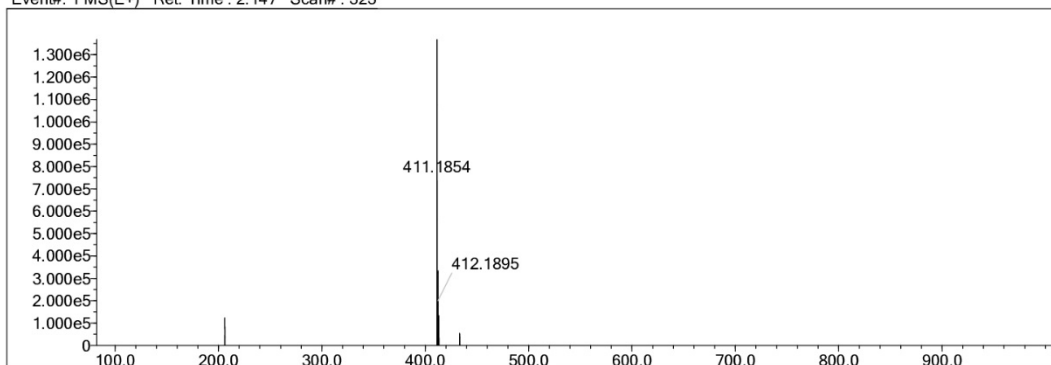
Figure S34. ¹³C-NMR spectra of compounds 4i

Data File: C:\LabSolutions\Data\Analyze\dera\MBS-2_167.lcd

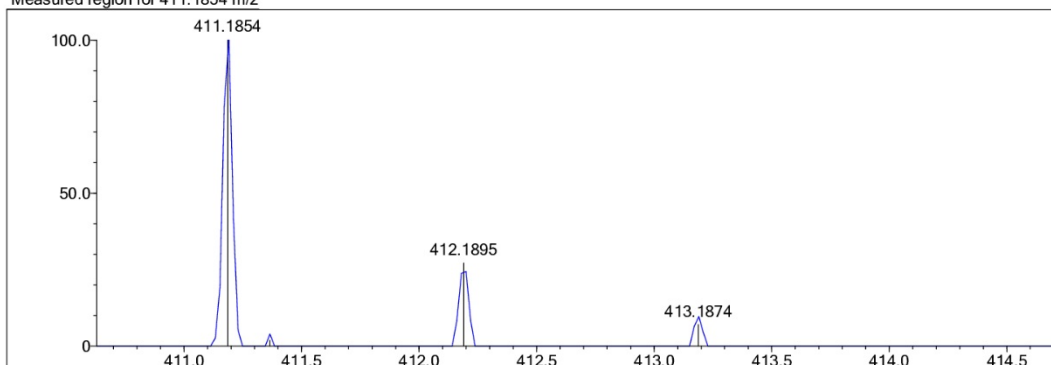
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	10	40	O	2	0	5	S	2	0	1	Ru	2	0	0	H
C	4	10	40	F	1	0	0	Cl	1	0	0	Pd	2	0	0	
N	3	2	5	P	3	0	0	Br	1	0	0	I	3	0	0	

Error Margin (ppm): 5
 DBE Range: 5.0 - 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
 Max Results: 150

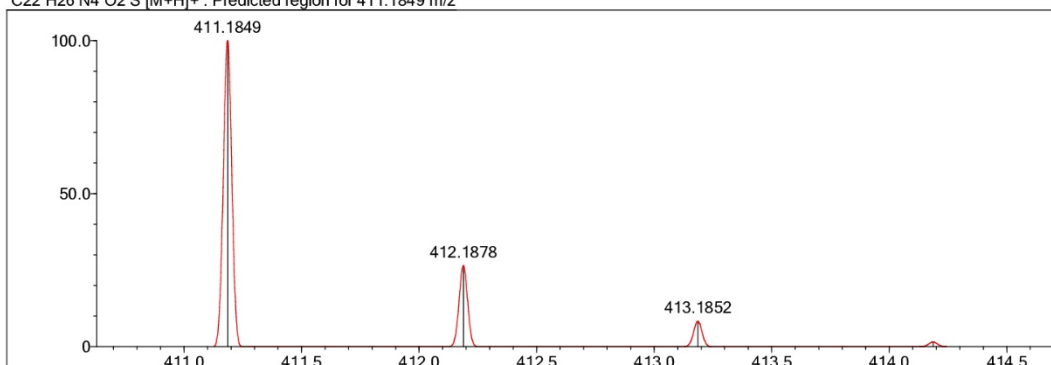
Event#: 1 MS(E+) Ret. Time : 2.147 Scan# : 323



Measured region for 411.1854 m/z



C22 H26 N4 O2 S [M+H]⁺ : Predicted region for 411.1849 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	79.48	C22 H26 N4 O2 S	[M+H] ⁺	411.1854	411.1849	0.5	1.22	79.91	12.0

Figure S35. HRMS spectra of compounds 4i

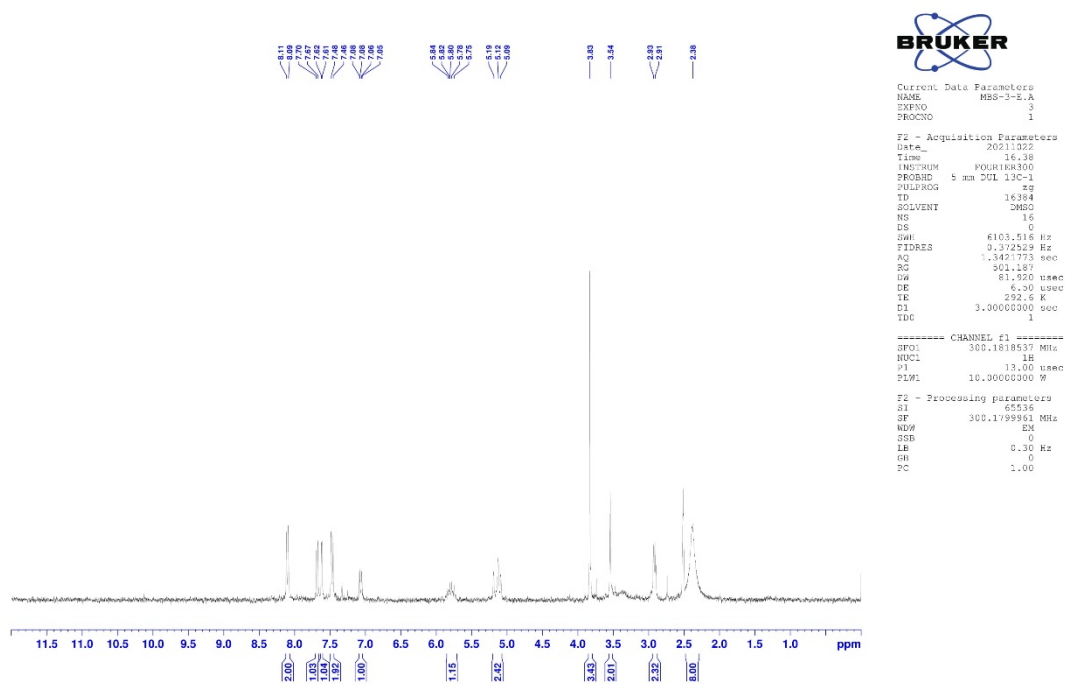


Figure S36. ¹H-NMR spectra of compounds 4j

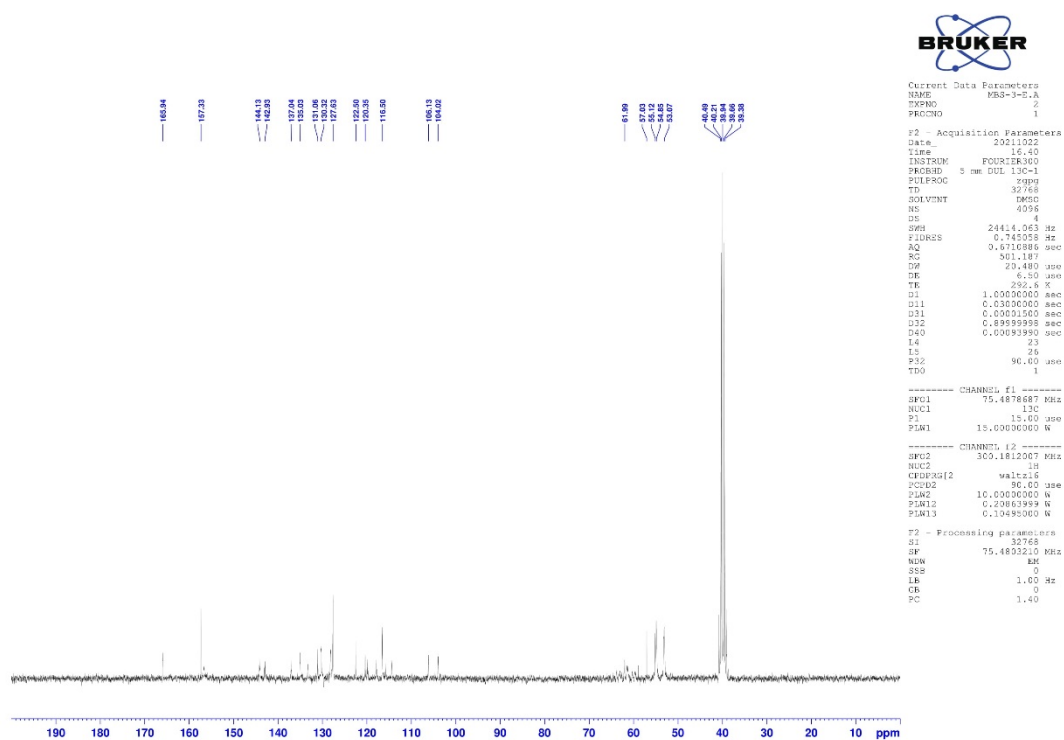


Figure S37. ¹³C-NMR spectra of compounds 4j

Data File: C:\LabSolutions\Data\Analiz\derya\MBS-3_168.lcd

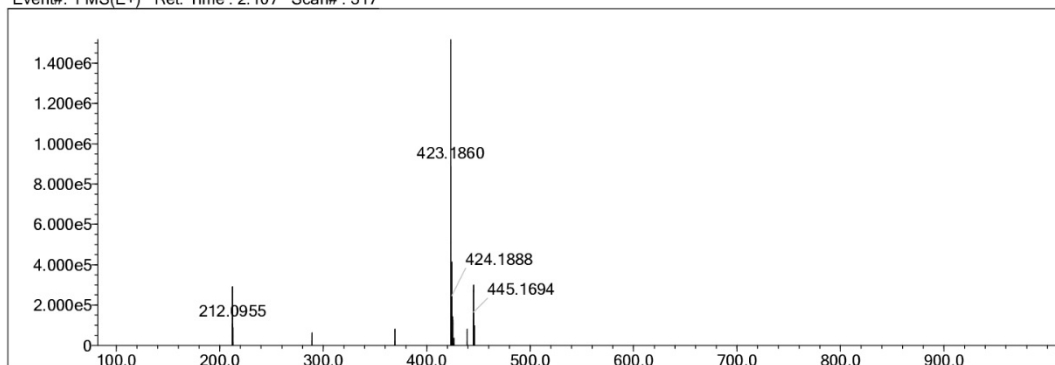
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	10	40	O	2	0	5	S	2	0	1	Ru	2	0	0	H
C	4	10	40	F	1	0	0	Cl	1	0	0	Pd	2	0	0	
N	3	2	5	P	3	0	0	Br	1	0	0	I	3	0	0	

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

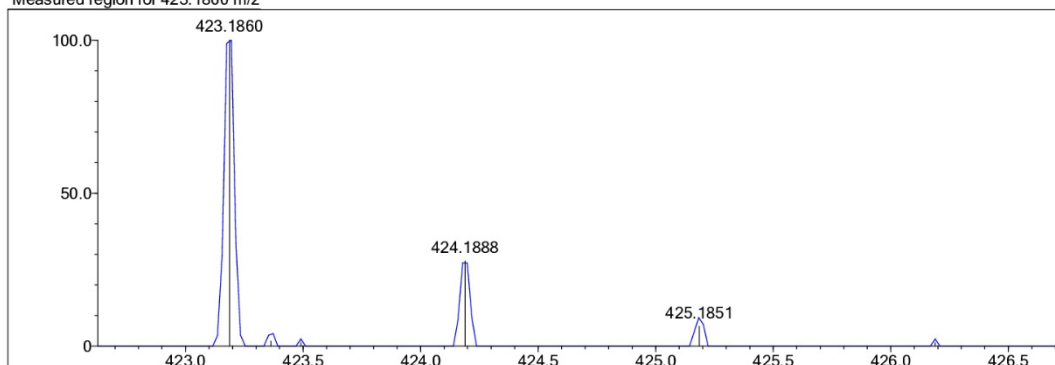
DBE Range: 5.0 - 15.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

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

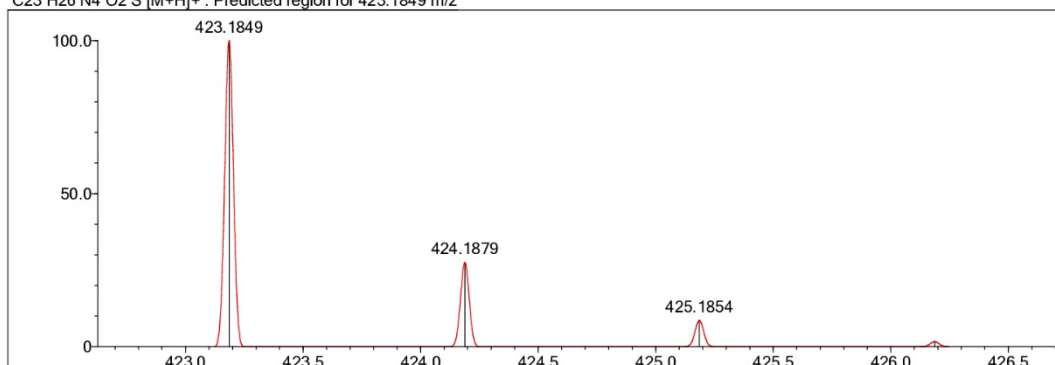
Event#: 1 MS(E+) Ret. Time : 2.107 Scan# : 317



Measured region for 423.1860 m/z



C23 H26 N4 O2 S [M+H]⁺ : Predicted region for 423.1849 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	96.00	C23 H26 N4 O2 S	[M+H] ⁺	423.1860	423.1849	1.1	2.60	100.00	13.0

Figure S38. HRMS spectra of compounds 4j

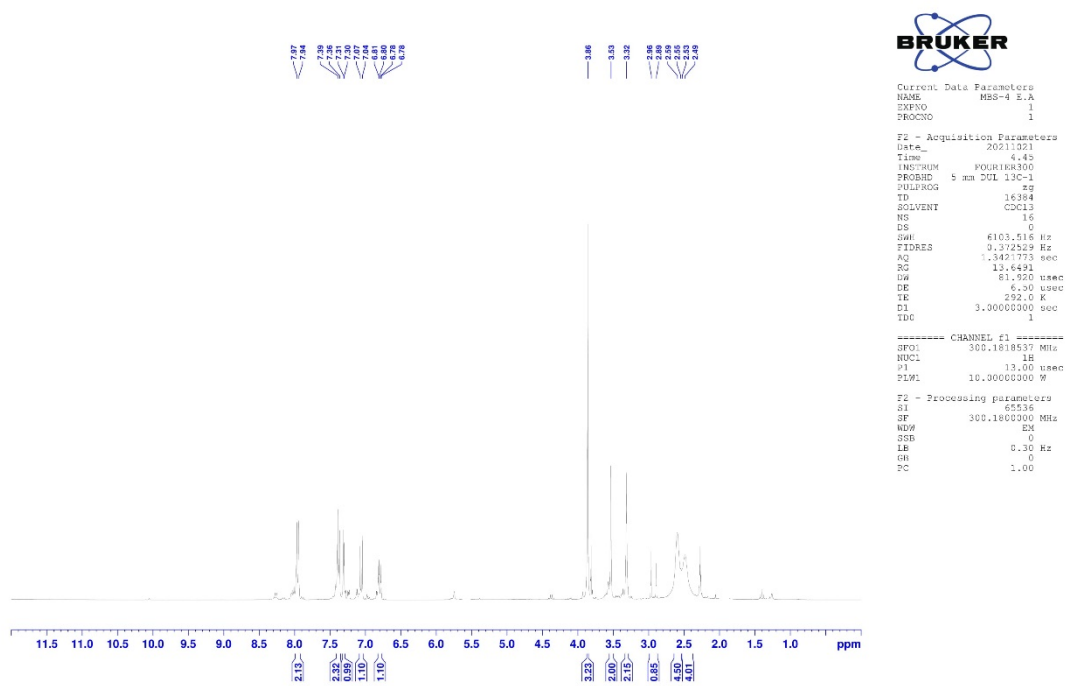


Figure S39. ¹H-NMR spectra of compounds 4k

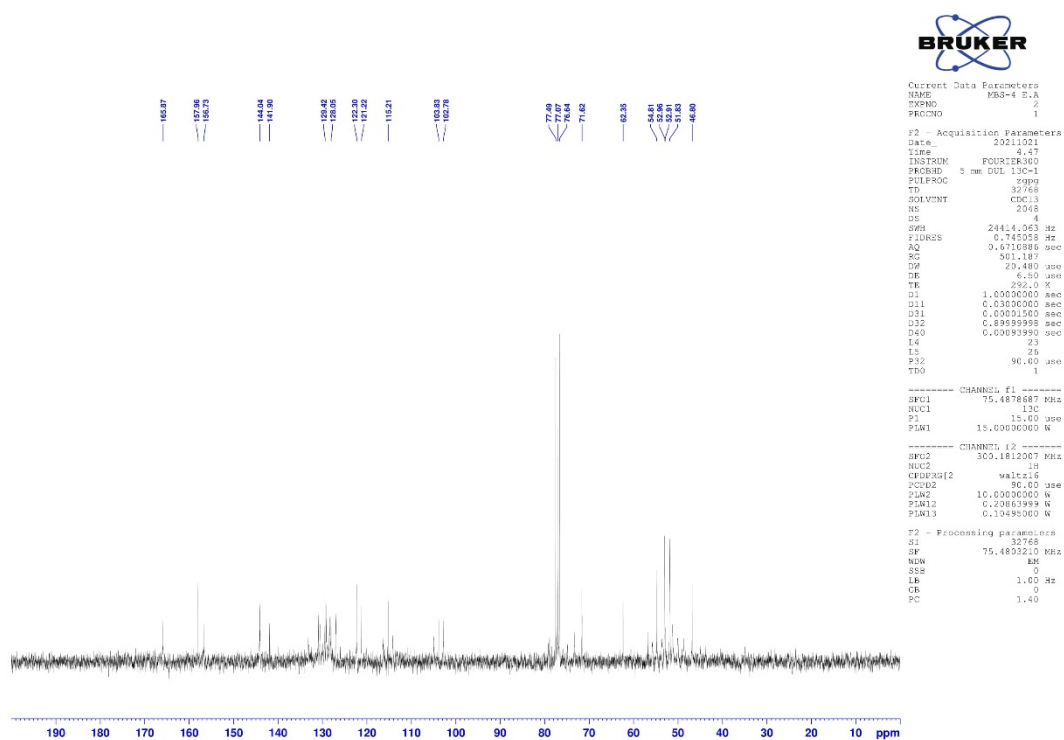


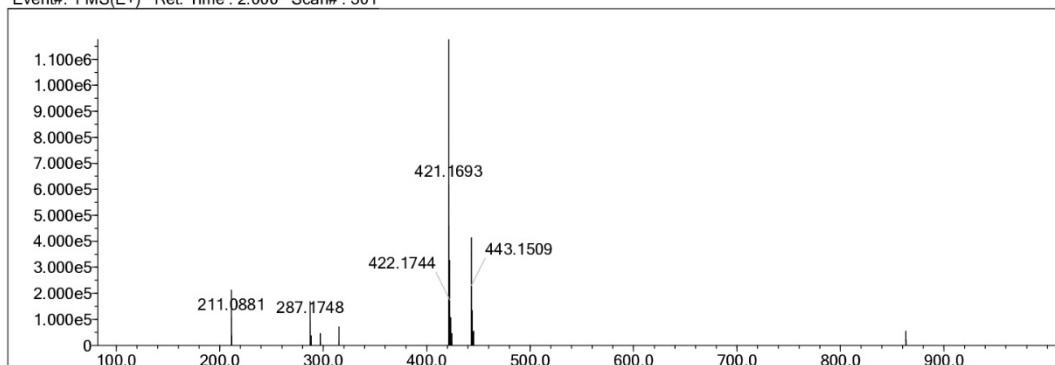
Figure S40. ¹³C-NMR spectra of compounds 4k

Data File: C:\LabSolutions\Data\Analiz\dera\MBS-4_169.lcd

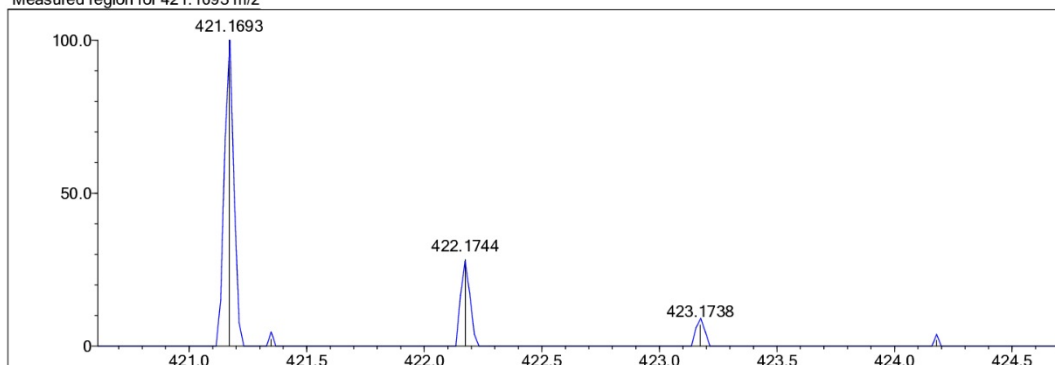
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	10	40	O	2	0	5	S	2	0	1	Ru	2	0	0	H
C	4	10	40	F	1	0	0	Cl	1	0	0	Pd	2	0	0	
N	3	2	5	P	3	0	0	Br	1	0	0	I	3	0	0	

Error Margin (ppm): 5
 DBE Range: 5.0 - 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: 150

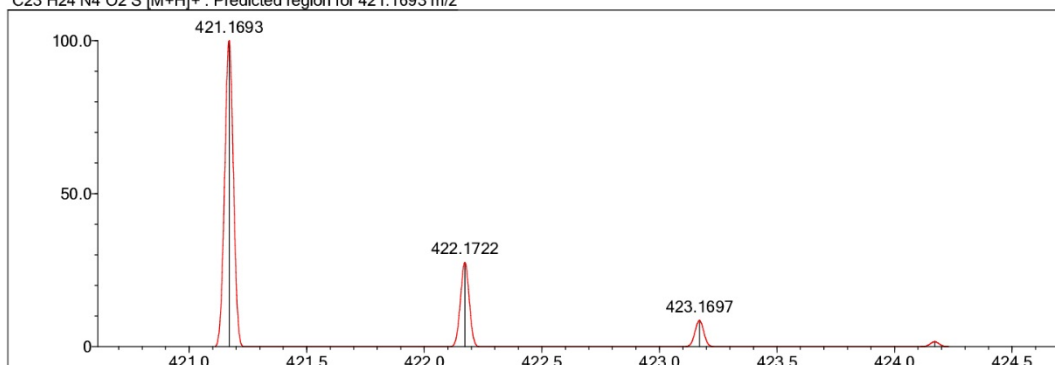
Event#: 1 MS(E+) Ret. Time : 2.000 Scan# : 301



Measured region for 421.1693 m/z



C23 H24 N4 O2 S [M+H]⁺ : Predicted region for 421.1693 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	77.64	C23 H24 N4 O2 S	[M+H] ⁺	421.1693	421.1693	0.0	0.00	77.64	14.0

Figure S41. HRMS spectra of compounds 4k

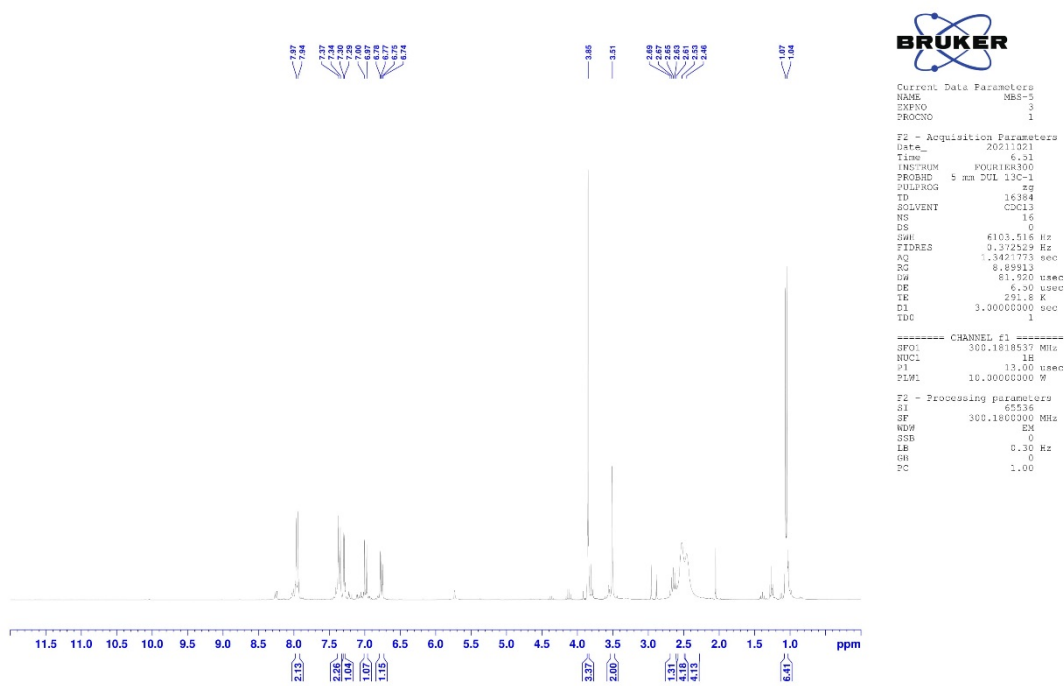


Figure S42. ¹H-NMR spectra of compounds 4I

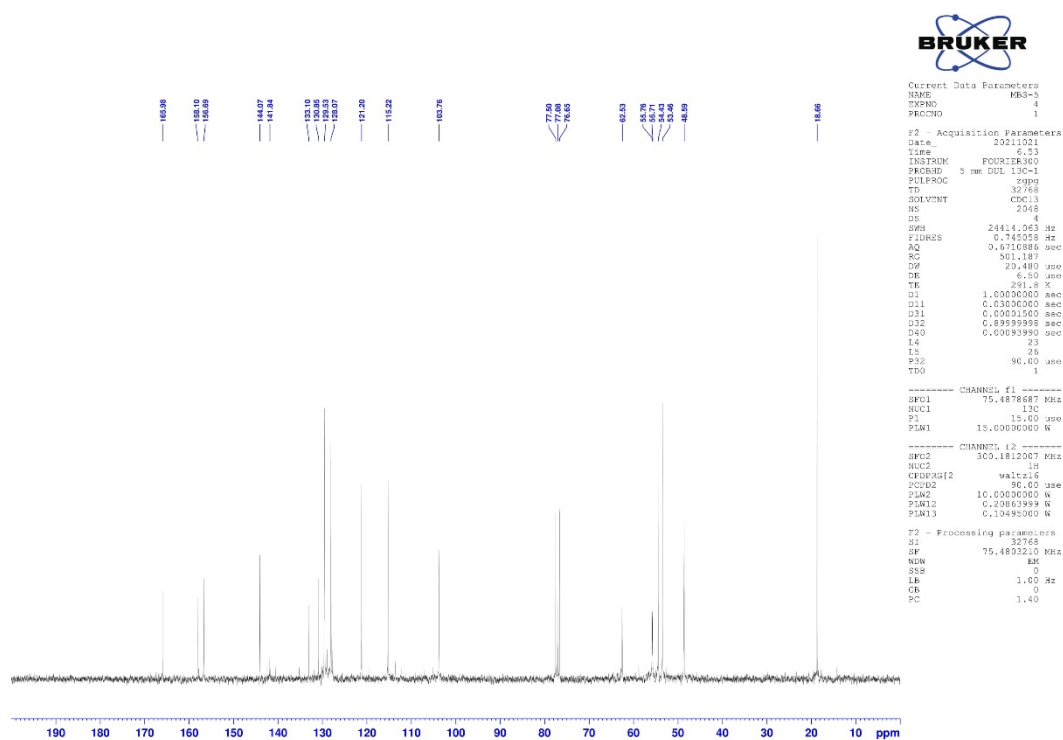


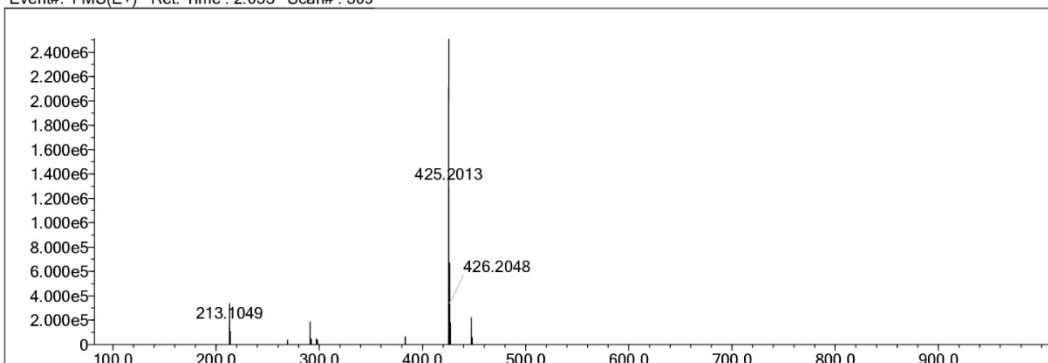
Figure S43. ¹³C-NMR spectra of compounds 4I

Data File: C:\LabSolutions\Data\Analiz\derya\MBS-5_170.lcd

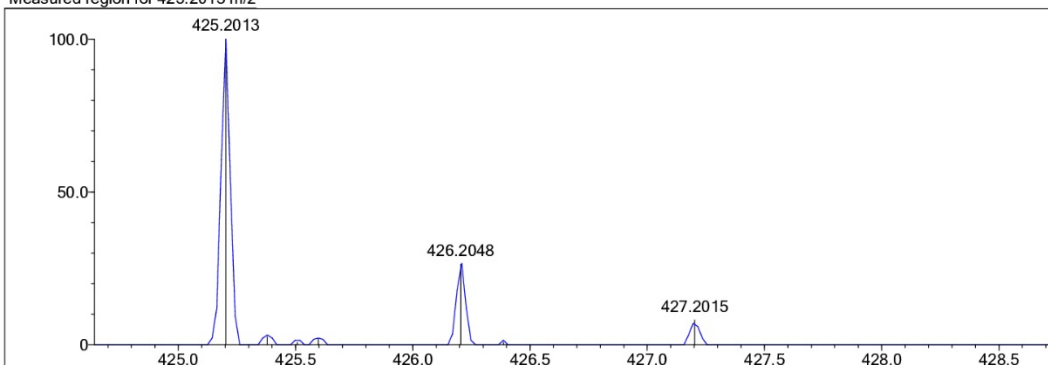
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	10	40	O	2	0	5	S	2	0	1	Ru	2	0	0	H
C	4	10	40	F	1	0	0	Cl	1	0	0	Pd	2	0	0	
N	3	2	5	P	3	0	0	Br	1	0	0	I	3	0	0	

Error Margin (ppm): 5
 DBE Range: 5.0 - 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
 Max Results: 150

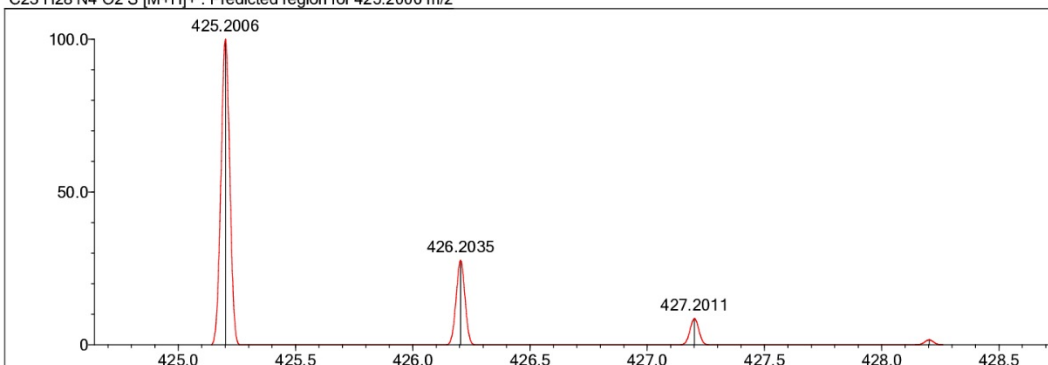
Event#: 1 MS(E+) Ret. Time : 2.053 Scan# : 309



Measured region for 425.2013 m/z



C23 H28 N4 O2 S [M+H]+ : Predicted region for 425.2006 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	83.75	C23 H28 N4 O2 S	[M+H] ⁺	425.2013	425.2006	0.7	1.65	85.13	12.0

Figure S44. HRMS spectra of compounds 4l

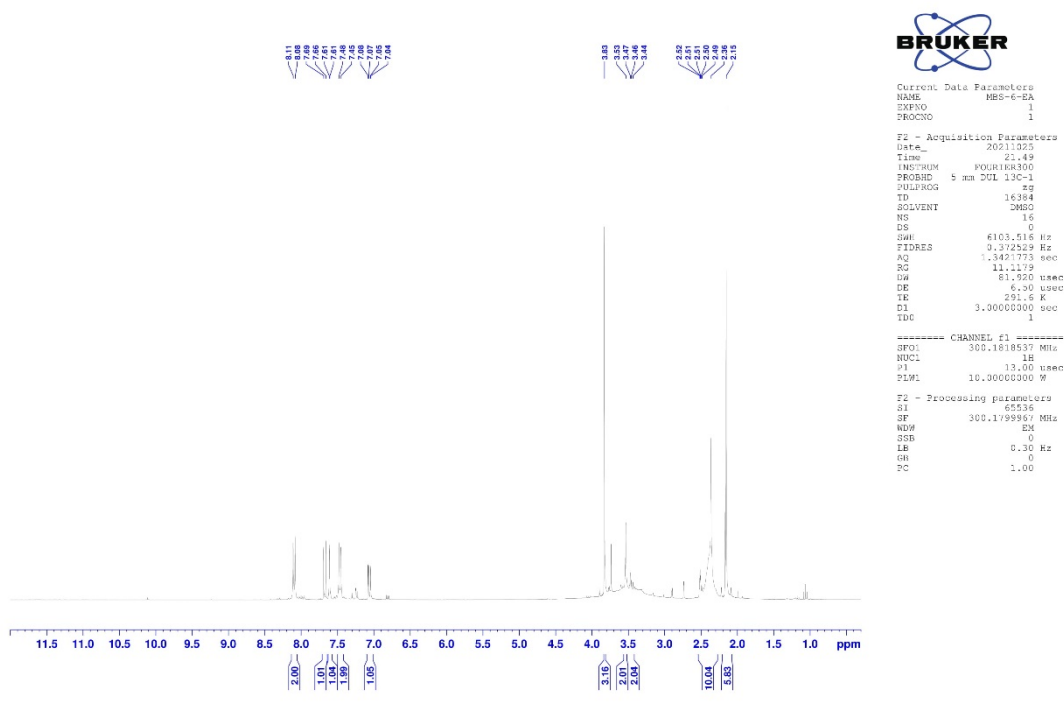


Figure S45. ¹H-NMR spectra of compounds **4m**

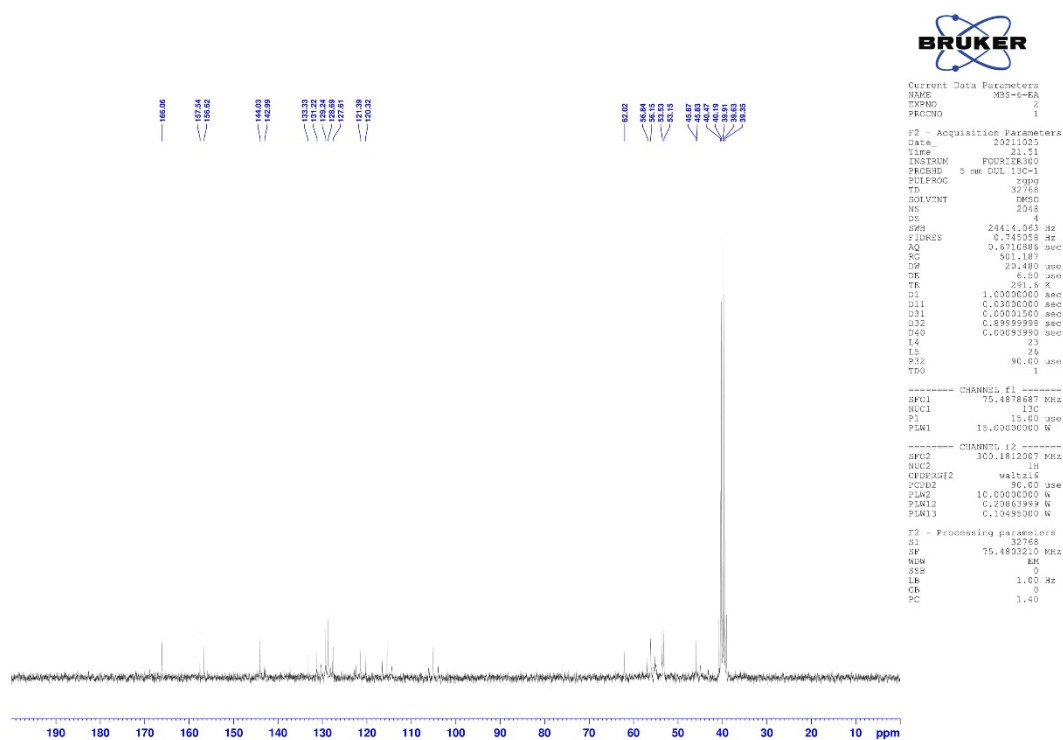


Figure S46. ¹³C-NMR spectra of compounds **4m**

Data File: C:\LabSolutions\Data\Analyze\dera\MBS-6_171.lcd

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	10	40	O	2	0	5	S	2	0	1	Ru	2	0	0	H
C	4	10	40	F	1	0	0	Cl	1	0	0	Pd	2	0	0	
N	3	2	5	P	3	0	0	Br	1	0	0	I	3	0	0	

Error Margin (ppm): 5

DBE Range: 5.0 - 15.0

Electron Ions: both

HC Ratio: unlimited

Apply N Rule: yes

Use MSn Info: yes

Max Isotopes: 3

Isotope RI (%): 1.00

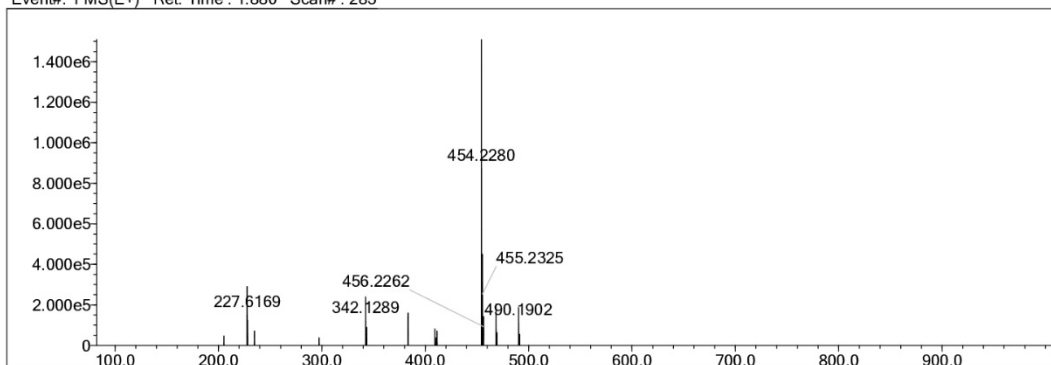
Isotope Res: 9000

MSn Iso RI (%): 10.00

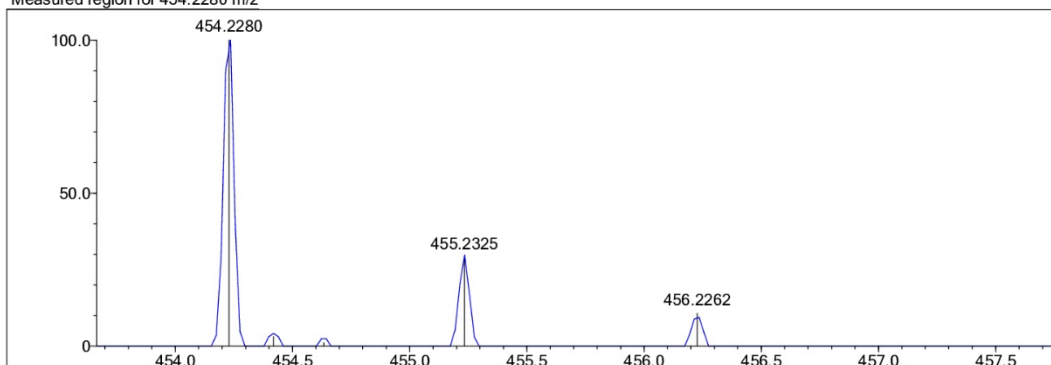
MSn Logic Mode: AND

Max Results: 150

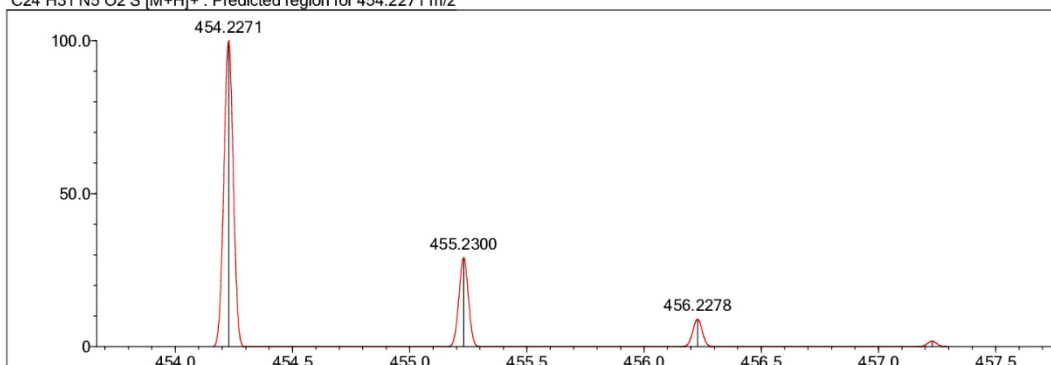
Event#: 1 MS(E+) Ret. Time: 1.880 Scan#: 283



Measured region for 454.2280 m/z



C24 H31 N5 O2 S [M+H]+ : Predicted region for 454.2271 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	87.16	C24 H31 N5 O2 S	[M+H] ⁺	454.2280	454.2271	0.9	1.98	89.35	12.0

Figure S47. HRMS spectra of compounds 4m

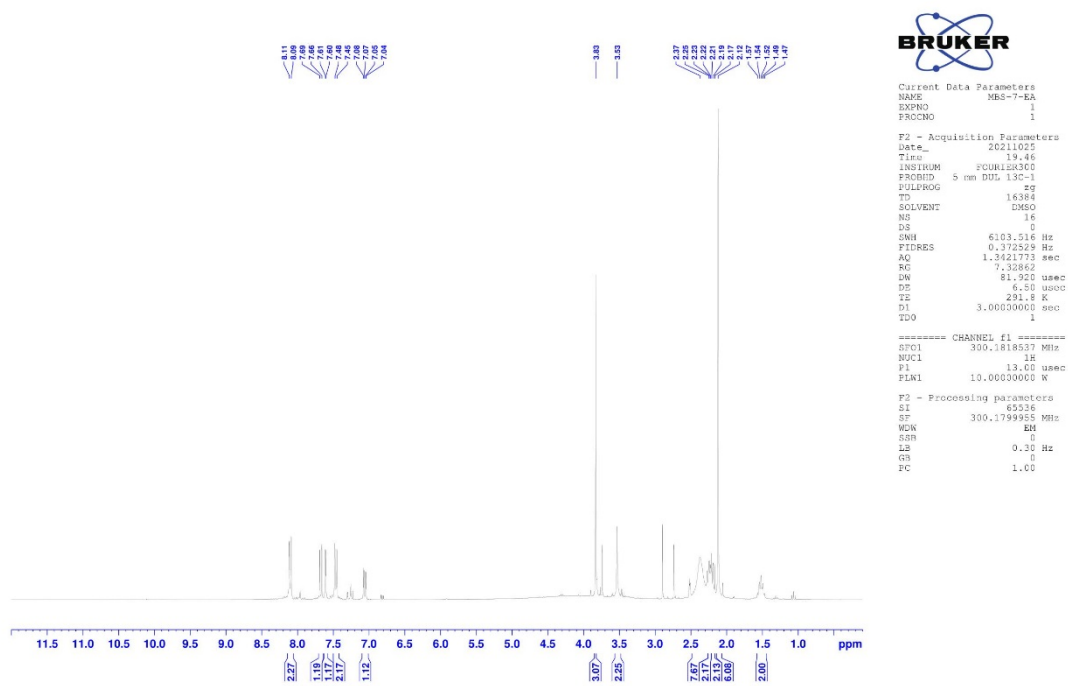


Figure S48. ¹H-NMR spectra of compounds 4n

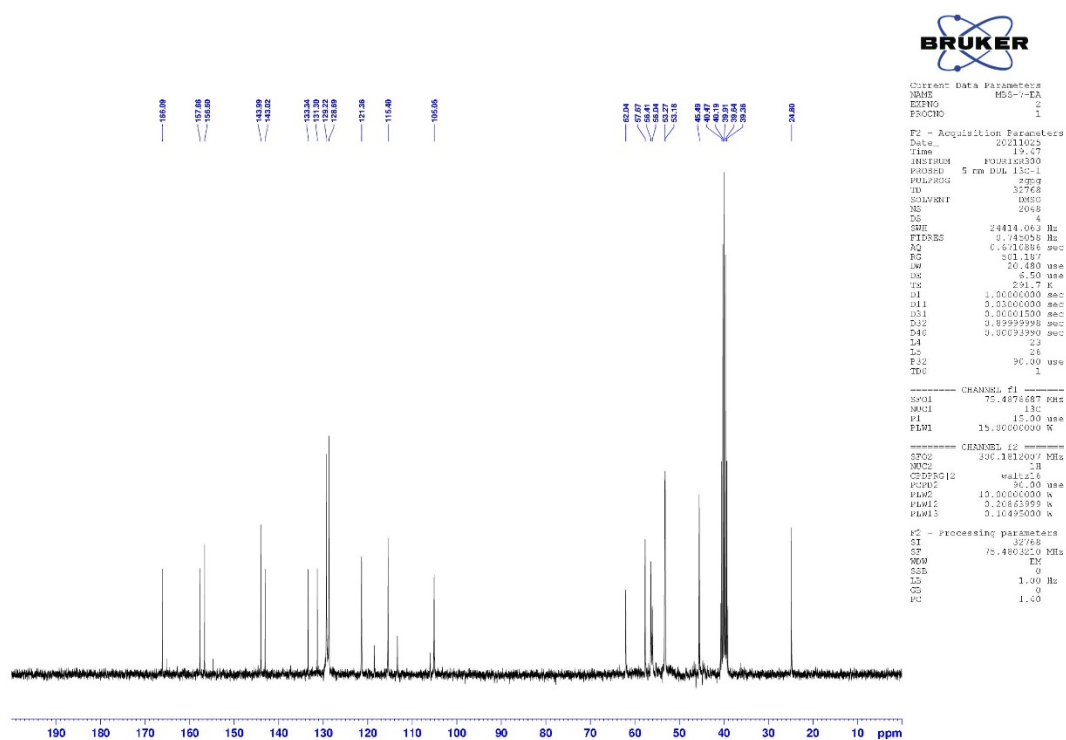


Figure S49. ¹³C-NMR spectra of compounds 4n

Data File: C:\LabSolutions\Data\Analiz\derya\MBS-7_172.lcd

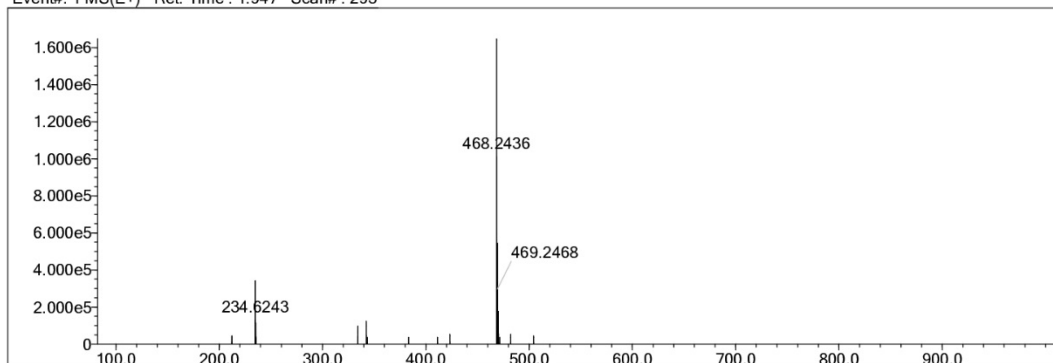
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	10	40	O	2	0	5	S	2	0	1	Ru	2	0	0	H
C	4	10	40	F	1	0	0	Cl	1	0	0	Pd	2	0	0	
N	3	2	5	P	3	0	0	Br	1	0	0	I	3	0	0	

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

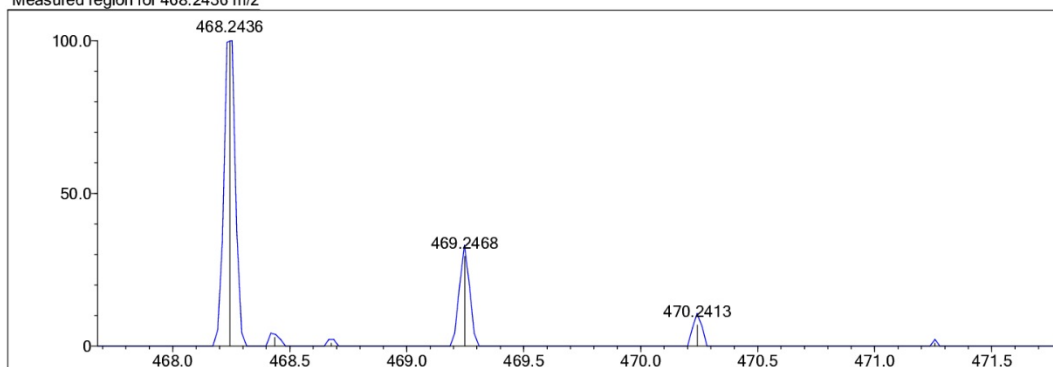
DBE Range: 5.0 - 15.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

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

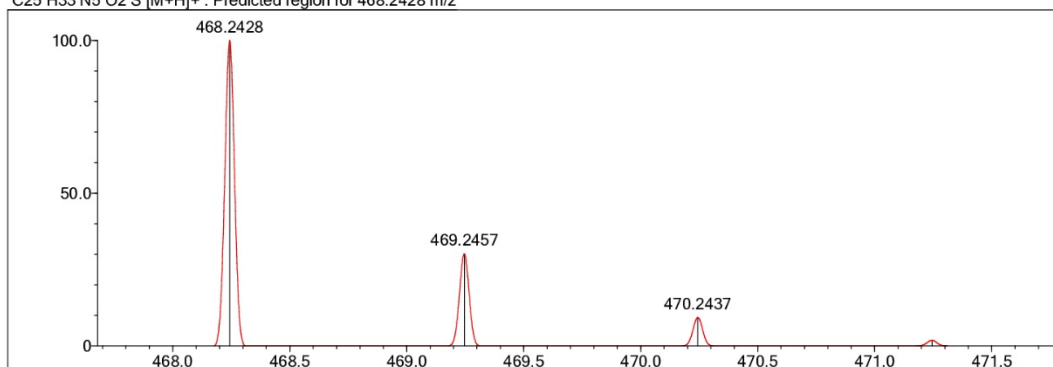
Event#: 1 MS(E+) Ret. Time: 1.947 Scan#: 293



Measured region for 468.2436 m/z



C25 H33 N5 O2 S [M+H]⁺ : Predicted region for 468.2428 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	77.52	C25 H33 N5 O2 S	[M+H] ⁺	468.2436	468.2428	0.8	1.71	78.92	12.0

Figure S50. HRMS spectra of compounds **4n**

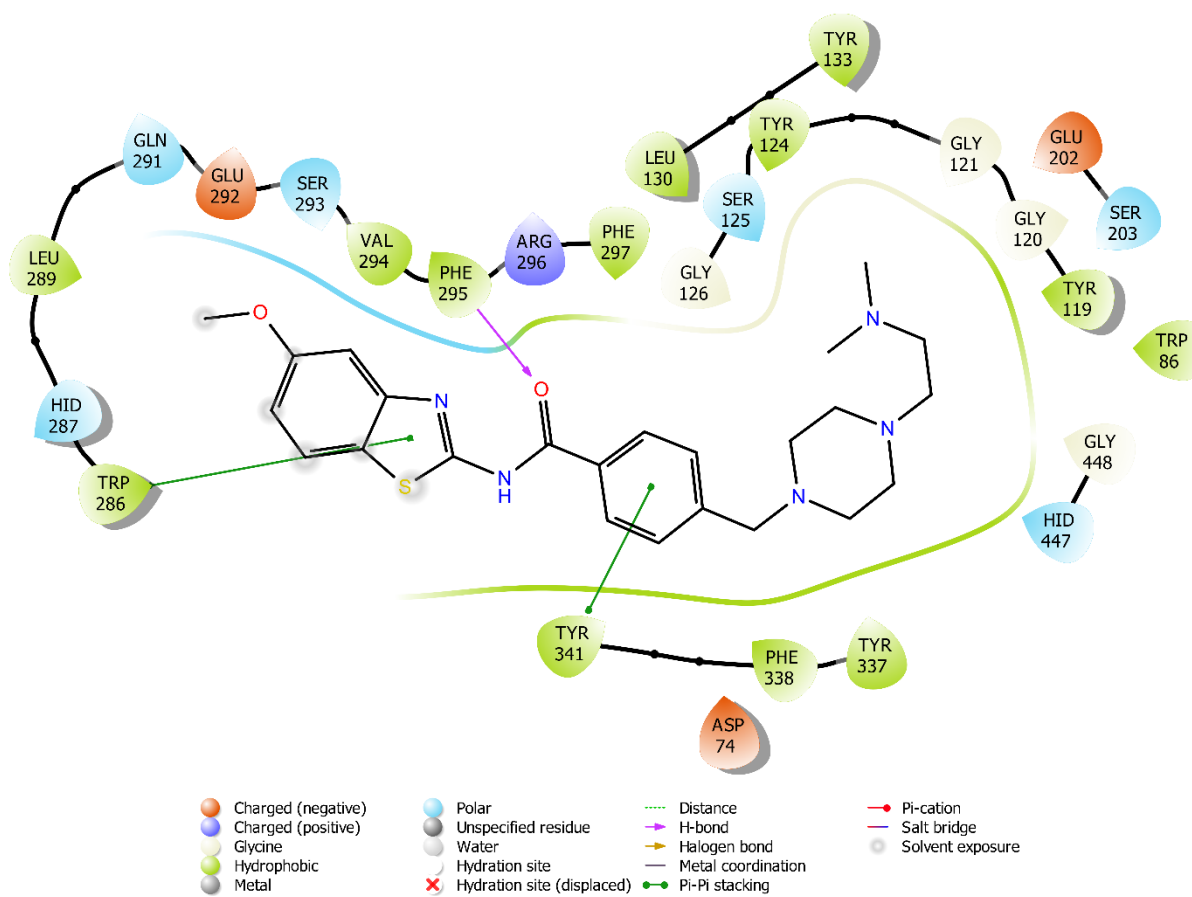


Figure S51. 2D interaction of compound **4m** at binding region (PBDID: 4EY7).

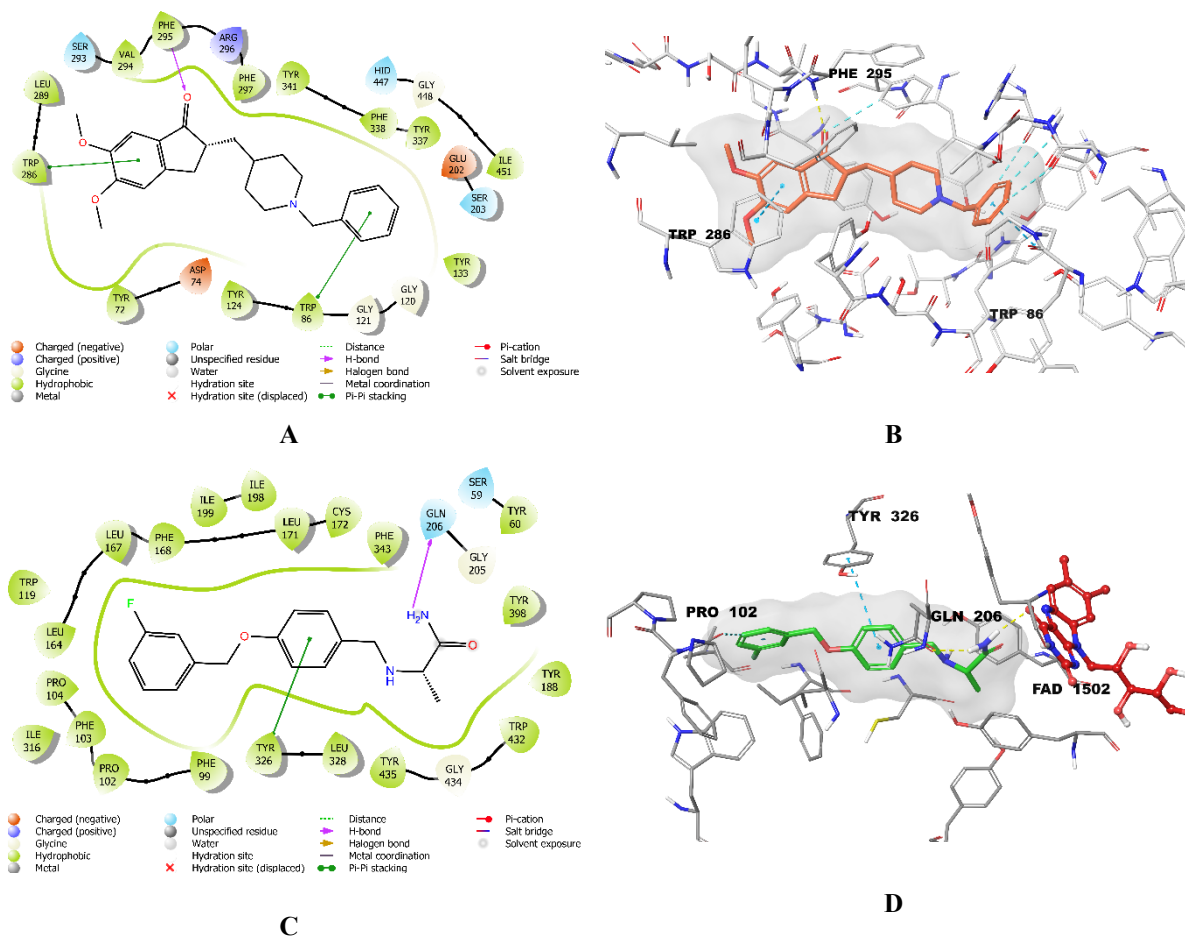
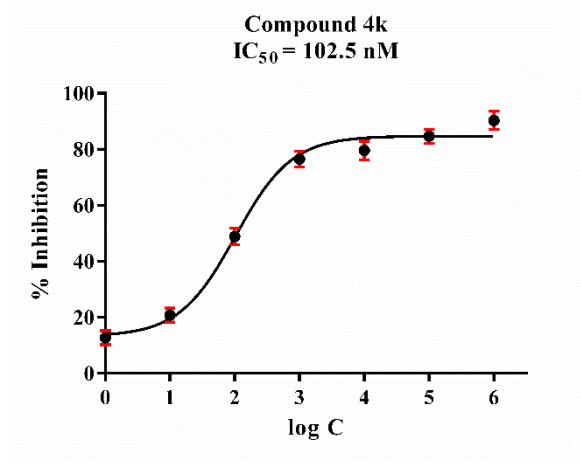
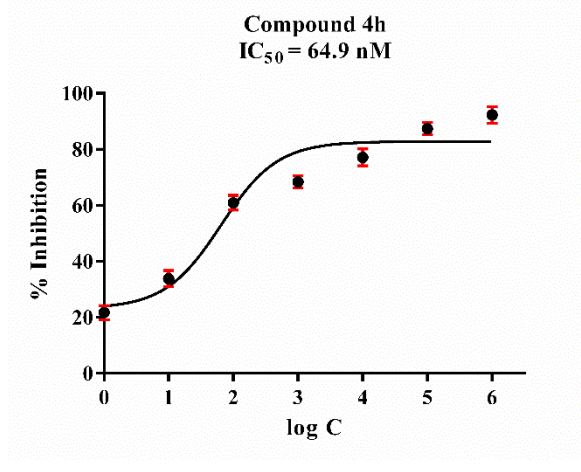
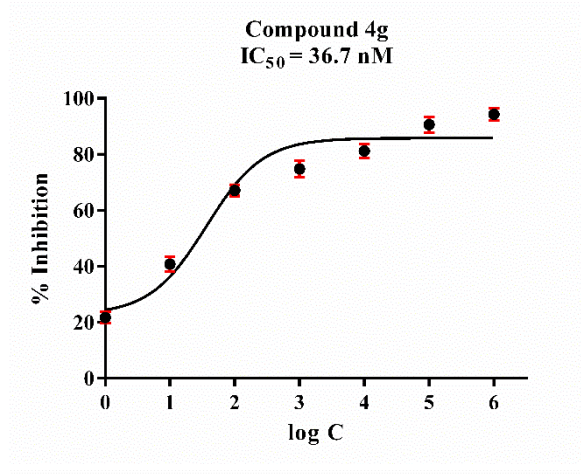
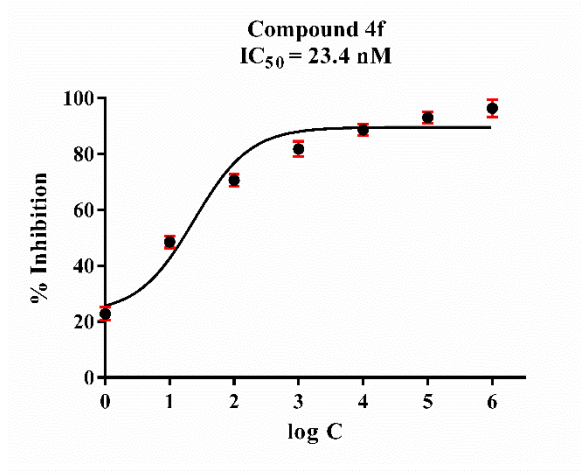
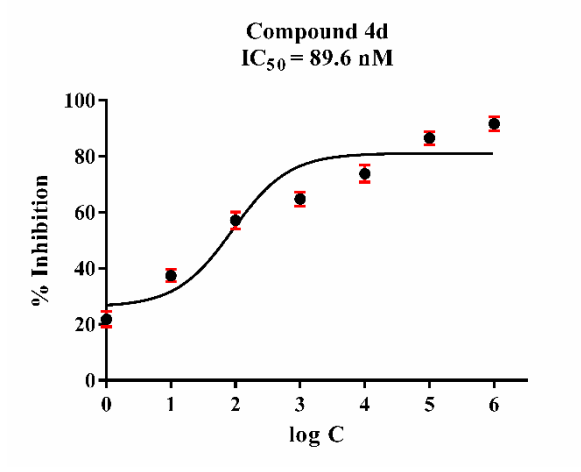
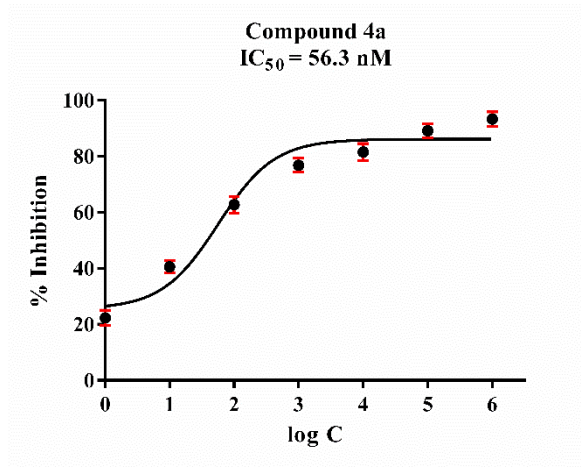


Figure S52. The 2D (A) and 3D (B) interacting modes of donepezil (colored with orange) in the active region the AChE (PDB ID: 4EY7). The 2D (C) and 3D (D) interacting modes of safinamide (colored with green) in the active region the MAO-B (PDB ID: 2V5Z).



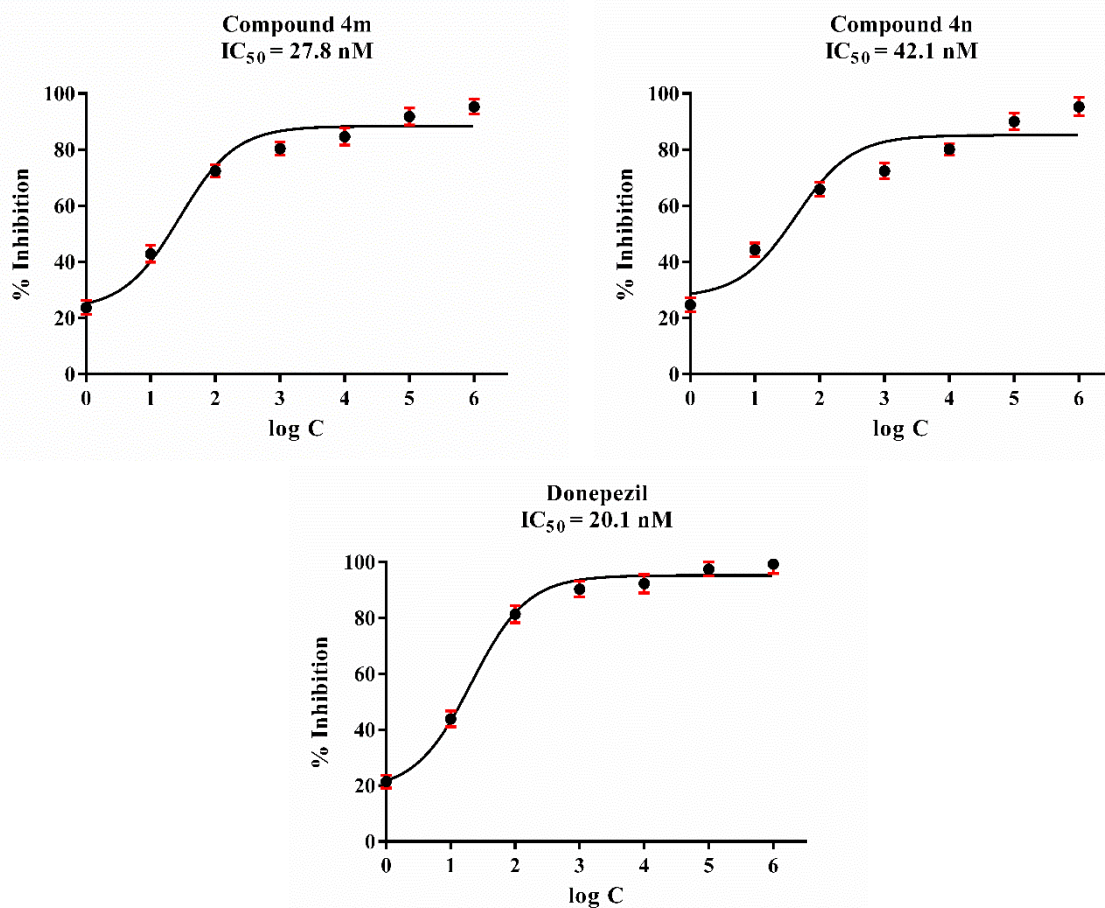
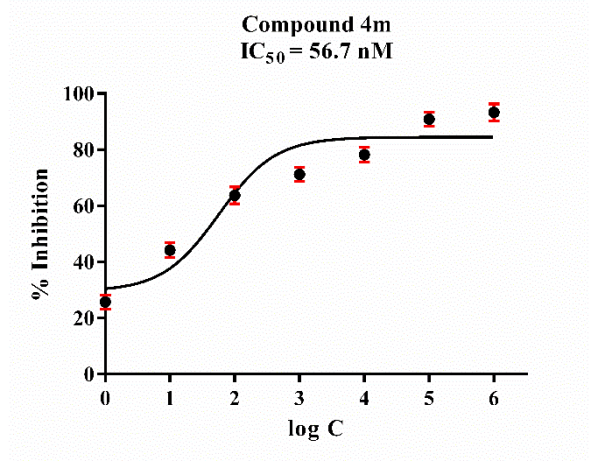
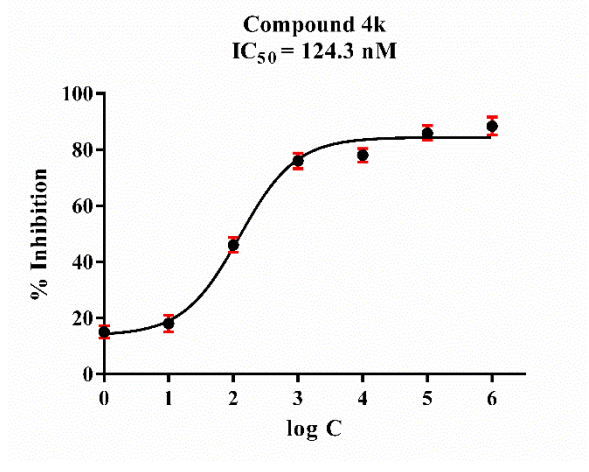
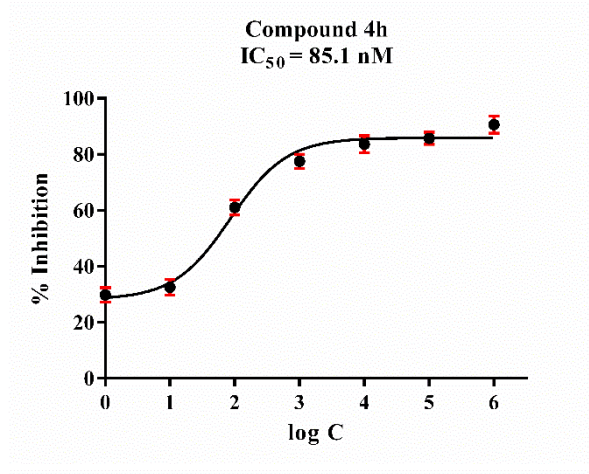
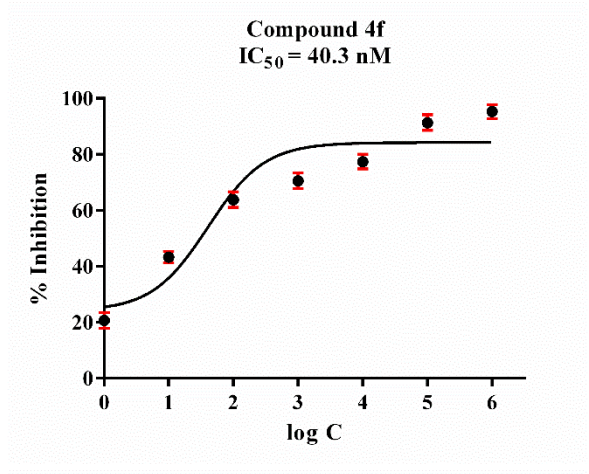
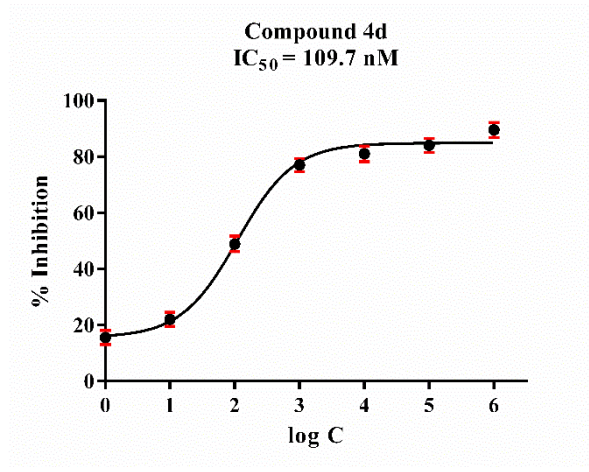
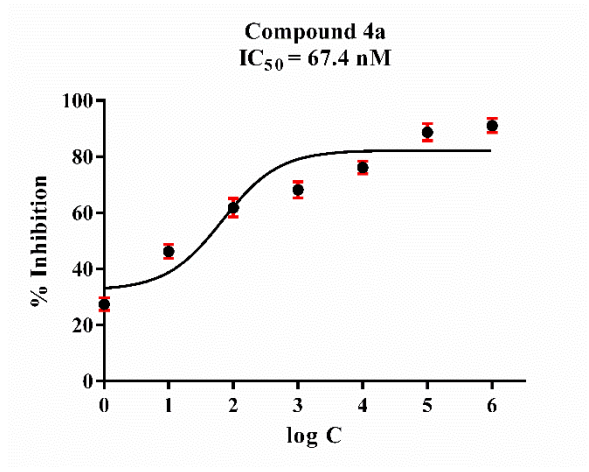


Figure S53. The IC_{50} graphs of compounds **4a**, **4d**, **4f**, **4g**, **4h**, **4k**, **4m**, **4n** and donepezil on AChE enzyme (The graphs are formed using GraphPad Prism Version 6 via regression analyses).



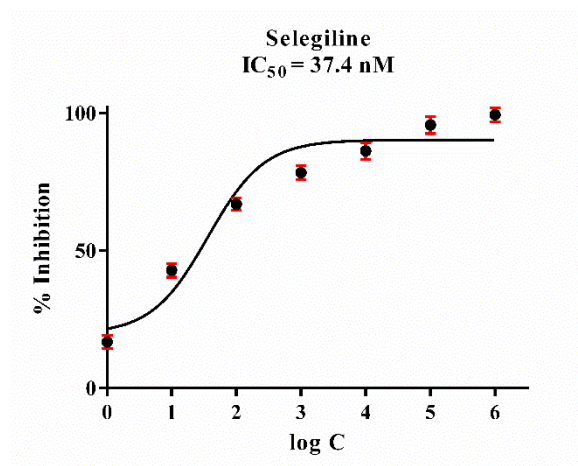


Figure S54. The IC_{50} graphs of compounds **4a**, **4d**, **4f**, **4h**, **4k**, **4m** and selegiline on MAO-B enzyme (The graphs are formed using GraphPad Prism Version 6 via regression analyses).