

Formula Predictor Report - ARZ-1_119.lcd

Page 1 of 1

Data File: C:\LabSolutions\Data\Analiz\derya\ARZ-1_119.lcd

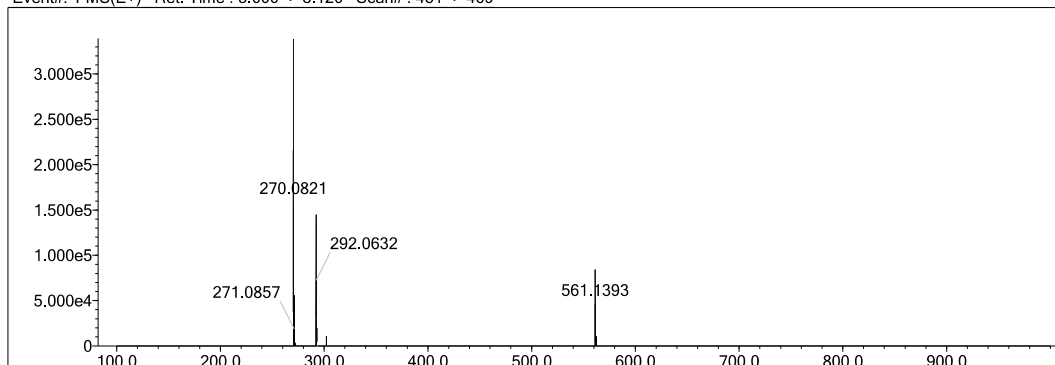
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C	4	10	40	F	1	0	0	Cl	1	0	0	Pd	2	0	0	
N	3	3	5	P	3	0	0	Br	1	0	0	I	3	0	0	

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

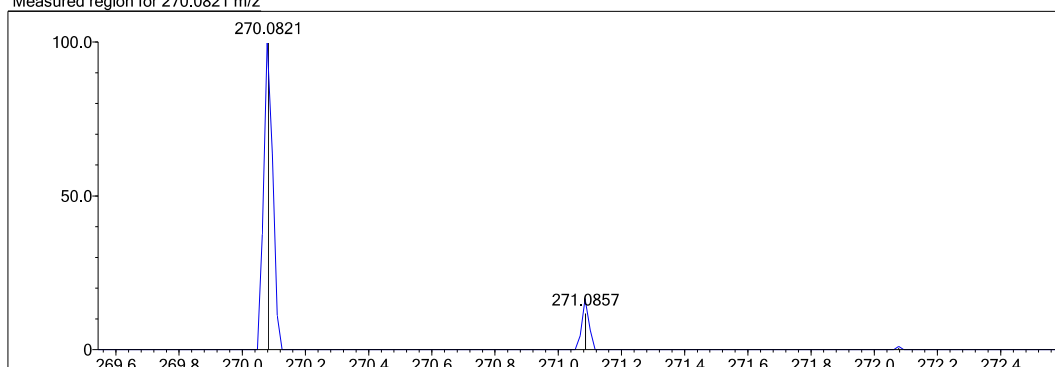
DBE Range: 5.0 - 25.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

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

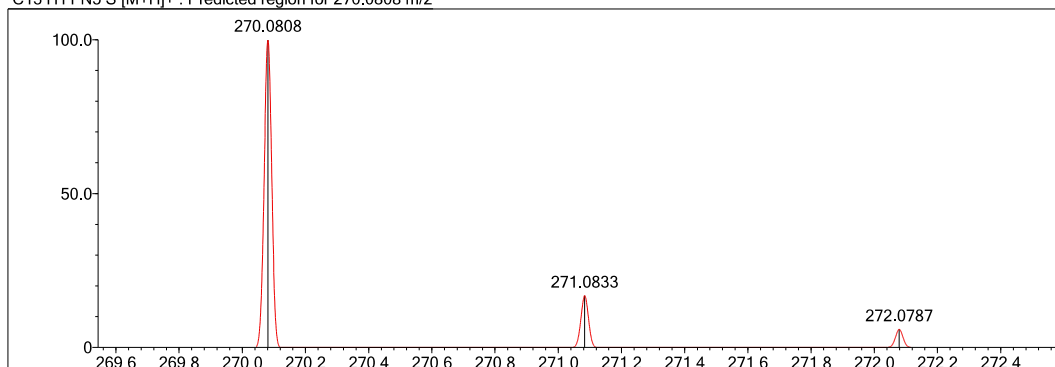
Event#: 1 MS(E+) Ret. Time : 3.000 -> 3.120 Scan# : 451 -> 469



Measured region for 270.0821 m/z



C13 H11 N5 S [M+H]⁺ : Predicted region for 270.0808 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	67.39	C13 H11 N5 S	[M+H] ⁺	270.0821	270.0808	1.3	4.81	74.48	11.0

Figure S1. Compound 2a HRMS report

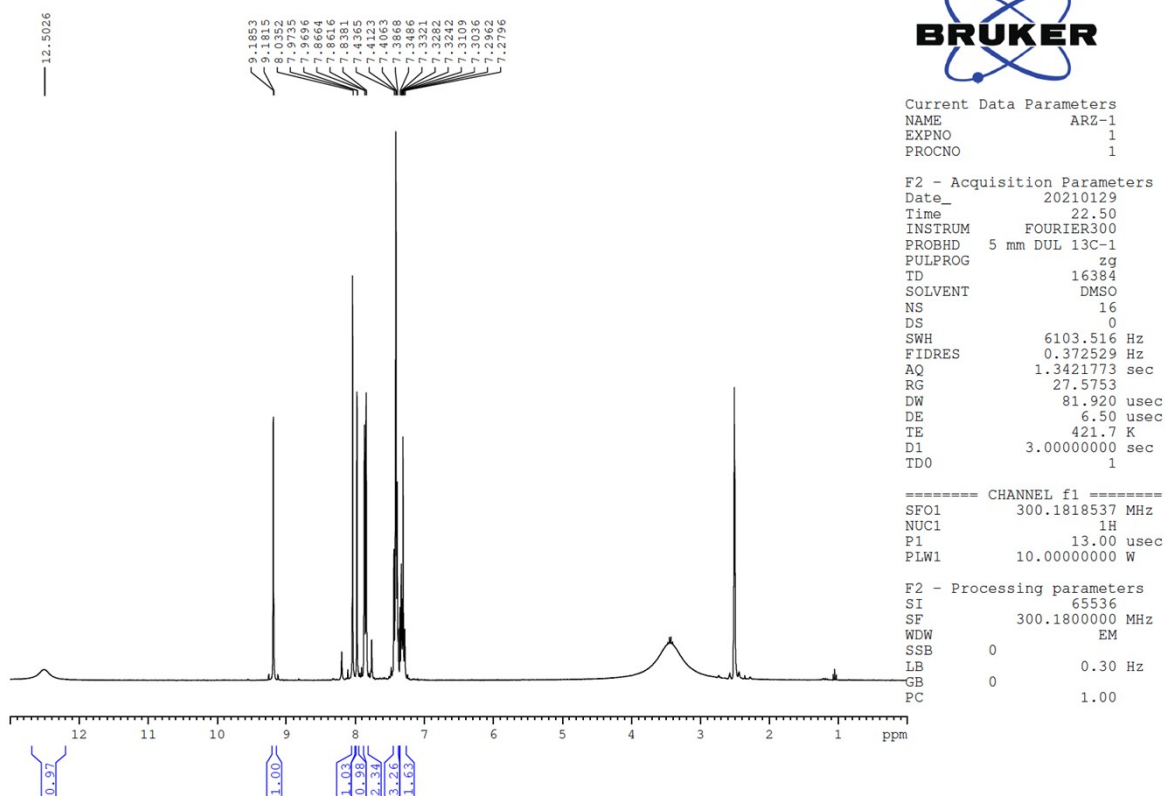


Figure S2. Compound 2a ¹H-NMR spectrum

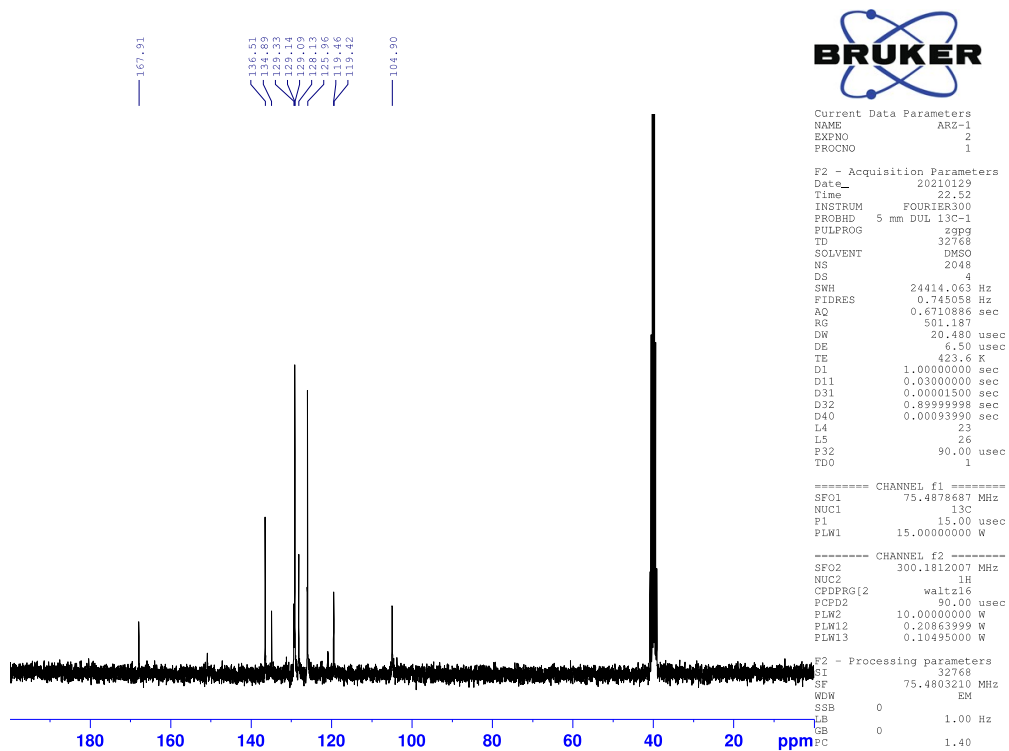


Figure S3. Compound 2a ¹³C-NMR spectrum

Data File: C:\LabSolutions\Data\Analiz\derya\ARZ-2_120.lcd

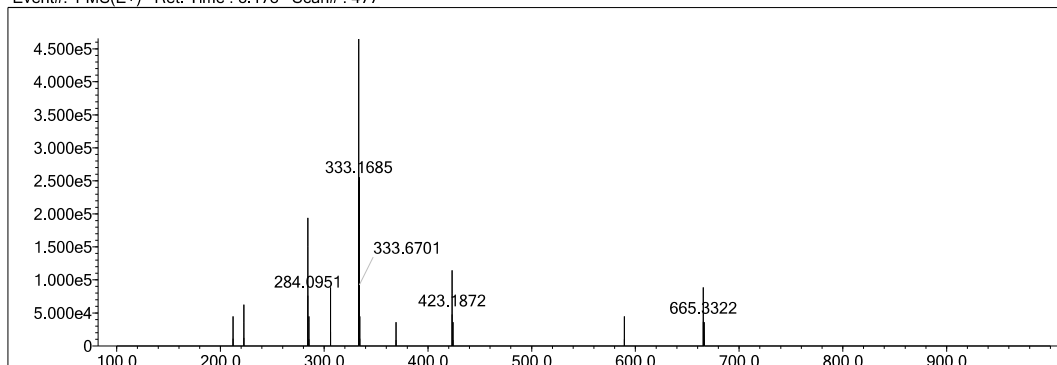
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	10	40	O	2	0	4	S	2	1	2	Ru	2	0	0	H
C	4	10	40	F	1	0	0	Cl	1	0	0	Pd	2	0	0	
N	3	3	5	P	3	0	0	Br	1	0	0	I	3	0	0	

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

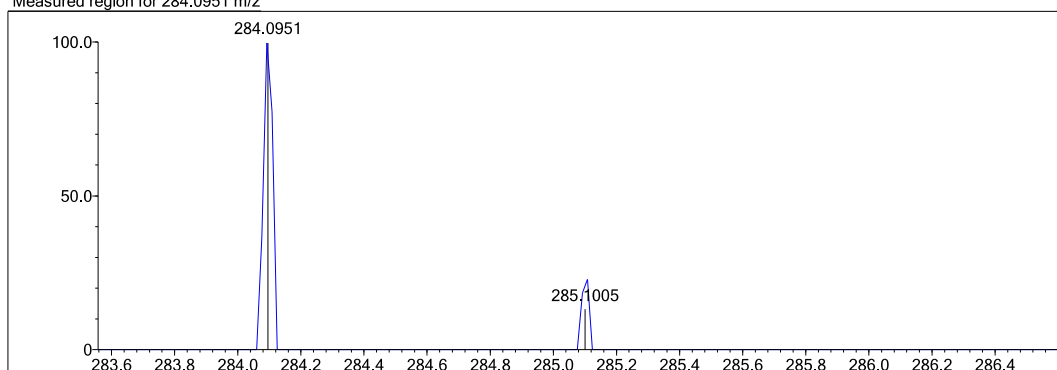
DBE Range: 5.0 - 25.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

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

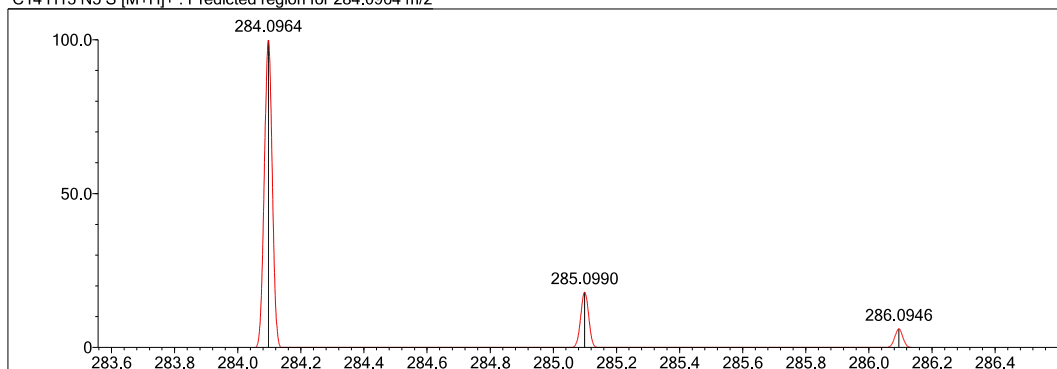
Event#: 1 MS(E+) Ret. Time : 3.173 Scan# : 477



Measured region for 284.0951 m/z



C14 H13 N5 S [M+H]⁺: Predicted region for 284.0964 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	56.74	C14 H13 N5 S	[M+H] ⁺	284.0951	284.0964	-1.3	-4.58	62.32	11.0

Figure S4. Compound 2b HRMS report

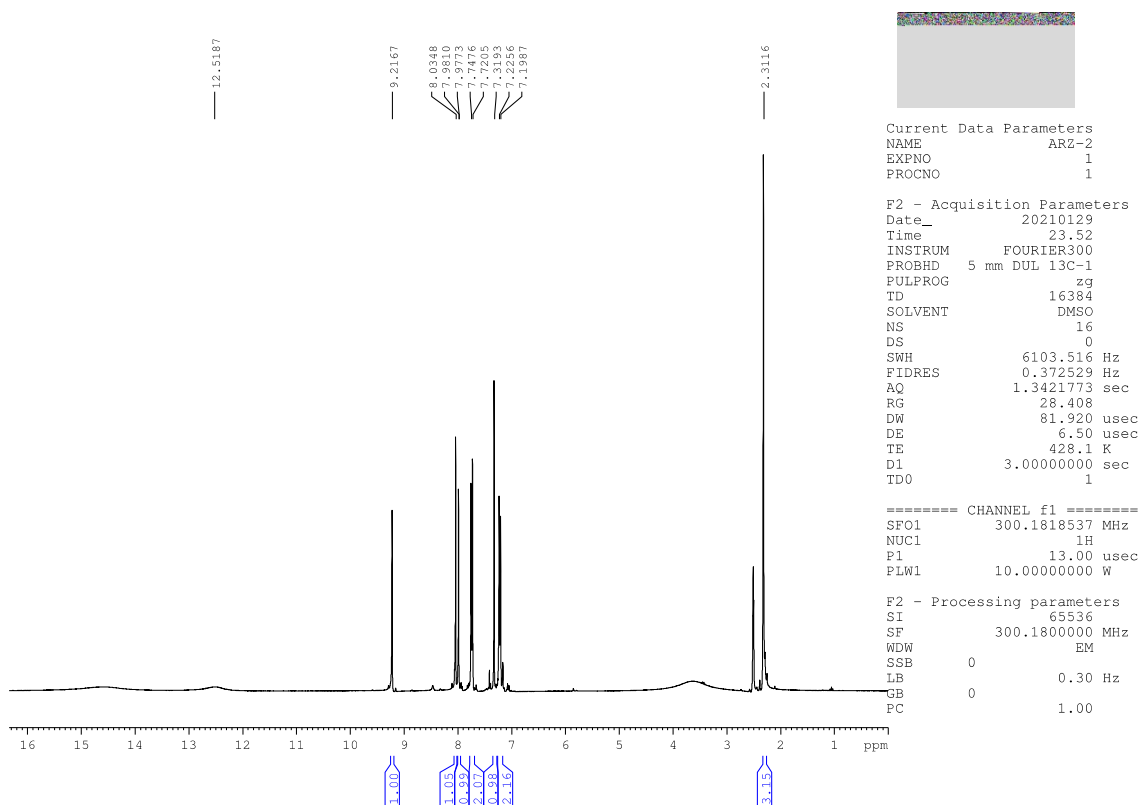


Figure S5. Compound 2b ¹H-NMR spectrum

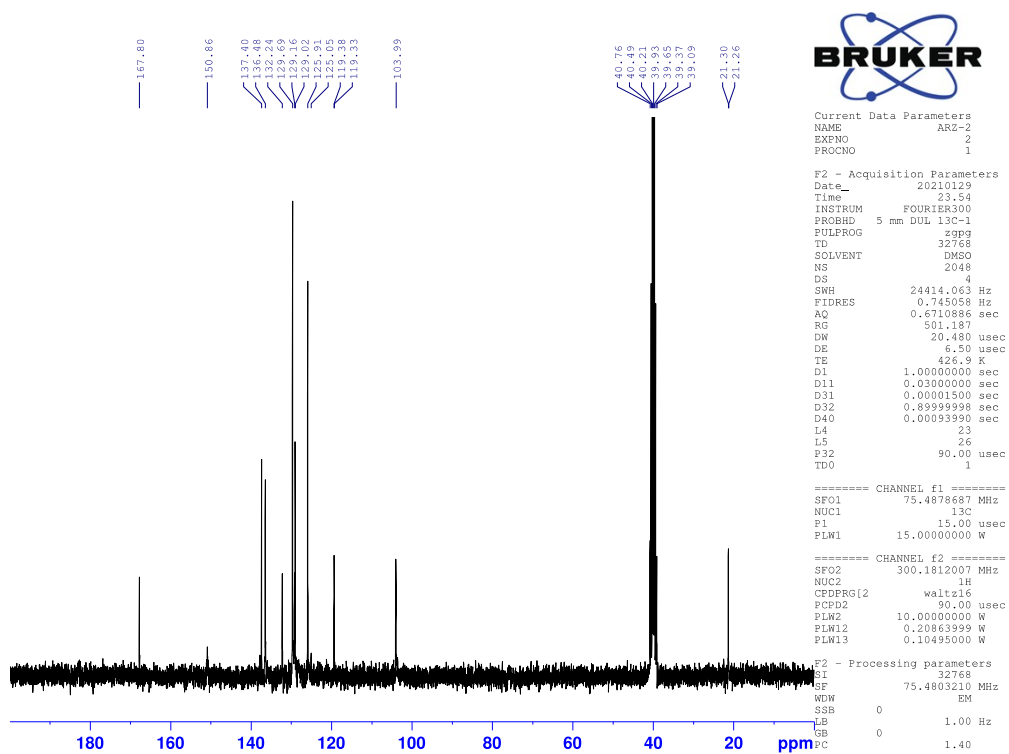


Figure S6. Compound 2b ¹³C-NMR spectrum

Data File: C:\LabSolutions\Data\Analiz\derya\ARZ-3_121.lcd

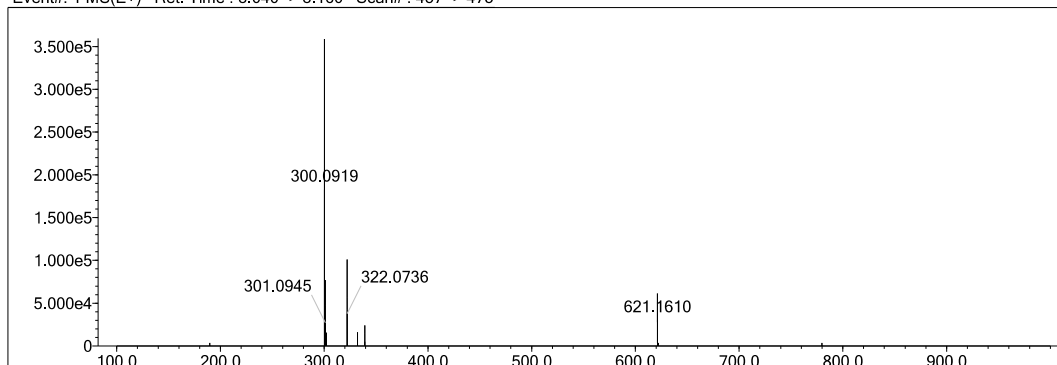
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	10	40	O	2	0	4	S	2	1	2	Ru	2	0	0	H
C	4	10	40	F	1	0	0	Cl	1	0	0	Pd	2	0	0	
N	3	3	5	P	3	0	0	Br	1	0	0	I	3	0	0	

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

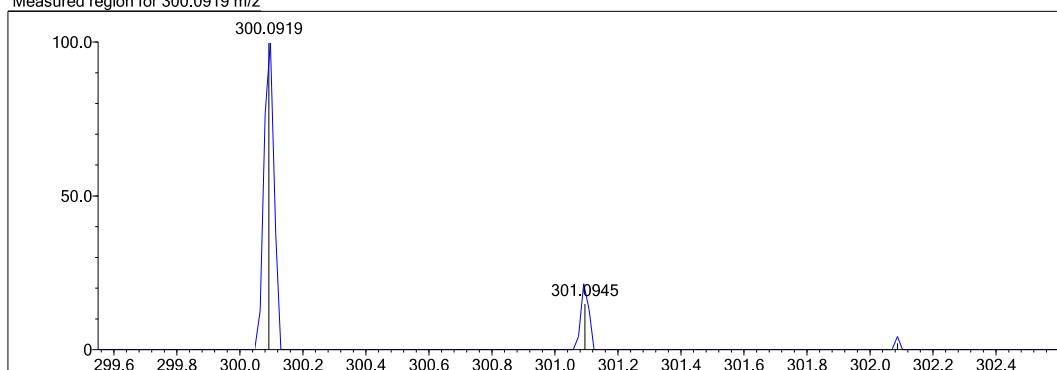
DBE Range: 5.0 - 25.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

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

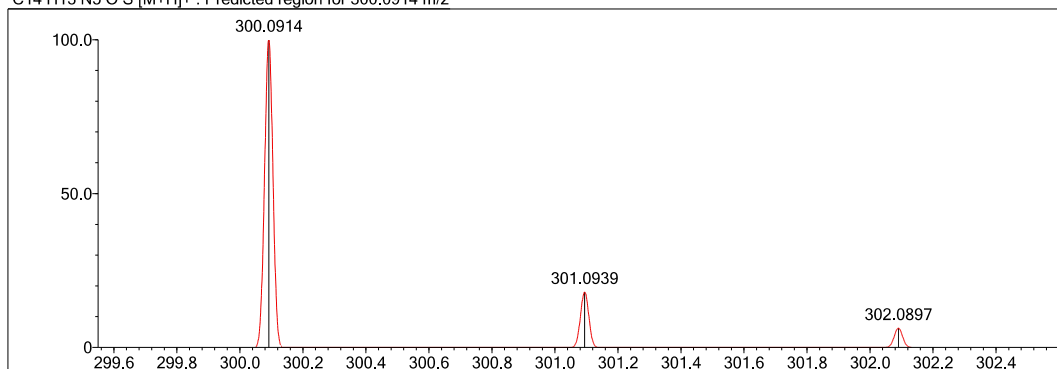
Event#: 1 MS(E+) Ret. Time : 3.040 -> 3.160 Scan# : 457 -> 475



Measured region for 300.0919 m/z



C14 H13 N5 O S [M+H]⁺ : Predicted region for 300.0914 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	72.00	C14 H13 N5 O S	[M+H] ⁺	300.0919	300.0914	0.5	1.67	73.23	11.0

Figure S7. Compound 2c HRMS report

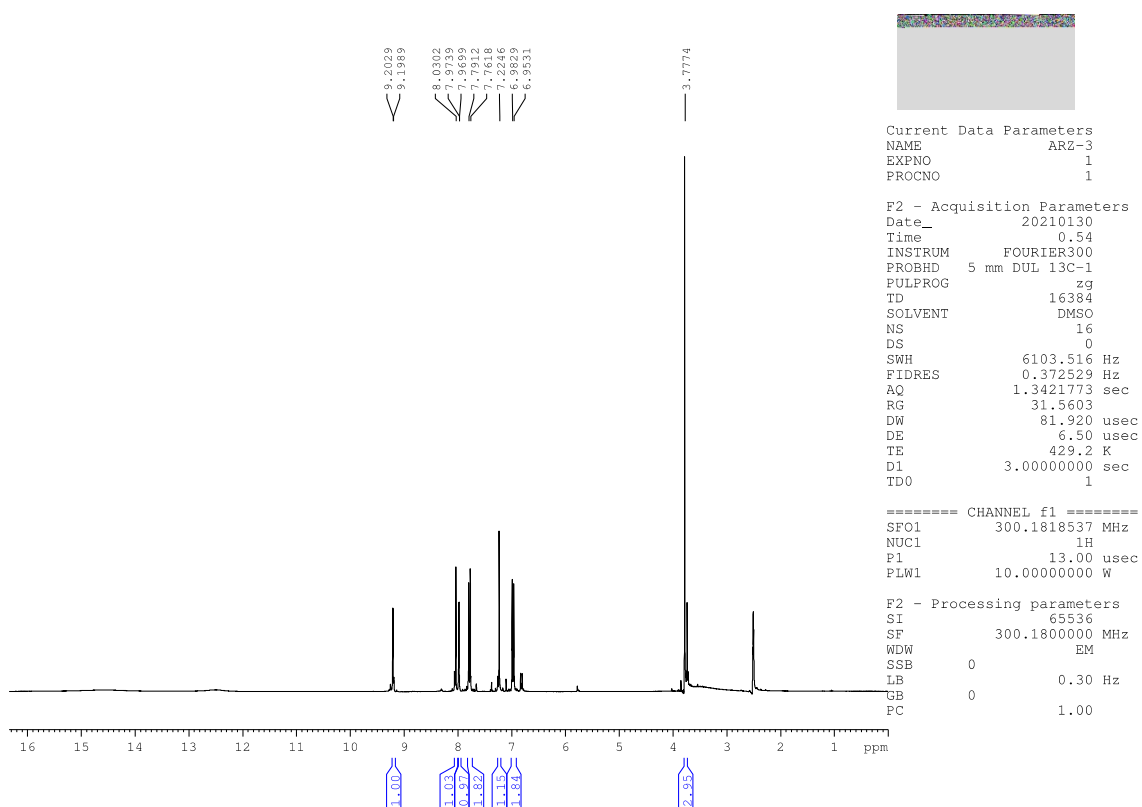


Figure S8. Compound 2c ¹H-NMR spectrum

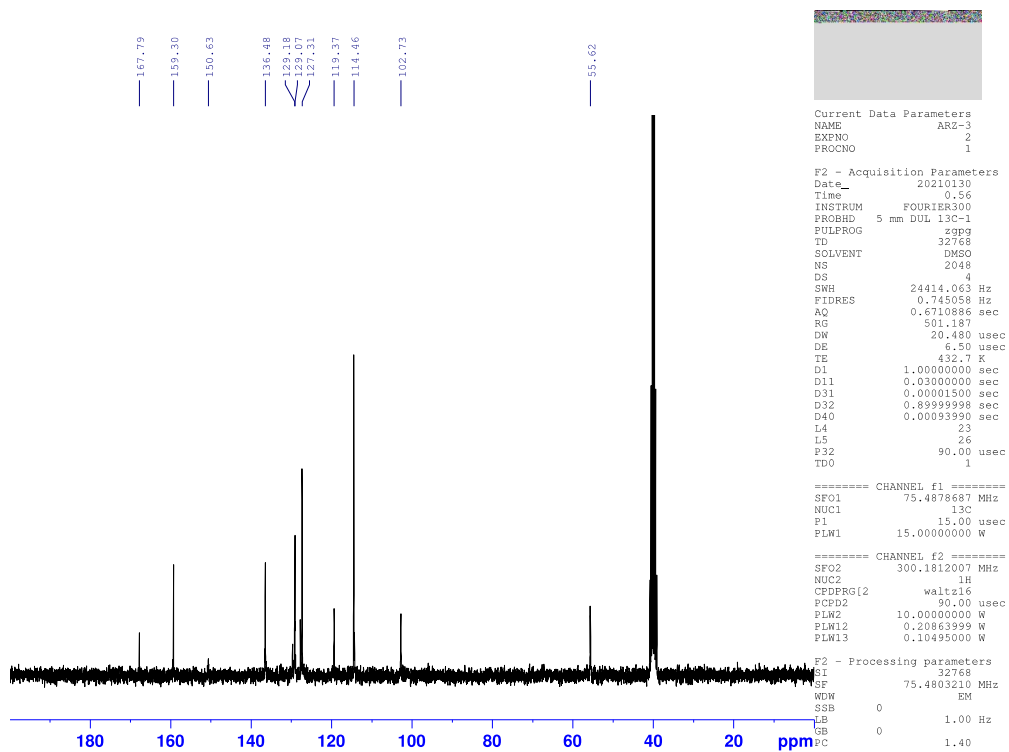


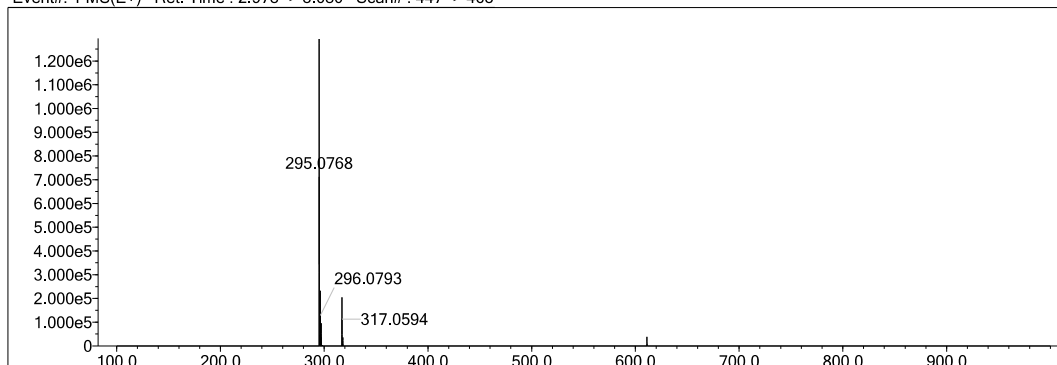
Figure S9. Compound 2c ¹³C-NMR spectrum

Data File: C:\LabSolutions\Data\Analiz\derya\ARZ-4_122.lcd

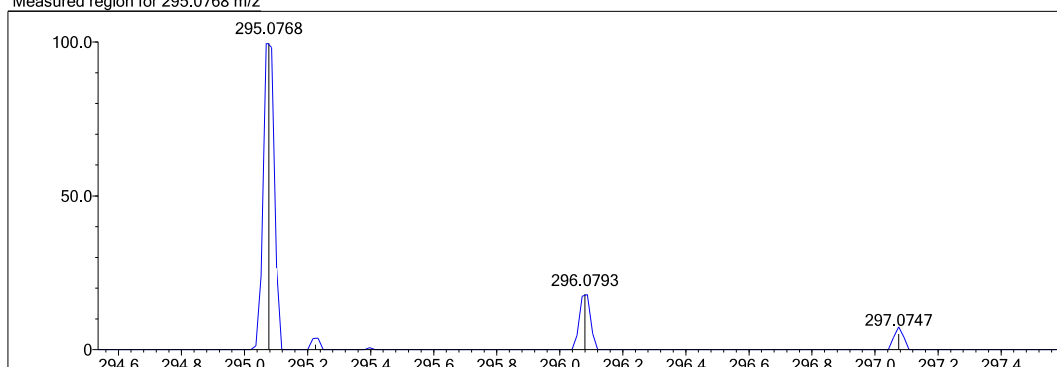
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	10	40	O	2	0	4	S	2	1	2	Ru	2	0	0	H
C	4	10	40	F	1	0	0	Cl	1	0	0	Pd	2	0	0	
N	3	3	6	P	3	0	0	Br	1	0	0	I	3	0	0	

Error Margin (ppm): 5
 DBE Range: 5.0 - 25.0
 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

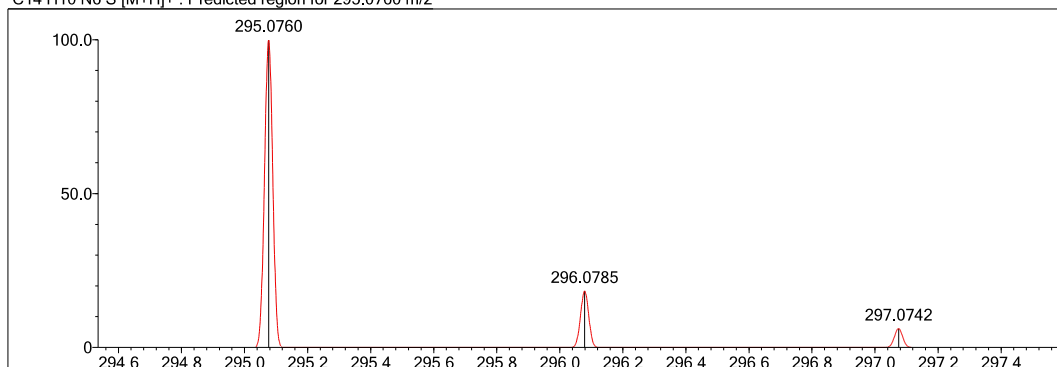
Event#: 1 MS(E+) Ret. Time : 2.973 -> 3.080 Scan# : 447 -> 463



Measured region for 295.0768 m/z



C14 H10 N6 S [M+H]⁺ : Predicted region for 295.0760 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	95.72	C14 H10 N6 S	[M+H] ⁺	295.0768	295.0760	0.8	2.71	100.00	13.0

Figure S10. Compound 2d HRMS report

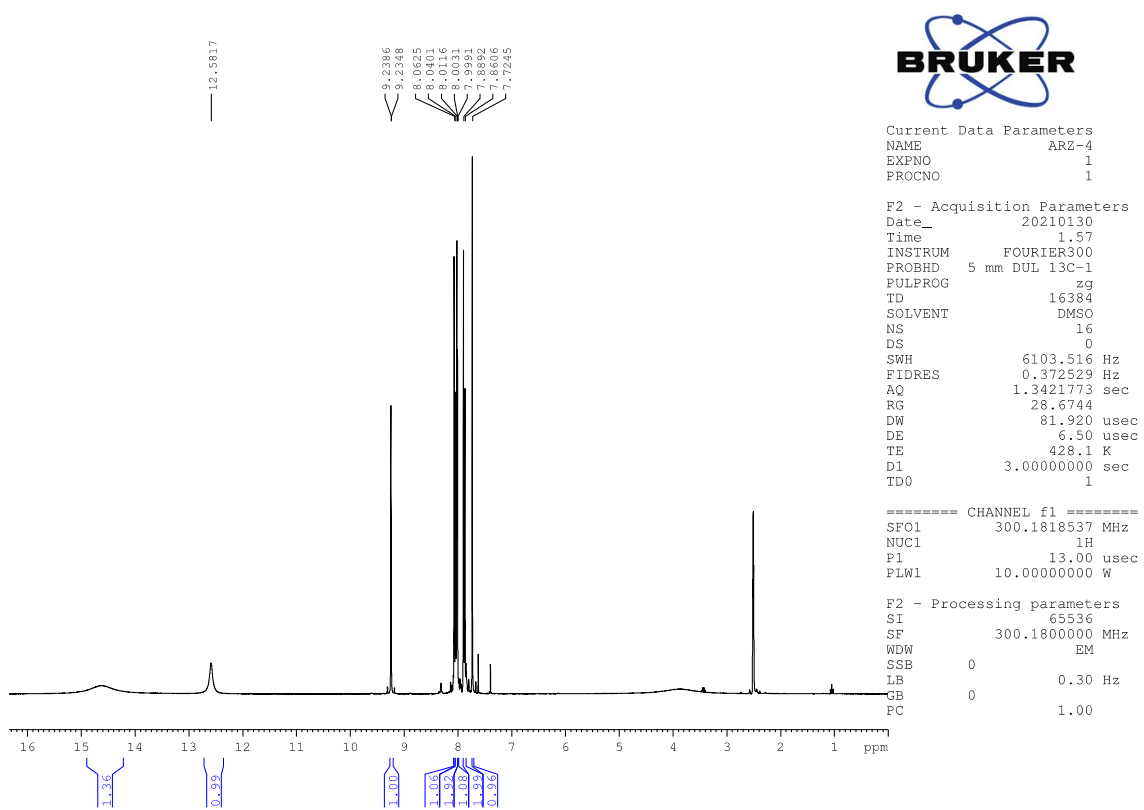


Figure S11. Compound 2d ¹H-NMR spectrum

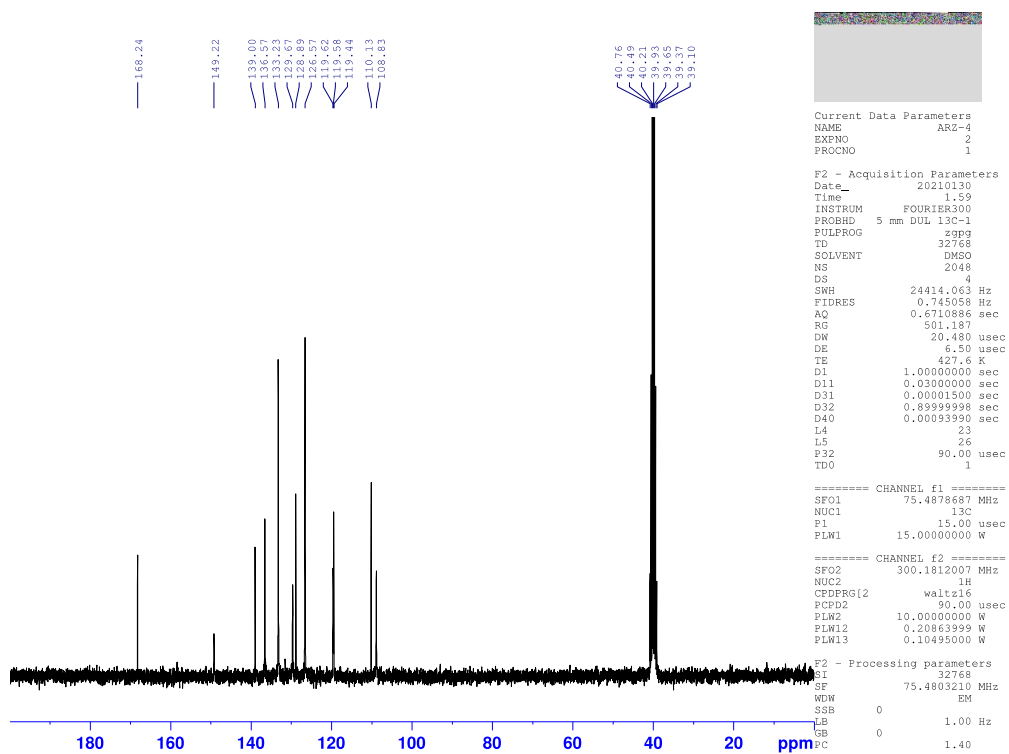


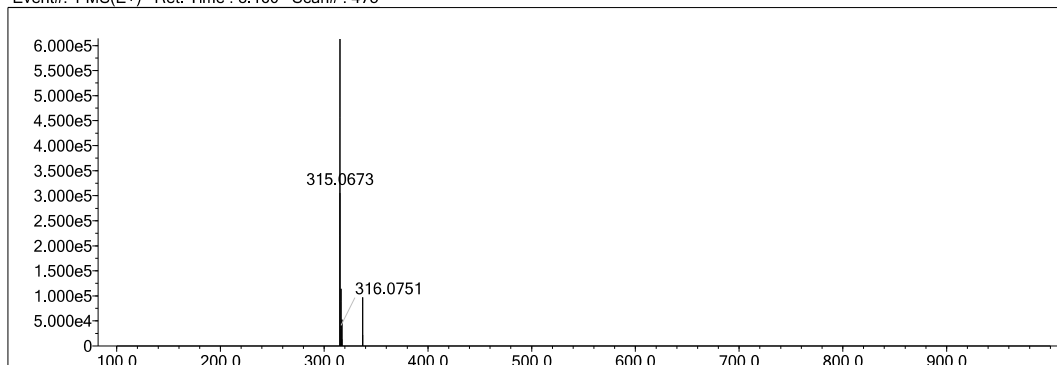
Figure S12. Compound 2d ¹³C-NMR spectrum

Data File: C:\LabSolutions\Data\Analiz\derya\ARZ-5_123.lcd

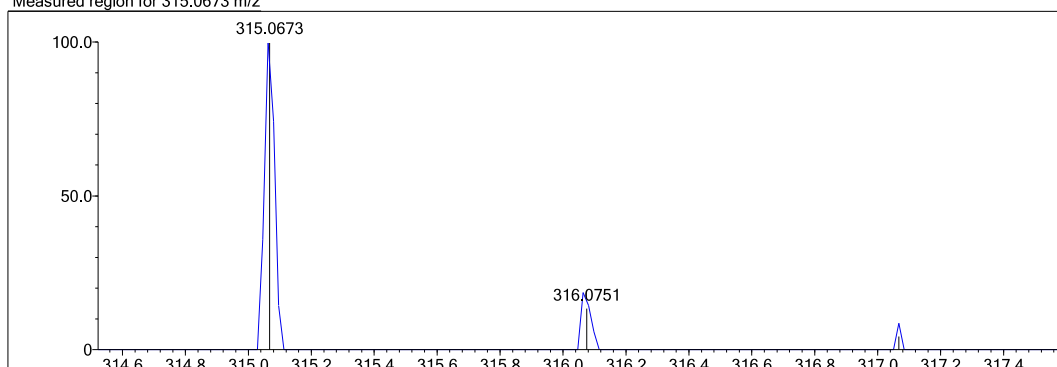
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	10	40	O	2	0	4	S	2	1	2	Ru	2	0	0	H
C	4	10	40	F	1	0	0	Cl	1	0	0	Pd	2	0	0	
N	3	3	6	P	3	0	0	Br	1	0	0	I	3	0	0	

Error Margin (ppm): 5
 DBE Range: 5.0 - 25.0
 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

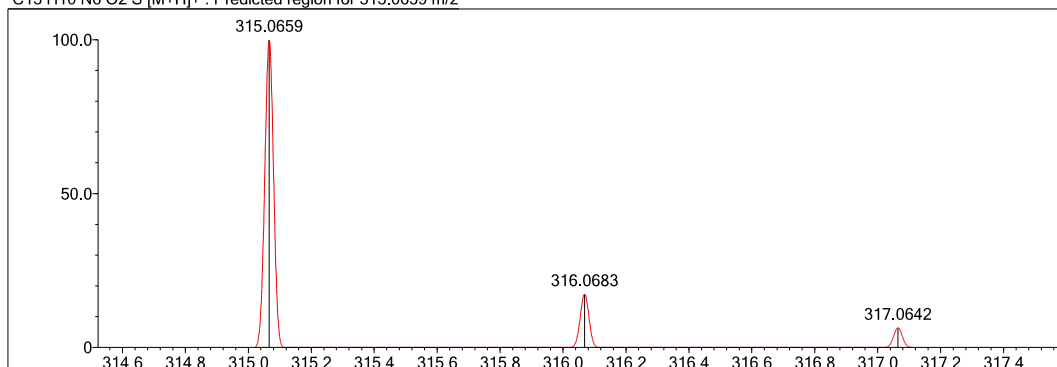
Event#: 1 MS(E+) Ret. Time : 3.160 Scan# : 475



Measured region for 315.0673 m/z



C13 H10 N6 O2 S [M+H]+ : Predicted region for 315.0659 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	64.79	C13 H10 N6 O2 S	[M+H]+	315.0673	315.0659	1.4	4.44	70.89	12.0

Figure S13. Compound 2e HRMS report

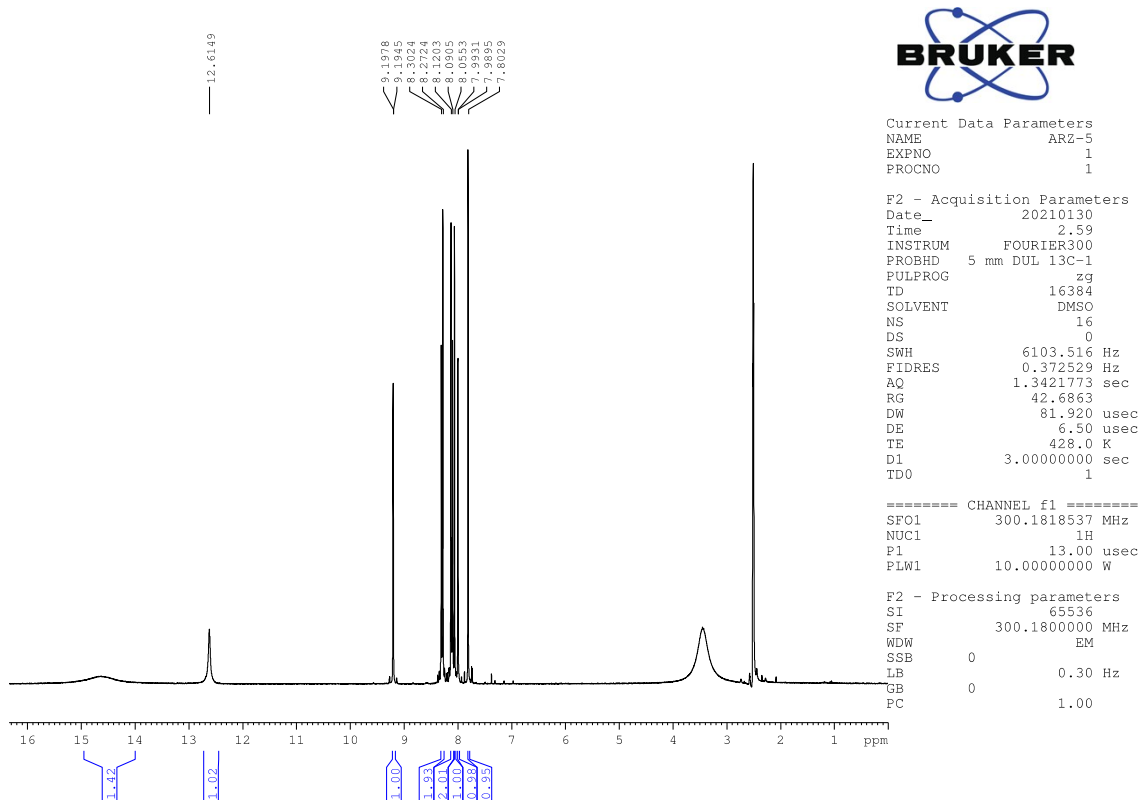


Figure S14. Compound 2e ¹H-NMR spectrum

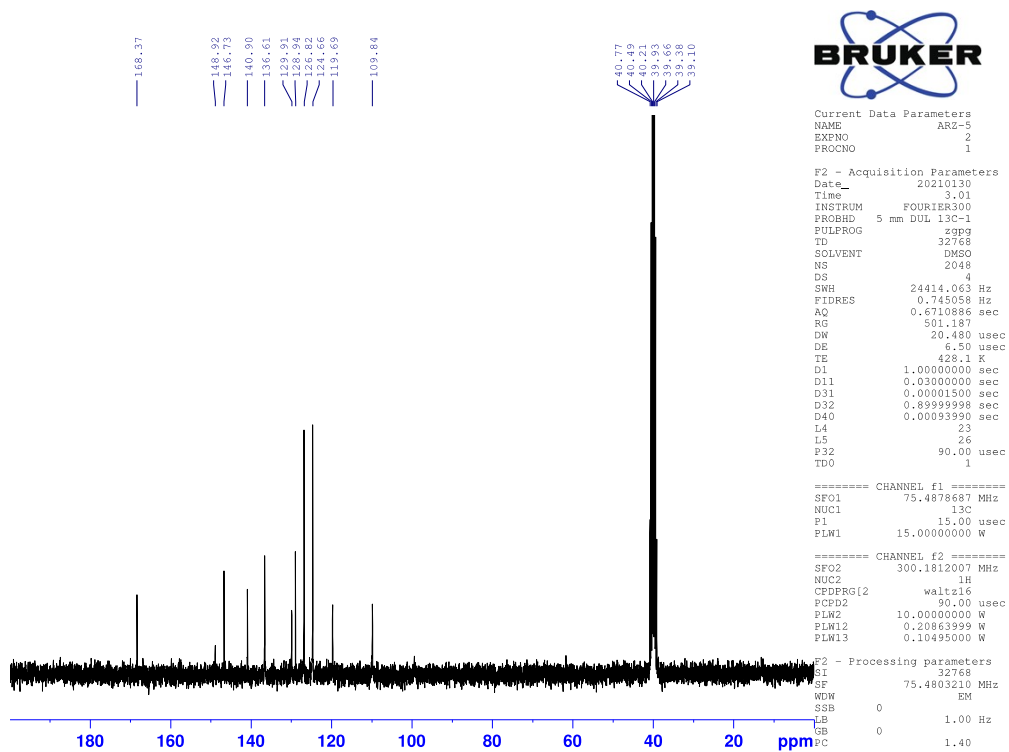


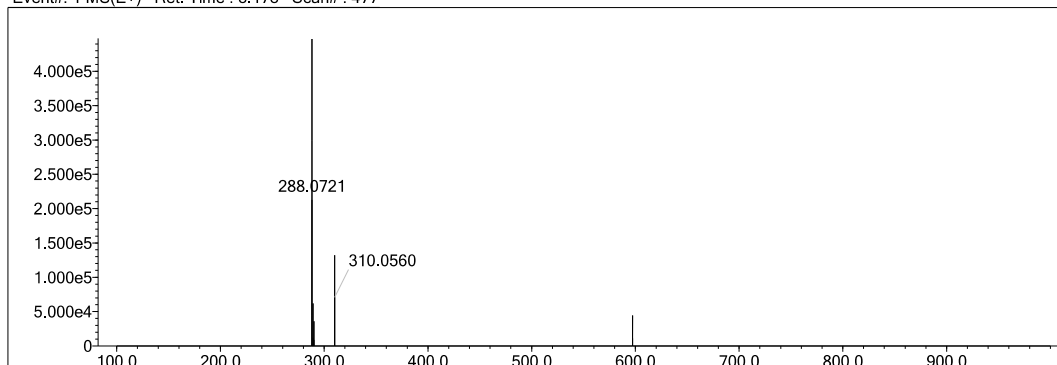
Figure S15. Compound 2e ¹³C-NMR spectrum

Data File: C:\LabSolutions\Data\Analiz\derya\ARZ-6_124.lcd

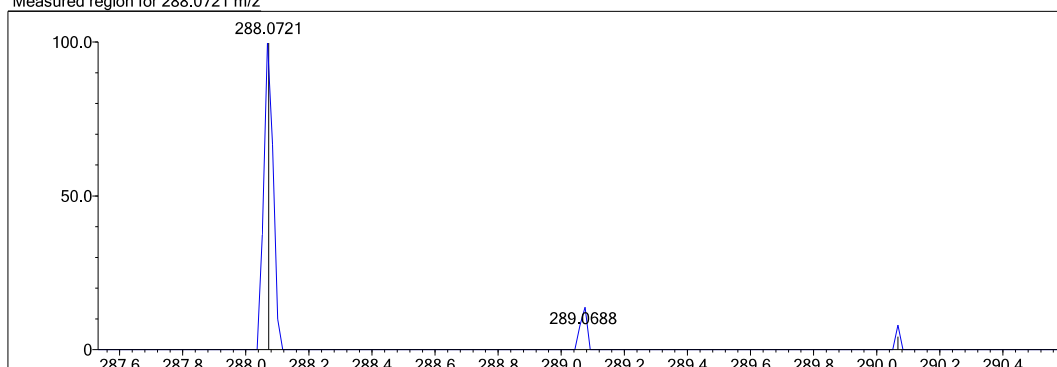
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	10	40	O	2	0	4	S	2	1	2	Ru	2	0	0	H
C	4	10	40	F	1	0	1	Cl	1	0	0	Pd	2	0	0	
N	3	3	6	P	3	0	0	Br	1	0	0	I	3	0	0	

Error Margin (ppm): 5
 DBE Range: 5.0 - 25.0
 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

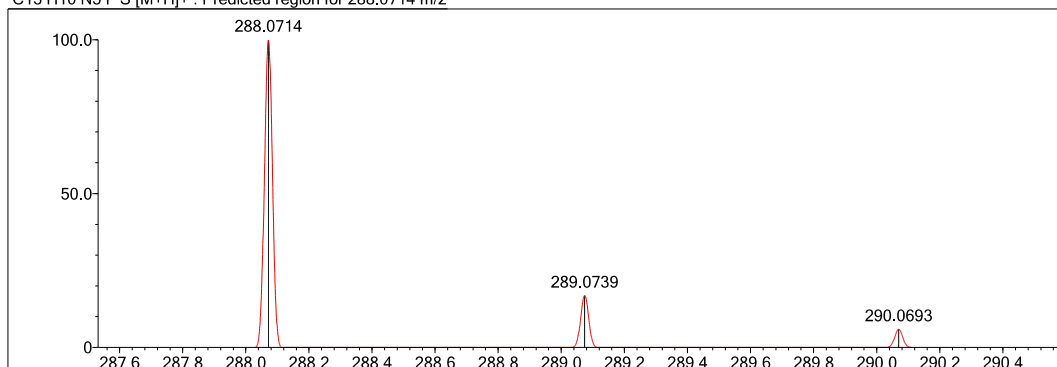
Event#: 1 MS(E+) Ret. Time : 3.173 Scan# : 477



Measured region for 288.0721 m/z



C13 H10 N5 F S [M+H]+ : Predicted region for 288.0714 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	67.92	C13 H10 N5 F S	[M+H] ⁺	288.0721	288.0714	0.7	2.43	70.44	11.0

Figure S16. Compound 2f HRMS report

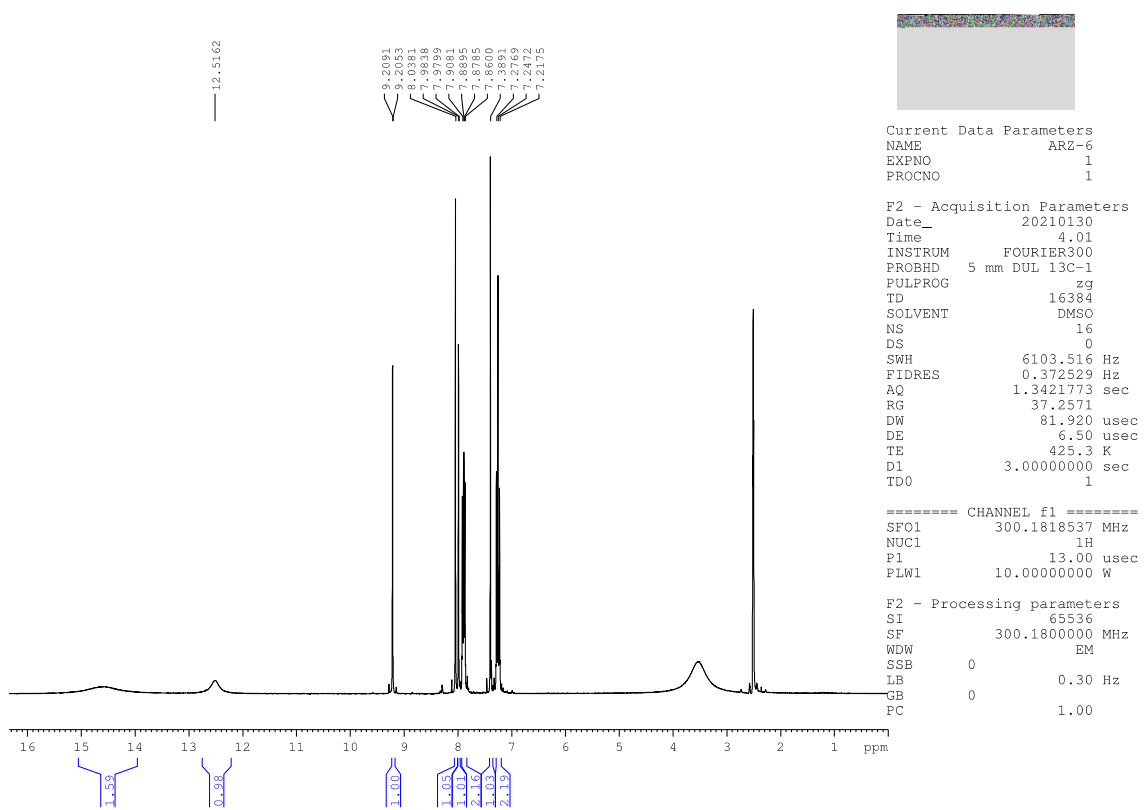


Figure S17. Compound 2f ¹H-NMR spectrum

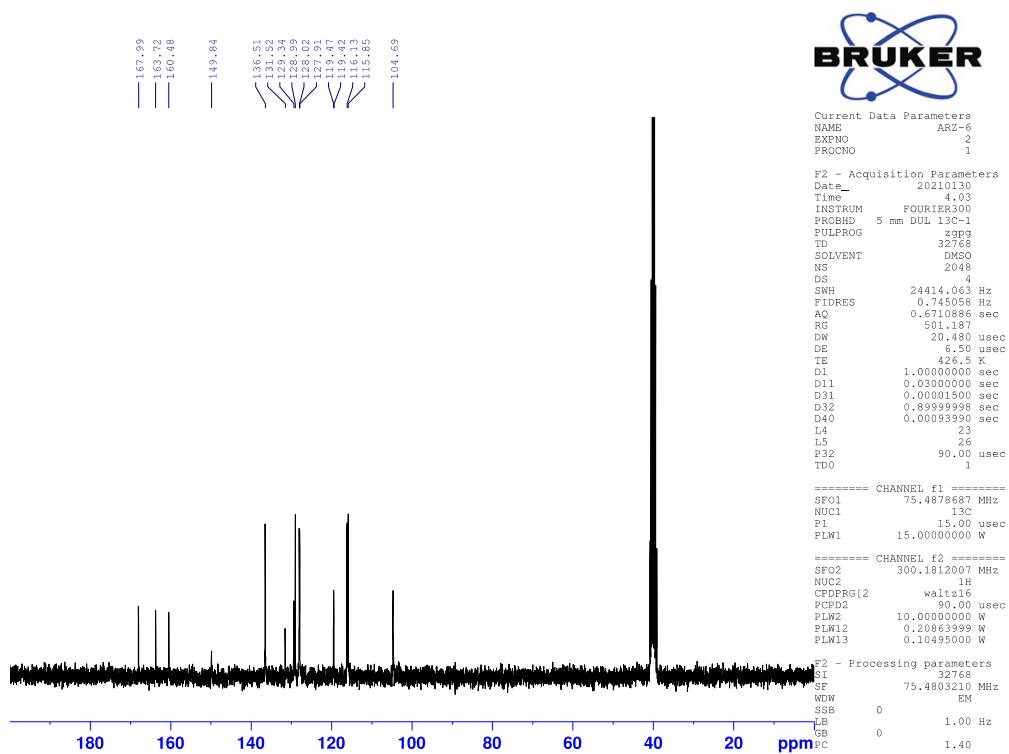


Figure S18. Compound 2f ¹³C-NMR spectrum

Data File: C:\LabSolutions\Data\Analiz\derya\ARZ-7_125.lcd

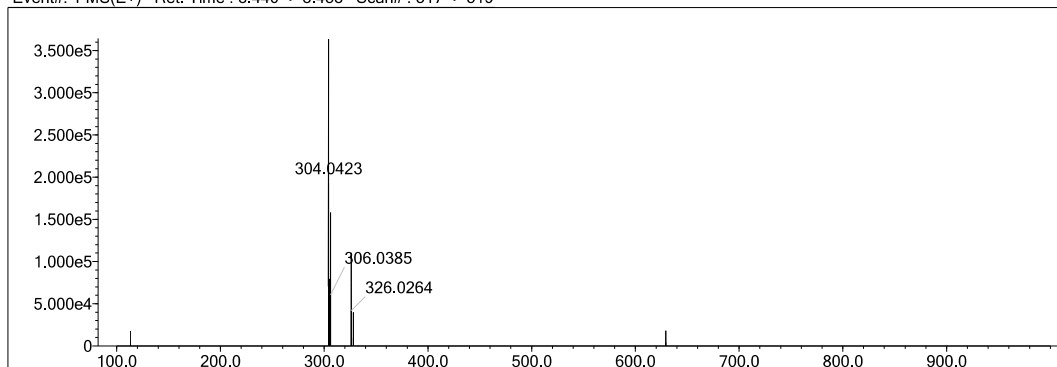
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	10	40	O	2	0	4	S	2	1	2	Ru	2	0	0	H
C	4	10	40	F	1	0	1	Cl	1	0	1	Pd	2	0	0	
N	3	3	6	P	3	0	0	Br	1	0	0	I	3	0	0	

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

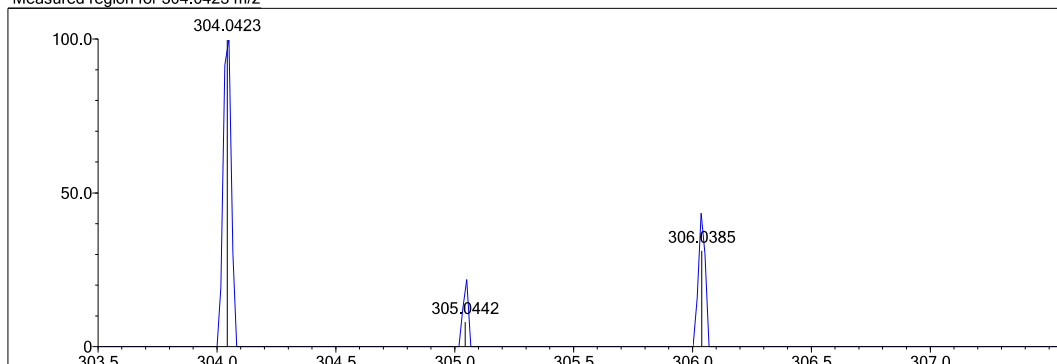
DBE Range: 8.0 - 25.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

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

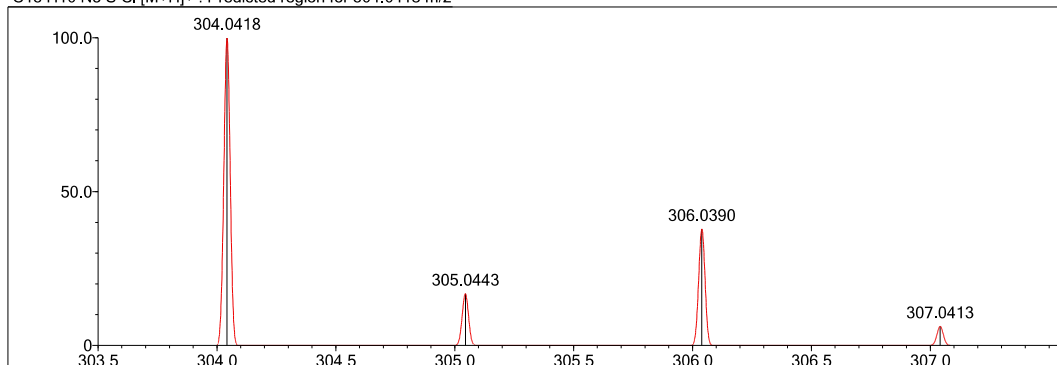
Event#: 1 MS(E+) Ret. Time : 3.440 -> 3.453 Scan# : 517 -> 519



Measured region for 304.0423 m/z



C13 H10 N5 S Cl [M+H]⁺ : Predicted region for 304.0418 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	79.56	C13 H10 N5 S Cl	[M+H] ⁺	304.0423	304.0418	0.5	1.64	80.85	11.0

Figure S19. Compound 2g HRMS report

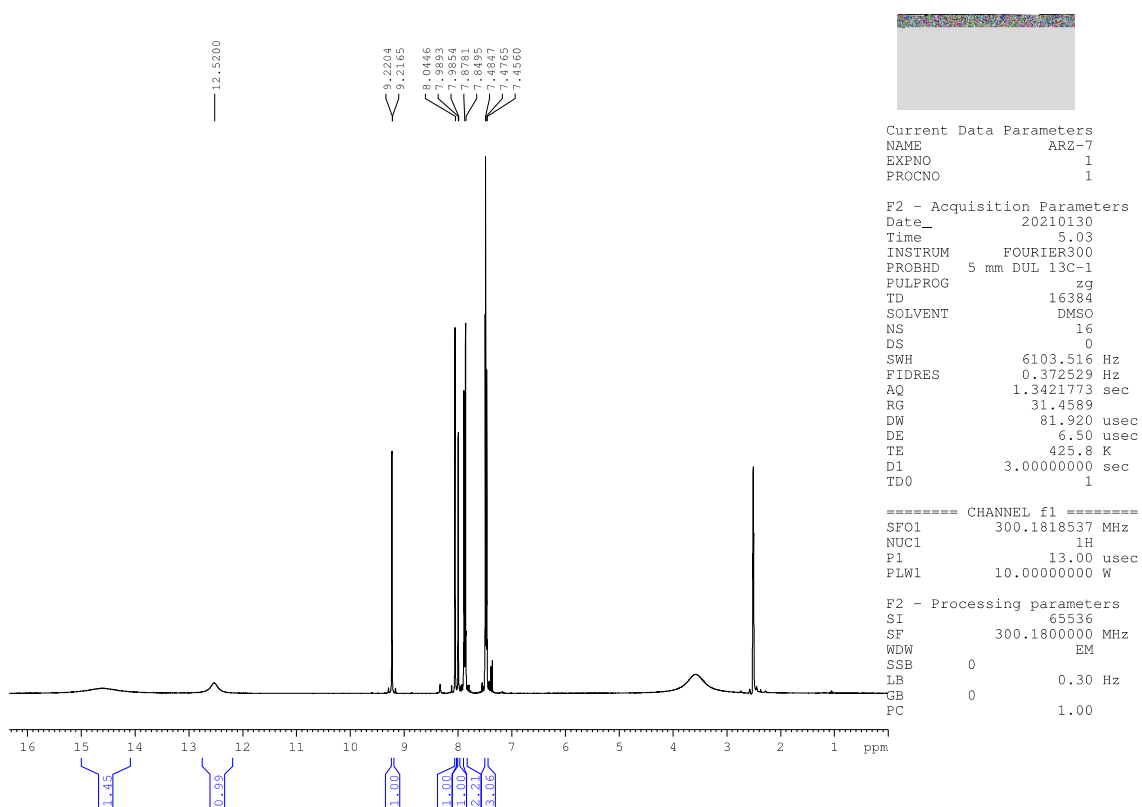


Figure S20. Compound 2g ¹H-NMR spectrum

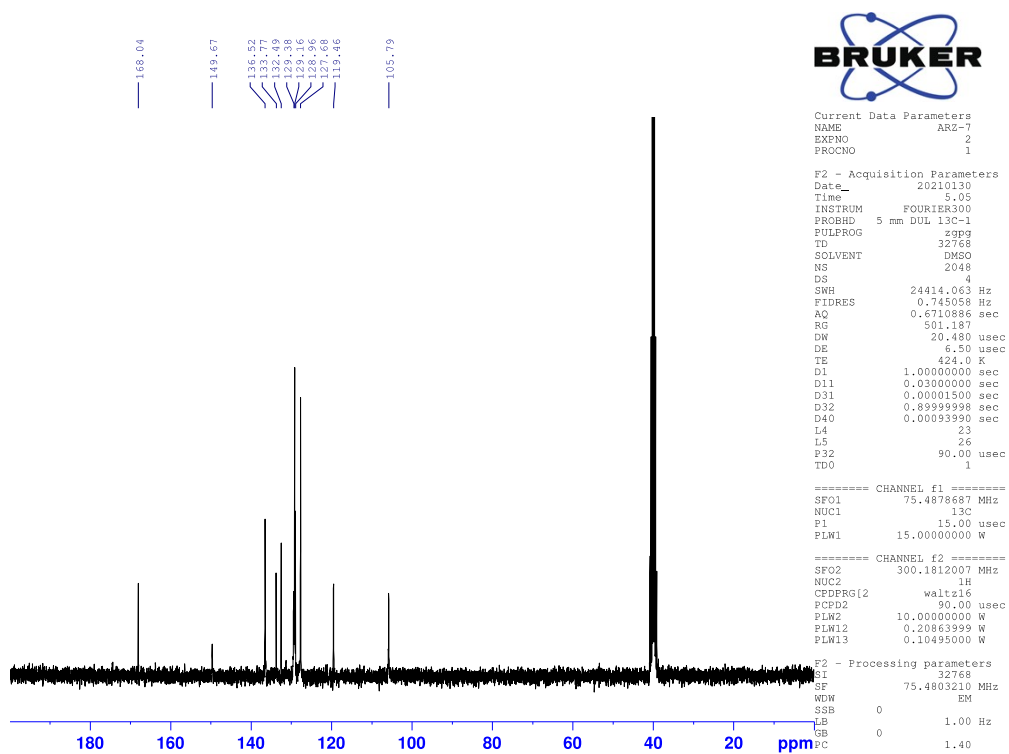


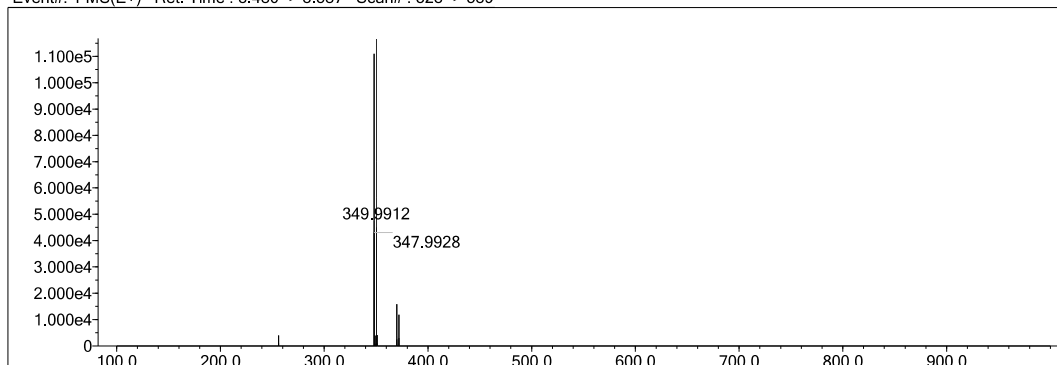
Figure S21. Compound 2g ¹³C-NMR spectrum

Data File: C:\LabSolutions\Data\Analiz\derya\ARZ-8_126.lcd

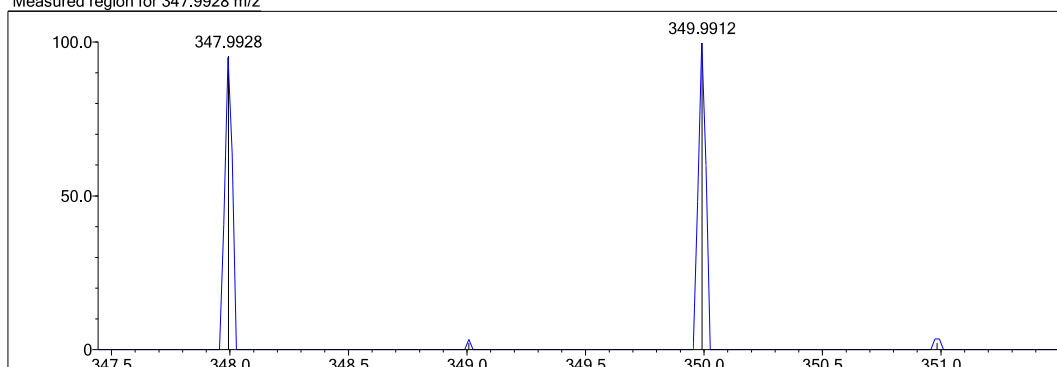
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	10	40	O	2	0	4	S	2	1	2	Ru	2	0	0	H
C	4	10	40	F	1	0	1	Cl	1	0	1	Pd	2	0	0	
N	3	3	6	P	3	0	0	Br	1	0	1	I	3	0	0	

Error Margin (ppm): 5
 DBE Range: 8.0 - 25.0
 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

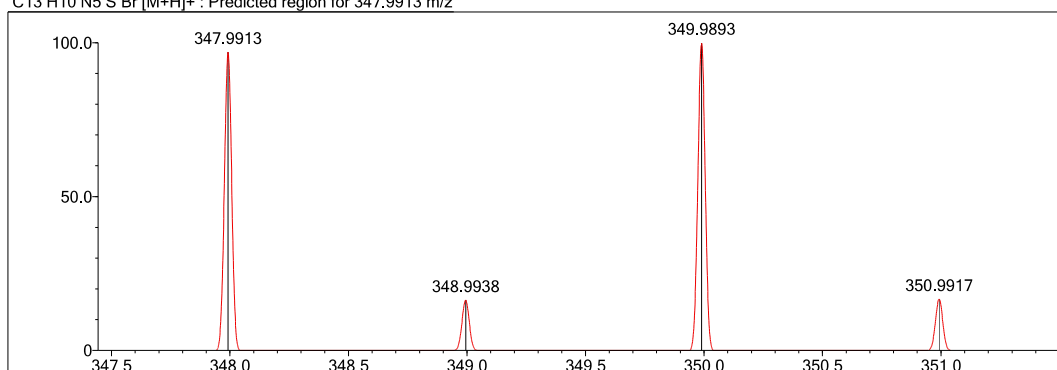
Event#: 1 MS(E+) Ret. Time : 3.480 -> 3.587 Scan# : 523 -> 539



Measured region for 347.9928 m/z



C13 H10 N5 S Br [M+H]⁺ : Predicted region for 347.9913 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	21.64	C13 H10 N5 S Br	[M+H] ⁺	347.9928	347.9913	1.5	4.31	23.59	11.0

Figure S22. Compound 2h HRMS report

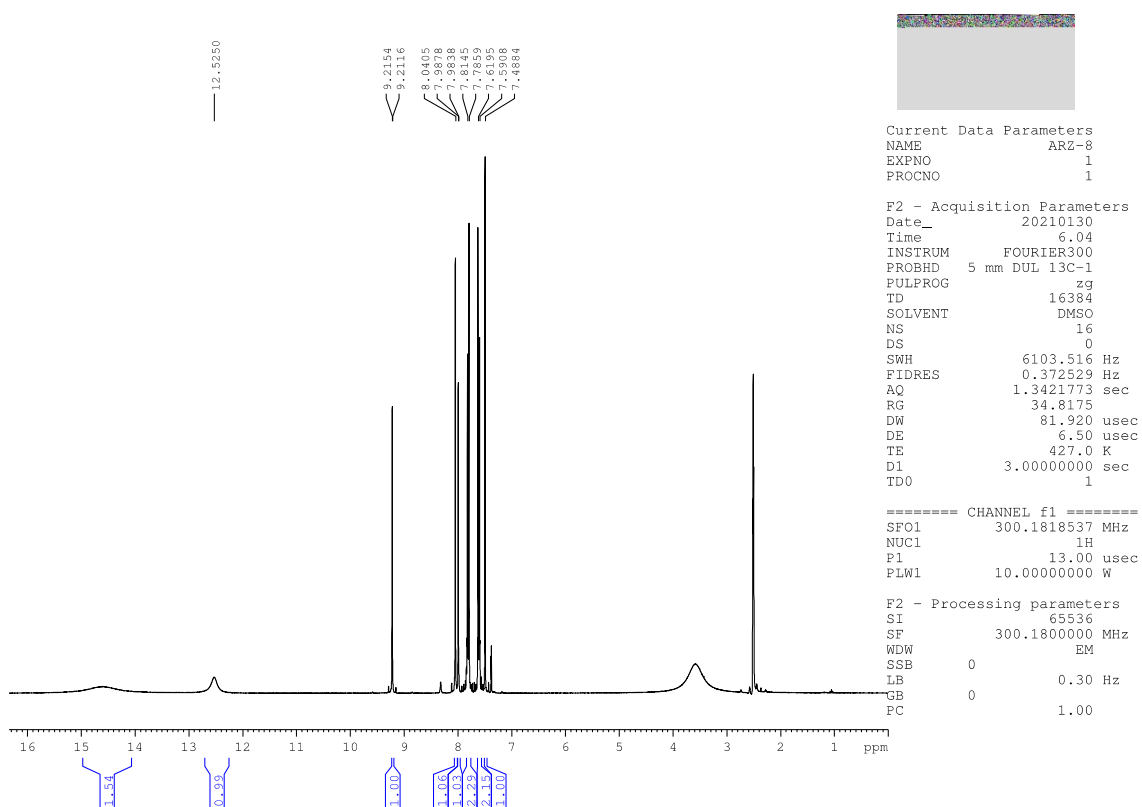


Figure S23. Compound 2h ¹H-NMR spectrum

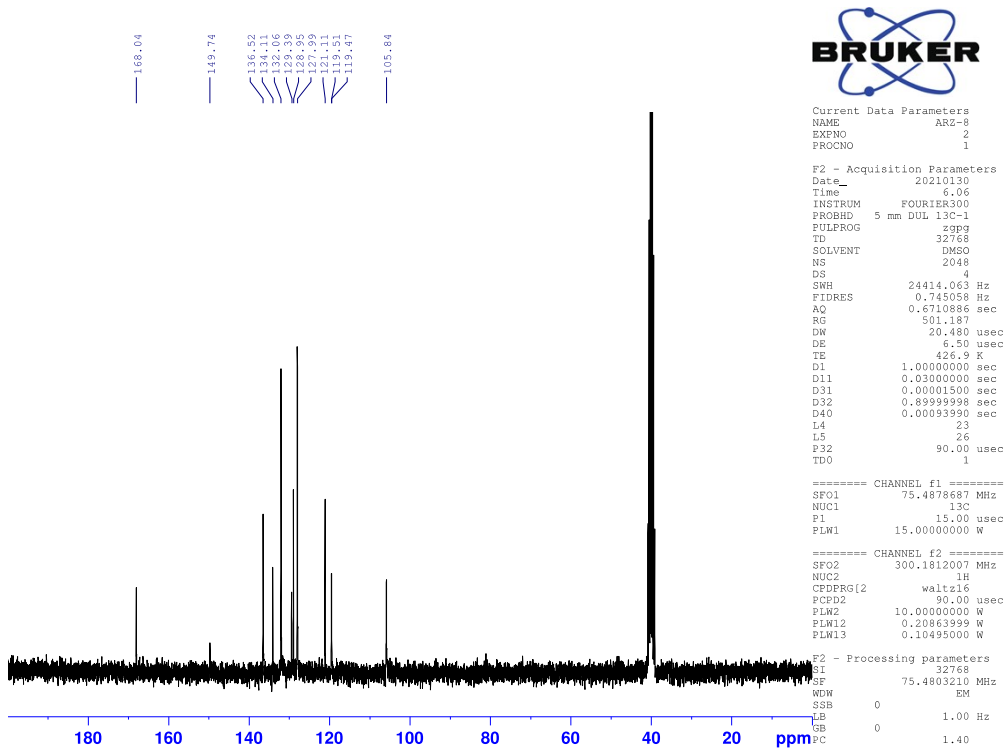


Figure S24. Compound 2h ¹³C-NMR spectrum

Data File: C:\LabSolutions\Data\Analiz\derya\ARZ-9_127.lcd

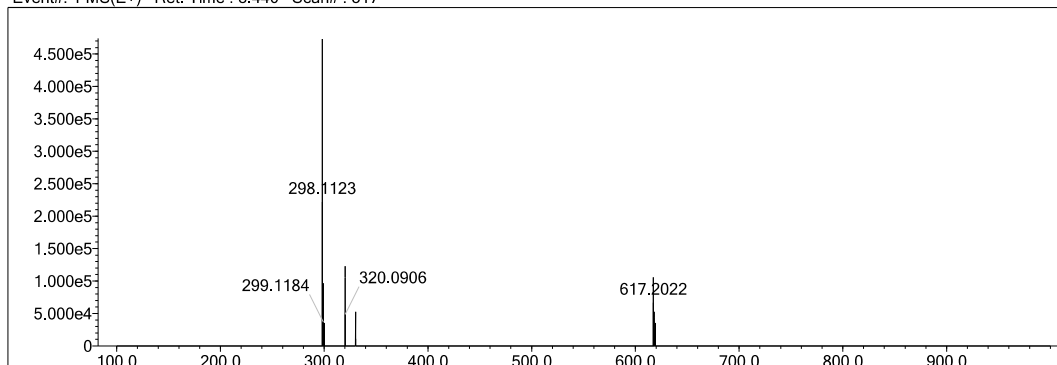
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	10	40	O	2	0	4	S	2	1	2	Ru	2	0	0	H
C	4	10	40	F	1	0	1	Cl	1	0	1	Pd	2	0	0	
N	3	3	6	P	3	0	0	Br	1	0	1	I	3	0	0	

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

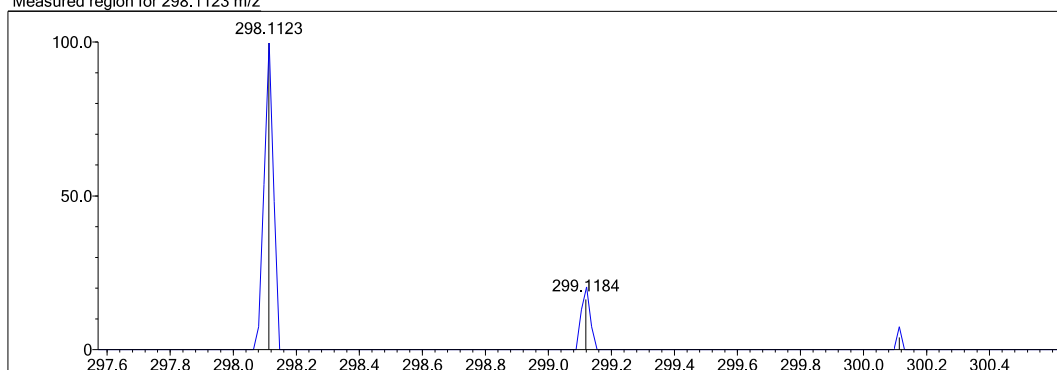
DBE Range: 8.0 - 25.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

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

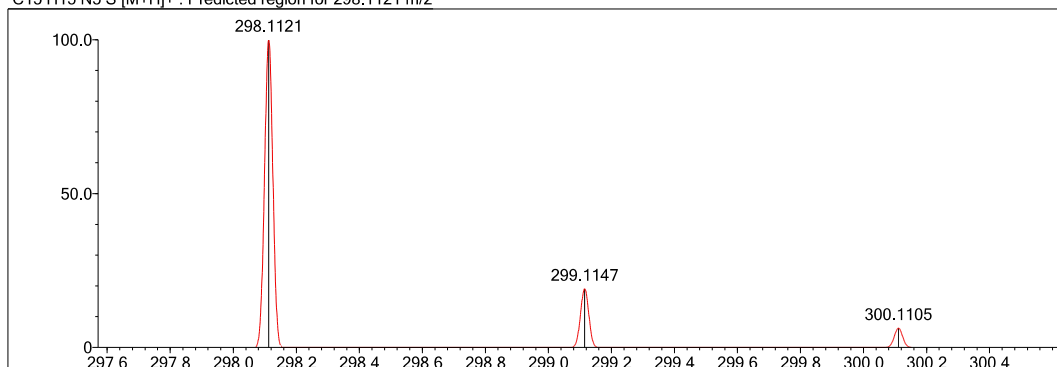
Event#: 1 MS(E+) Ret. Time : 3.440 Scan# : 517



Measured region for 298.1123 m/z



C15 H15 N5 S [M+H]⁺: Predicted region for 298.1121 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	87.13	C15 H15 N5 S	[M+H] ⁺	298.1123	298.1121	0.2	0.67	87.13	11.0

Figure S25. Compound 2i HRMS report

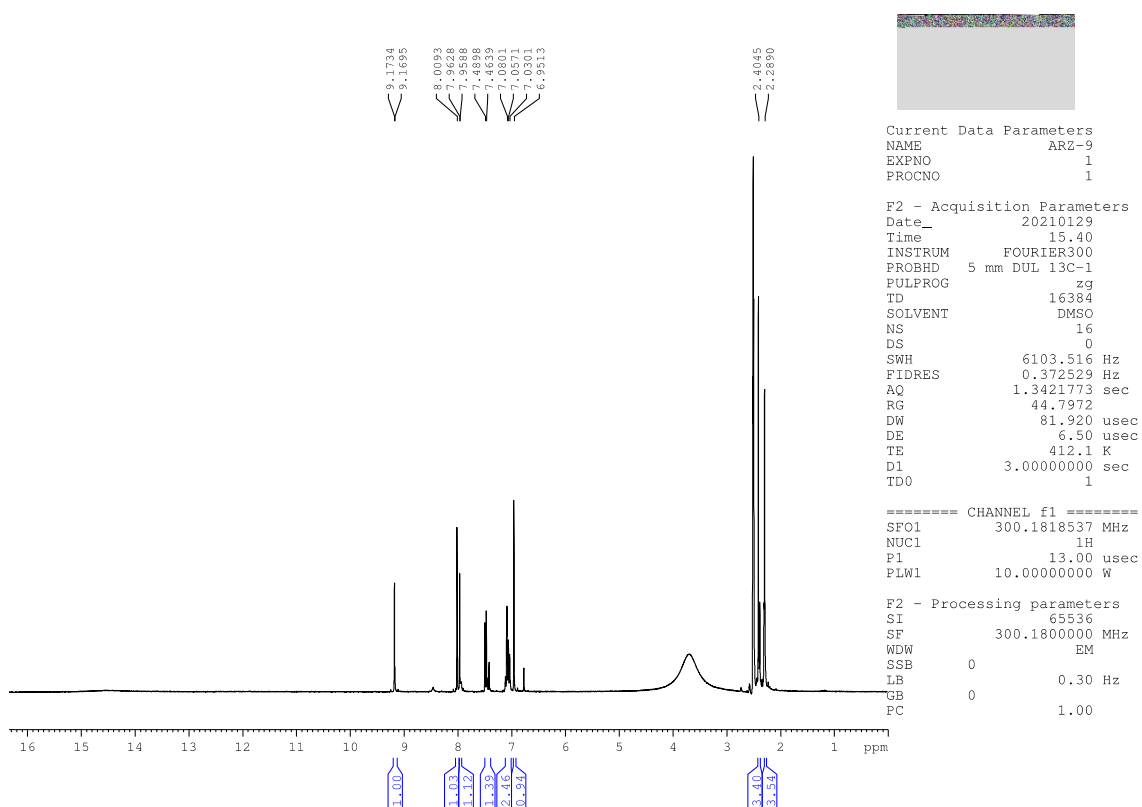


Figure S26. Compound 2i ¹H-NMR spectrum

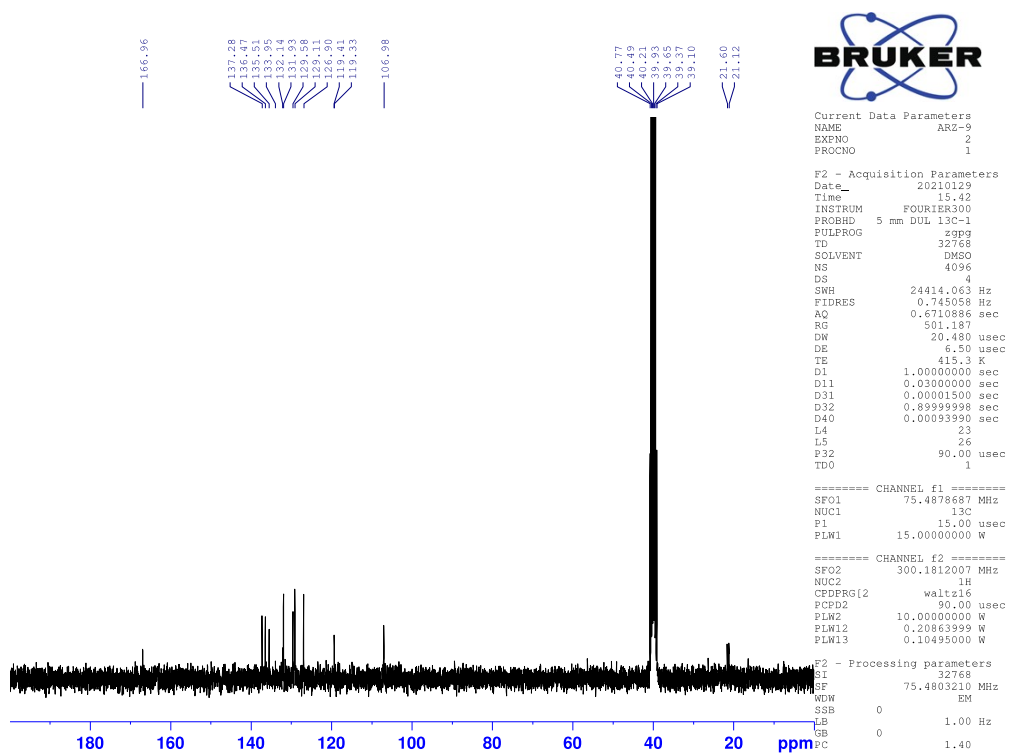


Figure S27. Compound 2i ¹³C-NMR spectrum

Data File: C:\LabSolutions\Data\Analiz\derya\ARZ-11_128.lcd

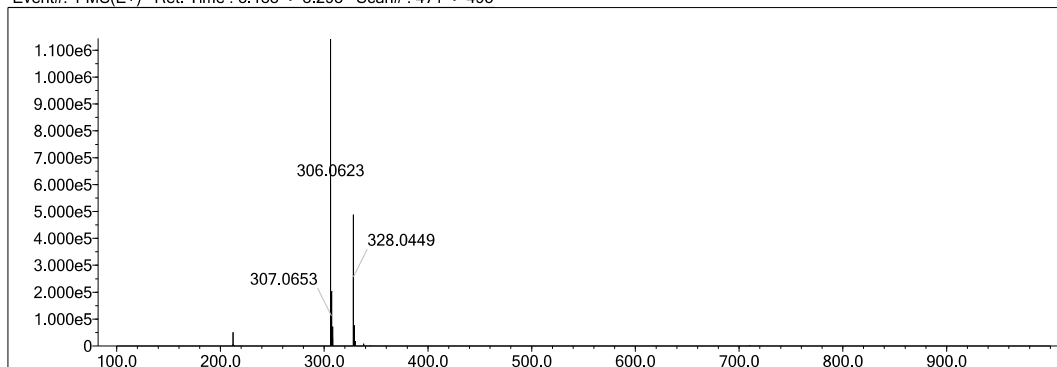
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	9	40	O	2	0	4	S	2	1	2	Ru	2	0	0	H
C	4	10	40	F	1	0	2	Cl	1	0	1	Pd	2	0	0	
N	3	3	6	P	3	0	0	Br	1	0	1	I	3	0	0	

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

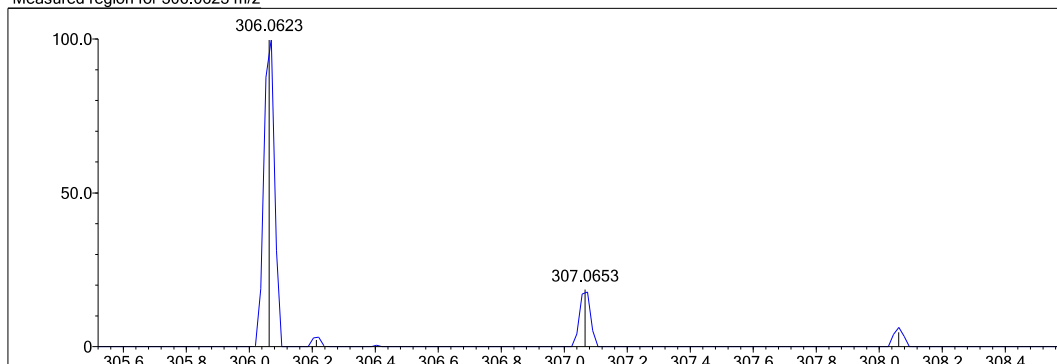
DBE Range: 8.0 - 25.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

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

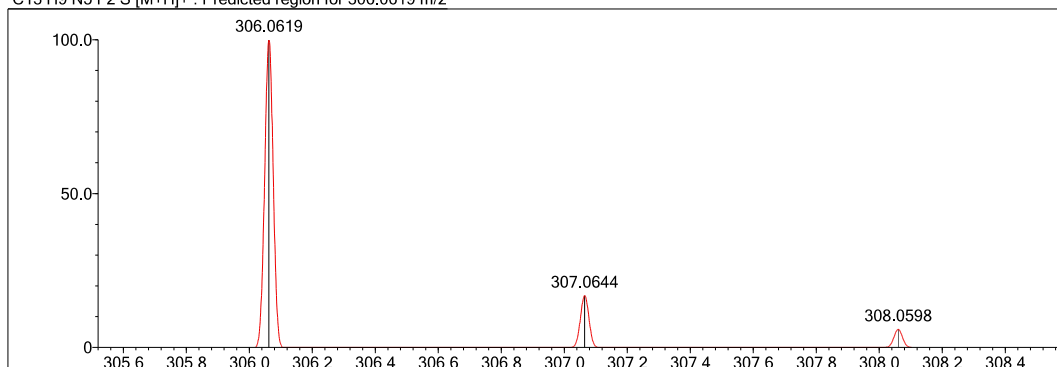
Event#: 1 MS(E+) Ret. Time : 3.133 -> 3.293 Scan# : 471 -> 495



Measured region for 306.0623 m/z



C13 H9 N5 F2 S [M+H]⁺ : Predicted region for 306.0619 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	92.03	C13 H9 N5 F2 S	[M+H] ⁺	306.0623	306.0619	0.4	1.31	92.75	11.0

Figure S28. Compound 2j HRMS report

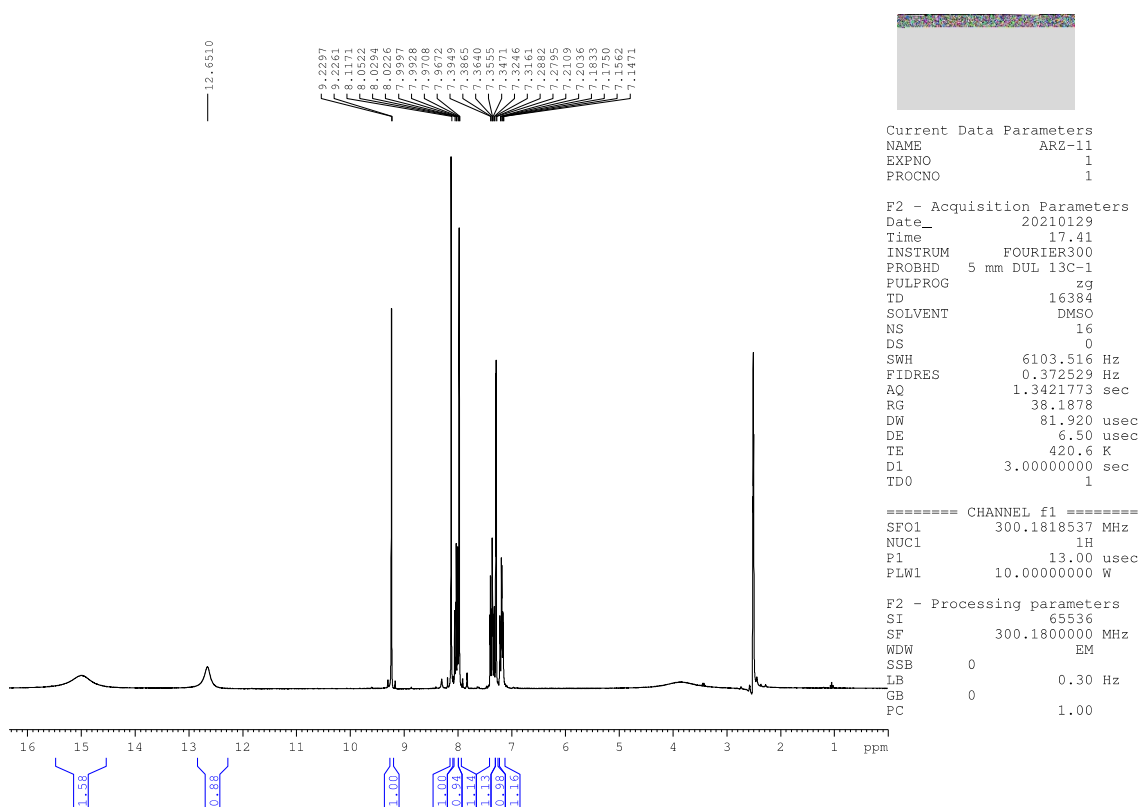


Figure S29. Compound 2j ¹H-NMR spectrum

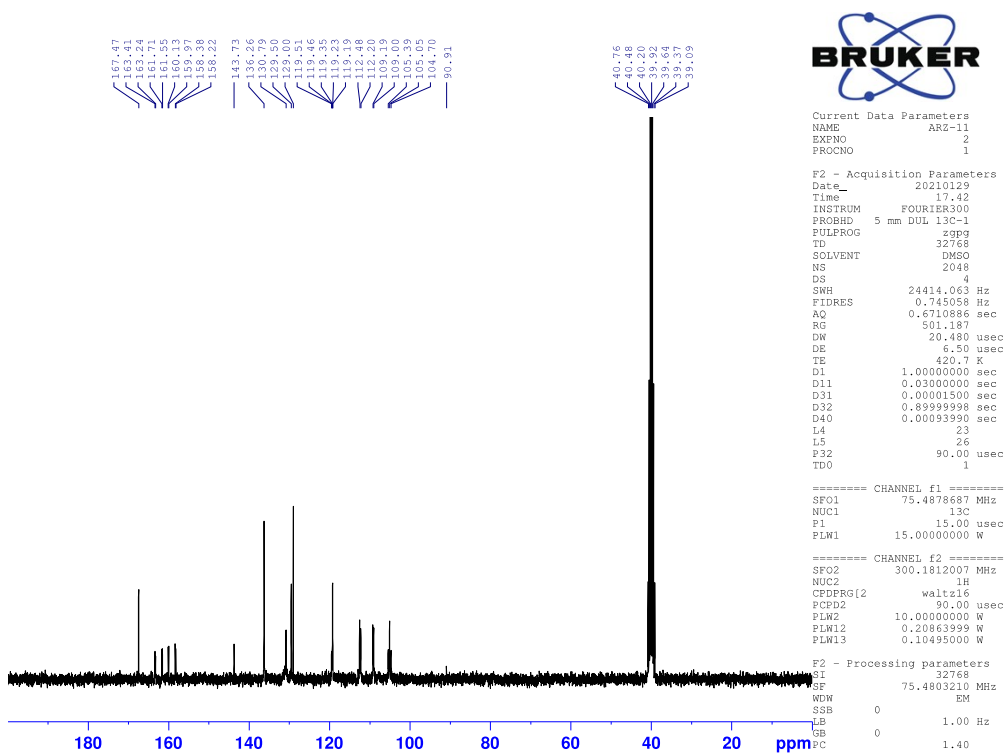


Figure S30. Compound 2j ¹³C-NMR spectrum

Data File: C:\LabSolutions\Data\Analiz\derya\ARZ-12_129.Icd

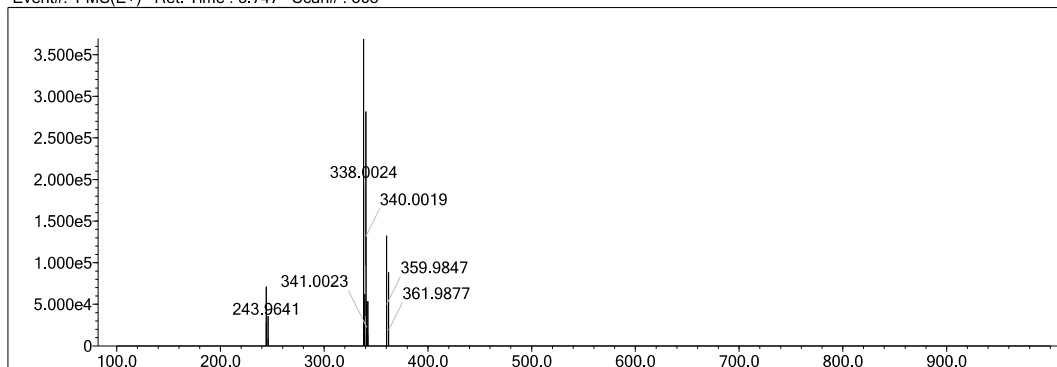
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	9	40	O	2	0	4	S	2	1	2	Ru	2	0	0	H
C	4	10	40	F	1	0	2	Cl	1	0	2	Pd	2	0	0	
N	3	3	6	P	3	0	0	Br	1	0	1	I	3	0	0	

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

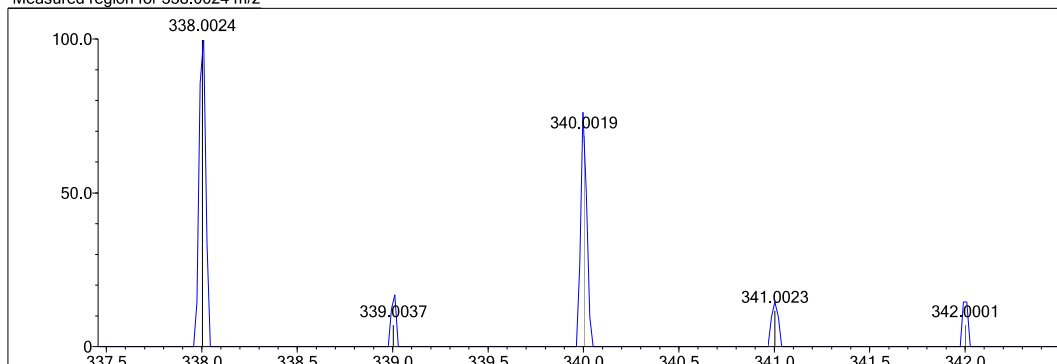
DBE Range: 8.0 - 25.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

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

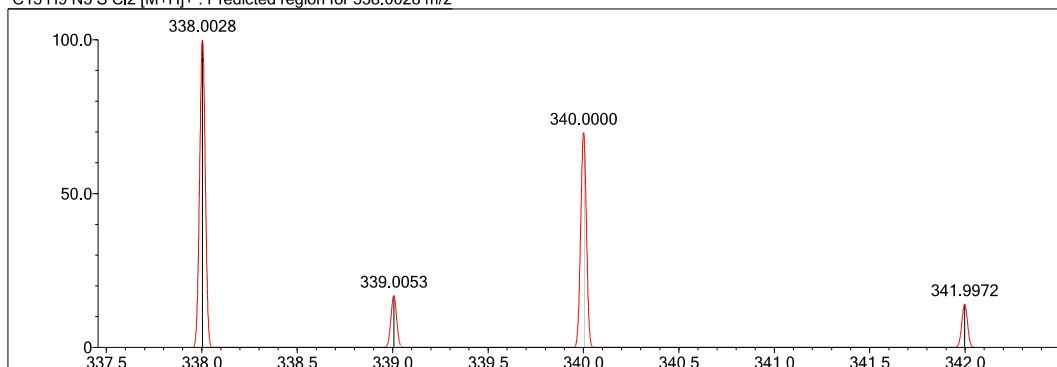
Event#: 1 MS(E+) Ret. Time : 3.747 Scan# : 563



Measured region for 338.0024 m/z



C13 H9 N5 S Cl2 [M+H]⁺ : Predicted region for 338.0028 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	89.11	C13 H9 N5 S Cl2	[M+H] ⁺	338.0024	338.0028	-0.4	-1.18	89.51	11.0

Figure S31. Compound 2k HRMS report

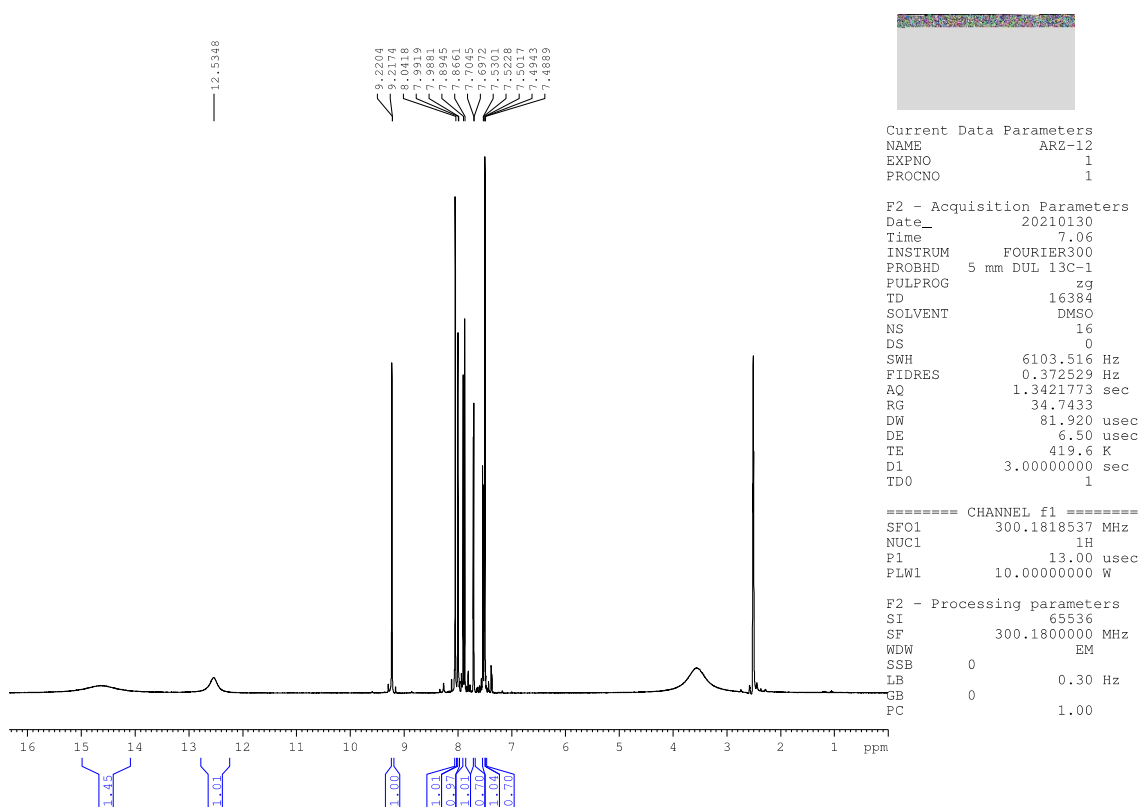


Figure S32. Compound 2k ¹H-NMR spectrum

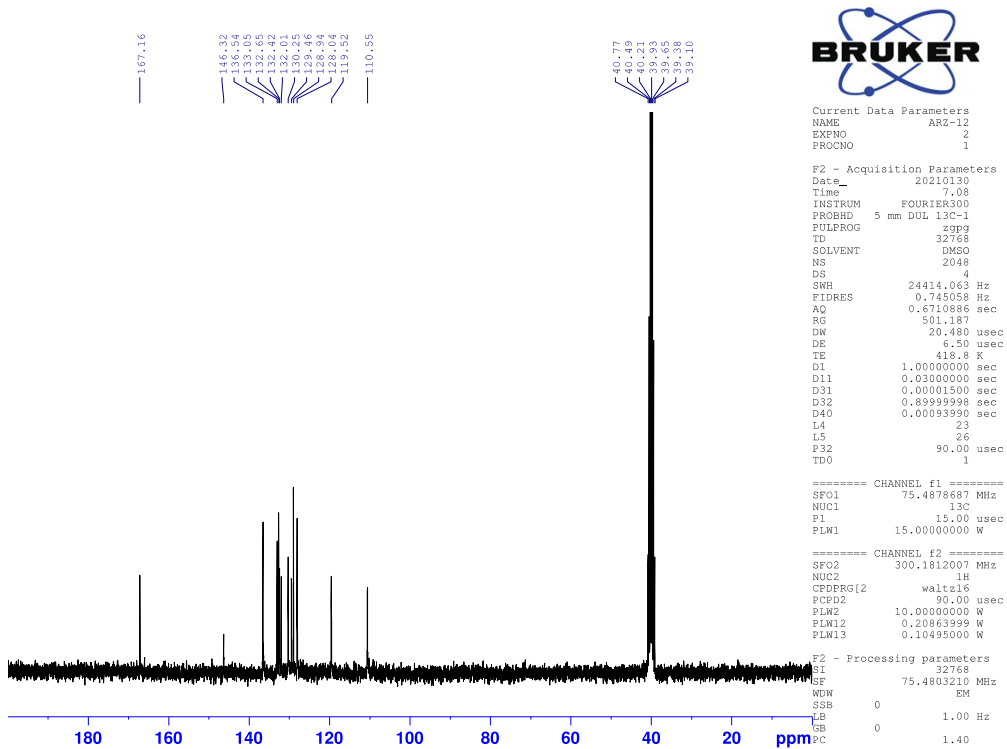


Figure S33. Compound 2k ¹³C-NMR spectrum

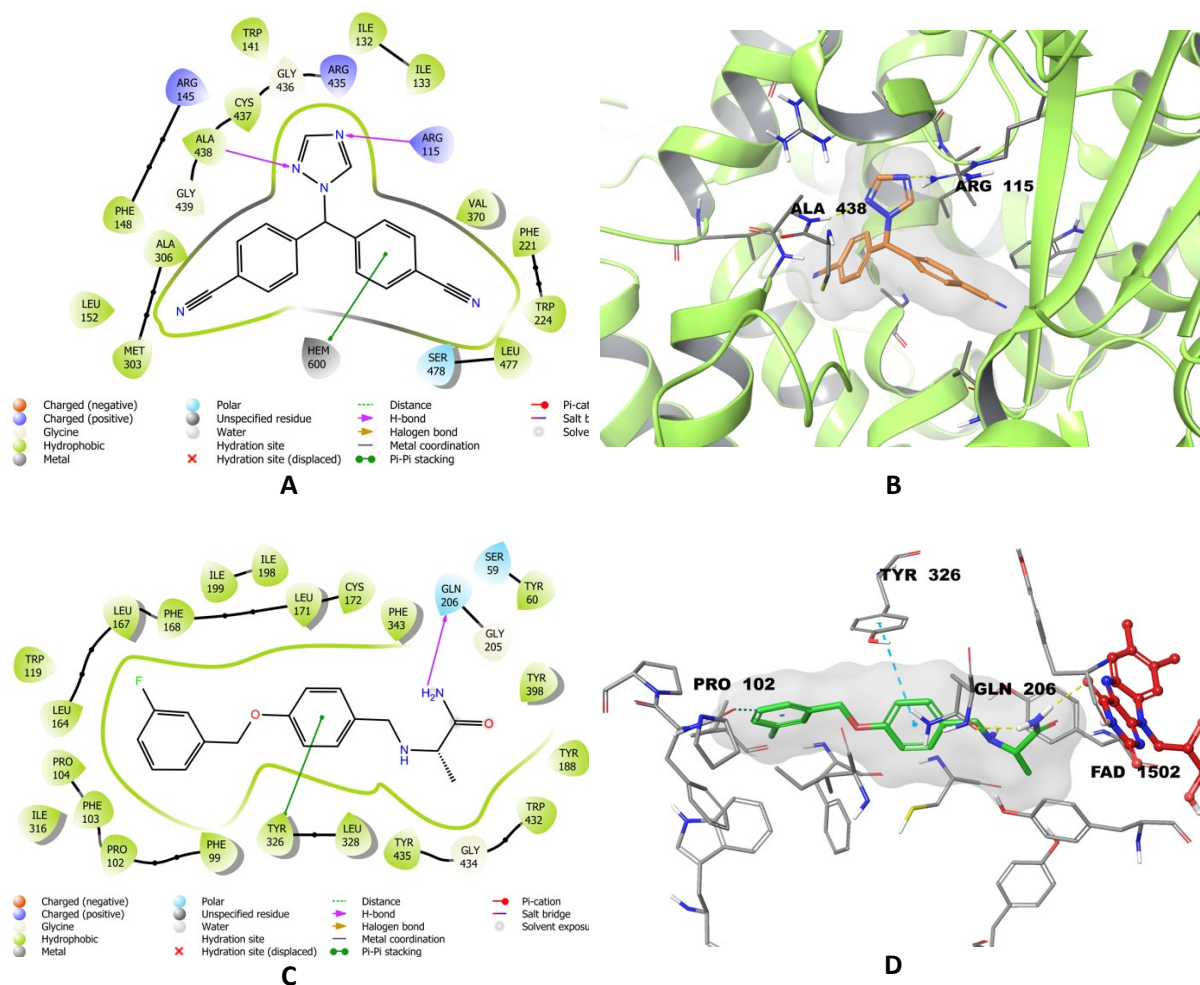


Figure S34: The 2D (A) and 3D (B) interacting modes of letrozole (colored with orange) in the active region the human aromatase (PDB ID: 3EQM). The 2D (C) and 3D (D) interacting modes of safinamide (colored with green) in the active region the MAO-B (PDB ID: 2V5Z).