Supplementary Material

Discovery of small molecule COX-1 and Akt inhibitors as anti-NSCLC agents endowed with anti-inflammatory action

Mehlika Dilek Altıntop [1], Gülşen Akalın Çiftçi [2,3], Nalan Yılmaz Savaş [3], İpek Ertorun [4], Betül Can [4], Belgin Sever [1], Halide Edip Temel [2], Özkan Alataş [4] and Ahmet Özdemir [1,*]

[1] Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Anadolu University, 26470 Eskişehir, Turkey; mdaltintop@anadolu.edu.tr (M.D.A.), belginsever@anadolu.edu.tr (B.S.)
[2] Department of Biochemistry, Faculty of Pharmacy, Anadolu University, 26470 Eskişehir, Turkey; gakalin@anadolu.edu.tr (G.A.Ç.), heincedal@anadolu.edu.tr (H.E.T.)
[3] Graduate School of Health Sciences, Anadolu University, 26470 Eskişehir, Turkey; nalan_y@anadolu.edu.tr (N.Y.S.)
[4] Department of Medical Biochemistry, Faculty of Medicine, Eskisehir Osmangazi University, 26480 Eskişehir, Turkey; erdoganipek@gmail.com (İ.E.), bcan@ogu.edu.tr (B.C.), oalatas@ogu.edu.tr (Ö.A.)

* Correspondence: mdaltintop@anadolu.edu.tr (M.D.A.); ahmeto@anadolu.edu.tr (A.Ö.); Tel.: +90-222-335-0580 (ext. 3772) (M.D.A); Tel.: +90-222-335-0580 (ext. 3780) (A.Ö.).

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Figure S1. IR spectrum of compound **3a**

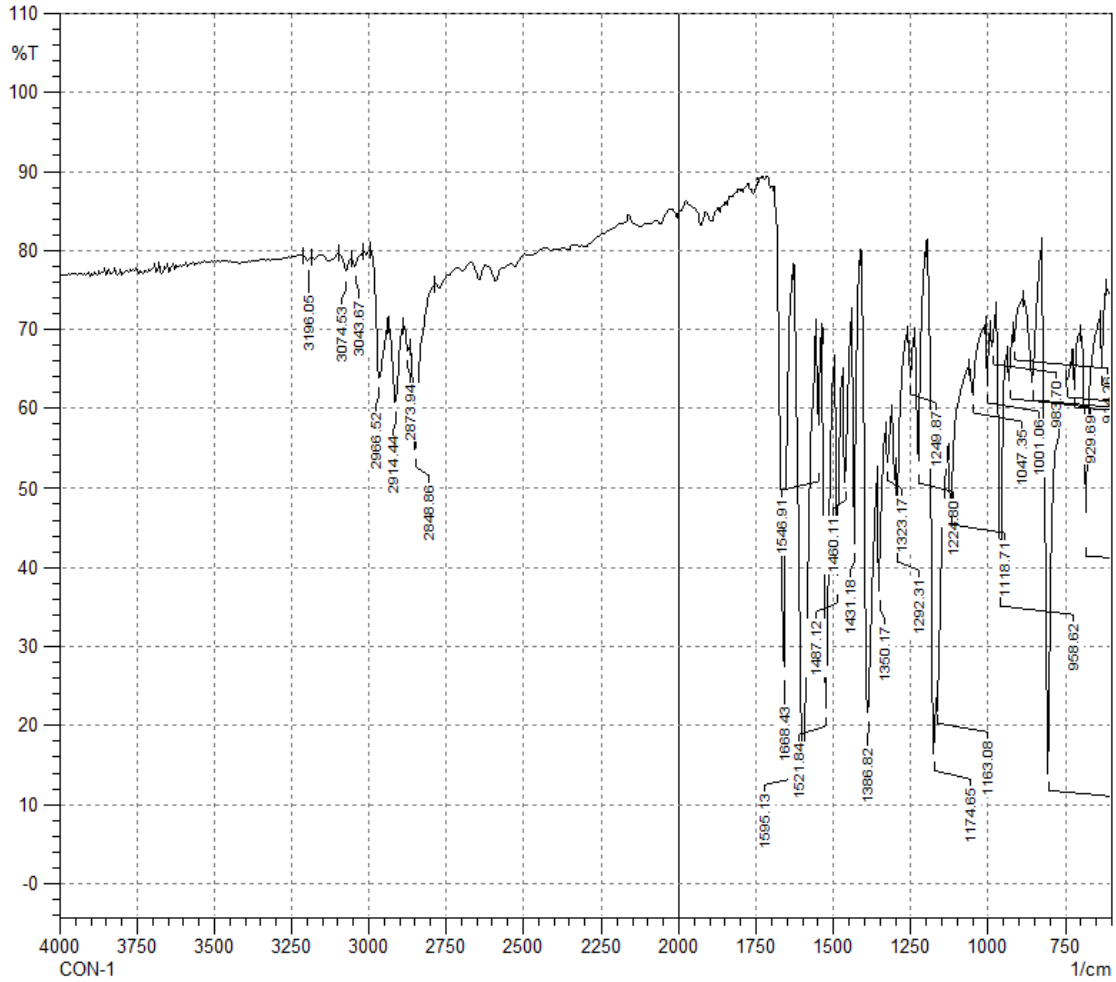

Figure S2. ^{1}H NMR spectrum of compound **3a**

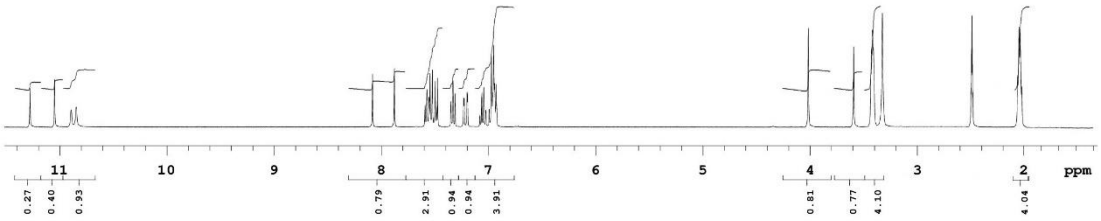

Figure S3. ^{13}C NMR spectrum of compound **3a**

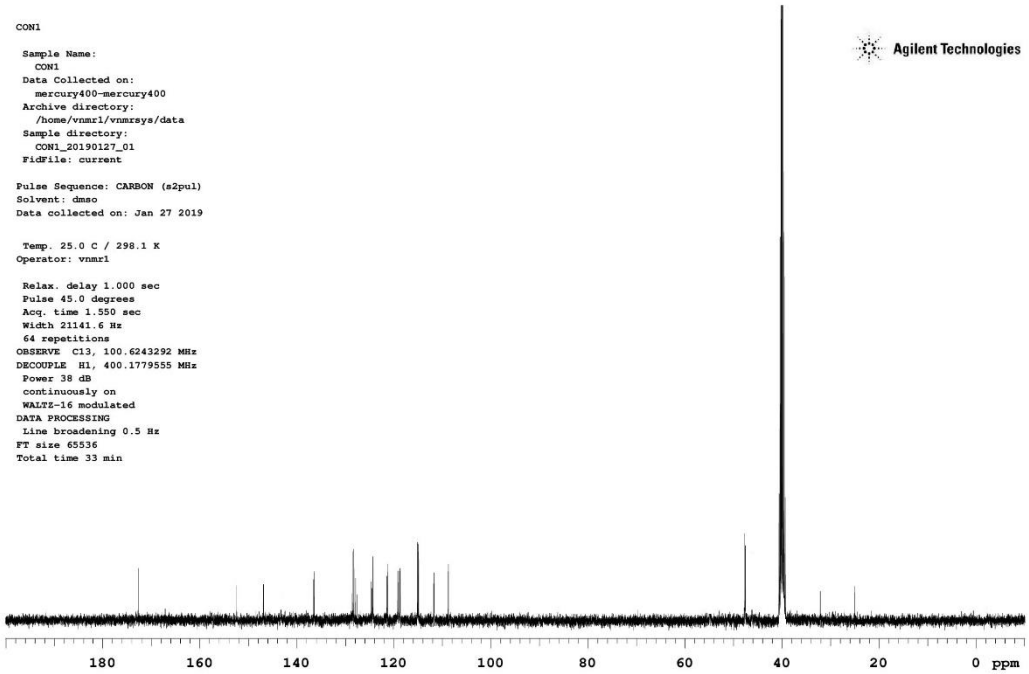

Figure S4. HRMS spectrum of compound **3a**

Formula Predictor Report - CON-1_2.lcd

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Data File: C:\LabSolutions\Data\Analiz\AOzdemir\CON-1_2.lcd

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
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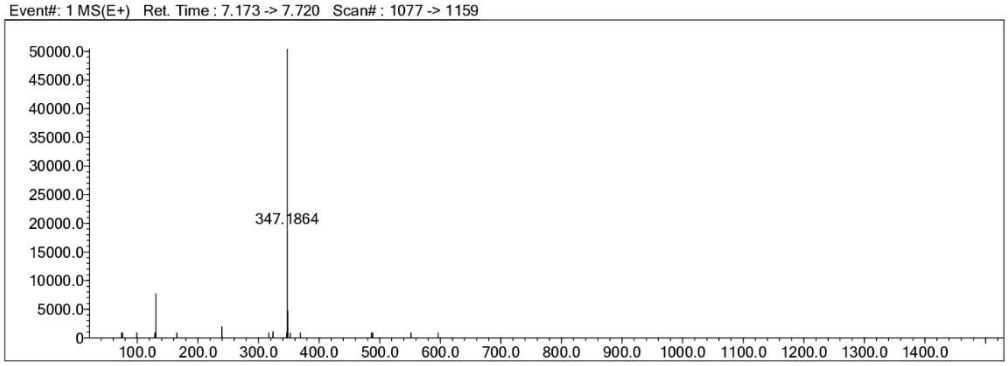
C	4	15	25	F	1	0	0	Cl	1	0	0	Pd	2	0	0	
N	3	1	4	P	3	0	0	Br	1	0	0	I	3	0	0	

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

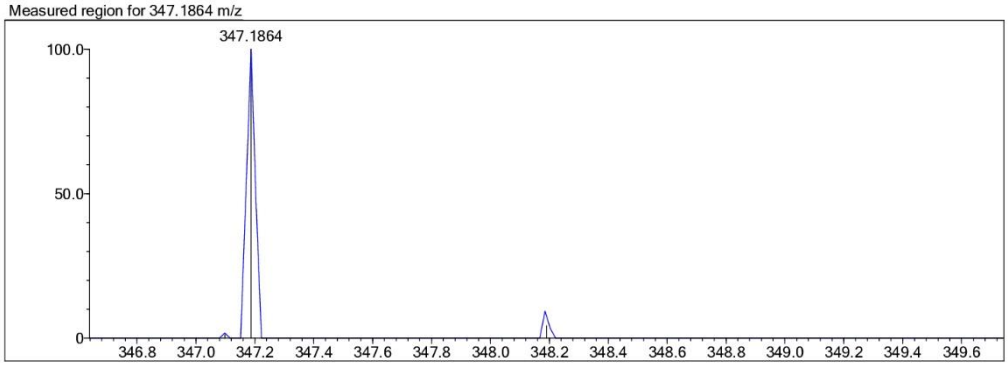
DBE Range: 10.0 - 20.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

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

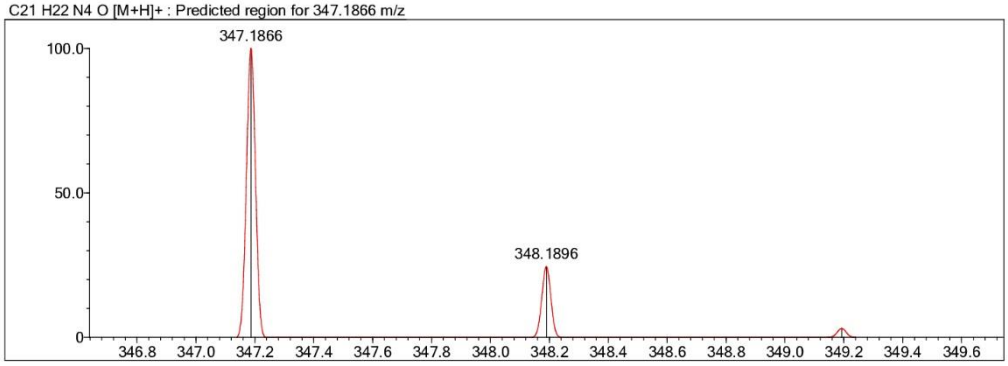
Event#: 1 MS(E+) Ret. Time : 7.173 -> 7.720 Scan# : 1077 -> 1159



Measured region for 347.1864 m/z



C21 H22 N4 O [M+H]+ : Predicted region for 347.1866 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	51.62	C21 H22 N4 O	[M+H]+	347.1864	347.1866	-0.2	-0.58	51.62	13.0

Figure S5. IR spectrum of compound **3b**

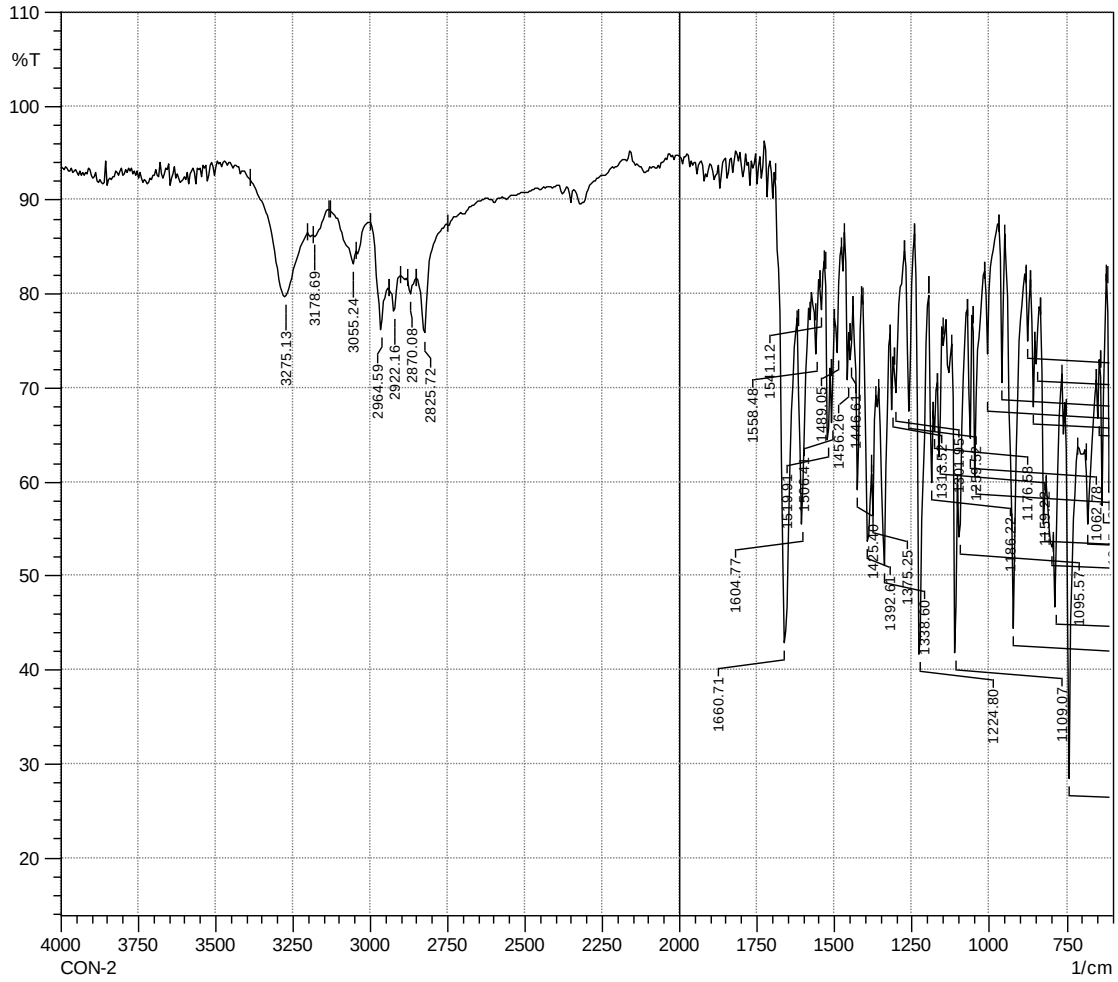


Figure S6. ^{1}H NMR spectrum of compound **3b**

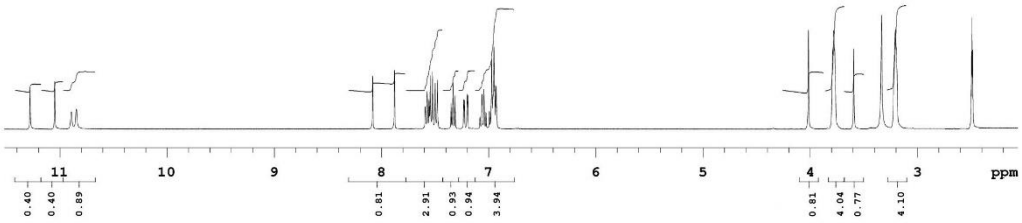


Figure S7. ^{13}C NMR spectrum of compound **3b**

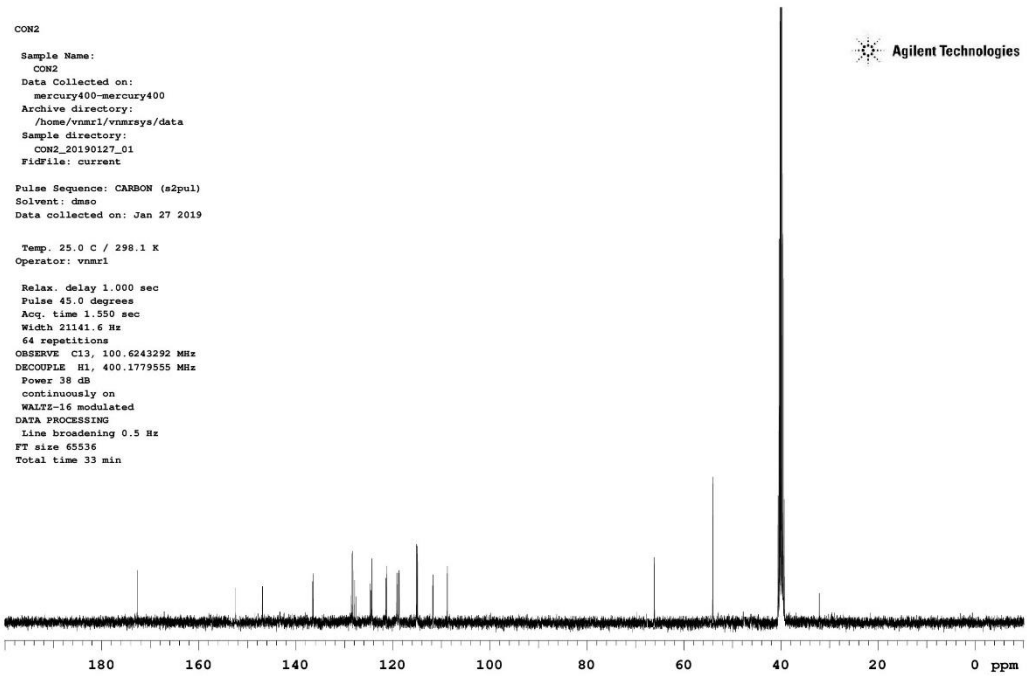


Figure S8. HRMS spectrum of compound **3b**

Formula Predictor Report - CON-2_6.lcd

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Data File: C:\LabSolutions\Data\Analiz\AOzdemir\CON-2_6.lcd

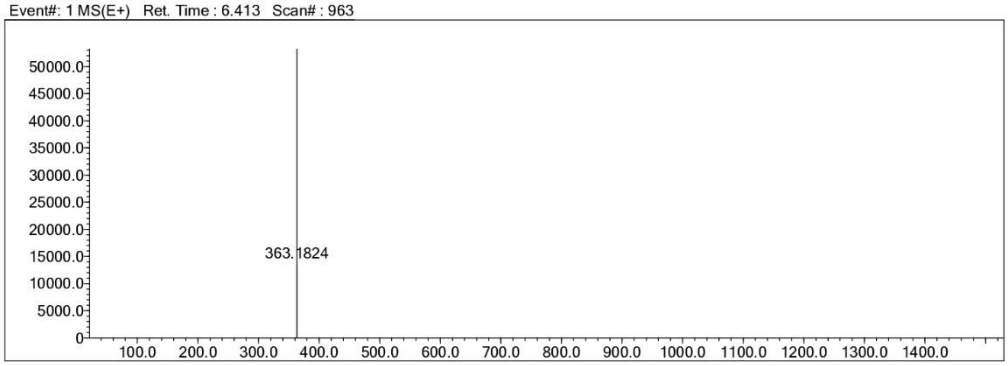
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	30	O	2	1	4	S	2	0	2	Ru	2	0	0	H
C	4	15	25	F	1	0	0	Cl	1	0	0	Pd	2	0	0	
N	3	1	4	P	3	0	0	Br	1	0	0	I	3	0	0	

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

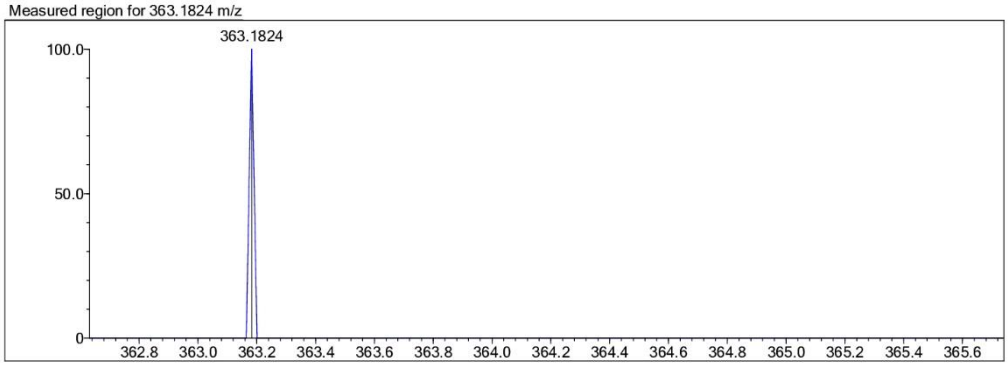
DBE Range: 10.0 - 20.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

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

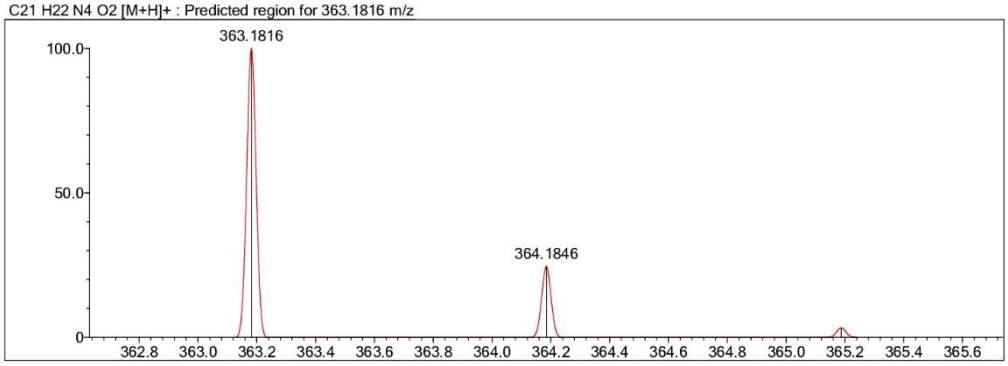
Event#: 1 MS(E+) Ret. Time : 6.413 Scan# : 963



Measured region for 363.1824 m/z



C21 H22 N4 O2 [M+H]+ : Predicted region for 363.1816 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	0.00	C21 H22 N4 O2	[M+H]+	363.1824	363.1816	0.8	2.20	0.00	13.0

Figure S9. IR spectrum of compound **3c**

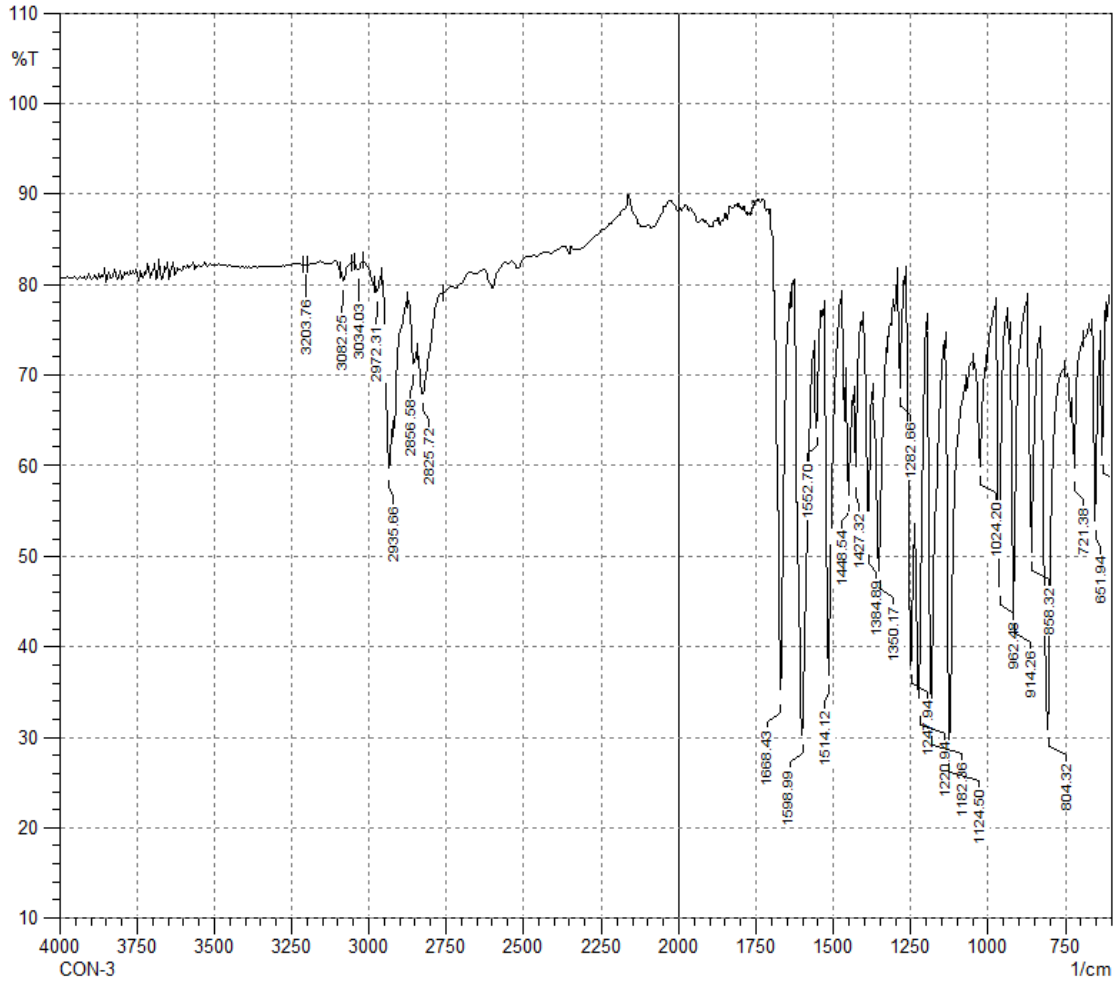


Figure S10. ^{1}H NMR spectrum of compound **3c**

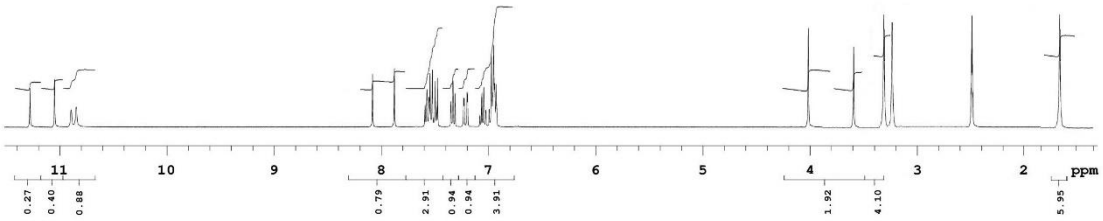


Figure S11. ^{13}C NMR spectrum of compound **3c**

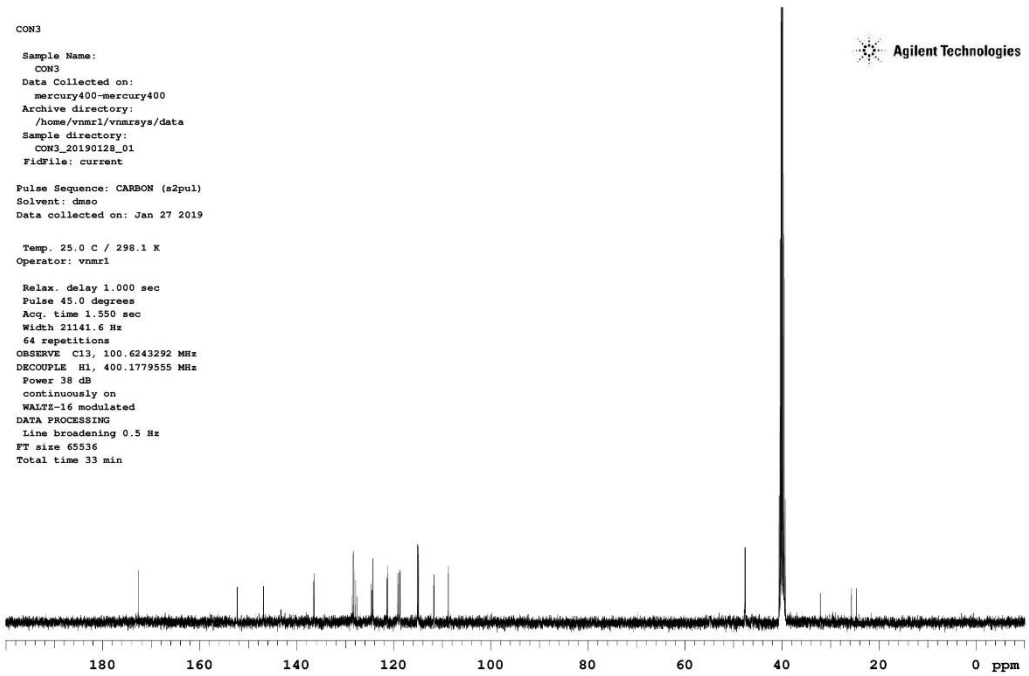


Figure S12. HRMS spectrum of compound **3c**

Formula Predictor Report - CON-3_7.lcd

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Data File: C:\LabSolutions\Data\Analiz\AOzdemir\CON-3_7.lcd

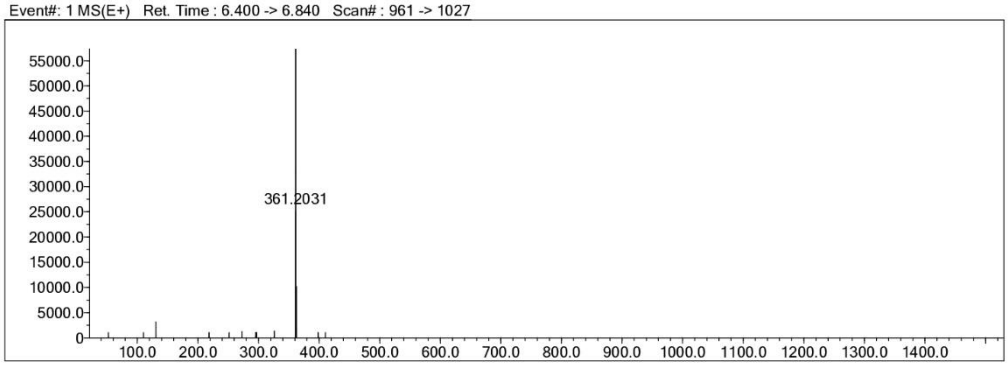
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	30	O	2	1	4	S	2	0	2	Ru	2	0	0	H
C	4	15	25	F	1	0	0	Cl	1	0	0	Pd	2	0	0	
N	3	1	4	P	3	0	0	Br	1	0	0	I	3	0	0	

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

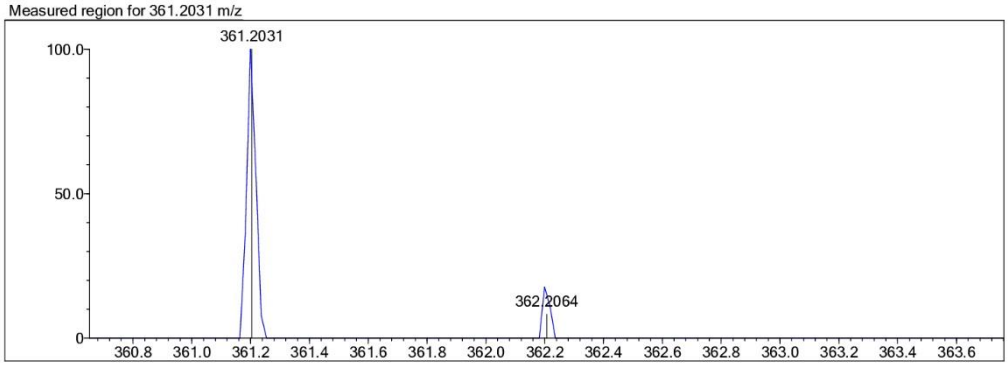
DBE Range: 10.0 - 20.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

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

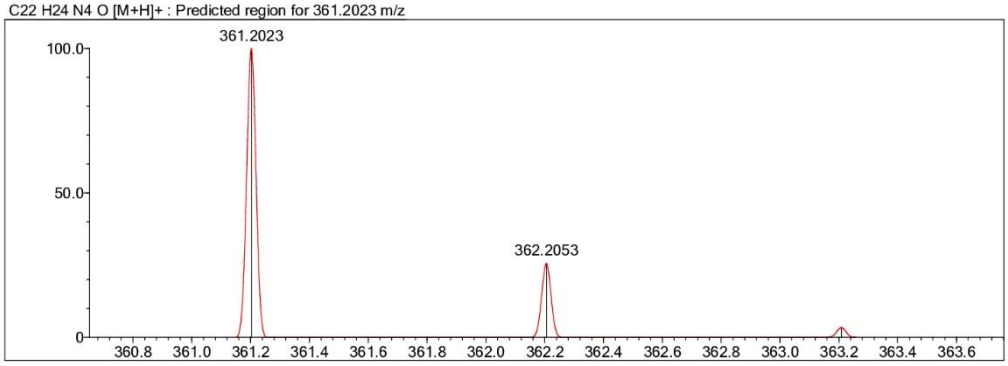
Event#: 1 MS(E+) Ret. Time : 6.400 -> 6.840 Scan# : 961 -> 1027



Measured region for 361.2031 m/z



C22 H24 N4 O [M+H]+ : Predicted region for 361.2023 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	57.85	C22 H24 N4 O	[M+H]+	361.2031	361.2023	0.8	2.21	59.65	13.0

Figure S13. IR spectrum of compound **3d**

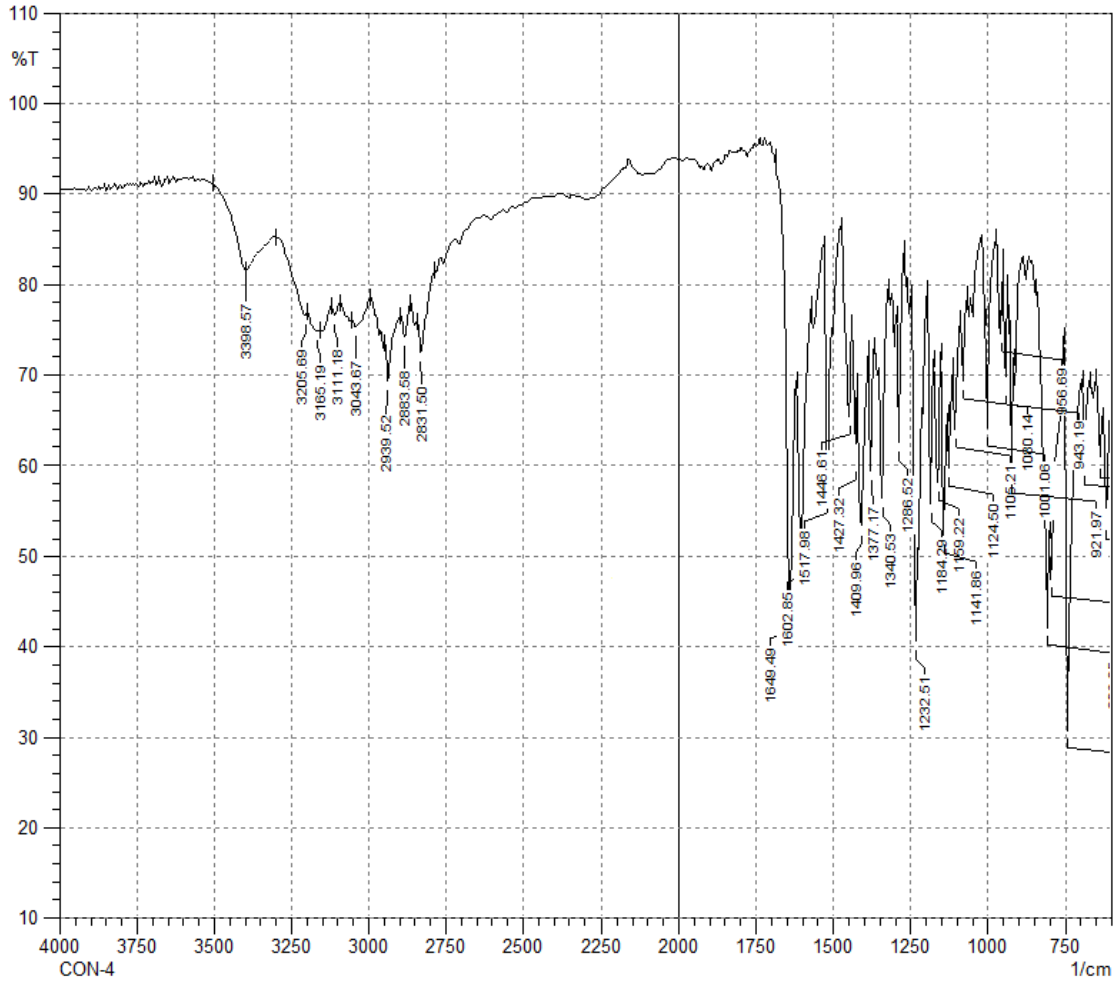


Figure S14. ^{1}H NMR spectrum of compound **3d**

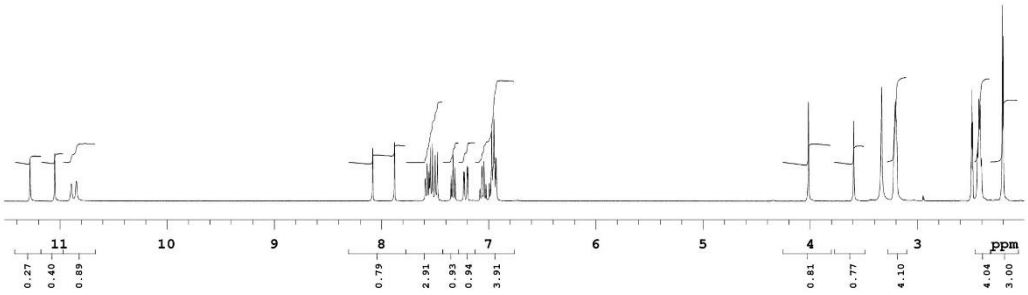


Figure S15. ^{13}C NMR spectrum of compound **3d**

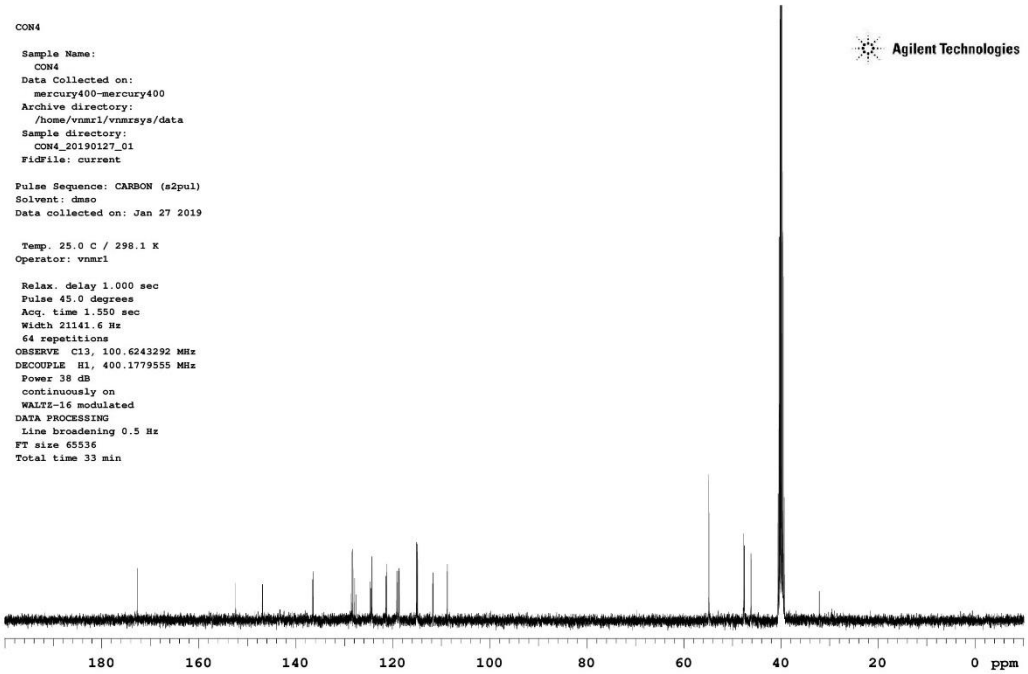


Figure S16. HRMS spectrum of compound **3d**

Formula Predictor Report - CON-5_7.lcd

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Data File: C:\LabSolutions\Data\Analiz\AOzdemir\CON-5_7.lcd

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
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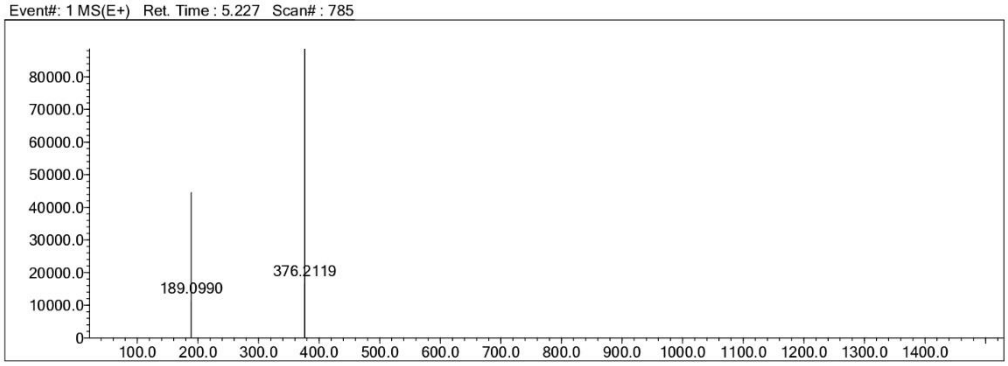
C	4	15	25	F	1	0	0	Cl	1	0	0	Pd	2	0	0	
N	3	1	5	P	3	0	0	Br	1	0	0	I	3	0	0	

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

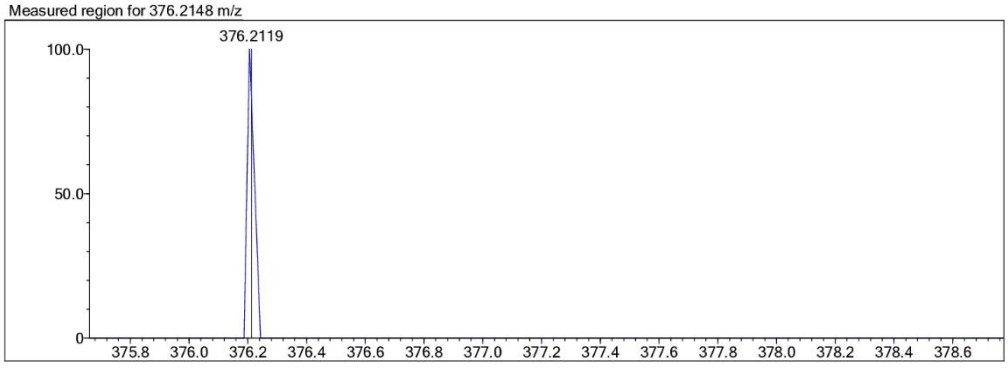
DBE Range: 8.0 - 17.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

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

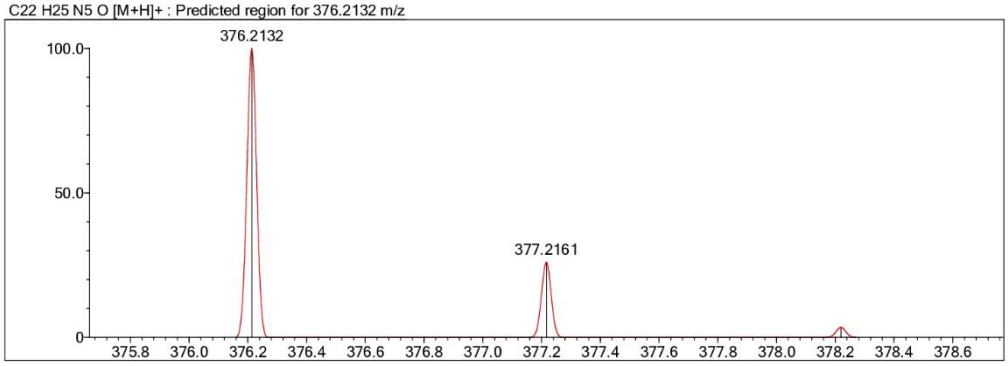
Event#: 1 MS(E+) Ret. Time : 5.227 Scan# : 785



Measured region for 376.2148 m/z



C22 H25 N5 O [M+H]+ : Predicted region for 376.2132 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	0.00	C22 H25 N5 O	[M+H]+	376.2148	376.2132	1.6	4.25	0.00	13.0

Figure S17. IR spectrum of compound **3e**

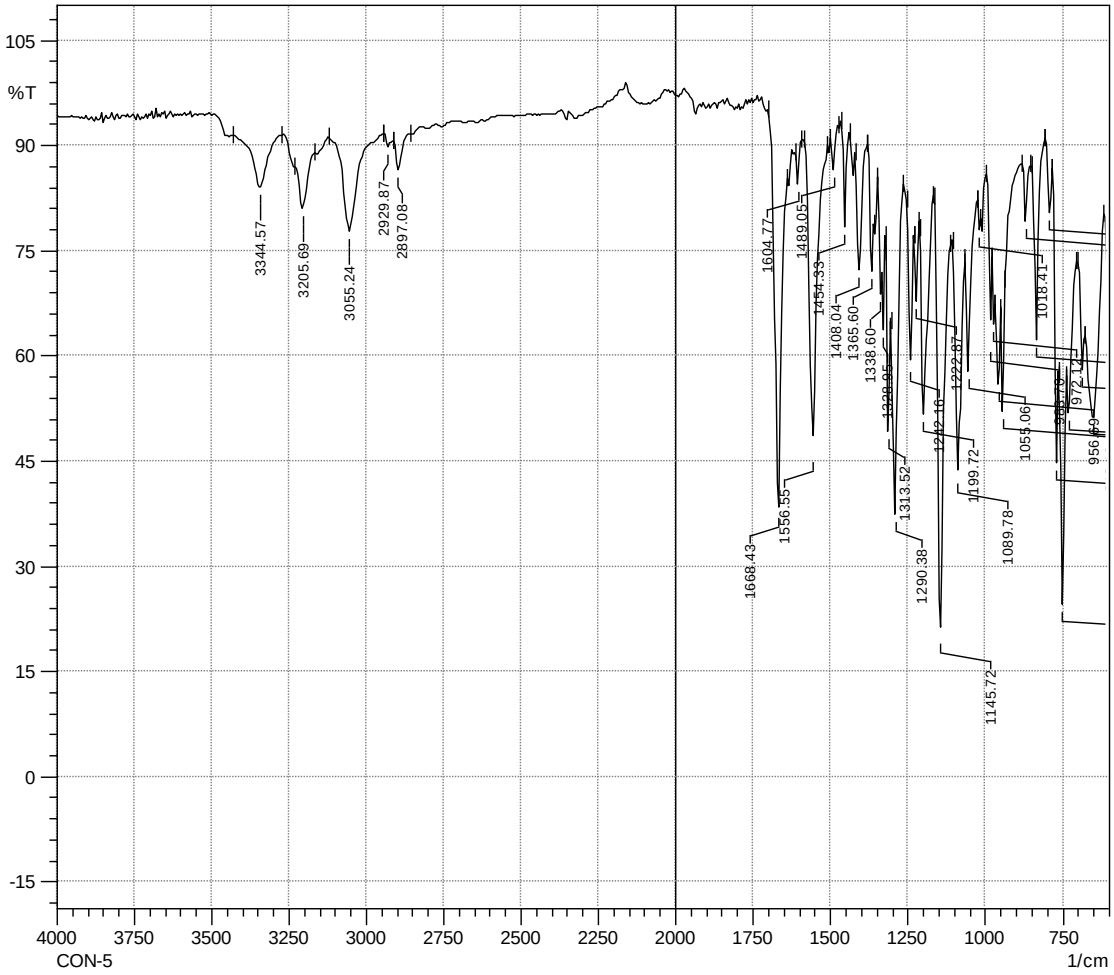


Figure S18. ^{1}H NMR spectrum of compound **3e**

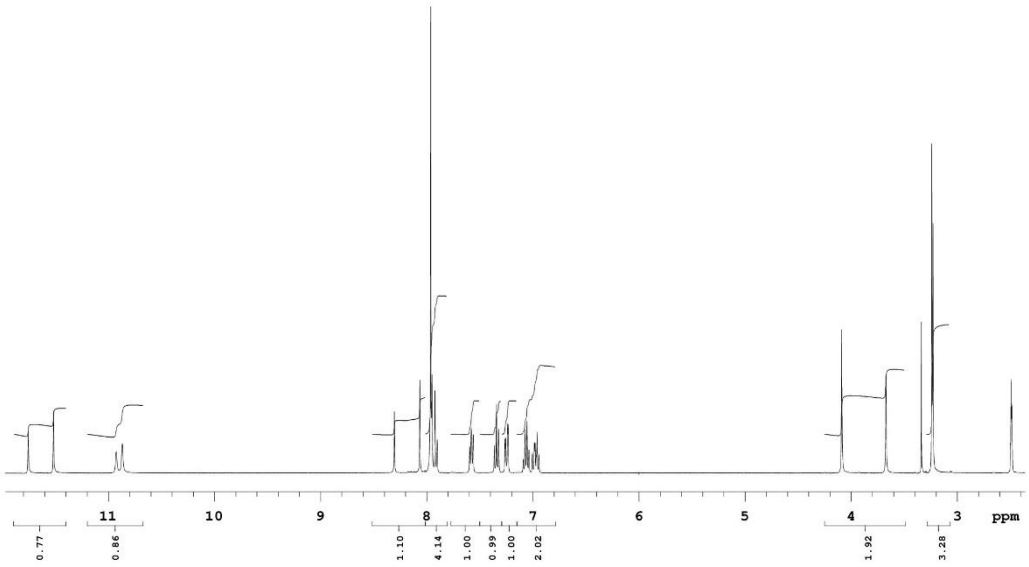


Figure S19. ^{13}C NMR spectrum of compound **3e**

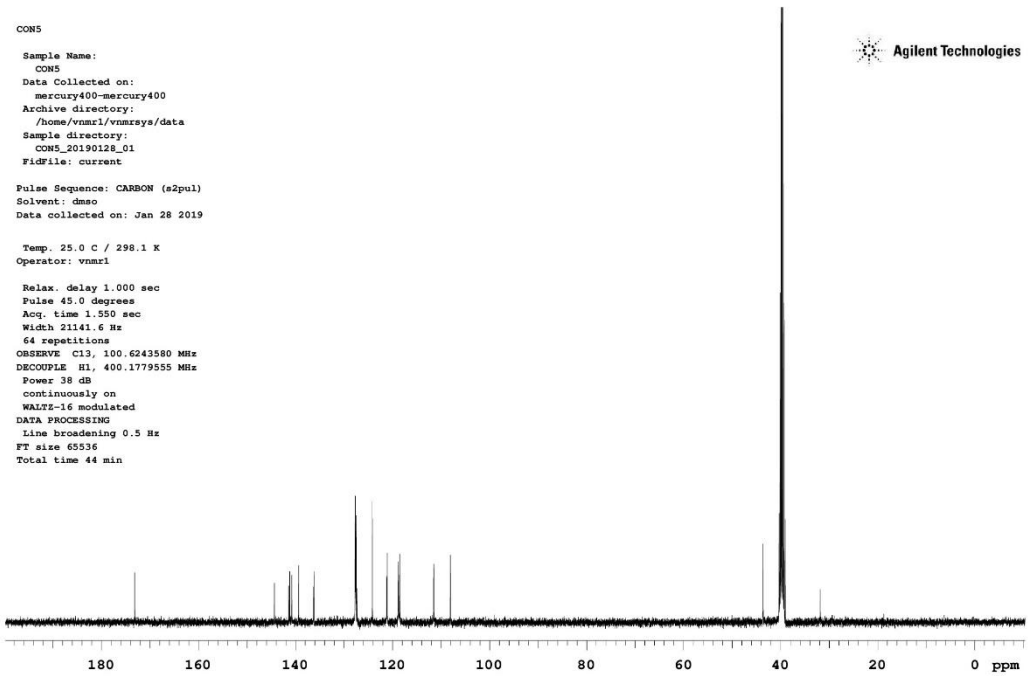


Figure S20. HRMS spectrum of compound **3e**

Formula Predictor Report - CON-7_8.lcd

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Data File: C:\LabSolutions\Data\Analiz\AOzdemir\CON-7_8.lcd

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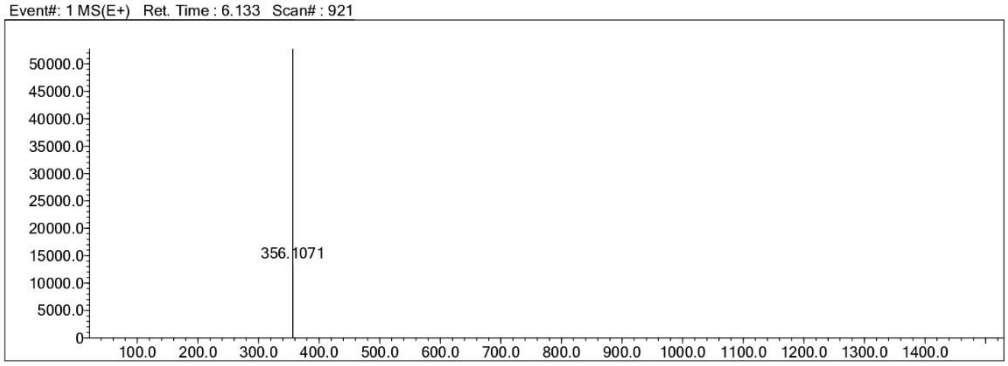
C	4	15	25	F	1	0	0	Cl	1	0	0	Pd	2	0	0	
N	3	1	5	P	3	0	0	Br	1	0	0	I	3	0	0	

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

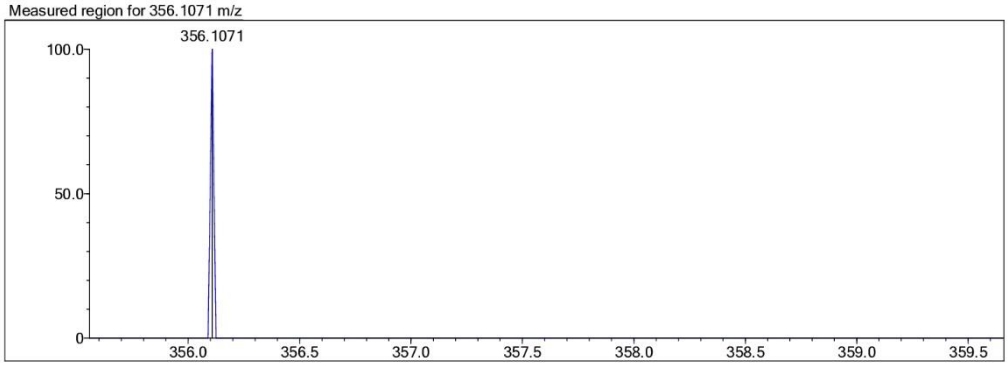
DBE Range: 8.0 - 17.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

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

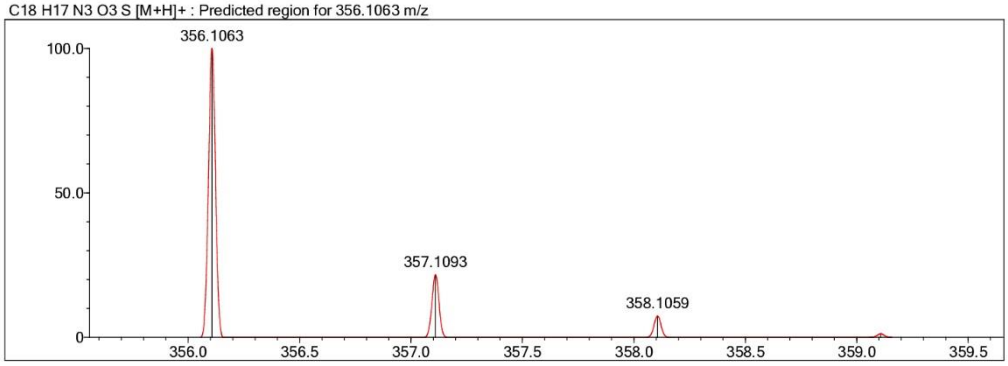
Event#: 1 MS(E+) Ret. Time : 6.133 Scan# : 921



Measured region for 356.1071 m/z



C18 H17 N3 O3 S [M+H]+ : Predicted region for 356.1063 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	0.00	C18 H17 N3 O3 S	[M+H]+	356.1071	356.1063	0.8	2.25	0.00	12.0

Figure S21. IR spectrum of compound **3f**

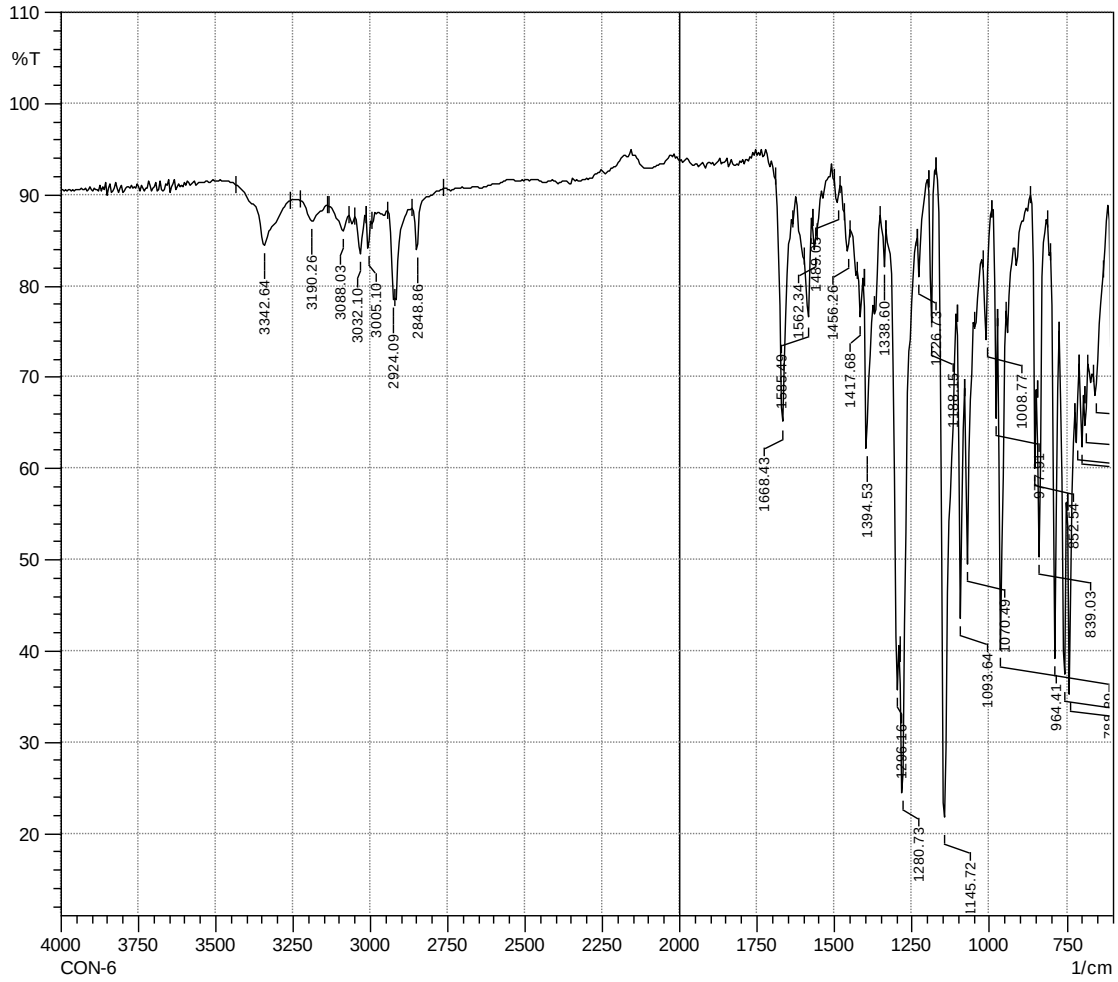


Figure S22. ^{1}H NMR spectrum of compound **3f**

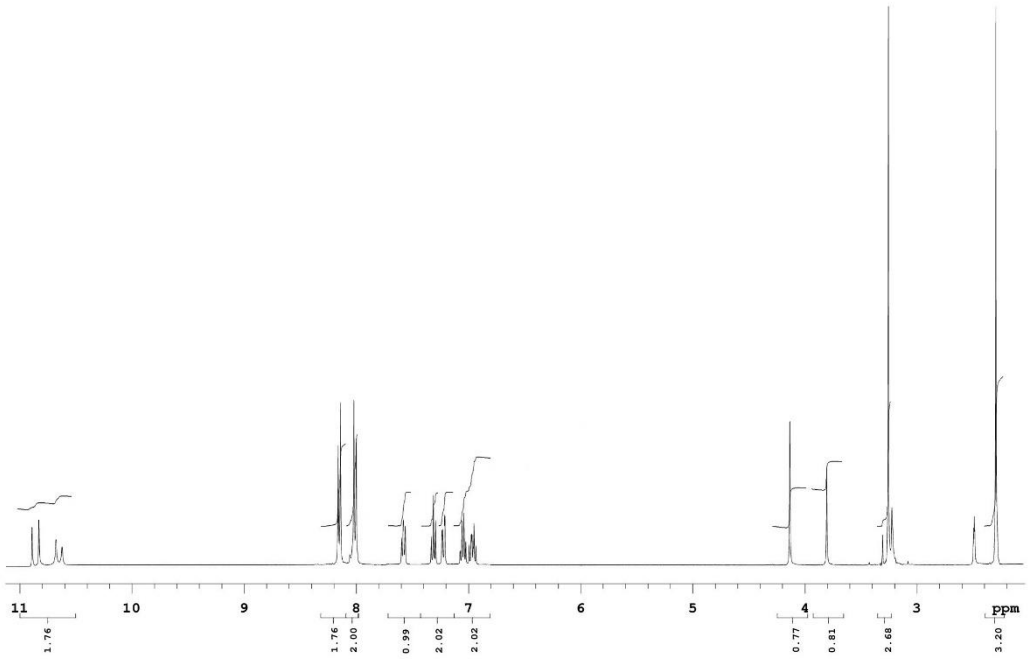


Figure S23. ^{13}C NMR spectrum of compound **3f**

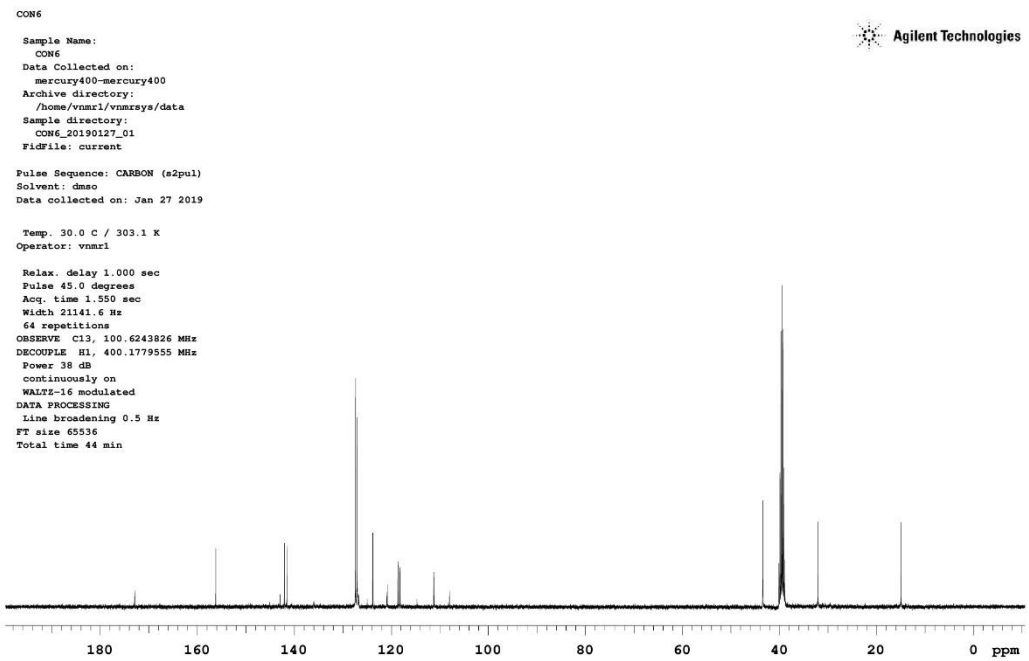


Figure S24. HRMS spectrum of compound **3f**

Formula Predictor Report - CON-8_9.lcd

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Data File: C:\LabSolutions\Data\Analiz\AOzdemir\CON-8_9.lcd

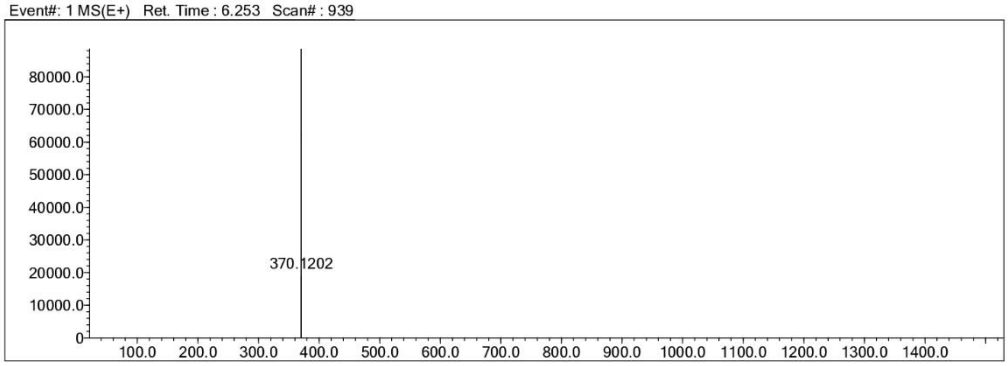
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	30	O	2	0	5	S	2	1	1	Ru	2	0	0	H
C	4	15	25	F	1	0	0	Cl	1	0	0	Pd	2	0	0	
N	3	1	5	P	3	0	0	Br	1	0	0	I	3	0	0	

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

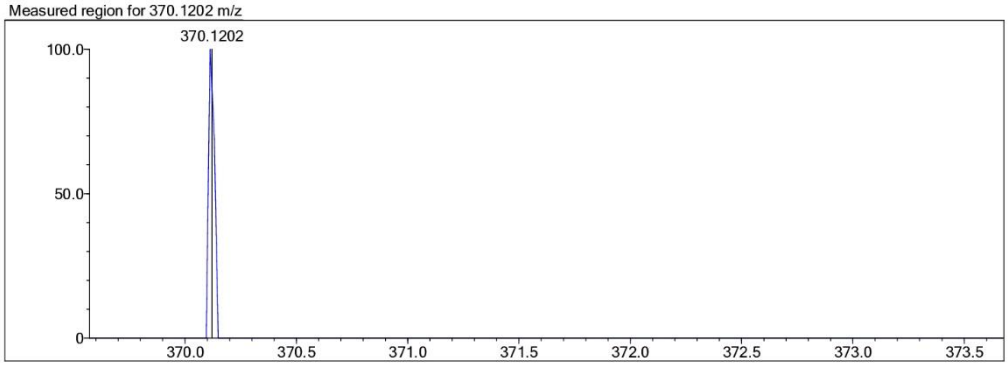
DBE Range: 8.0 - 17.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

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

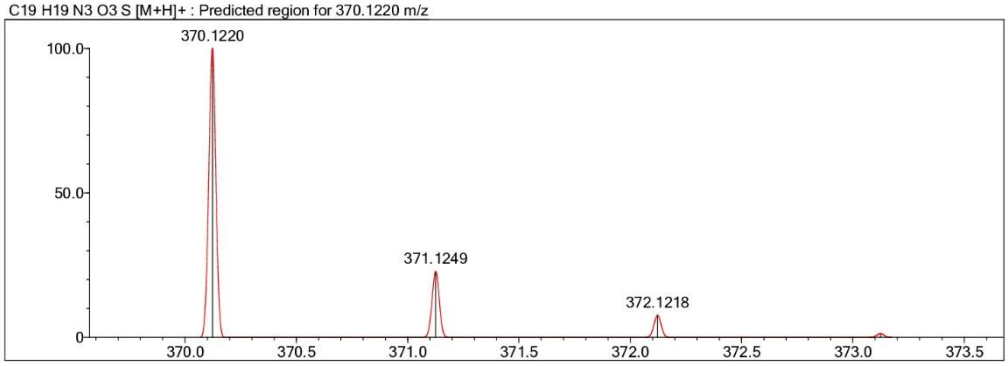
Event#: 1 MS(E+) Ret. Time : 6.253 Scan# : 939



Measured region for 370.1202 m/z



C19 H19 N3 O3 S [M+H]+ : Predicted region for 370.1220 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	0.00	C19 H19 N3 O3 S	[M+H]+	370.1202	370.1220	-1.8	-4.86	0.00	12.0

Figure S25. IR spectrum of compound **3g**

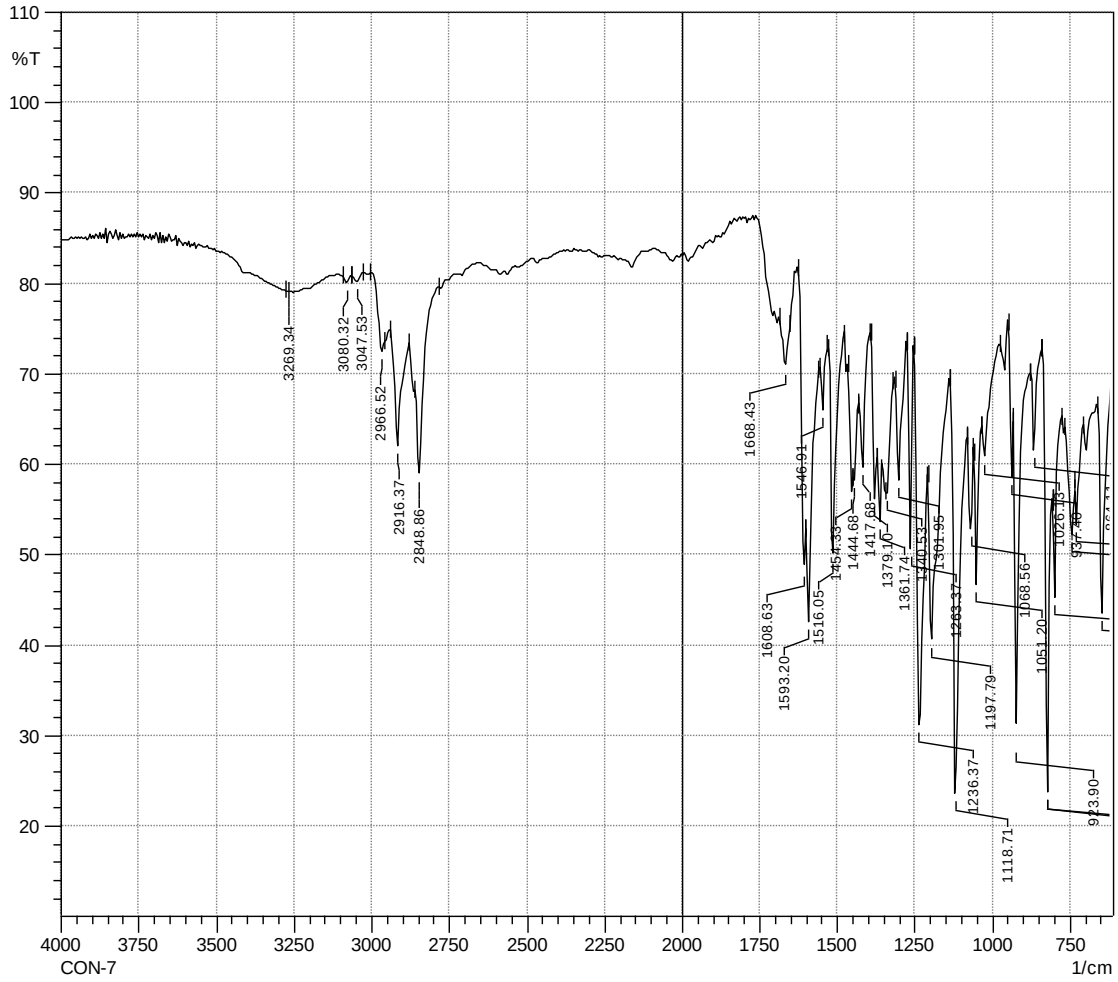


Figure S26. ^{1}H NMR spectrum of compound **3g**

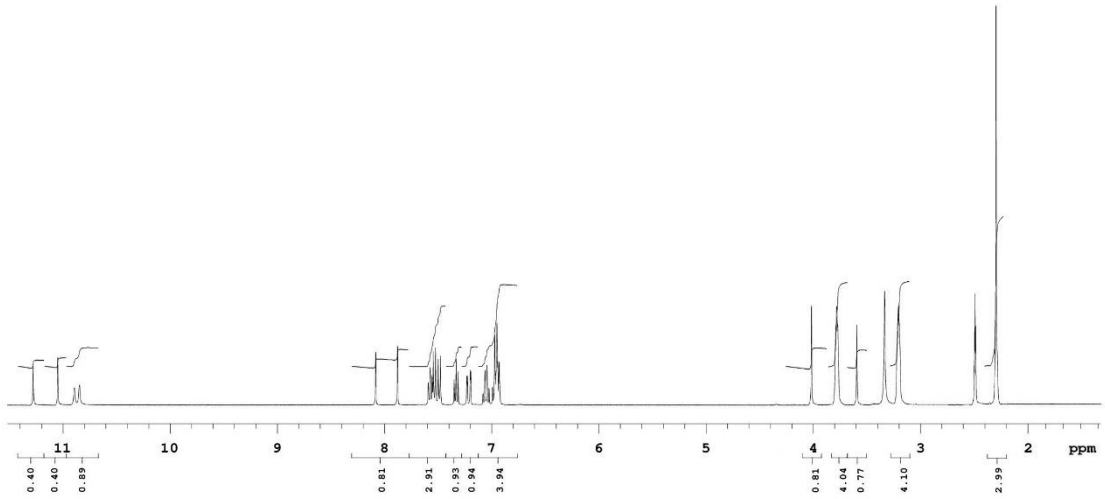


Figure S27. ^{13}C NMR spectrum of compound **3g**

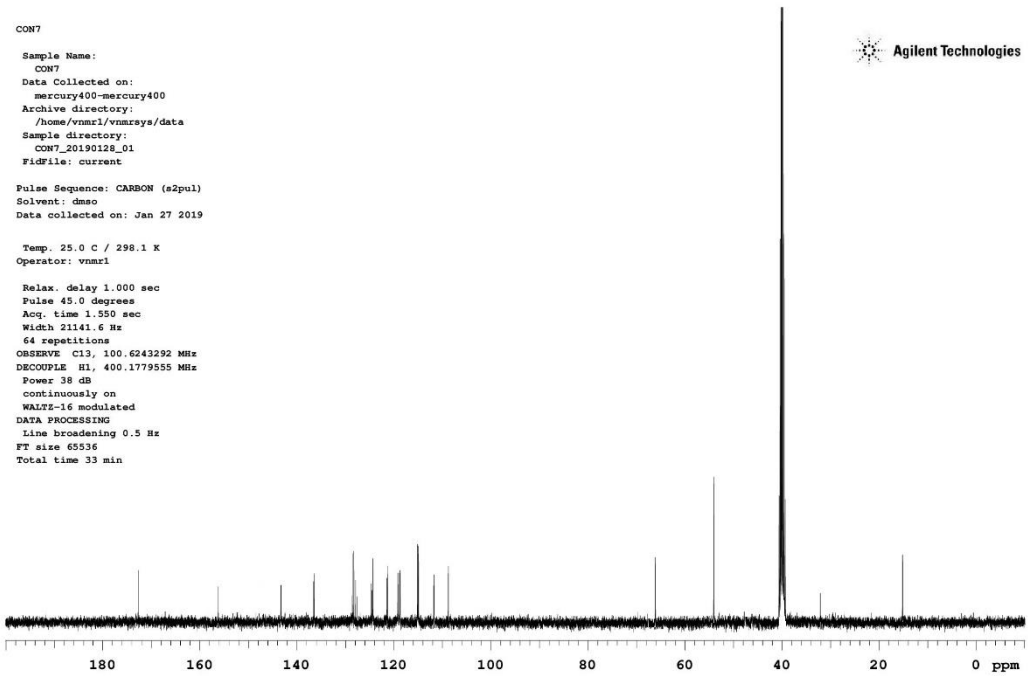


Figure S28. HRMS spectrum of compound **3g**

Formula Predictor Report - CON-9_8.lcd

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Data File: C:\LabSolutions\Data\Analiz\AOzdemir\CON-9_8.lcd

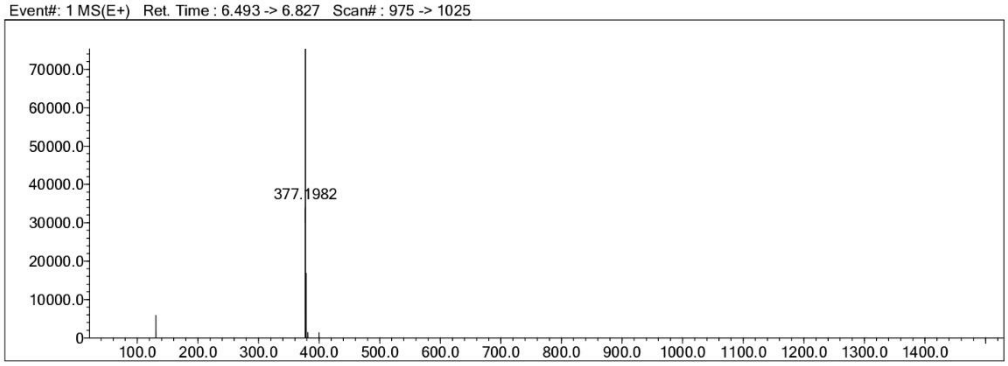
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	30	O	2	1	4	S	2	0	2	Ru	2	0	0	H
C	4	15	25	F	1	0	0	Cl	1	0	0	Pd	2	0	0	
N	3	1	4	P	3	0	0	Br	1	0	0	I	3	0	0	

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

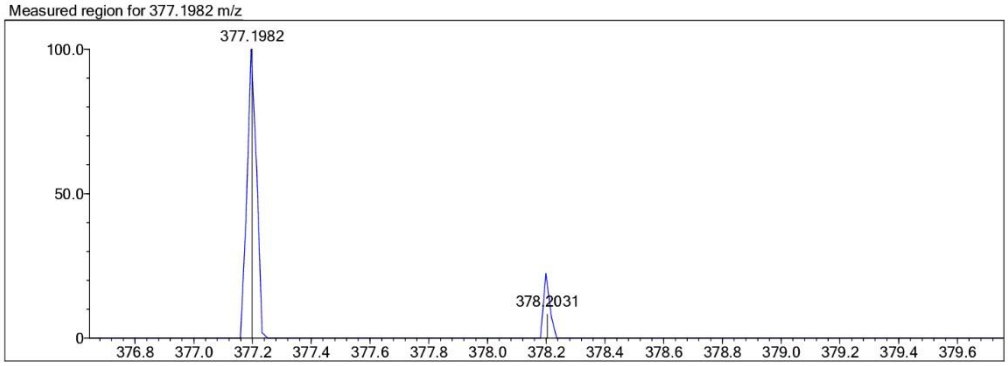
DBE Range: 10.0 - 20.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

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

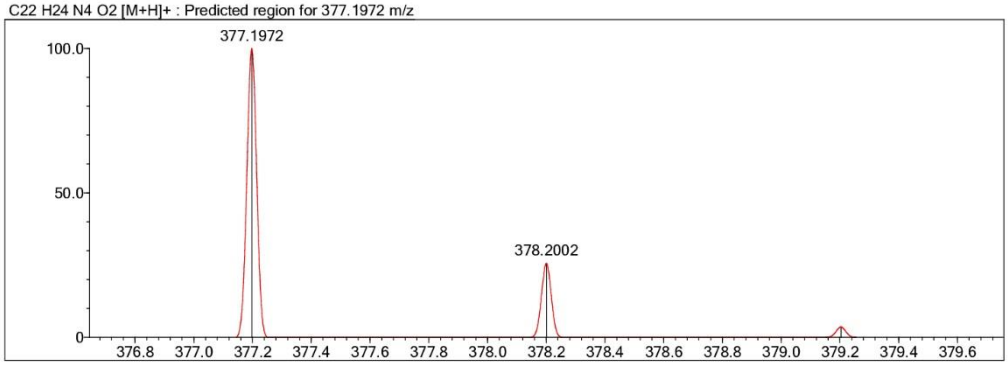
Event#: 1 MS(E+) Ret. Time : 6.493 -> 6.827 Scan# : 975 -> 1025



Measured region for 377.1982 m/z



C22 H24 N4 O2 [M+H]+ : Predicted region for 377.1972 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	69.48	C22 H24 N4 O2	[M+H]+	377.1982	377.1972	1.0	2.65	72.47	13.0

Figure S29. IR spectrum of compound **3h**

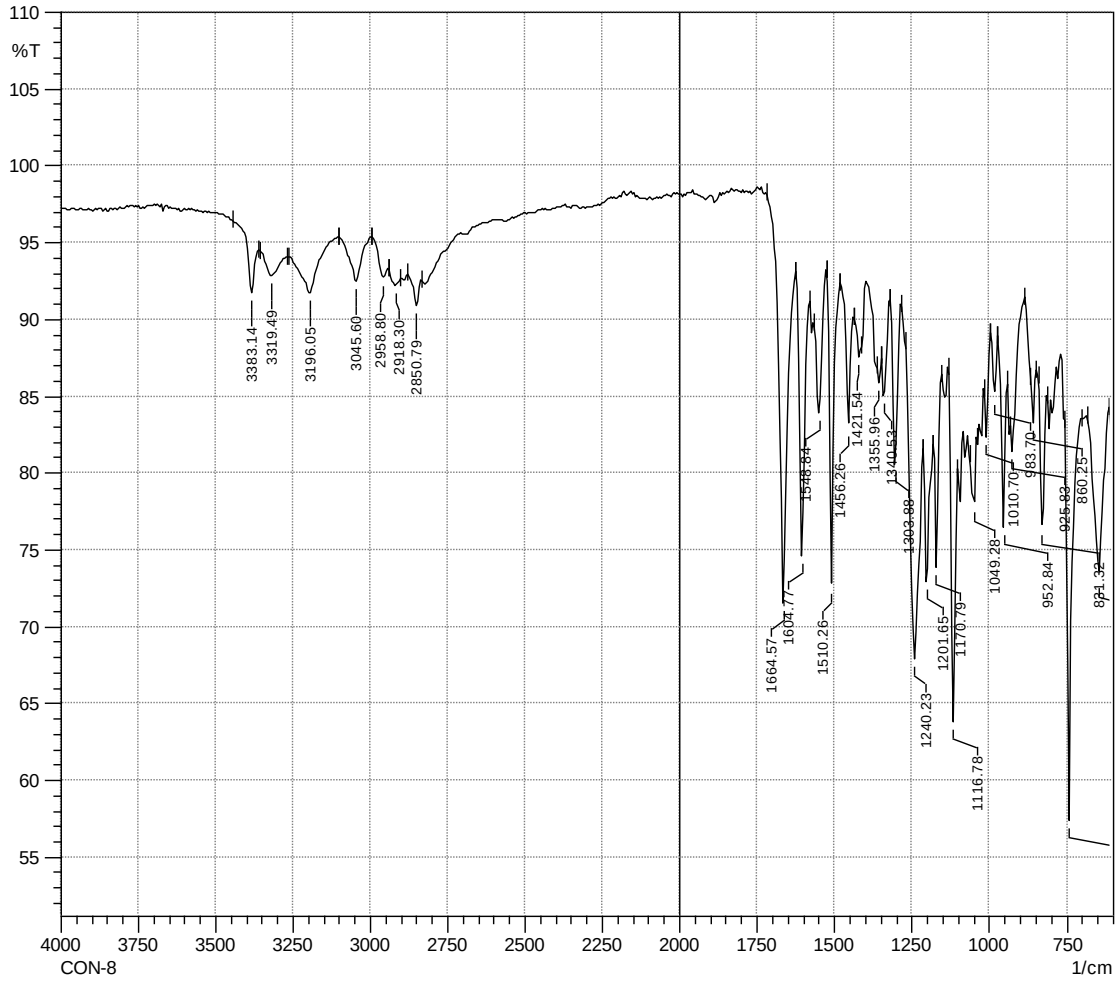


Figure S30. ^{1}H NMR spectrum of compound **3h**

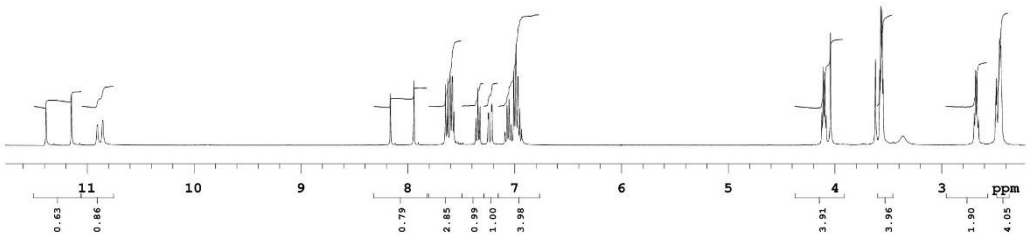


Figure S31. ^{13}C NMR spectrum of compound **3h**

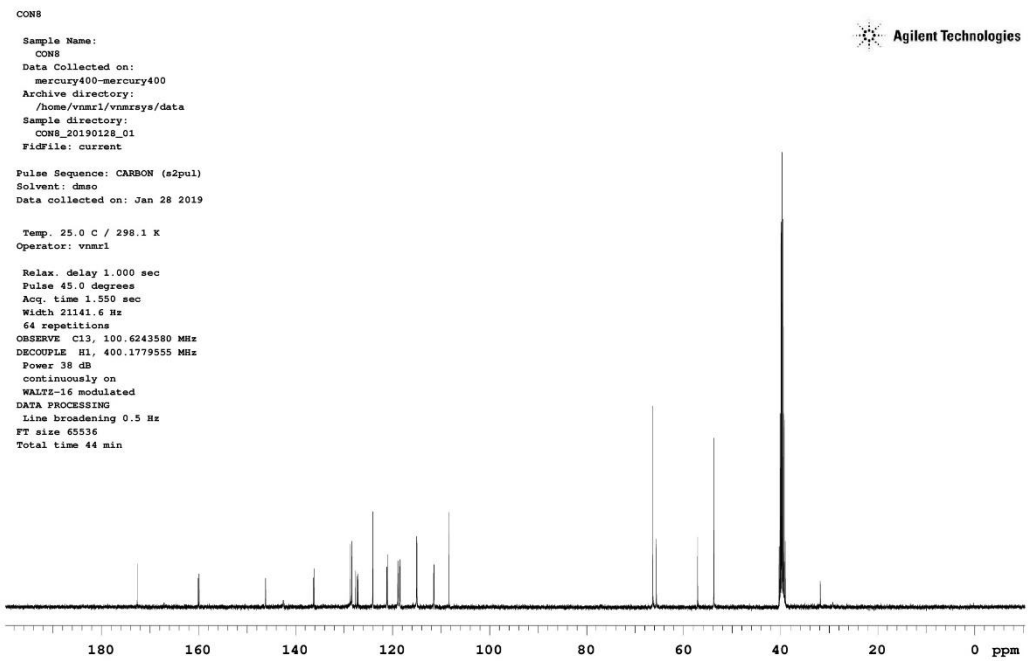


Figure S32. HRMS spectrum of compound **3h**

Formula Predictor Report - CON-12_11.lcd

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Data File: C:\LabSolutions\Data\Analiz\AOzdemir\CON-12_11.lcd

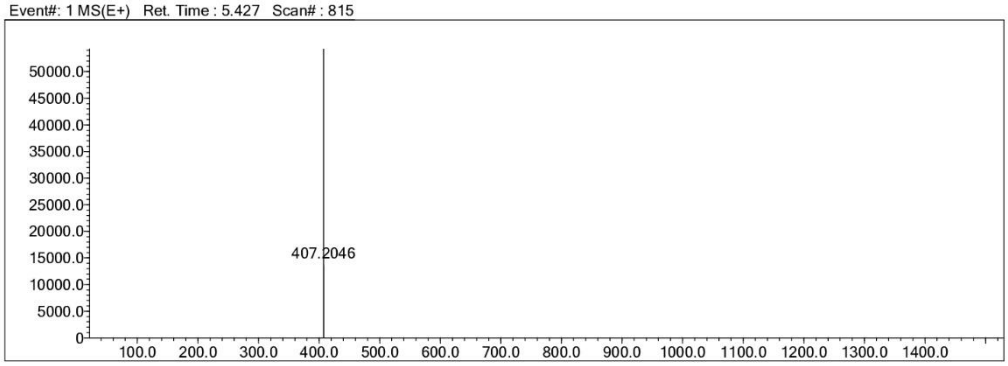
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	30	O	2	0	5	S	2	0	1	Ru	2	0	0	H
C	4	15	25	F	1	0	0	Cl	1	0	0	Pd	2	0	0	
N	3	1	5	P	3	0	0	Br	1	0	0	I	3	0	0	

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

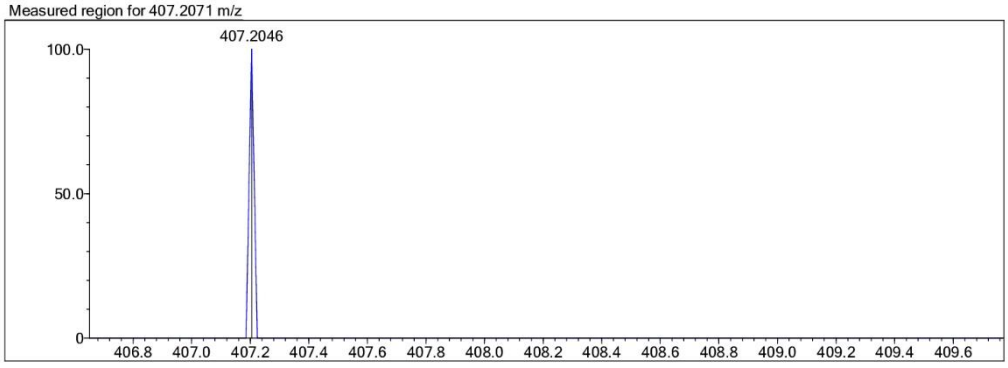
DBE Range: 5.0 - 20.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

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

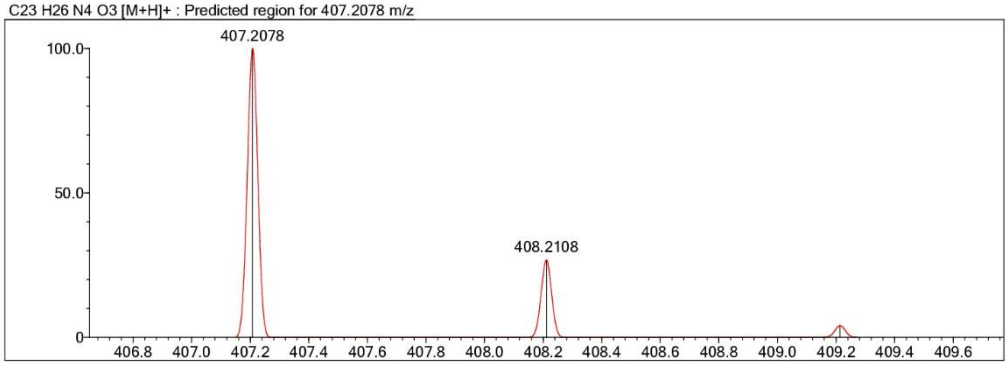
Event#: 1 MS(E+) Ret. Time : 5.427 Scan# : 815



Measured region for 407.2071 m/z



C23 H26 N4 O3 [M+H]+ : Predicted region for 407.2078 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	0.00	C23 H26 N4 O3	[M+H]+	407.2071	407.2078	-0.7	-1.72	0.00	13.0

Figure S33. IR spectrum of compound **3i**

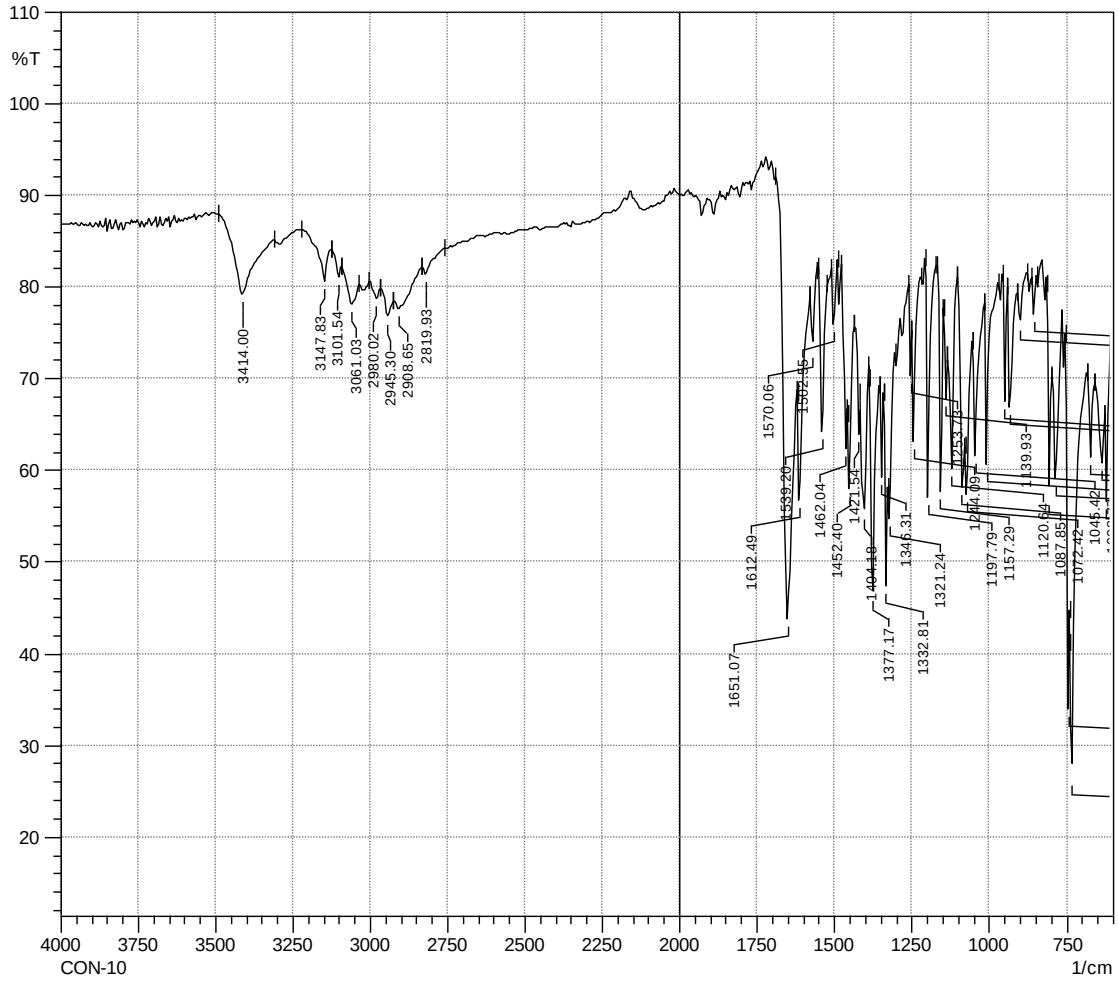


Figure S34. ^{1}H NMR spectrum of compound **3i**

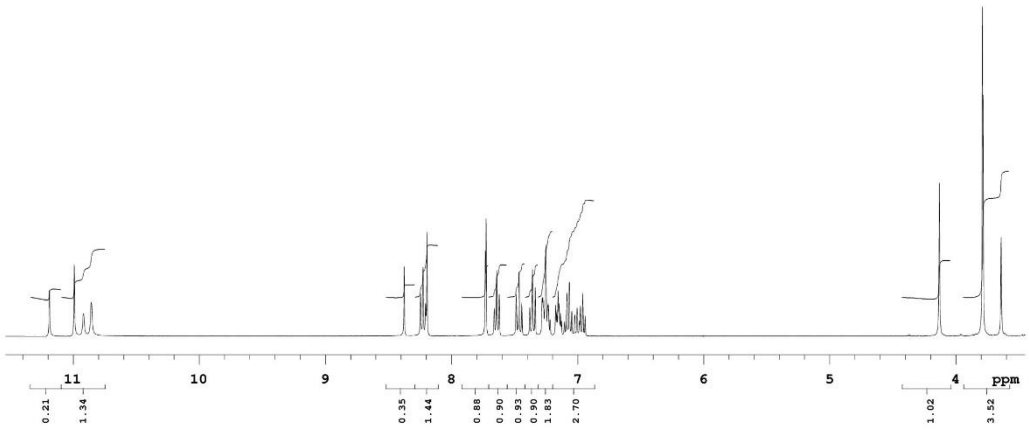


Figure S35. ^{13}C NMR spectrum of compound **3i**

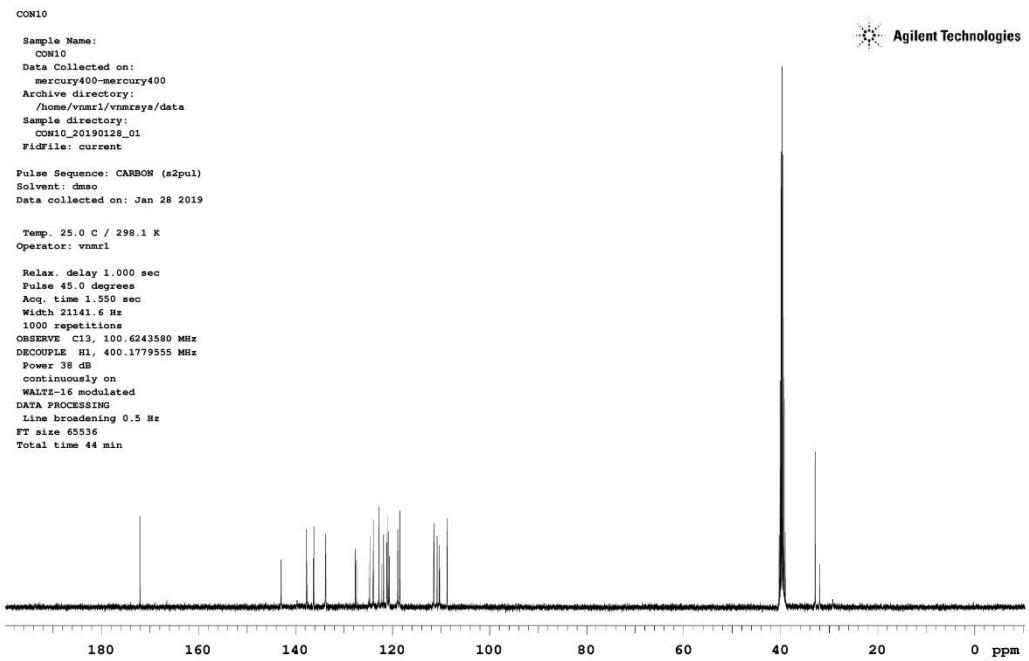


Figure S36. HRMS spectrum of compound **3i**

Formula Predictor Report - CON-15_13.lcd

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Data File: C:\LabSolutions\Data\Analiz\AOzdemir\CON-15_13.lcd

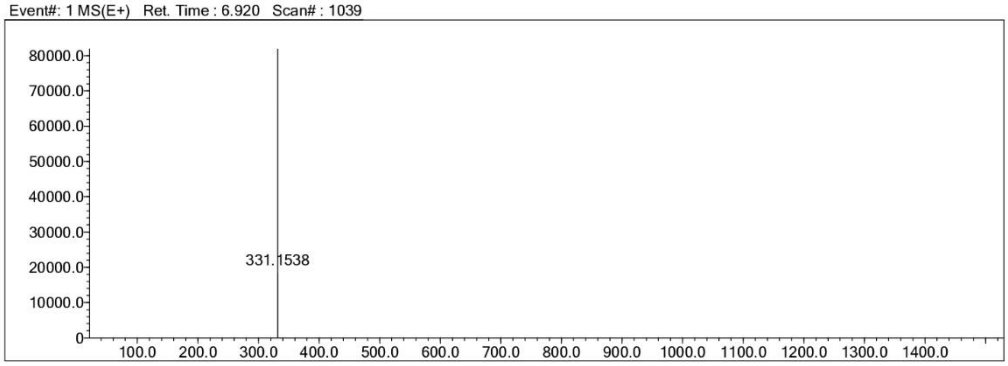
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	30	O	2	0	4	S	2	0	2	Ru	2	0	0	H
C	4	15	25	F	1	0	0	Cl	1	0	1	Pd	2	0	0	
N	3	1	6	P	3	0	0	Br	1	0	0	I	3	0	0	

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

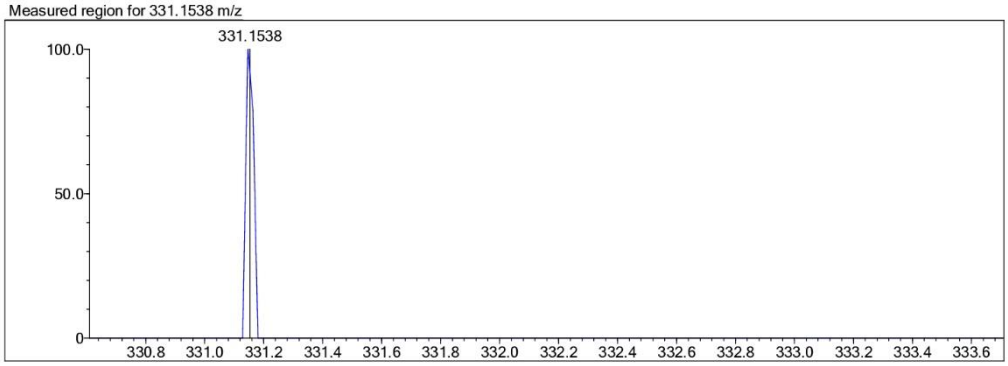
DBE Range: 10.0 - 20.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

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

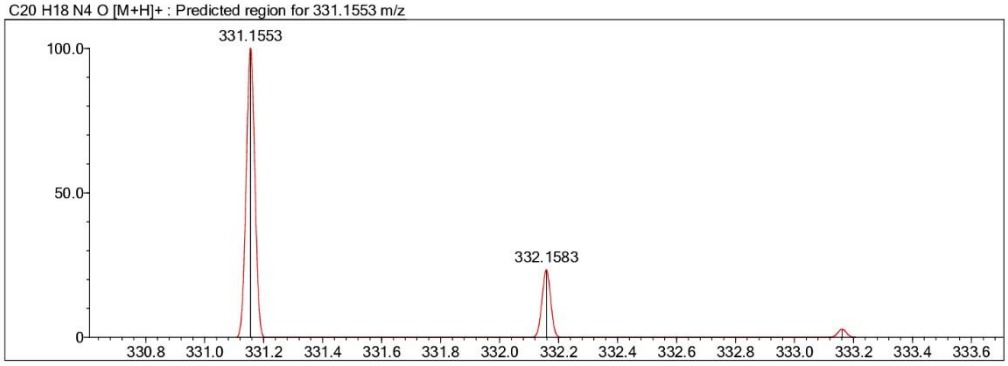
Event#: 1 MS(E+) Ret. Time : 6.920 Scan# : 1039



Measured region for 331.1538 m/z



C20 H18 N4 O [M+H]+ : Predicted region for 331.1553 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	0.00	C20 H18 N4 O	[M+H]+	331.1538	331.1553	-1.5	-4.53	0.00	14.0

Figure S37. IR spectrum of compound **3j**

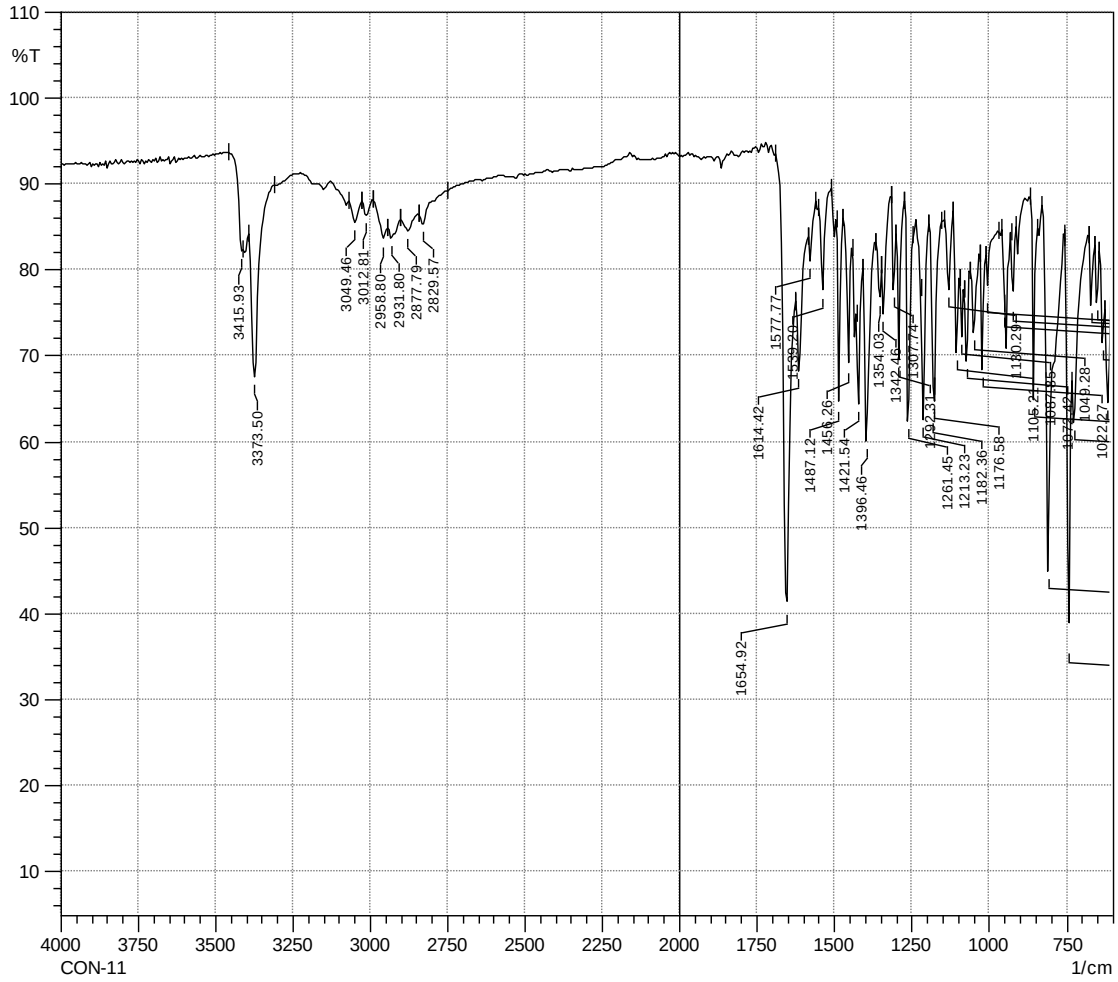


Figure S38. ^{1}H NMR spectrum of compound **3j**

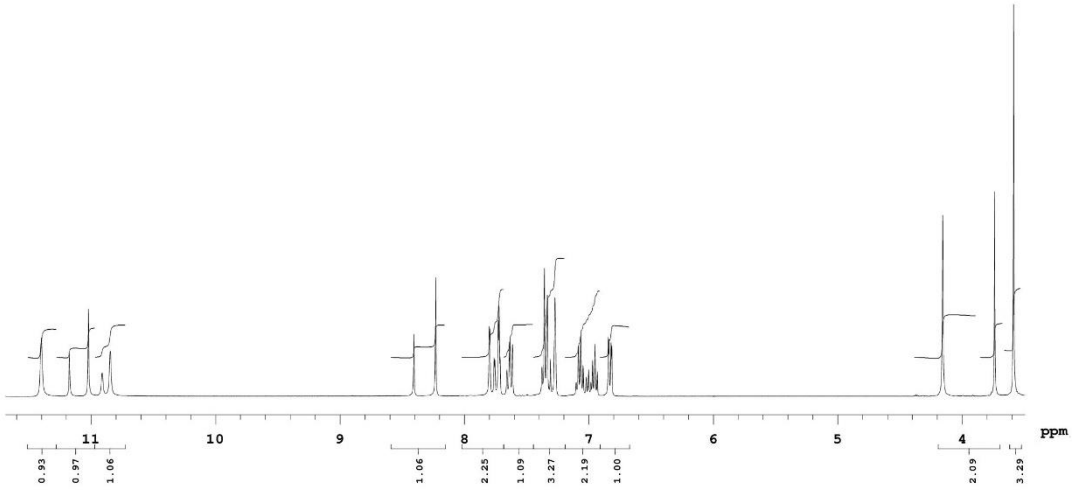


Figure S39. ^{13}C NMR spectrum of compound **3j**

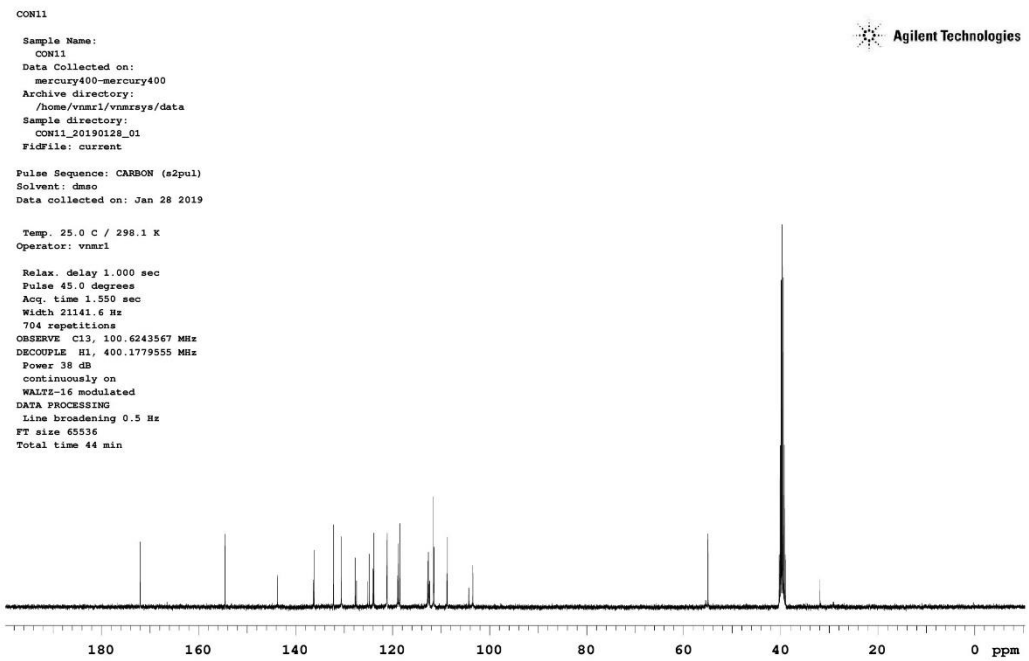


Figure S40. HRMS spectrum of compound **3j**

Formula Predictor Report - CON-16_14.lcd

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Data File: C:\LabSolutions\Data\Analiz\AOzdemir\CON-16_14.lcd

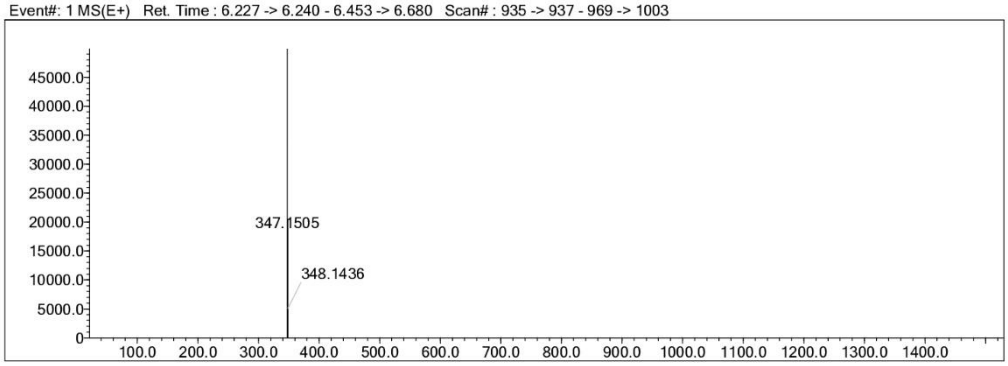
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	30	O	2	1	4	S	2	0	2	Ru	2	0	0	H
C	4	15	25	F	1	0	0	Cl	1	0	1	Pd	2	0	0	
N	3	1	6	P	3	0	0	Br	1	0	0	I	3	0	0	

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

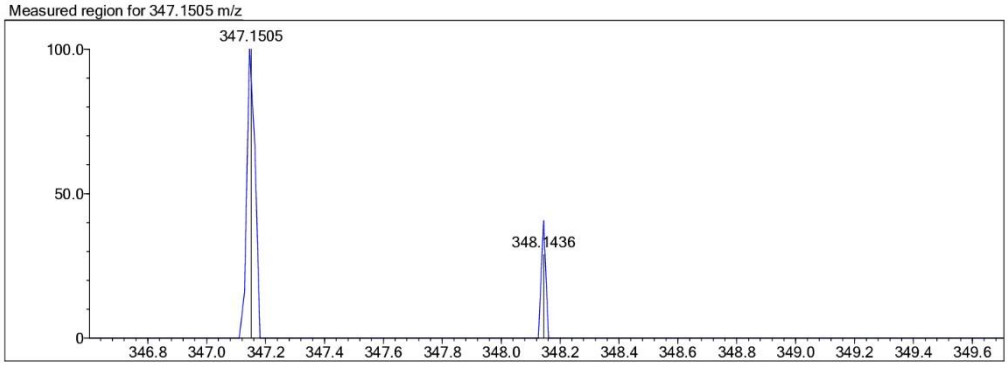
DBE Range: 10.0 - 20.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

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

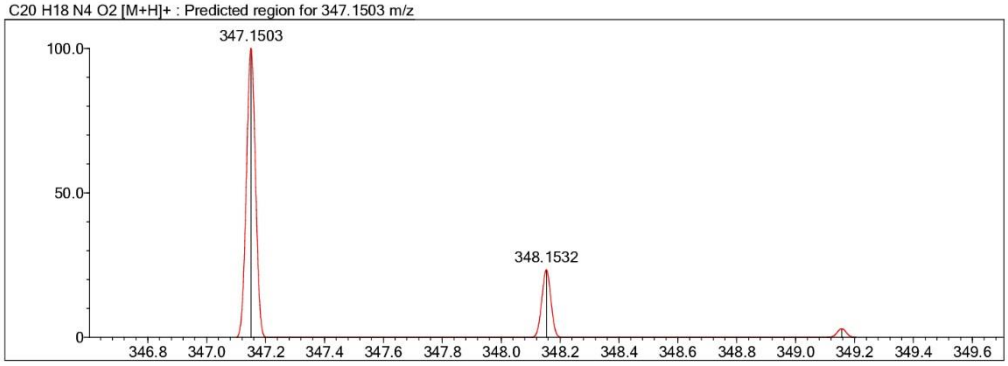
Event#: 1 MS(E+) Ret. Time : 6.227 -> 6.240 - 6.453 -> 6.680 Scan# : 935 -> 937 - 969 -> 1003



Measured region for 347.1505 m/z



C20 H18 N4 O2 [M+H]+ : Predicted region for 347.1503 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	38.14	C20 H18 N4 O2	[M+H]+	347.1505	347.1503	0.2	0.58	38.14	14.0

Figure S41. IR spectrum of compound **4a**

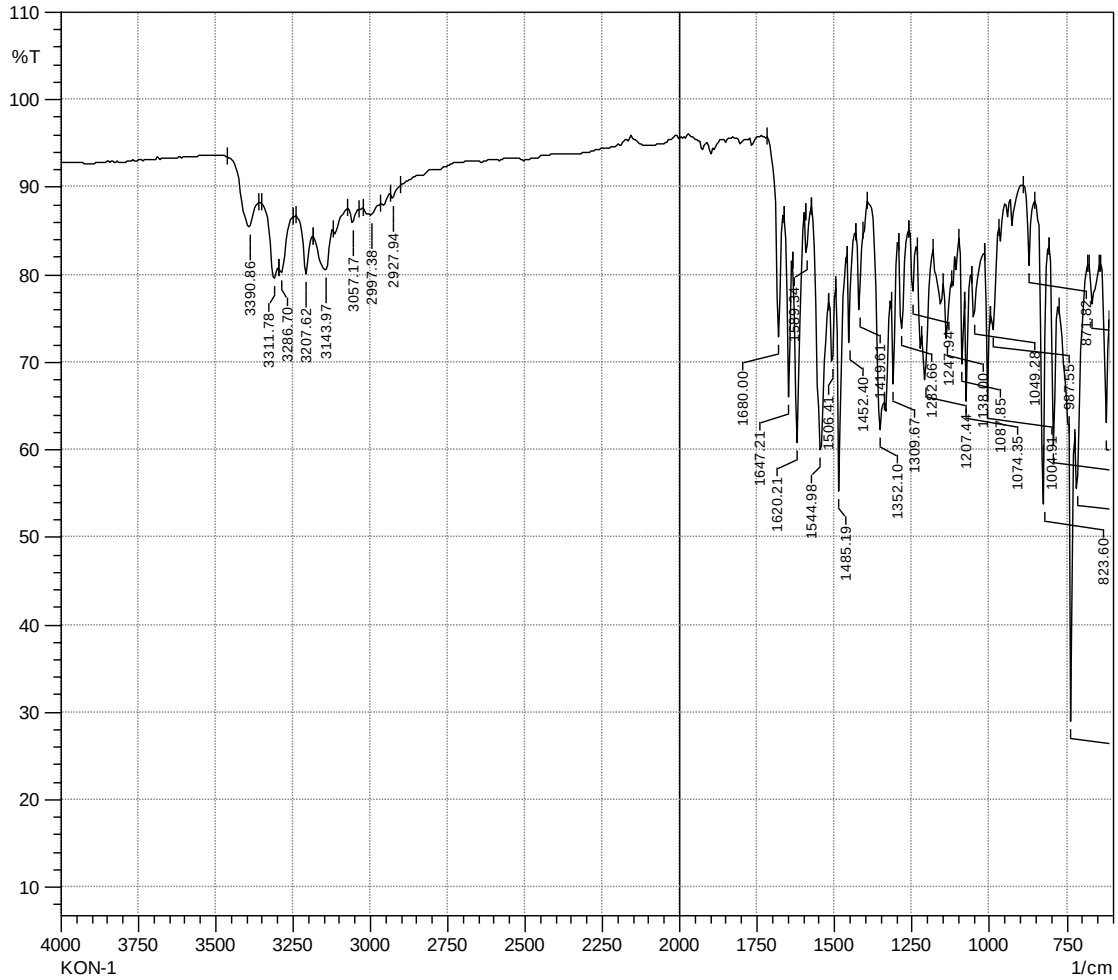


Figure S42. ^{1}H NMR spectrum of compound **4a**

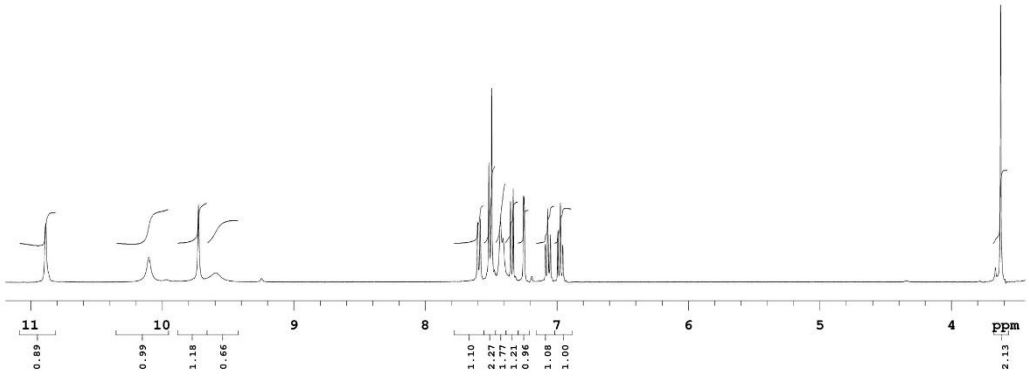


Figure S43. ^{13}C NMR spectrum of compound **4a**

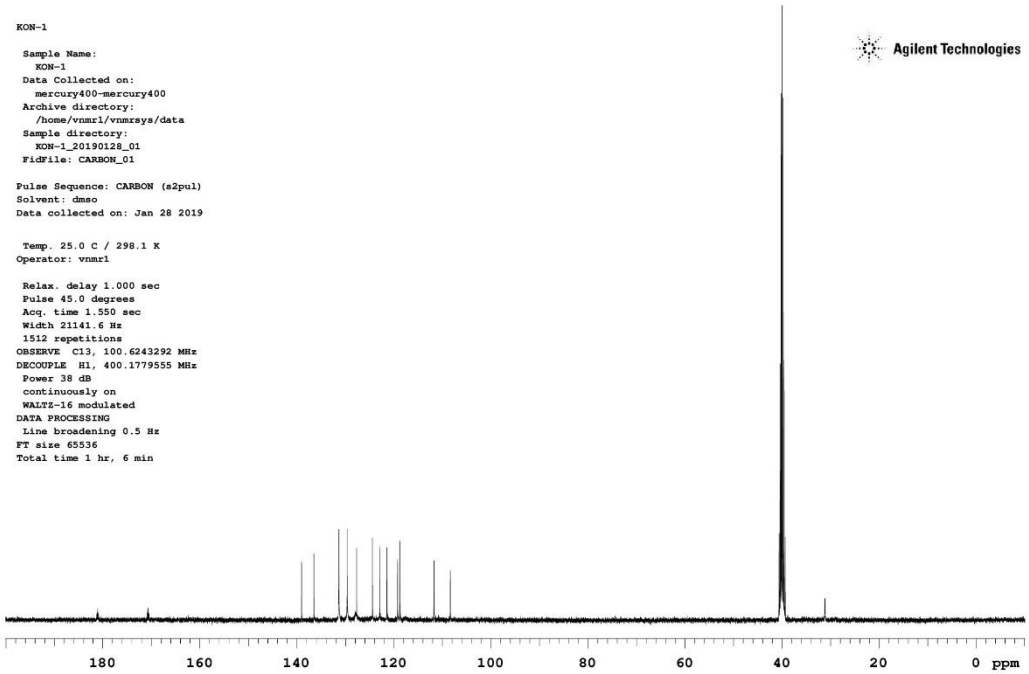


Figure S44. HRMS spectrum of compound **4a**

Formula Predictor Report - KON-1_17.lcd

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Data File: C:\LabSolutions\Data\Analiz\AOzdemir\KON-1_17.lcd

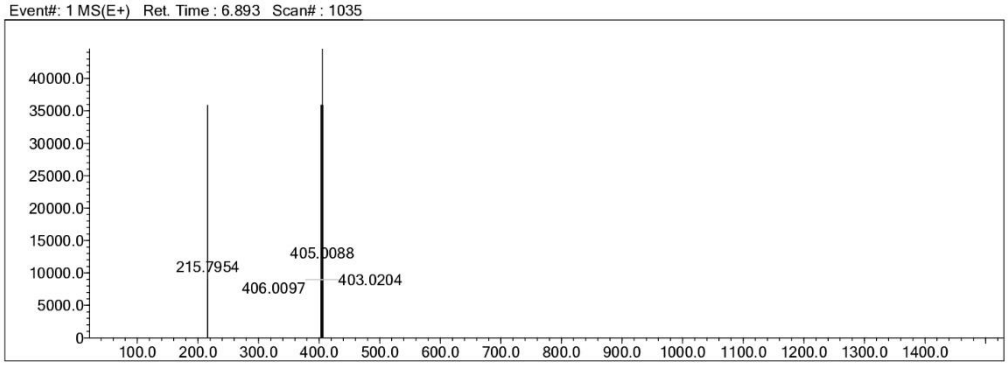
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	30	O	2	0	5	S	2	0	1	Ru	2	0	0	H
C	4	15	25	F	1	0	0	Cl	1	0	0	Pd	2	0	0	
N	3	1	5	P	3	0	0	Br	1	0	1	I	3	0	0	

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

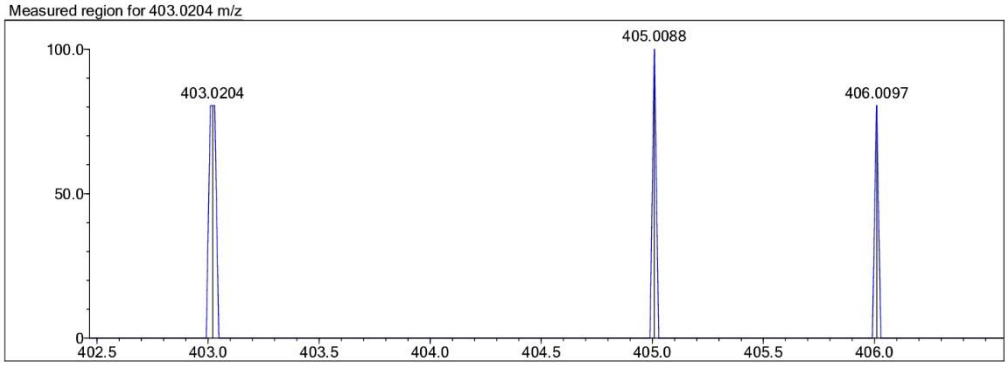
DBE Range: 5.0 - 15.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

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

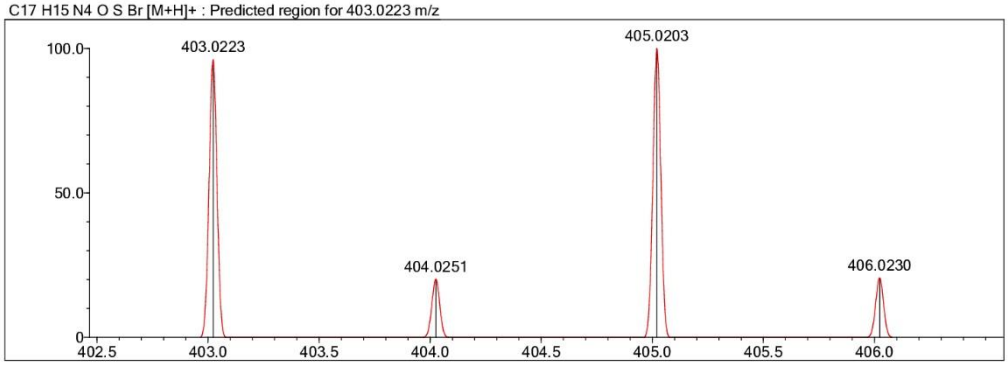
Event#: 1 MS(E+) Ret. Time : 6.893 Scan# : 1035



Measured region for 403.0204 m/z



C17 H15 N4 O S Br [M+H]+ : Predicted region for 403.0223 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	14.06	C17 H15 N4 O S Br	[M+H]+	403.0204	403.0223	-1.9	-4.71	15.50	12.0

Figure S45. IR spectrum of compound **4b**

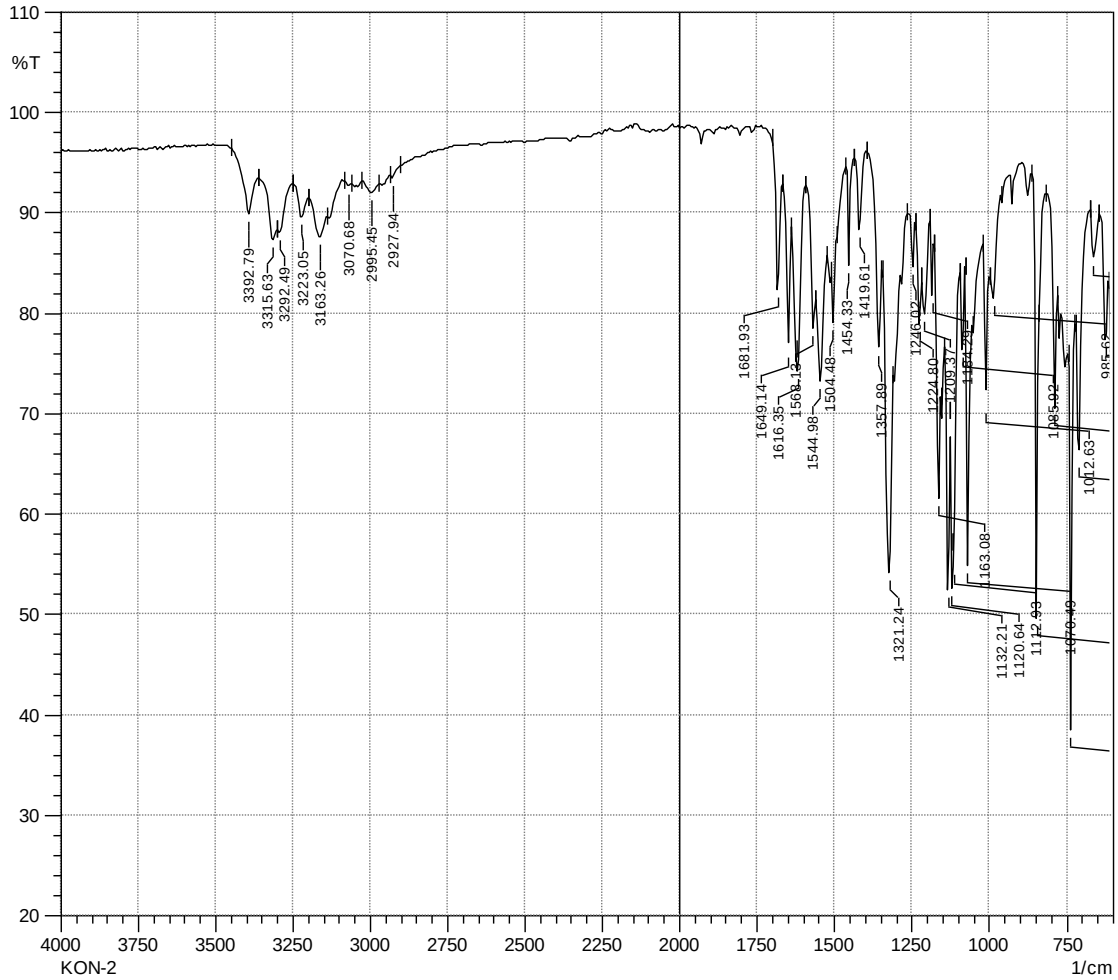


Figure S46. ^{1}H NMR spectrum of compound **4b**

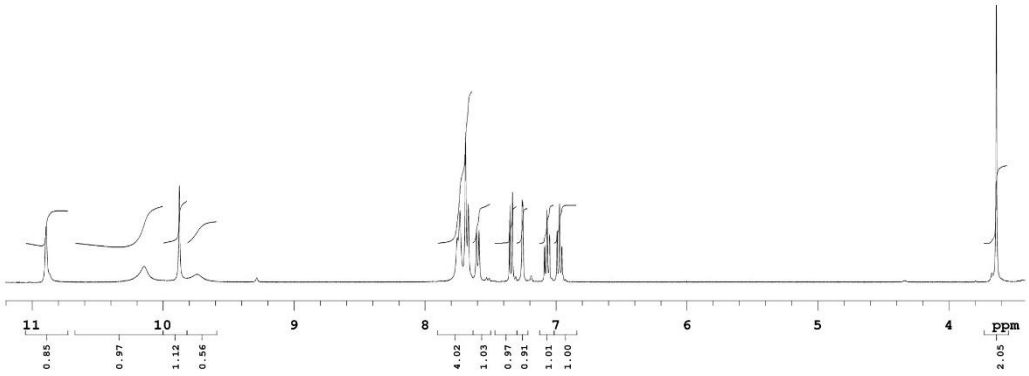


Figure S47. ^{13}C NMR spectrum of compound **4b**

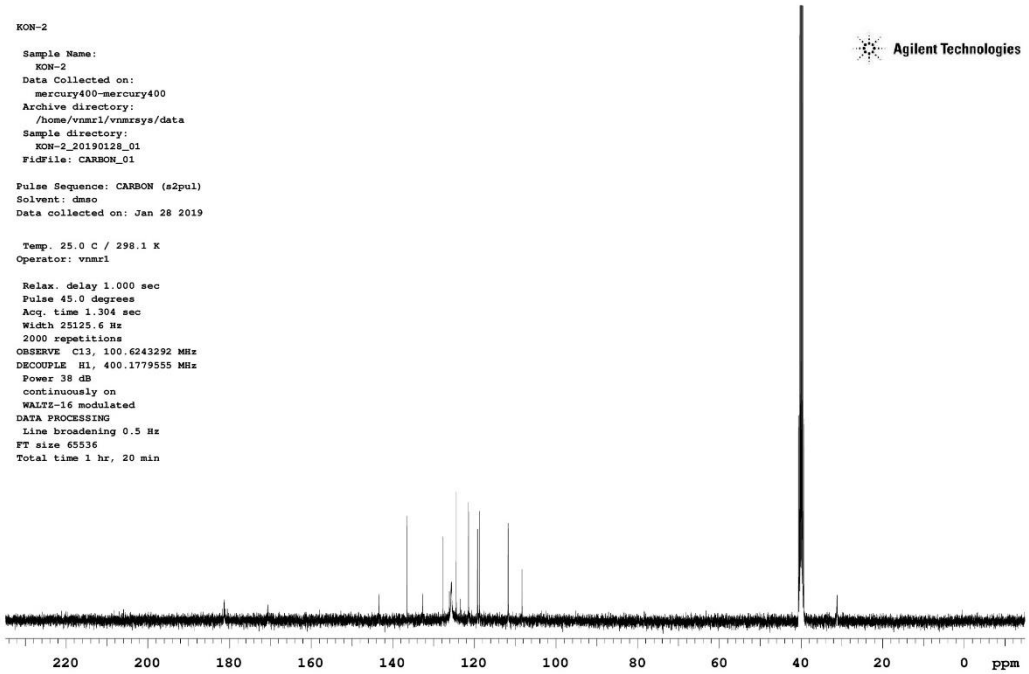


Figure S48. HRMS spectrum of compound **4b**

Formula Predictor Report - KON-2_18.lcd

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Data File: C:\LabSolutions\Data\Analiz\AOzdemir\KON-2_18.lcd

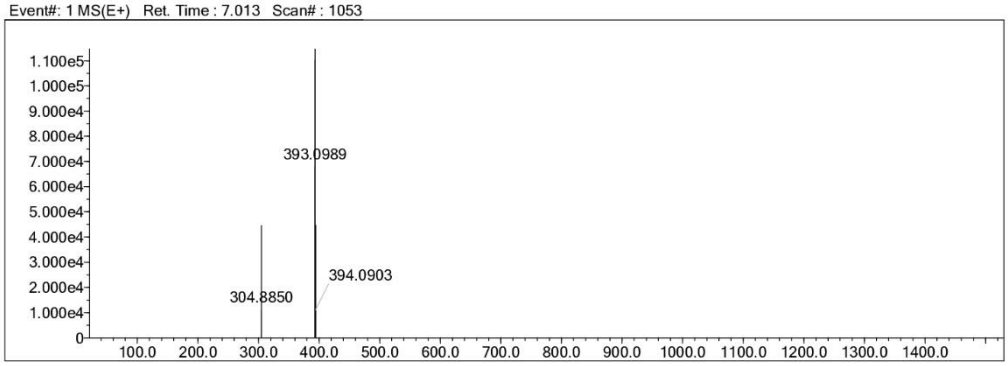
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	30	O	2	0	4	S	2	0	1	Ru	2	0	0	H
C	4	15	25	F	1	0	3	Cl	1	0	0	Pd	2	0	0	
N	3	1	5	P	3	0	0	Br	1	0	0	I	3	0	0	

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

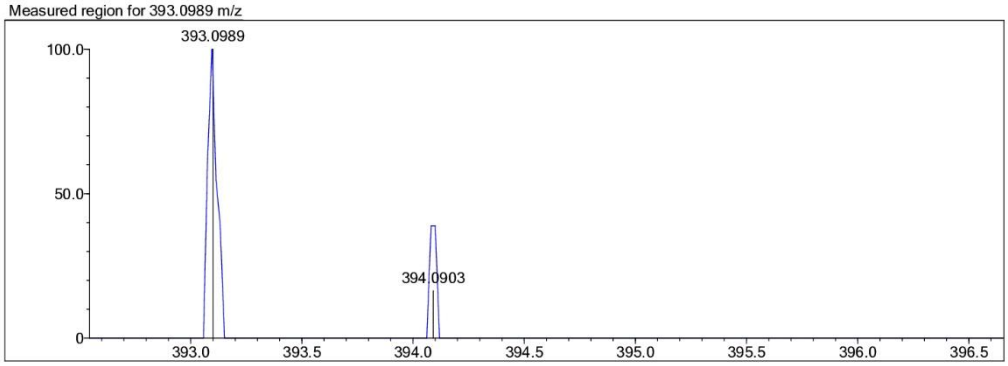
DBE Range: 5.0 - 15.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

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

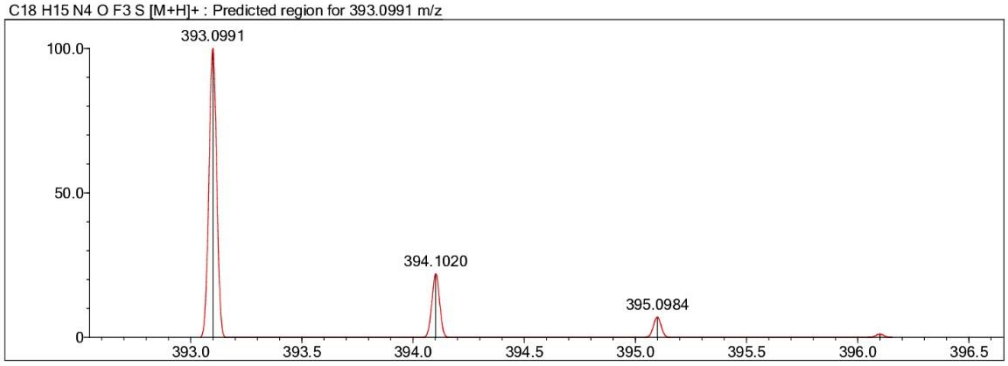
Event#: 1 MS(E+) Ret. Time : 7.013 Scan# : 1053



Measured region for 393.0989 m/z



C18 H15 N4 O F3 S [M+H]+ : Predicted region for 393.0991 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	0.00	C18 H15 N4 O F3 S	[M+H]+	393.0989	393.0991	-0.2	-0.51	0.00	12.0

Figure S49. IR spectrum of compound **4c**

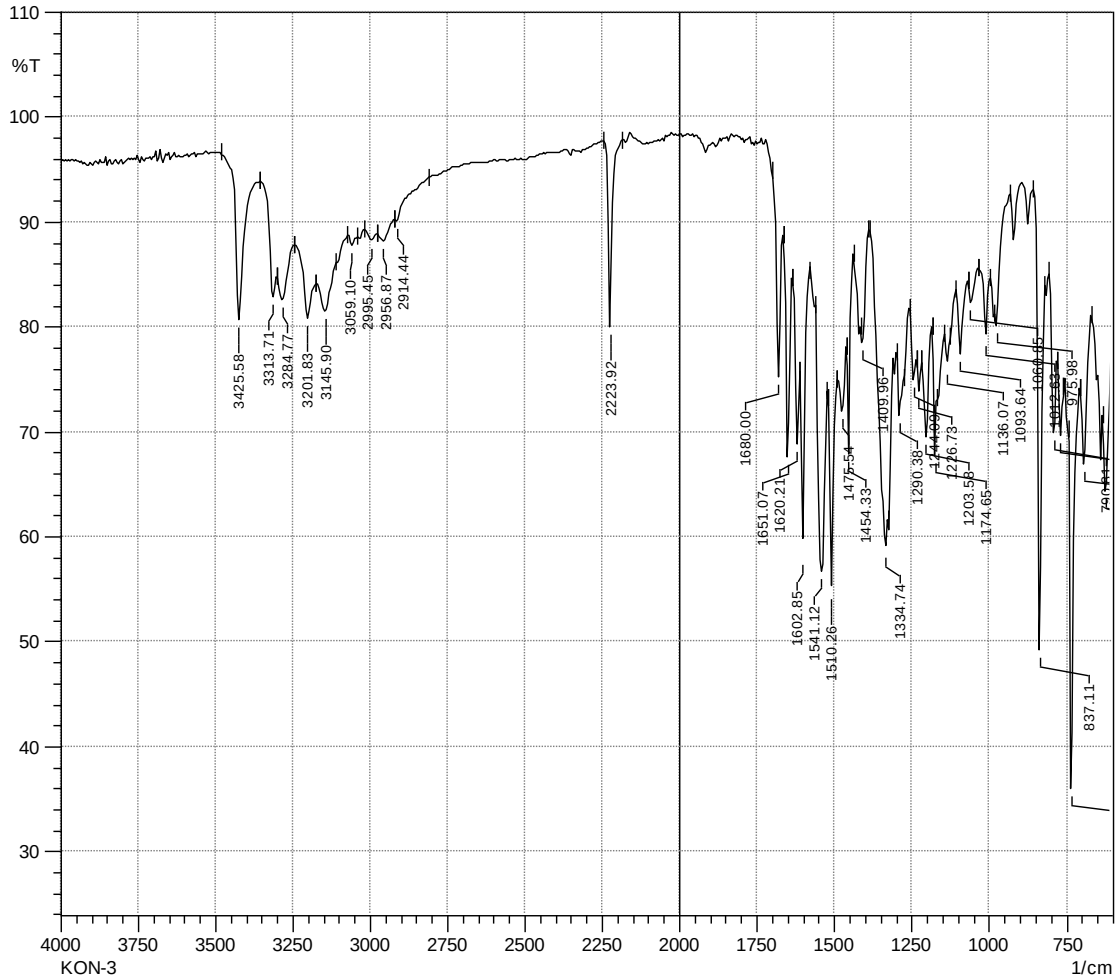


Figure S50. ^{1}H NMR spectrum of compound **4c**

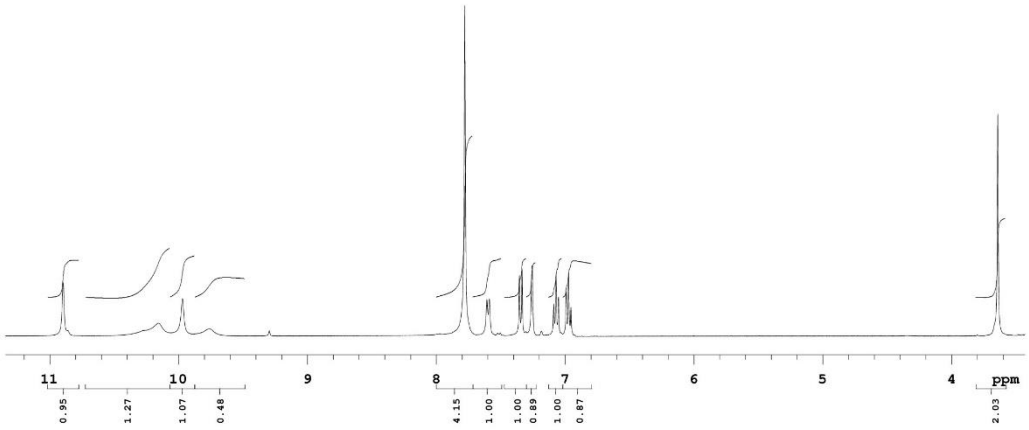


Figure S51. ^{13}C NMR spectrum of compound **4c**

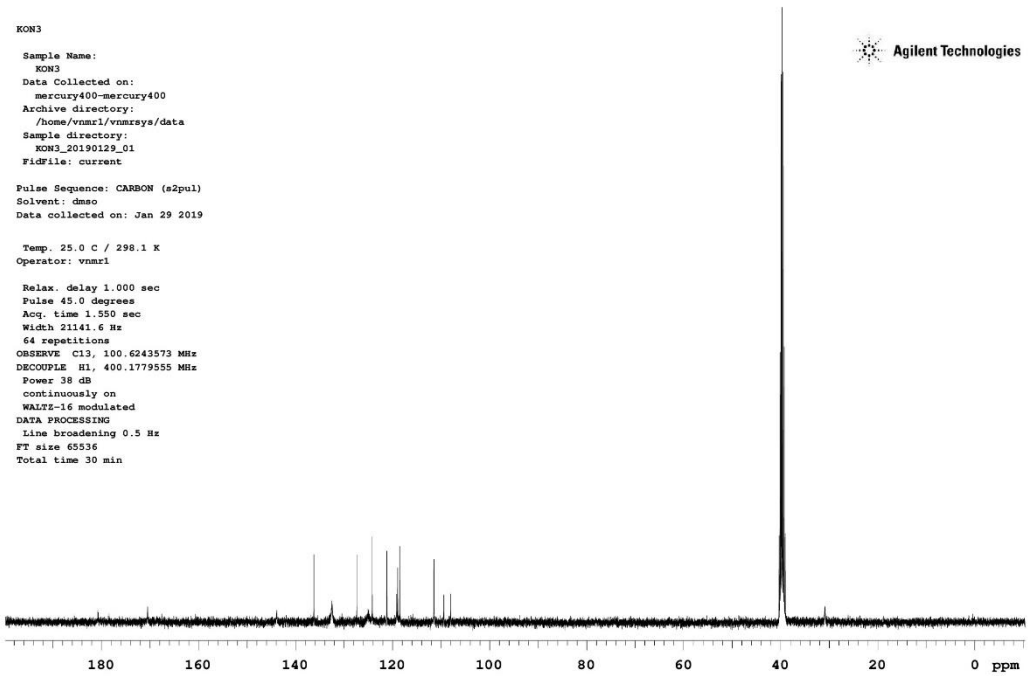


Figure S52. HRMS spectrum of compound **4c**

Formula Predictor Report - KON-3_19.lcd

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Data File: C:\LabSolutions\Data\Analiz\AOzdemir\KON-3_19.lcd

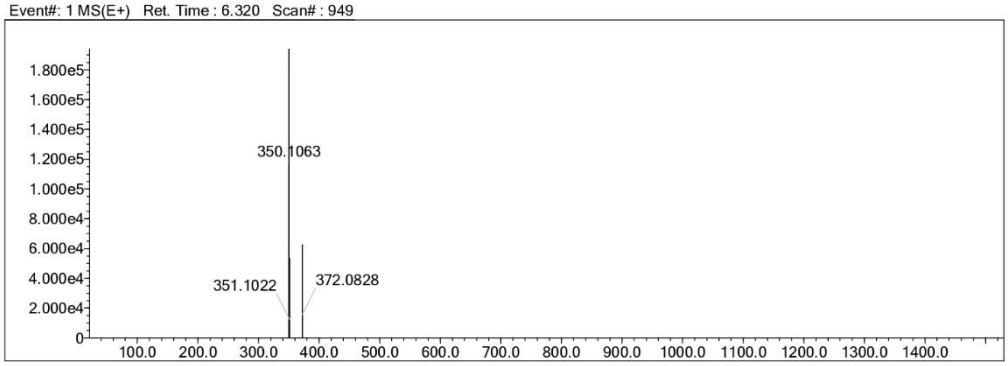
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	30	O	2	0	4	S	2	0	1	Ru	2	0	0	H
C	4	15	25	F	1	0	0	Cl	1	0	0	Pd	2	0	0	
N	3	1	5	P	3	0	0	Br	1	0	0	I	3	0	0	

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

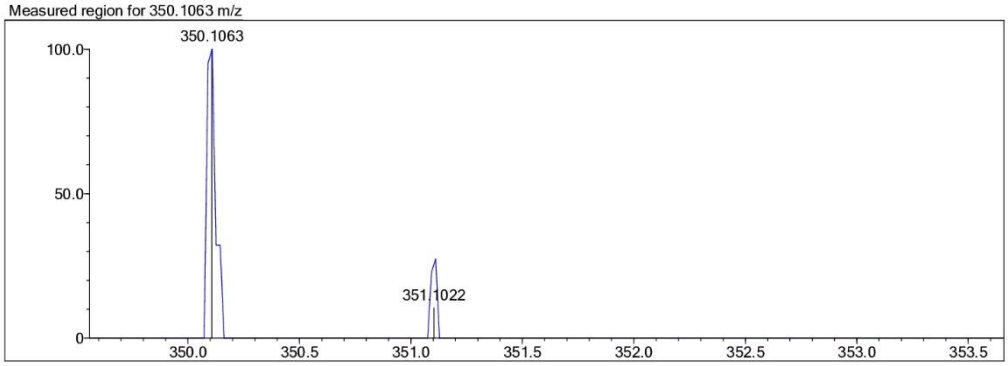
DBE Range: 5.0 - 15.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

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

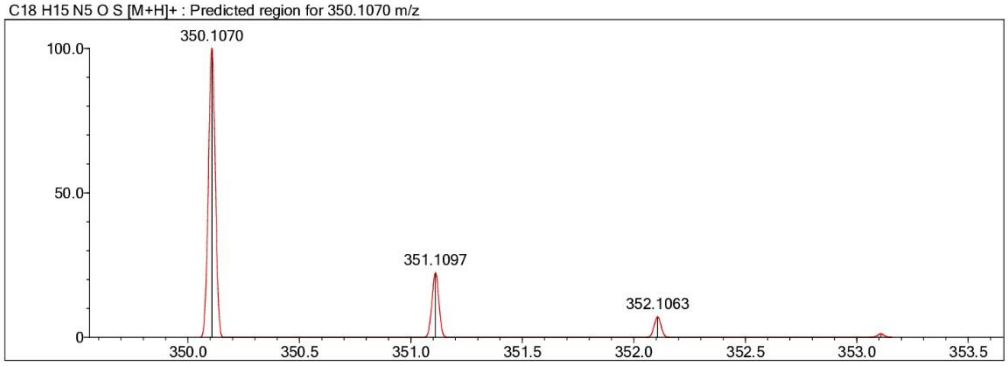
Event#: 1 MS(E+) Ret. Time : 6.320 Scan# : 949



Measured region for 350.1063 m/z



C18 H15 N5 O S [M+H]+ : Predicted region for 350.1070 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	0.00	C18 H15 N5 O S	[M+H]+	350.1063	350.1070	-0.7	-2.00	0.00	14.0

Figure S53. IR spectrum of compound **4d**

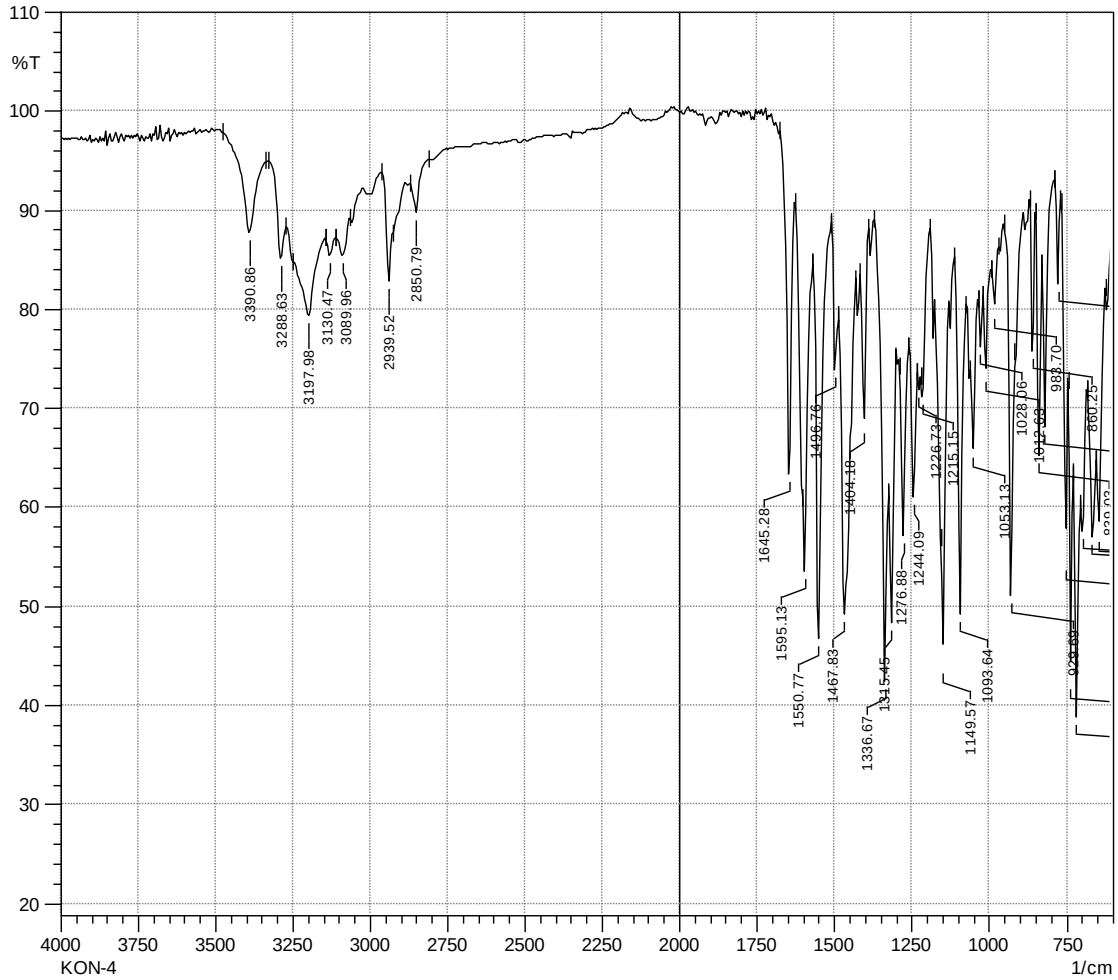


Figure S54. ^{1}H NMR spectrum of compound **4d**

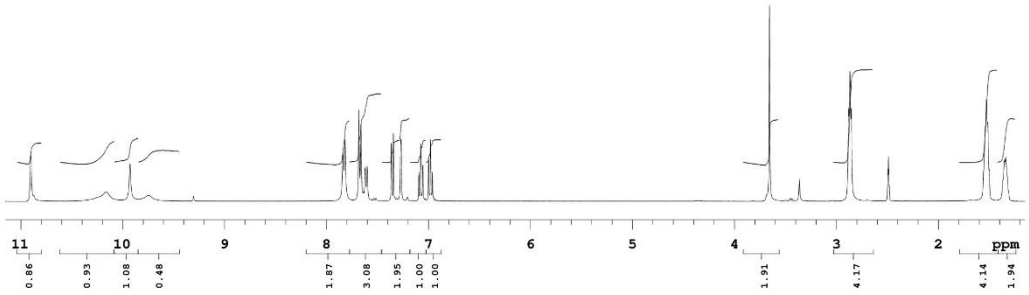


Figure S55. ^{13}C NMR spectrum of compound **4d**

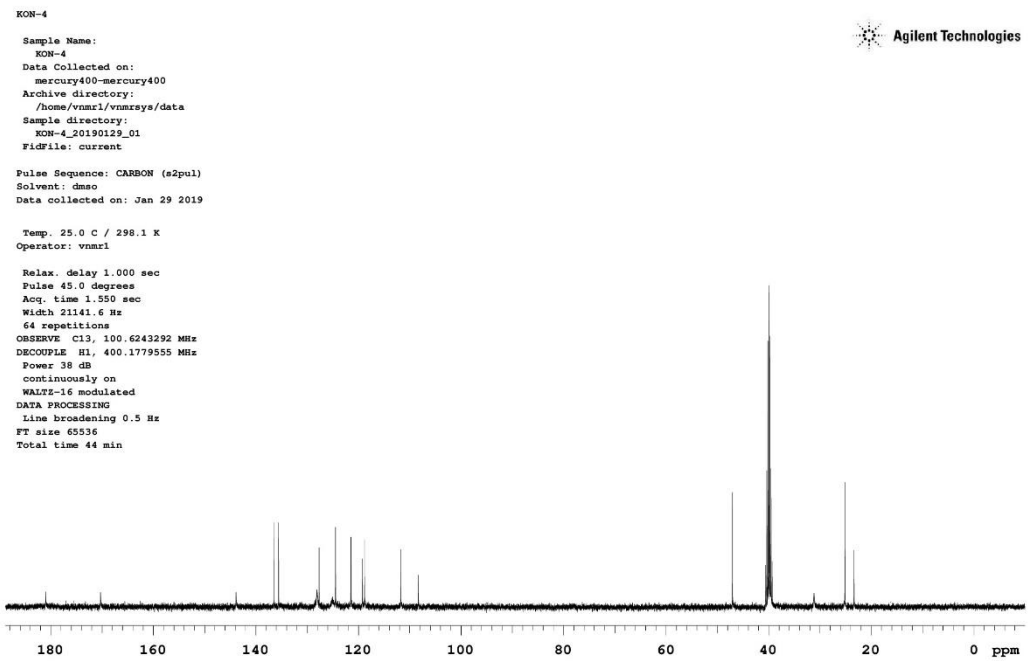


Figure S56. HRMS spectrum of compound **4d**

Formula Predictor Report - KON-4_20.lcd

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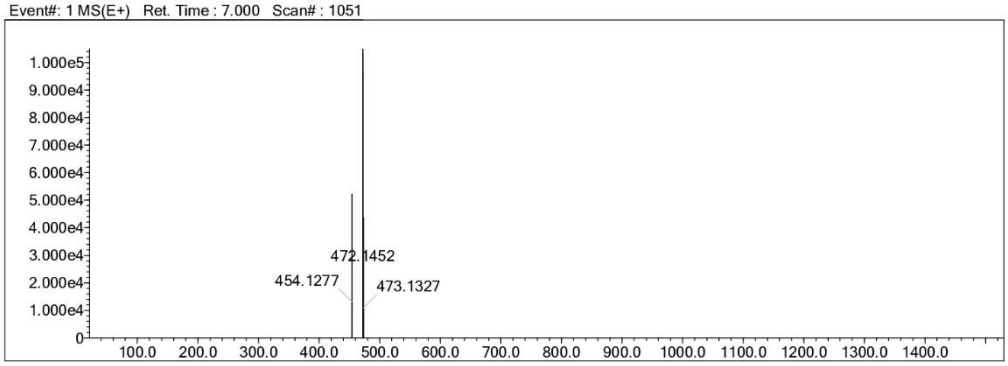
Data File: C:\LabSolutions\Data\Analiz\AOzdemir\KON-4_20.lcd

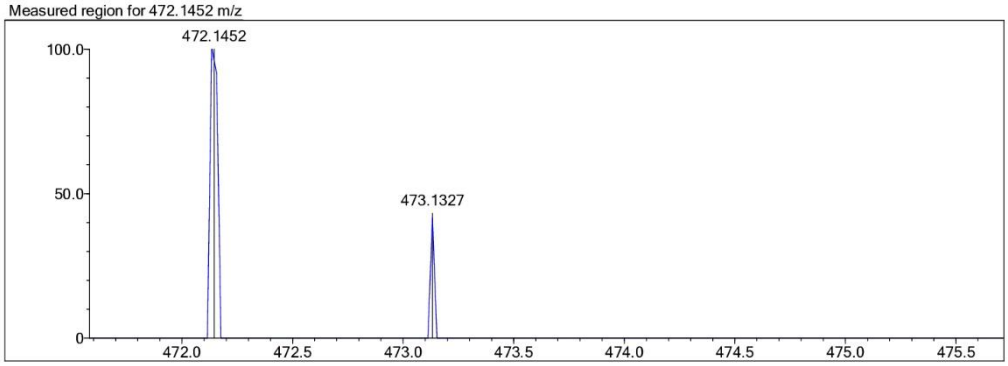
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	30	O	2	0	4	S	2	0	2	Ru	2	0	0	H
C	4	15	25	F	1	0	0	Cl	1	0	0	Pd	2	0	0	
N	3	1	5	P	3	0	0	Br	1	0	0	I	3	0	0	

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:	500

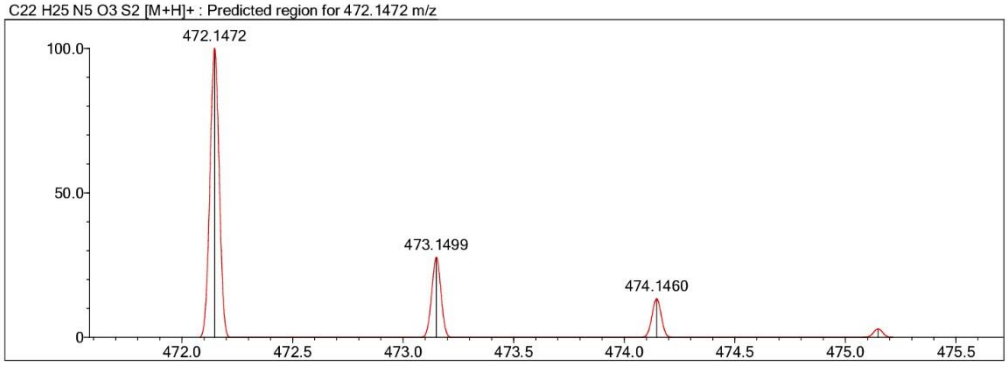
Event#: 1 MS(E+) Ret. Time : 7.000 Scan# : 1051



Measured region for 472.1452 m/z



C22 H25 N5 O3 S2 [M+H]+ : Predicted region for 472.1472 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	0.00	C22 H25 N5 O3 S2	[M+H]+	472.1452	472.1472	-2.0	-4.24	0.00	13.0

Figure S57. IR spectrum of compound **4e**

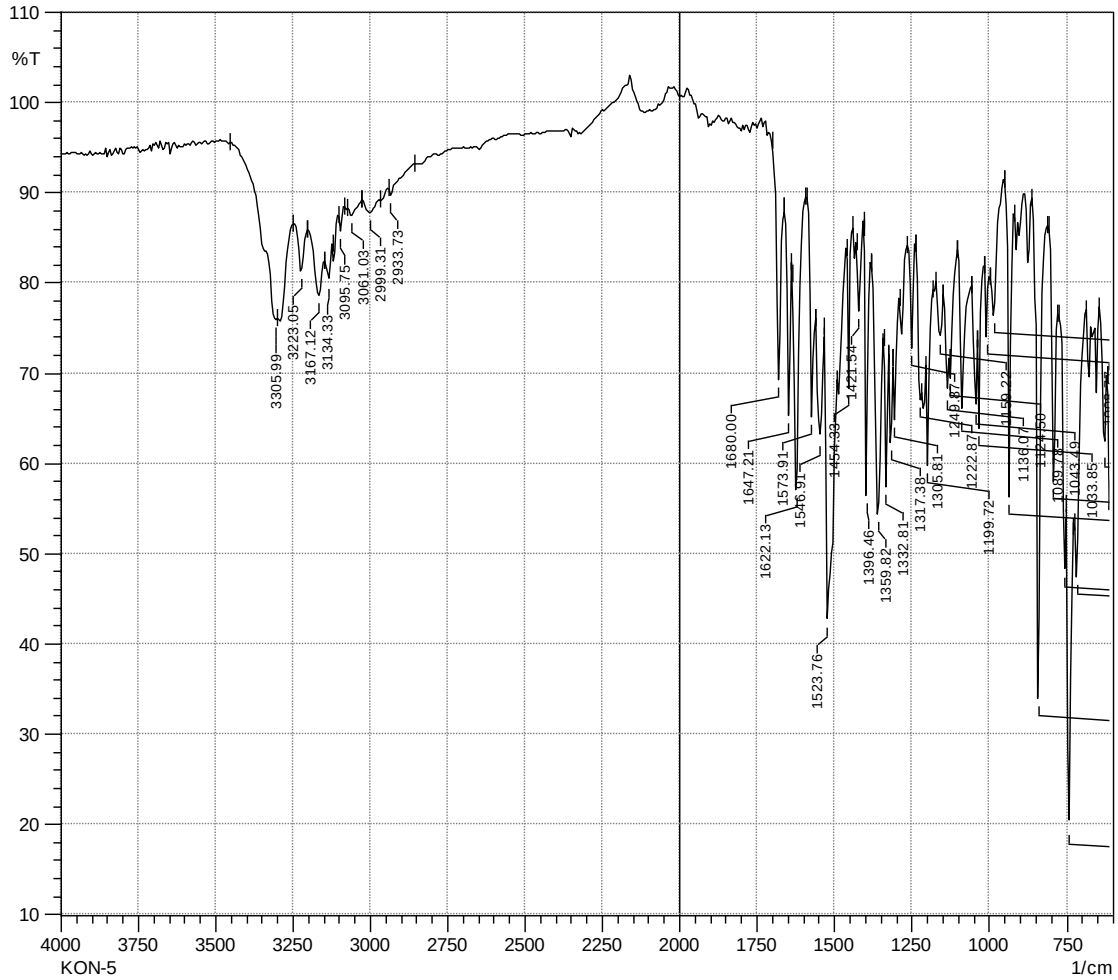


Figure S58. ^{1}H NMR spectrum of compound **4e**

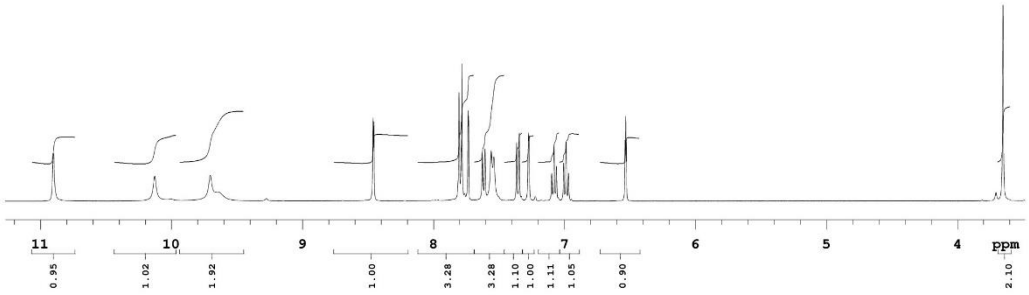


Figure S59. ^{13}C NMR spectrum of compound **4e**

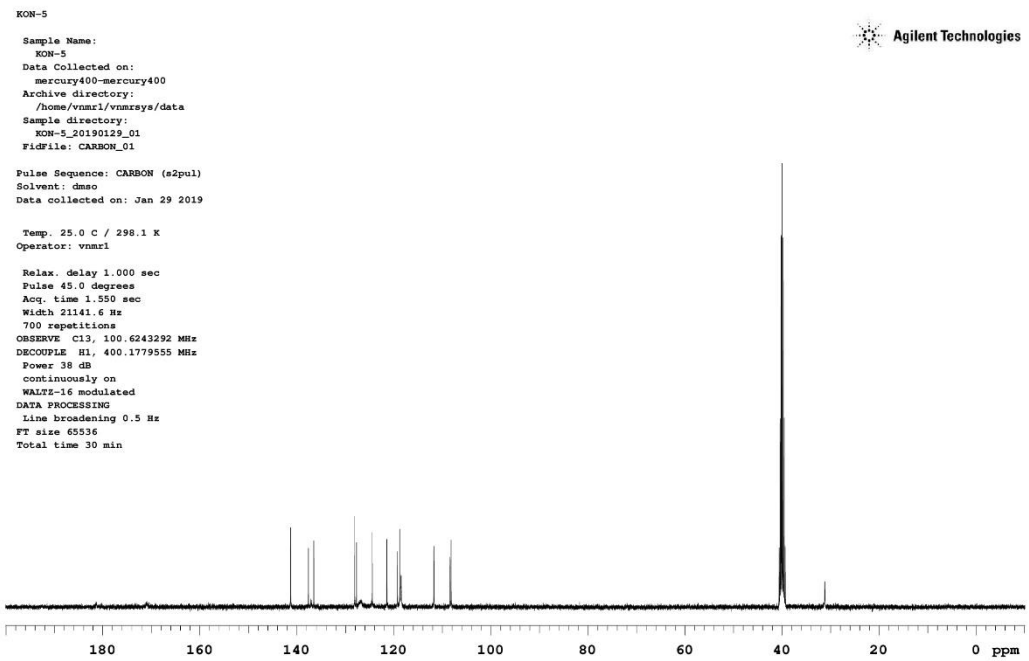


Figure S60. HRMS spectrum of compound **4e**

Formula Predictor Report - KON-5_2.lcd

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Data File: C:\LabSolutions\Data\Analiz\mdaltintop\KON-5_2.lcd

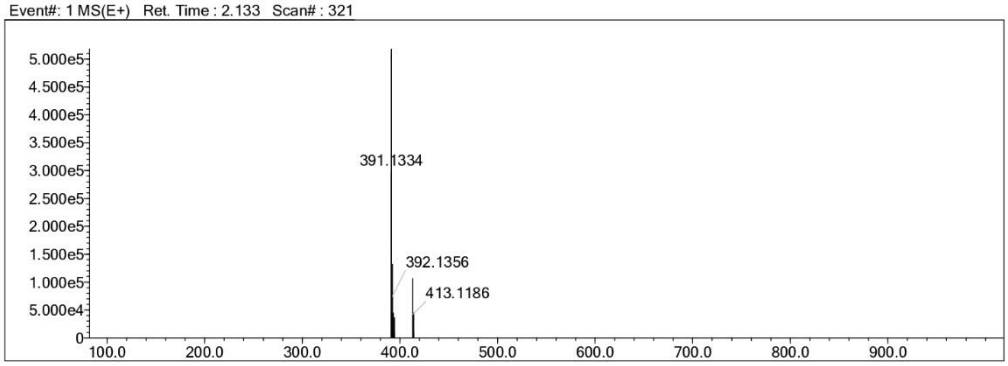
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	10	40	O	2	1	2	S	2	0	1	Ru	2	0	0	H
C	4	10	40	F	1	0	0	Cl	1	0	0	Pd	2	0	0	
N	3	2	6	P	3	0	0	Br	1	0	0	I	3	0	0	

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

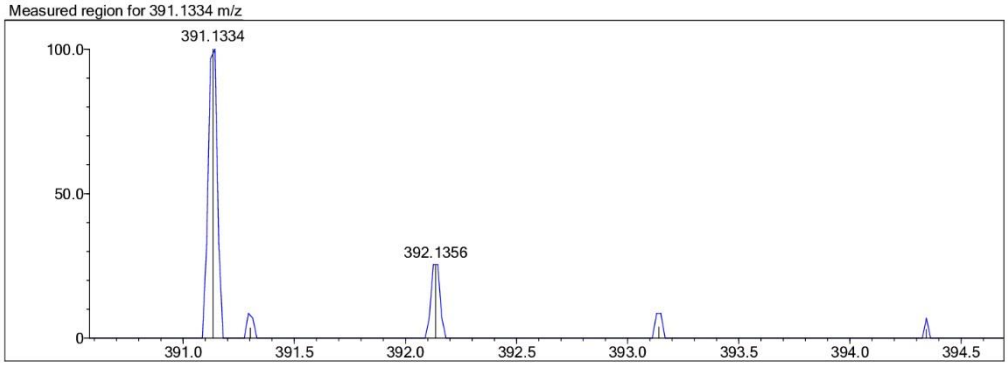
DBE Range: 5.0 - 25.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

Electron Ions: both
Use MSn Info: yes
Isotope Res: 9000
Max Results: 200

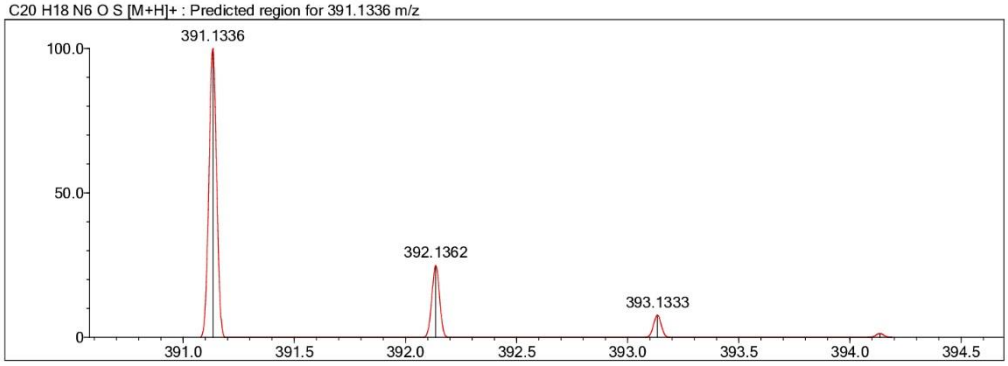
Event#: 1 MS(E+) Ret. Time : 2.133 Scan# : 321



Measured region for 391.1334 m/z



C20 H18 N6 O S [M+H]+ : Predicted region for 391.1336 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	88.29	C20 H18 N6 O S	[M+H]+	391.1334	391.1336	-0.2	-0.51	88.29	15.0

Figure S61. IR spectrum of compound **4f**

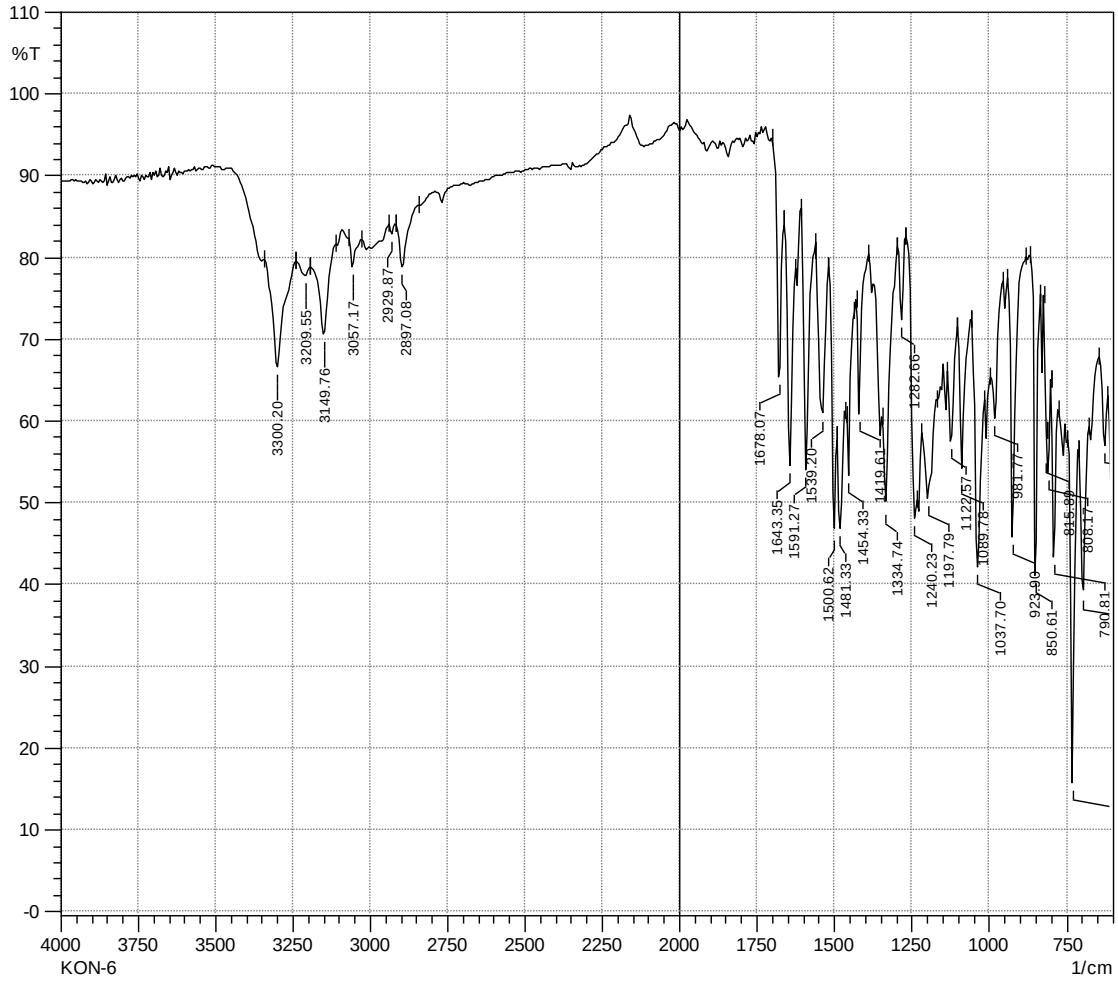


Figure S62. ^{1}H NMR spectrum of compound **4f**

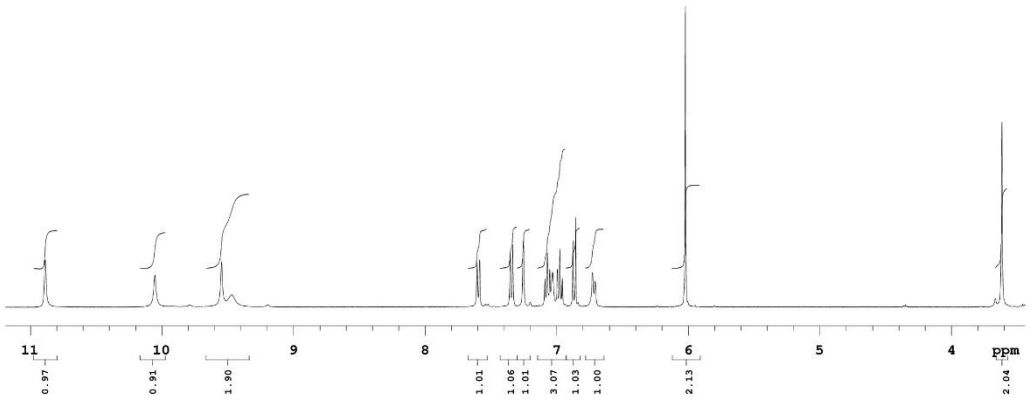


Figure S63. ^{13}C NMR spectrum of compound **4f**

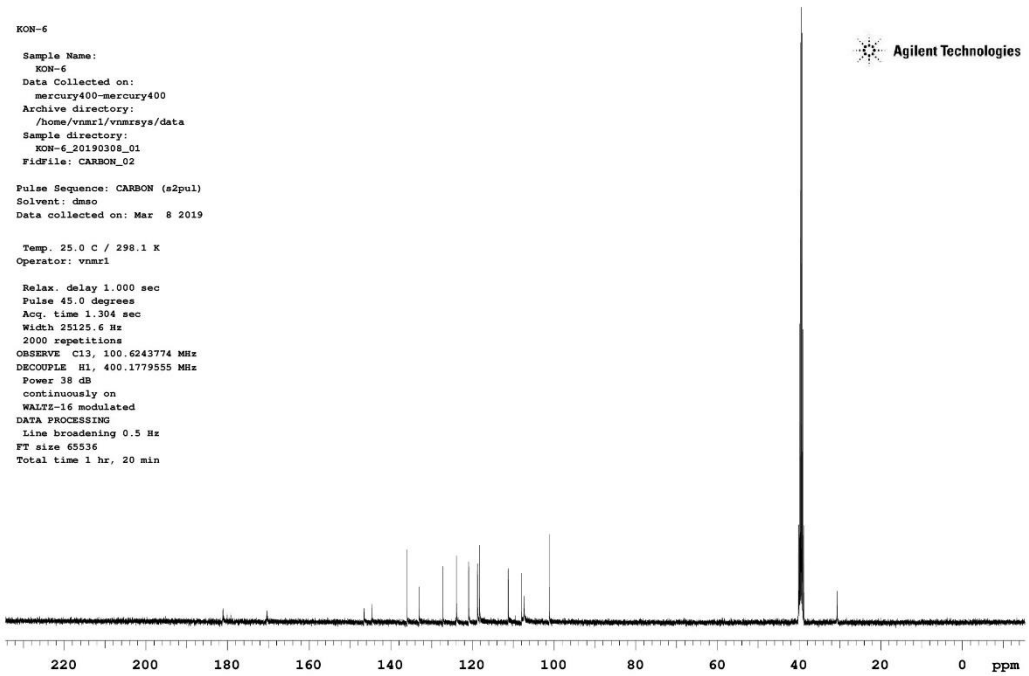


Figure S64. HRMS spectrum of compound **4f**

Formula Predictor Report - KON-6_58.lcd

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Data File: C:\LabSolutions\Data\Analiz\AOzdemir\KON-6_58.lcd

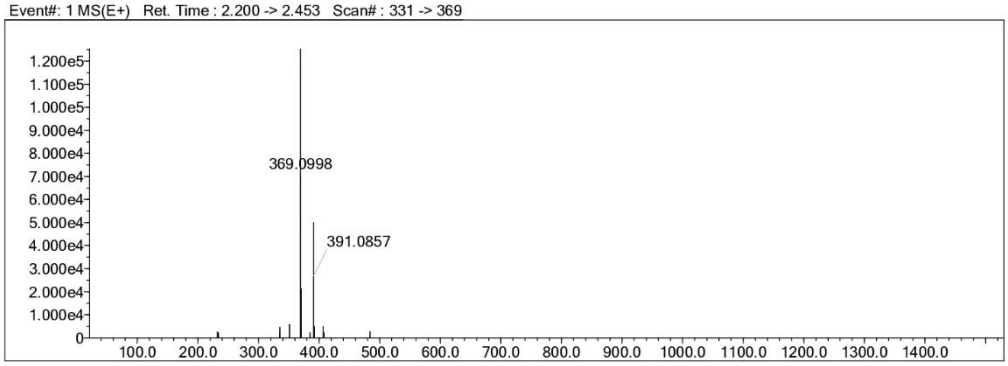
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	10	40	O	2	1	5	S	2	1	2	Ru	2	0	0	H
C	4	18	30	F	1	0	0	Cl	1	0	0	Pd	2	0	0	
N	3	4	7	P	3	0	0	Br	1	0	1	I	3	0	0	

Error Margin (ppm): 20
HC Ratio: unlimited
Max Isotopes: 3
MSn Iso RI (%): 10.00

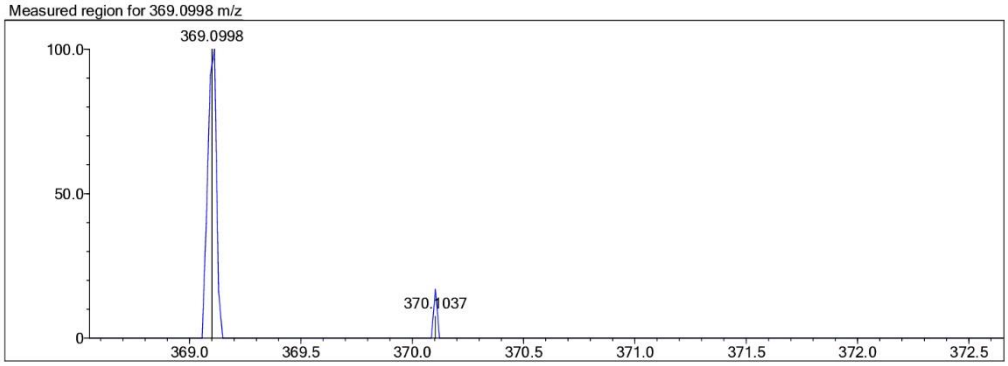
DBE Range: 10.0 - 21.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

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

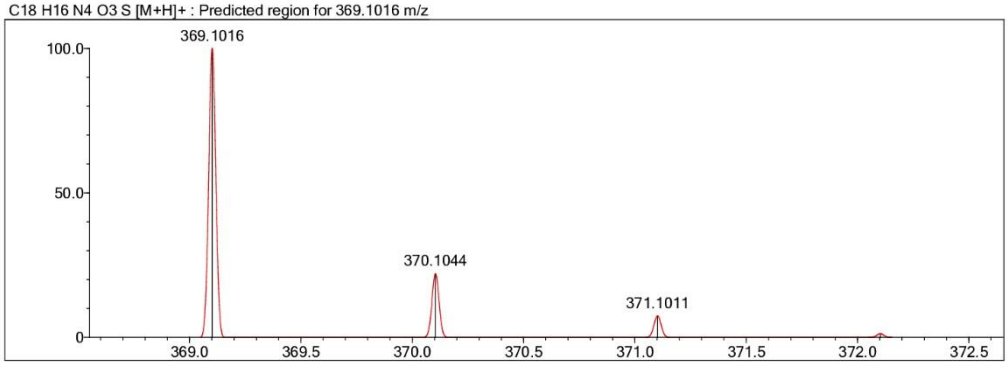
Event#: 1 MS(E+) Ret. Time : 2.200 -> 2.453 Scan# : 331 -> 369



Measured region for 369.0998 m/z



C18 H16 N4 O3 S [M+H]+ : Predicted region for 369.1016 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	0.00	C18 H16 N4 O3 S	[M+H]+	369.0998	369.1016	-1.8	-4.88	0.00	13.0

Figure S65. IR spectrum of compound **4g**

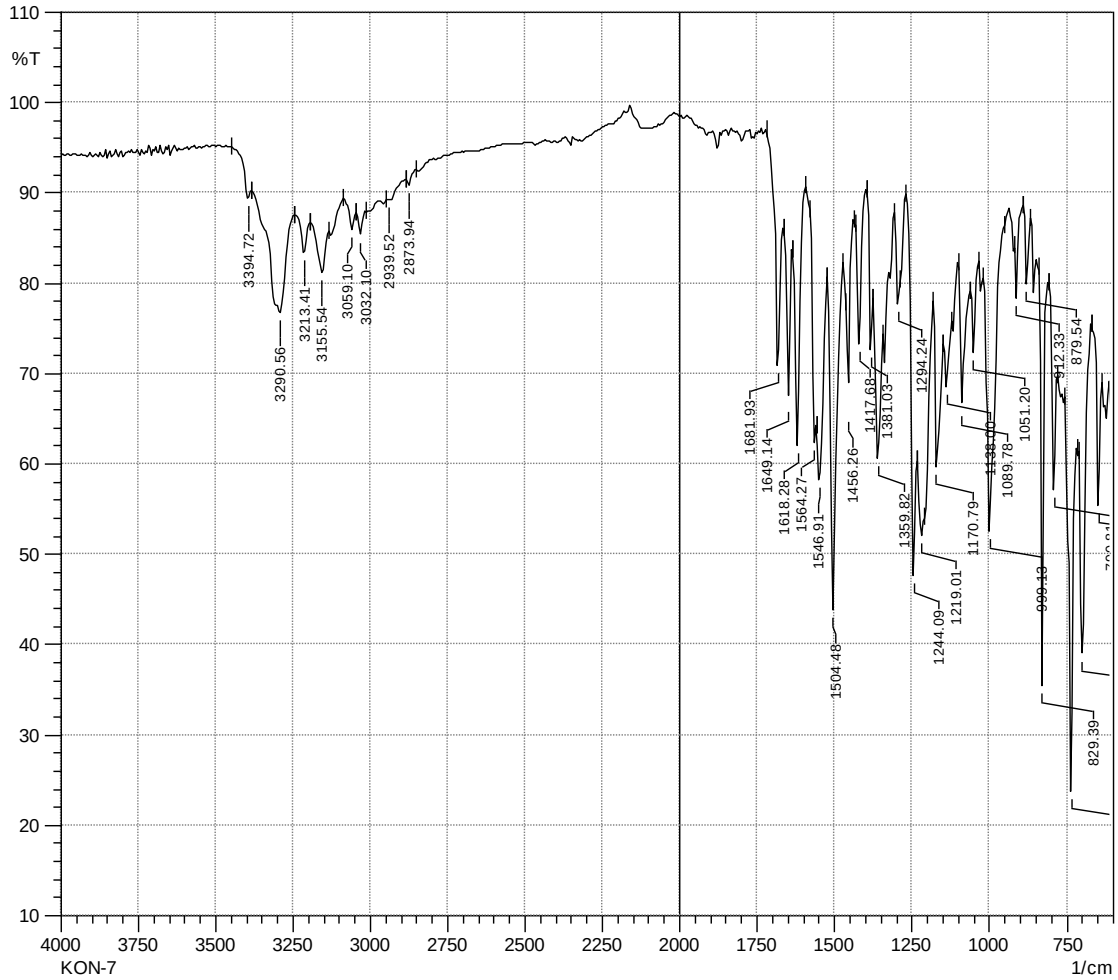


Figure S66. ^{1}H NMR spectrum of compound **4g**

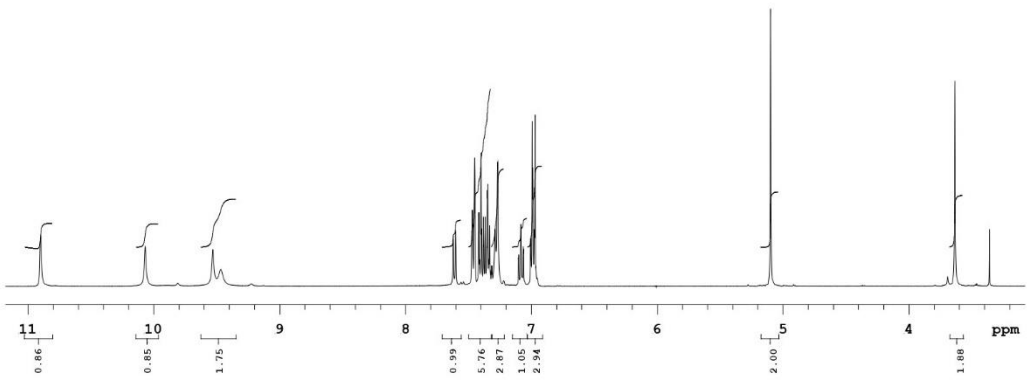


Figure S67. ^{13}C NMR spectrum of compound **4g**

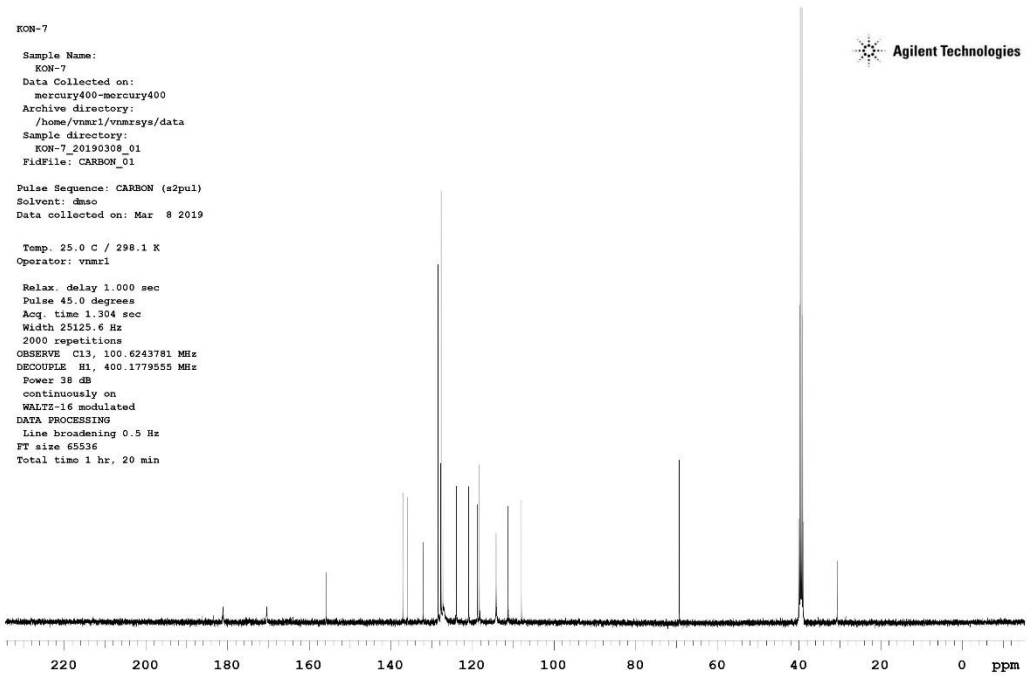


Figure S68. HRMS spectrum of compound **4g**

Formula Predictor Report - KON-7_59.lcd

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Data File: C:\LabSolutions\Data\Analiz\AOzdemir\KON-7_59.lcd

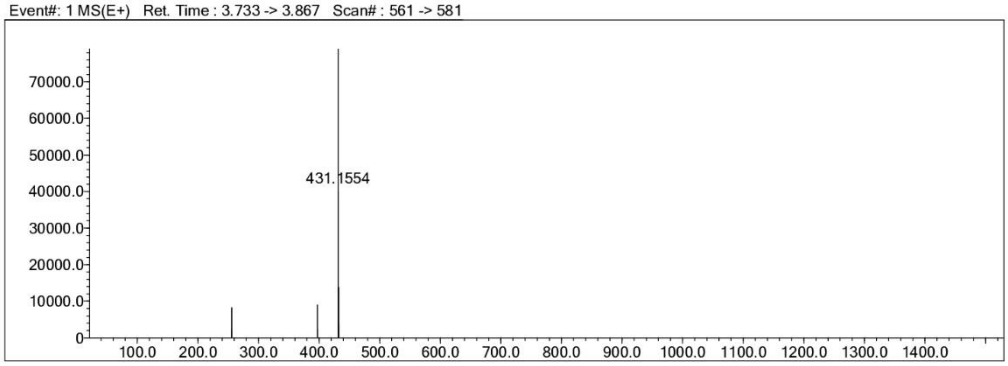
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	10	40	O	2	1	5	S	2	1	2	Ru	2	0	0	H
C	4	18	30	F	1	0	0	Cl	1	0	0	Pd	2	0	0	
N	3	4	7	P	3	0	0	Br	1	0	1	I	3	0	0	

Error Margin (ppm): 20
HC Ratio: unlimited
Max Isotopes: 3
MSn Iso RI (%): 10.00

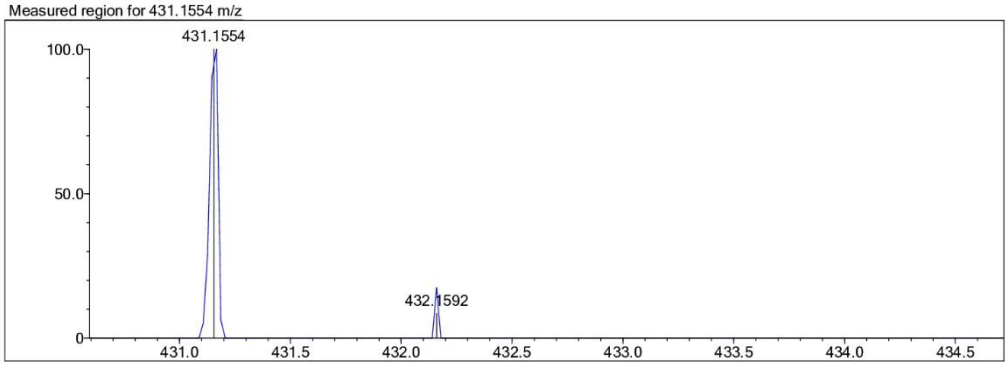
DBE Range: 13.0 - 21.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

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

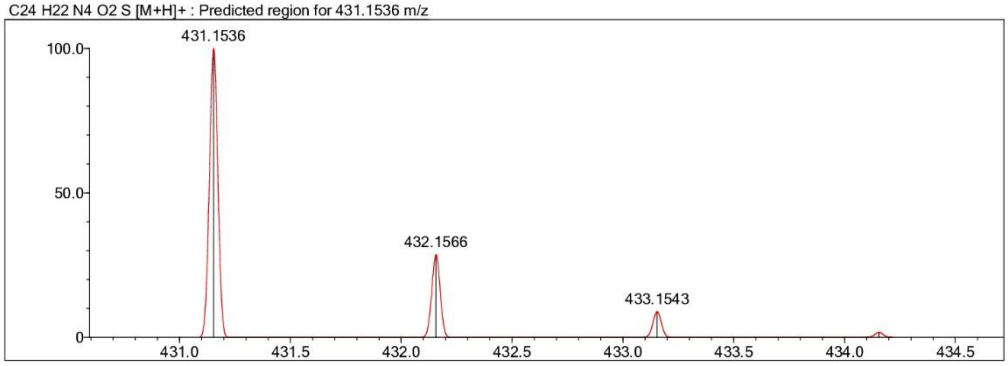
Event#: 1 MS(E+) Ret. Time : 3.733 -> 3.867 Scan# : 561 -> 581



Measured region for 431.1554 m/z



C24 H22 N4 O2 S [M+H]+ : Predicted region for 431.1536 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	0.00	C24 H22 N4 O2 S	[M+H]+	431.1554	431.1536	1.8	4.17	0.00	16.0