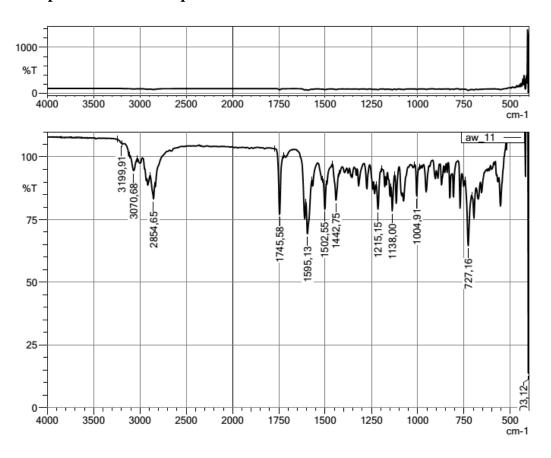
# **Supplementary document**

OHN N 
$$R_2$$
  $R_3$   $R_4$   $R_4$ 

Compounds	$\mathbf{R}_1$	R <sub>2</sub>	R <sub>3</sub>	R <sub>4</sub>
4a	Cyclohexyl	Н	Н	Н
<b>4b</b>	Cyclohexyl	Н	Н	$OCH_3$
<b>4c</b>	Phenyl	Н	Н	Н
<b>4d</b>	Phenyl	Н	Н	$CH_3$
<b>4e</b>	Phenyl	Н	Н	$OCH_3$
4f	Phenyl	Н	Н	Br
<b>4</b> g	Phenyl	Н	Н	Cl
4h	Phenyl	Н	Н	F
4i	Phenyl	Н	$NO_2$	Н
<b>4</b> j	Phenyl	Н	Н	$NO_2$
4k	Phenyl	Cl	Cl	Н

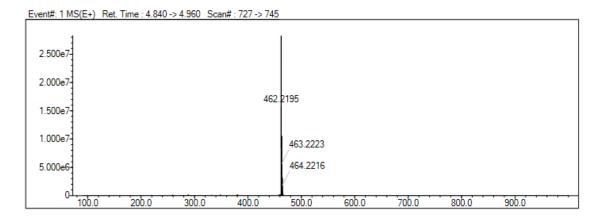
## -IR spectrum of the compound 4a



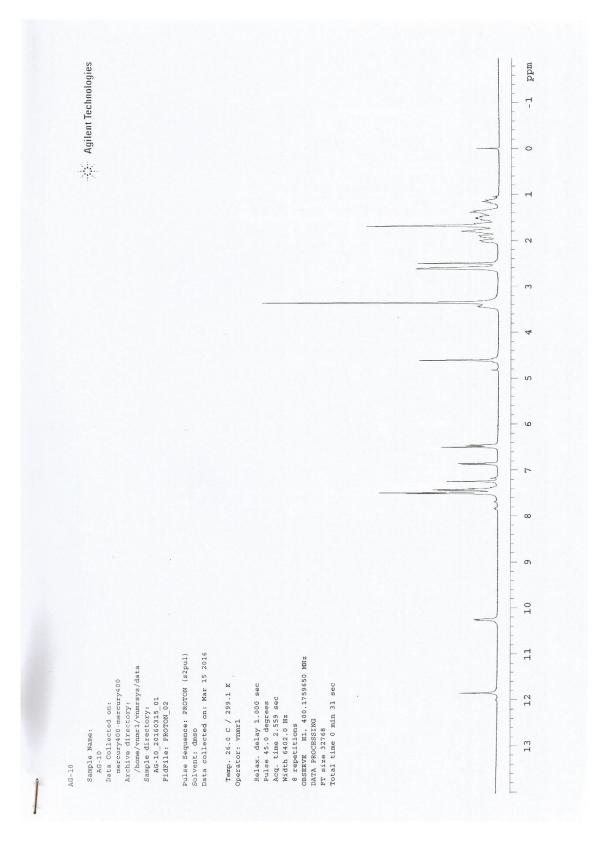
#### - HRMS spectrum of the compound4a

Data File: C:\LabSolutions\Data\Analiz\Lyuttas\A\W-1\_1.lcd

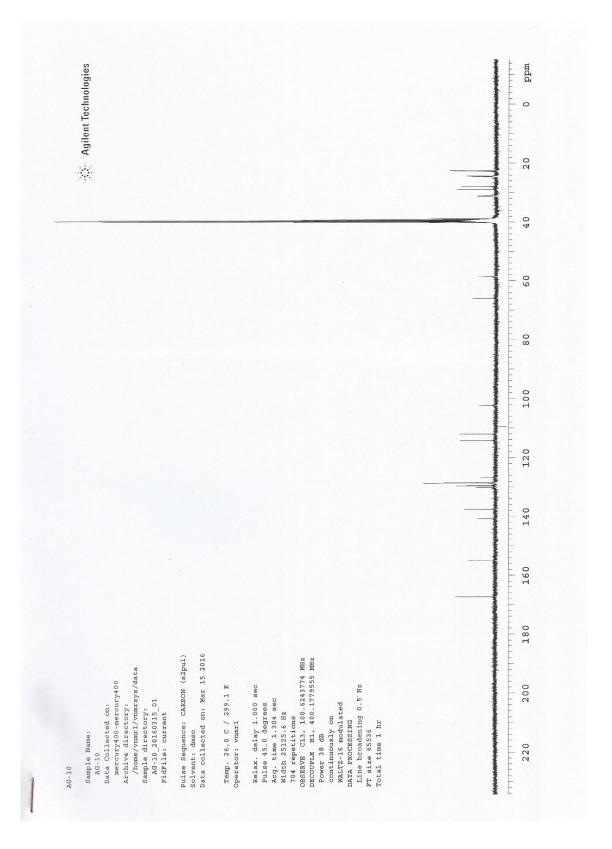
Elmt Val. Min Max Elmt	Val. Min Max	Elmt Val.	Min Max	Elmt Val.	Min Max	Use Adduct
H 1 20 35 O	2 2 4	CI 1	0 1	I 3	0 0	Н
C 4 25 30 F	1 0 1	Br   1	0 1			
N 3 3 4 S	2 1 1	Ru 2	0 0			
Error Margin (ppm): 5	DBE Rang	ge: not fixed		Electron lons:	both	
HC Ratio: unlimited	Apply N Ru	ıle: yes		Use MSn Info:	no	
Max Isotopes: 3	Isotope RI (%	%): 1.00		Isotope Res:	10000	
MSn Iso RI (%): 10.00	MSn Logic Mod			Max Results:	500	



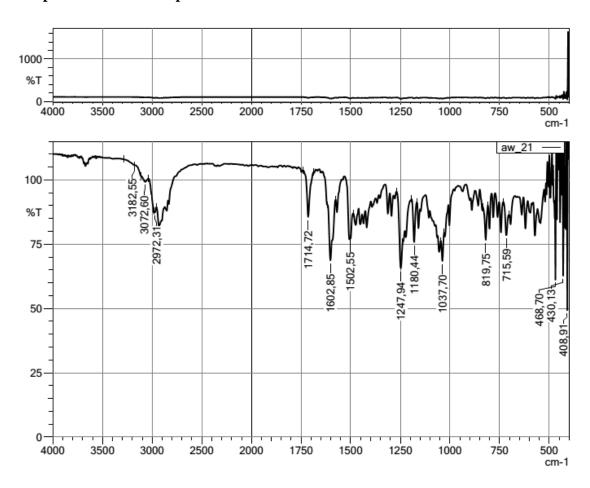
## -¹H NMR spectrum of the compound 4a



## -13C NMR spectrum of the compound 4a



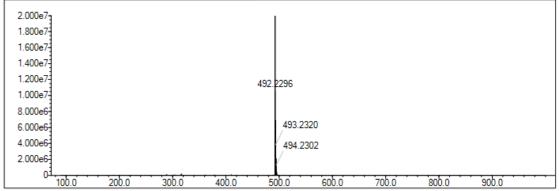
## -IR spectrum of the compound 4b



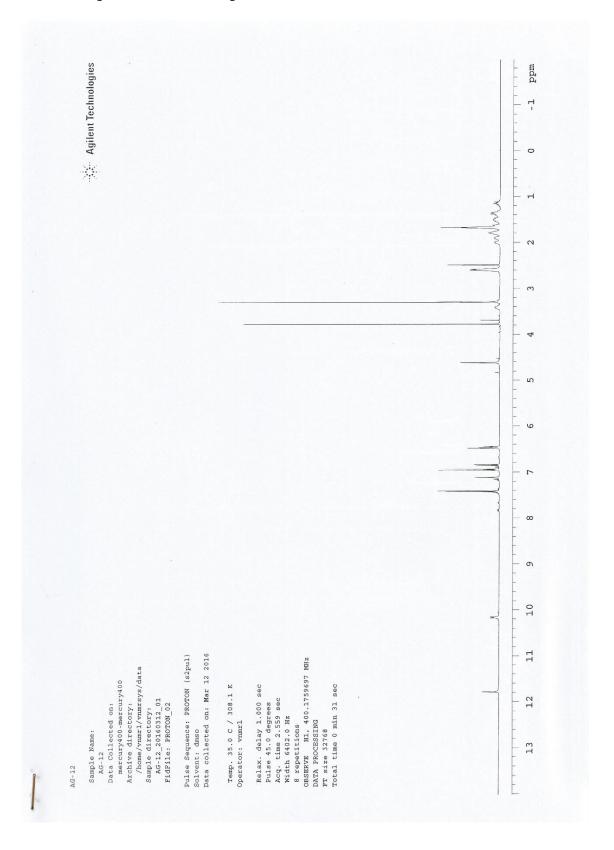
#### -HRMS spectrum of the compound 4b

Data File: C:\LabSolutions\Data\Analiz\Lyuttas\AW-2\_2.lcd

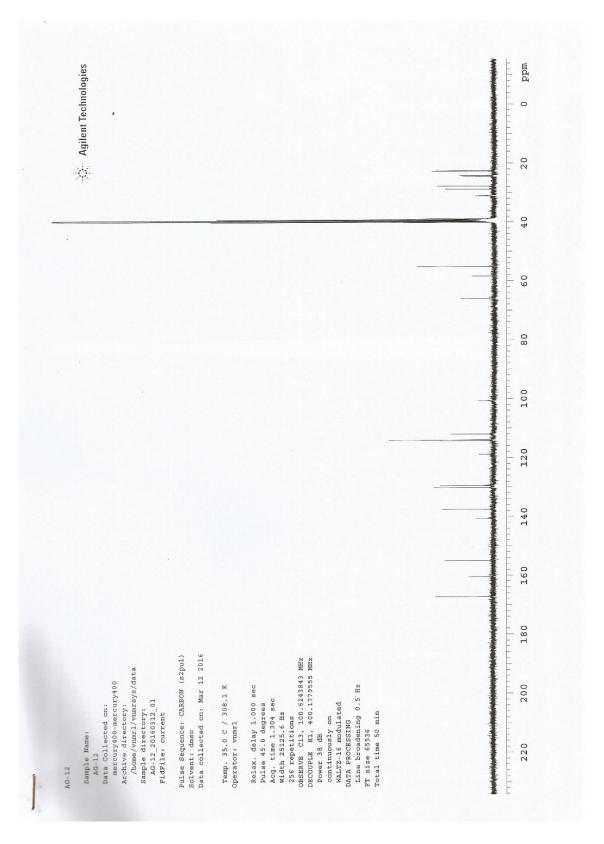
	-			
Elmt Val. Min Max Elmt	Val. Min Max	Elmt Val. Min Max	c Elmt Val. Min Max	Use Adduct
H 1 20 35 O C 4 25 30 F	2 2 4	CI 1 0 1	1 3 0 0	H
C 4 25 30 F	1 0 1	Br   1   0   1	1	
N 3 3 4 S	2 1 1	Ru 2 0 0	)	
Error Margin (ppm): 5	DBE Rar	nge: not fixed	Electron lons: both	
HC Ratio: unlimited	Apply N R		Use MSn Info: no	
Max Isotopes: 3	Isotope RI		Isotope Res: 10000	
MSn Iso RI (%): 10.00	MSn Logic Mo		Max Results: 500	
14011100111 (10). 10.00	Mon Logic M	ode. Para	Max Modalis. God	
Event#: 1 MS(E+) Ret. Time : 4.933	-> 5 107   Soap# - 74	11 -> 767		
Evenia. 1 Mo(E+) Net. Time . 4.333	-20.107 3CdH# . 74	+1-> /0/		
2 000 7				
2.000e7 <sub>3</sub>		1		



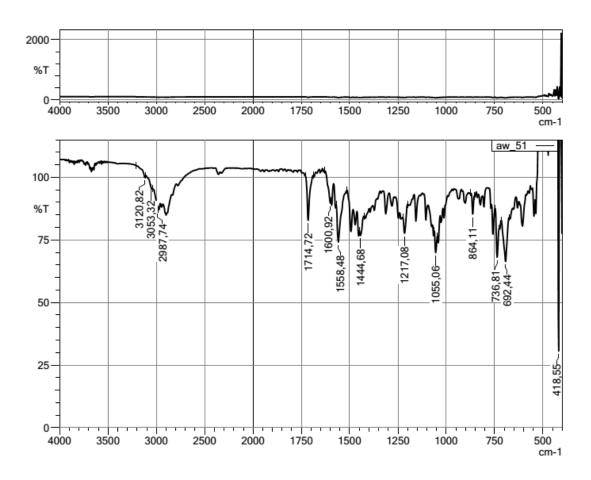
## -¹H NMR spectrum of the compound 4b



## -13C NMR spectrum of the compound 4b



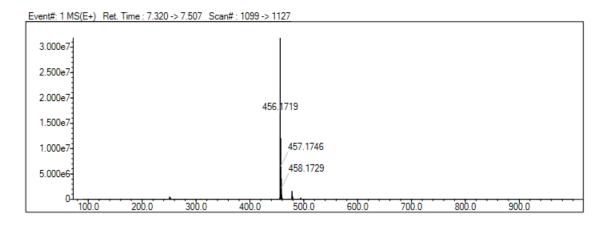
## - IR spectrum of the compound 4c



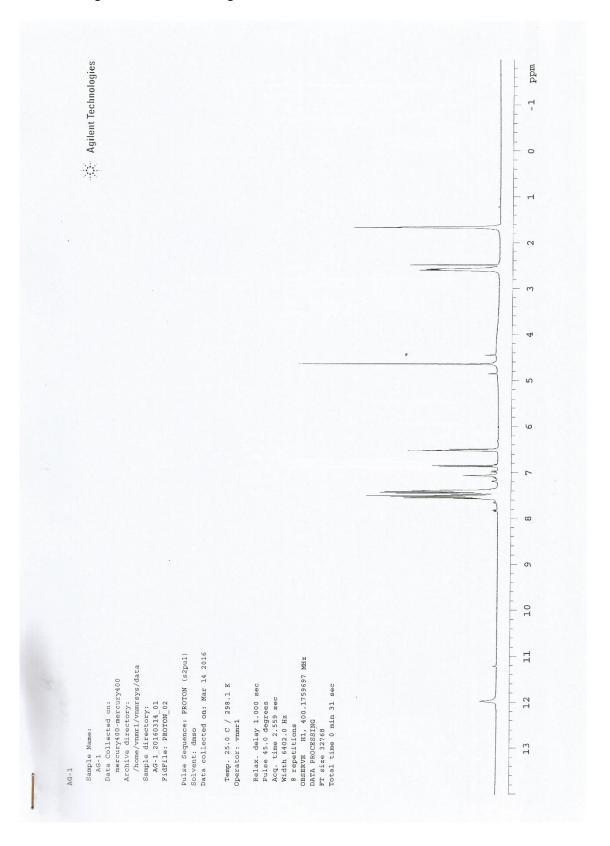
#### HRMS spectrum of the compound4c

Data File: C:\LabSolutions\Data\Analiz\Lyuttas\A\V-5\_3.lcd

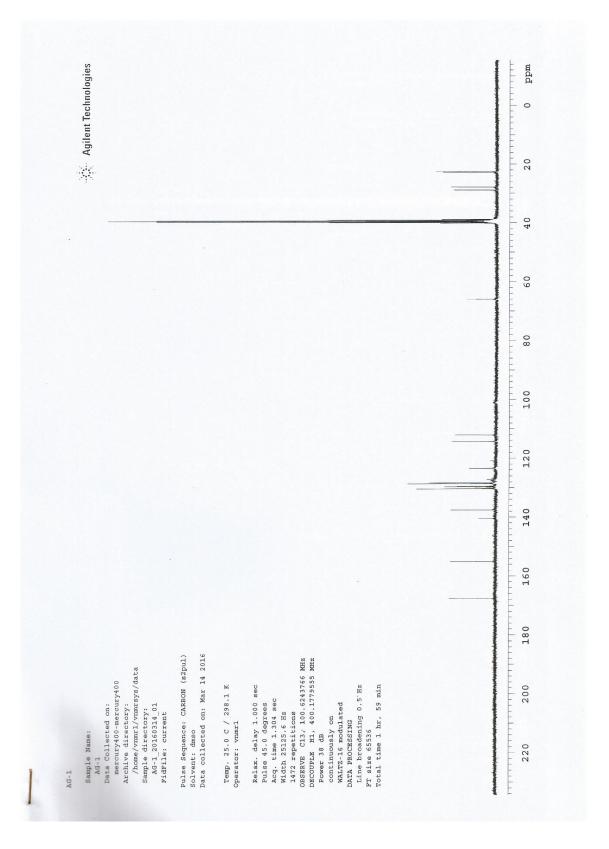
	mt Val. Min Max	Elmt Val. M	in Max Elm	t Val. Min	Max Use Adduct
H   1   20   35 (	) 2 2 4	CI 1	0 1 1	3 0	0 H
C 4 25 30	=   1   0   1	Br 1	0 1		
N 3 3 4	6 2 1 1 1	Ru 2	0 0		
Error Margin (ppm): 5 HC Ratio: unlimited	DBE Rai Apply N F	nge: not fixed Rule: yes		ron lons: both 4Sn Info: no	
Max Isotopes: 3 MSn Iso RI (%): 10.00	Isotope RI MSn Logic M			ope Res: 1000 :Results: 500	00



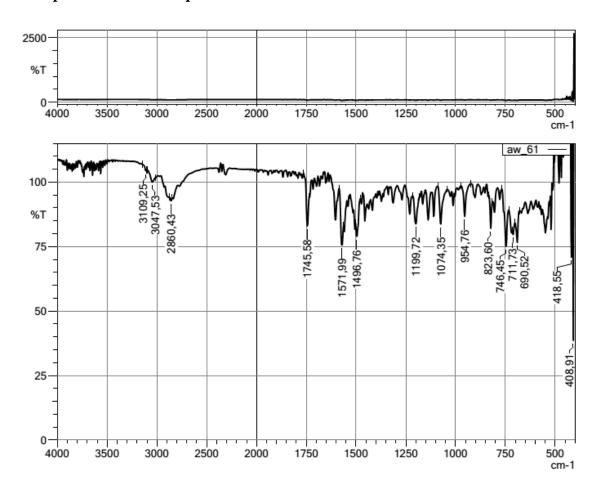
## ${}^{-1}H$ NMR spectrum of the compound 4c



## $-^{13}$ C NMR spectrum of the compound 4c



## - IR spectrum of the compound 4d

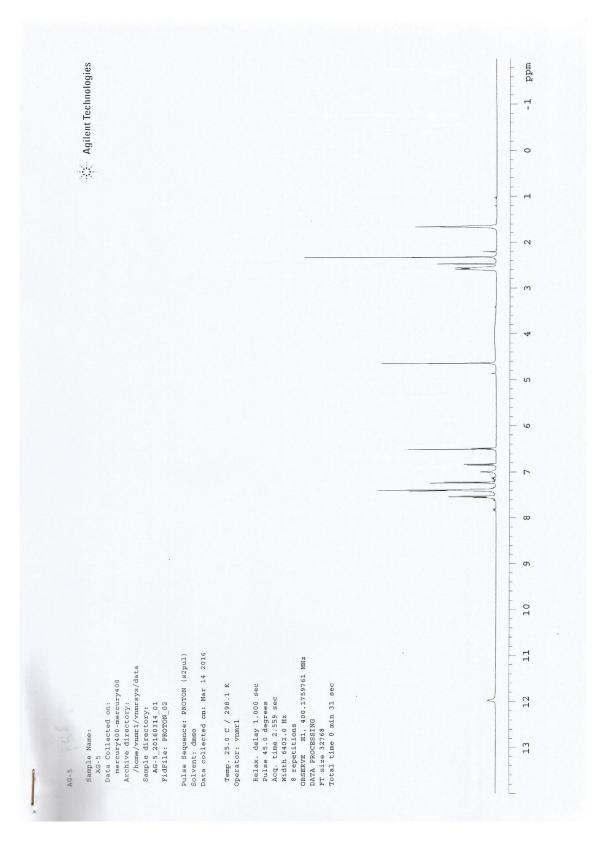


#### -HRMS spectrum of the compound 4d

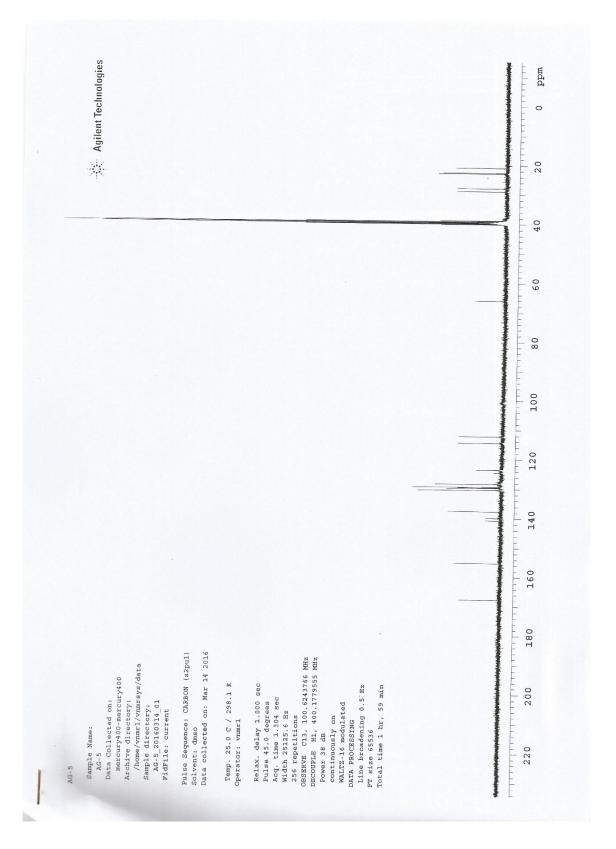
Data File: C:\LabSolutions\Data\Analiz\Lyuttas\AW-6\_4.lcd

Elmt         Val.         Min         Max         Eln           H         1         20         35         O           C         4         26         30         F           N         3         3         4         S	2 2 4 CI 1 0 1 Br	Val.         Min         Max           1         0         1           1         0         1           2         0         0	Elmt Val. Min Max	Use Adduct H
Error Margin (ppm): 5 HC Ratio: unlimited Max Isotopes: 3 MSn Iso RI (%): 10.00	DBE Range: not fix Apply N Rule: yes Isotope RI (%): 1.00 MSn Logic Mode: AND	ked	Electron Ions: both Use MSn Info: no Isotope Res: 10000 Max Results: 500	
Event#: 1 MS(E+) Ret. Time : 7.5	20 -> 7.733 Scan#: 1129 -> 1161	1		
2.400e7- 2.200e7- 2.000e7- 1.800e7-				
1.600e7- 1.400e7- 1.200e7- 1.000e7- 8.000e6-	470.	471.1906		
6.000e6 4.000e6 2.000e6		472.1886		
100.0 200.0	300.0 400.0	500.0 600	.0 70b.0 80b.	0 900.0

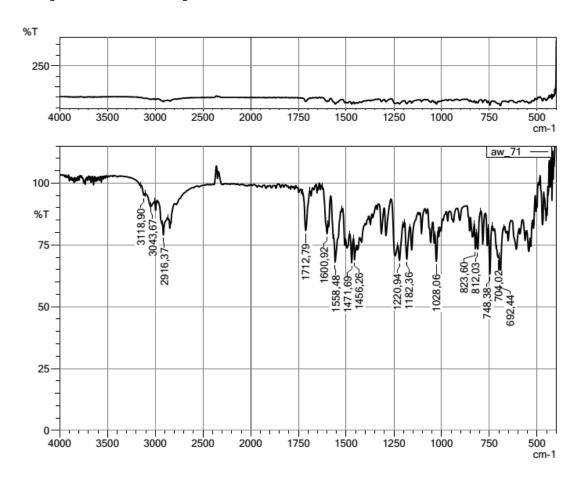
## $-^{1}H$ NMR spectrum of the compound 4d



## $-^{13}$ C NMR spectrum of the compound 4d



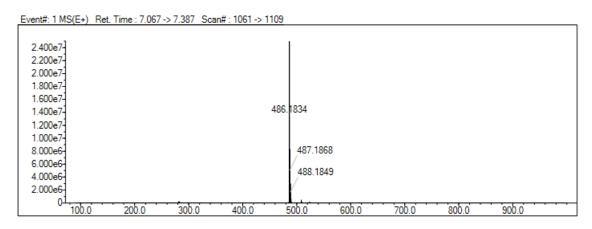
## -IR spectrum of the compound 4e



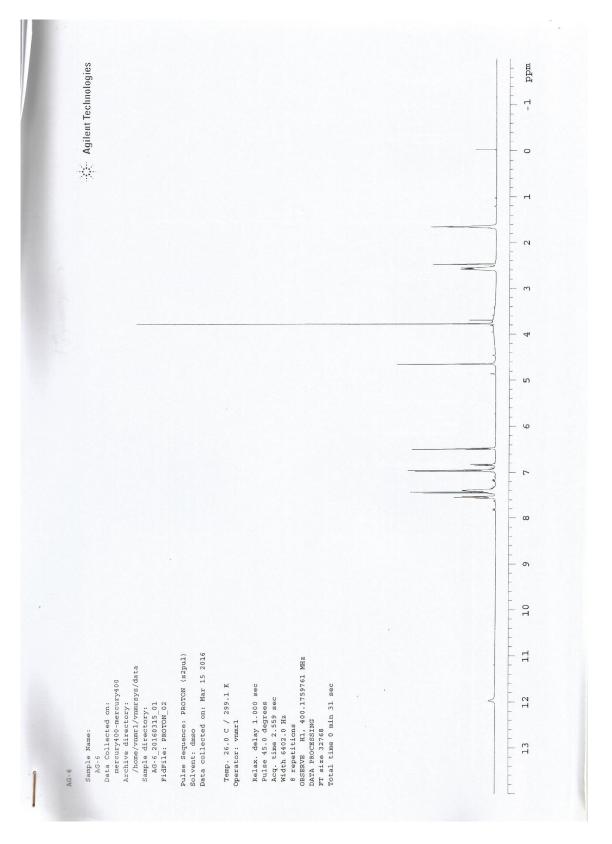
#### -HRMS spectrum of the compound 4e

Data File: C:\LabSolutions\Data\Analiz\Lyuttas\AW-7\_5.lcd

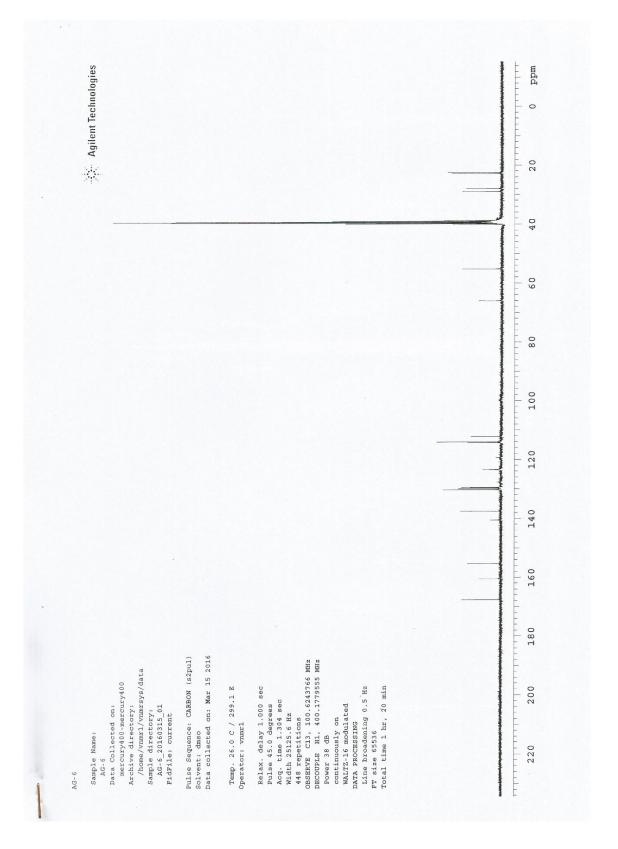
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt Val.	Min N	Max	Use Adduct
H	1	20	35	0	2	2	4	CI	1	0	1	1 3	0	0	Н
С	4	26	30	F	1	0	1	Br	1	0	1				
N	3	3	4	S	2	1	1	Ru	2	0	0				
		Ratio: opes:	unlimite 3	d		App Isotor	lyNRi beRl(	ge: noti ule: yes %): 1.00 de: ANI	)			Electron Ions: Use MSn Info: Isotope Res: Max Results:	no 10000		



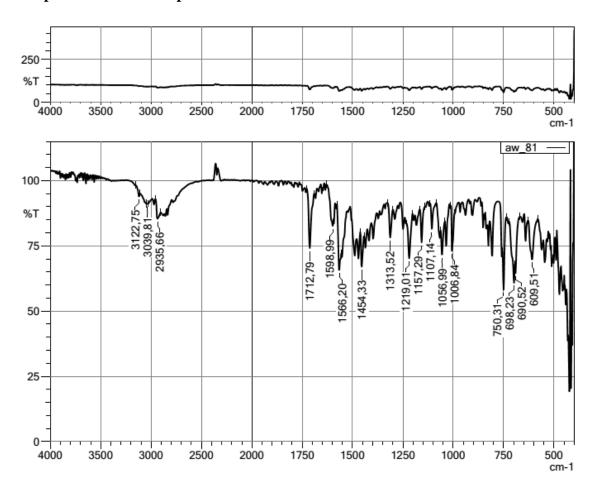
## -¹H NMR spectrum of the compound 4e



<sup>13</sup>C NMR spectrum of the compound 4e



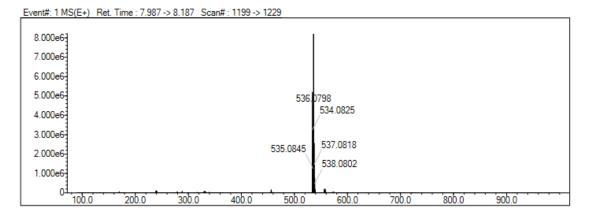
## -IR spectrum of the compound 4f



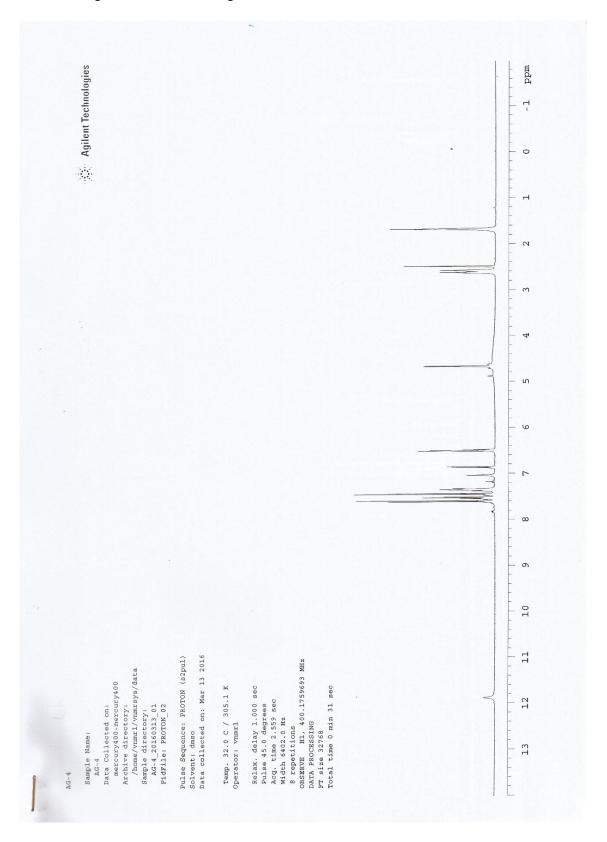
#### -HRMS spectrum of the compound 4f

Data File: C:\LabSolutions\Data\Analiz\Lyuttas\A\W-8\_9.lcd

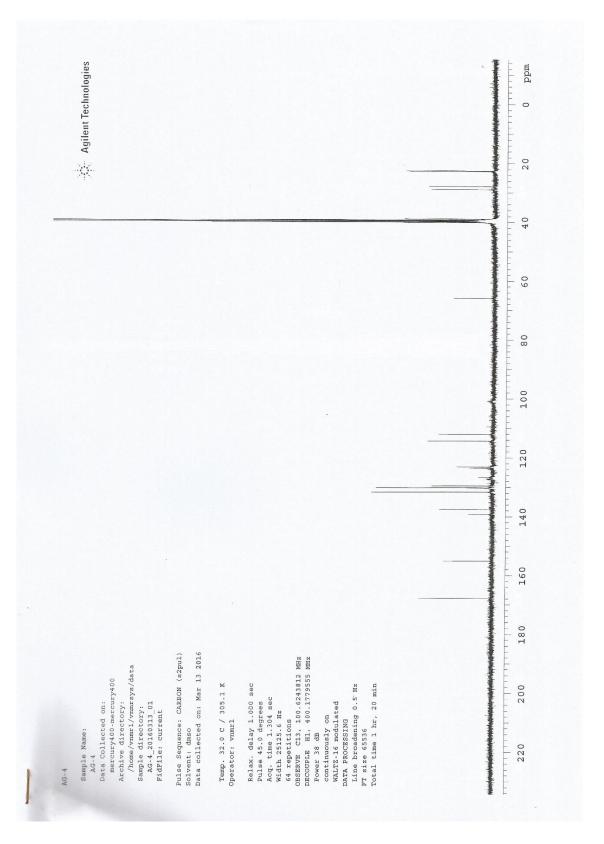
Elmt	Val.	Min		Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt Val.	Min	Max	Use Adduct
H	1	20	35	0	2	2	4	CI	1	0	1	I 3	0	0	H
С	4	26	30	F	1	0	1	Br	1	0	1	, ,			
N	3	3	4	S	2	1	1	Ru	2	0	0				
	HC ax Isot		unlimite 3	d		App Isoto	oly N Ri pe RI (	ge: noti ule: yes %): 1.00 de: ANE	)			Electron Ions: Use MSn Info: Isotope Res: Max Results:	no 1000	0	



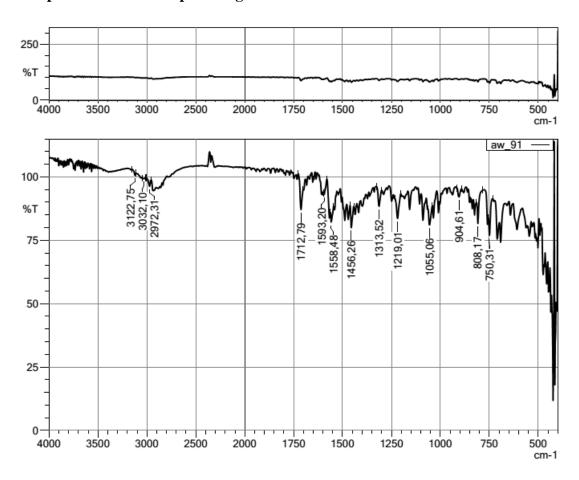
## -¹H NMR spectrum of the compound 4f



## -13C NMR spectrum of the compound 4f



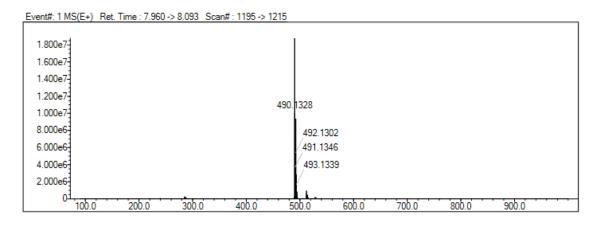
## -IR spectrum of the compound 4g



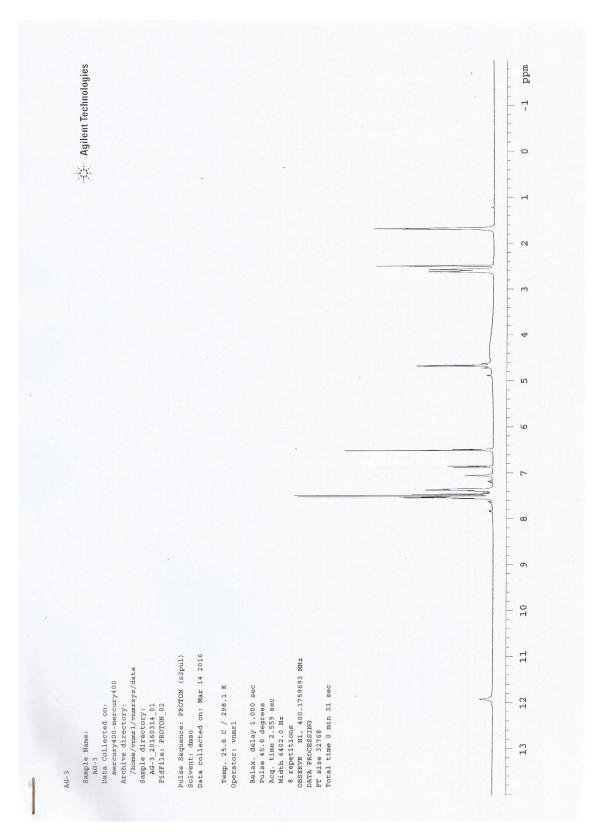
#### -HRMS spectrum of the compound 4g

Data File: C:\LabSolutions\Data\Analiz\Lyuttas\AW-9\_10.lcd

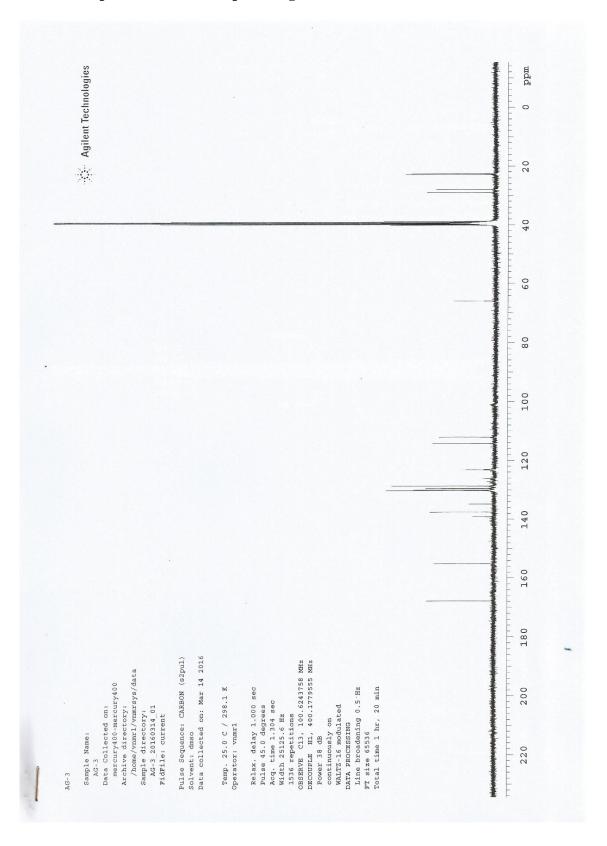
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	20	35	0	2	2	4	CI	1	0	1		3	0	0	H
С	4	26	30	F	1	0	1	Br	1	0	1					
N	3	3	4	S	2	1	1	Ru	2	0	0					
Error M	argin (	nom).	5			DE	E Dar	nge: noti	fived			Electro	n lone:	both		
LITOI M			unlimite	d				ule: yes				Use MS				
M	ax Isot							(%): 1.00					e Res:		n	
	n Iso R							ode: ANE					esults:			



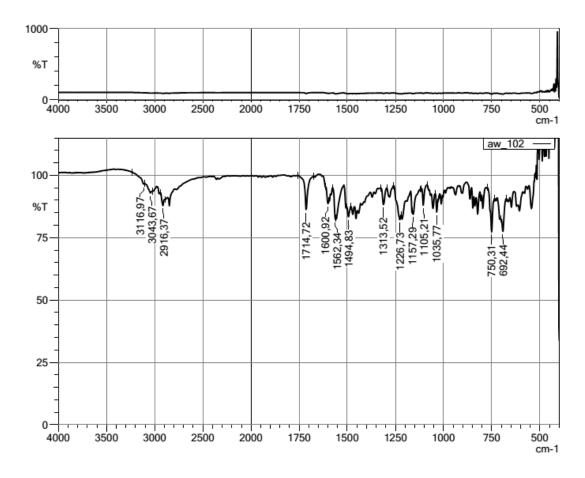
## -¹H NMR spectrum of the compound 4g



## -13C NMR spectrum of the compound 4g



## -IR spectrum of the compound 4h

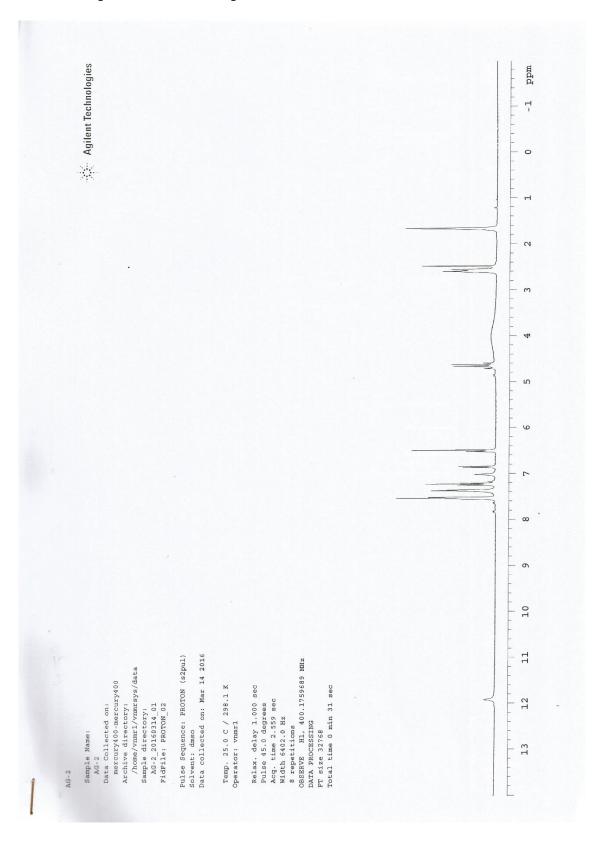


## -HRMS spectrum of the compound 4h

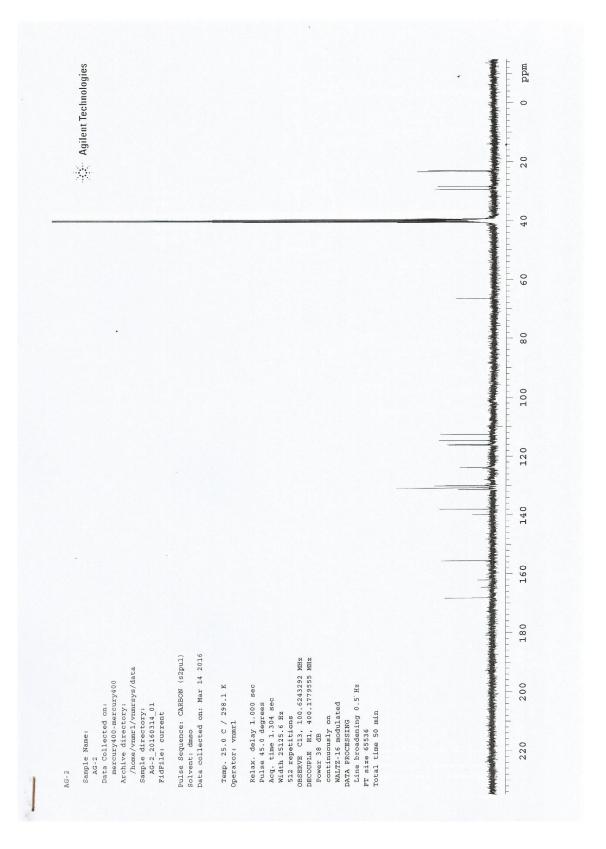
Data File: C:\LabSolutions\Data\Analiz\Lyuttas\A\W-10\_13.lcd

Elmt   Val.   Min   Max   Elm   H   1   20   35   O   C   4   26   30   F   N   3   3   4   S	t Val. Min Max Elmt 2 2 4 Cl 1 0 1 Br 2 1 1 Ru	Val.         Min         Max           1         0         2           1         0         1           2         0         0	Elmt Val. Min Max	Use Adduct H
Error Margin (ppm): 5 HC Ratio: unlimited Max Isotopes: 3 MSn Iso RI (%): 10.00	DBE Range: not fix Apply N Rule: yes Isotope RI (%): 1.00 MSn Logic Mode: AND	ced	Electron lons: both Use MSn Info: no Isotope Res: 10000 Max Results: 500	
Event#: 1 MS(E+) Ret. Time : 7.48	30 -> 7.720 Scan# : 1123 -> 1159	)		
2.000e7				
1.800e7				
1.600e7- 1.400e7-				
1.200e7-	474.	1629		
1.000e7				
8.000e6		475.1654		
6.000e6- 4.000e6-		476.1637		
2.000e6		/ 4/0.103/		
0 100.0 200.0	300.0 400.0	500.0 600.	.0 700.0 800.	0 900.0
.55.0	3333 100.0	555.5	.5 .55.6 500.	

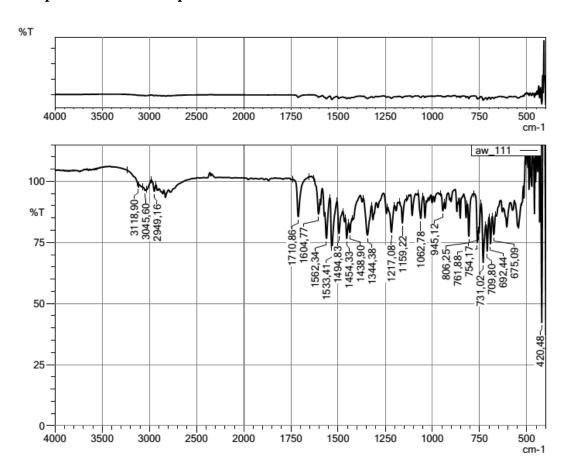
## - <sup>1</sup>H NMR spectrum of the compound 4h



## -13C NMR spectrum of the compound 4h



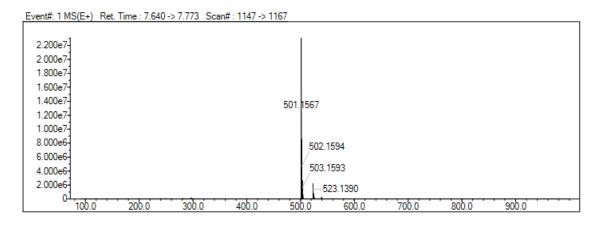
## -IR spectrum of the compound 4i



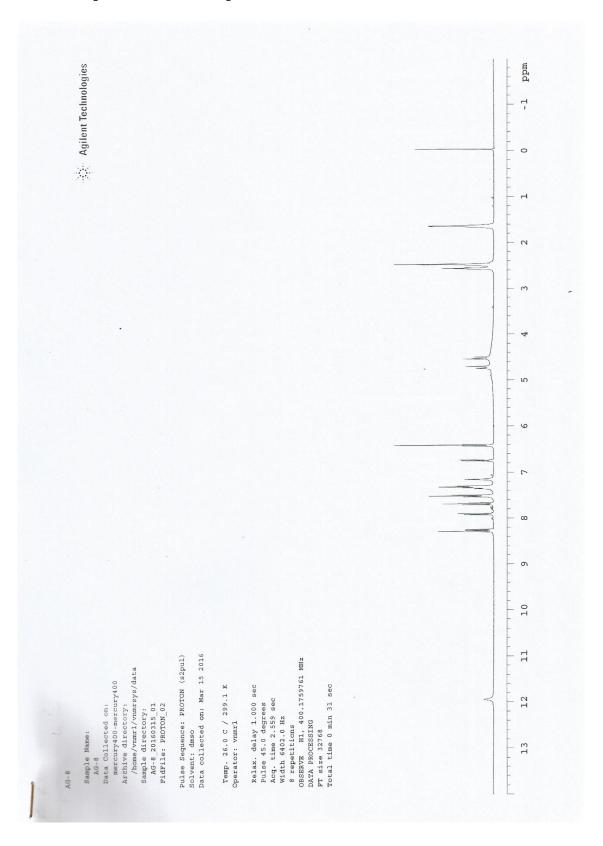
#### -HRMS spectrum of the compound 4i

Data File: C:\LabSolutions\Data\Analiz\Lyuttas\A\W-11\_10.lcd

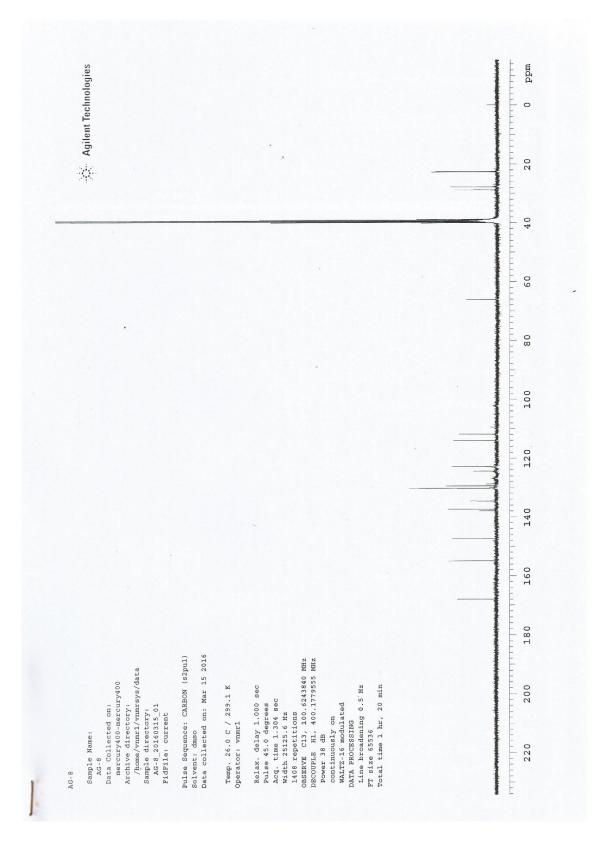
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	20	35	0	2	2	4	CI	1	0	1		3	0	0	H
C	4	26	30	F	1	0	1	Br	1	0	1					
N	3	3	4	S	2	1	1	Ru	2	0	0					
		Ratio: opes:	unlimite 3	d		App Isoto	lyNRi peRl(	ge: not: ule: yes %): 1.00 de: ANI	)					no 1000	0	



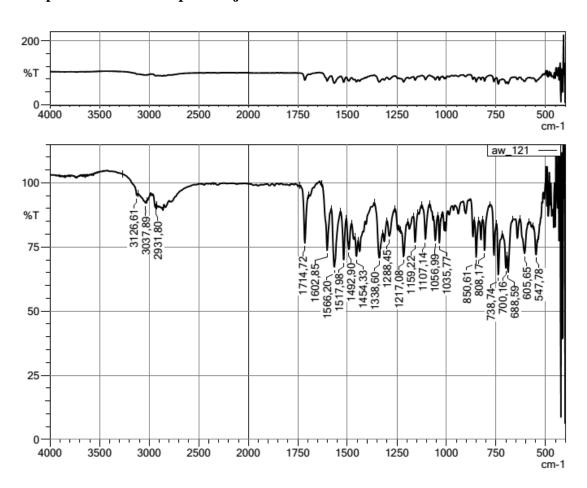
## -¹H NMR spectrum of the compound 4i



## $-^{13}$ C NMR spectrum of the compound 4i



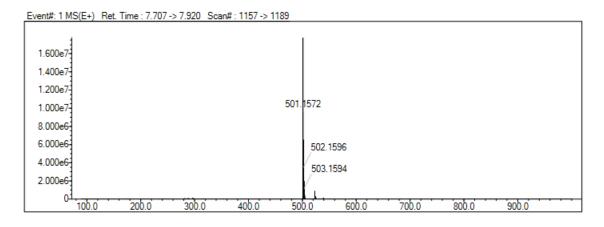
## -IR spectrum of the compound 4j



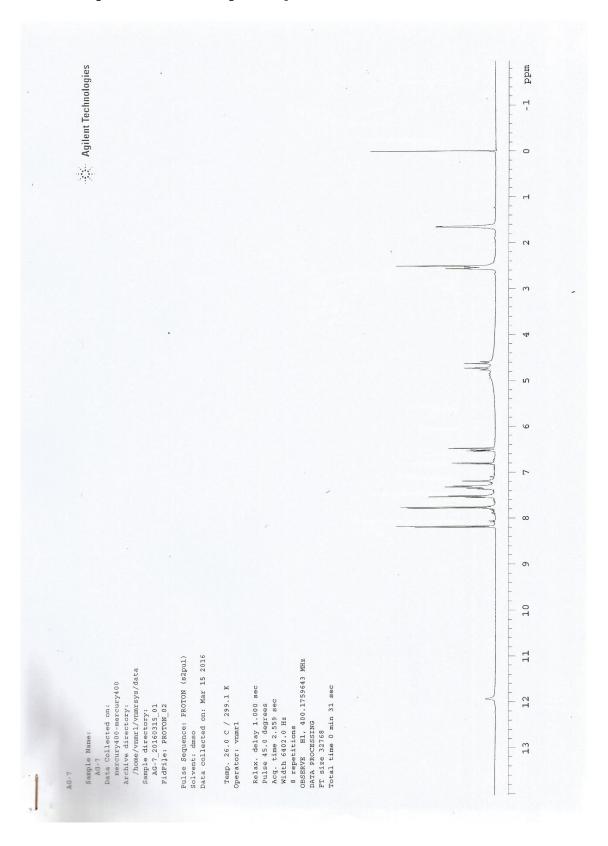
#### -HRMS spectrum of the compound 4j

Data File: C:\LabSolutions\Data\Analiz\Lyuttas\AW-12\_11.lcd

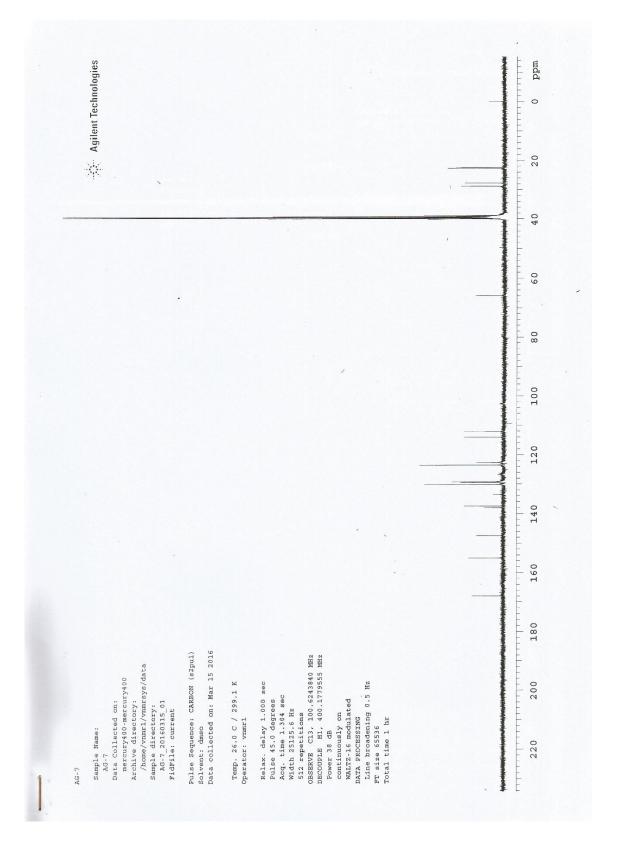
Elmt Va	l. Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H 1	20	35		2	2	4	CI	1	0	1		3	0	0	Н
C 4	26	30	F	1	0	1	Br	1	0	1					
N 3	3	4	S	2	1	1	Ru	2	0	0					
Error Margir	(ppm):	5			DE	E Ran	ige: not f	ixed			Electro	n lons:	both		
Н	C Ratio:	unlimite	d		App	ly N R	ule: yes				Use MS	in Info:	no		
Max Is	otopes:	3			Isoto	oe RI (	%): 1.00				Isotop	e Res:	10000	0	
MSn Iso	RI (%):	10.00			MSn Lo	gic Mo	dé: AND	)			Max R	esults:	500		



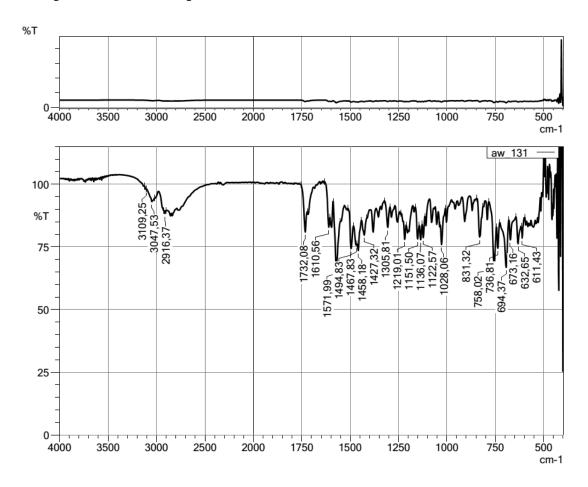
## -¹H NMR spectrum of the compound 4j



## -13C NMR spectrum of the compound 4j



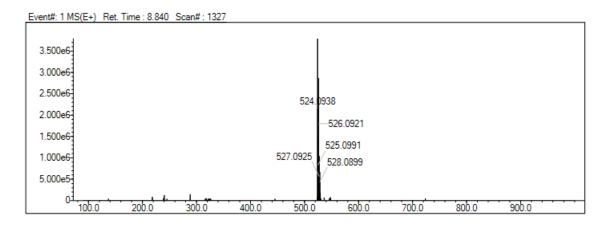
## - IR spectrum of the compound 4k



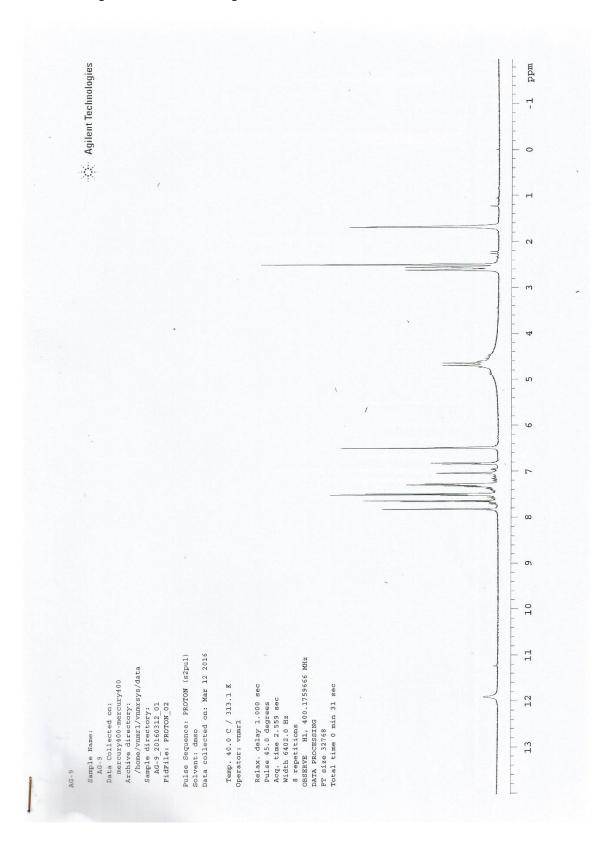
## -HRMS spectrum of the compound 4k

Data File: C:\LabSolutions\Data\Analiz\Lyuttas\AW-13\_12.lcd

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	20	35		2	2	4	CI	1	0	2		3	0	0	H
С	4	26	30	F	1	0	1	Br	1	0	1		,			
N	3	3	4	S	2	1	1	Ru	2	0	0					
Error M	argin (	ppm):	5			DE	BE Rar	ige: not	fixed			Electro	n lons:	both		
	HC I	Ratio:	unlimite	d		App	ly NR	ule: yes				Use MS	in Info:	no		
M	ax Isot	opes:	3			Isoto	pe RI (	(%): 1.00	)			Isotop	e Res:	10000	0	
MSi	n Iso R	1 (%):	10.00			MSn Lo	gic Mo	de: ANI	)			Max Ř	esults:	500		



## -¹H NMR spectrum of the compound 4k



## $-^{13}$ C NMR spectrum of the compound4k

