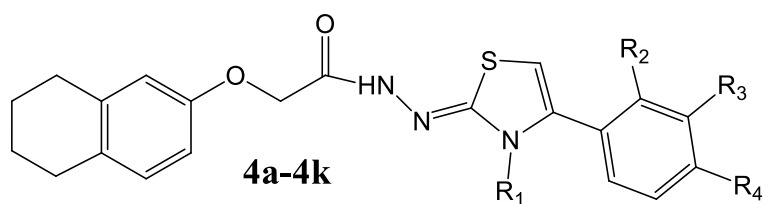
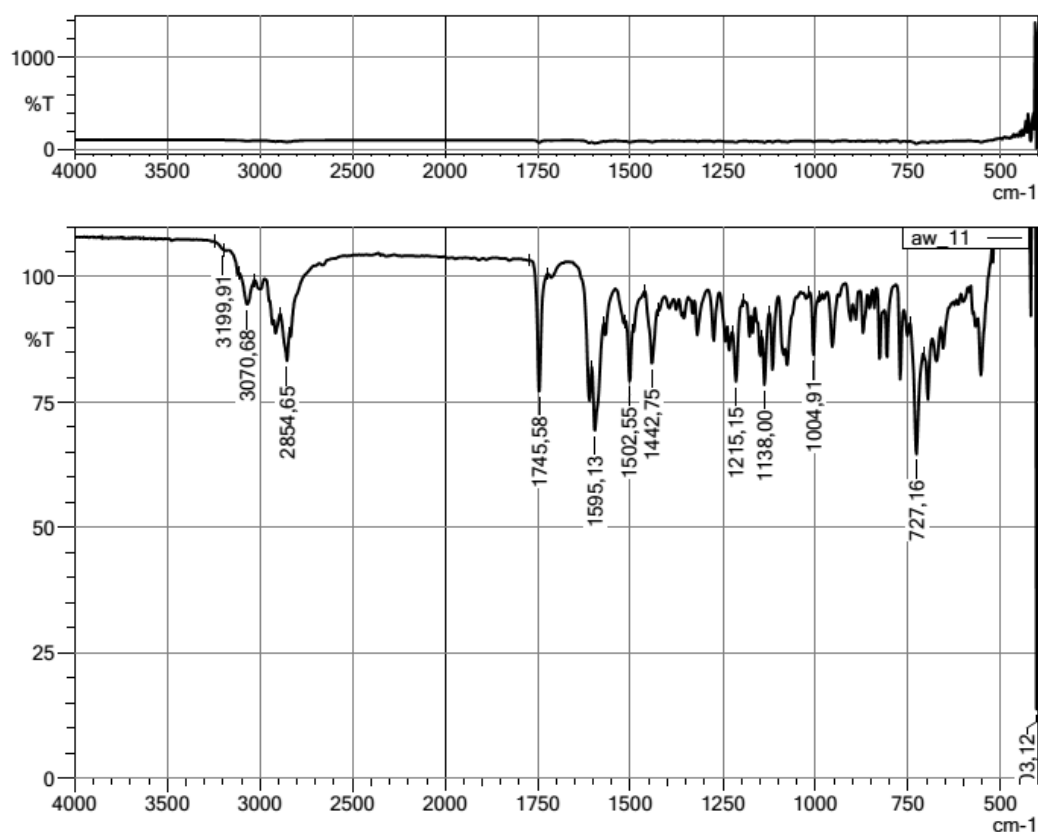


Supplementary document



Compounds	R ₁	R ₂	R ₃	R ₄
4a	Cyclohexyl	H	H	H
4b	Cyclohexyl	H	H	OCH ₃
4c	Phenyl	H	H	H
4d	Phenyl	H	H	CH ₃
4e	Phenyl	H	H	OCH ₃
4f	Phenyl	H	H	Br
4g	Phenyl	H	H	Cl
4h	Phenyl	H	H	F
4i	Phenyl	H	NO ₂	H
4j	Phenyl	H	H	NO ₂
4k	Phenyl	Cl	Cl	H

-IR spectrum of the compound 4a



- HRMS spectrum of the compound 4a

Data File: C:\LabSolutions\Data\Analiz\Lyuttas\AW-1_1 lod

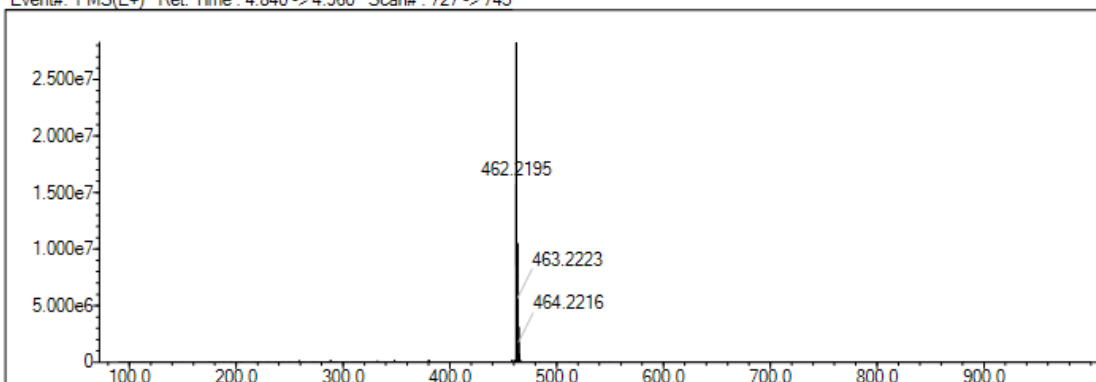
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	20	35	O	2	2	4	Cl	1	0	1	I	3	0	0	H
C	4	25	30	F	1	0	1	Br	1	0	1					
N	3	3	4	S	2	1	1	Ru	2	0	0					

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

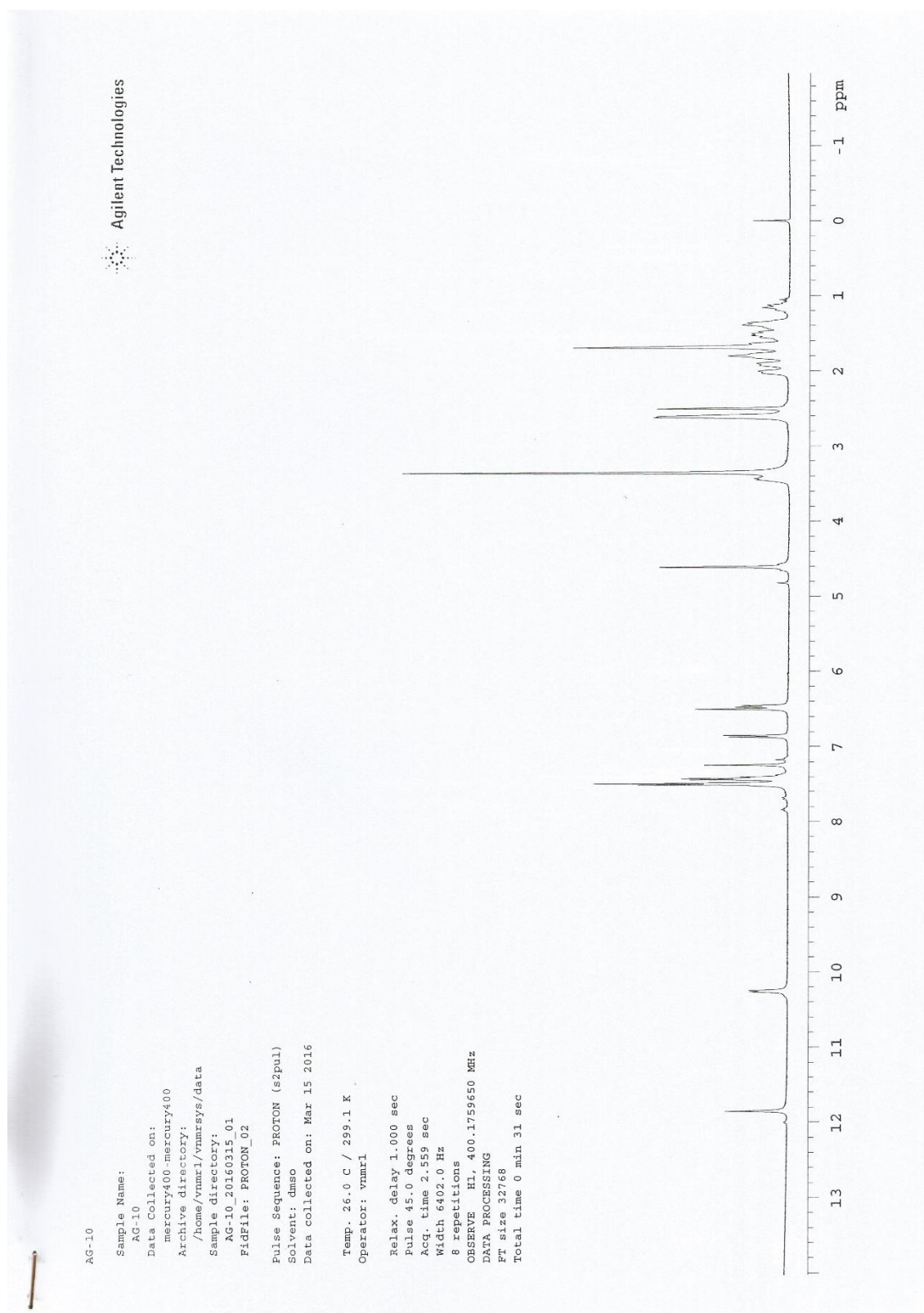
DBE Range: not fixed
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

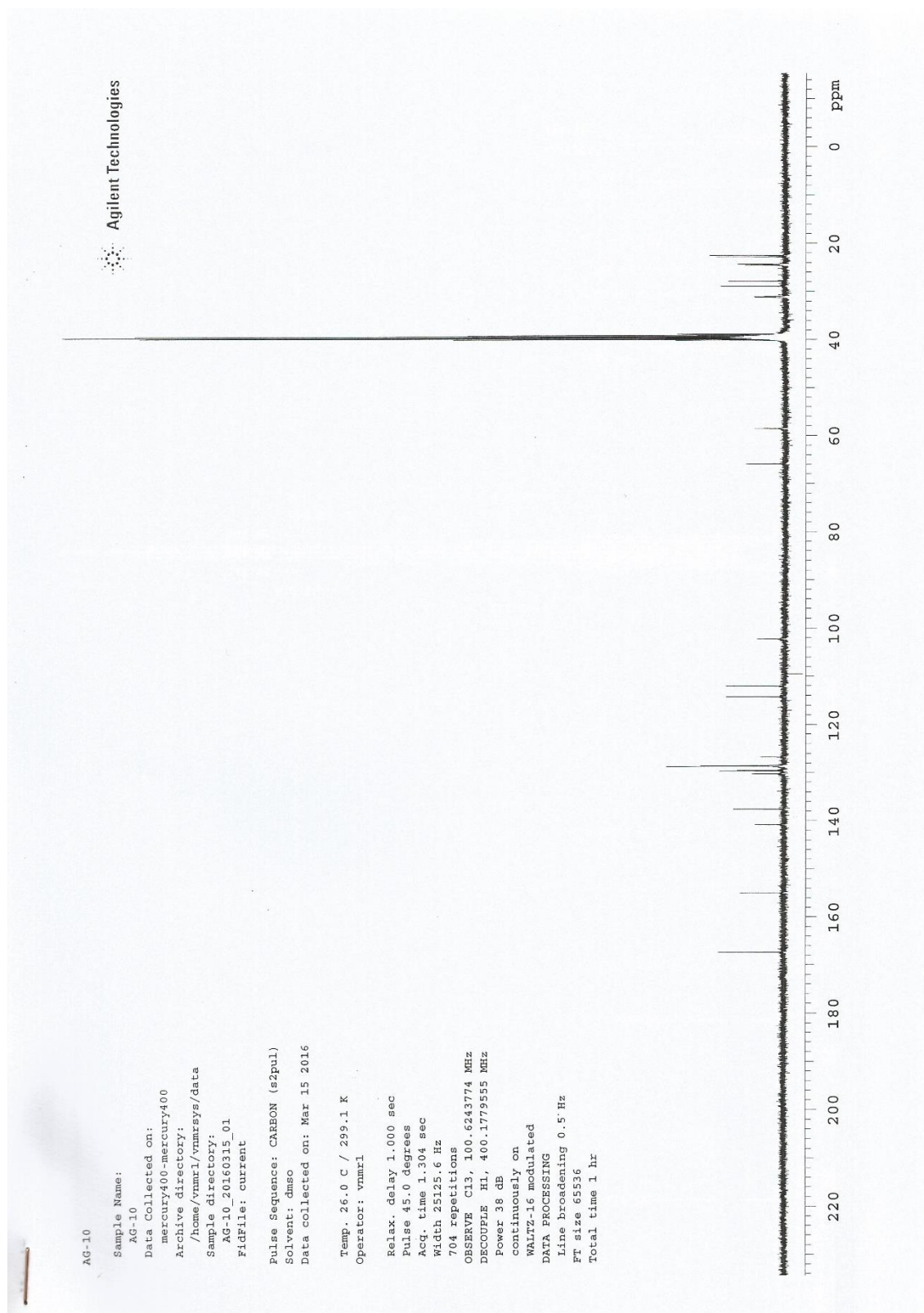
Event#: 1 MS(E+) Ret. Time: 4.840 -> 4.960 Scan#: 727 -> 745



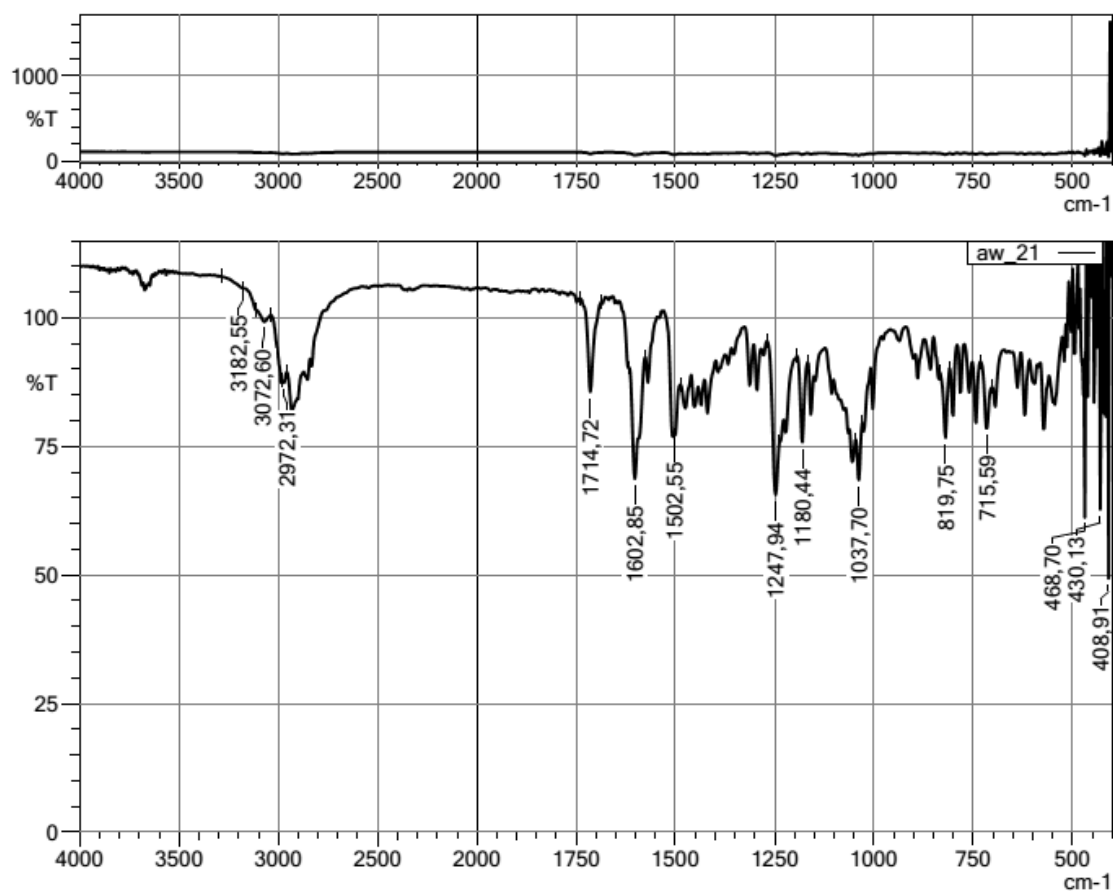
^1H NMR spectrum of the compound 4a



^{13}C 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

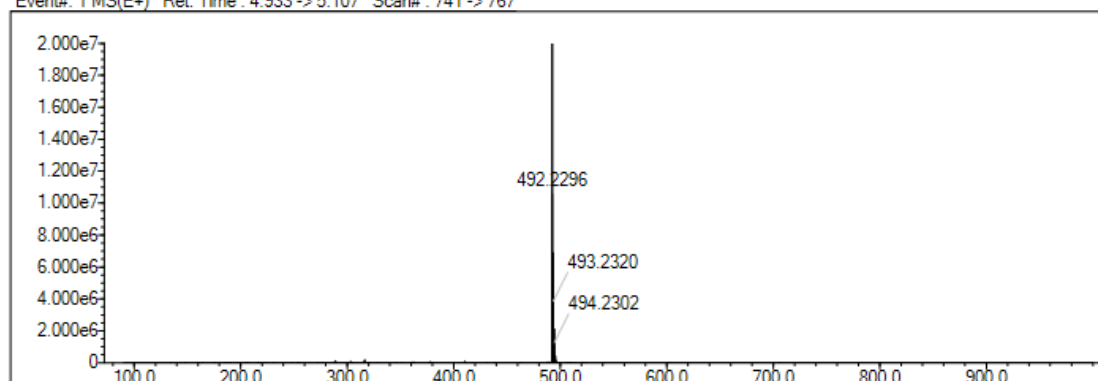
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	20	35	O	2	2	4	Cl	1	0	1	I	3	0	0	H
C	4	25	30	F	1	0	1	Br	1	0	1					
N	3	3	4	S	2	1	1	Ru	2	0	0					

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

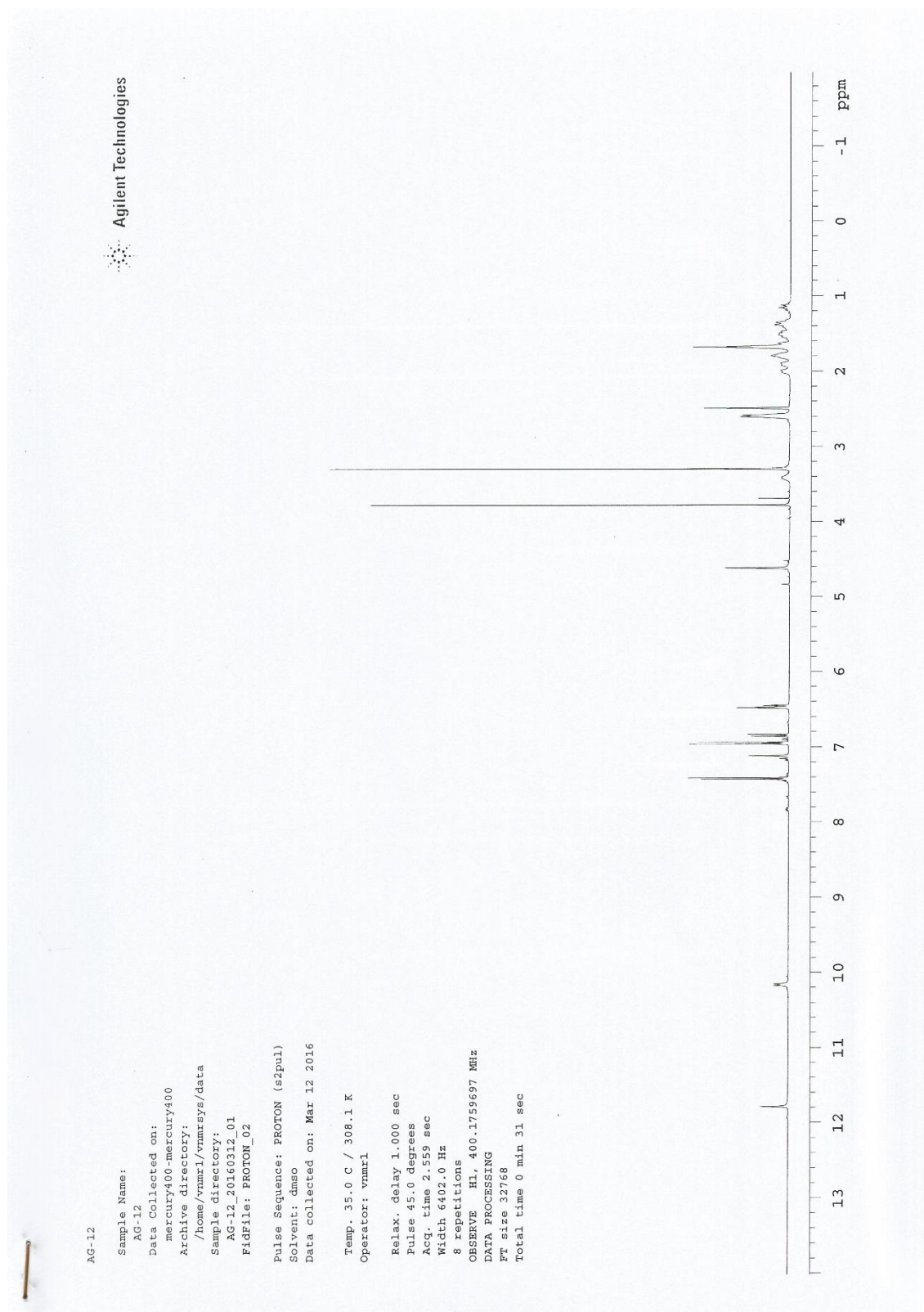
DBE Range: not fixed
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

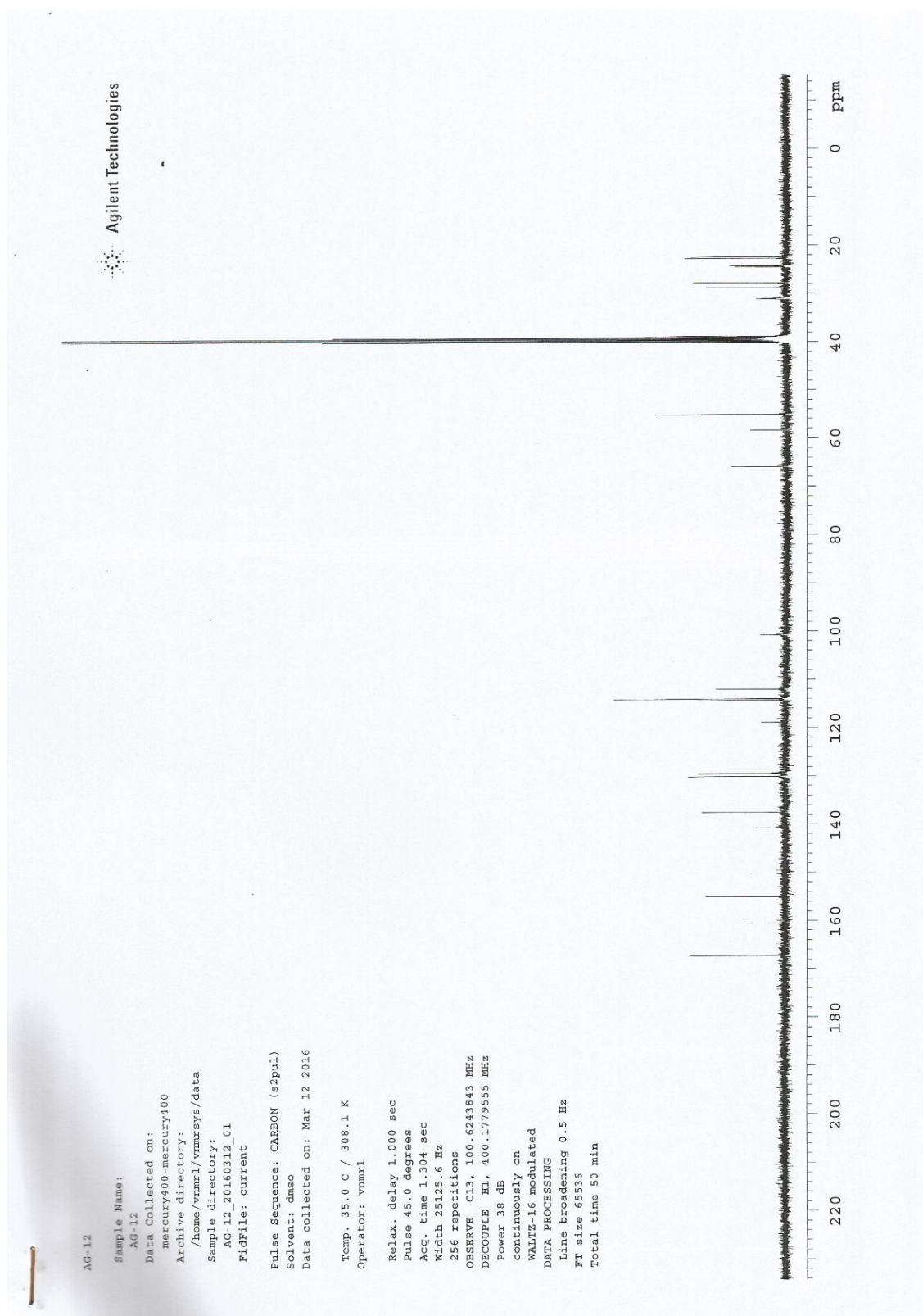
Event#: 1 MS(E+) Ret. Time : 4.933 -> 5.107 Scan#: 741 -> 767



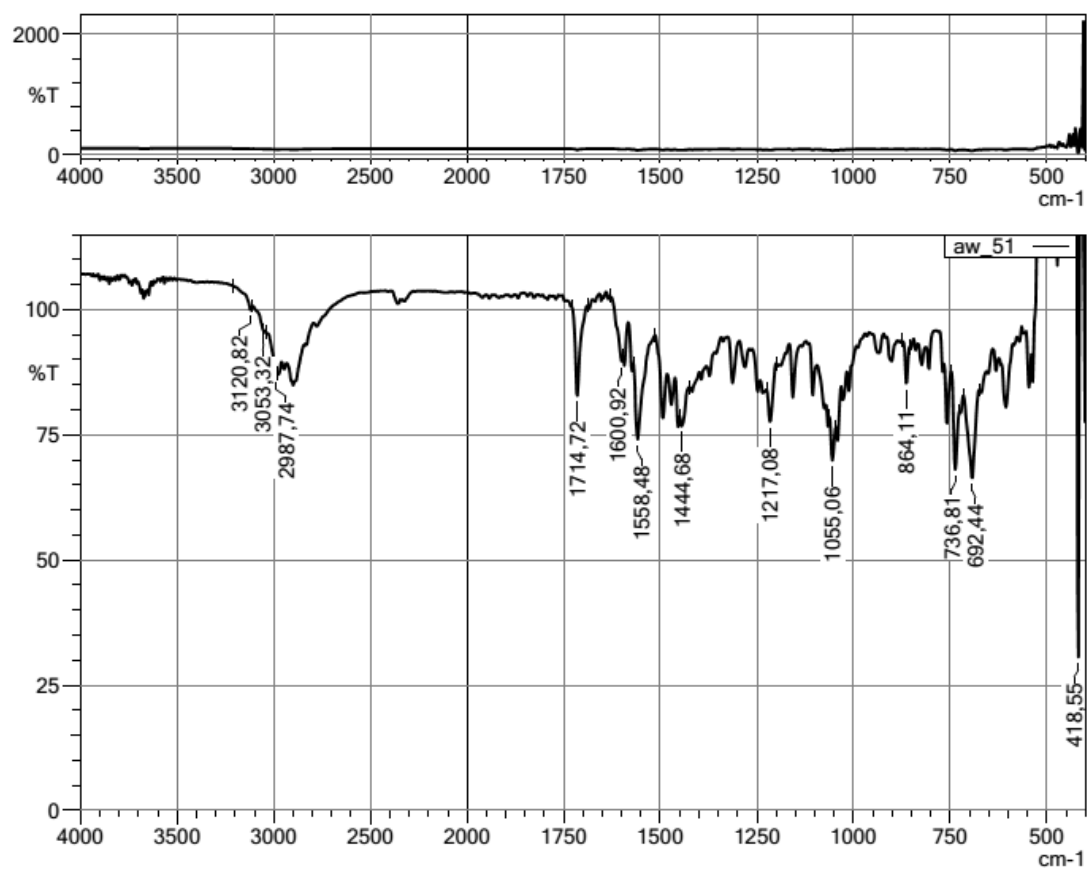
^1H NMR spectrum of the compound 4b



^{13}C NMR spectrum of the compound 4b



- IR spectrum of the compound 4c



HRMS spectrum of the compound 4c

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

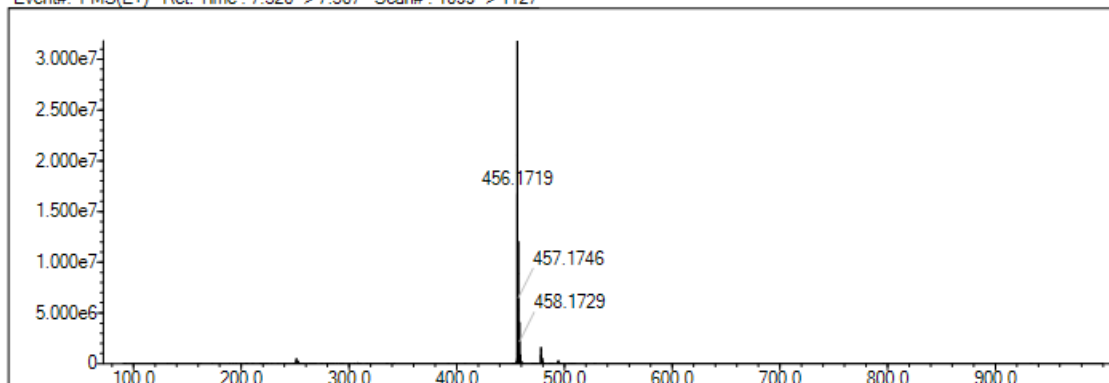
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	20	35	O	2	2	4	Cl	1	0	1	I	3	0	0	H
C	4	25	30	F	1	0	1	Br	1	0	1					
N	3	3	4	S	2	1	1	Ru	2	0	0					

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

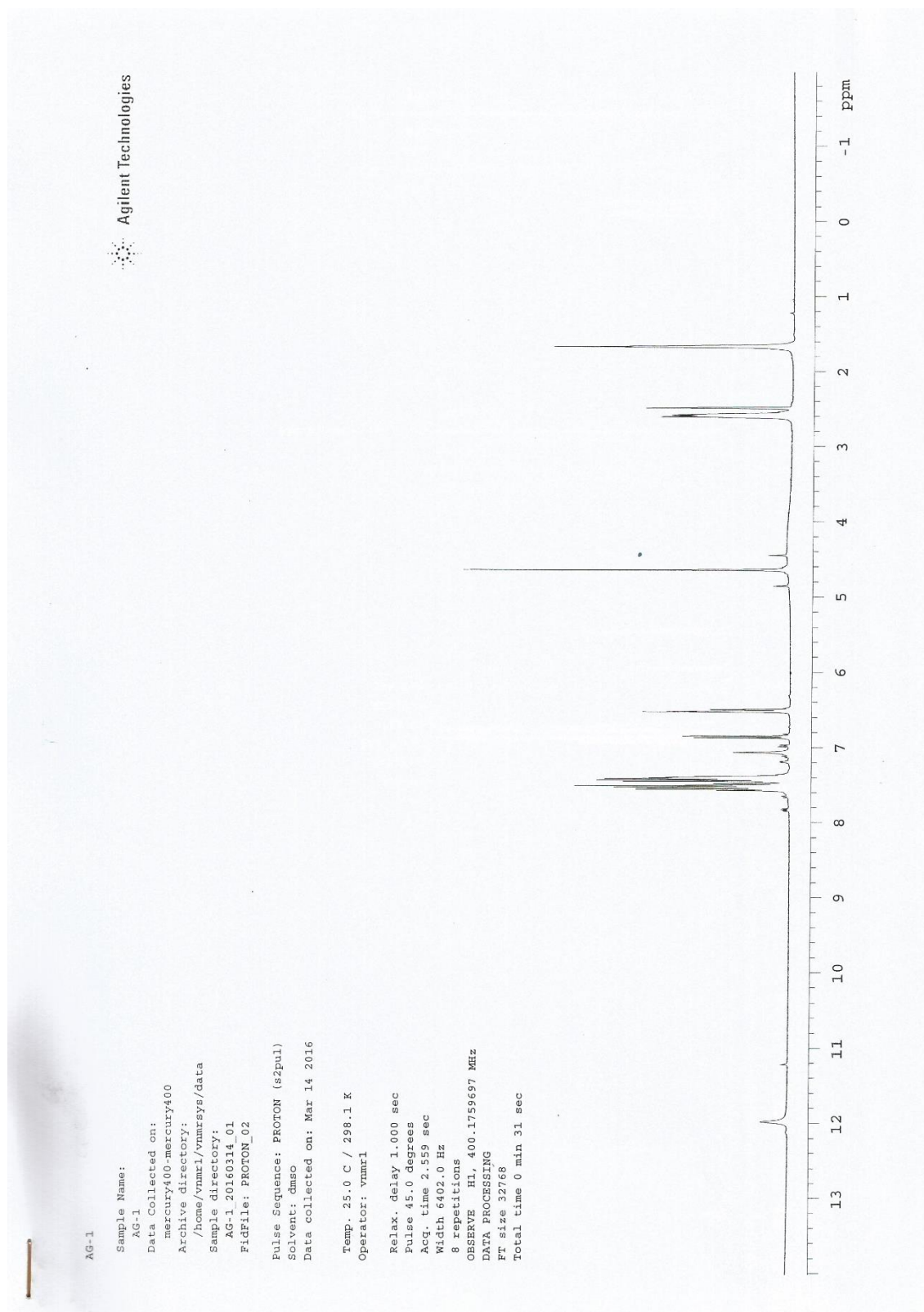
DBE Range: not fixed
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

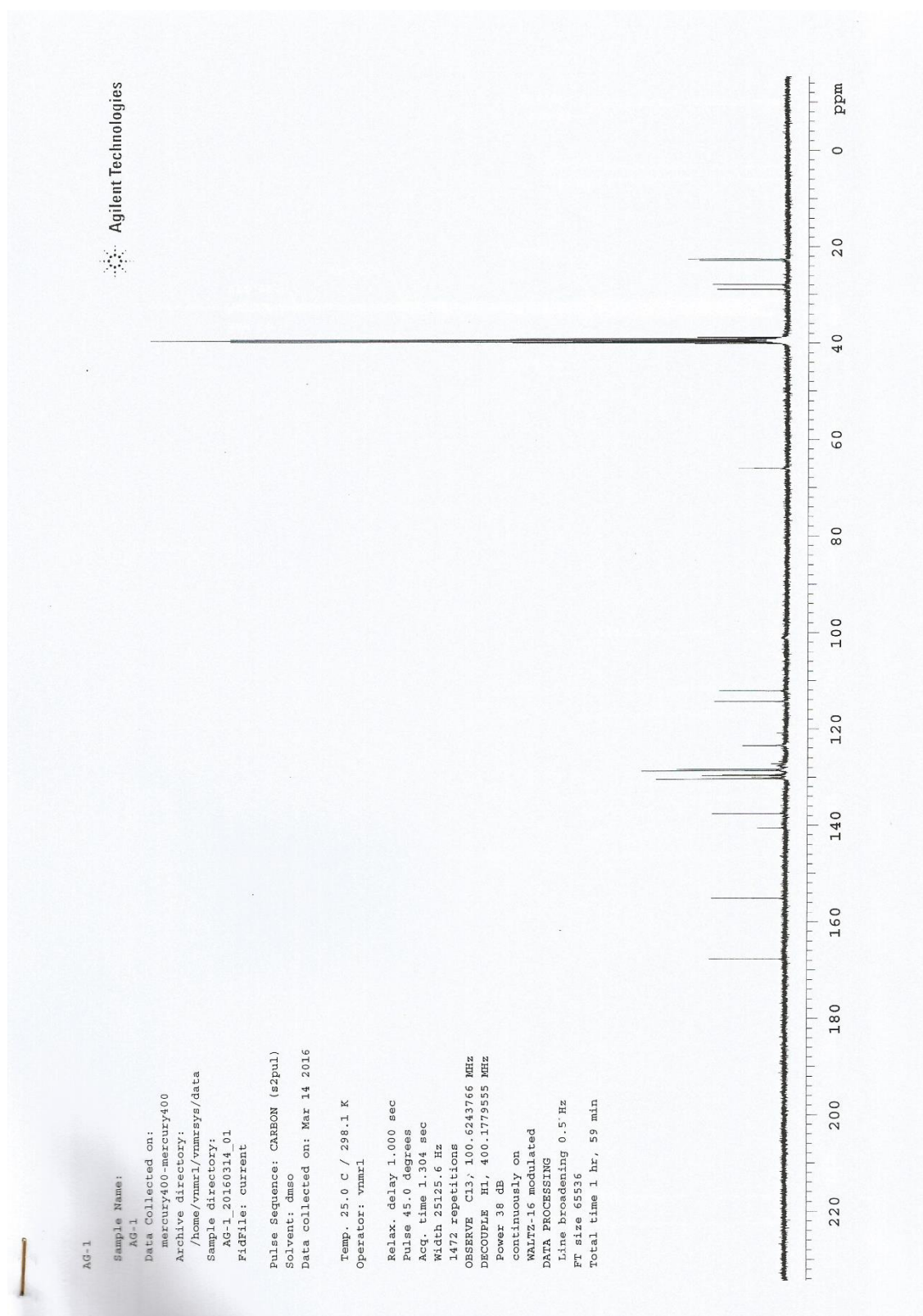
Event#: 1 MS(E+) Ret. Time: 7.320 -> 7.507 Scan#: 1099 -> 1127



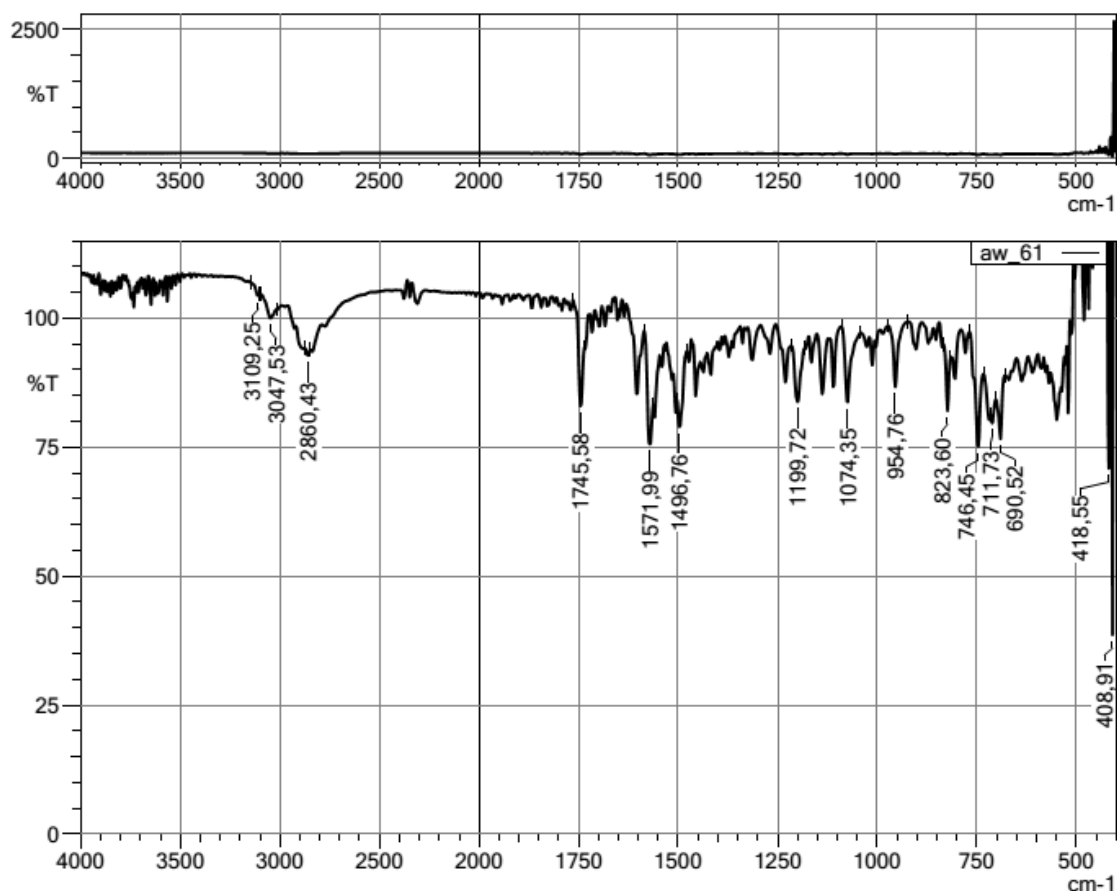
^1H NMR spectrum of the compound 4c



^{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

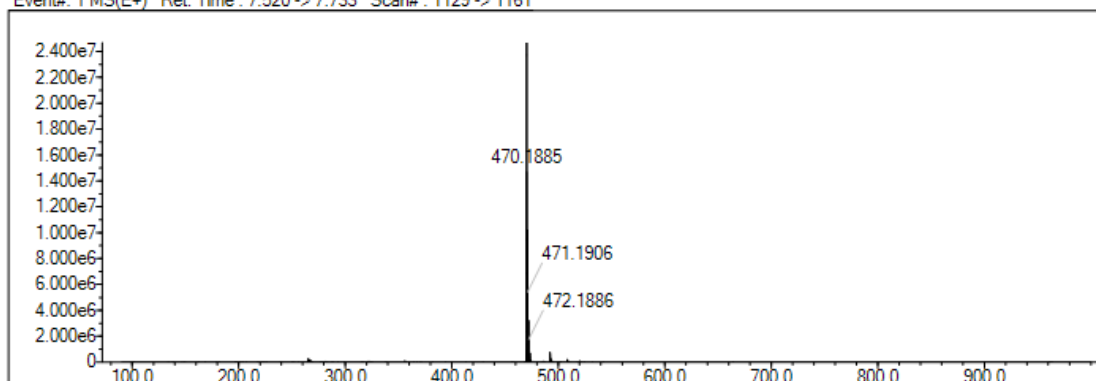
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	20	35	O	2	2	4	Cl	1	0	1	I	3	0	0	H
C	4	26	30	F	1	0	1	Br	1	0	1					
N	3	3	4	S	2	1	1	Ru	2	0	0					

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

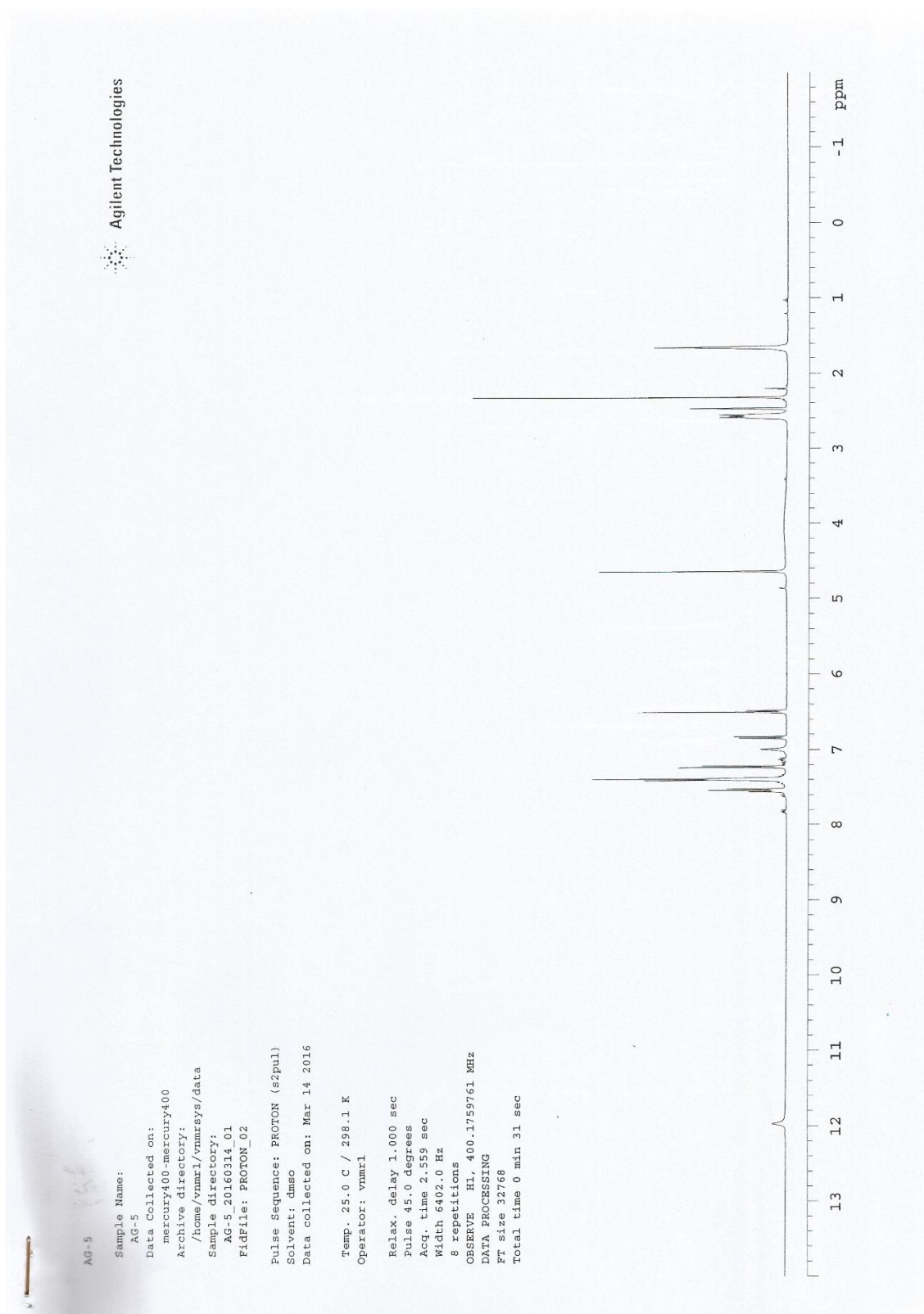
DBE Range: not fixed
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

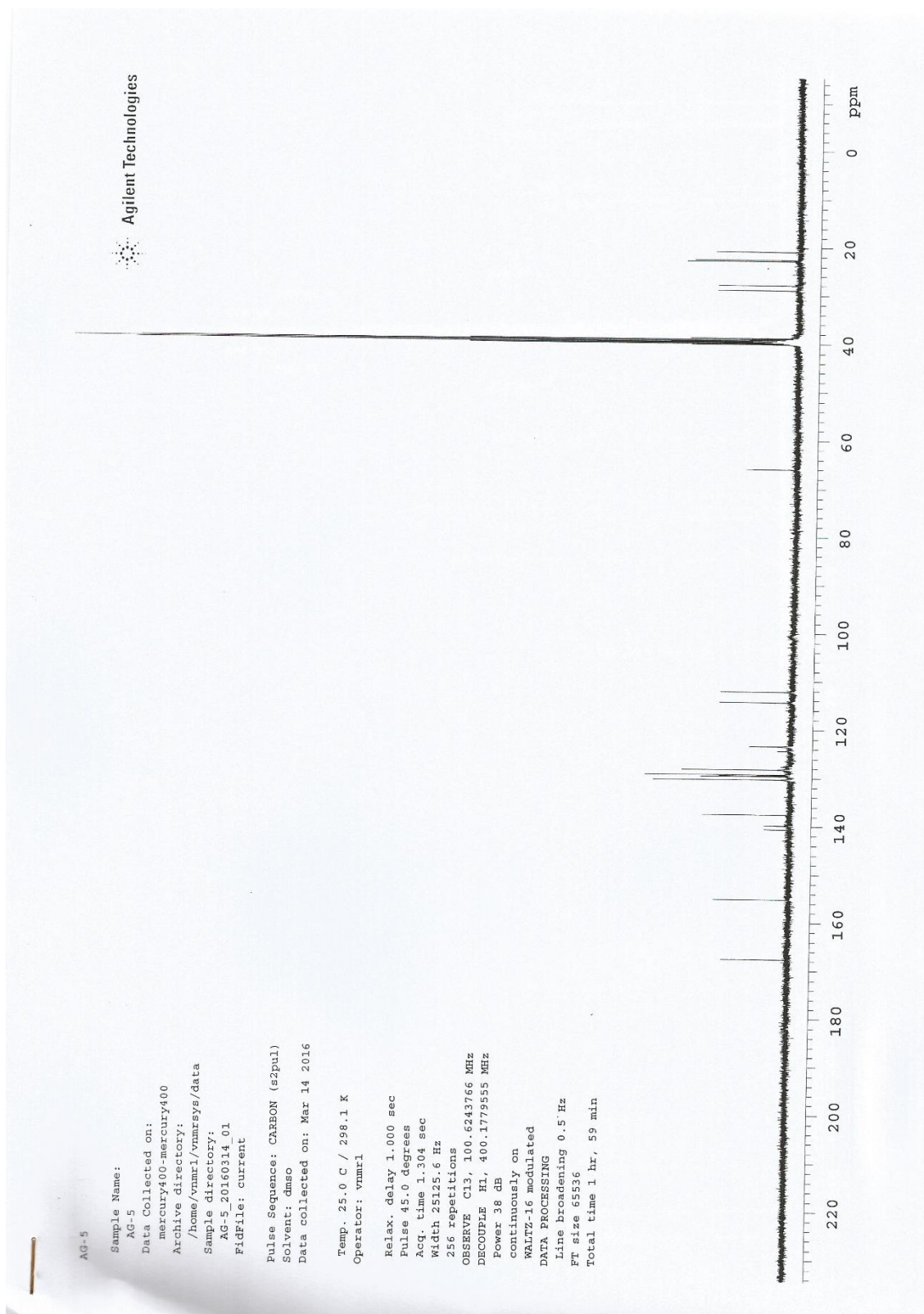
Event#: 1 MS(E+) Ret. Time : 7.520 -> 7.733 Scan#: 1129 -> 1161



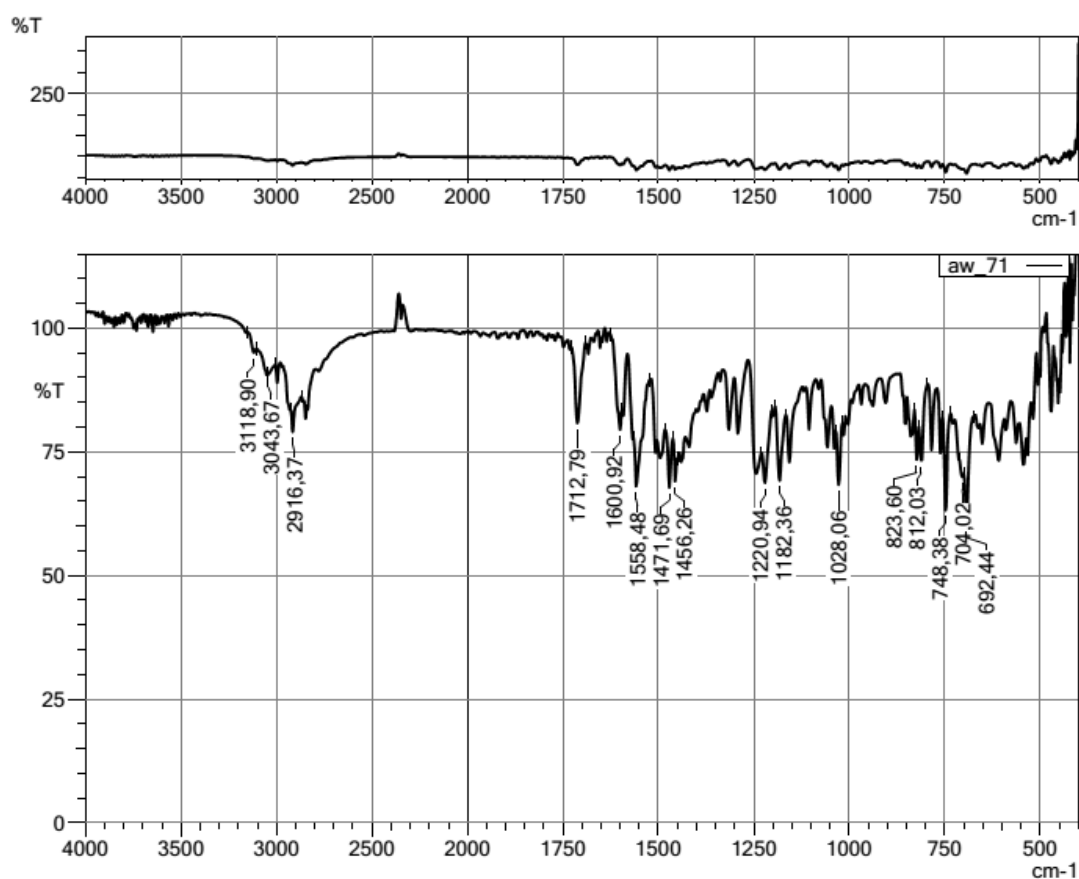
^1H NMR spectrum of the compound 4d



^{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

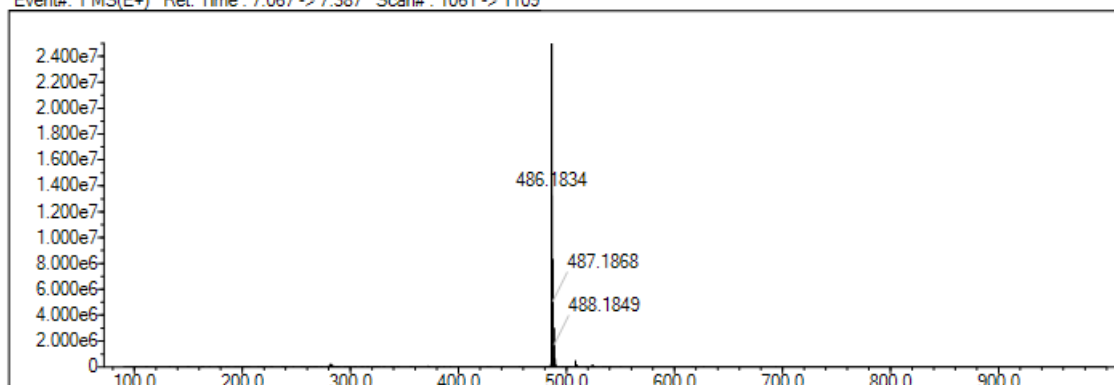
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	20	35	O	2	2	4	Cl	1	0	1	I	3	0	0	H
C	4	26	30	F	1	0	1	Br	1	0	1					
N	3	3	4	S	2	1	1	Ru	2	0	0					

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

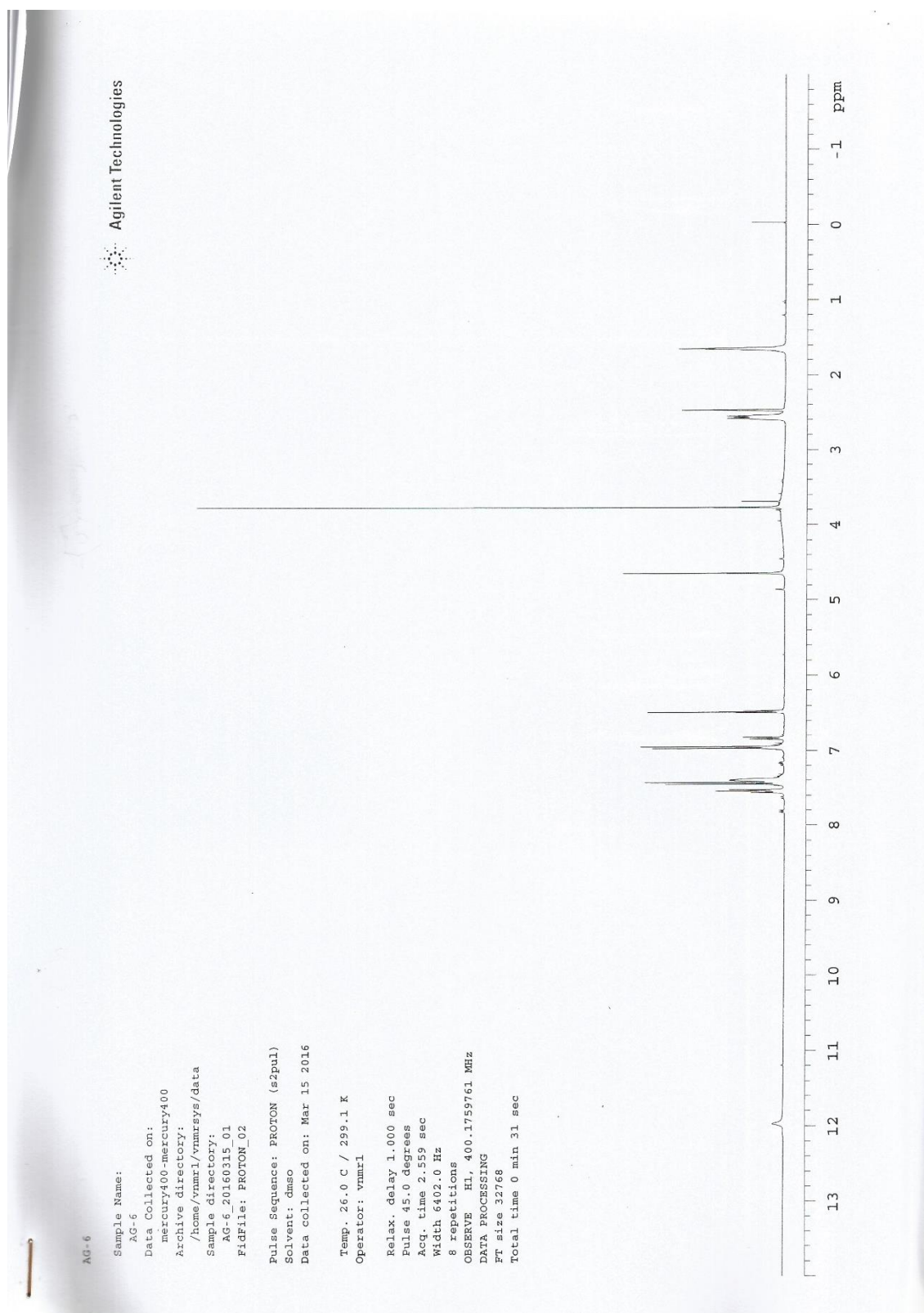
DBE Range: not fixed
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

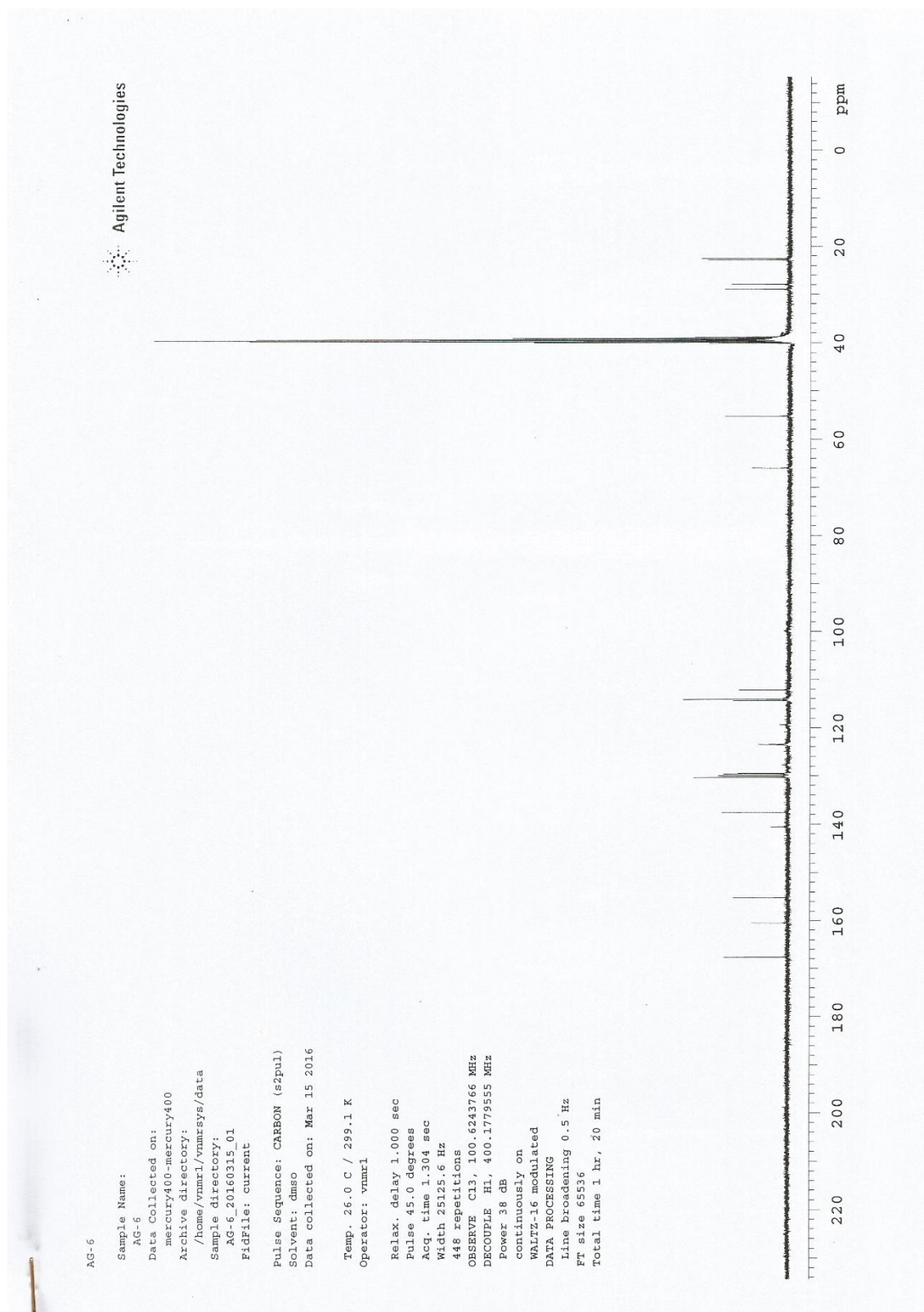
Event#: 1 MS(E+) Ret. Time : 7.067 -> 7.387 Scan#: 1061 -> 1109



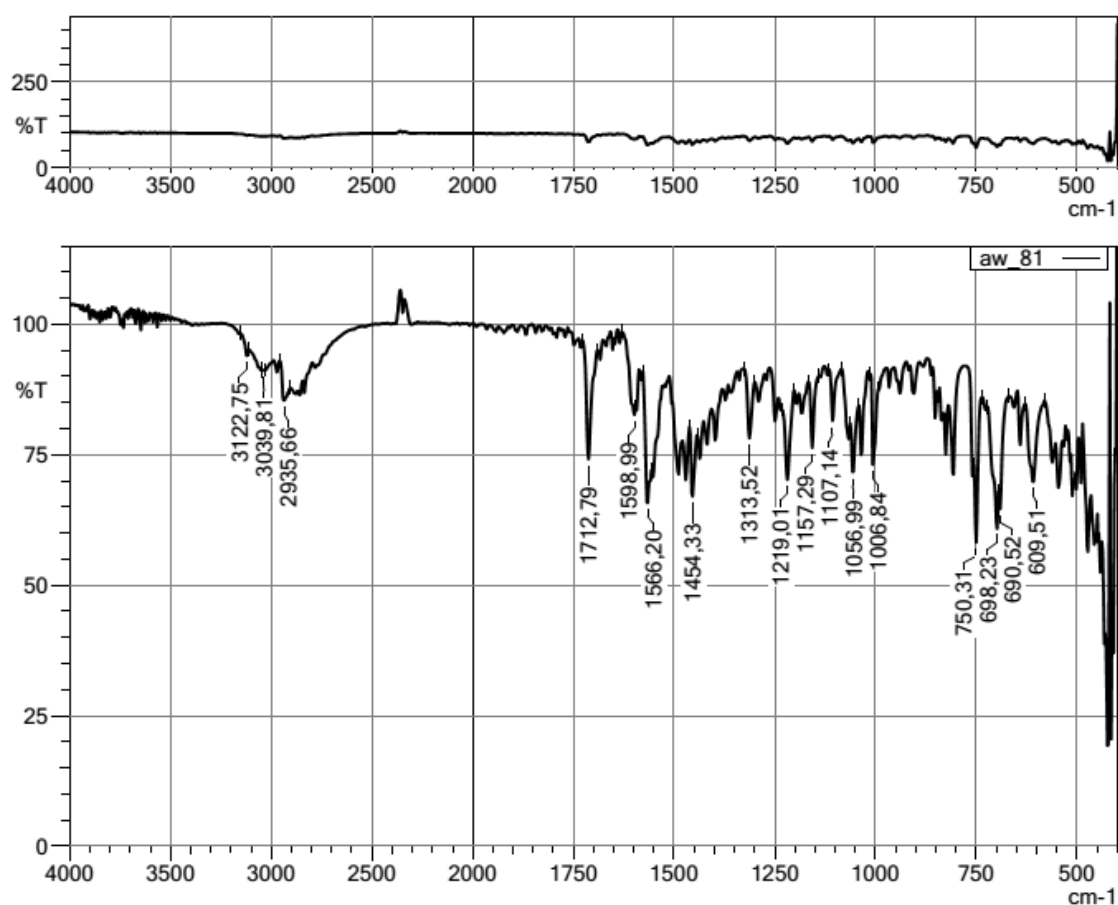
^1H NMR spectrum of the compound 4e



^{13}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\AW-8_9.lcd

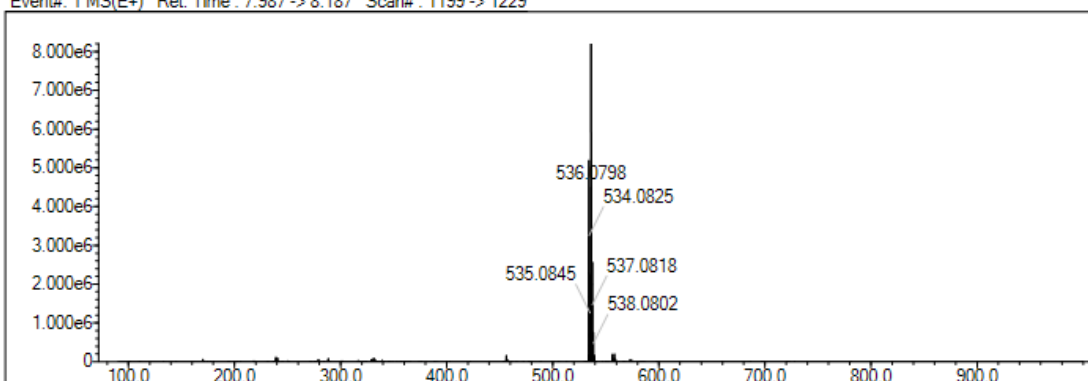
Elmt	Val	Mini	Max	Elmt	Val	Mini	Max	Elmt	Val	Mini	Max	Elmt	Val	Mini	Max	Use Adduct
H	1	20	35	O	2	2	4	Cl	1	0	1	I	3	0	0	H
C	4	26	30	F	1	0	1	Br	1	0	1					
N	3	3	4	S	2	1	1	Ru	2	0	0					

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

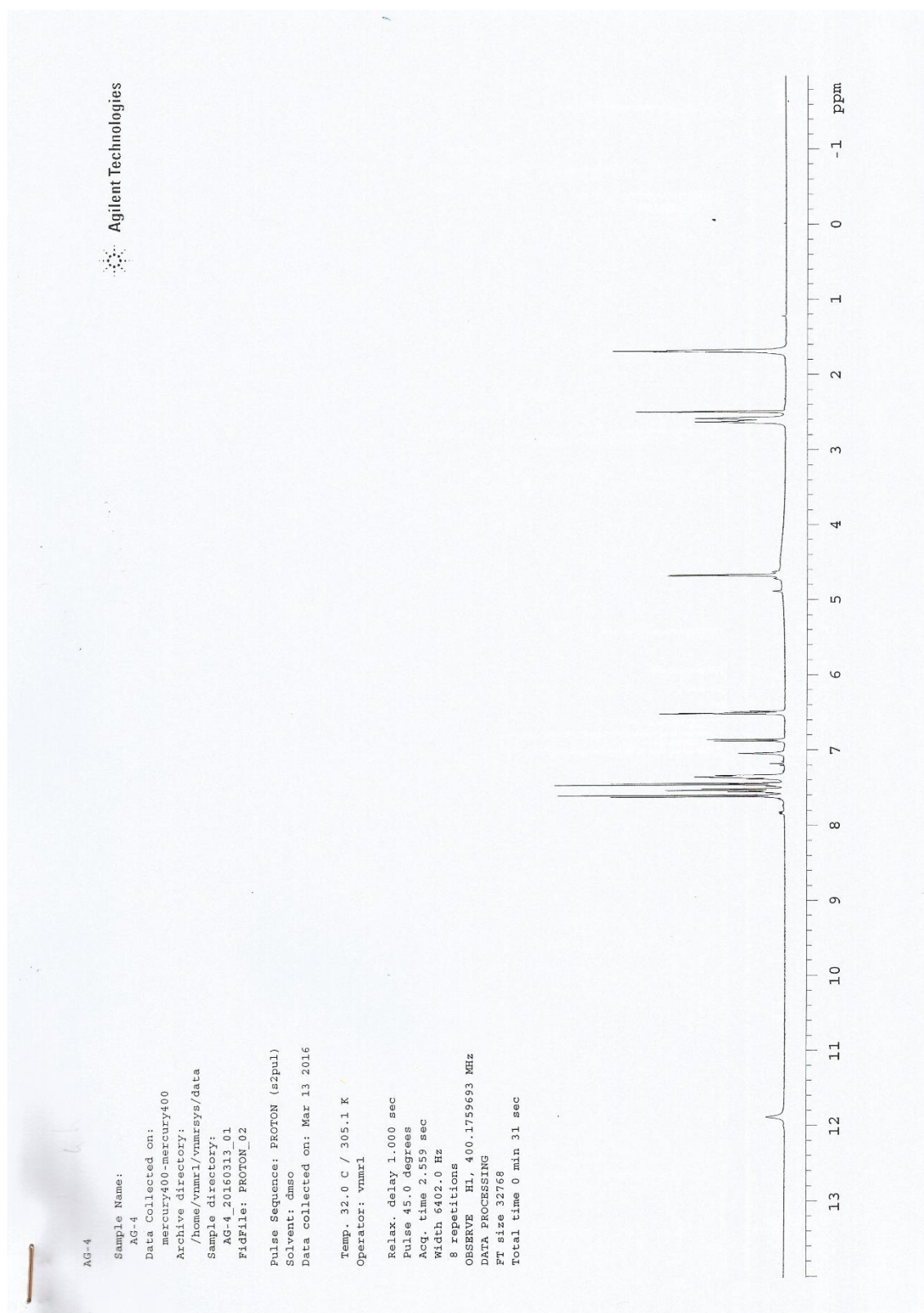
DBE Range: not fixed
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

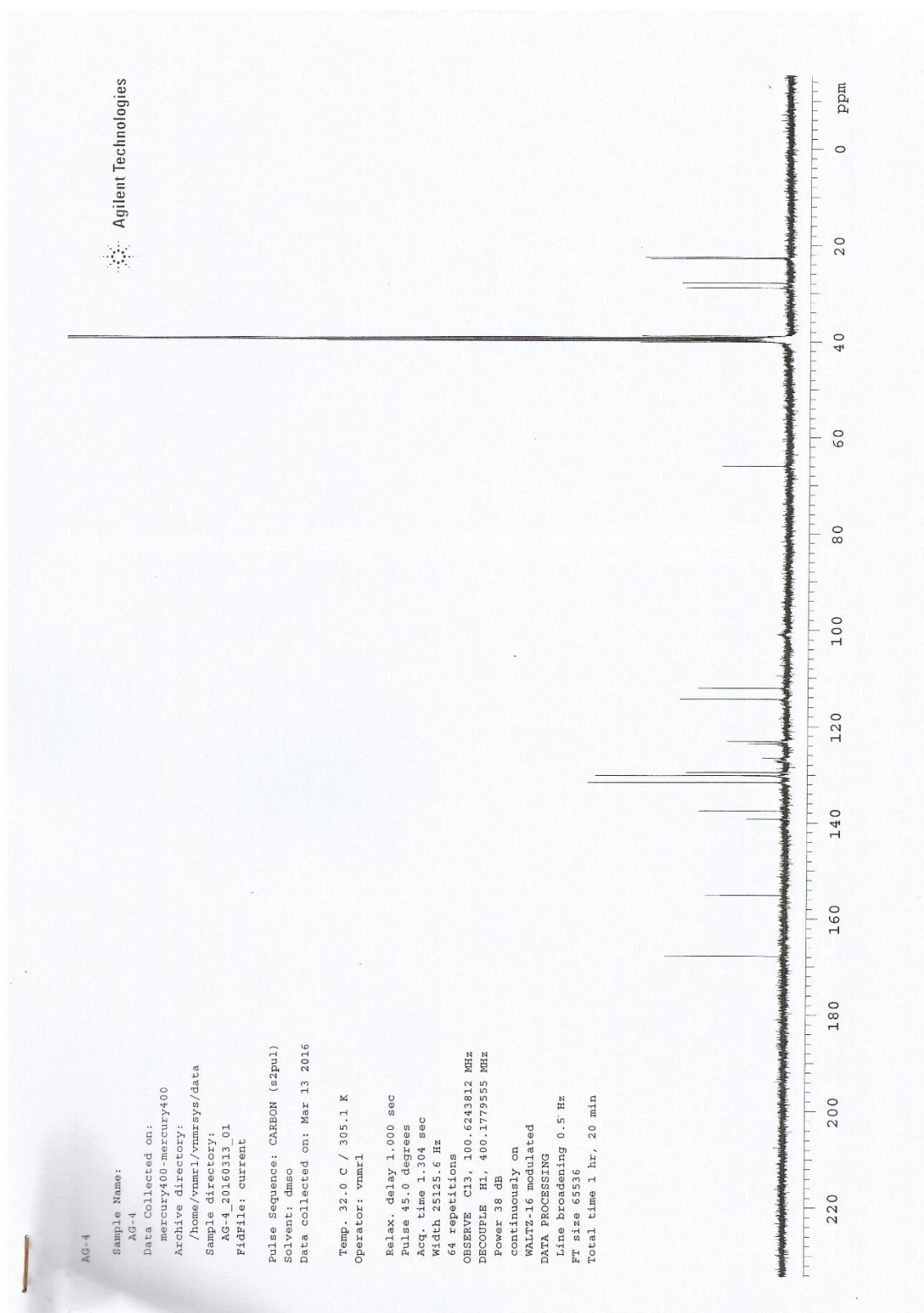
Event#: 1 MS(E+) Ret. Time: 7.987 -> 8.187 Scan#: 1199 -> 1229



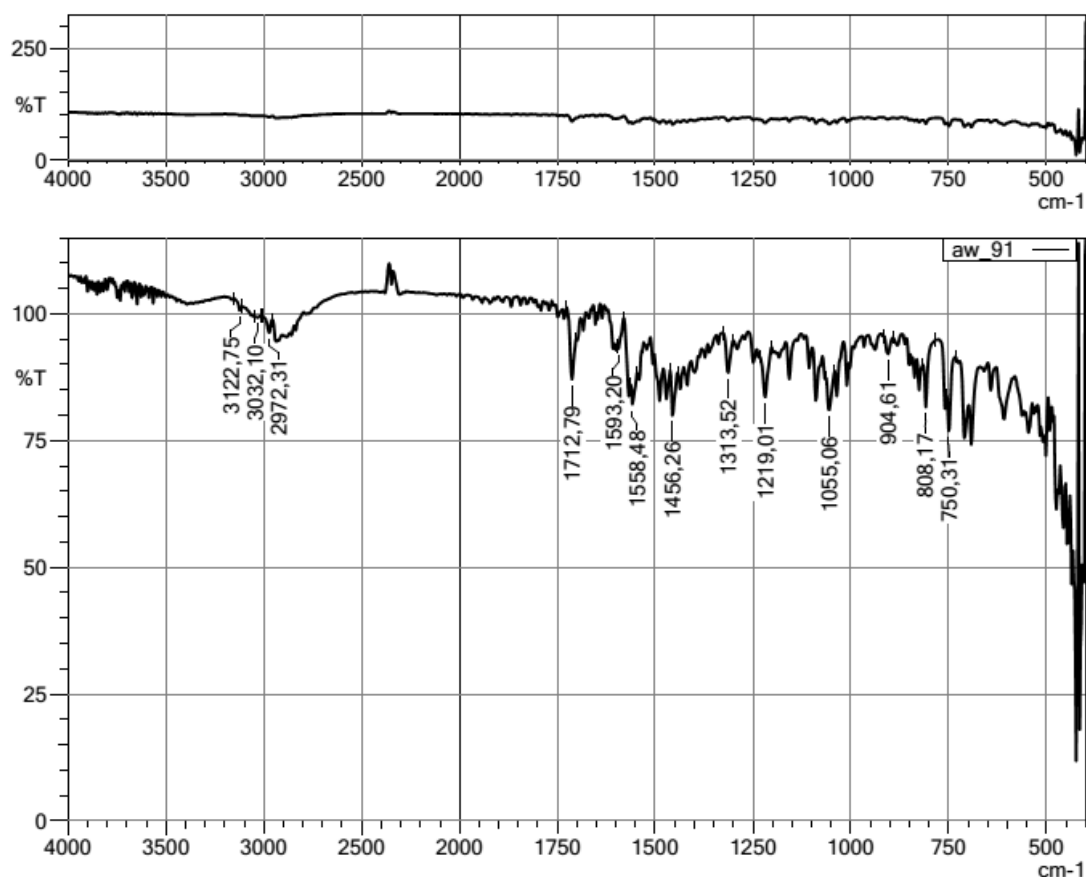
^1H NMR spectrum of the compound 4f



^{13}C 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

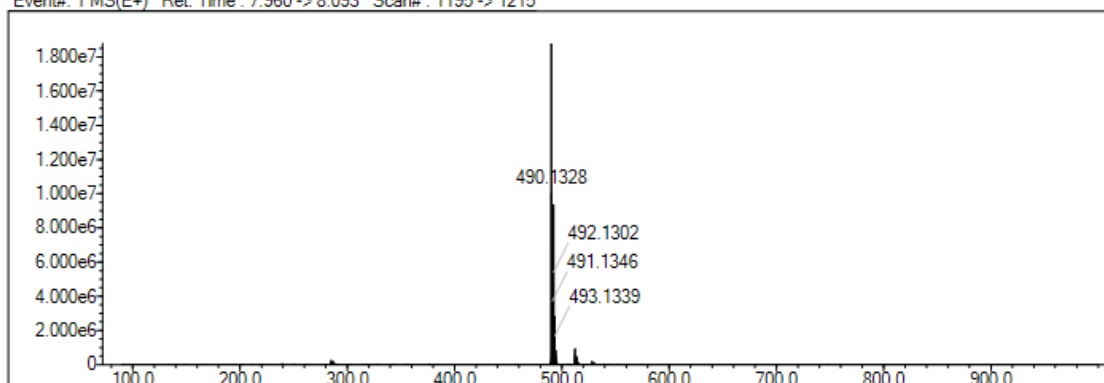
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	20	35	O	2	2	4	Cl	1	0	1	I	3	0	0	H
C	4	26	30	F	1	0	1	Br	1	0	1					
N	3	3	4	S	2	1	1	Ru	2	0	0					

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

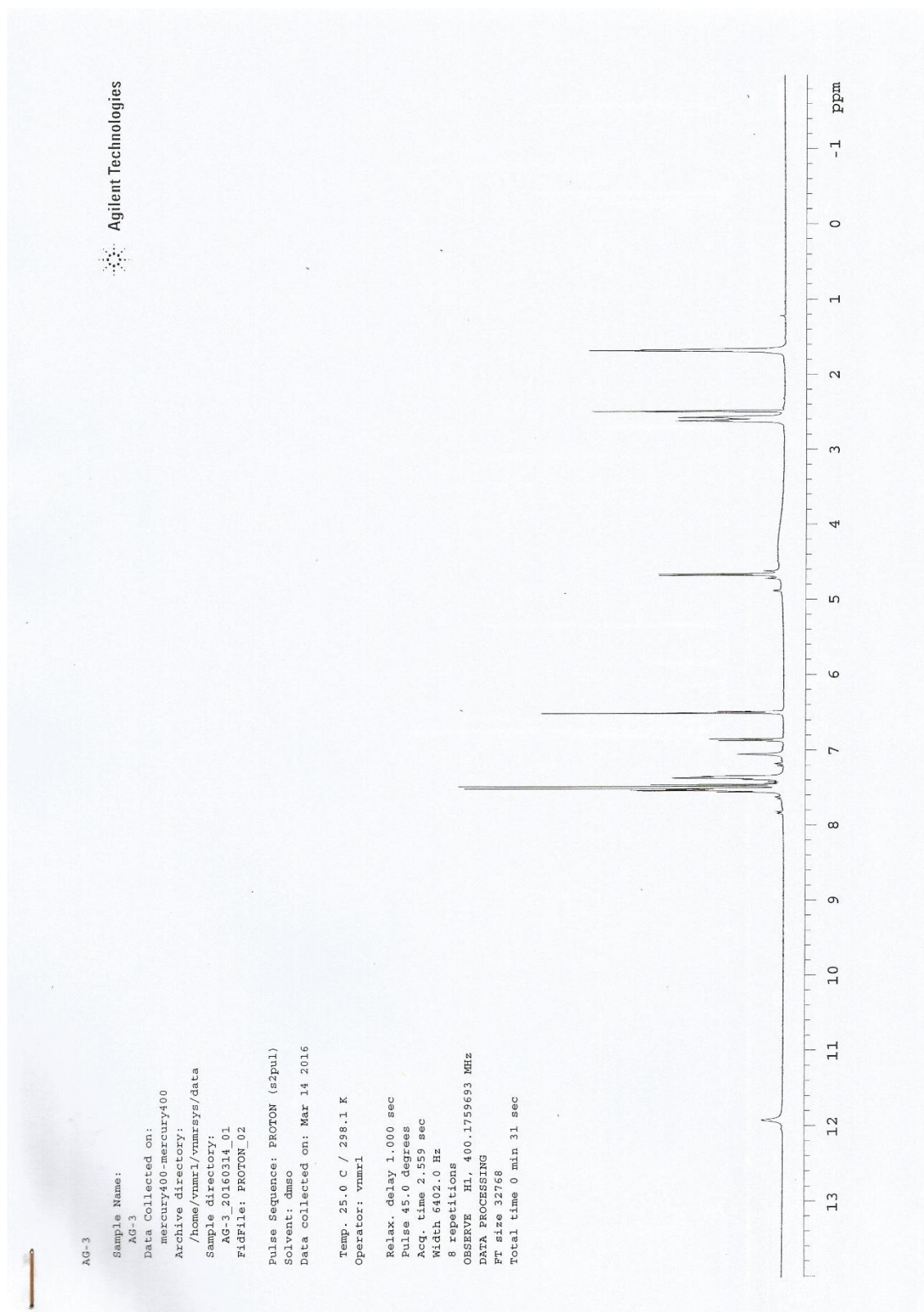
DBE Range: not fixed
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

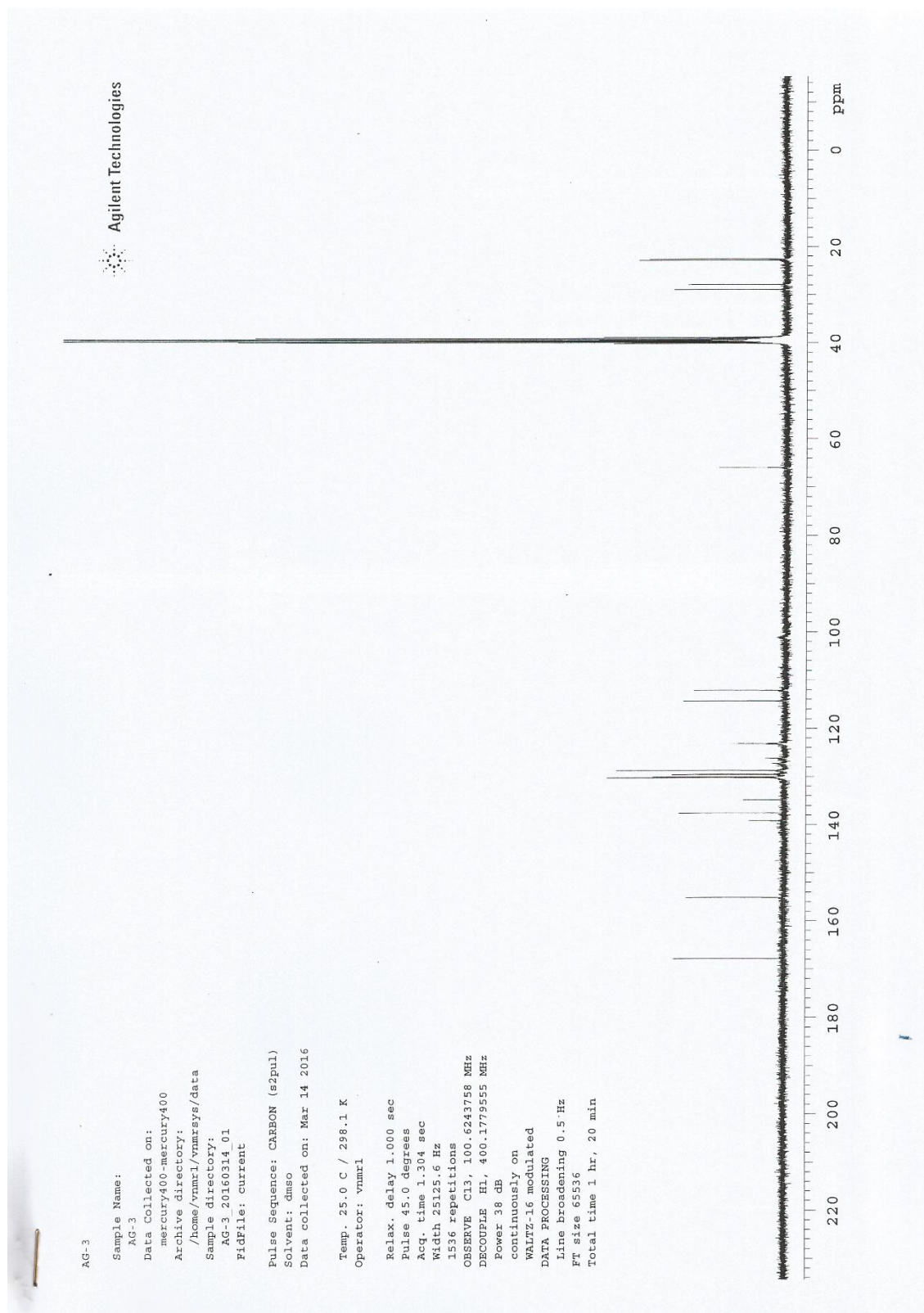
Event#: 1 MS(E+) Ret. Time : 7.960 -> 8.093 Scan# : 1195 -> 1215



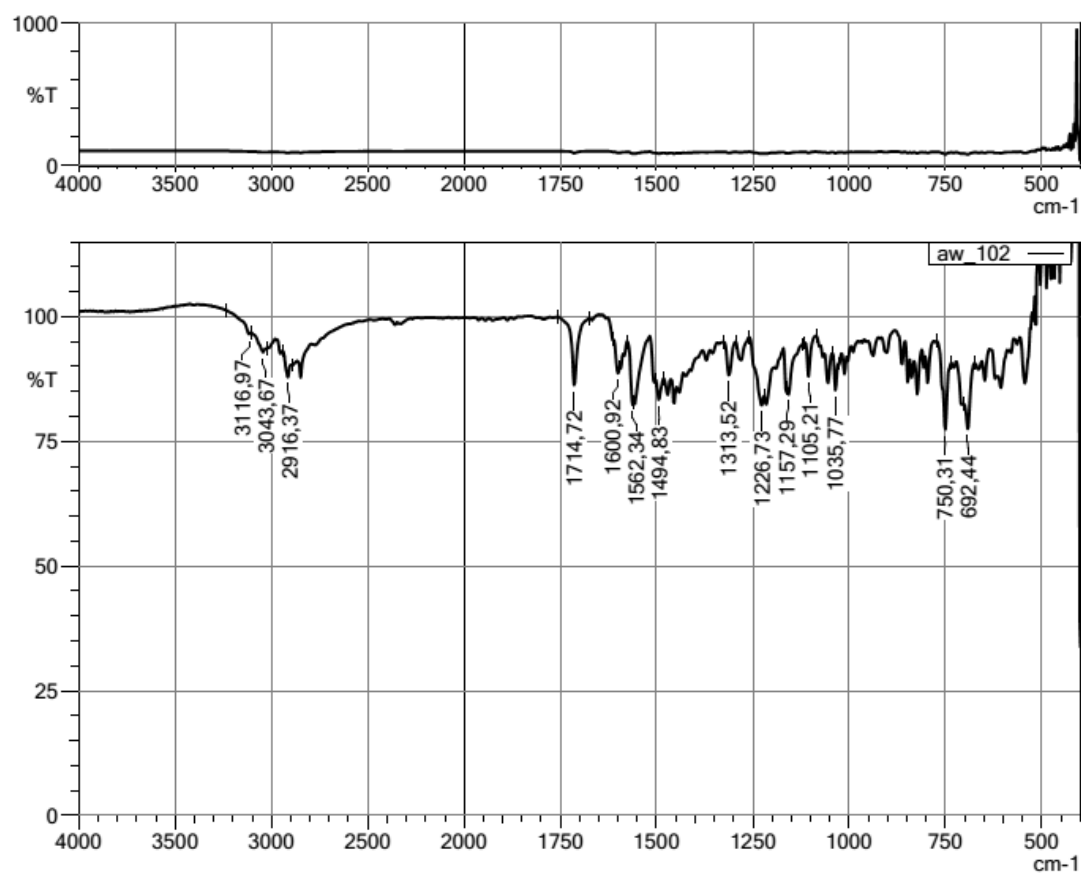
^1H NMR spectrum of the compound 4g



^{13}C 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\AW-10_13.lcd

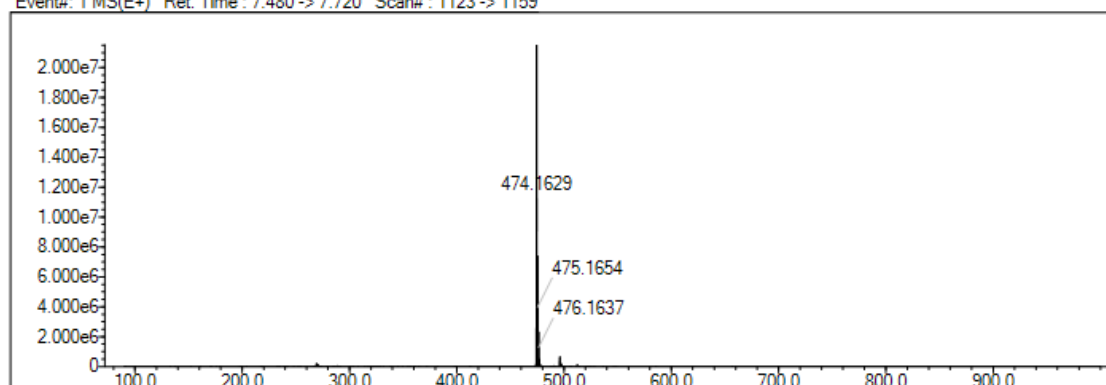
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	20	35	O	2	2	4	Cl	1	0	2	I	3	0	0	H
C	4	26	30	F	1	0	1	Br	1	0	1					
N	3	3	4	S	2	1	1	Ru	2	0	0					

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

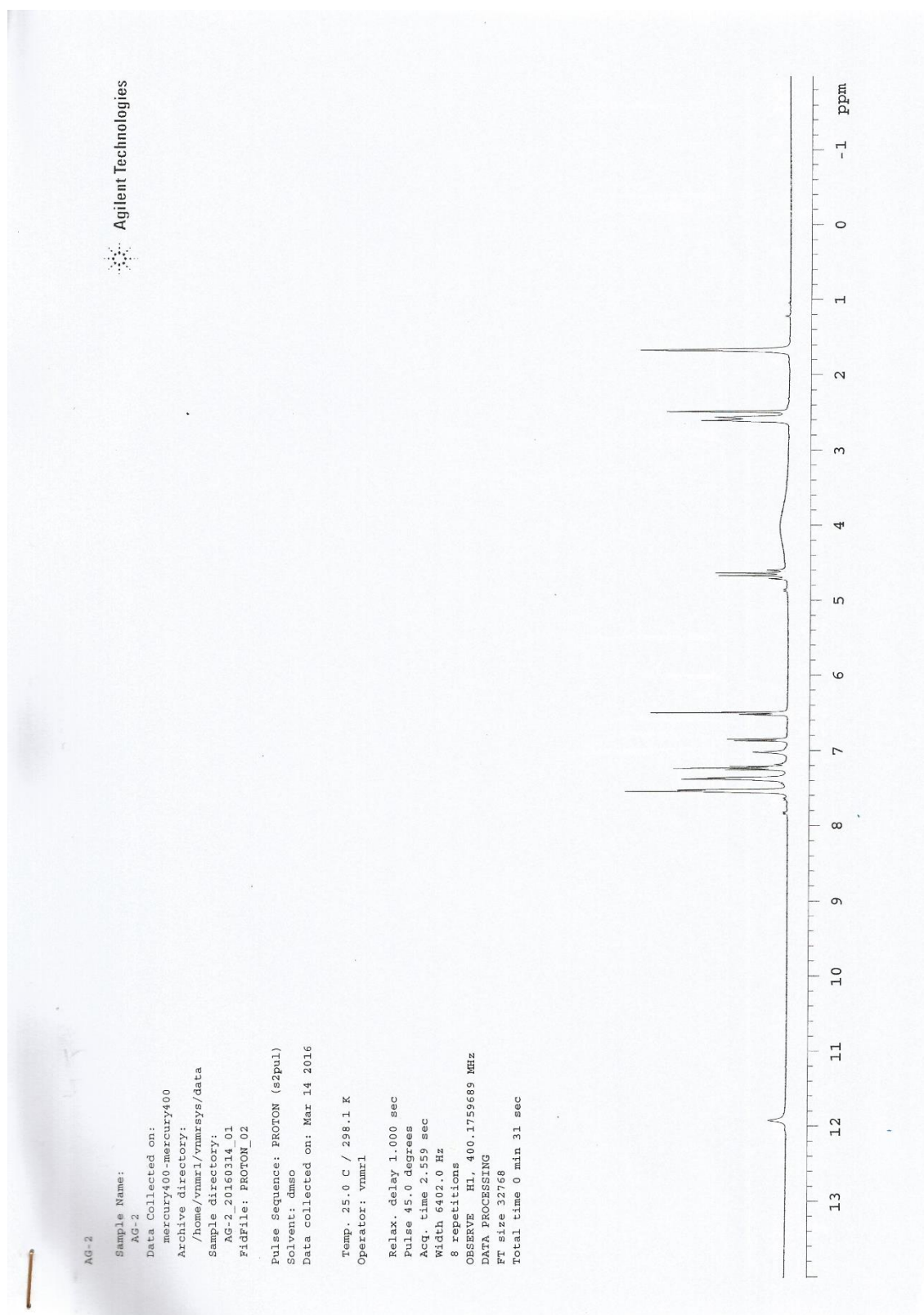
DBE Range: not fixed
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

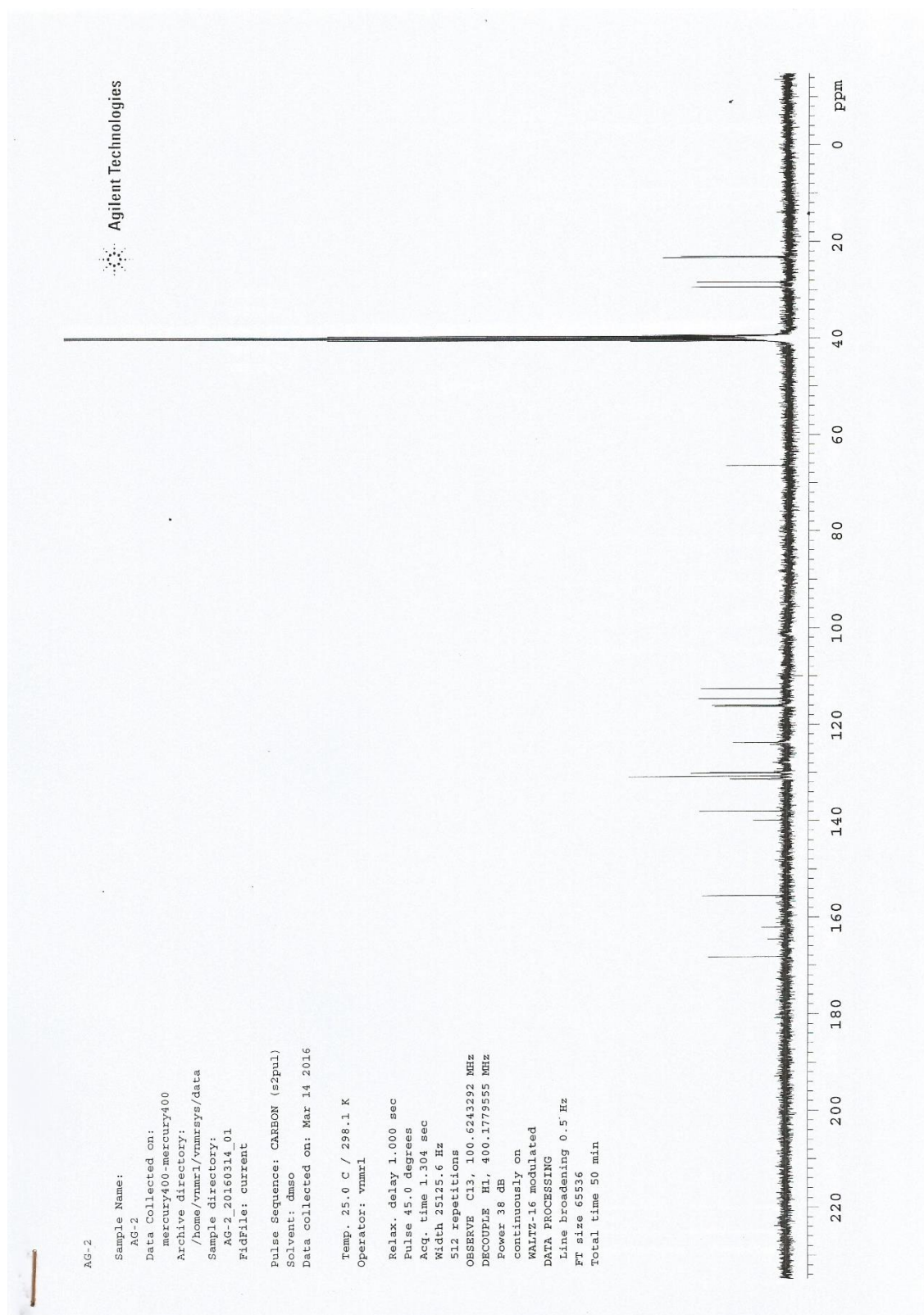
Event#: 1 MS(E+) Ret. Time : 7.480 -> 7.720 Scan#: 1123 -> 1159



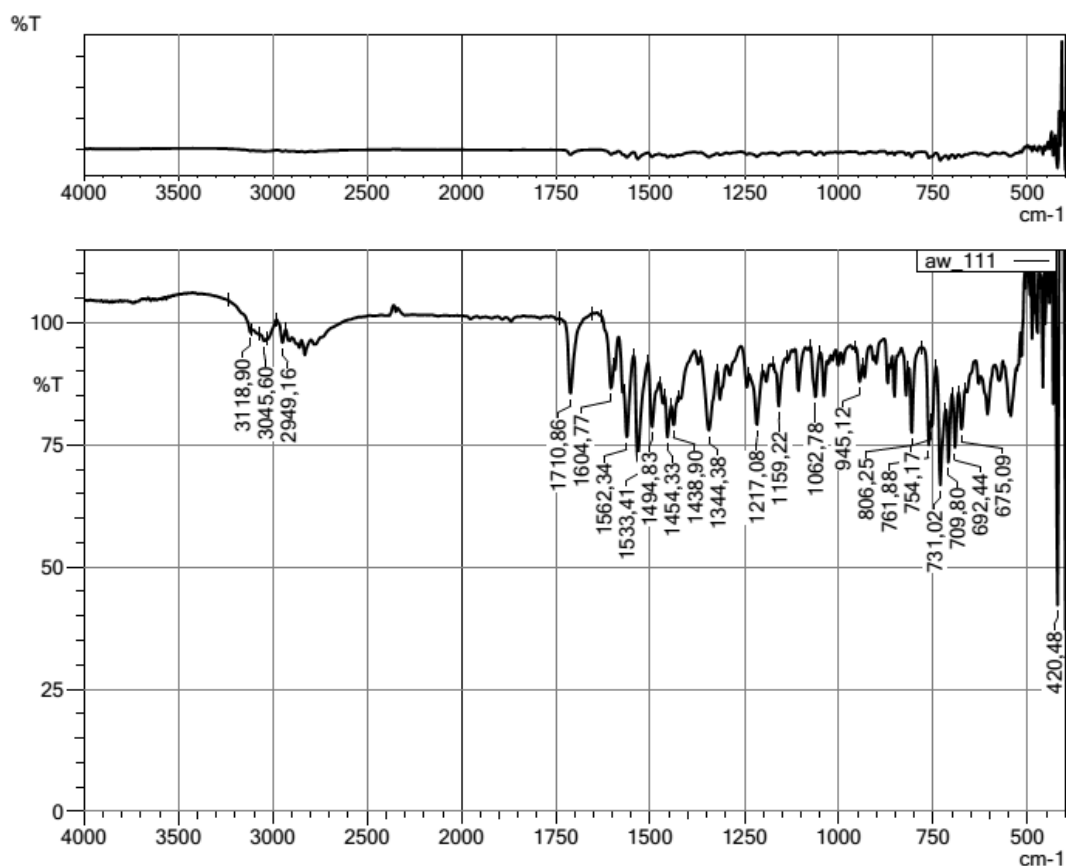
- ^1H NMR spectrum of the compound 4h



^{13}C NMR spectrum of the compound 4h



-IR spectrum of the compound 4i



-HRMS spectrum of the compound 4i

Data File: C:\LabSolutions\Data\Analiz\Lyuittas\AW-11_10.lcd

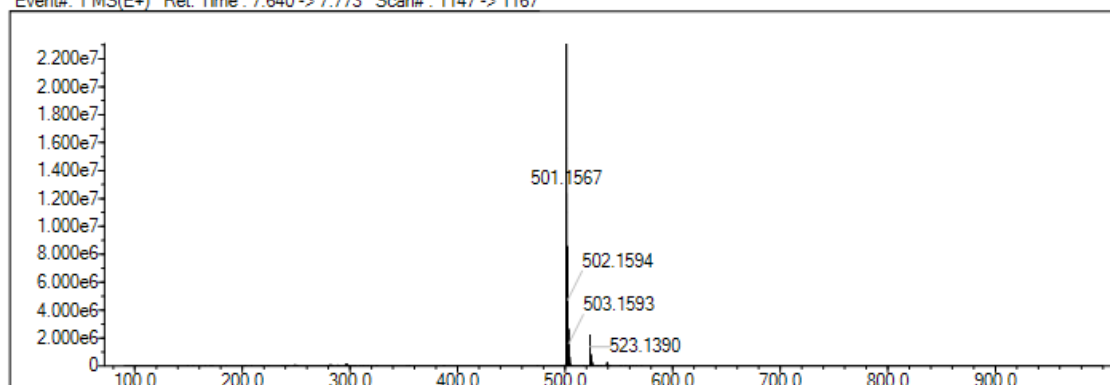
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	20	35	O	2	2	4	Cl	1	0	1	I	3	0	0	H
C	4	26	30	F	1	0	1	Br	1	0	1					
N	3	3	4	S	2	1	1	Ru	2	0	0					

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

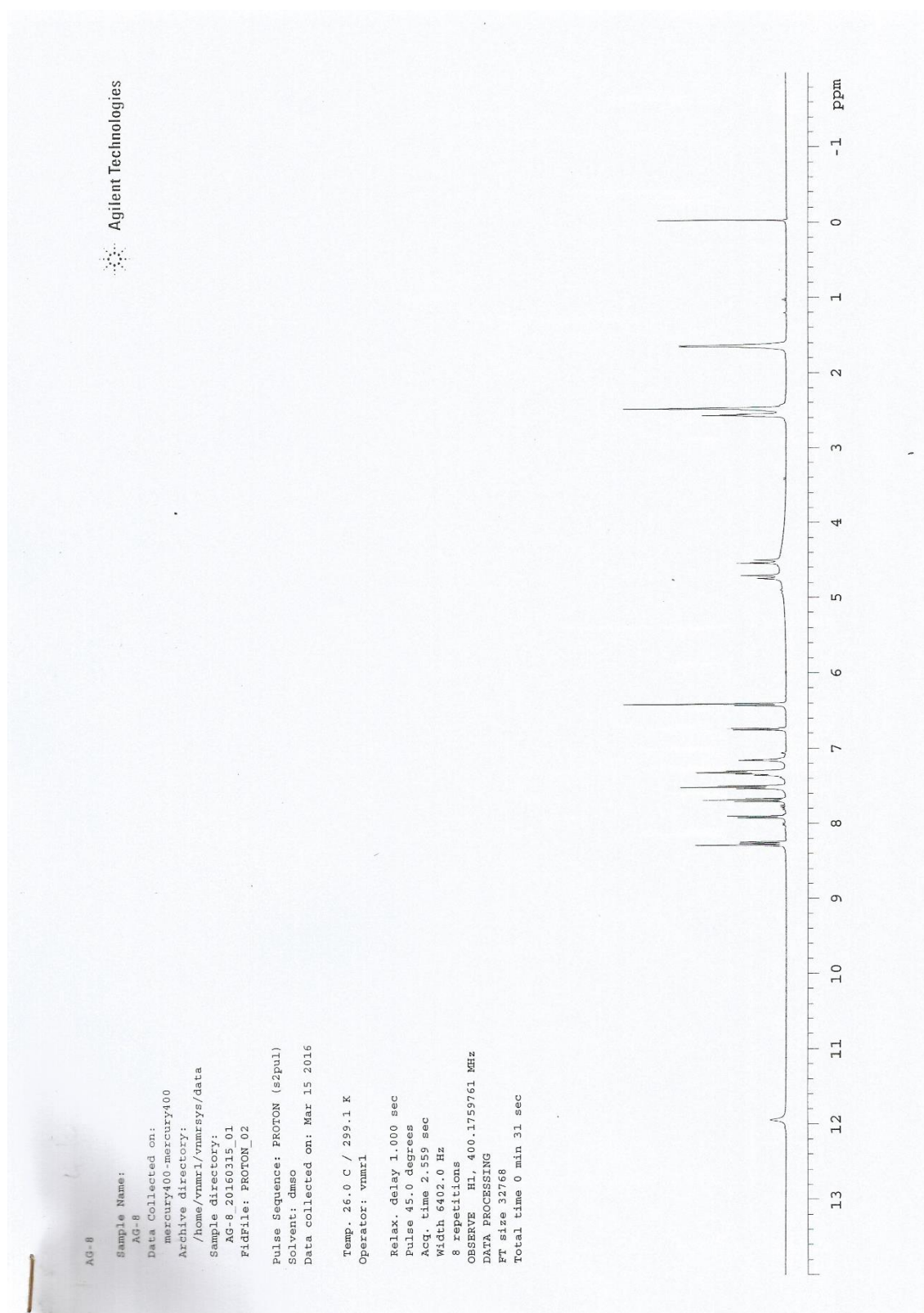
DBE Range: not fixed
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

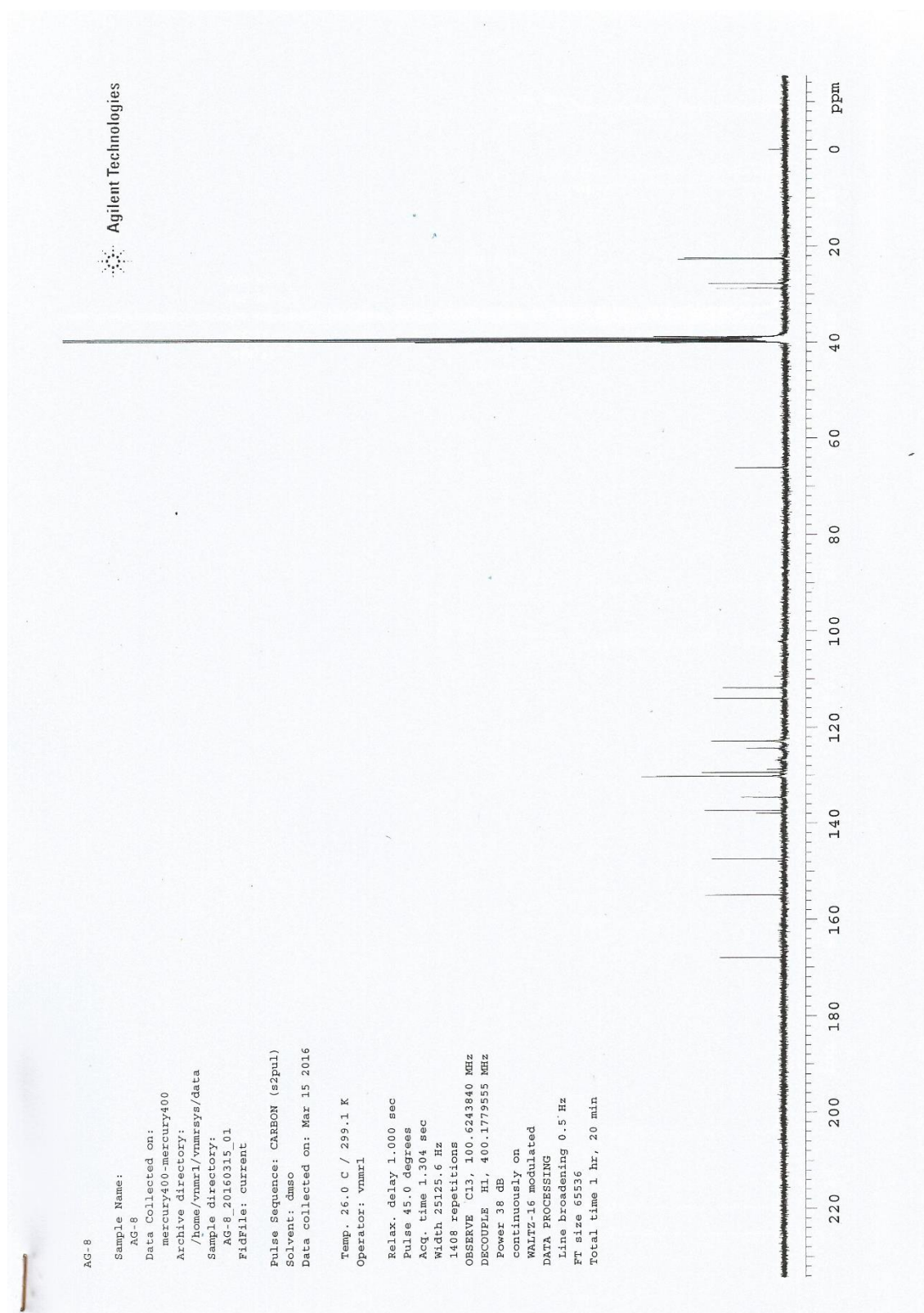
Event#: 1 MS(E+) Ret. Time: 7.640 -> 7.773 Scan#: 1147 -> 1167



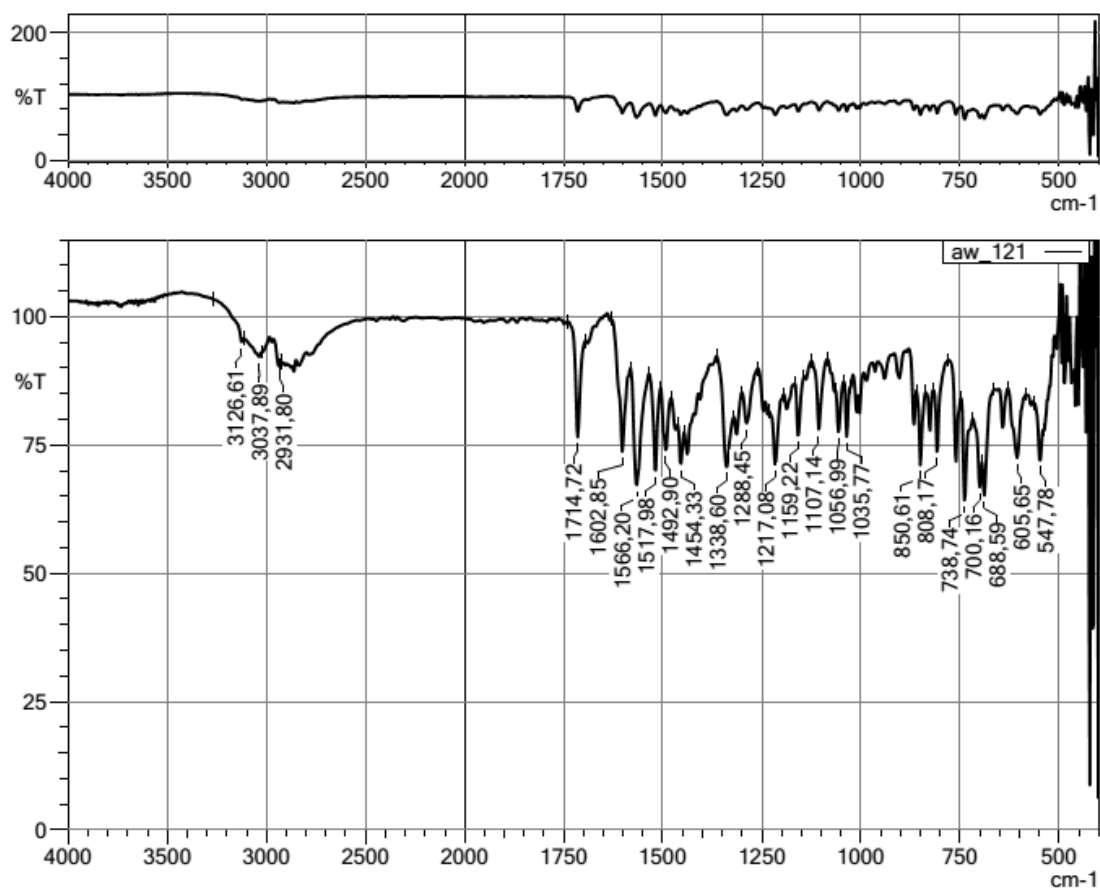
^1H NMR spectrum of the compound 4i



^{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\Lyttas\AW-12_11.lcd

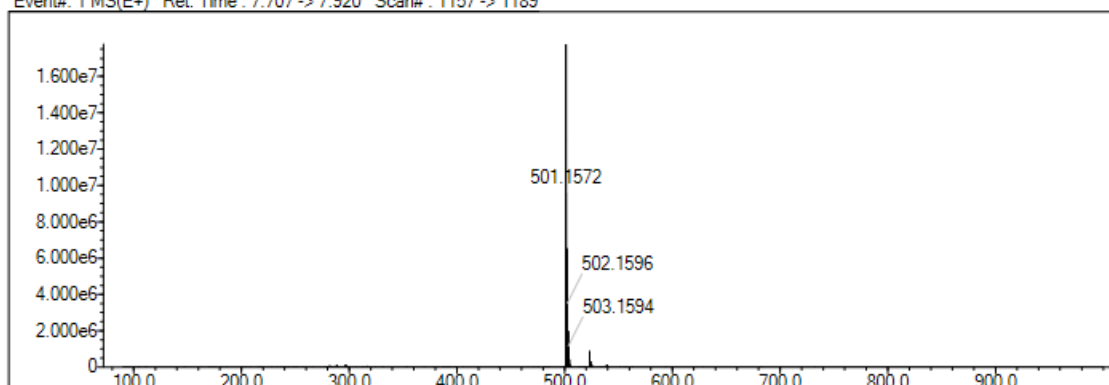
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	20	35	O	2	2	4	Cl	1	0	1	I	3	0	0	H
C	4	26	30	F	1	0	1	Br	1	0	1					
N	3	3	4	S	2	1	1	Ru	2	0	0					

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

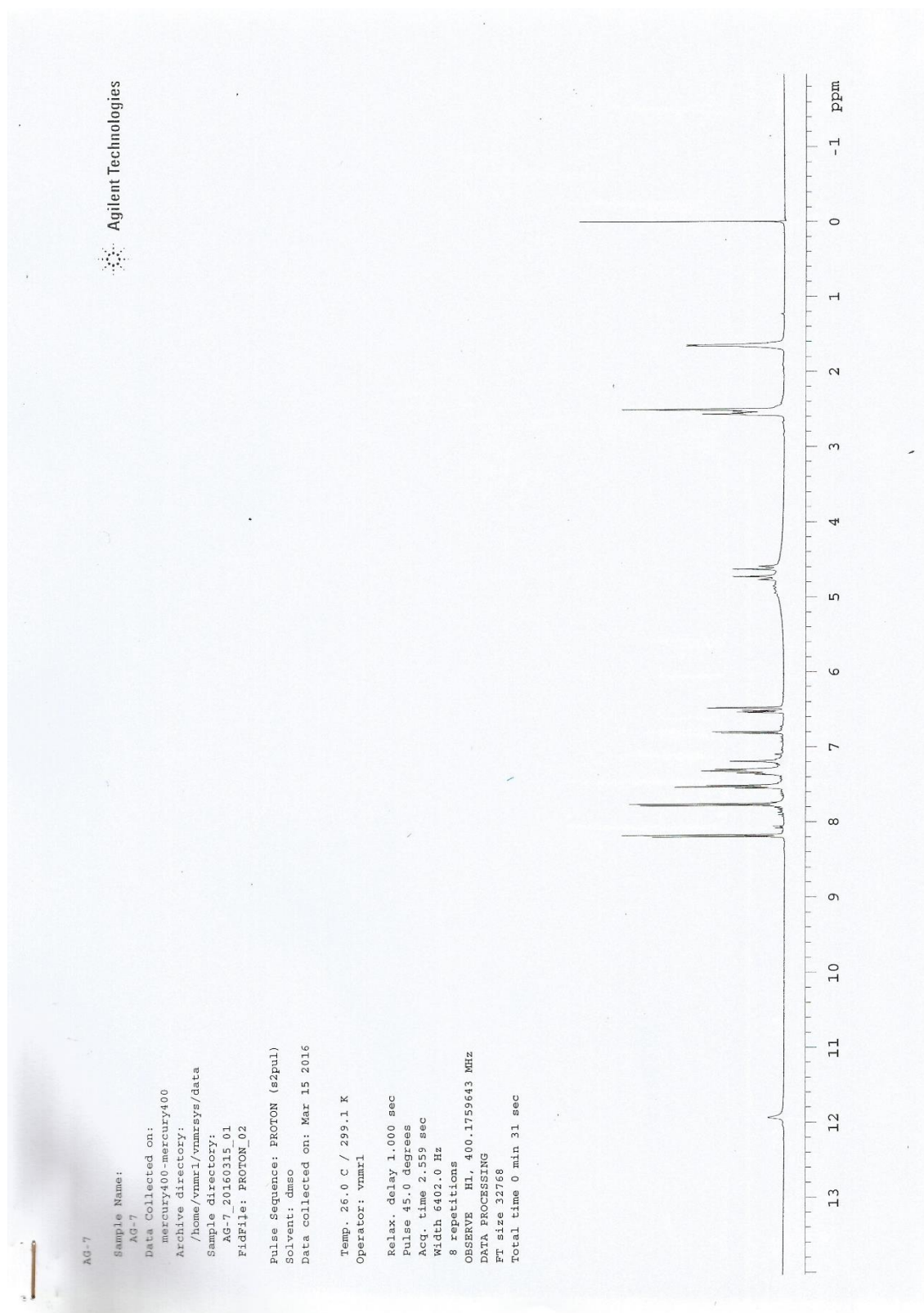
DBE Range: not fixed
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

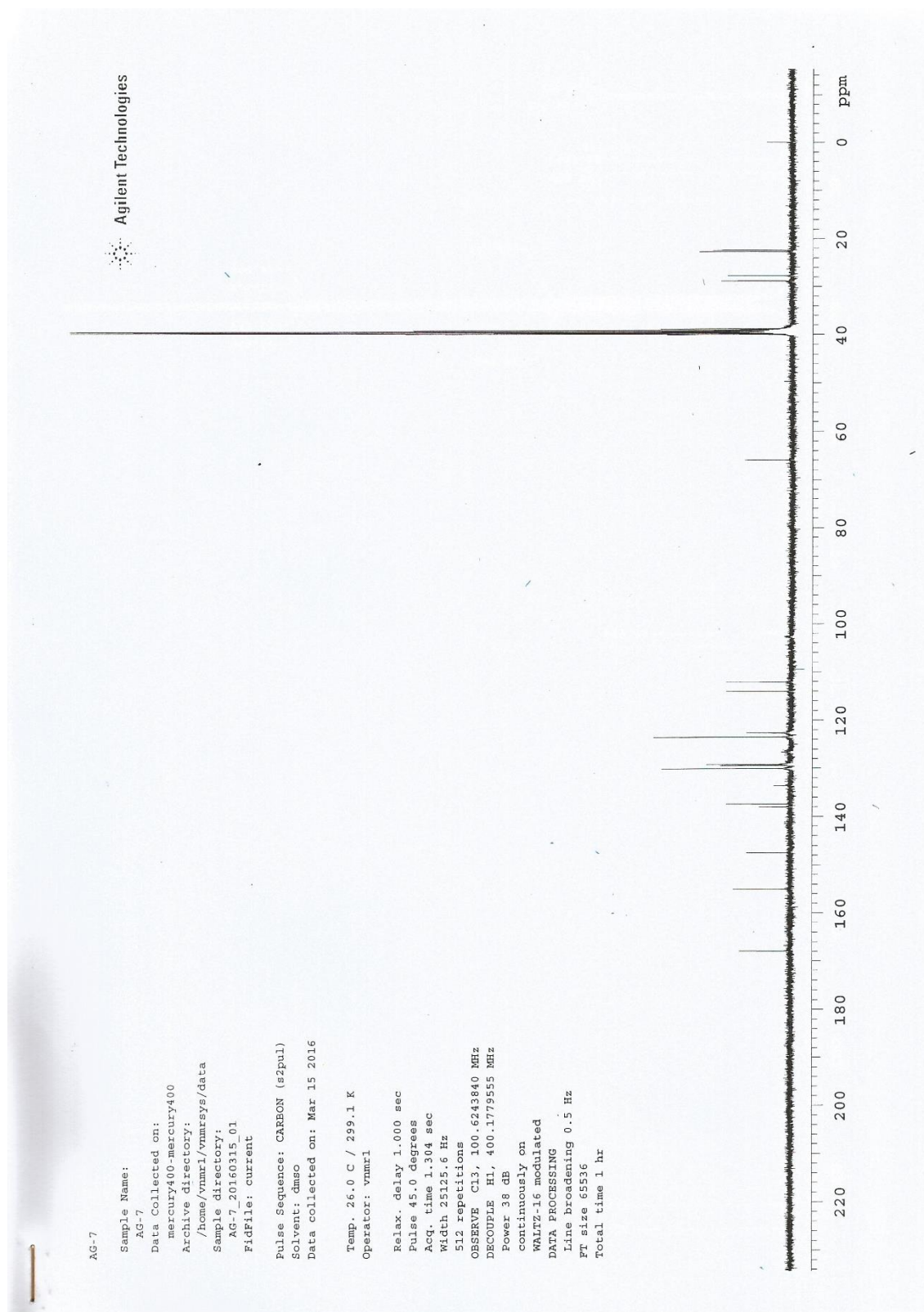
Event#: 1 MS(E+) Ret. Time : 7.707 -> 7.920 Scan# : 1157 -> 1189



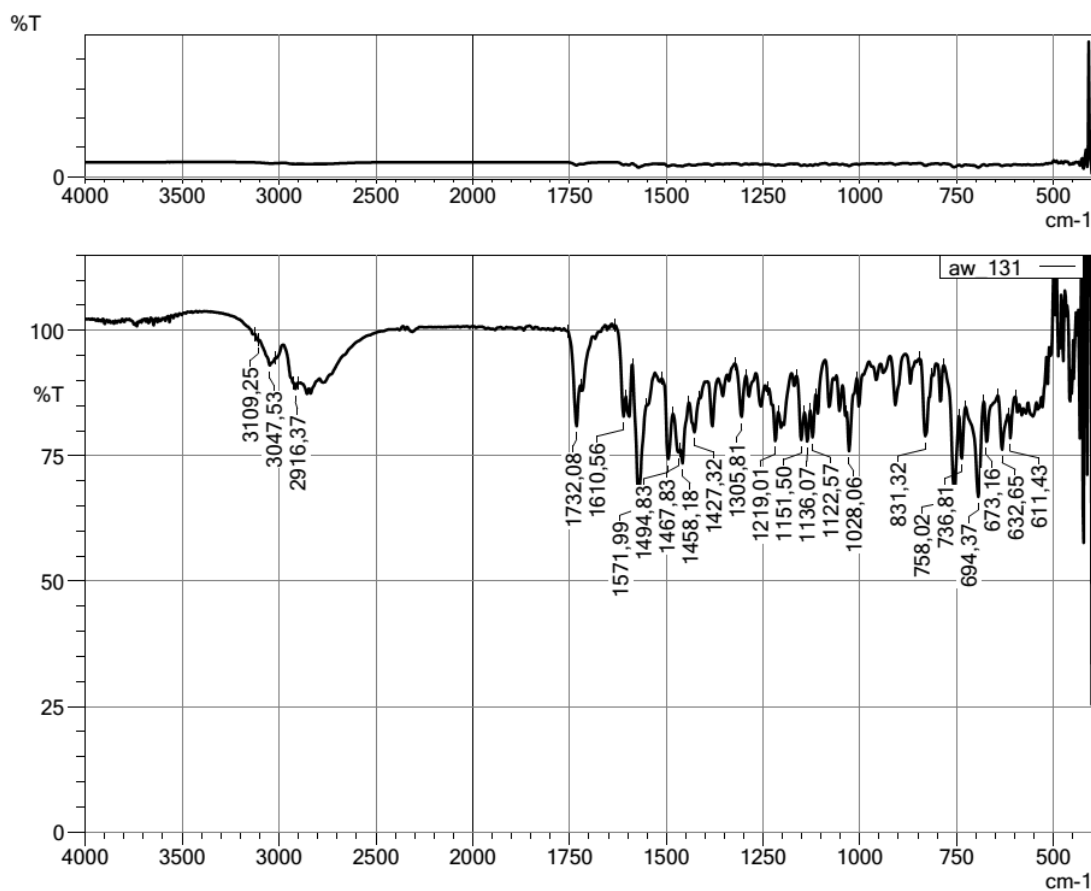
^1H NMR spectrum of the compound 4j



^{13}C NMR spectrum of the compound 4j



- IR spectrum of the compound 4k



-HRMS spectrum of the compound 4k

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

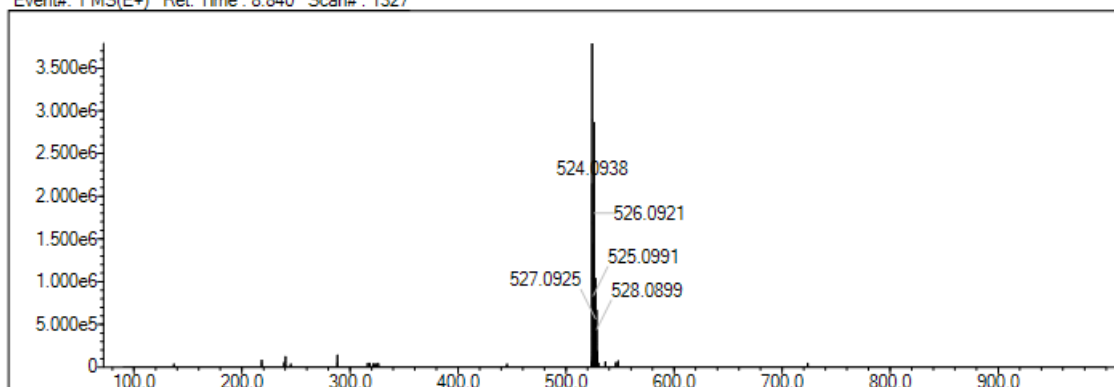
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	20	35	O	2	2	4	Cl	1	0	2	I	3	0	0	H
C	4	26	30	F	1	0	1	Br	1	0	1					
N	3	3	4	S	2	1	1	Ru	2	0	0					

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

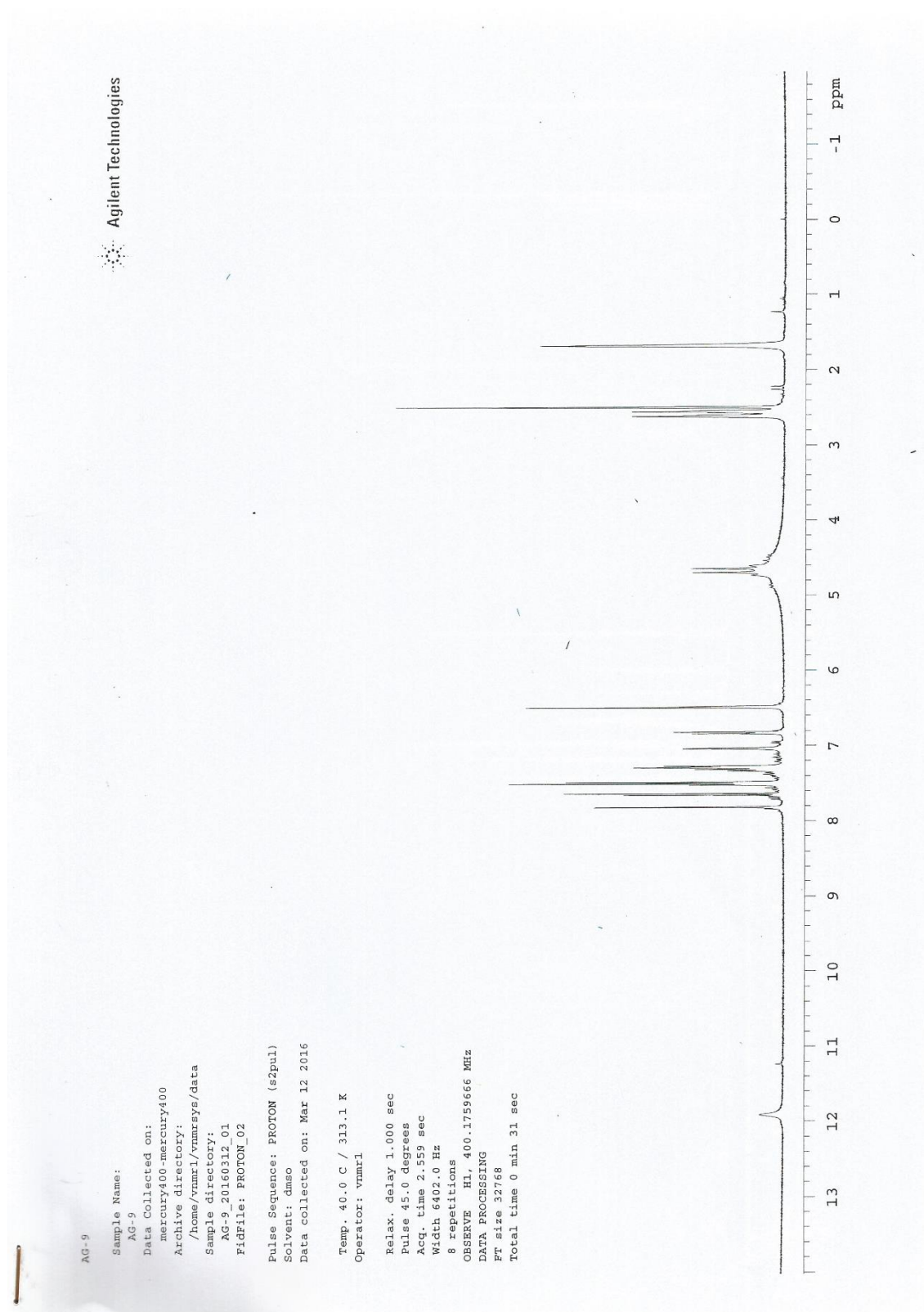
DBE Range: not fixed
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

Event#: 1 MS(E+) Ret. Time: 8.840 Scan#: 1327



^1H NMR spectrum of the compound 4k



^{13}C NMR spectrum of the compound 4k

