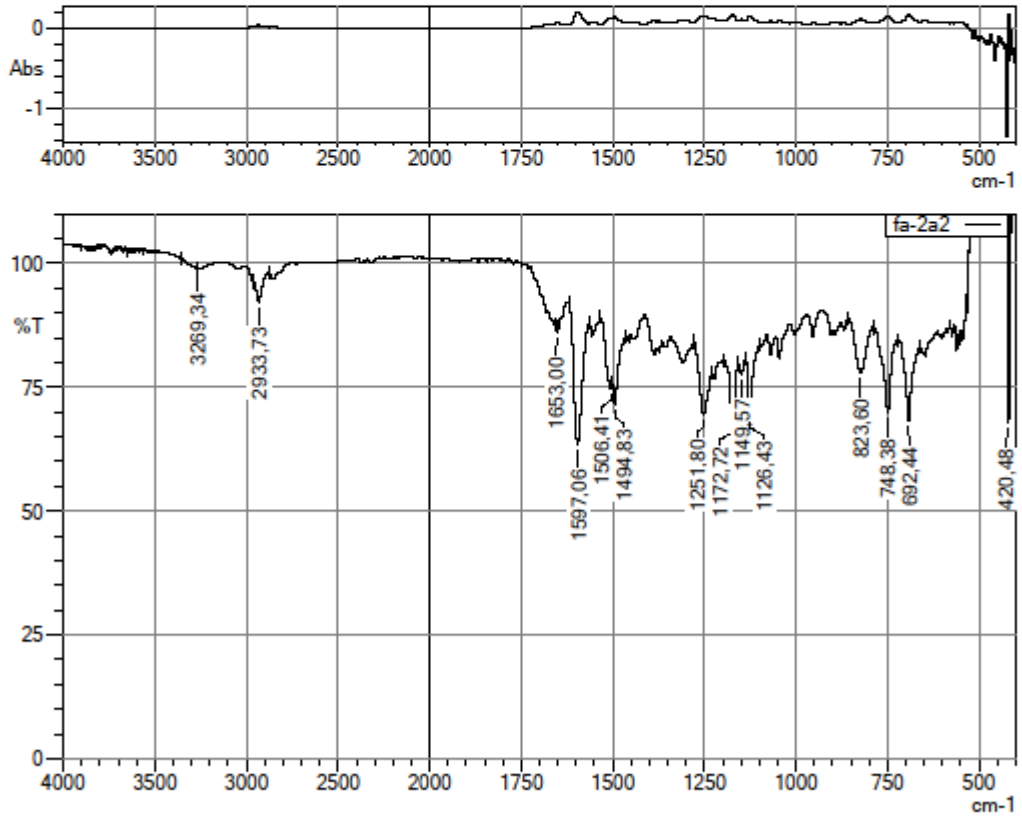
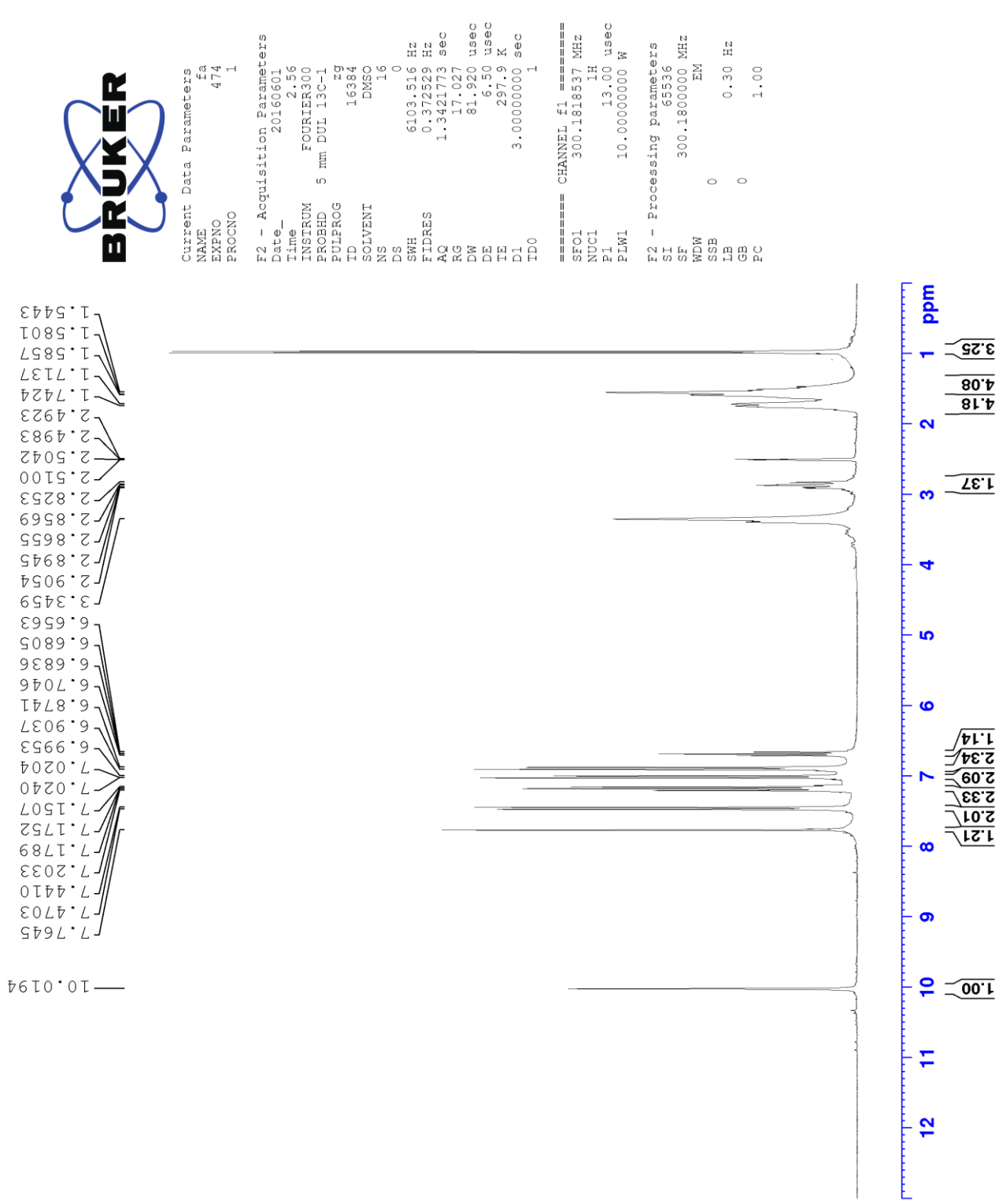
DOPNALAB

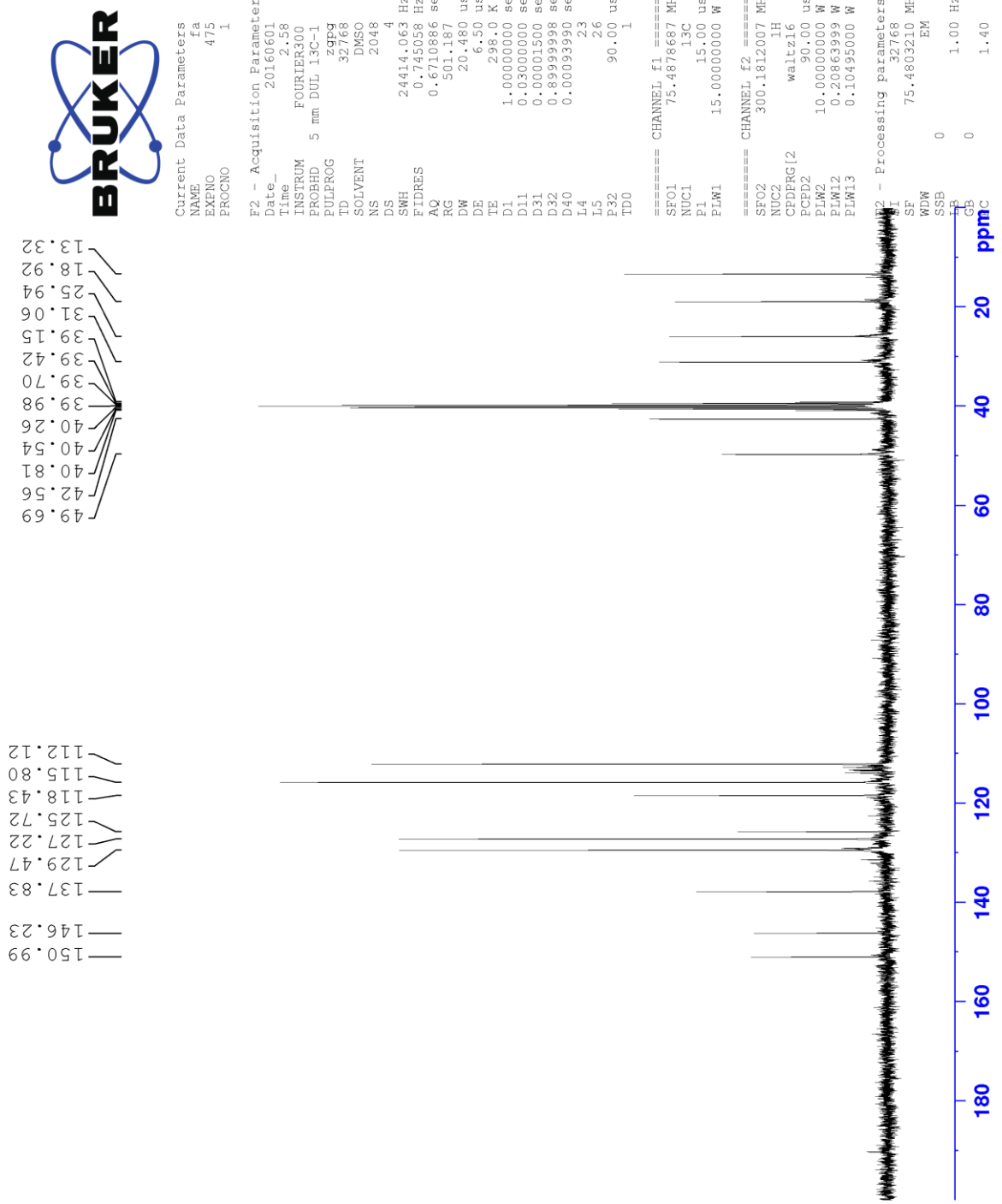
Item	Value
Acquired Date&Time	5.10.2016 09:43:26
Acquired by	System Administrator
Filename	C:\Users\dopnalab\Desktop\derya\fa\fa-2a2.ispd
Spectrum name	fa-2a2
Sample name	fa_2a
Sample ID	
Option	
Comment	
No. of Scans	10
Resolution	4 [cm-1]
Apodization	Happ-Genzel



Spectra 1. IR spectra of the compound 2a



Spectra 2. ^{1}H NMR spectra of the compound 2a



Spectra 3. ^{13}C NMR spectra of the compound 2a

Data File: C:\ LabSolutions\ Data\Analiz\derya\ FA-1_1.lcd

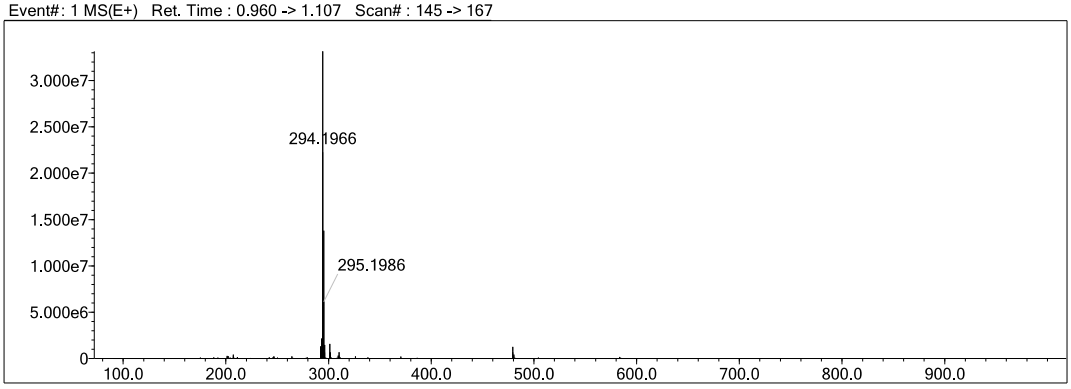
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	50	O	2	0	6	Cl	1	0	0	H
C	4	0	50	F	1	0	0	Br	1	0	0	
N	3	0	3	S	2	0	0	Pd	2	0	0	

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

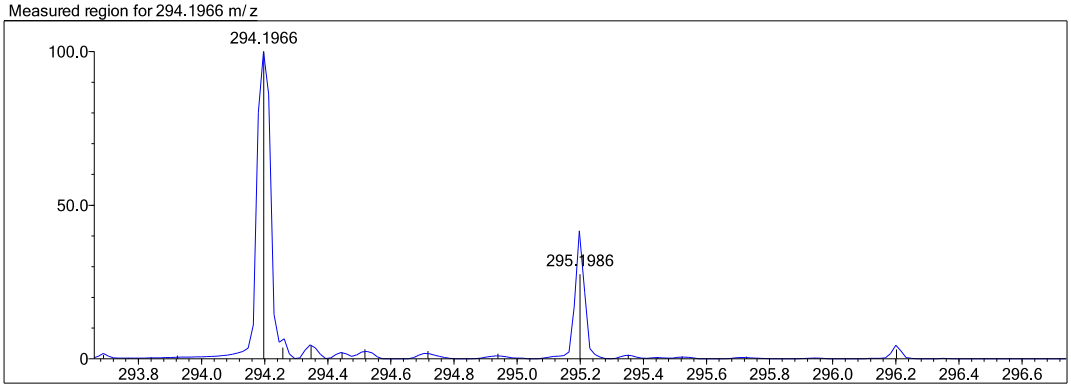
DBE Range: 10.0 - 20.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

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

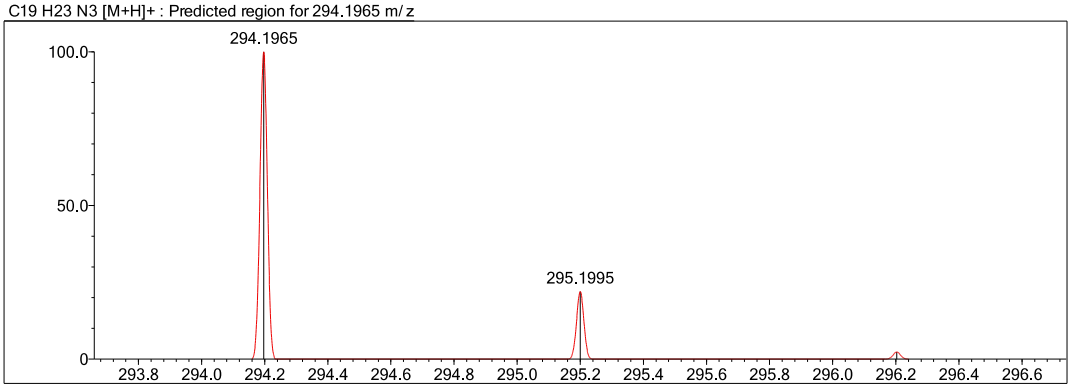
Event#: 1 MS(E+) Ret. Time : 0.960 -> 1.107 Scan# : 145 -> 167



Measured region for 294.1966 m/z



C19 H23 N3 [M+H]+ : Predicted region for 294.1965 m/z

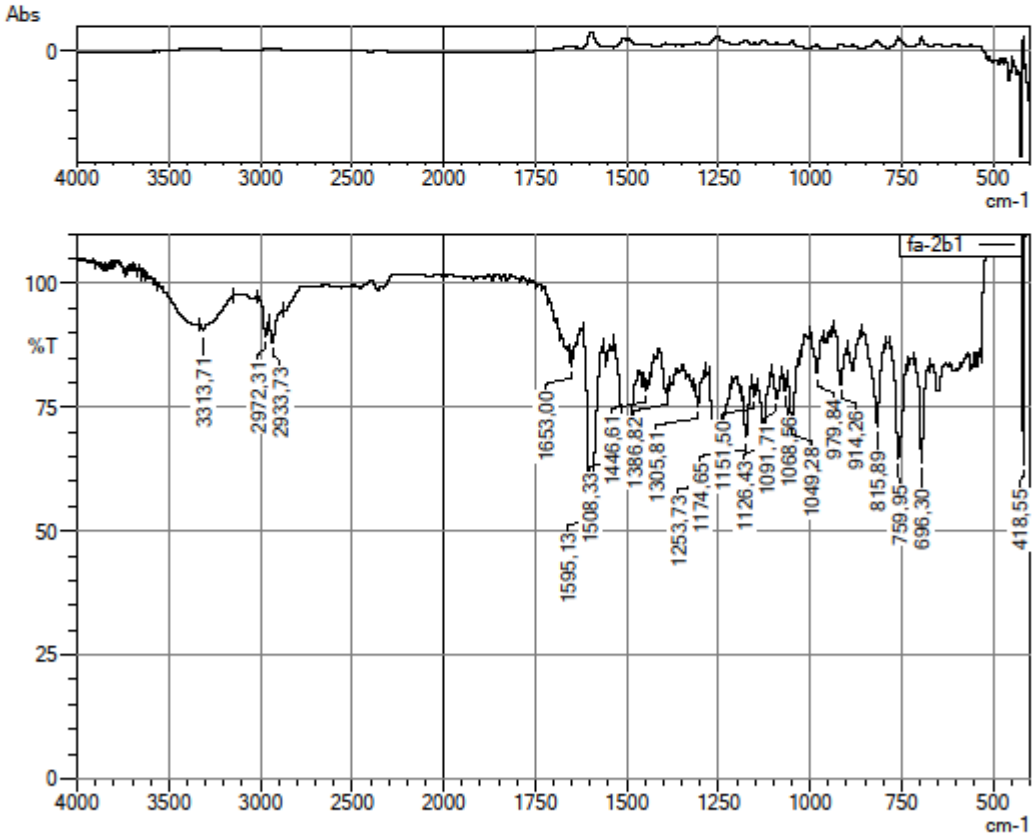


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	68.06	C19 H23 N3	[M+H]+	294.1966	294.1965	0.1	0.34	68.06	10.0

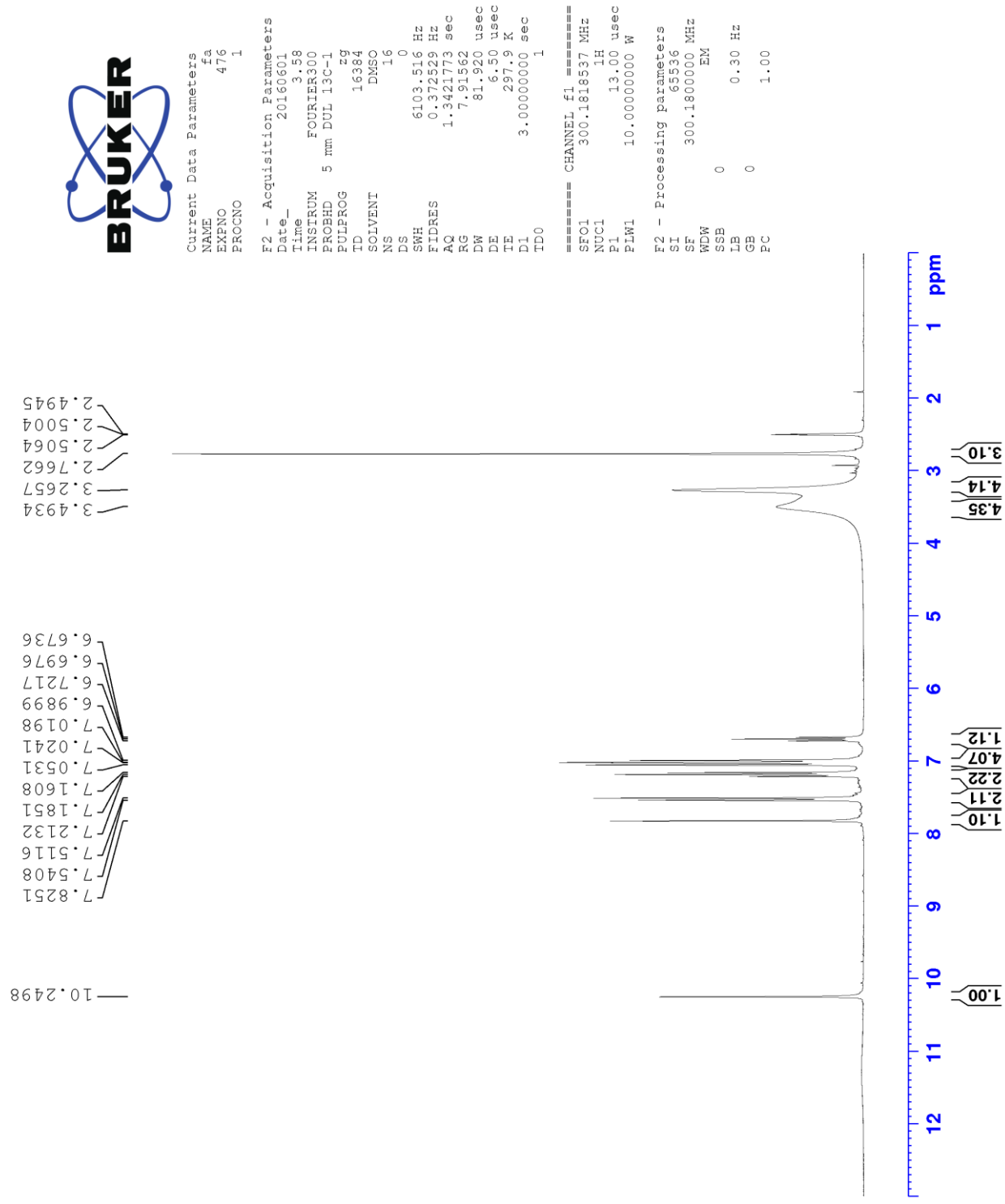
Spectra 4. HRMS spectra of the compound 2a

DOPNALAB

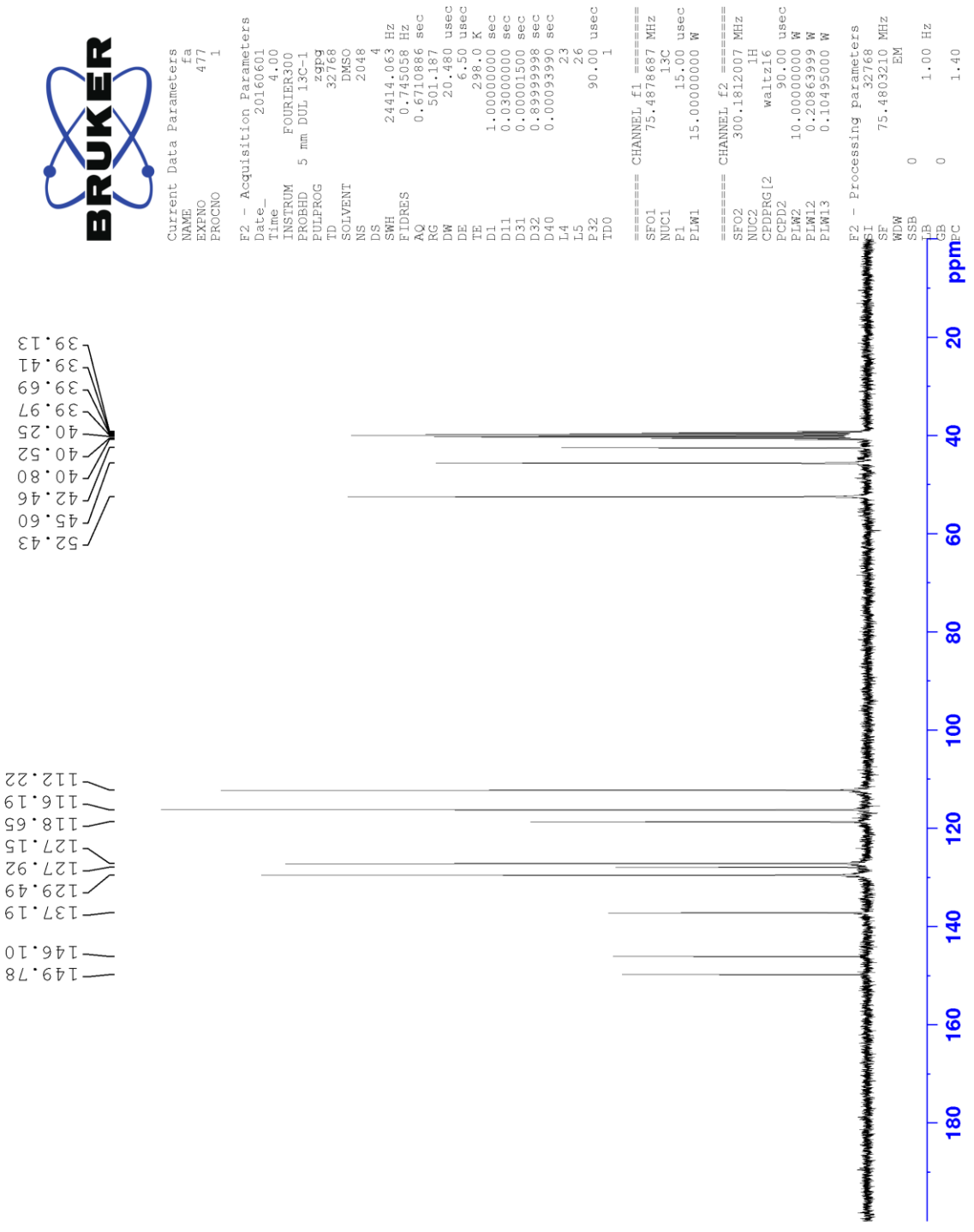
Item	Value
Acquired Date&Time	5.10.2016 09:48:36
Acquired by	System Administrator
Filename	C:\Users\dopnalab\Desktop\derya\fa\fa-2b1.ispd
Spectrum name	fa-2b1
Sample name	fa_2b
Sample ID	
Option	
Comment	
No. of Scans	10
Resolution	4 [cm-1]
Apodization	Happ-Genzel



Spectra 5. IR spectra of the compound 2b



Spectra 6. ^{1}H NMR spectra of the compound 2b



Spectra 7. ^{13}C NMR spectra of the compound 2b

Data File: C:\ LabSolutions\ Data\Analiz\derya\ FA-2_2.lcd

Elmt	Val.	Min	Max
H	1	0	50
C	4	0	50
N	3	0	4

Elmt	Val.	Min	Max
O	2	0	6
F	1	0	0
S	2	0	0

Elmt	Val.	Min	Max
Cl	1	0	0
Br	1	0	0
Pd	2	0	0

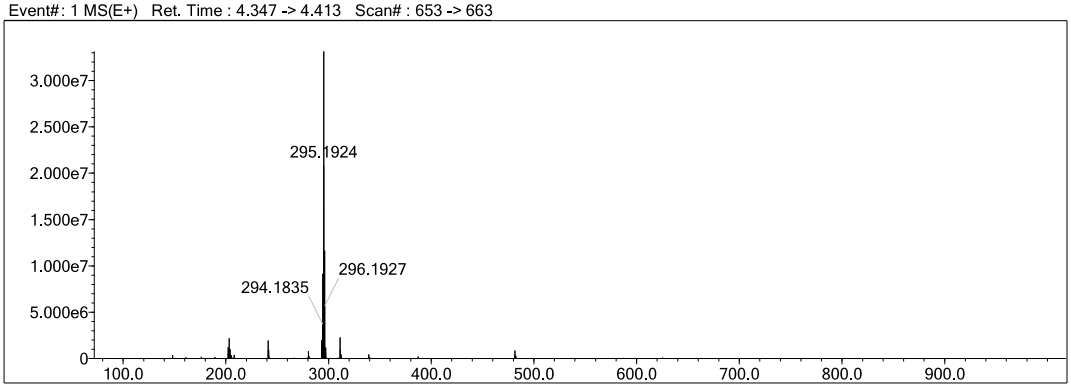
Use Adduct
H

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

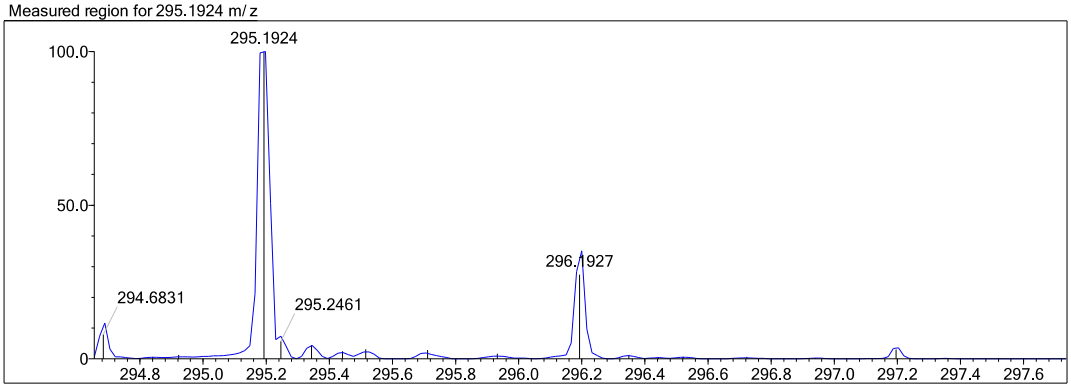
DBE Range: 10.0 - 20.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

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

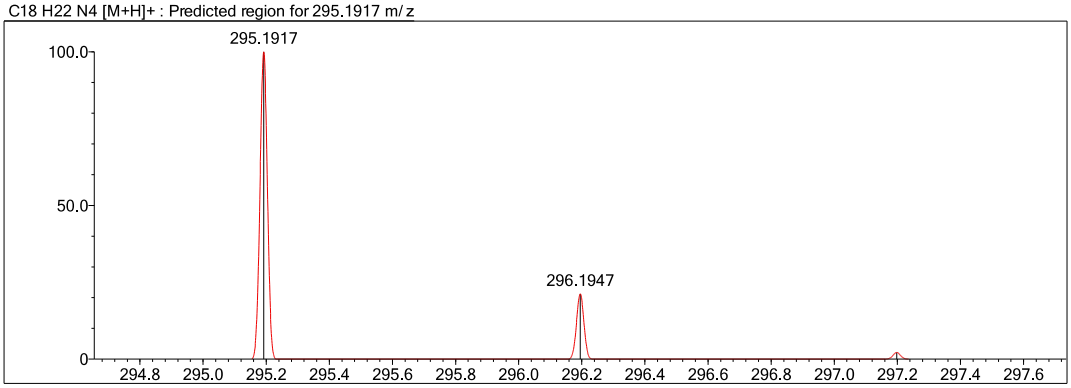
Event#: 1 MS(E+) Ret. Time : 4.347 -> 4.413 Scan# : 653 -> 663



Measured region for 295.1924 m/z



C18 H22 N4 [M+H]+ : Predicted region for 295.1917 m/z

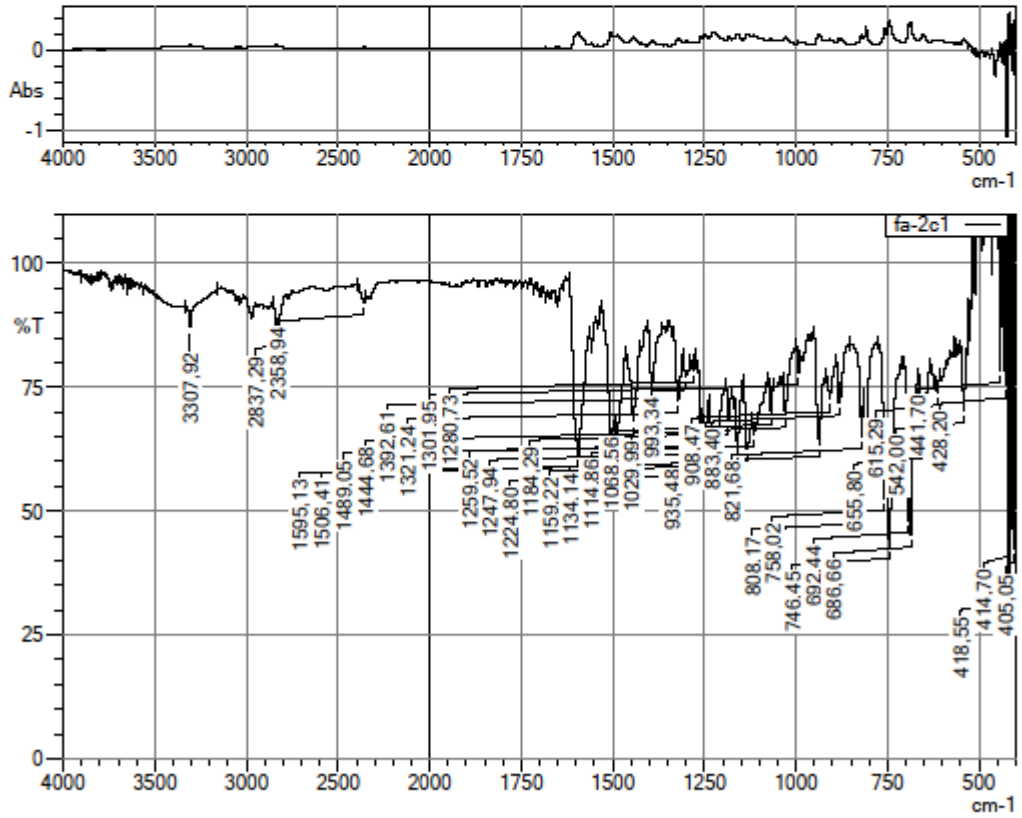


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	64.39	C18 H22 N4	[M+H]+	295.1924	295.1917	0.7	2.37	66.68	10.0

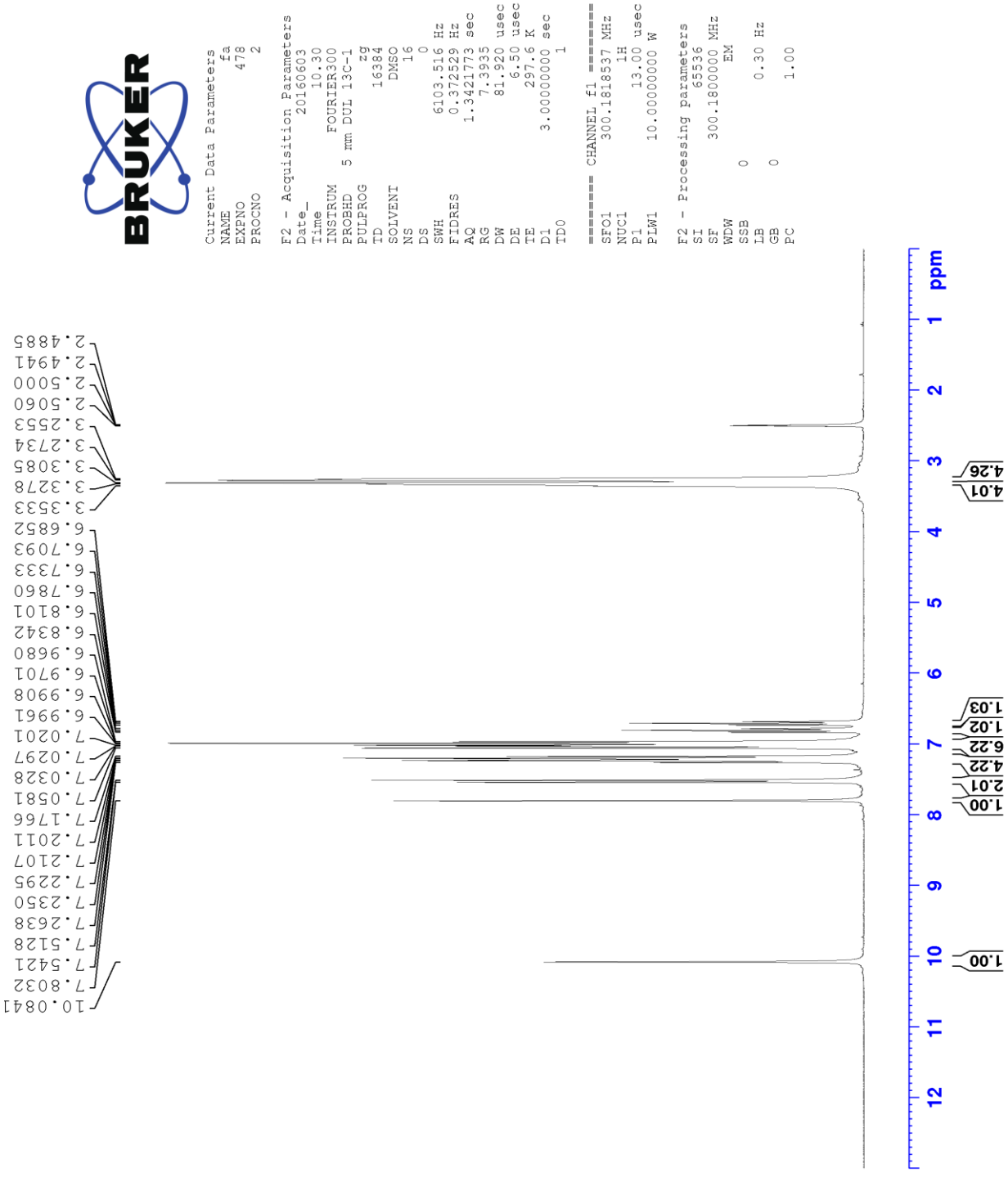
Spectra 8. HRMS spectra of the compound 2b

DOPNALAB

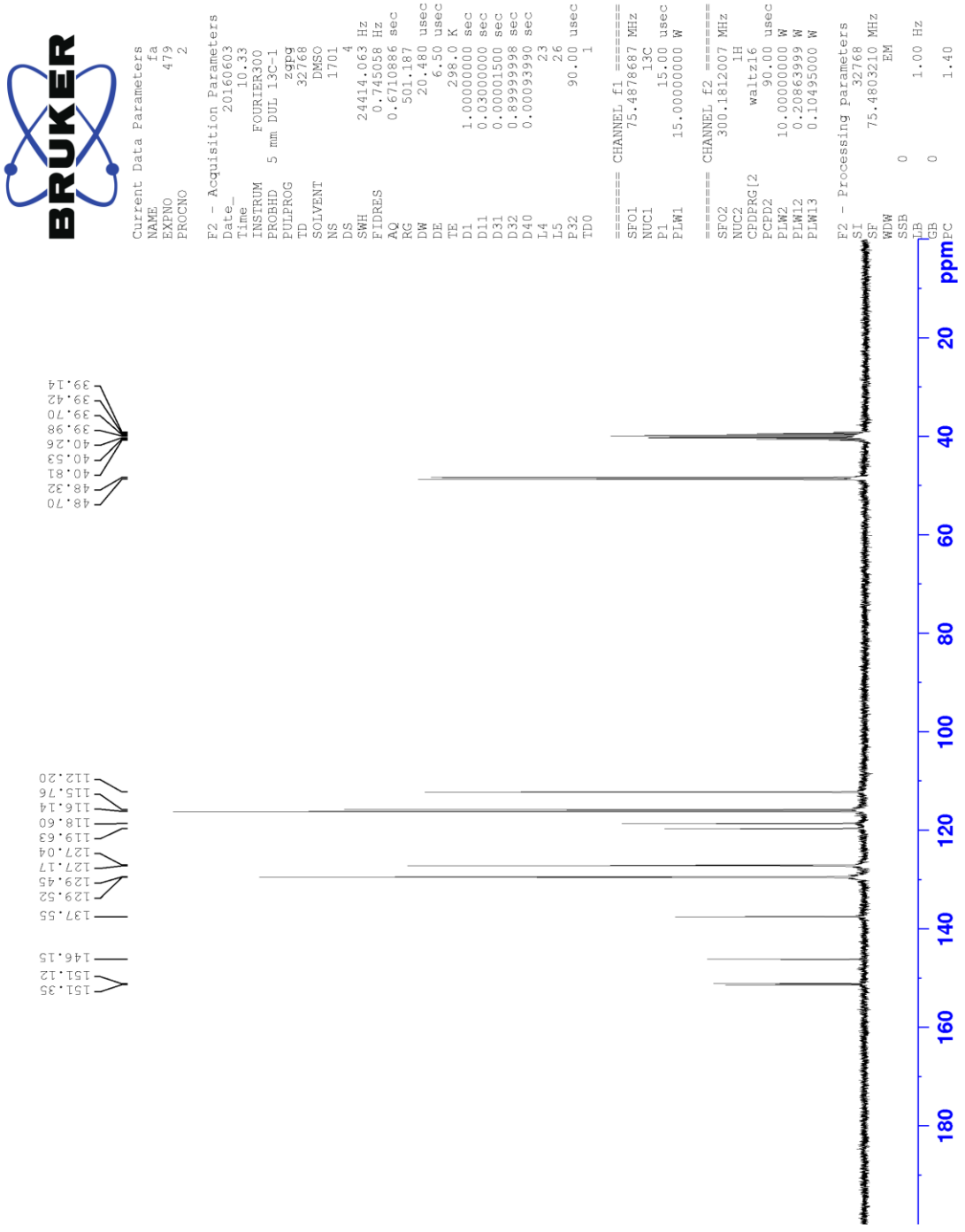
Item	Value
Acquired Date&Time	5.10.2016 09:53:15
Acquired by	System Administrator
Filename	C:\Users\dopnalab\Desktop\derya\fa\fa-2c1.ispd
Spectrum name	fa-2c1
Sample name	fa_2c
Sample ID	
Option	
Comment	
No. of Scans	10
Resolution	4 [cm-1]
Apodization	Happ-Genzel



Spectra 9. IR spectra of the compound 2c



Spectra 10. ^{1}H NMR spectra of the compound 2c



Spectra 11. ^{13}C NMR spectra of the compound 2c

Data File: C:\ LabSolutions\ Data\Analiz\derya\ FA-3_3.lcd

Elmt	Val.	Min	Max
H	1	0	50
C	4	0	50
N	3	0	4

Elmt	Val.	Min	Max
O	2	0	6
F	1	0	0
S	2	0	0

Elmt	Val.	Min	Max
Cl	1	0	0
Br	1	0	0
Pd	2	0	0

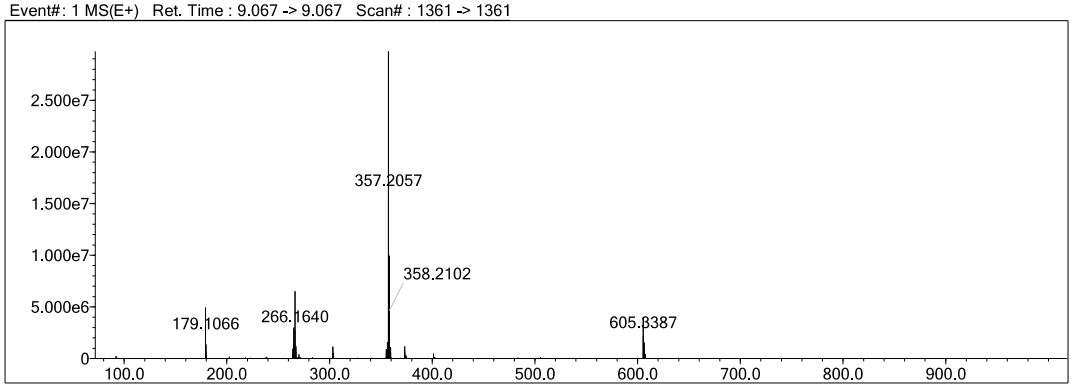
Use Adduct
H

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

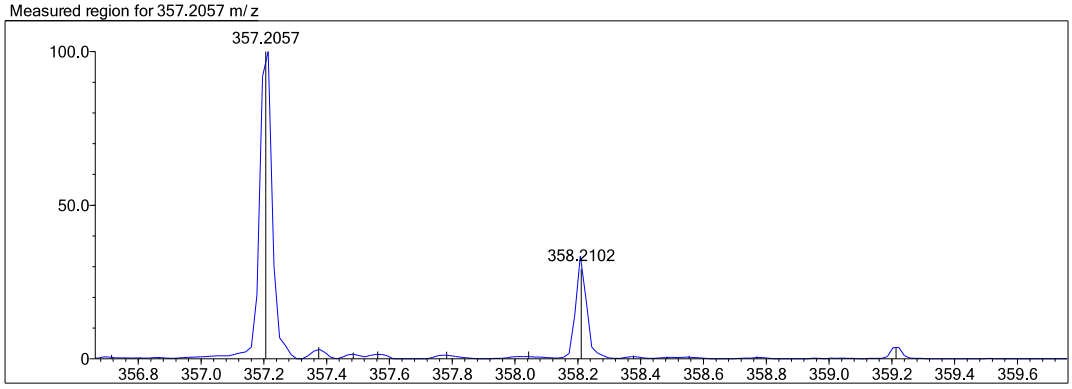
DBE Range: 10.0 - 20.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

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

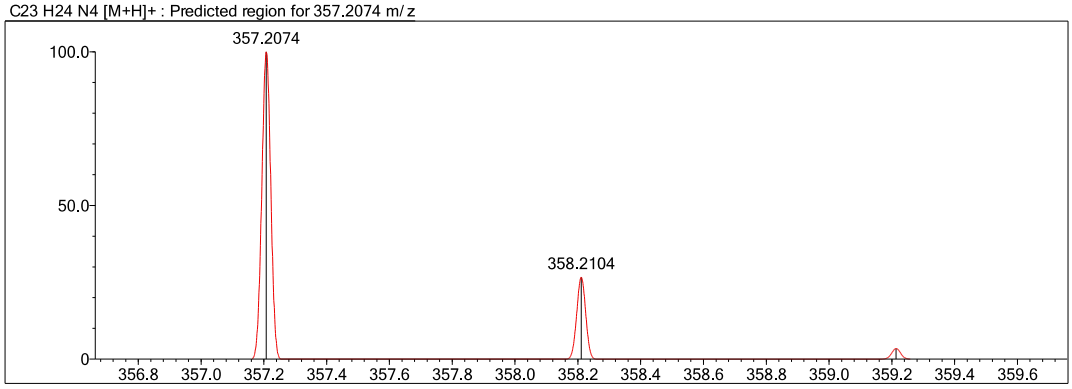
Event#: 1 MS(E+) Ret. Time : 9.067 -> 9.067 Scan# : 1361 -> 1361



Measured region for 357.2057 m/z



C23 H24 N4 [M+H]+ : Predicted region for 357.2074 m/z

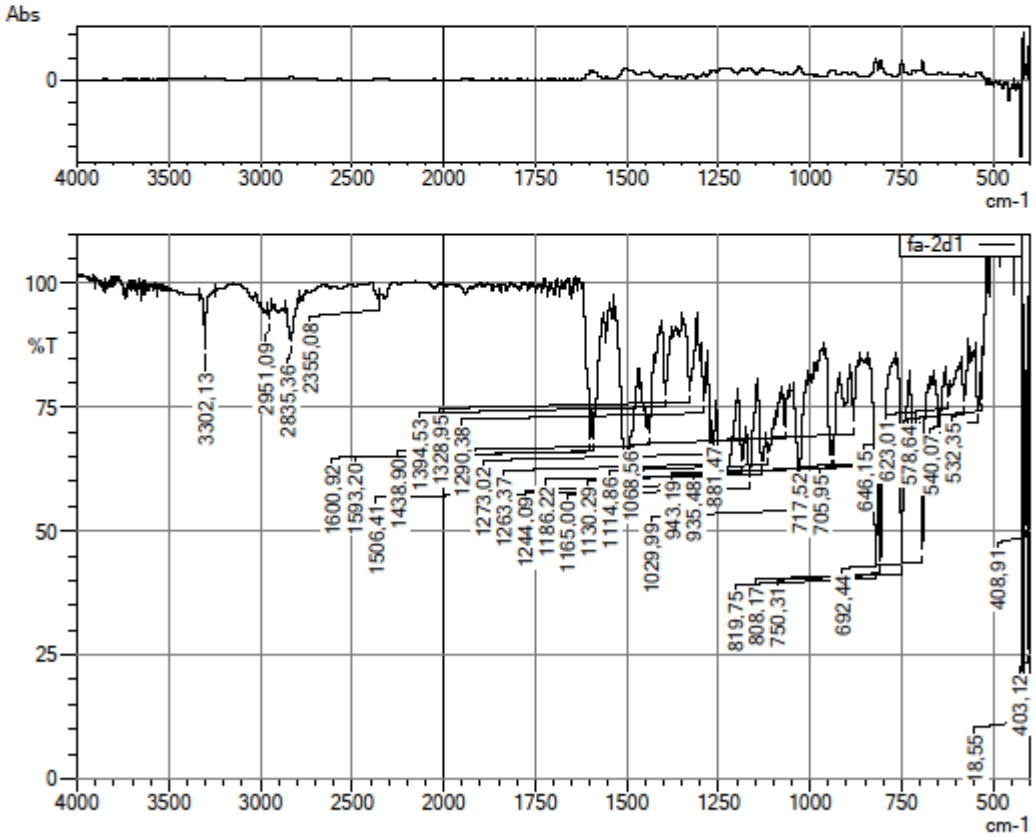


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	83.47	C23 H24 N4	[M+H]+	357.2057	357.2074	-1.7	-4.76	92.13	14.0

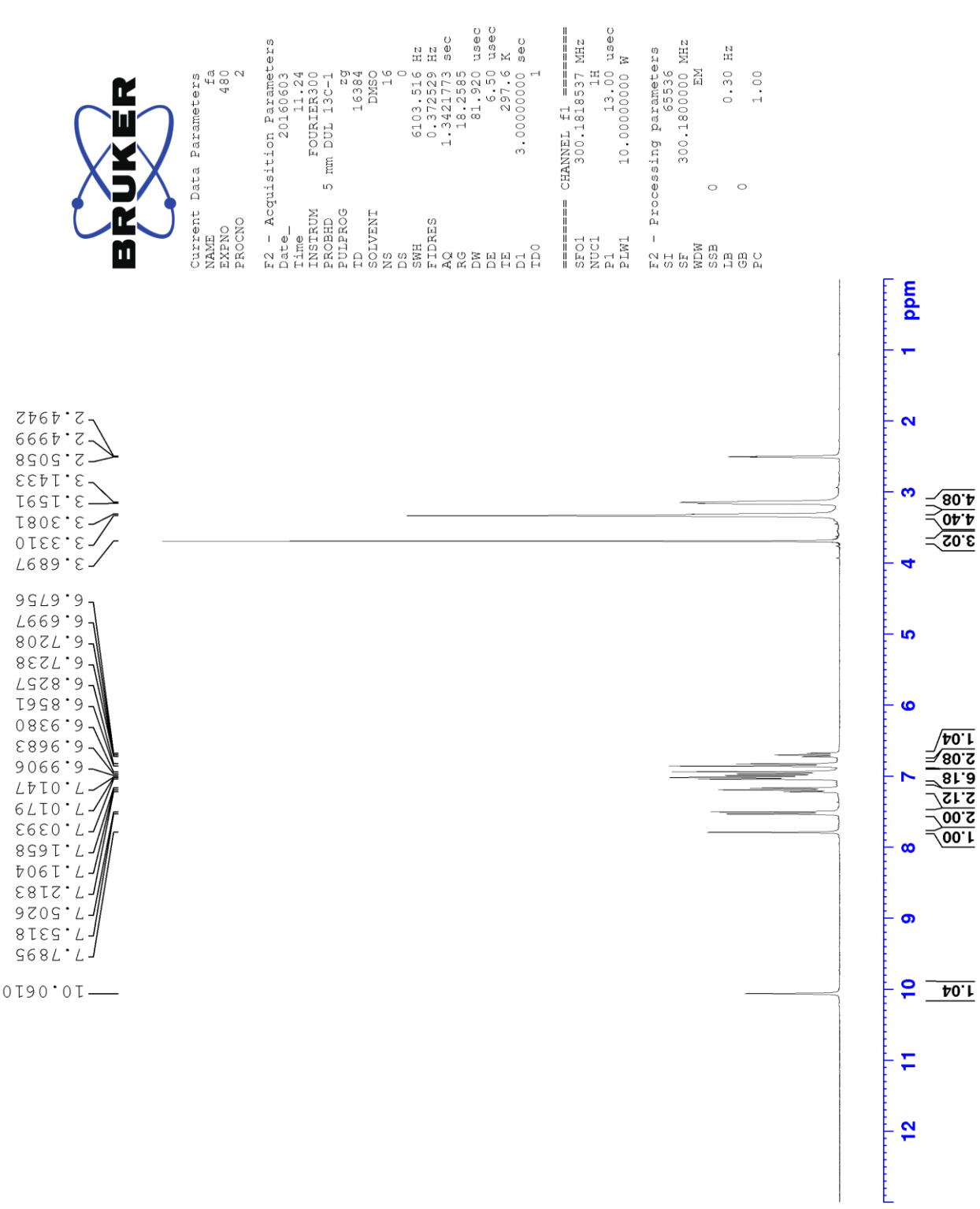
Spectra 12. HRMS spectra of the compound 2c

DOPNALAB

Item	Value
Acquired Date&Time	5.10.2016 09:56:50
Acquired by	System Administrator
Filename	C:\Users\dopnalab\Desktop\derya\fa\fa-2d1.ispd
Spectrum name	fa-2d1
Sample name	fa_2d
Sample ID	
Option	
Comment	
No. of Scans	10
Resolution	4 [cm-1]
Apodization	Happ-Genzel

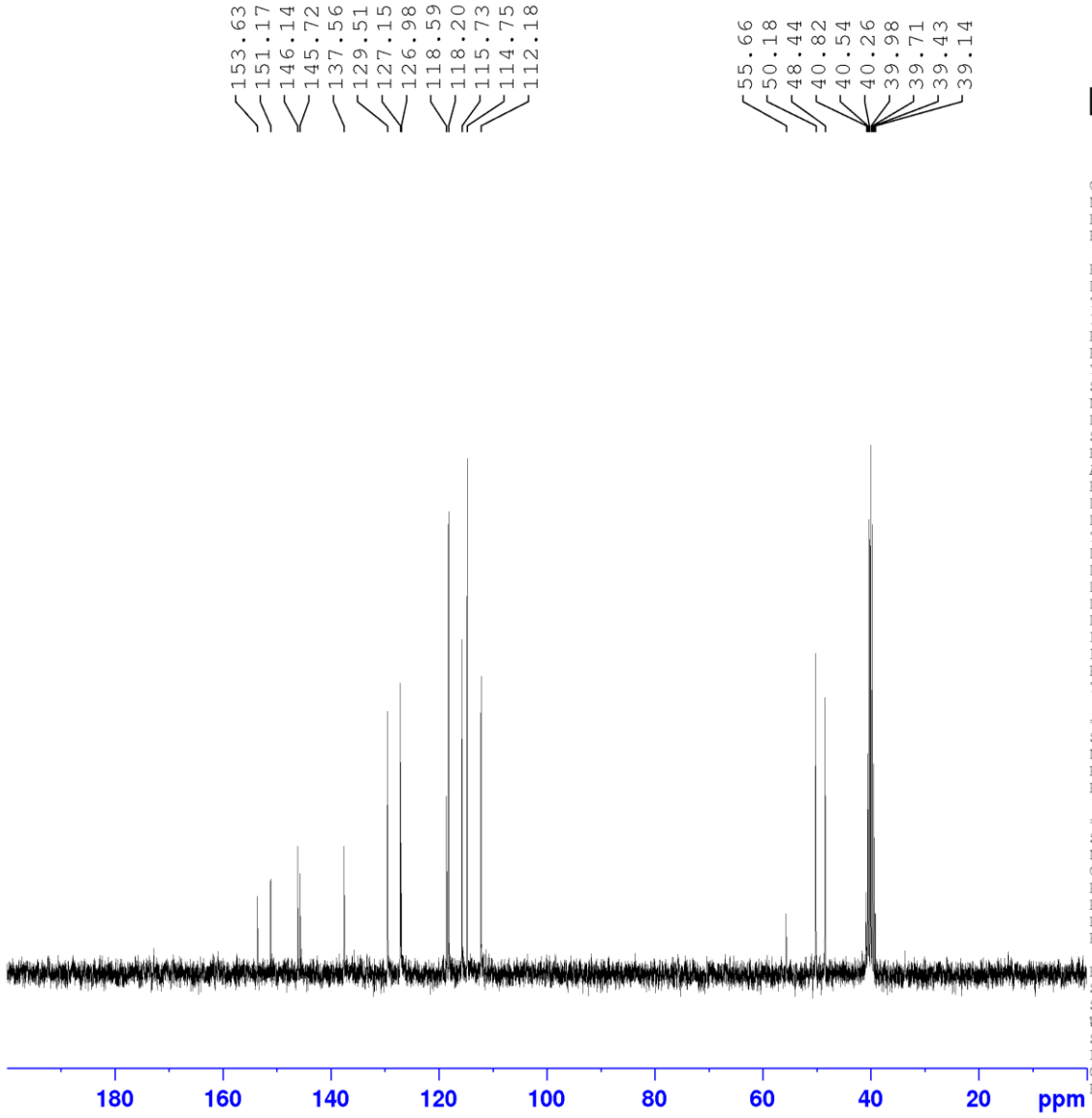


Spectra 13. IR spectra of the compound 2d



Spectra 14. [1]H NMR spectra of the compound 2d

Spectra 15. ^{13}C NMR spectra of the compound 2d



BRUKER

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Current Data Parameters
NAME                   fa
EXPNO                 481
PROCNO                  3

F2 - Acquisition Parameters
Date_           20160603
Time               11.28
INSTRUM       FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG             zgpg
TD                 32768
SOLVENT             DMSO
NS                   575
DS                     4
SWH            24414.063 Hz
FIDRES          0.745058 Hz
AQ              0.6710886 sec
RG                501.187
DW                 20.480 usec
DE                  6.50 usec
TE                 298.0 K
D1            1.00000000 sec
D11           0.03000000 sec
D31           0.00001500 sec
D32           0.89999998 sec
D40           0.00093990 sec
L4                    23
L5                    26
P32                90.00 usec
TD0                    1

======== CHANNEL f1 ========
SFO1          75.4878687 MHz
NUC1                 13C
P1                 15.00 usec
PLW1         15.00000000 W

======== CHANNEL f2 ========
SFO2         300.1812007 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2         10.00000000 W
PLW12         0.20863999 W
PLW13         0.10495000 W

F2 - Processing parameters
SI                 32768
SF            75.4803210 MHz
WDW                   EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
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Data File: C:\ LabSolutions\ Data\Analiz\derya\ FA-4_4.lcd

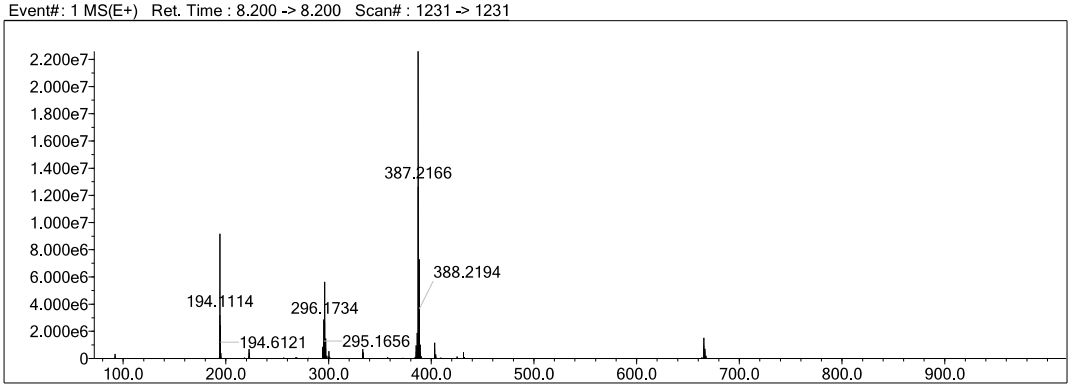
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	50	O	2	0	6	Cl	1	0	0	H
C	4	0	50	F	1	0	0	Br	1	0	0	
N	3	0	4	S	2	0	0	Pd	2	0	0	

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

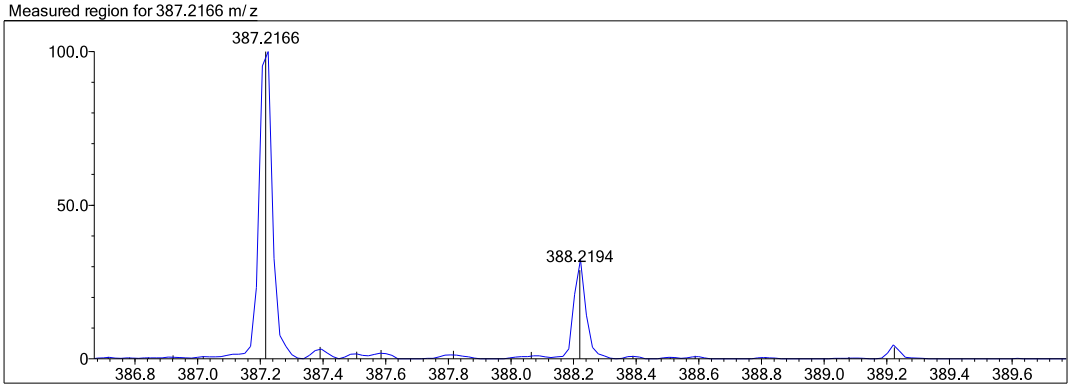
DBE Range: 10.0 - 20.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

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

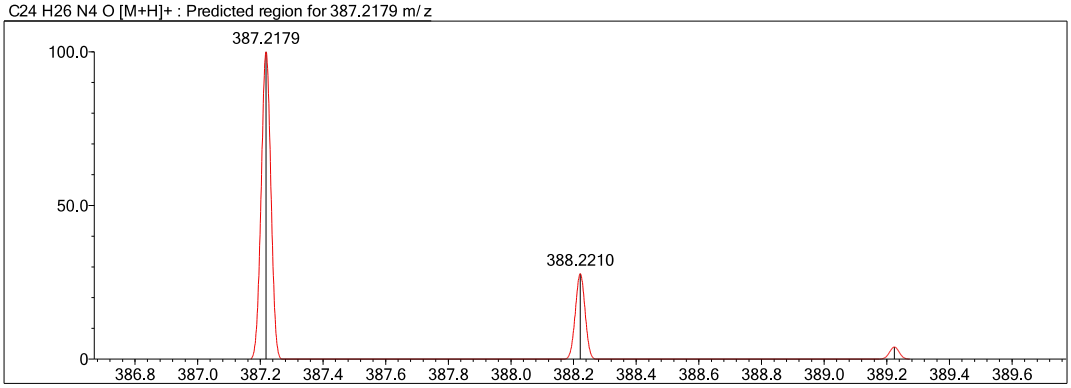
Event#: 1 MS(E+) Ret. Time : 8.200 -> 8.200 Scan# : 1231 -> 1231



Measured region for 387.2166 m/z



C24 H26 N4 O [M+H]+ : Predicted region for 387.2179 m/z

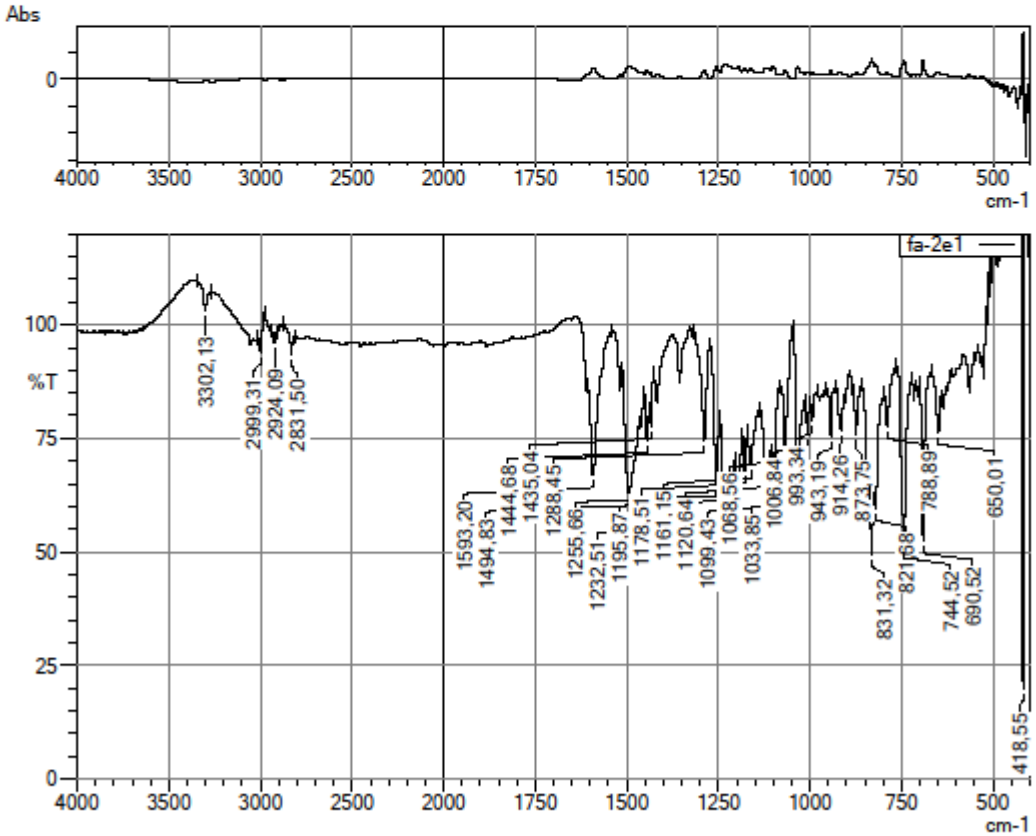


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	92.48	C24 H26 N4 O	[M+H]+	387.2166	387.2179	-1.3	-3.36	98.28	14.0

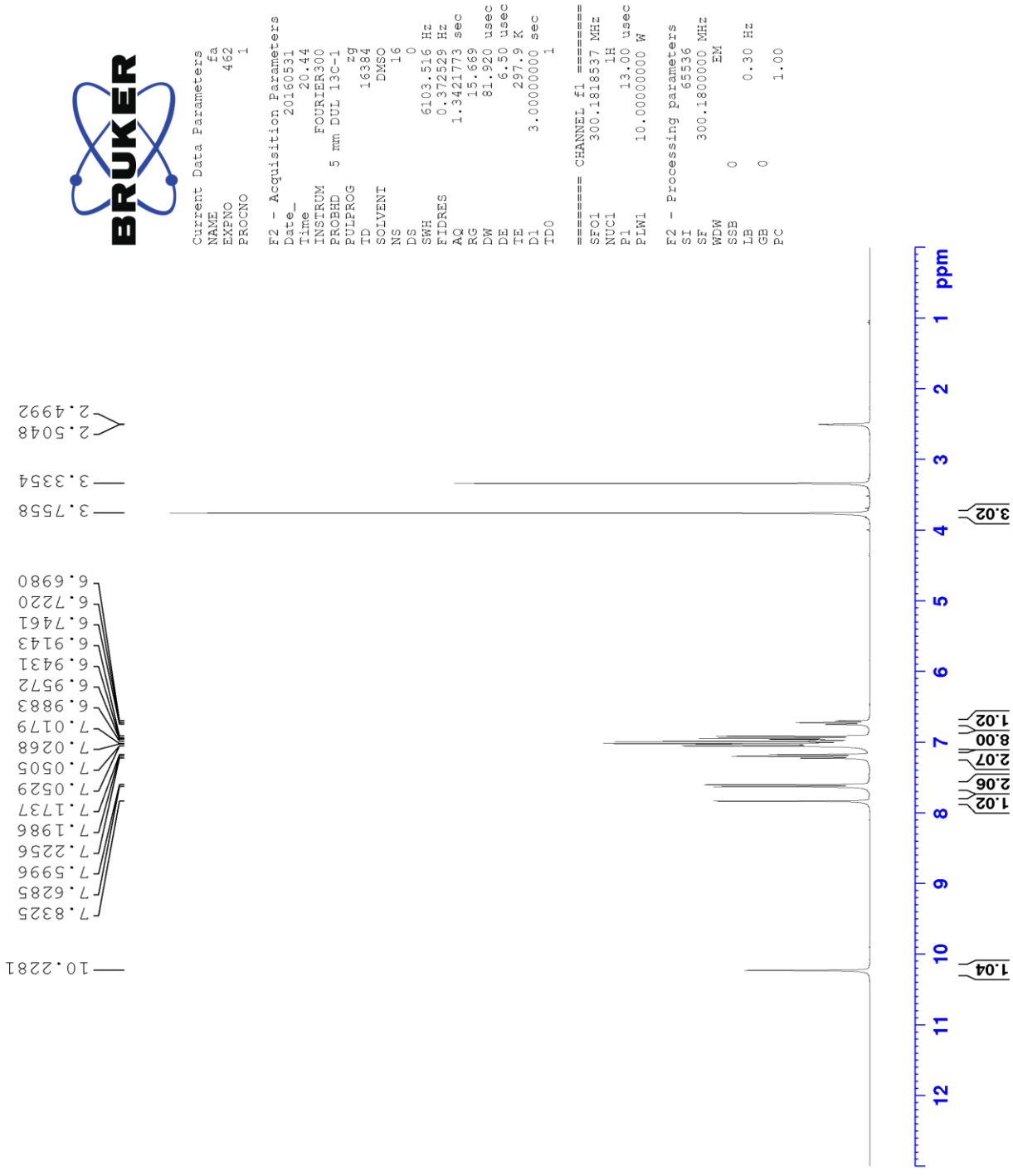
Spectra 16. HRMS spectra of the compound 2d

DOPNALAB

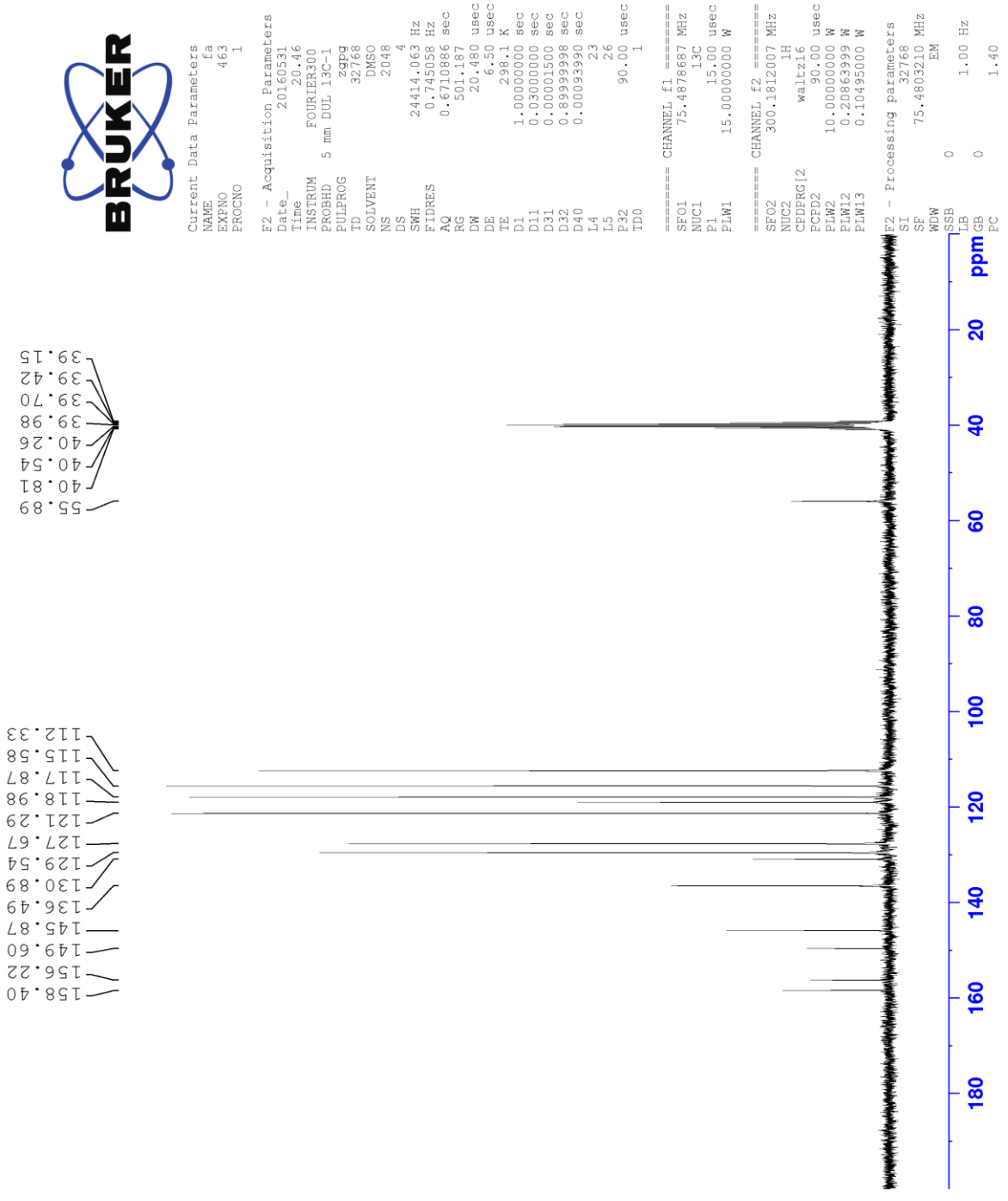
	Item	Value
	Acquired Date&Time	5.10.2016 10:00:28
	Acquired by	System Administrator
	Filename	C:\Users\dopnalab\Desktop\derya\fa\fa-2e1.ispd
	Spectrum name	fa-2e1
	Sample name	fa_2e
	Sample ID	
	Option	
	Comment	
	No. of Scans	10
	Resolution	4 [cm-1]
	Apodization	Happ-Genzel



Spectra 17. IR spectra of the compound 2e



Spectra 18. ^{1}H NMR spectra of the compound 2e



Spectra 19. ^{13}C NMR spectra of the compound 2e

Data File: C:\ LabSolutions\ Data\Analiz\derya\ FA-5_5.lcd

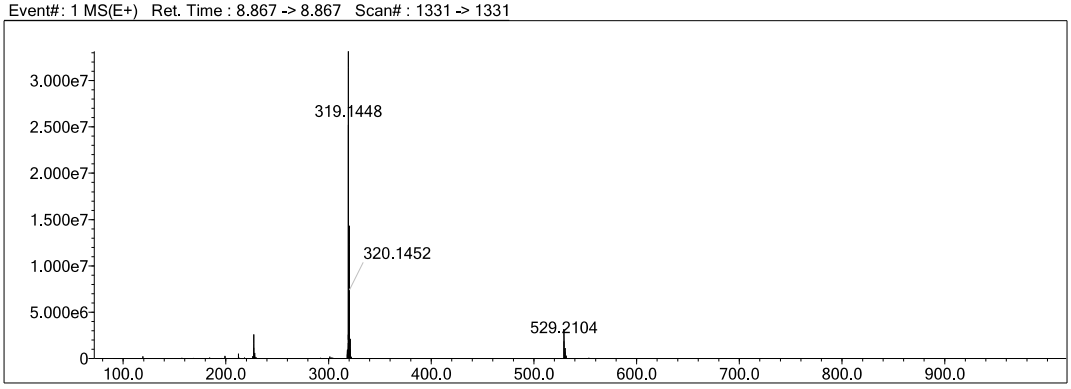
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	50	O	2	0	6	Cl	1	0	0	H
C	4	0	50	F	1	0	0	Br	1	0	0	
N	3	0	4	S	2	0	0	Pd	2	0	0	

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

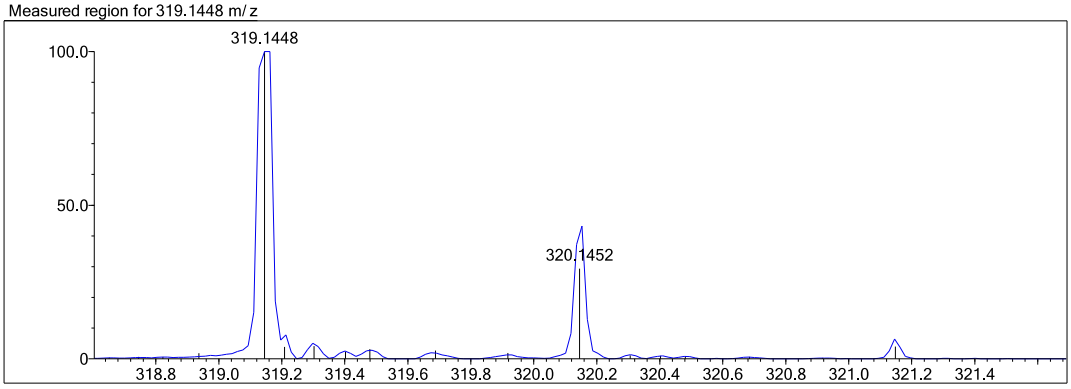
DBE Range: 10.0 - 20.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

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

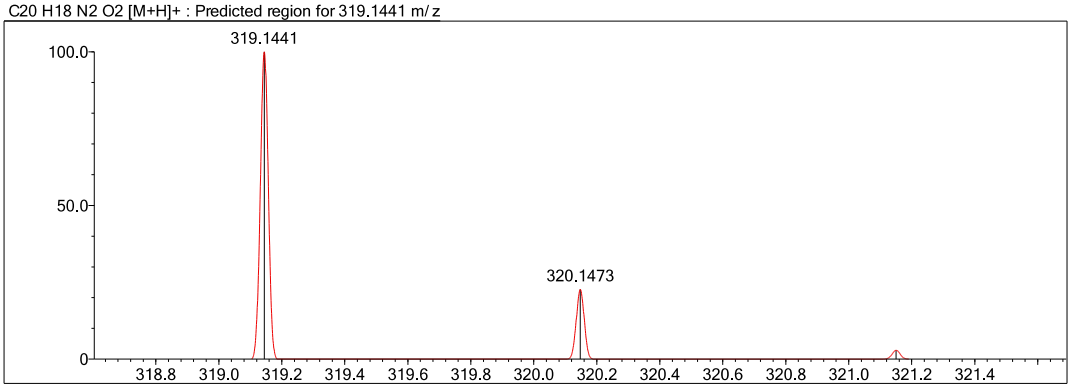
Event#: 1 MS(E+) Ret. Time : 8.867 -> 8.867 Scan# : 1331 -> 1331



Measured region for 319.1448 m/z



C20 H18 N2 O2 [M+H]+ : Predicted region for 319.1441 m/z

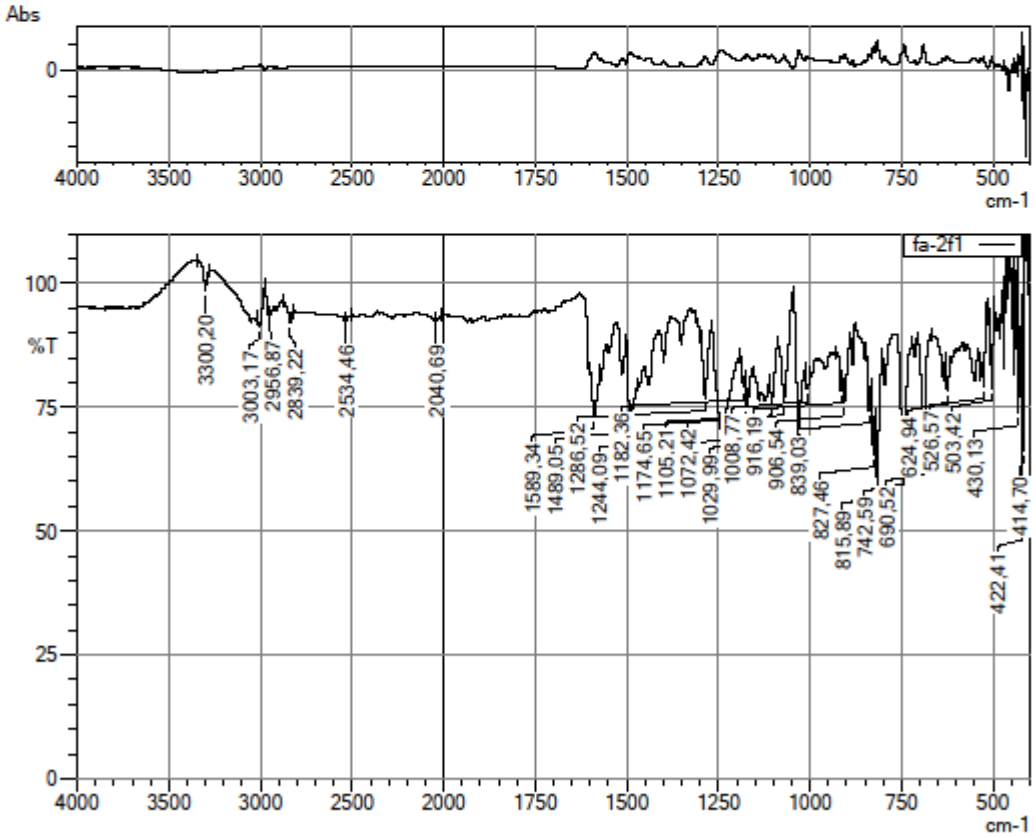


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	59.52	C20 H18 N2 O2	[M+H]+	319.1448	319.1441	0.7	2.19	61.35	13.0

Spectra 20. HRMS spectra of the compound 2e

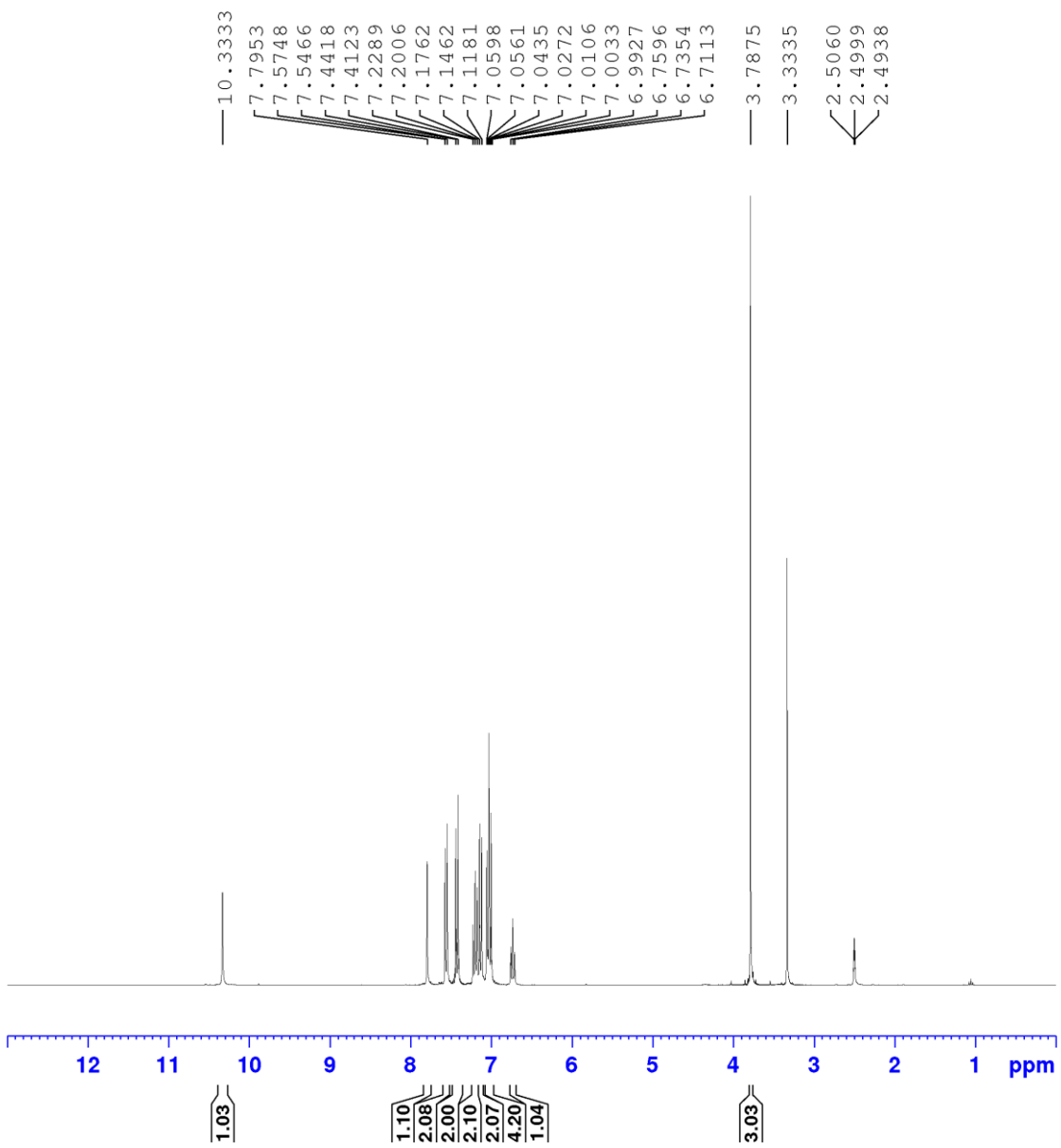
DOPNALAB

Item	Value
Acquired Date&Time	5.10.2016 10:03:22
Acquired by	System Administrator
Filename	C:\Users\dopnalab\Desktop\derya\fa\fa-2f1.lspd
Spectrum name	fa-2f1
Sample name	fa_2f
Sample ID	
Option	
Comment	
No. of Scans	10
Resolution	4 [cm-1]
Apodization	Happ-Genzel



Spectra 21. IR spectra of the compound 2f

Spectra 22. ^{1}H NMR spectra of the compound 2f



BRUKER

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Current Data Parameters
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EXPNO                464
PROCNO                 1

F2 - Acquisition Parameters
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Time               21.46
INSTRUM       FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG               zg
TD                 16384
SOLVENT             DMSO
NS                    16
DS                     0
SWH             6103.516 Hz
FIDRES          0.372529 Hz
AQ             1.3421773 sec
RG                17.237
DW                81.920 usec
DE                 6.50 usec
TE                298.1 K
D1            3.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         300.1818537 MHz
NUC1                   1H
P1                 13.00 usec
PLW1         10.00000000 W

F2 - Processing parameters
SI                 65536
SF           300.1800000 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
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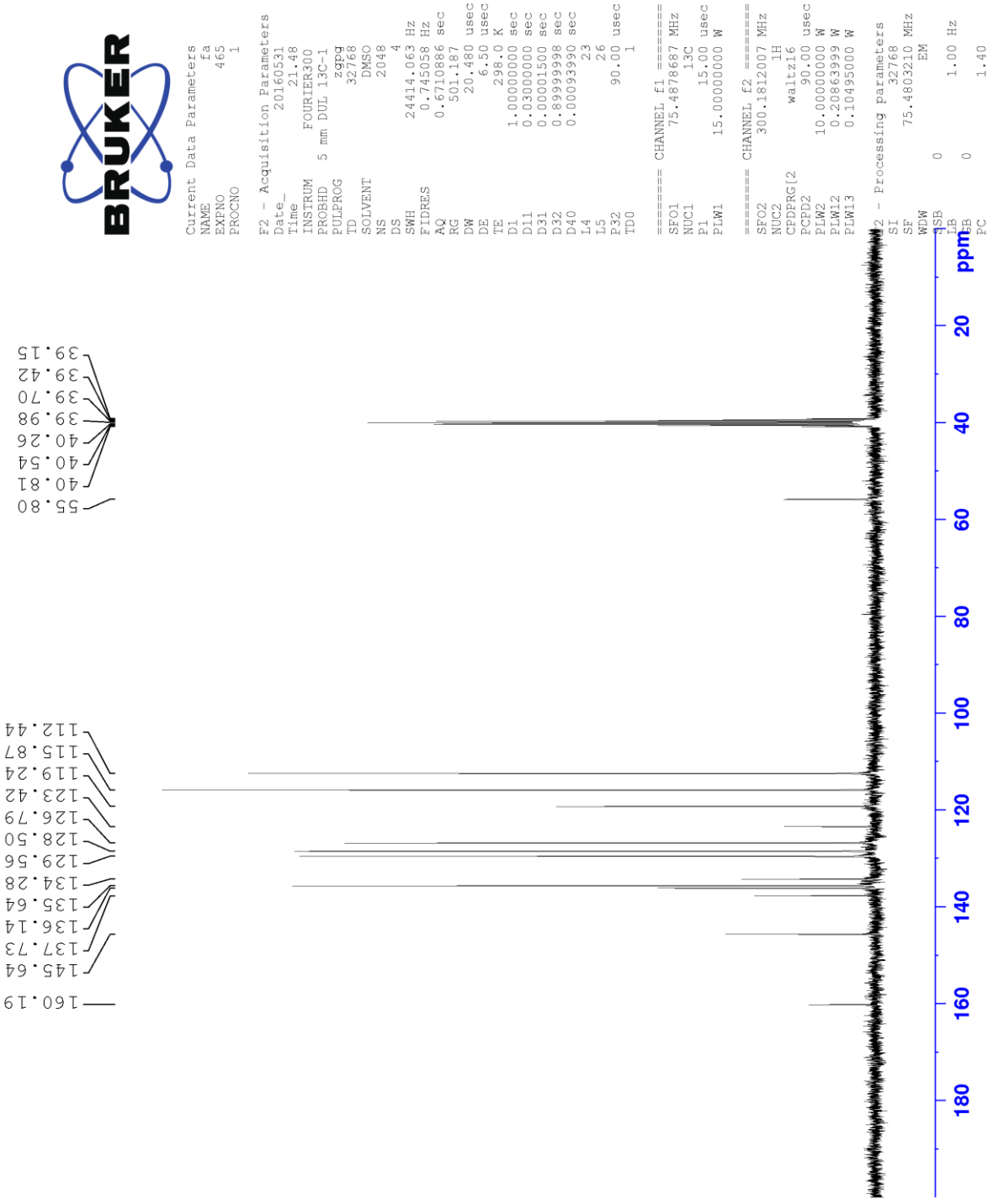


Spectra 23. ^{13}C NMR spectra of the compound 2f

Data File: C:\ LabSolutions\ Data\Analiz\derya\ FA-6_6.lcd

Elmt	Val.	Min	Max
H	1	0	50
C	4	0	50
N	3	0	4

Elmt	Val.	Min	Max
O	2	0	6
F	1	0	0
S	2	0	1

Elmt	Val.	Min	Max
Cl	1	0	0
Br	1	0	0
Pd	2	0	0

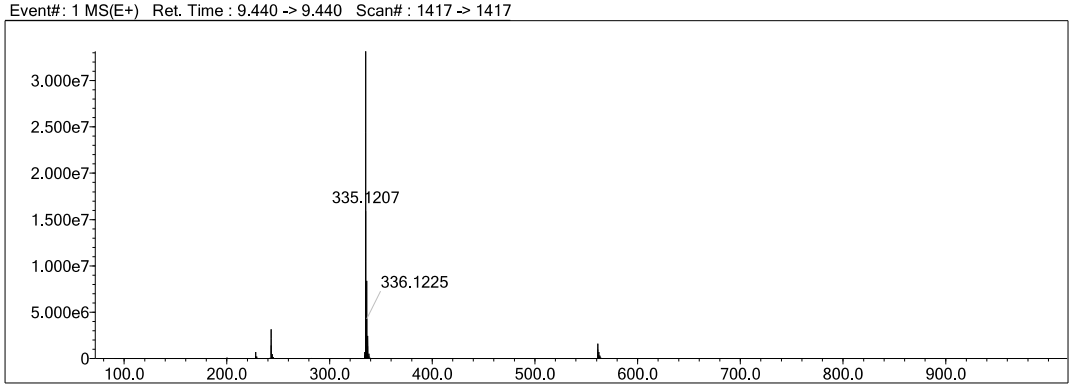
Use Adduct
H

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

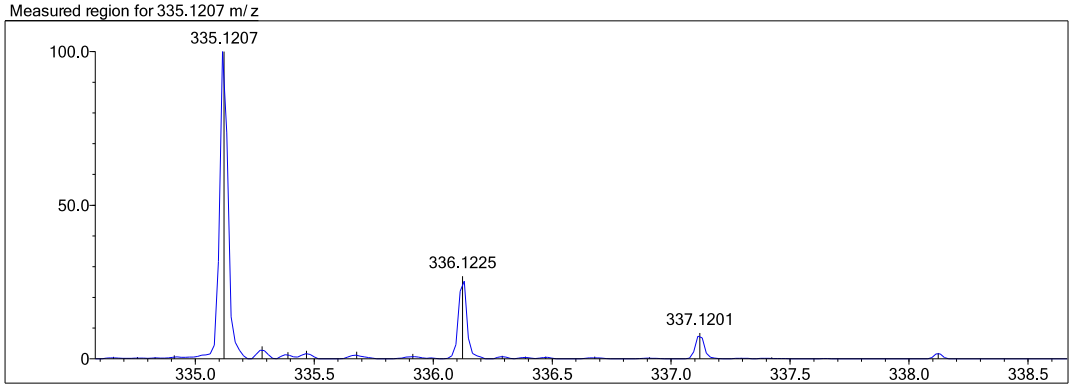
DBE Range: 10.0 - 20.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

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

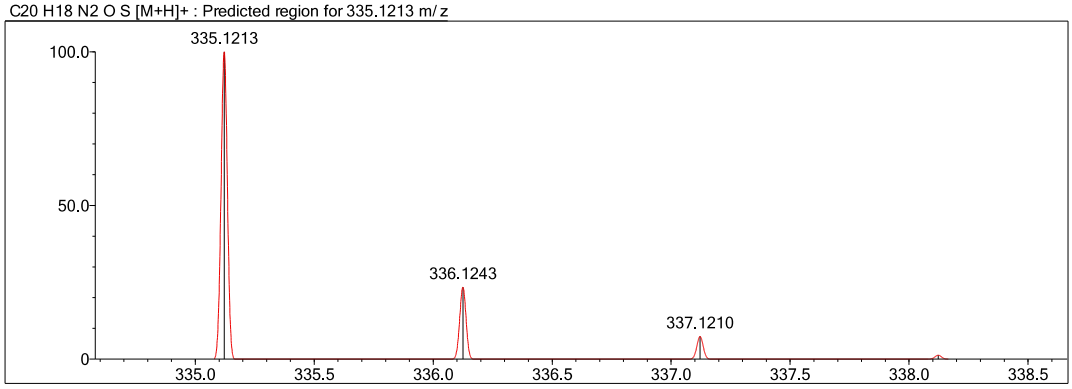
Event#: 1 MS(E+) Ret. Time : 9.440 -> 9.440 Scan# : 1417 -> 1417



Measured region for 335.1207 m/z



C20 H18 N2 O S [M+H]+ : Predicted region for 335.1213 m/z

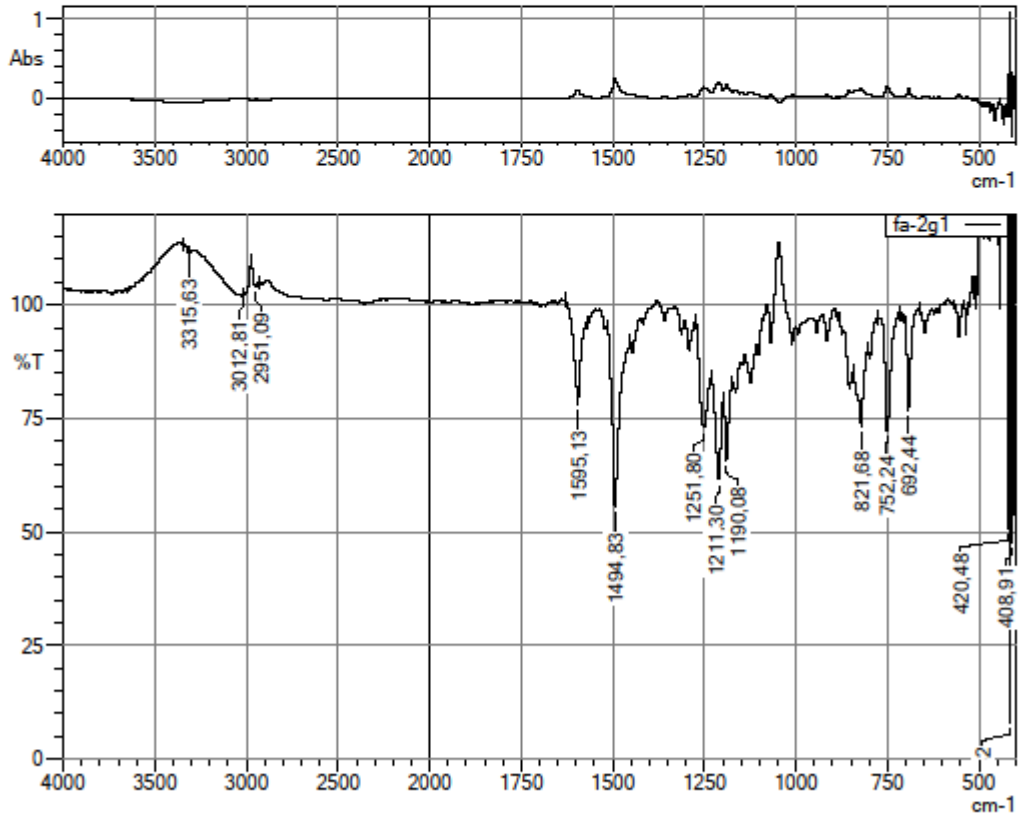


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	77.61	C20 H18 N2 O S	[M+H]+	335.1207	335.1213	-0.6	-1.79	79.17	13.0

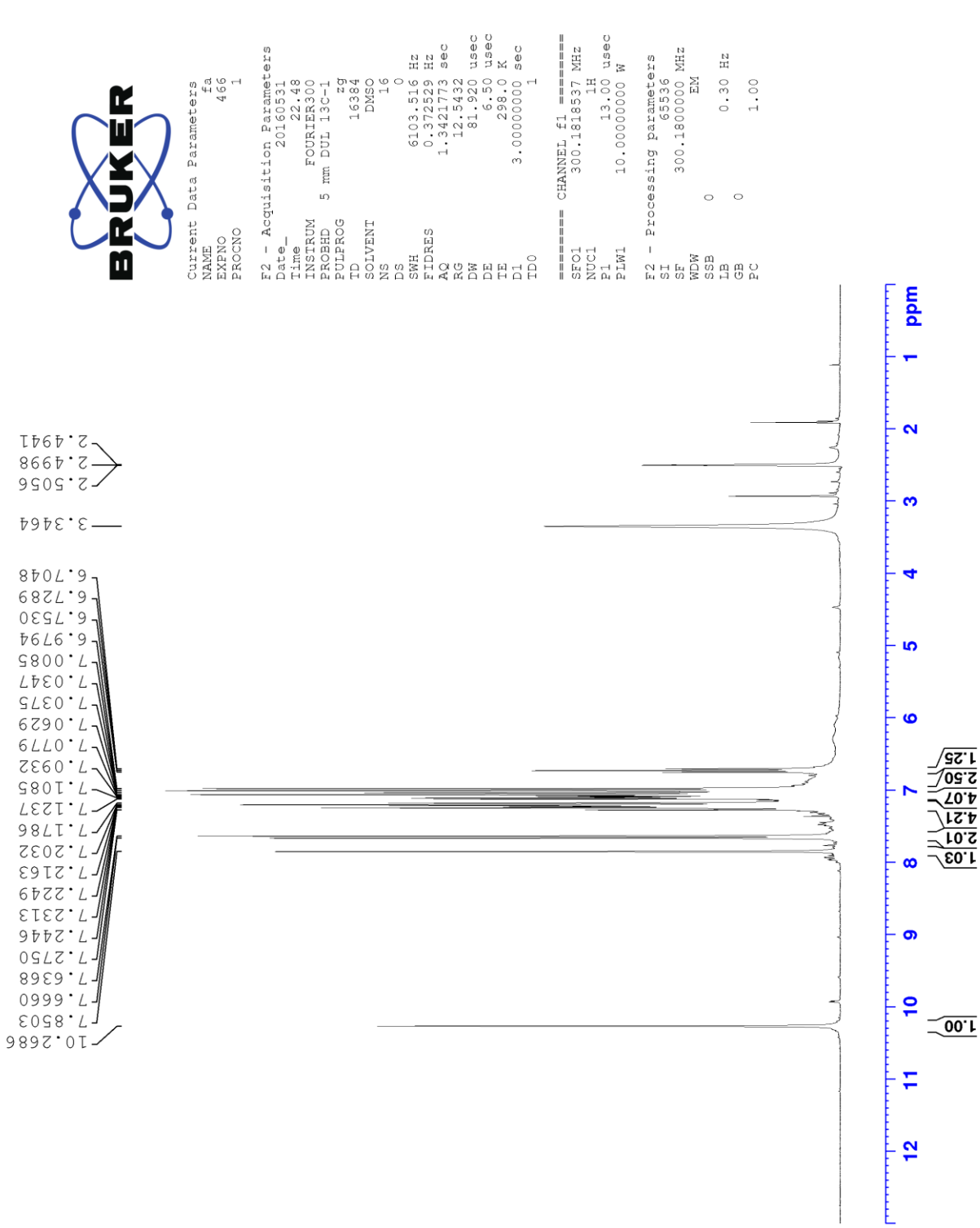
Spectra 24. HRMS spectra of the compound 2f

DOPNALAB

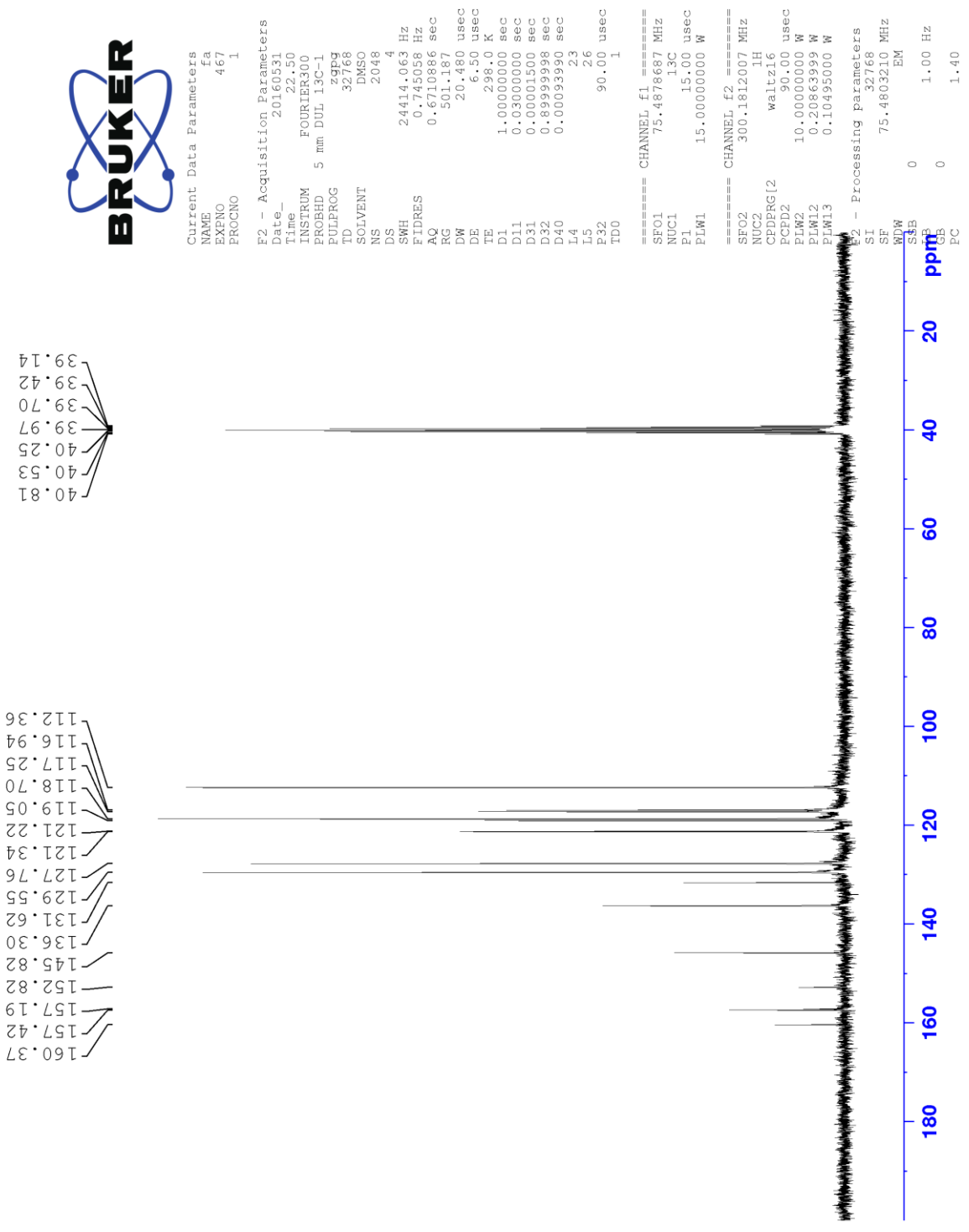
Item	Value
Acquired Date&Time	5.10.2016 10:06:35
Acquired by	System Administrator
Filename	C:\Users\dopnalab\Desktop\derya\fa\fa-2g1.ispd
Spectrum name	fa-2g1
Sample name	fa_2g
Sample ID	
Option	
Comment	
No. of Scans	10
Resolution	4 [cm-1]
Apodization	Happ-Genzel



Spectra 25. IR spectra of the compound 2g



Spectra 26. [1]H NMR spectra of the compound 2g



Spectra 27. ^{13}C NMR spectra of the compound 2g

Data File: C:\ LabSolutions\ Data\Analiz\derya\ FA-7_7.lcd

Elmt	Val.	Min	Max
H	1	0	50
C	4	0	50
N	3	0	4

Elmt	Val.	Min	Max
O	2	0	6
F	1	1	1
S	2	0	1

Elmt	Val.	Min	Max
Cl	1	0	0
Br	1	0	0
Pd	2	0	0

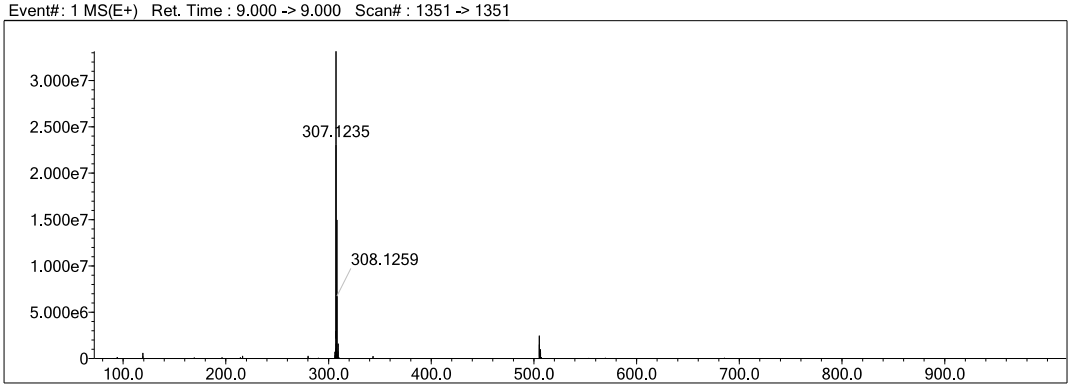
Use Adduct
H

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

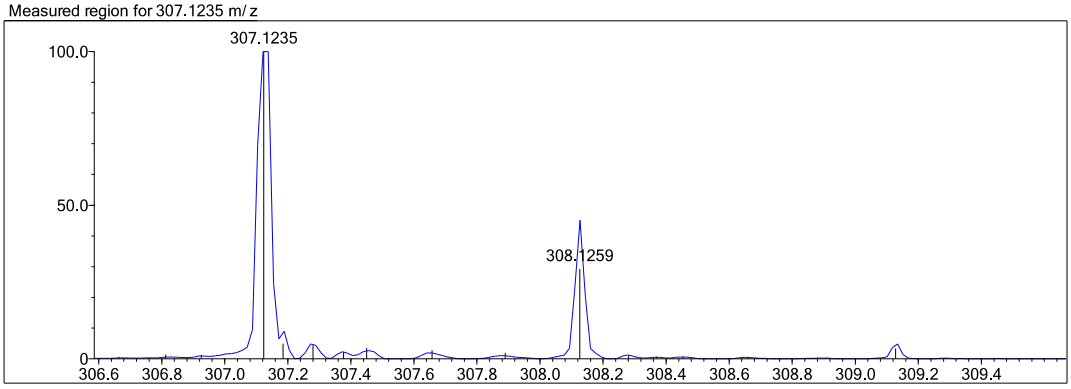
DBE Range: 10.0 - 20.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

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

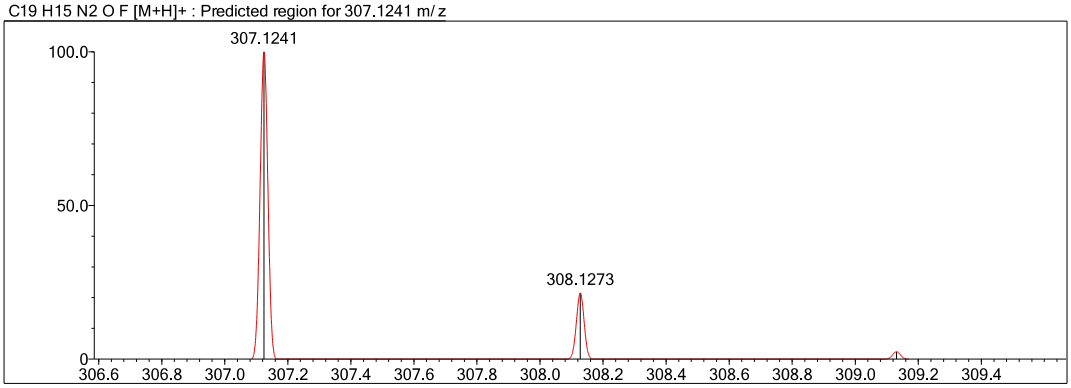
Event#: 1 MS(E+) Ret. Time : 9.000 -> 9.000 Scan# : 1351 -> 1351



Measured region for 307.1235 m/z



C19 H15 N2 O F [M+H]+ : Predicted region for 307.1241 m/z

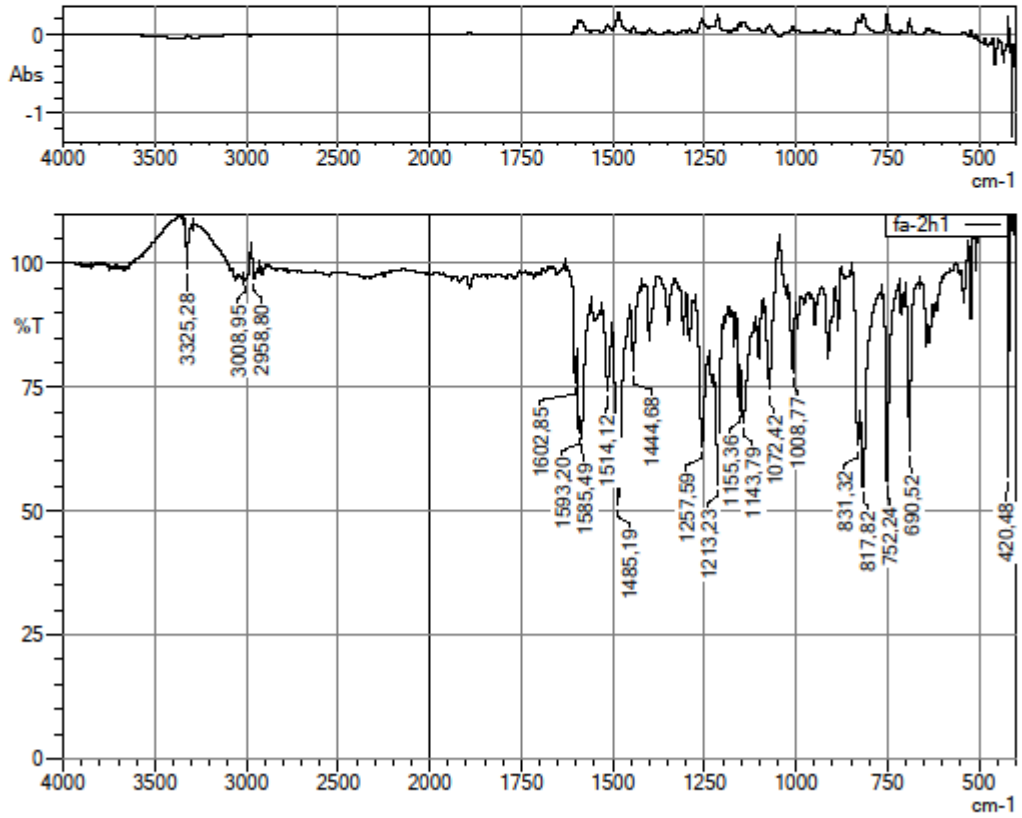


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	59.86	C19 H15 N2 O F	[M+H]+	307.1235	307.1241	-0.6	-1.95	61.32	13.0

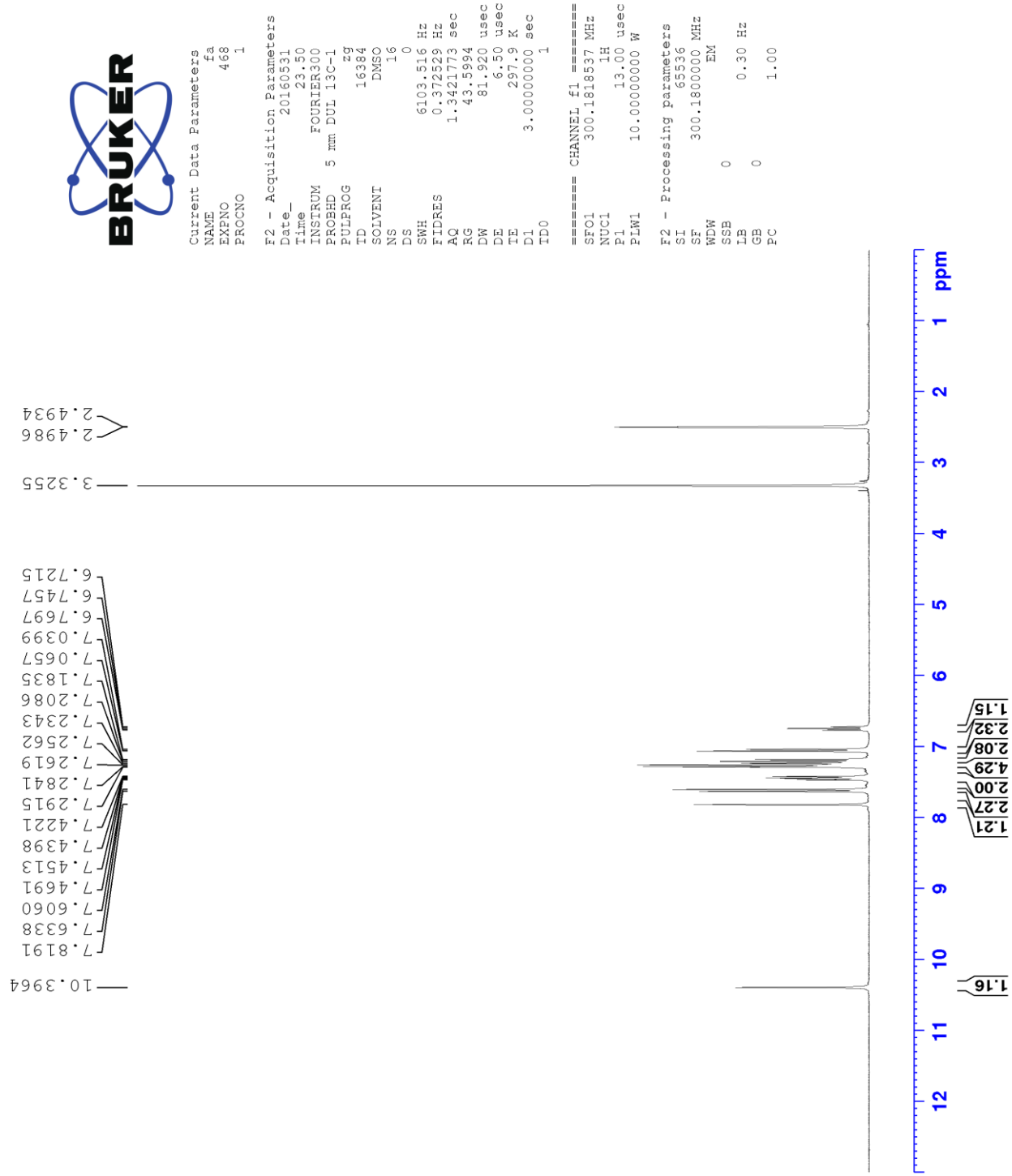
Spectra 28. HRMS spectra of the compound 2g

DOPNALAB

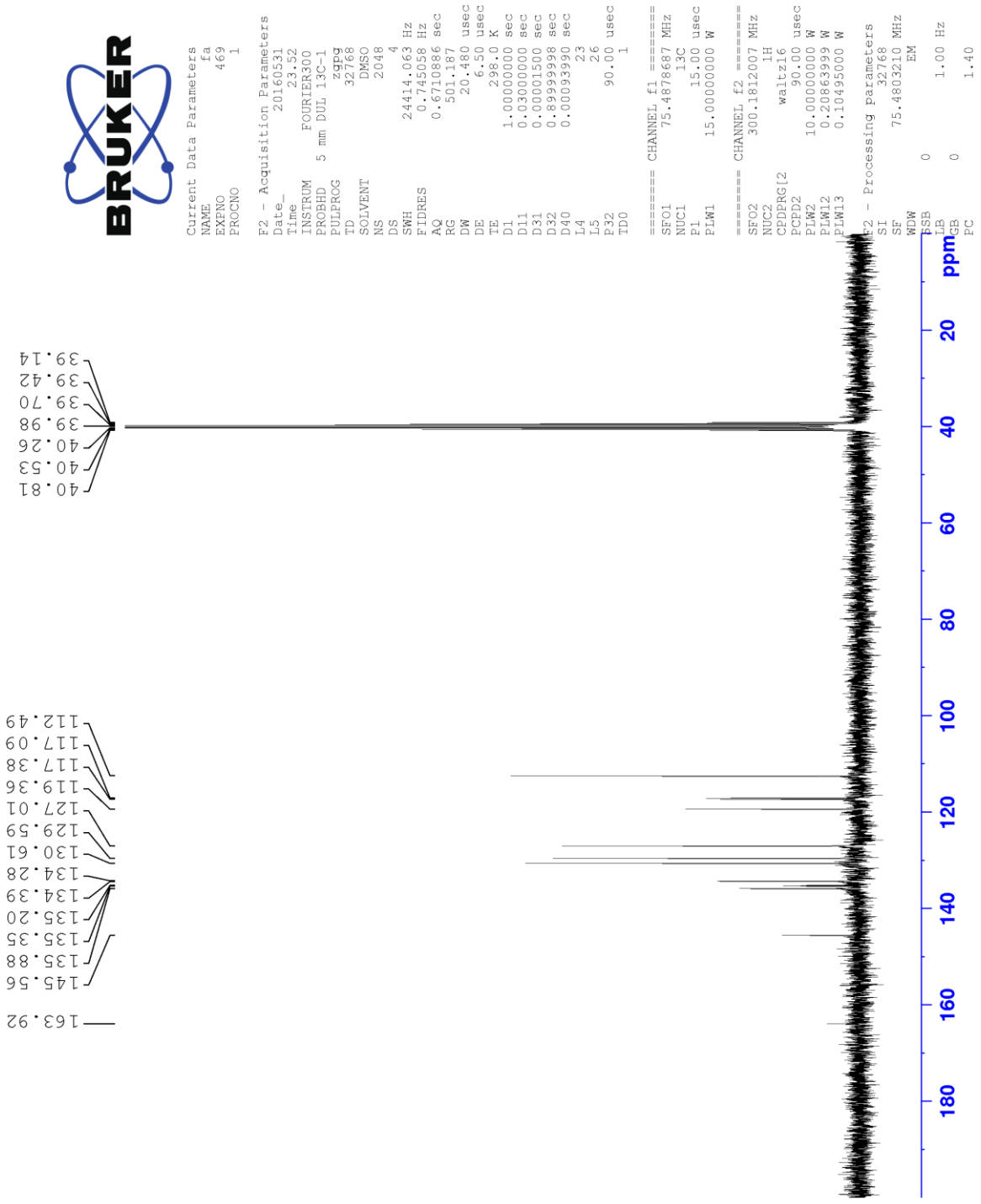
	Item	Value
	Acquired Date&Time	5.10.2016 10:09:19
	Acquired by	System Administrator
	Filename	C:\Users\dopnalab\Desktop\derya\fa\fa-2h1.ispd
	Spectrum name	fa-2h1
	Sample name	fa_2h
	Sample ID	
	Option	
	Comment	
	No. of Scans	10
	Resolution	4 [cm-1]
	Apodization	Happ-Genzel



Spectra 29. IR spectra of the compound 2h



Spectra 30. ^{1}H NMR spectra of the compound 2h



Spectra 31. ^{13}C NMR spectra of the compound 2h

Data File: C:\ LabSolutions\ Data\Analiz\derya\ FA-8_8.lcd

Elmt	Val.	Min	Max
H	1	0	50
C	4	0	50
N	3	0	4

Elmt	Val.	Min	Max
O	2	0	6
F	1	1	1
S	2	0	1

Elmt	Val.	Min	Max
Cl	1	0	0
Br	1	0	0
Pd	2	0	0

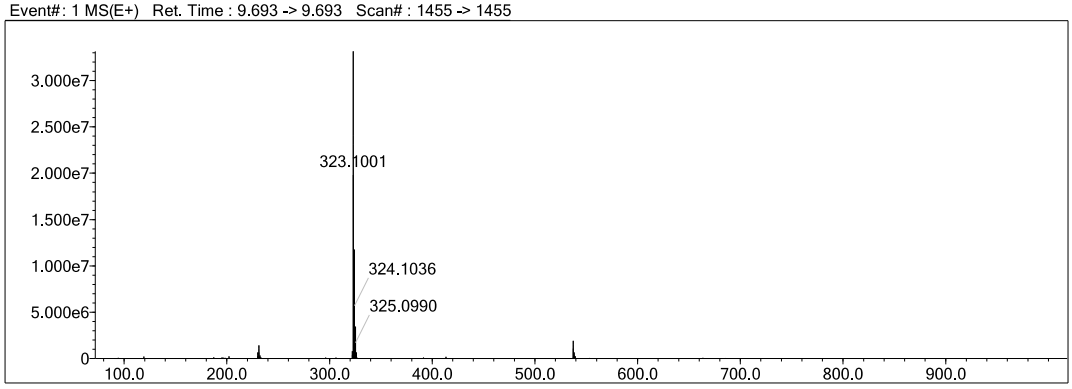
Use Adduct
H

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

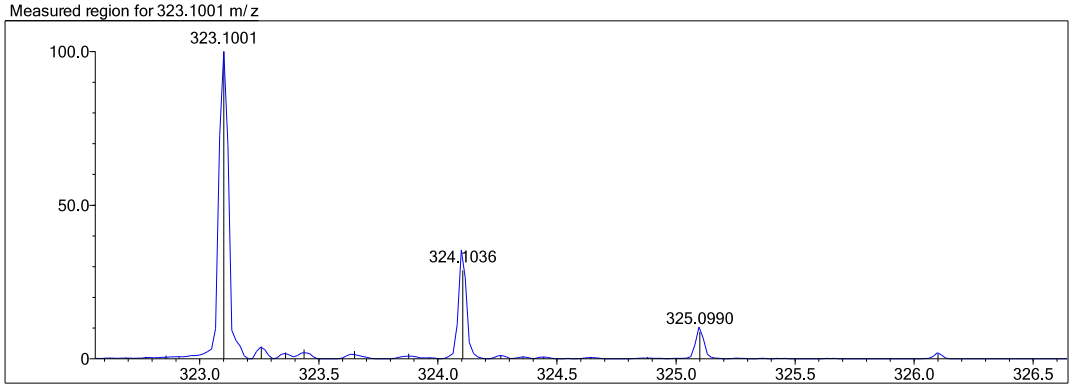
DBE Range: 10.0 - 20.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

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

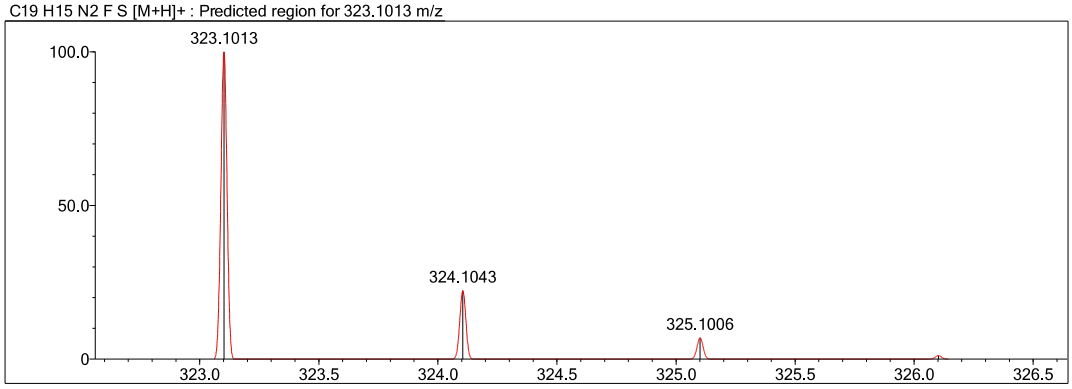
Event#: 1 MS(E+) Ret. Time : 9.693 -> 9.693 Scan# : 1455 -> 1455



Measured region for 323.1001 m/z



C19 H15 N2 F S [M+H]+ : Predicted region for 323.1013 m/z

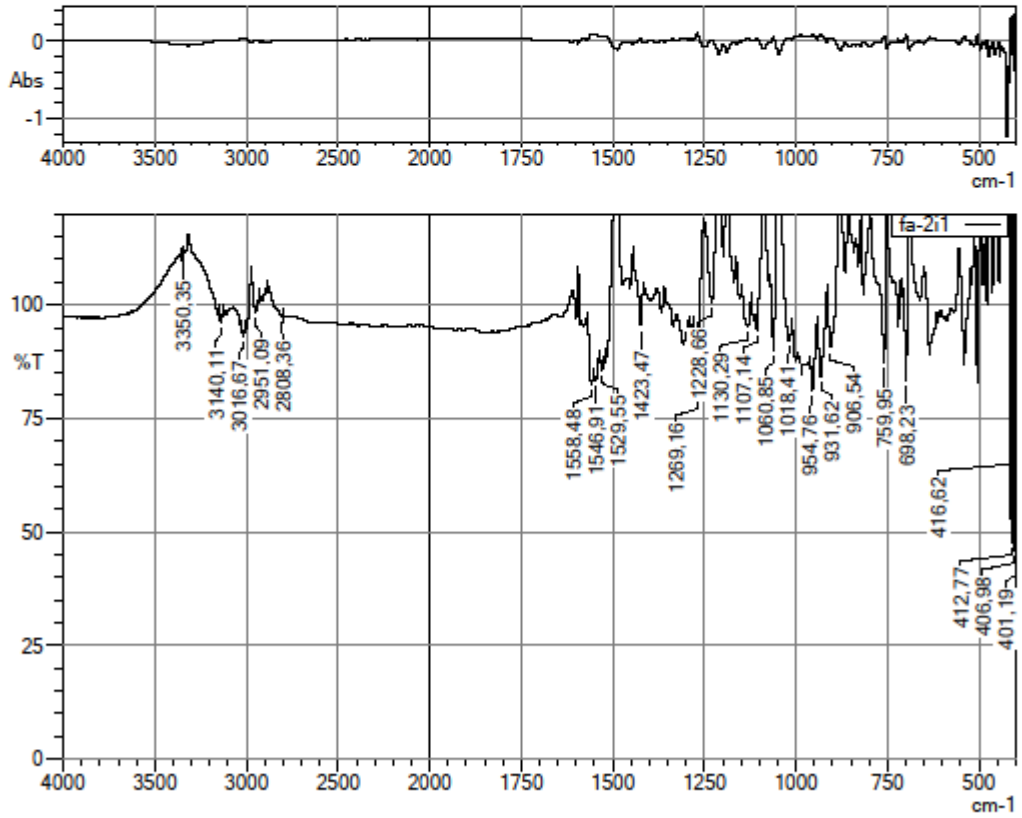


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	73.78	C19 H15 N2 F S	[M+H]+	323.1001	323.1013	-1.2	-3.71	79.14	13.0

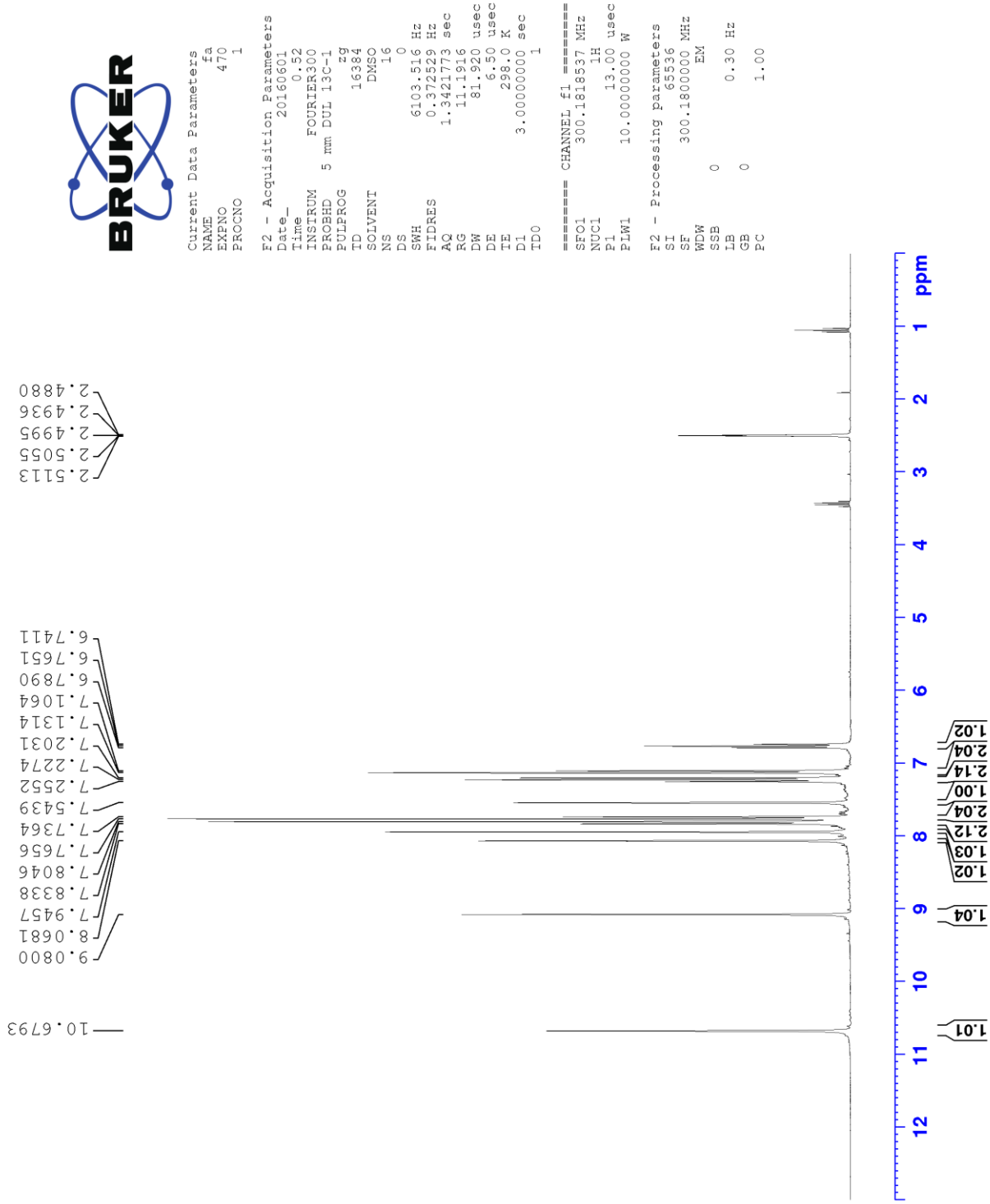
Spectra 32. HRMS spectra of the compound 2h

DOPNALAB

	Item	Value
	Acquired Date&Time	5.10.2016 10:17:07
	Acquired by	System Administrator
	Filename	C:\Users\dopnalab\Desktop\derya\fa\fa-2i1.lspd
	Spectrum name	fa-2i1
	Sample name	fa_2i
	Sample ID	
	Option	
	Comment	
	No. of Scans	10
	Resolution	4 [cm-1]
	Apodization	Happ-Genzel

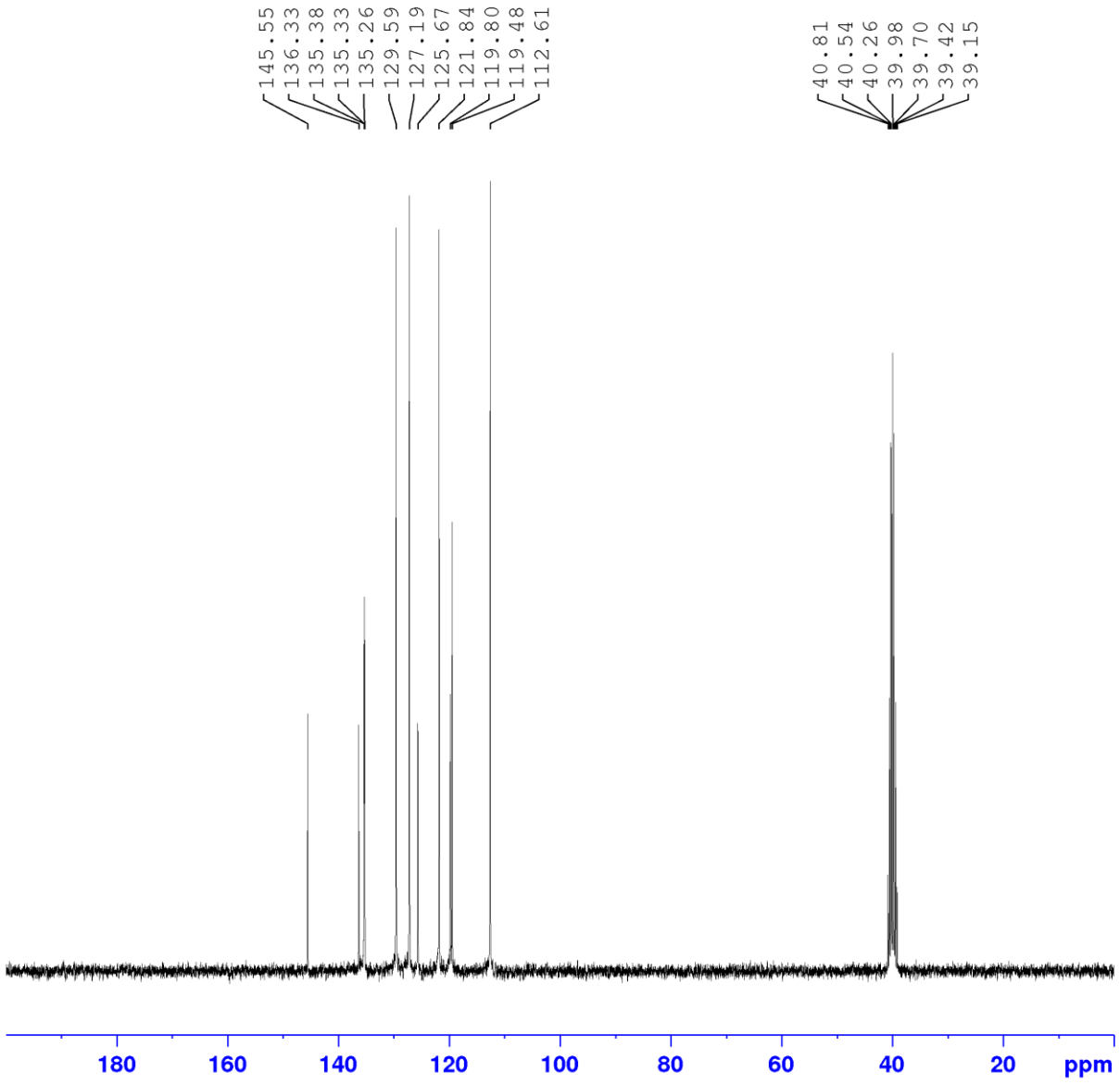


Spectra 33. IR spectra of the compound 2i



Spectra 34. ^{1}H NMR spectra of the compound 2i

Spectra 35. ^{13}C NMR spectra of the compound 2i



BRUKER

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Current Data Parameters
NAME                  fa
EXPNO                471
PROCNO                 1

F2 - Acquisition Parameters
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Time               0.53
INSTRUM      FOURIER300
PROBHD   5 mm DUL 13C-1
PULPROG            zgpg
TD                32768
SOLVENT             DMSO
NS                  2048
DS                     4
SWH           24414.063 Hz
FIDRES         0.745058 Hz
AQ            0.6710886 sec
RG              501.187
DW               20.480 usec
DE                6.50 usec
TE                298.1 K
D1           1.00000000 sec
D11          0.03000000 sec
D31          0.00001500 sec
D32          0.89999998 sec
D40          0.00093990 sec
L4                   23
L5                   26
P32               90.00 usec
TD0                   1

======== CHANNEL f1 ========
SFO1         75.4878687 MHz
NUC1                13C
P1                15.00 usec
PLW1        15.00000000 W

======== CHANNEL f2 ========
SFO2         300.1812007 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        10.00000000 W
PLW12        0.20863999 W
PLW13        0.10495000 W

F2 - Processing parameters
SI                 32768
SF           75.4803210 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
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Data File: C:\ LabSolutions\ Data\Analiz\derya\ FA-9_9.lcd

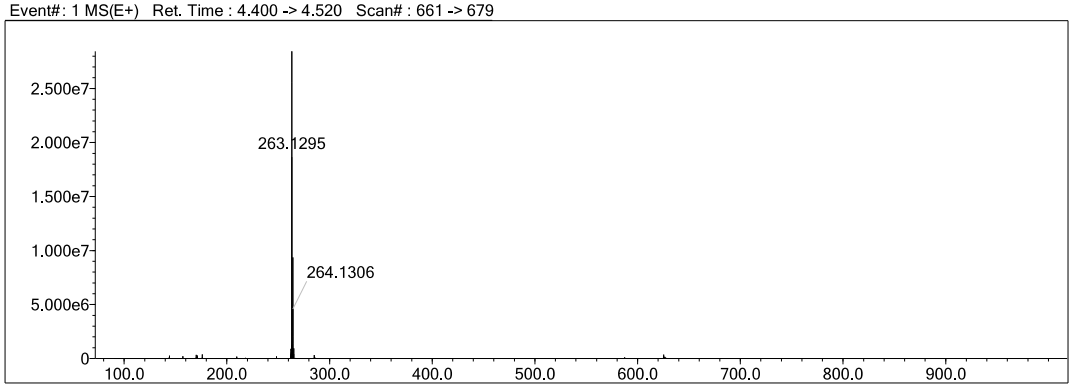
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	50	O	2	0	6	Cl	1	0	0	H
C	4	0	50	F	1	0	1	Br	1	0	0	
N	3	0	5	S	2	0	1	Pd	2	0	0	

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

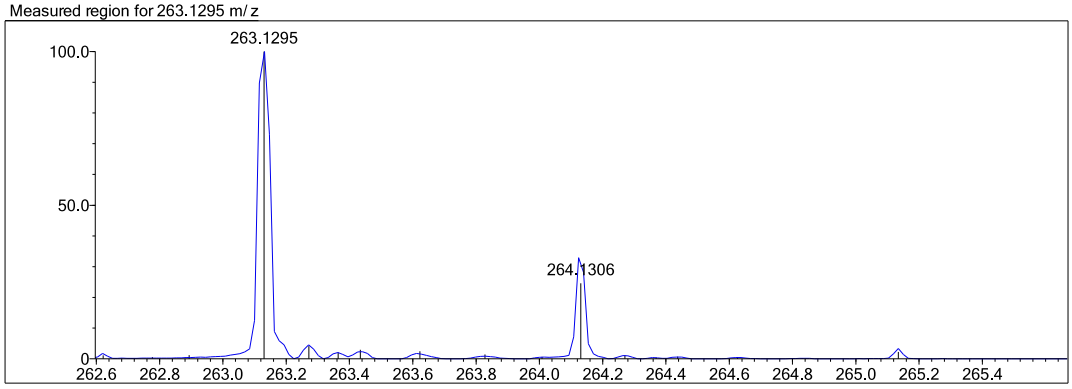
DBE Range: 10.0 - 20.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

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

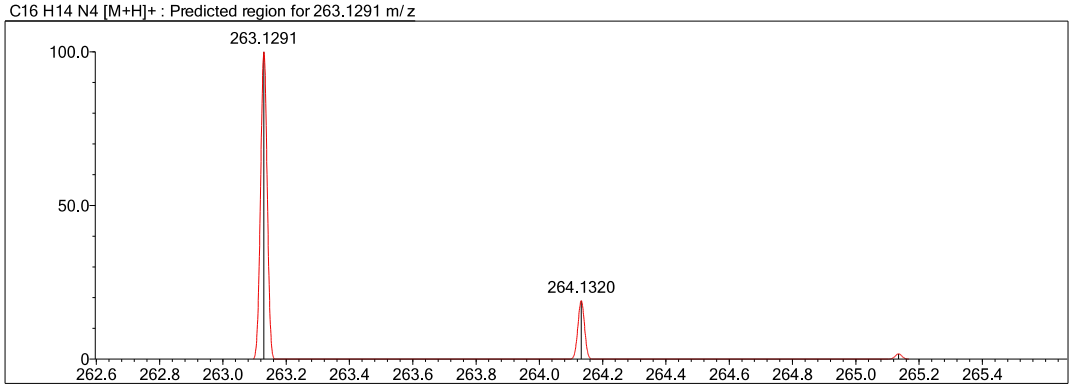
Event#: 1 MS(E+) Ret. Time : 4.400 -> 4.520 Scan# : 661 -> 679



Measured region for 263.1295 m/z



C16 H14 N4 [M+H]+ : Predicted region for 263.1291 m/z

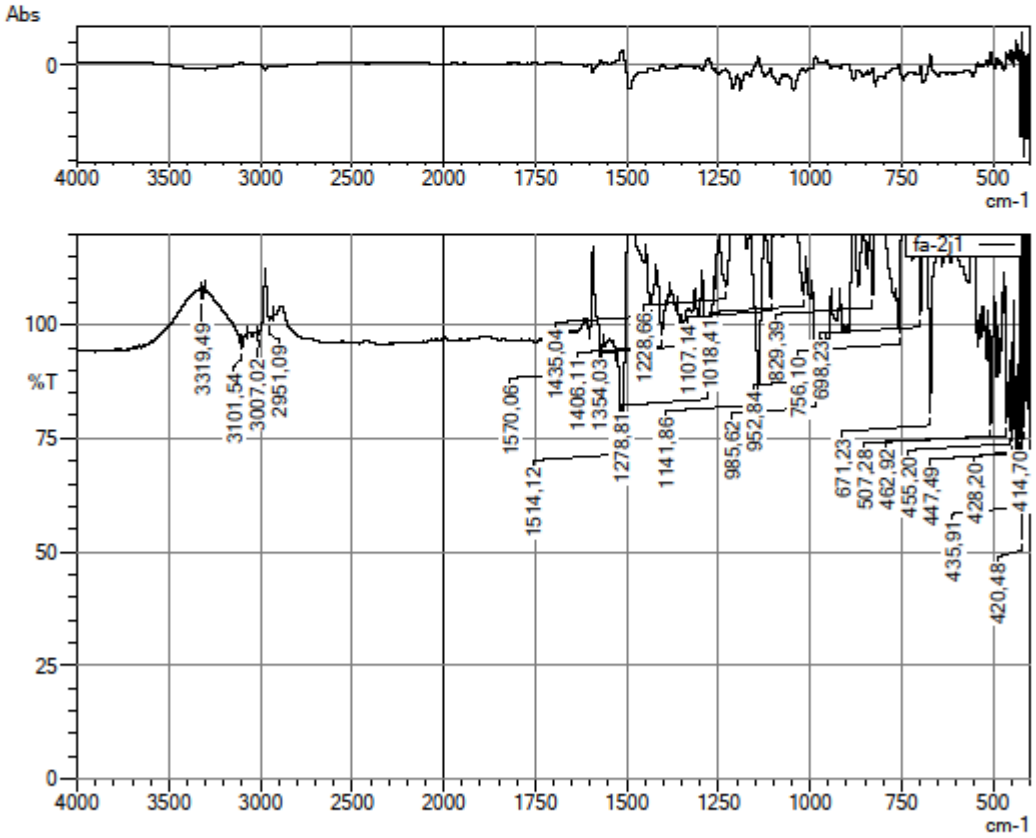


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	74.65	C16 H14 N4	[M+H]+	263.1295	263.1291	0.4	1.52	75.64	12.0

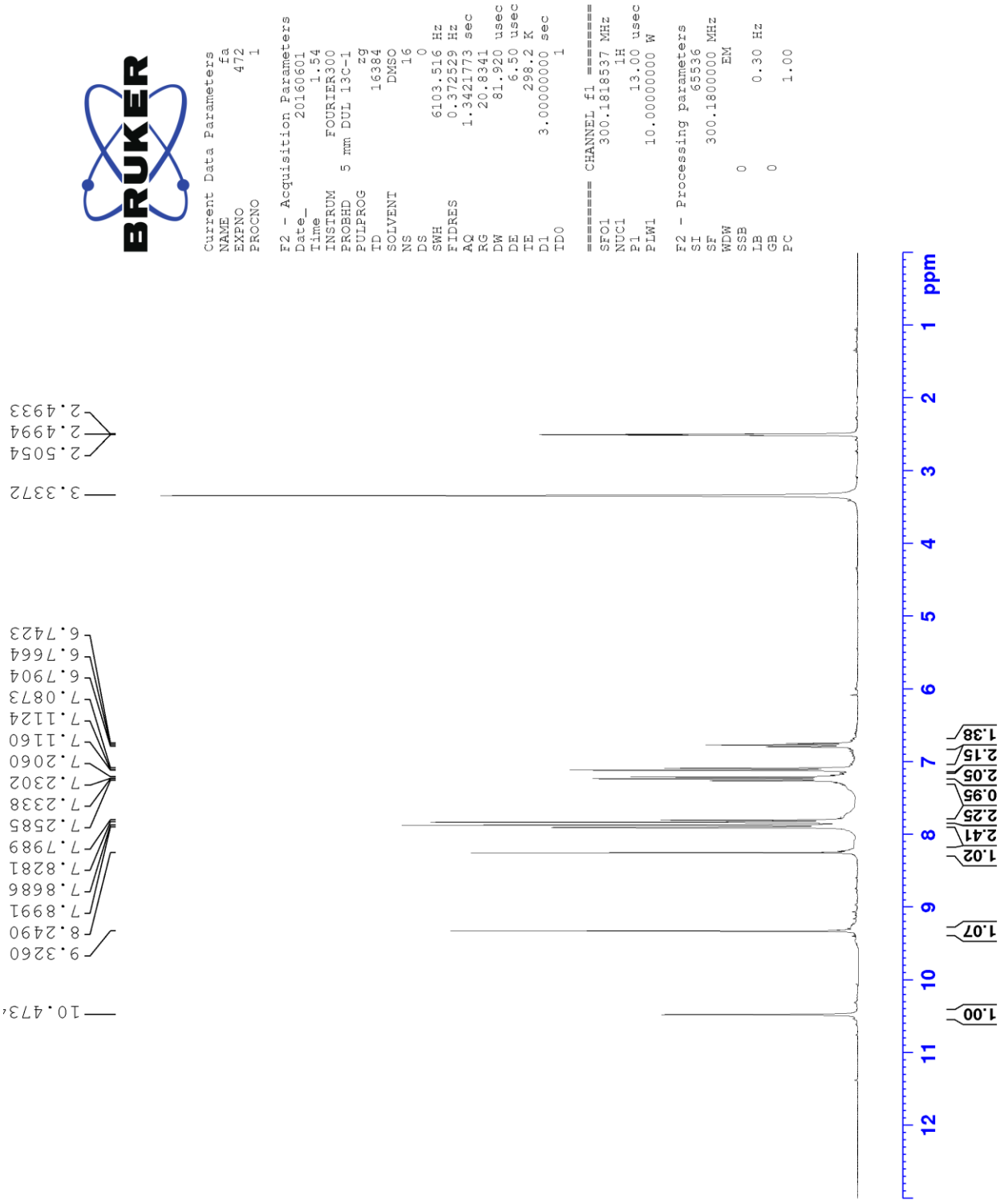
Spectra 36. HRMS spectra of the compound 2i

DOPNALAB

Item	Value
Acquired Date&Time	5.10.2016 10:21:39
Acquired by	System Administrator
Filename	C:\Users\dopnalab\Desktop\derya\fa\fa-2\1.lspd
Spectrum name	fa-2\1
Sample name	fa_2\
Sample ID	
Option	
Comment	
No. of Scans	10
Resolution	4 [cm-1]
Apodization	Happ-Genzel

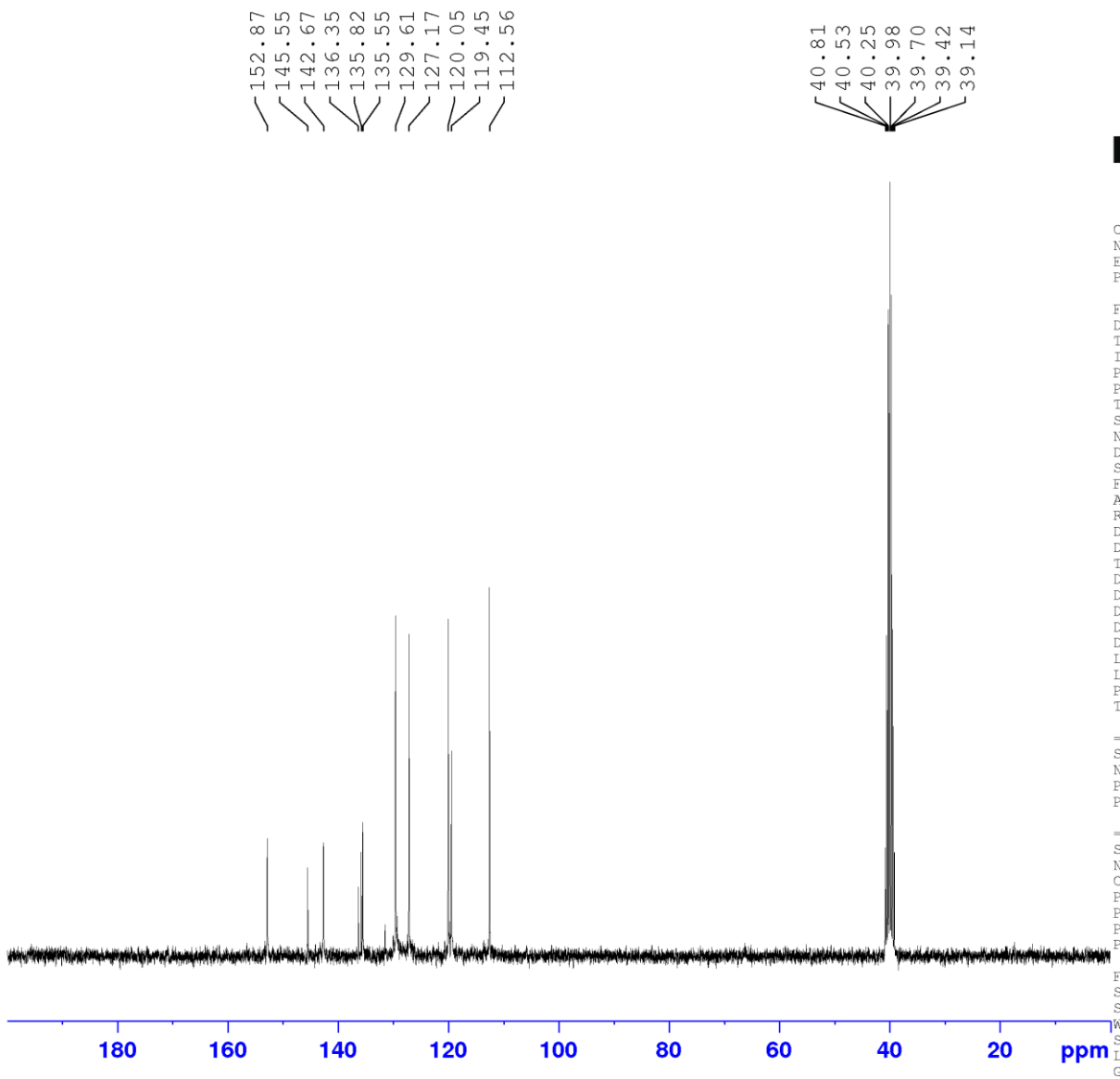


Spectra 37. IR spectra of the compound 2j



Spectra 38. ^{1}H NMR spectra of the compound 2j

Spectra 39. ^{13}C NMR spectra of the compound 2j



BRUKER

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Current Data Parameters
NAME                      fa
EXPNO                    473
PROCNO                     1

F2 - Acquisition Parameters
Date_              20160601
Time                   1.56
INSTRUM       FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG                zgpg
TD                    32768
SOLVENT                DMSO
NS                     2048
DS                        4
SWH               24414.063 Hz
FIDRES             0.745058 Hz
AQ                 0.6710886 sec
RG                   501.187
DW                  20.480 usec
DE                   6.50 usec
TE                   298.0 K
D1                1.00000000 sec
D11               0.03000000 sec
D31               0.00001500 sec
D32               0.89999998 sec
D40               0.00093990 sec
L4                        23
L5                        26
P32                  90.00 usec
TD0                        1

======== CHANNEL f1 ========
SFO1             75.4878687 MHz
NUC1                    13C
P1                   15.00 usec
PLW1            15.00000000 W

======== CHANNEL f2 ========
SFO2            300.1812007 MHz
NUC2                    1H
CPDPRG[2             waltz16
PCPD2                90.00 usec
PLW2            10.00000000 W
PLW12            0.20863999 W
PLW13            0.10495000 W

F2 - Processing parameters
SI                    32768
SF               75.4803210 MHz
WDW                      EM
SSB          0
LB                    1.00 Hz
GB           0
PC                    1.40
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Data File: C:\ LabSolutions\ Data\Analiz\derya\ FA-10_10.lcd

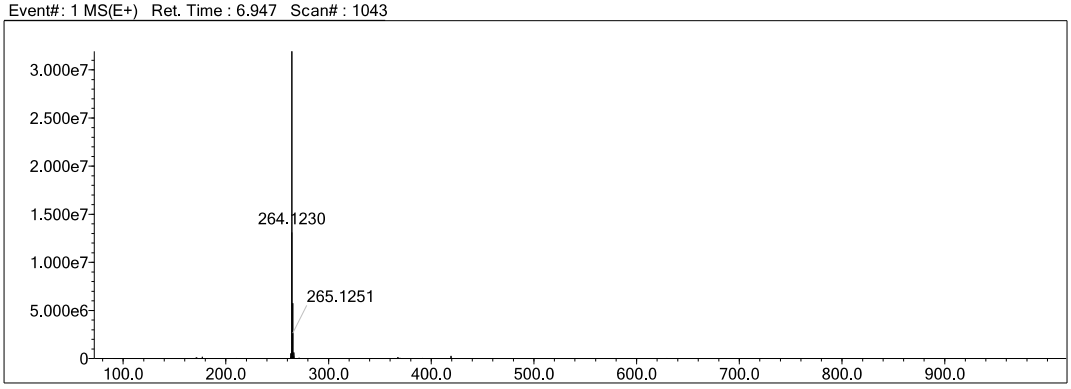
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	50	O	2	0	6	Cl	1	0	0	H
C	4	0	50	F	1	0	1	Br	1	0	0	
N	3	0	5	S	2	0	1	Pd	2	0	0	

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

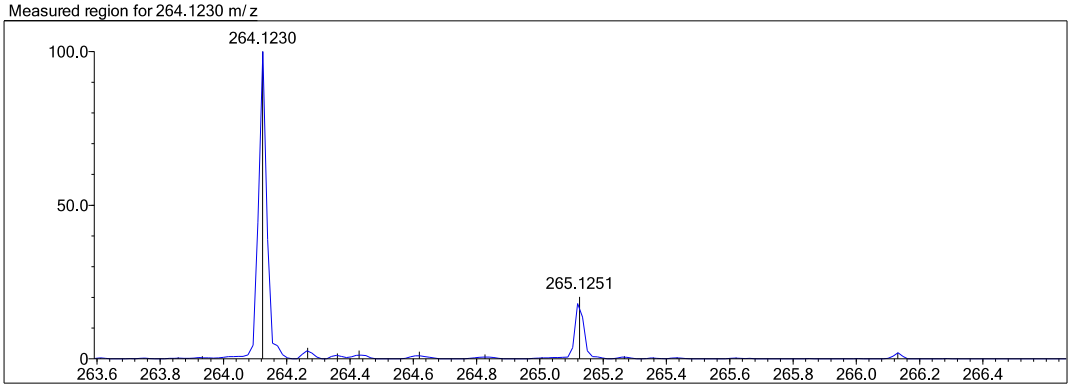
DBE Range: 10.0 - 20.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

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

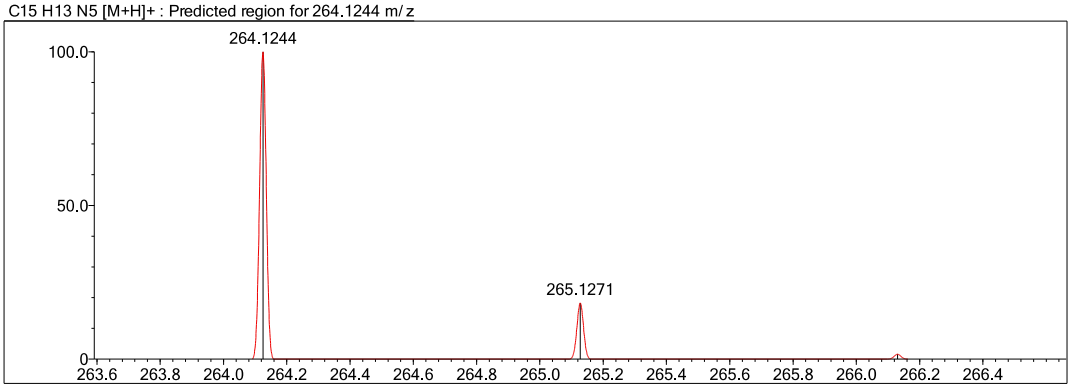
Event#: 1 MS(E+) Ret. Time : 6.947 Scan# : 1043



Measured region for 264.1230 m/z



C15 H13 N5 [M+H]+ : Predicted region for 264.1244 m/z

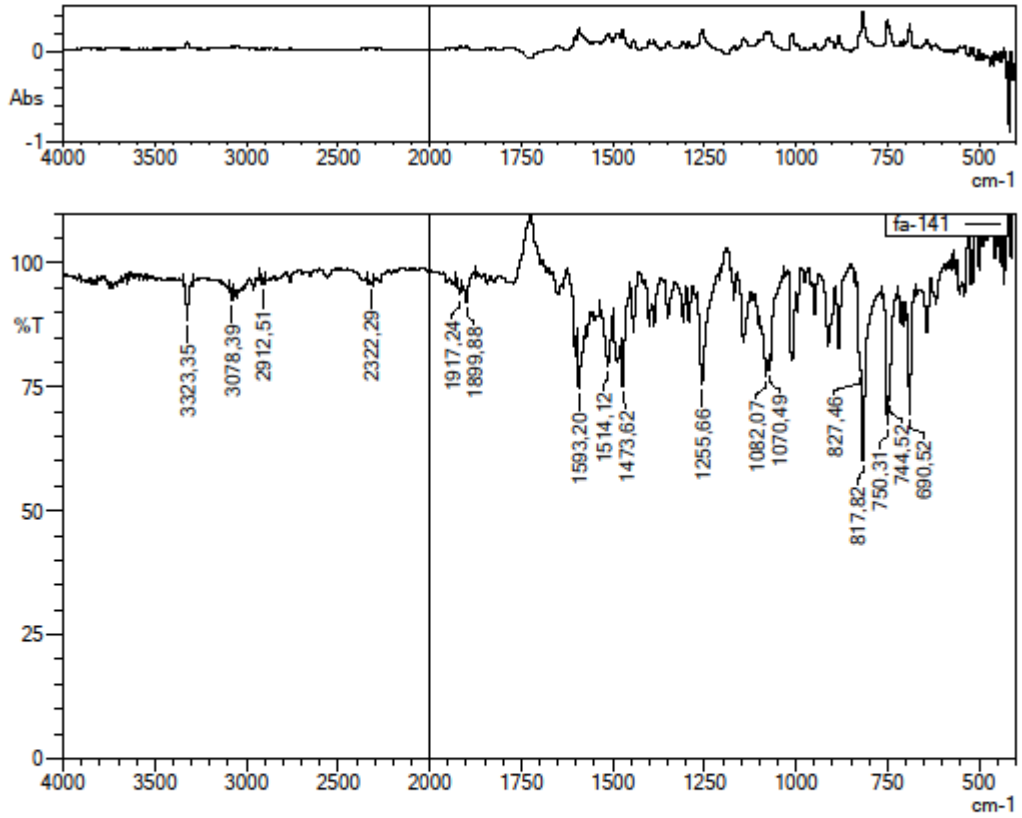


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	82.79	C15 H13 N5	[M+H]+	264.1230	264.1244	-1.4	-5.30	95.17	12.0

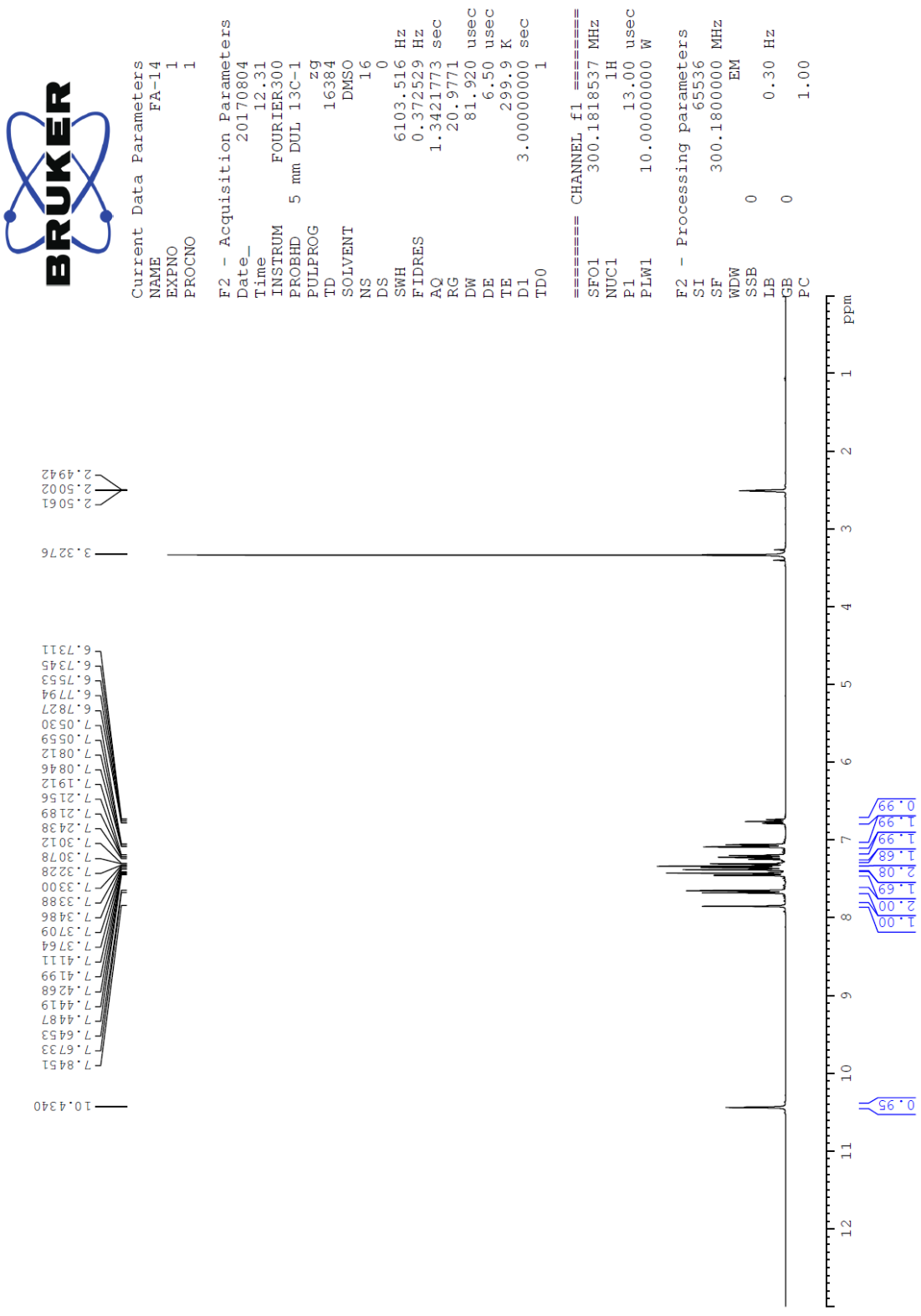
Spectra 40. HRMS spectra of the compound 2j

DOPNALAB

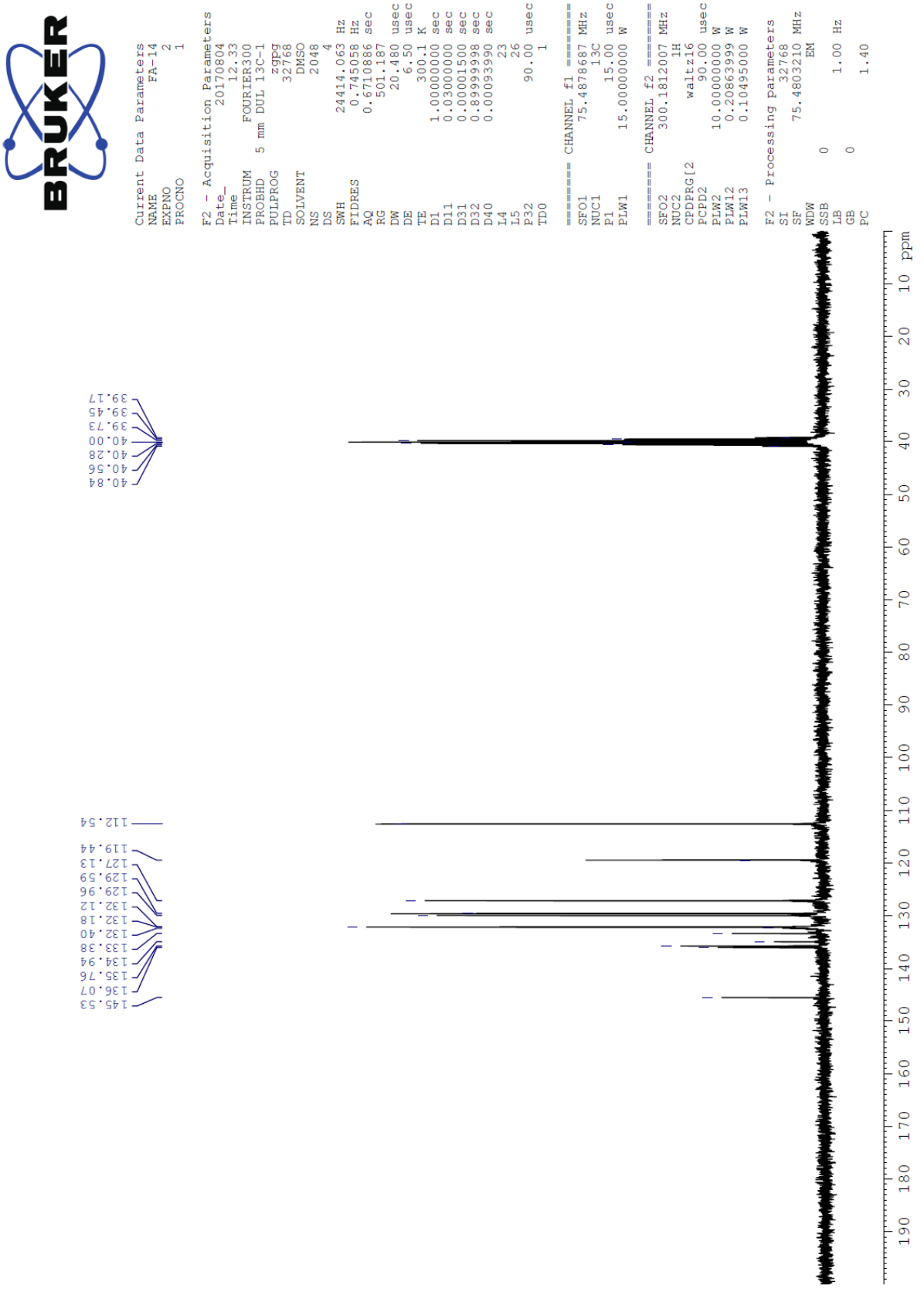
Item	Value
Acquired Date&Time	7.06.2017 10:39:00
Acquired by	System Administrator
Filename	C:\Users\dopnalab\Desktop\derya\fa\fa-141.ispd
Spectrum name	fa-141
Sample name	fa-14
Sample ID	
Option	
Comment	
No. of Scans	10
Resolution	4 [cm-1]
Apodization	Happ-Genzel



Spectra 41. IR spectra of the compound 2k



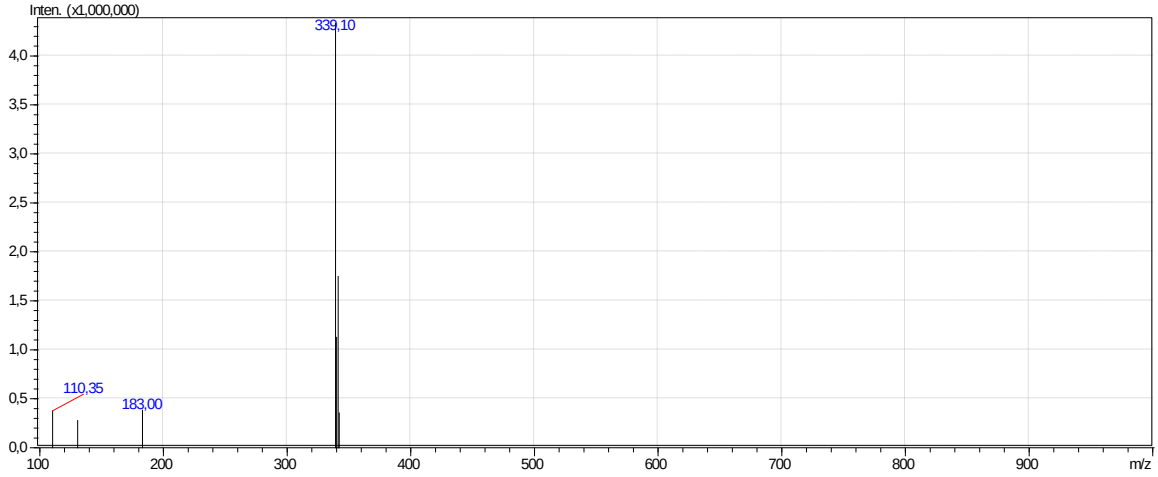
Spectra 42. ^{1}H NMR spectra of the compound 2k



Spectra 43. ^{13}C NMR spectra of the compound 2k

LCMSMS ANALYSIS REPORT

Sample Name	: FA-14		
Sample ID	:		
Data Filename	: FA-14_004.lcd		
Method Filename	: geneltarama.lcm		
Batch Filename	: batch.lcb		
Vial #	: 1-79		
Injection Volume	: 1 uL	Sample Type	: Unknown
Date Acquired	: 04.08.2017 14:52:32	Acquired by	: System Administrator
Date Processed	: 04.08.2017 14:54:35	Processed by	: System Administrator

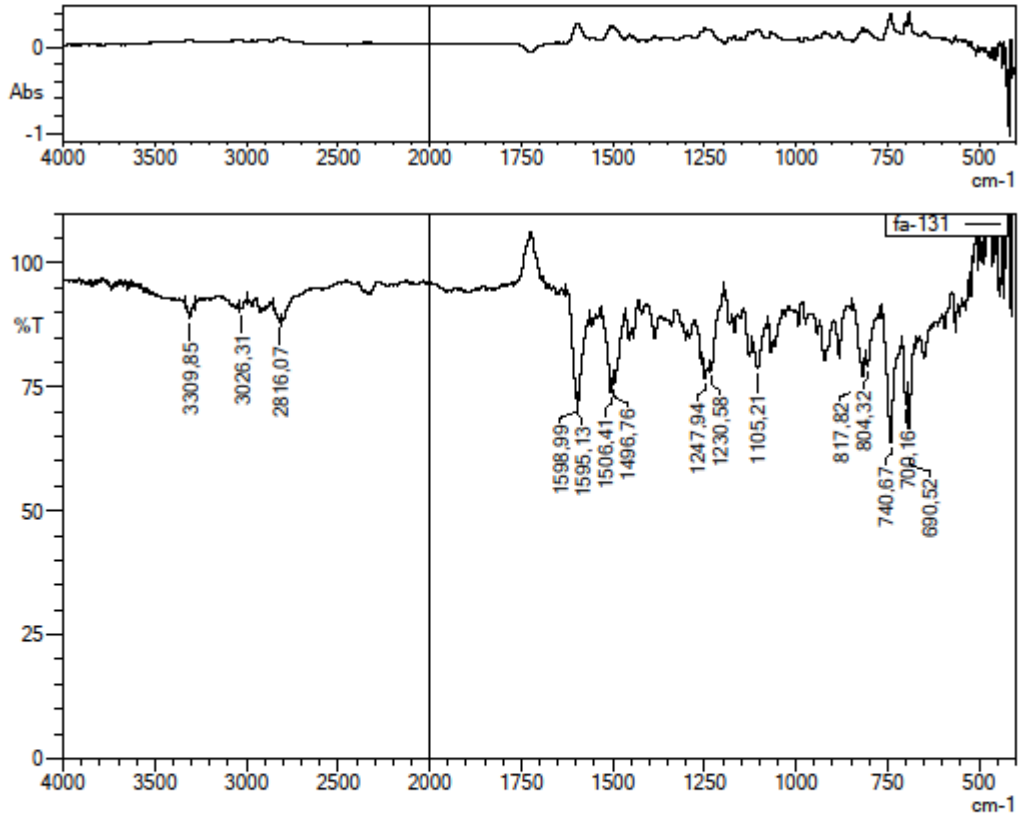


[MS Spectrum]		
# of Peaks	7	
Raw Spectrum	[1,590],(scan:[95])	
Background	[0,068->0,203],(scan:[5->13])	
Base Peak	m/z 339,10 (Inten : 4.335.027)	
m/z	Absolute Intensity	Relative Intensity
110,35	377521	8,71
130,70	279346	6,44
183,00	385160	8,88
339,10	4335027	100,00
340,10	1128654	26,04
341,20	1751529	40,40
342,15	357781	8,25
Event	1	

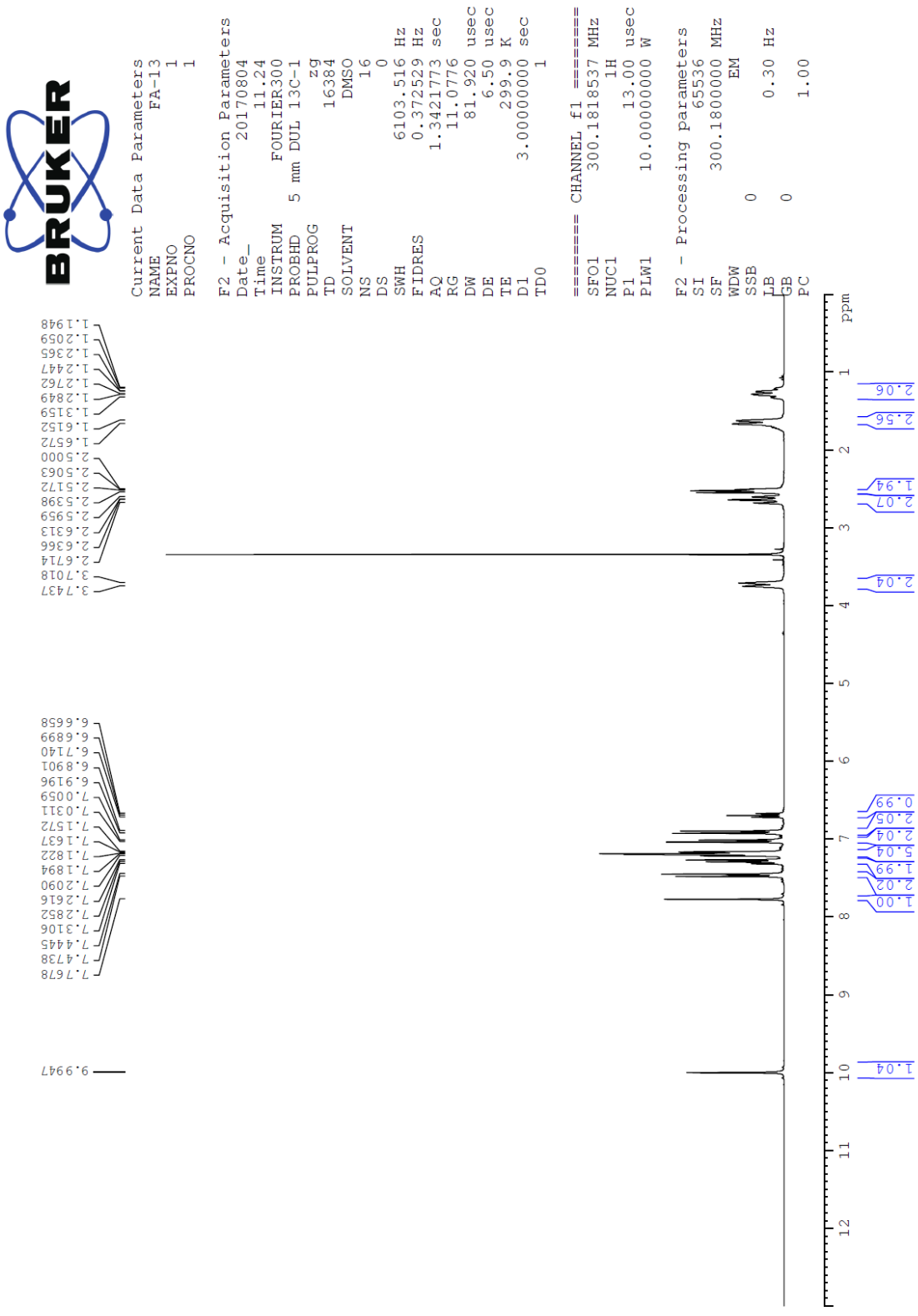
Spectra 44. LCMSMS spectra of the compound 2k

DOPNALAB

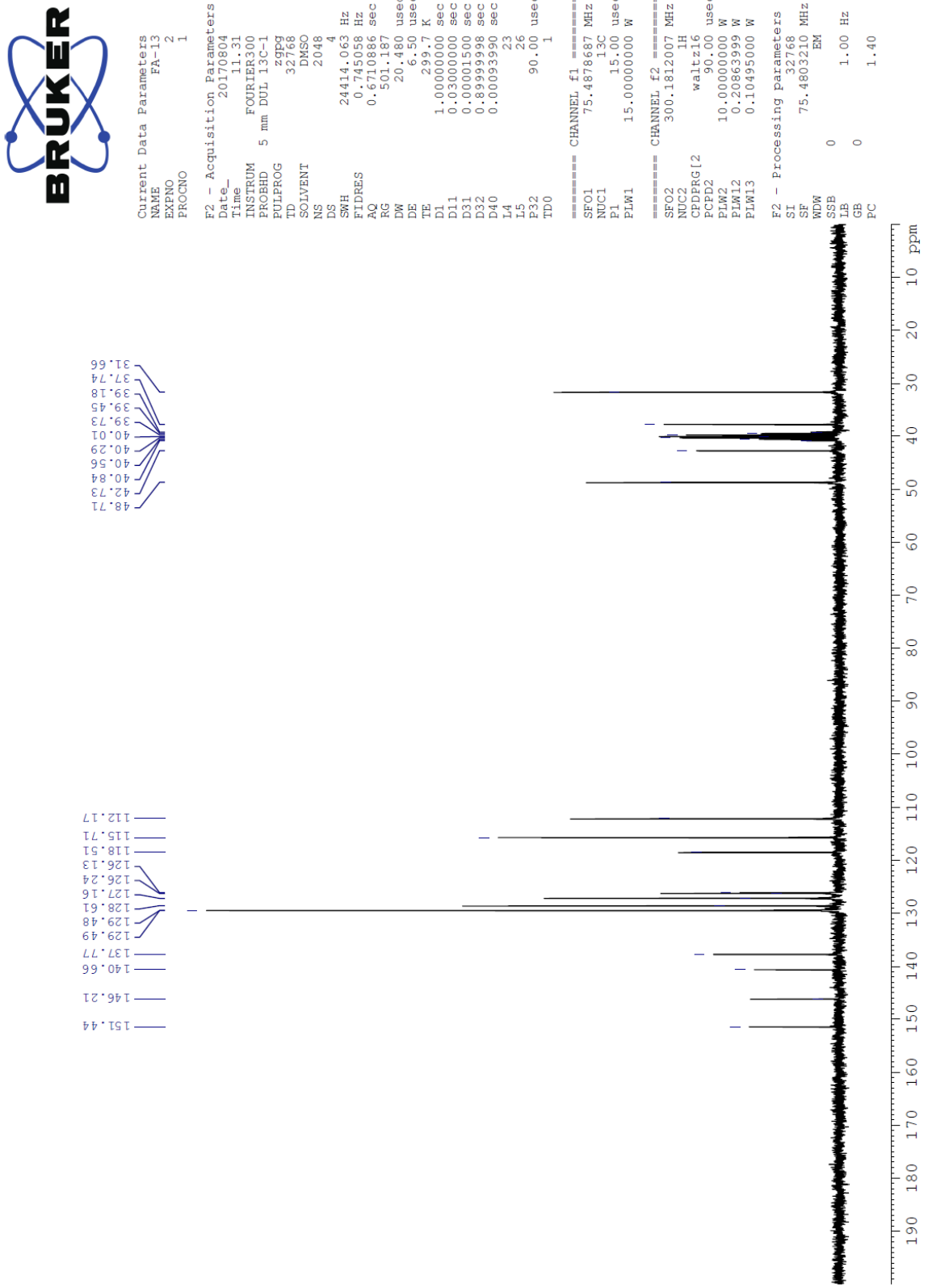
	Item	Value
	Acquired Date&Time	7.08.2017 10:36:28
	Acquired by	System Administrator
	Filename	C:\Users\dopnalab\Desktop\derya\fa\fa-131.ispd
	Spectrum name	fa-131
	Sample name	fa-13
	Sample ID	
	Option	
	Comment	
	No. of Scans	10
	Resolution	4 [cm-1]
	Apodization	Happ-Genzel



Spectra 45. IR spectra of the compound 2l



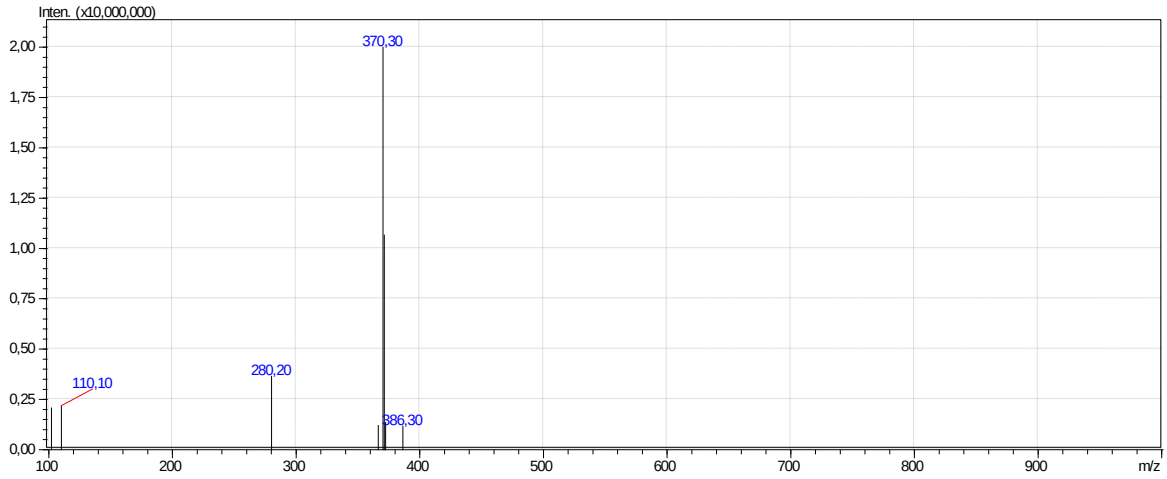
Spectra 46. ^{1}H NMR spectra of the compound 2l



Spectra 47. ^{13}C NMR spectra of the compound 2l

LCMSMS ANALYSIS REPORT

Sample Name	: FA-13		
Sample ID	:		
Data Filename	: FA-13_003.lcd		
Method Filename	: geneltarama.lcm		
Batch Filename	: batch.lcb		
Vial #	: 1-78		
Injection Volume	: 1 uL	Sample Type	: Unknown
Date Acquired	: 04.08.2017 14:49:53	Acquired by	: System Administrator
Date Processed	: 04.08.2017 14:51:56	Processed by	: System Administrator

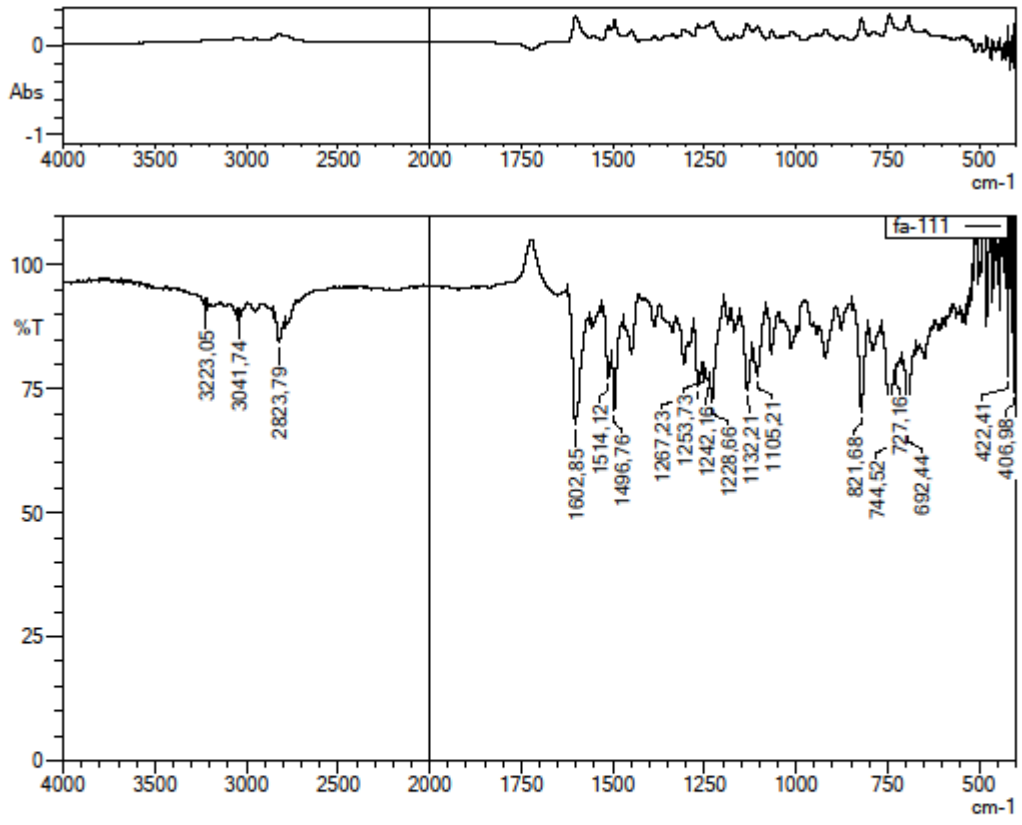


[MS Spectrum]		
# of Peaks	8	
Raw Spectrum	[1,590],(scan:[95])	
Background	No Background Spectrum	
Base Peak	m/z 370,30 (Inten : 20.000.000)	
m/z	Absolute Intensity	Relative Intensity
102,15	2086434	10,43
110,10	2194096	10,97
280,20	3659206	18,30
366,35	1214546	6,07
370,30	20000000	100,00
371,30	10672056	53,36
372,40	1362345	6,81
386,30	1181229	5,91
Event	1	

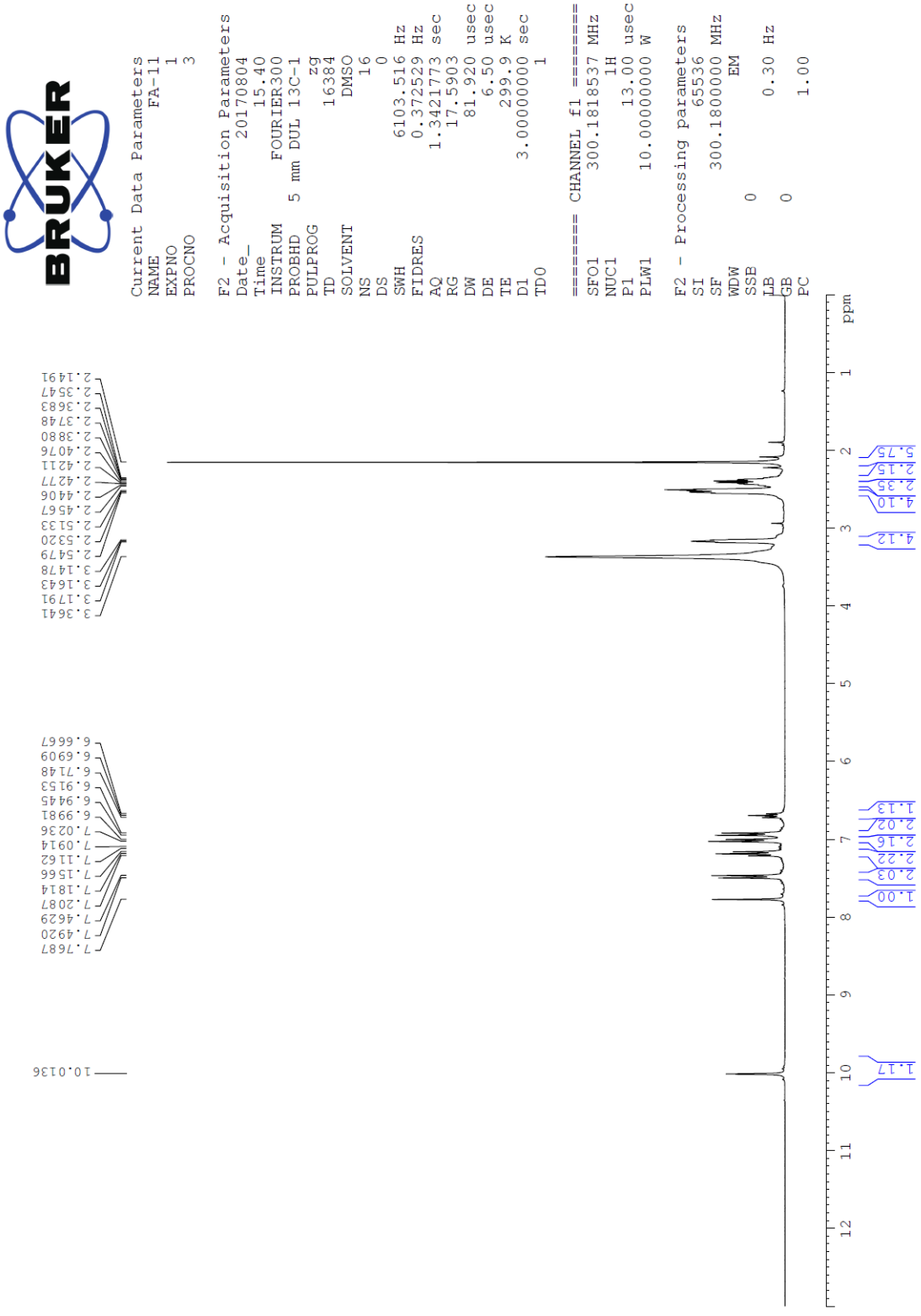
Spectra 48. LCMSMS spectra of the compound 2l

DOPNALAB

	Item	Value
	Acquired Date&Time	7.06.2017 10:28:53
	Acquired by	System Administrator
	Filename	C:\Users\dopnalab\Desktop\derya\fa\fa-111.ispd
	Spectrum name	fa-111
	Sample name	fa-11
	Sample ID	
	Option	
	Comment	
	No. of Scans	10
	Resolution	4 [cm-1]
	Apodization	Happ-Genzel

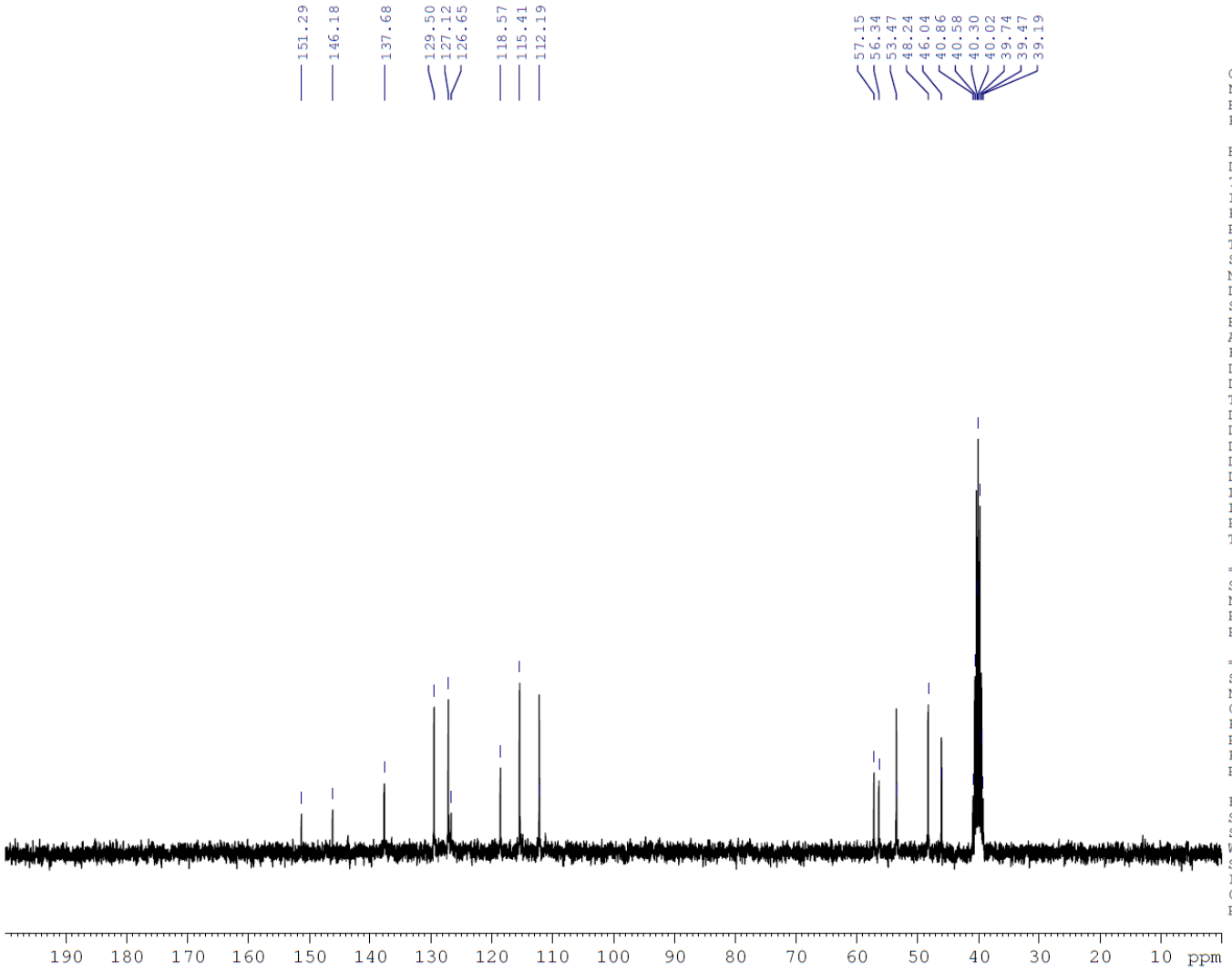


Spectra 49. IR spectra of the compound 2m



Spectra 50. ^{1}H NMR spectra of the compound 2m

Spectra 51. ^{13}C NMR spectra of the compound 2m

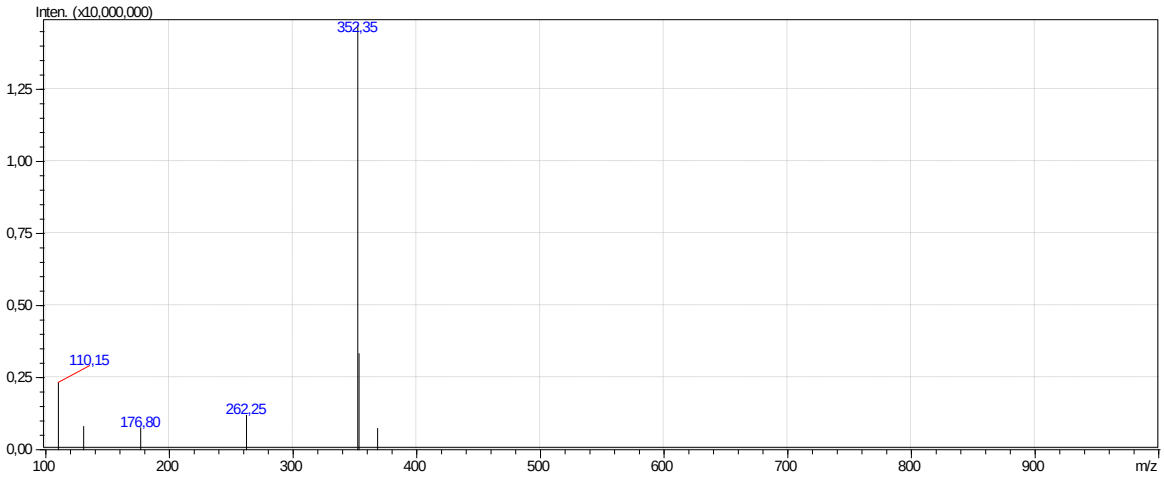


BRUKER

```
Current Data Parameters
NAME                  FA-11
EXPNO                     2
PROCNO                    2

F2 - Acquisition Parameters
Date_              20170804
Time                 14.04
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG                zgpg
TD                    32768
SOLVENT                DMSO
NS                     1829
DS                        4
SWH              24414.063 Hz
FIDRES            0.745058 Hz
AQ                0.6710886 sec
RG                  501.187
DW                   20.480 usec
DE                    6.50 usec
TE                   300.0 K
D1              1.00000000 sec
D11             0.03000000 sec
D31             0.00001500 sec
D32             0.89999998 sec
D40             0.00093990 sec
L4                       23
L5                       26
P32                   90.00 usec
TD0                       1

======== CHANNEL f1 ========
SFO1            75.4878687 MHz
NUC1                    13C
P1                    15.00 usec
PLW1           15.00000000 W

======== CHANNEL f2 ========
SFO2           300.1812007 MHz
NUC2                    1H
CPDPRG[2           waltz16
PCPD2                 90.00 usec
PLW2           10.00000000 W
PLW12           0.20863999 W
PLW13           0.10495000 W

F2 - Processing parameters
SI                    32768
SF              75.4803210 MHz
WDW                      EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```

LCMSMS ANALYSIS REPORT

Sample Name	: FA-11		
Sample ID	:		
Data Filename	: FA-11_001.lcd		
Method Filename	: geneltarama.lcm		
Batch Filename	: batch.lcb		
Vial #	: 1-76		
Injection Volume	: 1 uL	Sample Type	: Unknown
Date Acquired	: 04.08.2017 14:44:33	Acquired by	: System Administrator
Date Processed	: 04.08.2017 14:46:36	Processed by	: System Administrator

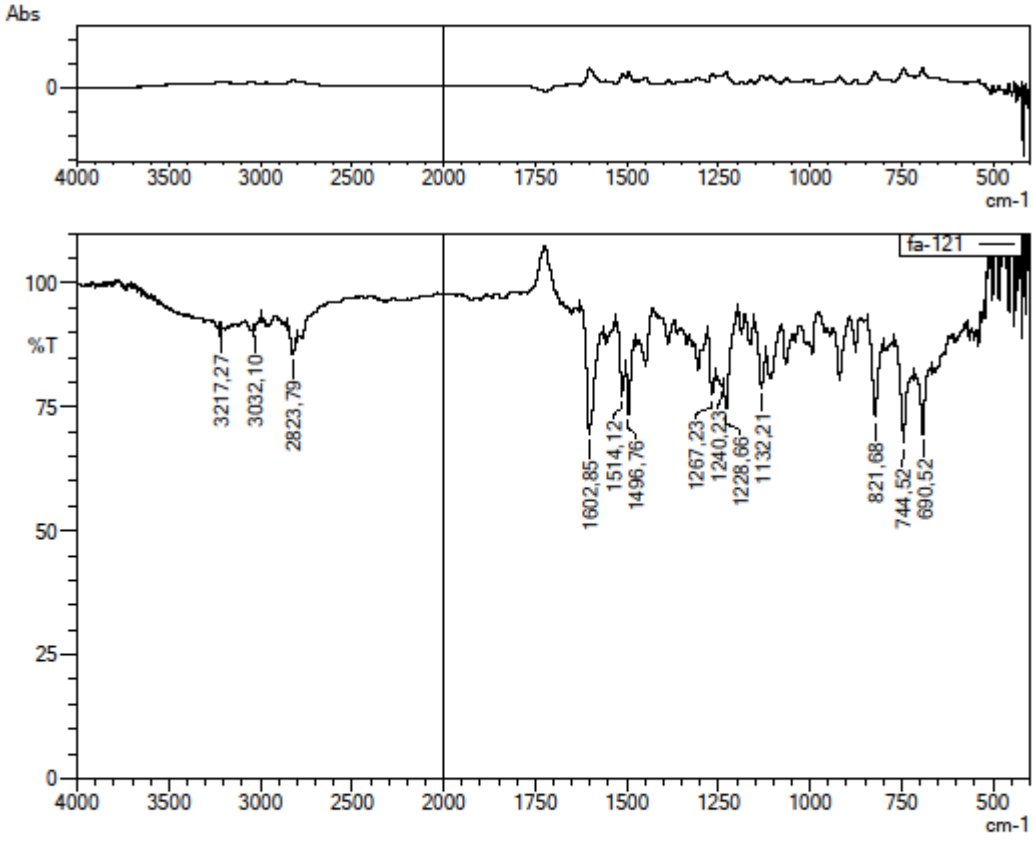


[MS Spectrum]		
# of Peaks	7	
Raw Spectrum	[1,624->1,759],(scan:[97->105])	
Background	[0,101->0,271],(scan:[7->17])	
Base Peak	m/z 352,35 (Inten : 14.730.228)	
m/z	Absolute Intensity	Relative Intensity
110,15	2341968	15,90
130,70	807890	5,48
176,80	761119	5,17
262,25	1201700	8,16
352,35	14730228	100,00
353,40	3336602	22,65
368,30	745511	5,06
Event	1	

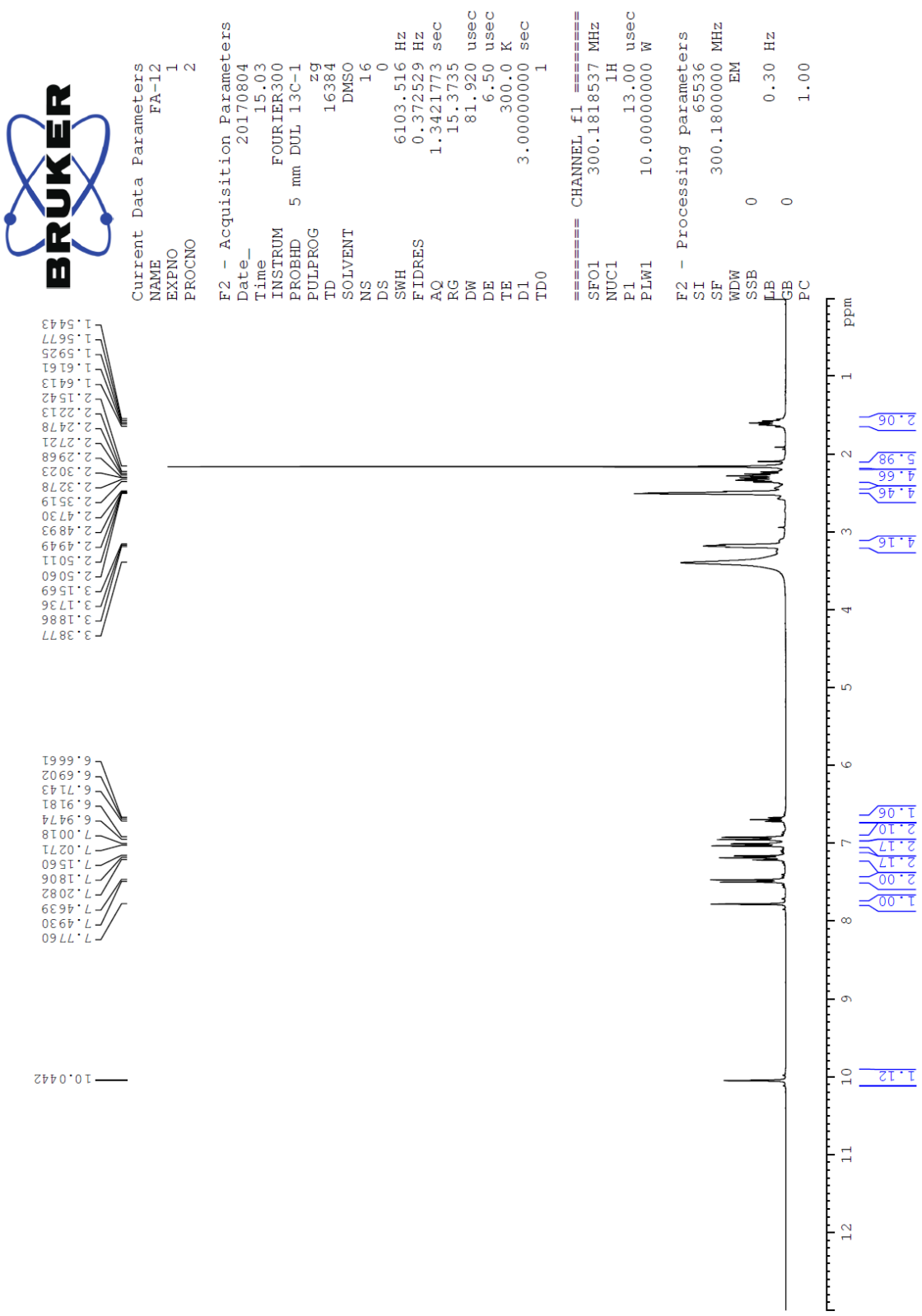
Spectra 52. LCMSMS spectra of the compound 2m

DOPNALAB

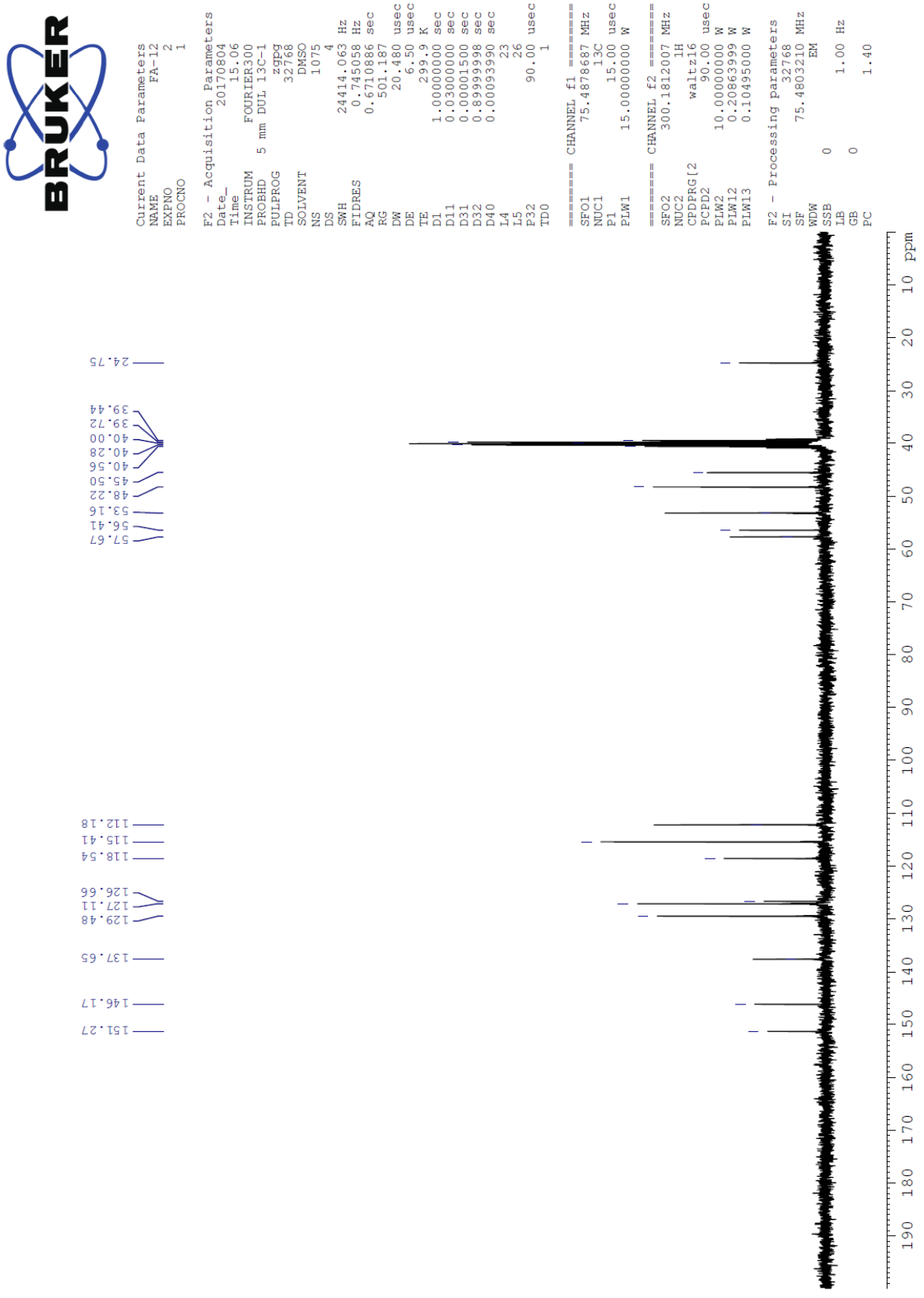
	Item	Value
	Acquired Date&Time	7.06.2017 10:33:21
	Acquired by	System Administrator
	Filename	C:\Users\dopnalab\Desktop\derya\fa\fa-121.ispd
	Spectrum name	fa-121
	Sample name	fa-12
	Sample ID	
	Option	
	Comment	
	No. of Scans	10
	Resolution	4 [cm-1]
	Apodization	Happ-Genzel



Spectra 53. IR spectra of the compound 2n



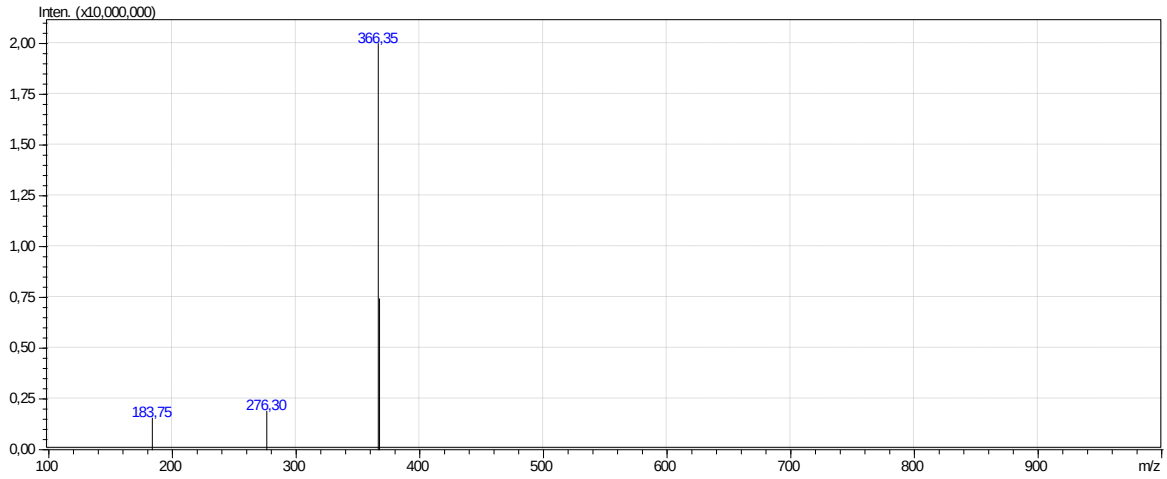
Spectra 54. ^{1}H NMR spectra of the compound 2n



Spectra 55. ^{13}C NMR spectra of the compound 2n

LCMSMS ANALYSIS REPORT

Sample Name	: FA-12		
Sample ID	:		
Data Filename	: FA-12_002.lcd		
Method Filename	: geneltarama.lcm		
Batch Filename	: batch.lcb		
Vial #	: 1-77		
Injection Volume	: 1 uL	Sample Type	: Unknown
Date Acquired	: 04.08.2017 14:47:13	Acquired by	: System Administrator
Date Processed	: 04.08.2017 14:49:17	Processed by	: System Administrator



[MS Spectrum]		
# of Peaks	4	
Raw Spectrum	[1,590],(scan:[95])	
Background	[0,034->0,135],(scan:[3->9])	
Base Peak	m/z 366,35 (Inten : 20.000.000)	
m/z	Absolute Intensity	Relative Intensity
183,75	1572286	7,86
276,30	1907242	9,54
366,35	20000000	100,00
367,40	7431947	37,16
Event	1	

Spectra 56. LCMSMS spectra of the compound 2n