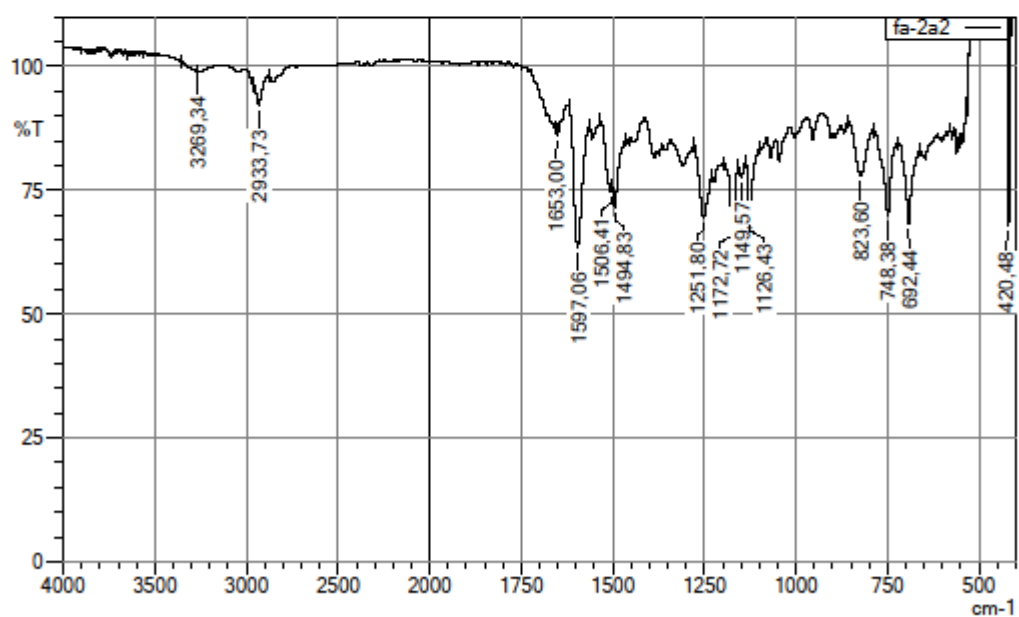
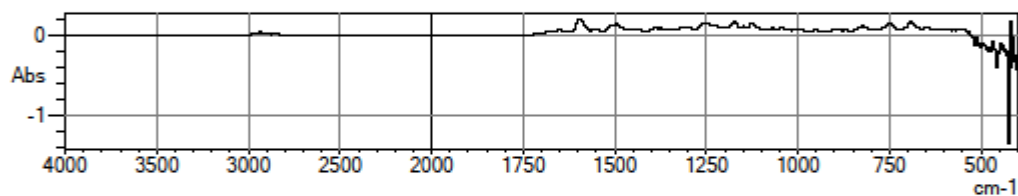


DOPNALAB

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

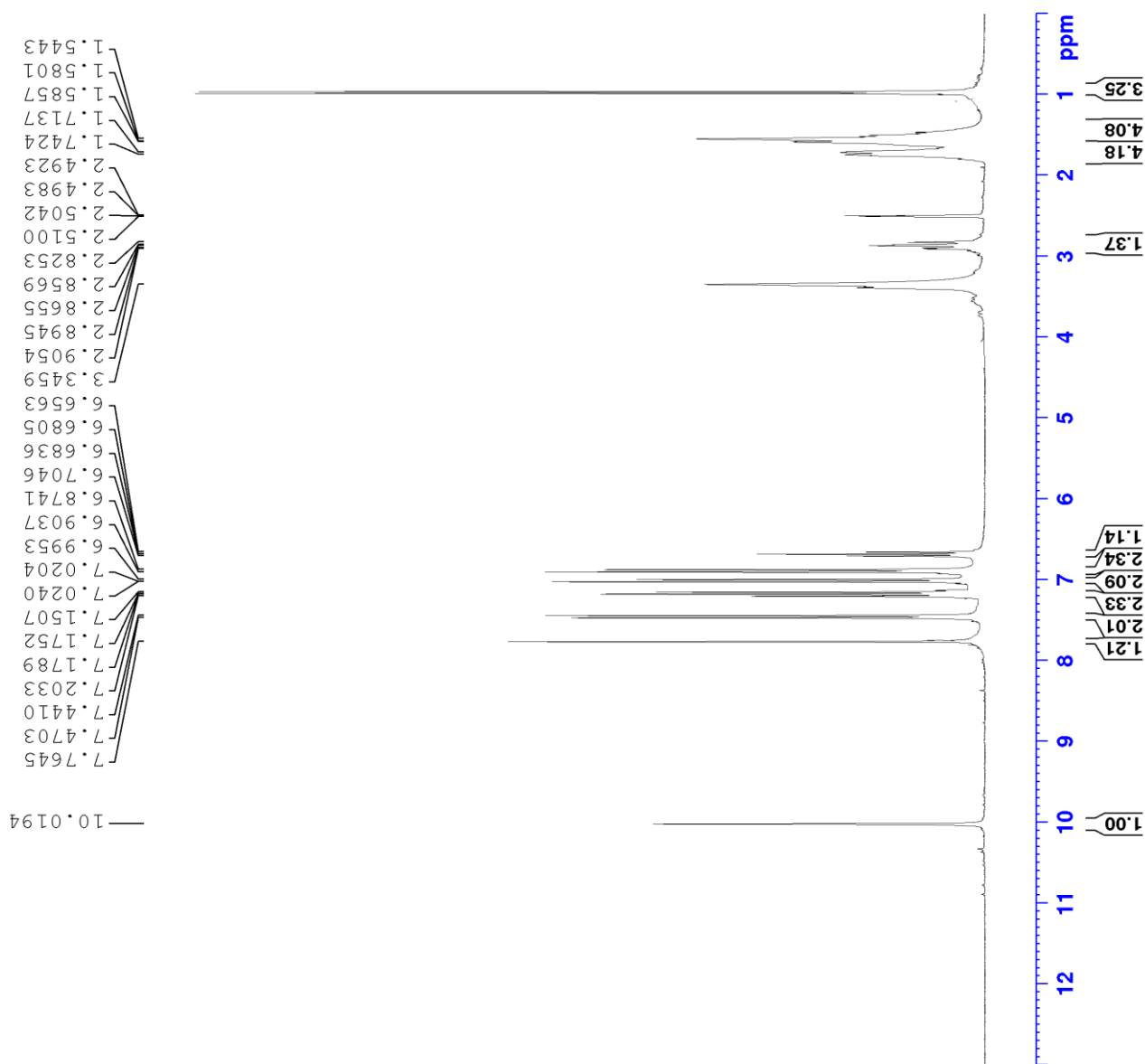


Current Data Parameters
NAME fa
EXPNO 474
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160601
Time 2.56
INSTRUM FOURIER300
PROBHD 5 mm DUL 13C-1
PULPROG zg
ID 16384
SOLVENT DMSO
NS 16
DS 0
SWH 6103.516 Hz
FIDRES 0.372529 Hz
AQ 1.3421773 sec
RG 17.027
DW 81.920 usec
DE 6.50 usec
TE 297.9 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 65836
SF 300.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

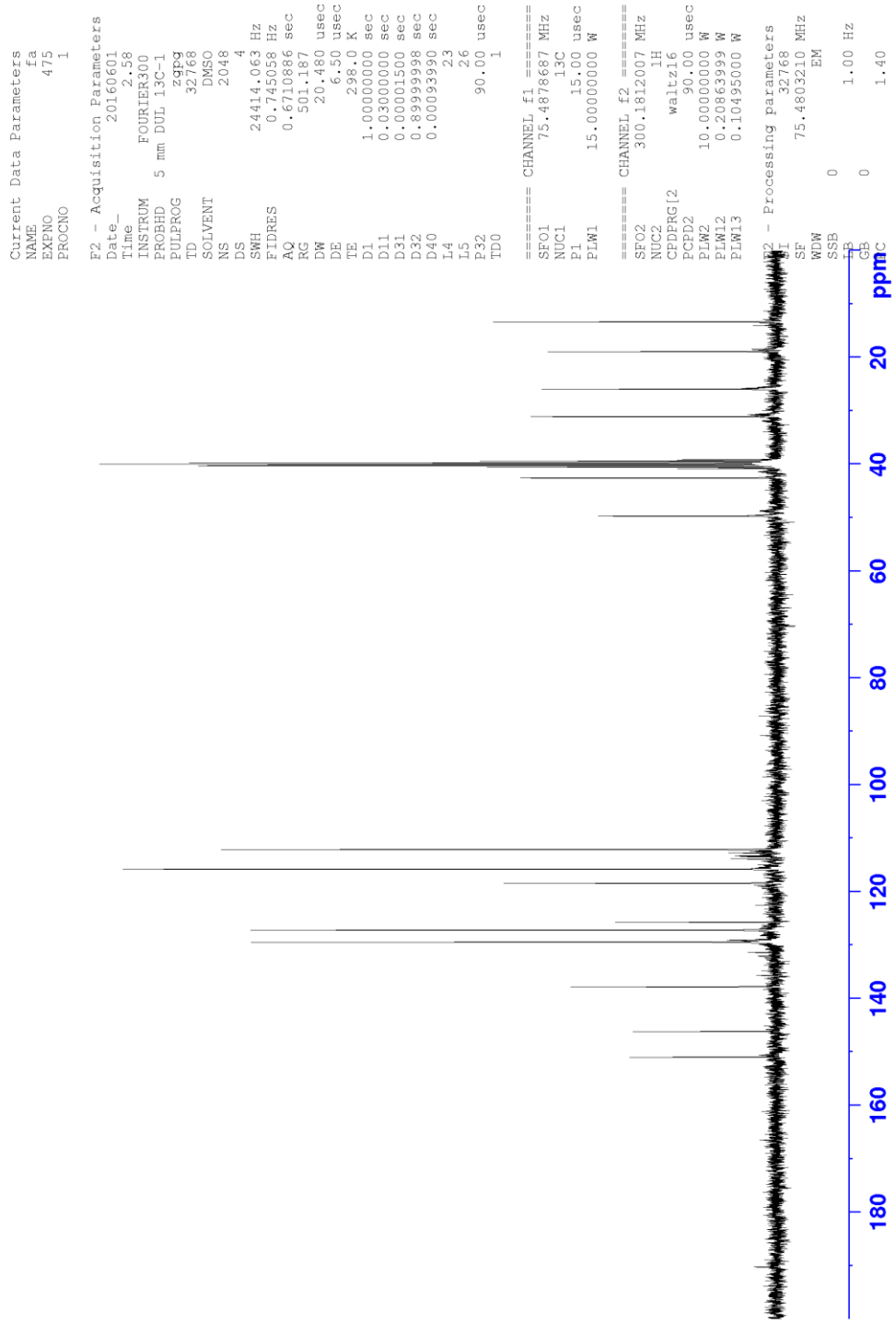


Spectra 2. ¹H NMR spectra of the compound 2a



49.69
42.56
40.81
40.54
40.26
39.98
39.70
39.42
39.15
31.06
25.94
18.92
13.32

150.99
146.23
137.83
129.47
127.22
125.72
118.43
115.80
112.12



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

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

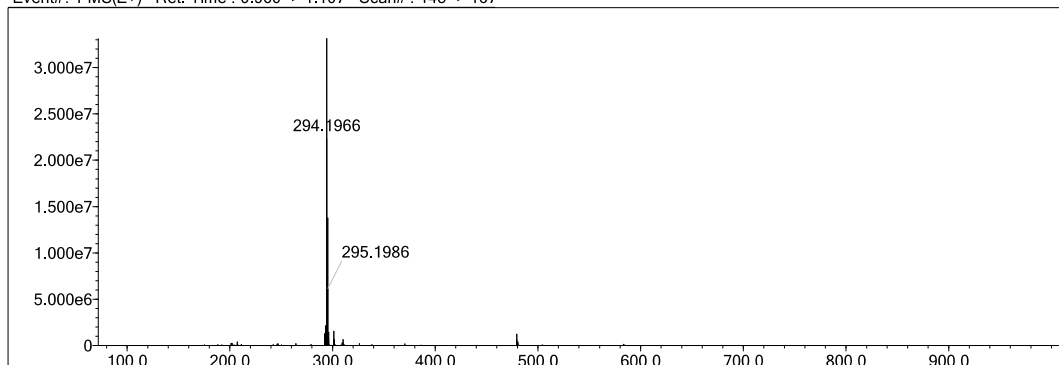
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	50	O	2	0	6	Cl	1	0	0	H
C	4	0	50	F	1	0	0	Br	1	0	0	
N	3	0	3	S	2	0	0	Pd	2	0	0	

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

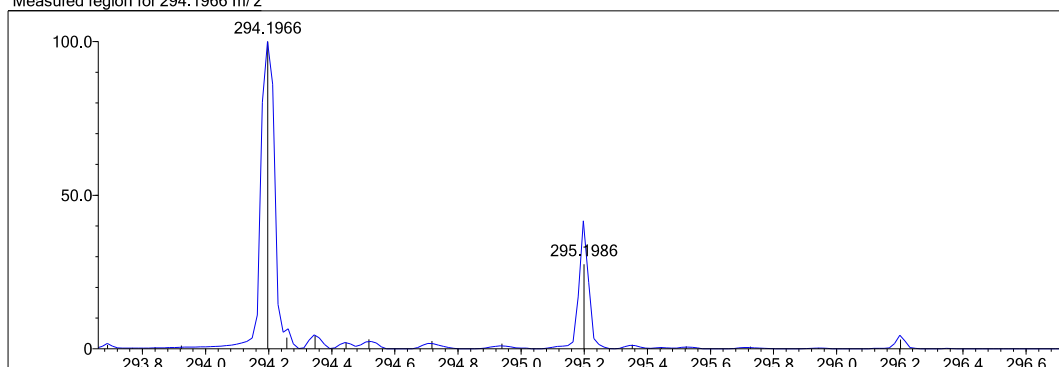
DBE Range: 10.0 - 20.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

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

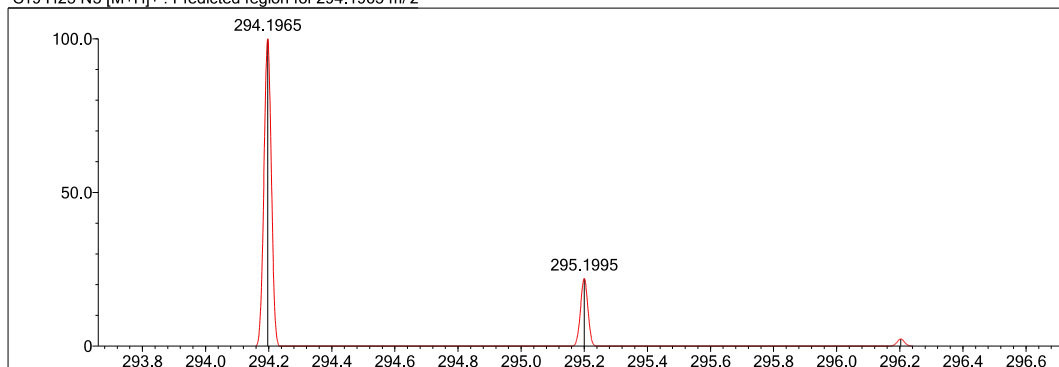
Event#: 1 MS(E+) Ret. Time : 0.960 -> 1.107 Scan#: 145 -> 167



Measured region for 294.1966 m/z



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

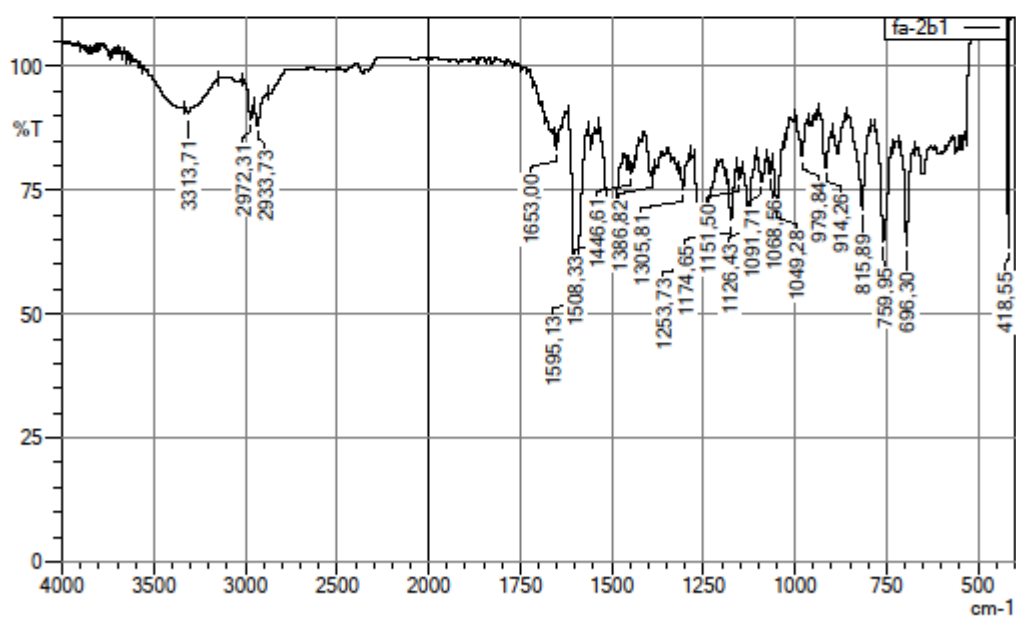
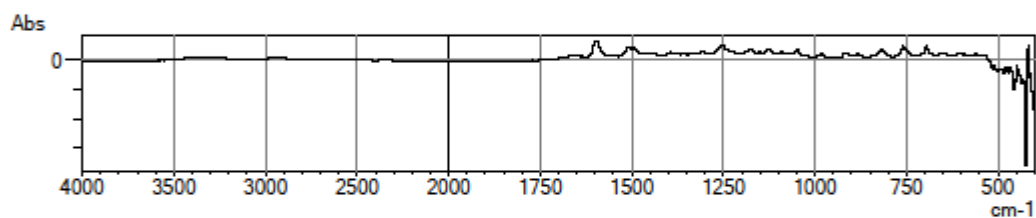


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	68.06	C19 H23 N3	[M+H]+	294.1966	294.1965	0.1	0.34	68.06	10.0

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-2b1.jspd
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



Current Data Parameters
NAME fa
EXPNO 476
PROCNO 1

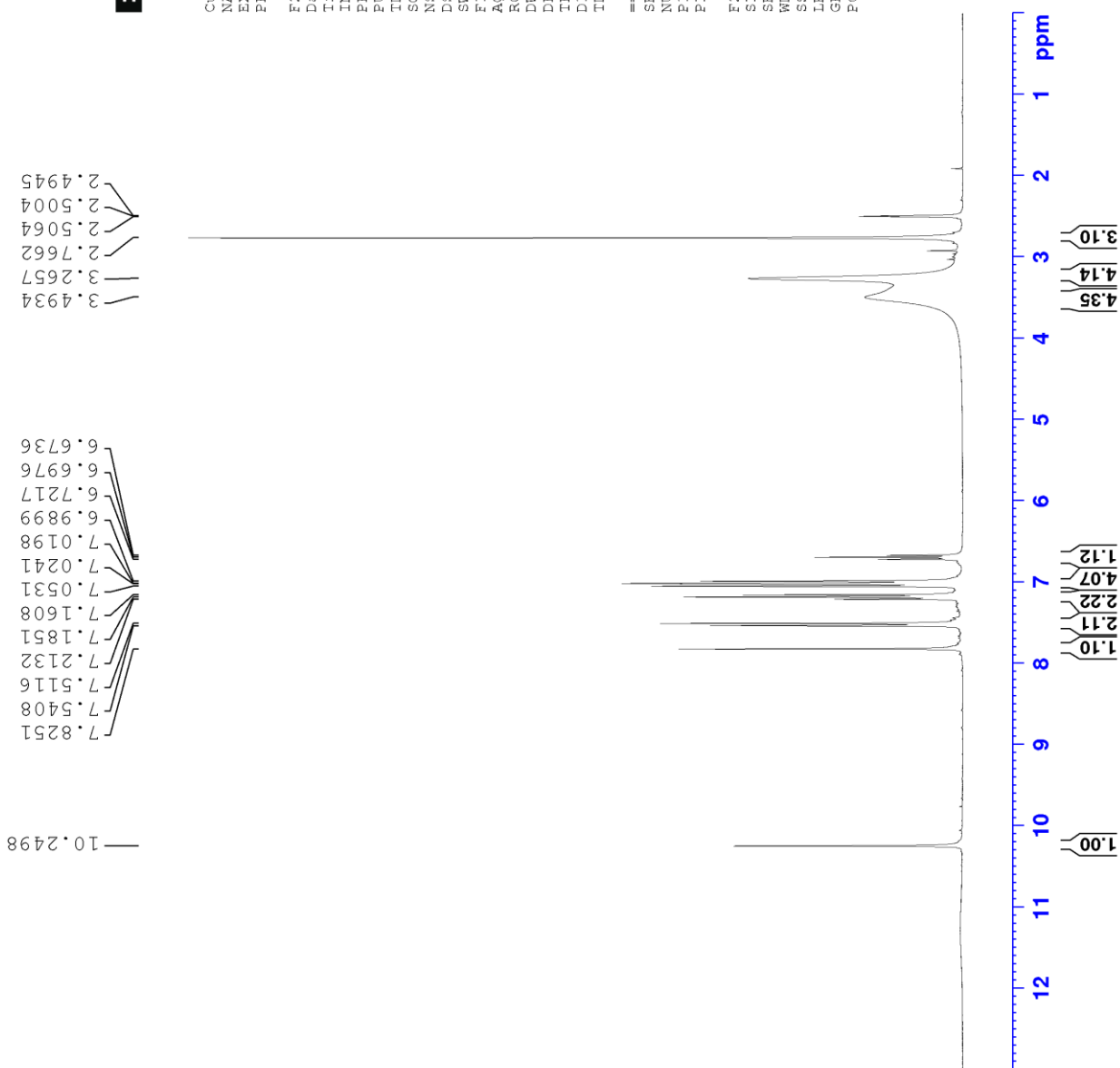
F2 - Acquisition Parameters

Date_ 20160601
Time_ 3.58
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 7.91562
DW 81.920 usec
DE 6.50 usec
TE 297.9 K
D1 3.00000000 sec
TD0 1

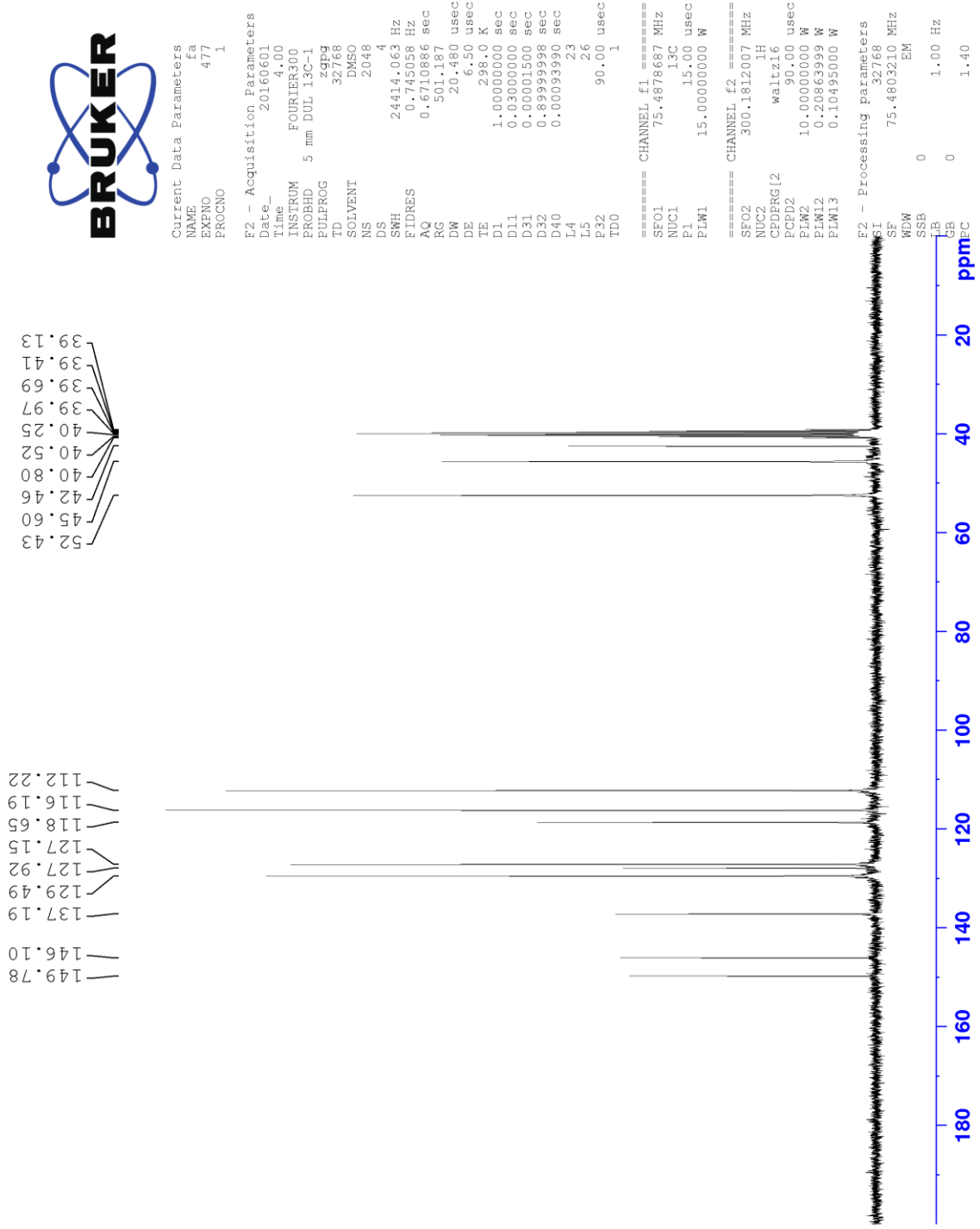
==== CHANNEL f1 =====
SFO1 300.1618537 MHz
NUC1 1H
P1 13.00 usec
PLW1 10.00000000 W

F2 - Processing parameters

SI 65536
SF 300.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



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



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

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

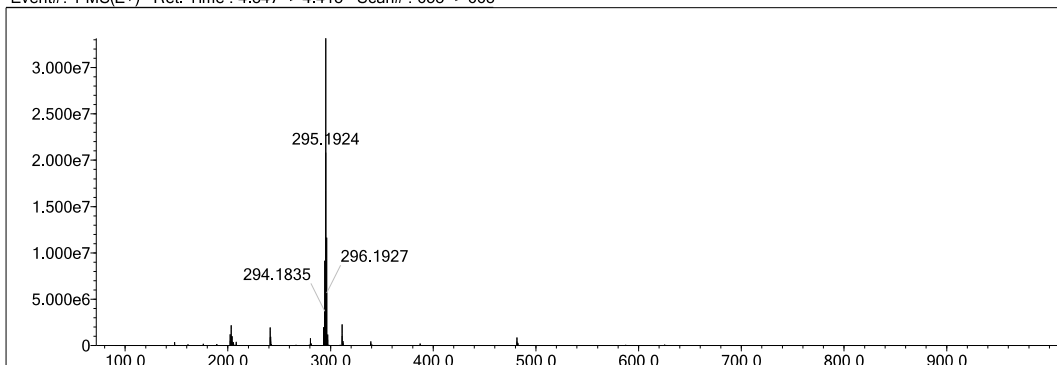
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	50	O	2	0	6	Cl	1	0	0	H
C	4	0	50	F	1	0	0	Br	1	0	0	
N	3	0	4	S	2	0	0	Pd	2	0	0	

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

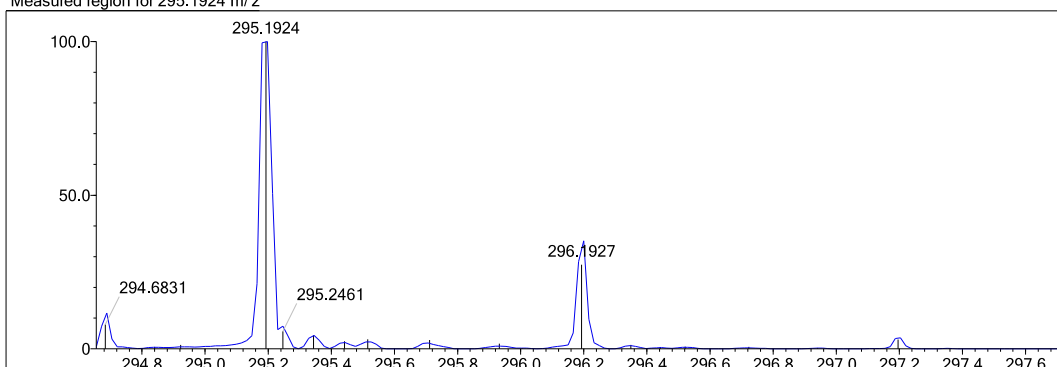
DBE Range: 10.0 - 20.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

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

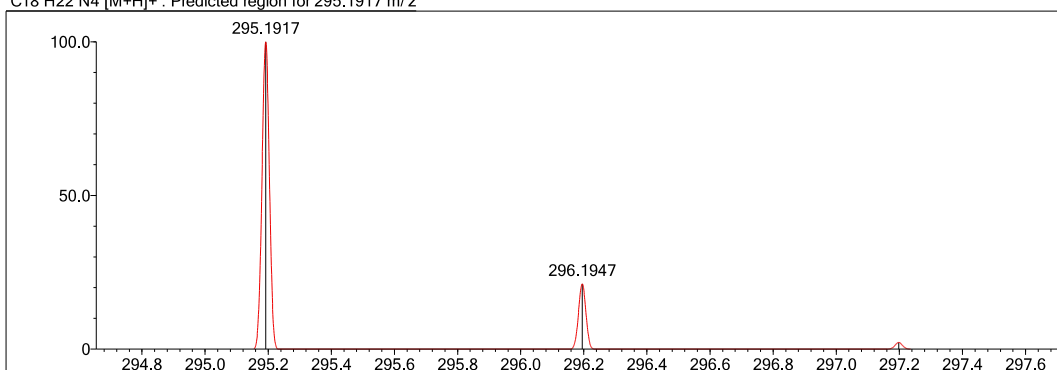
Event#: 1 MS(E+) Ret. Time : 4.347 -> 4.413 Scan# : 653 -> 663



Measured region for 295.1924 m/z



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

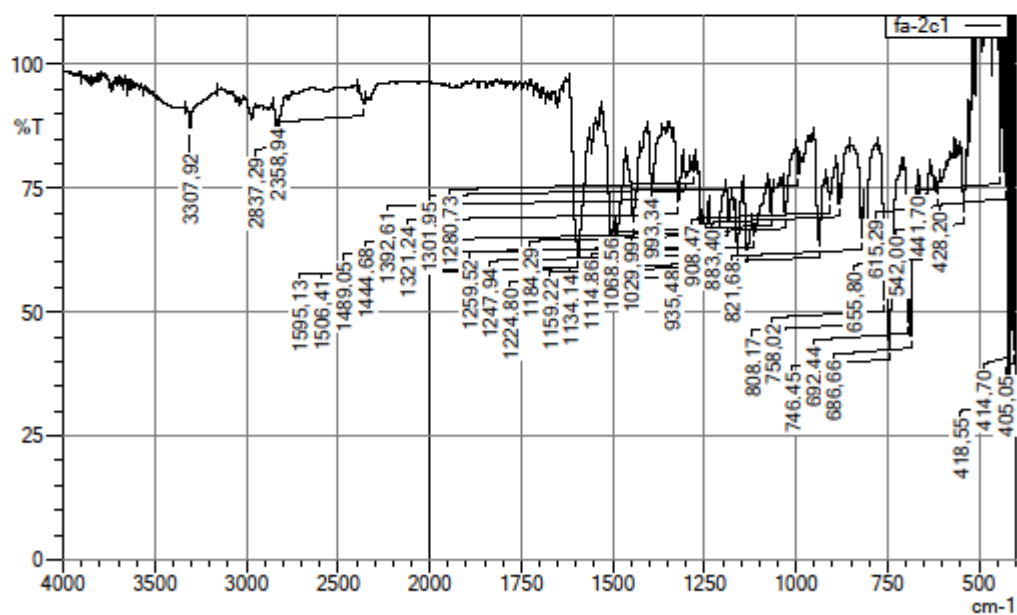
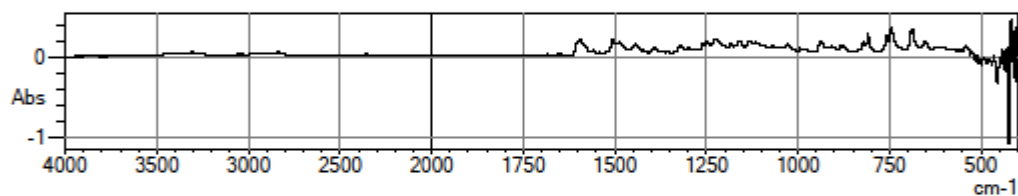


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	64.39	C18 H22 N4	[M+H] ⁺	295.1924	295.1917	0.7	2.37	66.68	10.0

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\faifa-2c1.jspd
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

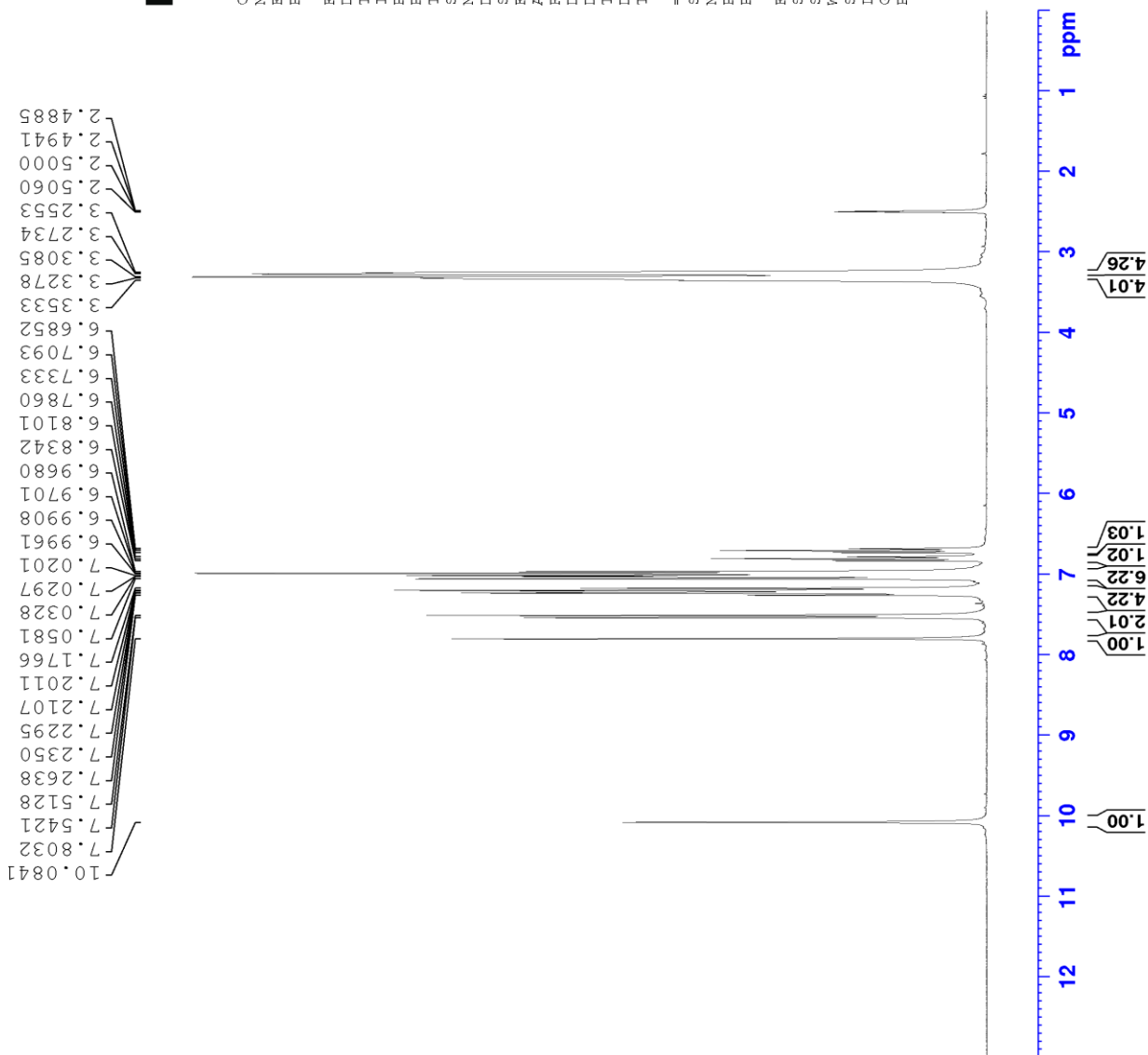


Current Data Parameters
NAME fa
EXPNO 478
PROCNO 2

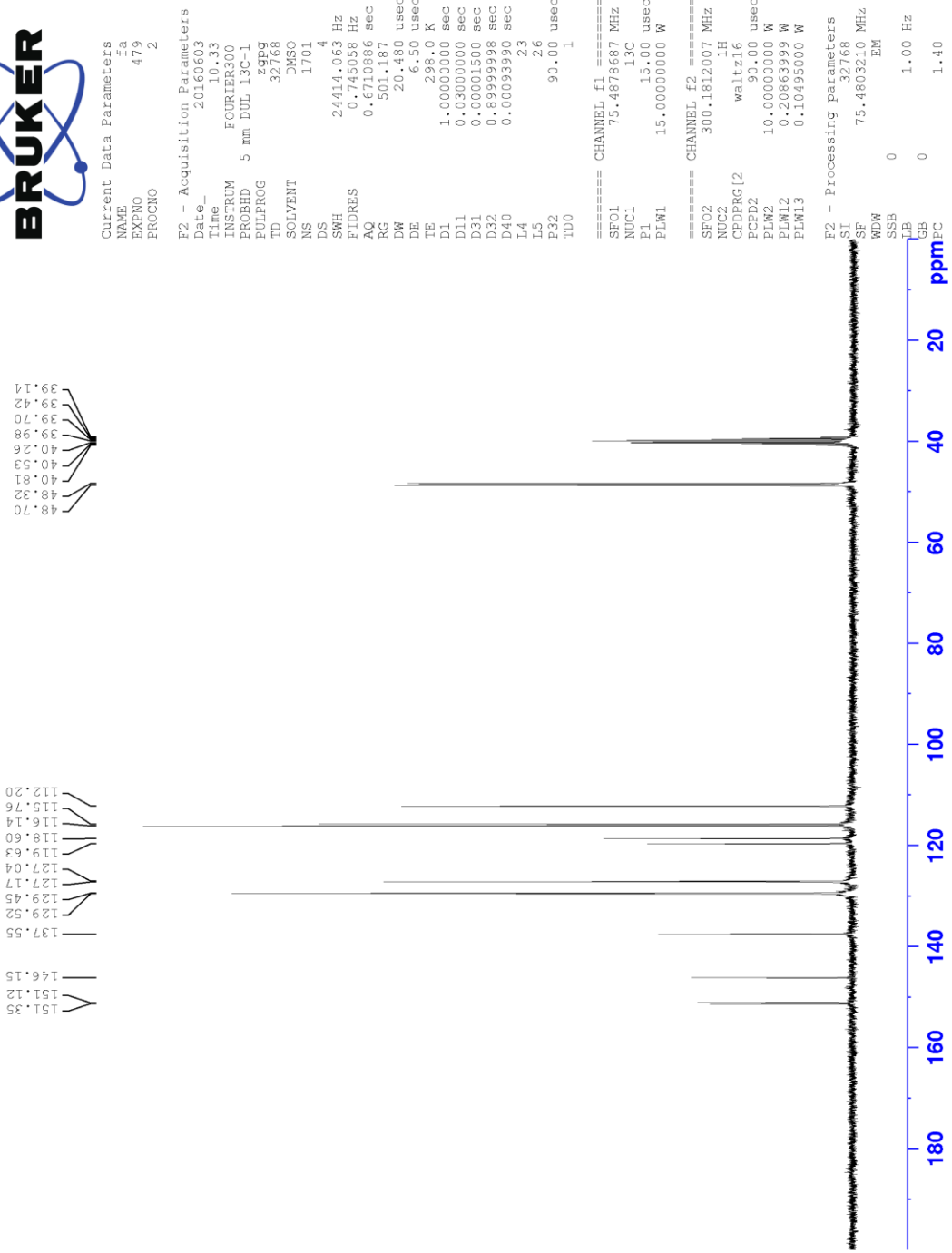
F2 - Acquisition Parameters
Date_ 20160603
Time_ 10.30
INSTRUM FOURIER300
PROBHD 5 mm DUL 13C-1
PULPROG zg
TD 16384
SOLVENT DMSO
NS 16
DS 0
SWH 6103.516 Hz
FIDRES 0.372529 Hz
AQ 1.3421773 sec
RG 7.3935
DW 81.920 usec
DE 6.50 usec
TE 297.6 K
D1 3.00000000 sec
TD0 1

===== 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



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



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

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

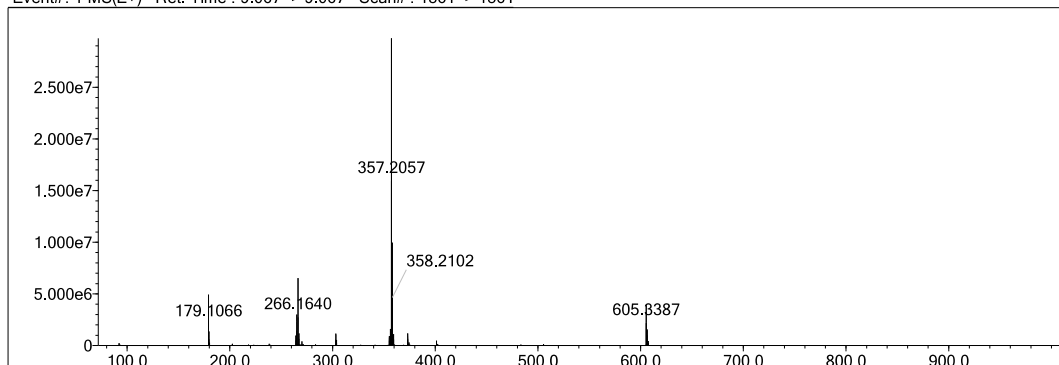
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	50	O	2	0	6	Cl	1	0	0	H
C	4	0	50	F	1	0	0	Br	1	0	0	
N	3	0	4	S	2	0	0	Pd	2	0	0	

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

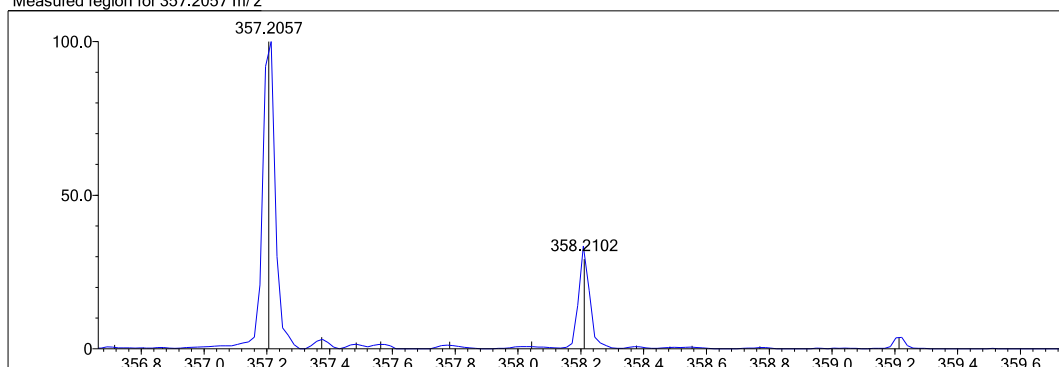
DBE Range: 10.0 - 20.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

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

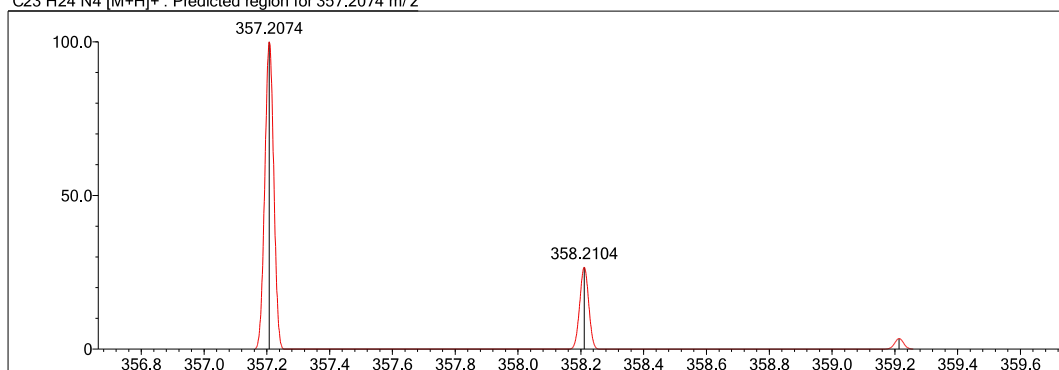
Event#: 1 MS(E+) Ret. Time : 9.067 -> 9.067 Scan#: 1361 -> 1361



Measured region for 357.2057 m/z



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

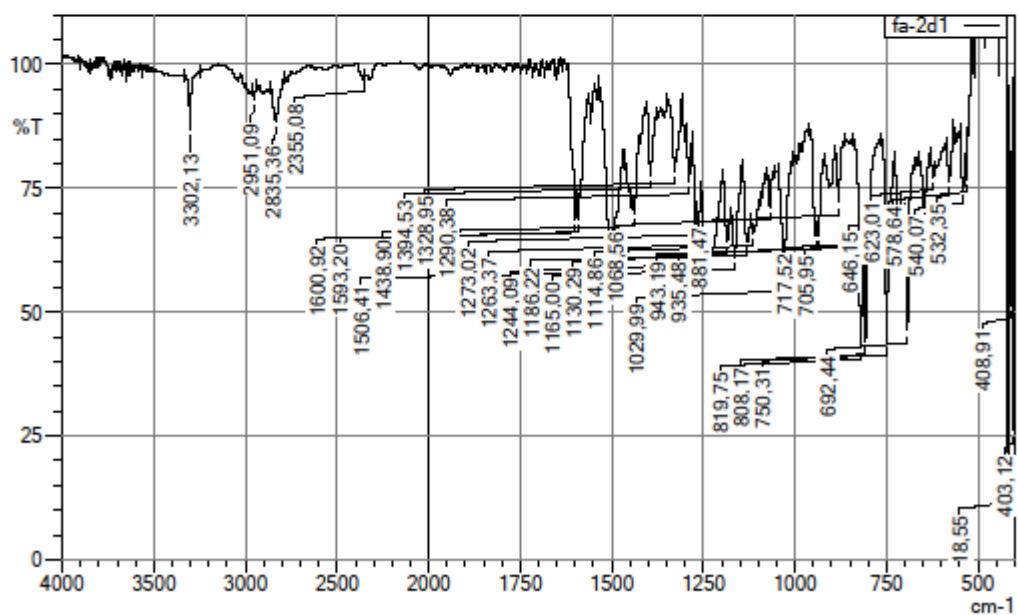
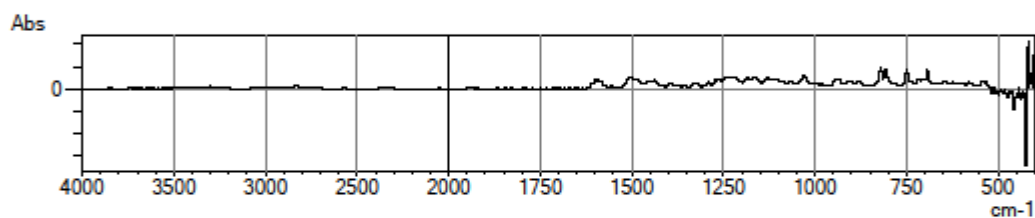


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	83.47	C23 H24 N4	[M+H] ⁺	357.2057	357.2074	-1.7	-4.76	92.13	14.0

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\faifa-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

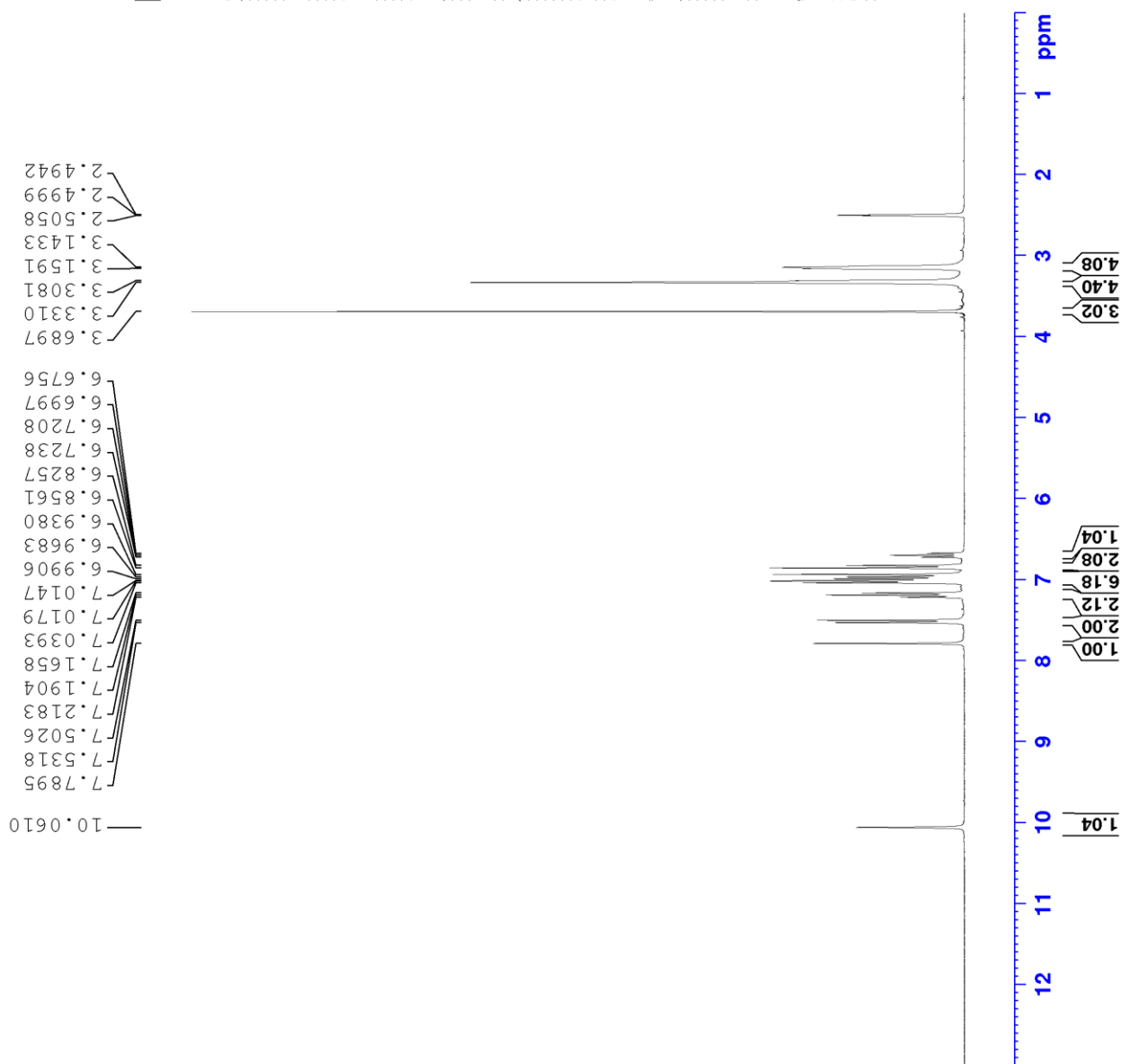


Current Data Parameters
NAME fa
EXPNO 480
PROCNO 2

F2 - Acquisition Parameters
Date_ 20160603
Time 11.24
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 1.342173 sec
RG 18.2585
DW 81.920 usec
DE 6.50 usec
TE 297.6 K
D1 3.0000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 300.1818537 MHz
NUC1 1H
PI 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



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



Current Data Parameters
NAME fa
EXPNO 481
PROCNO 3

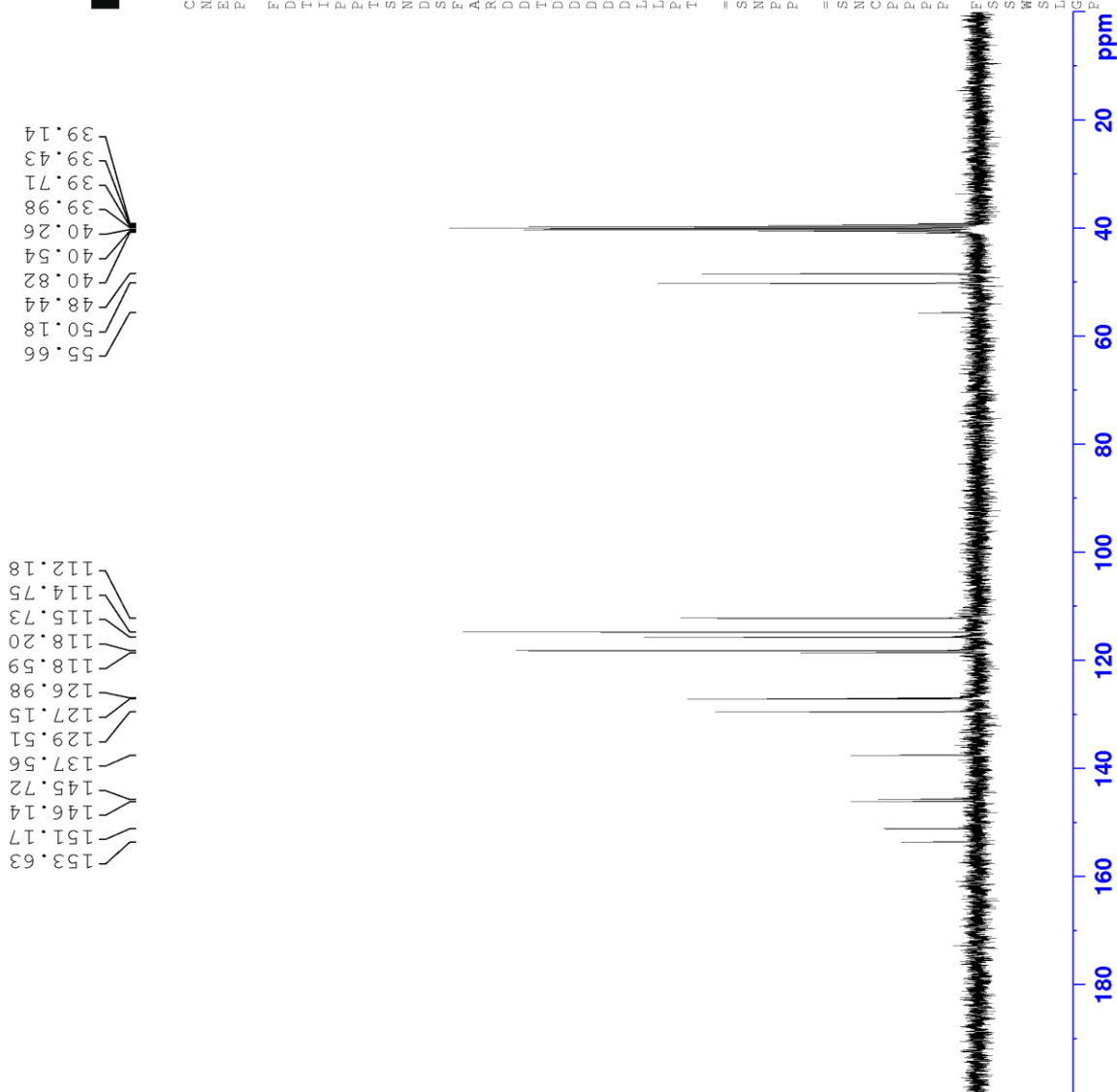
F2 - Acquisition Parameters

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 0.745056 Hz
AQ 0.6710866 sec
RG 501.187
DW 20.480 usec
DE 6.50 usec
TE 298.0 K
D1 1.0000000 sec
D11 0.0300000 sec
D31 0.0001500 sec
D32 0.8999998 sec
D40 0.0003390 sec
L4 23
L5 26
F32 90.00 usec
TD0 1

===== CHANNEL f1 =====
SFO1 75.4878687 MHz
NUC1 13C
P1 15.00 usec
PLW1 15.0000000 W

===== CHANNEL f2 =====
SFO2 300.1812007 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 10.0000000 W
PLW12 0.20863999 W
PLW13 0.10495000 W

F2 - Processing parameters
SI 32768
SF 75.4803210 MHz
WDW EM
SSE 0
LB 0
GB 0
PC 1.40



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

Data File: C:\LabSolutions\Data\Analiz\dera\FA-4_4.lcd

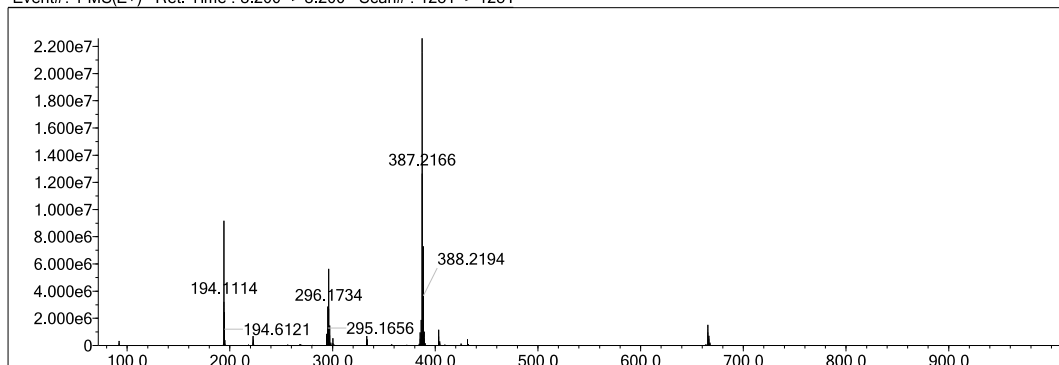
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	50	O	2	0	6	Cl	1	0	0	H
C	4	0	50	F	1	0	0	Br	1	0	0	
N	3	0	4	S	2	0	0	Pd	2	0	0	

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

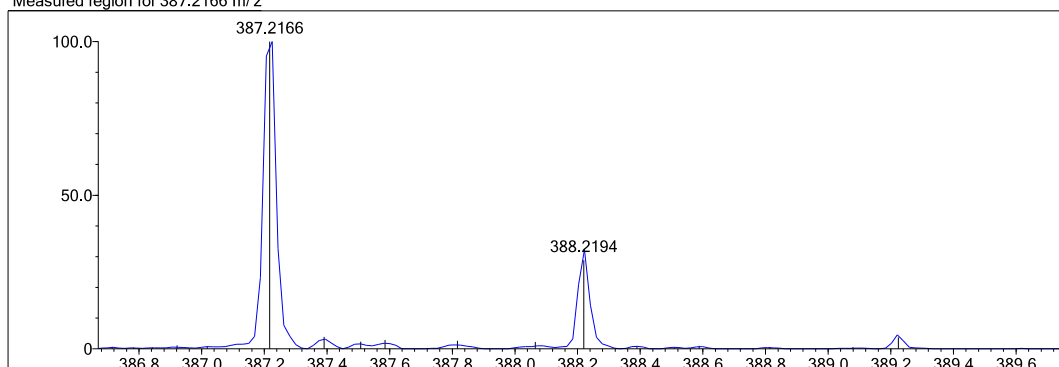
DBE Range: 10.0 - 20.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

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

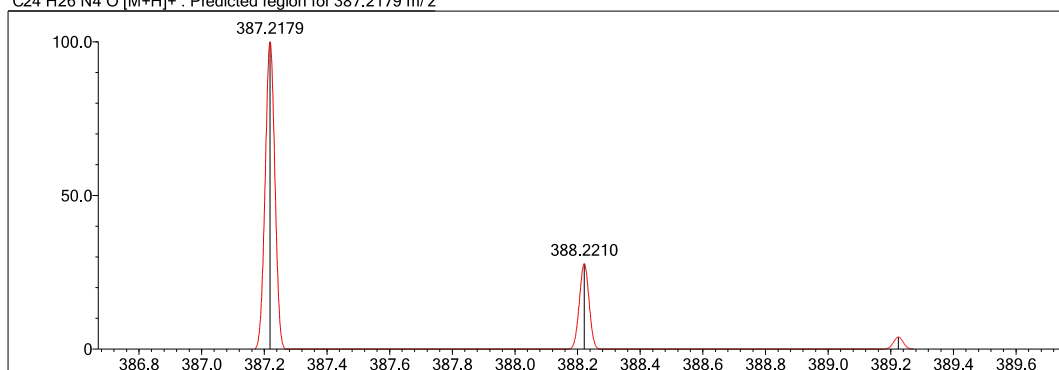
Event#: 1 MS(E+) Ret. Time : 8.200 -> 8.200 Scan# : 1231 -> 1231



Measured region for 387.2166 m/z



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

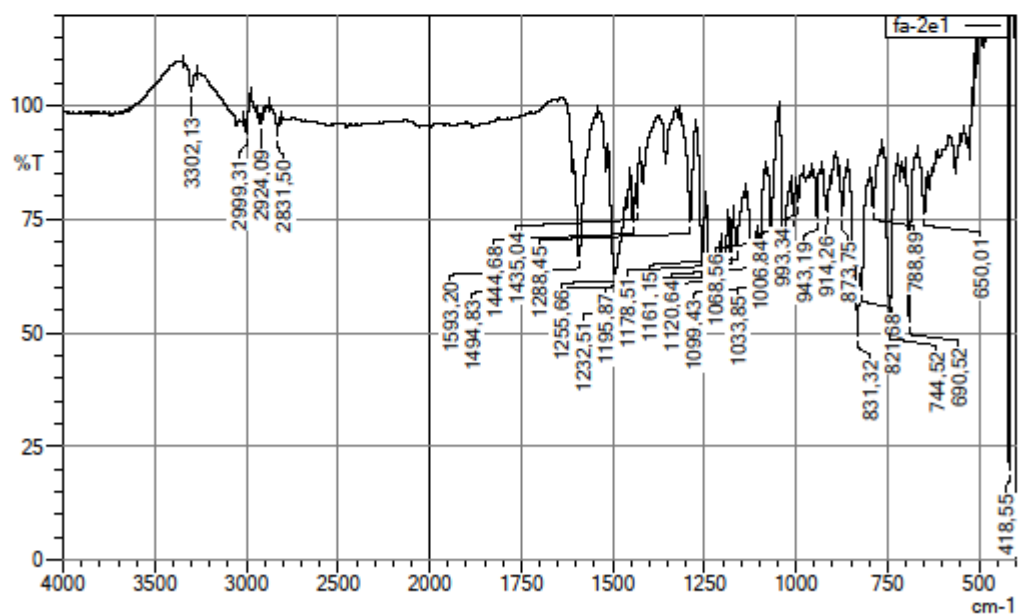
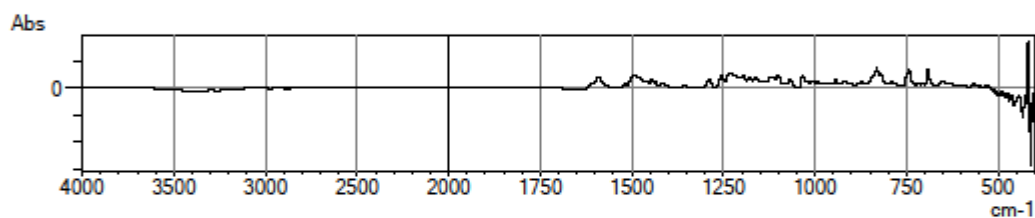


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	92.48	C24 H26 N4 O	[M+H] ⁺	387.2166	387.2179	-1.3	-3.36	98.28	14.0

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\faifa-2e1.jspd
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

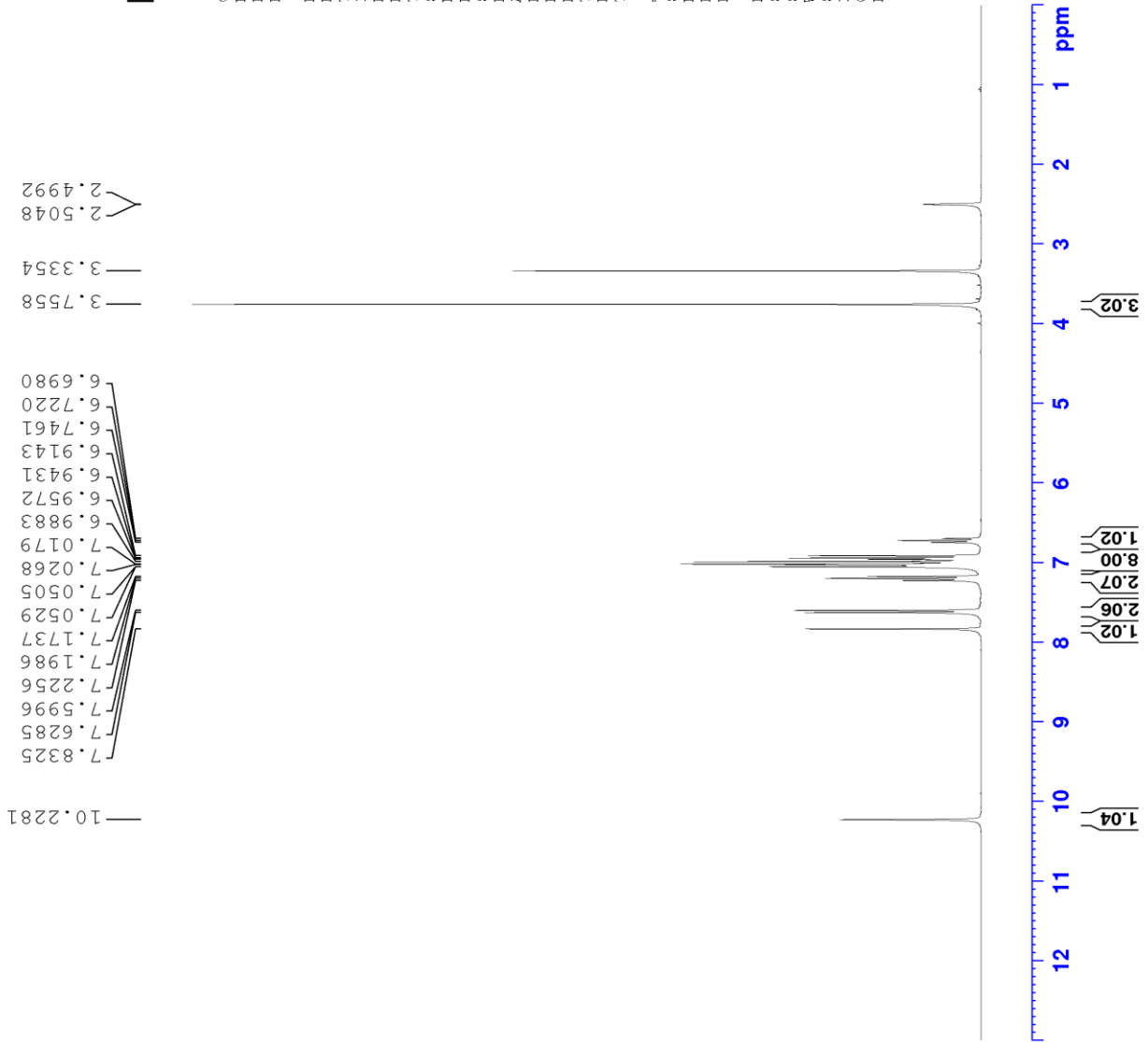


Current Data Parameters
NAME fa
EXPNO 462
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160531
Time 20.44
INSTRUM FOURIER300
PROBHD 5 mm DUL 13C-1
PULPROG zg
TD 16384
SOLVENT DMSO
NS 16
DS 0
SWH 6103.516 Hz
FIDRES 0.374529 Hz
AQ 1.342173 sec
RG 15.669
DW 81.920 usec
DE 6.50 usec
TE 297.9 K
D1 3.00000000 sec
TD0 1

===== CHANNEL f1 =====
SF01 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



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



Current Data Parameters
NAME fa
EXPNO 463
PROCNO 1

F2 - Acquisition Parameters

Date_ 20160531
Time 20.46
INSTRUM FOURIER300
PROBHD 5 mm DUL 13C-1
PULPROG zgpg
TD 32768
SOLVENT DMSO
NS 2048
DS 4
SMH 24414.063 Hz
FIDRES 0.745058 Hz
AQ 0.6710886 sec
RG 501.167
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
F2 90.00 usec
TD0 1

==== CHANNEL f1 =====
SF01 75.4878687 MHz
NUC1 13C
P1 15.00 usec
PLW1 15.0000000 W

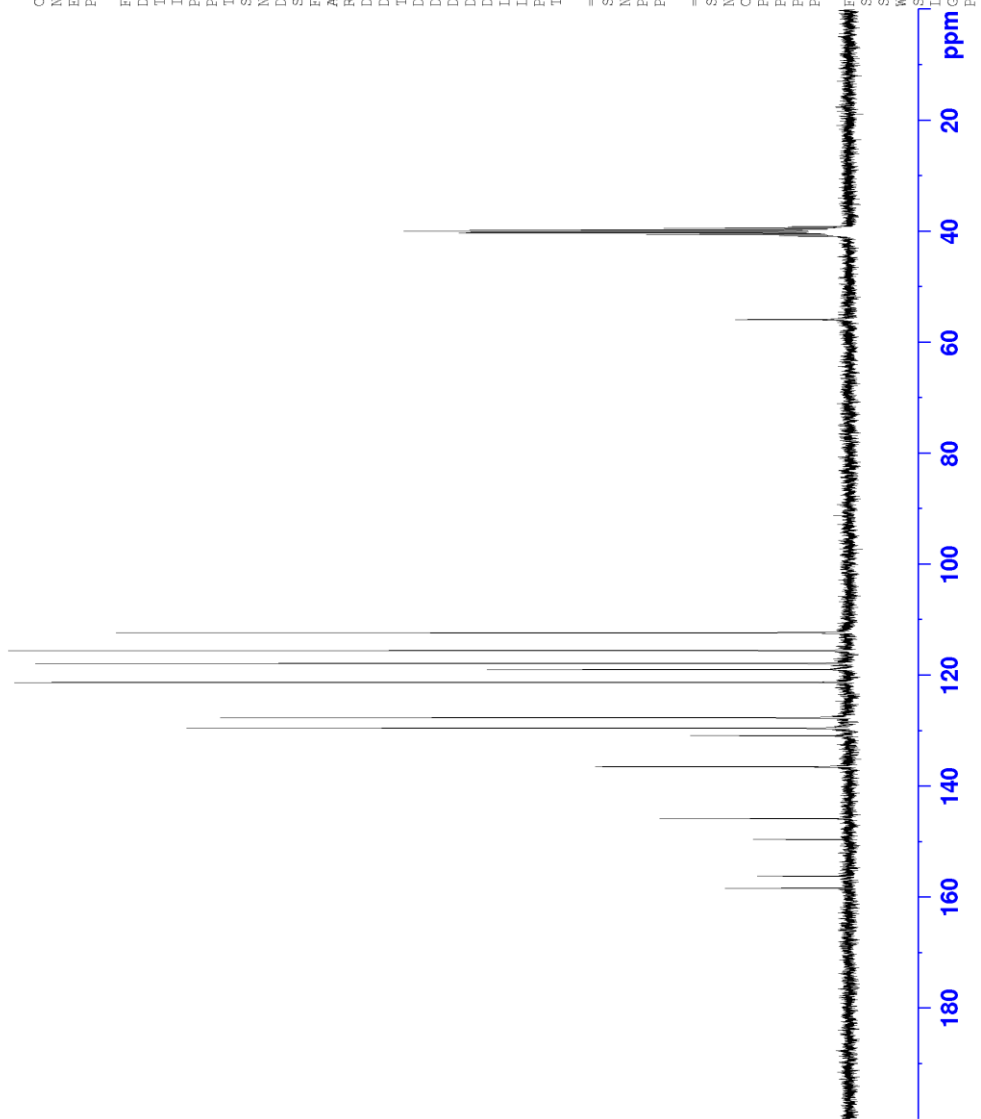
==== CHANNEL f2 =====
SF02 300.1812007 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 10.0000000 W
PLW12 0.2086399 W
PLW13 0.10495000 W

F2 - Processing parameters

SI 32768
SF 75.4803210 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
FC 1.40

55.89
40.81
40.54
40.26
39.98
39.70
39.42
39.15

158.40
156.22
149.60
145.87
136.49
130.89
129.54
127.67
121.29
118.98
117.87
115.58
112.33



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

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

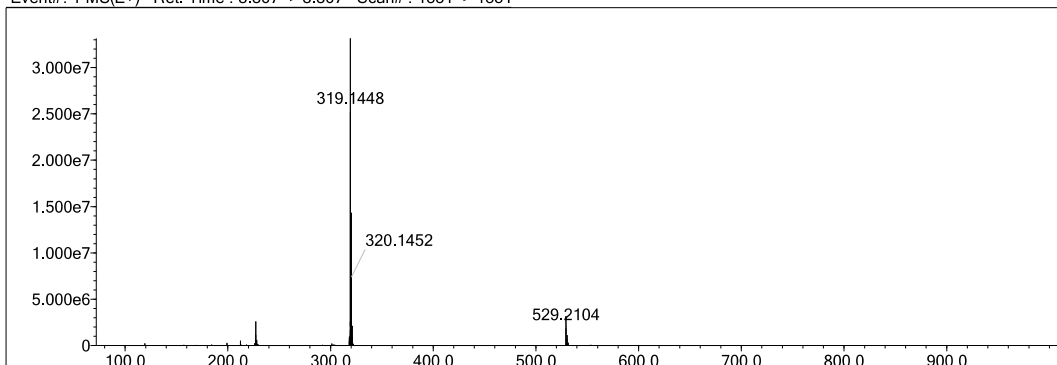
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	50	O	2	0	6	Cl	1	0	0	H
C	4	0	50	F	1	0	0	Br	1	0	0	
N	3	0	4	S	2	0	0	Pd	2	0	0	

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

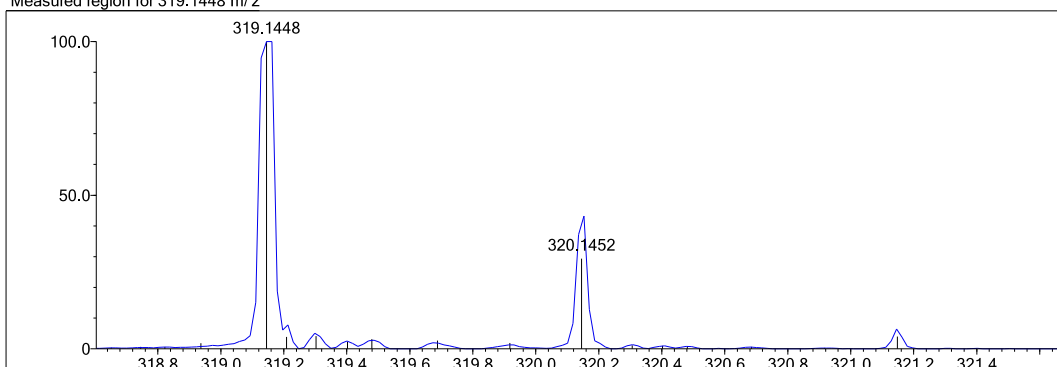
DBE Range: 10.0 - 20.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

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

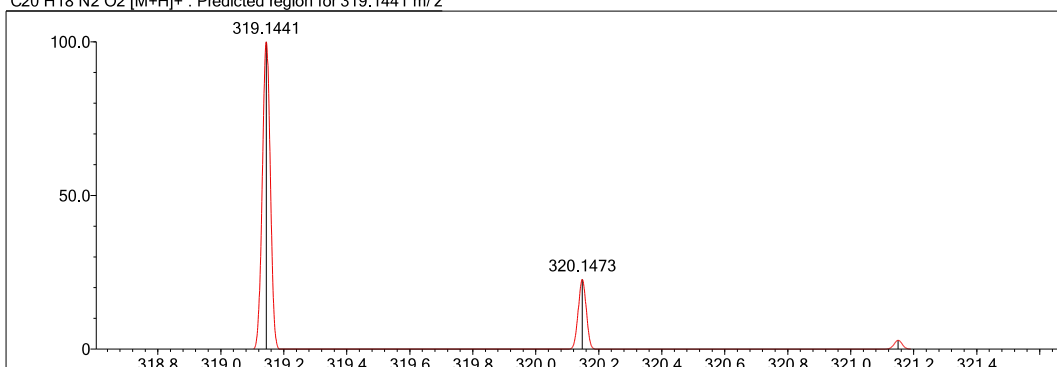
Event#: 1 MS(E+) Ret. Time : 8.867 -> 8.867 Scan#: 1331 -> 1331



Measured region for 319.1448 m/z



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

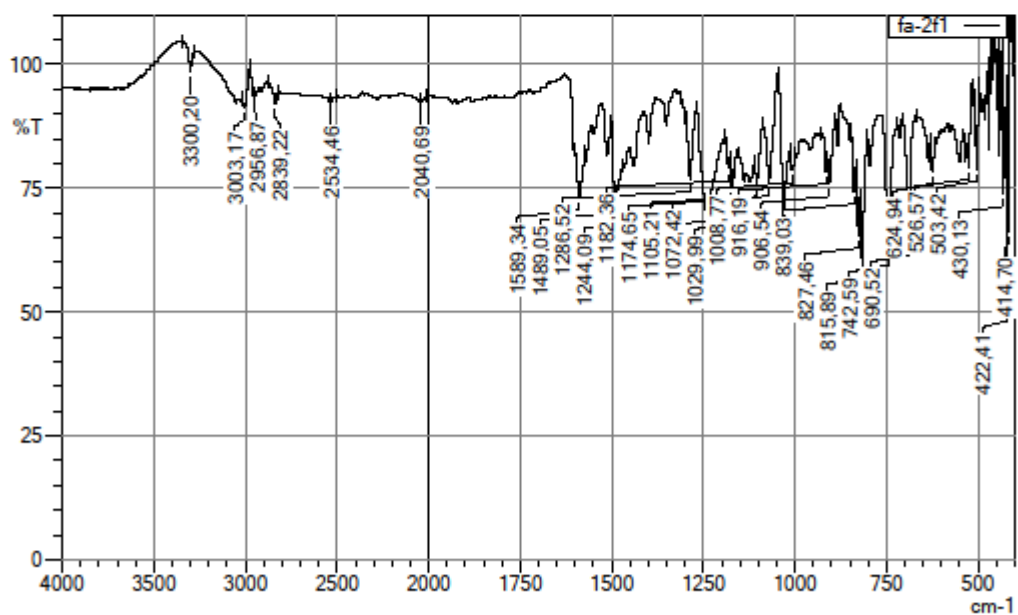
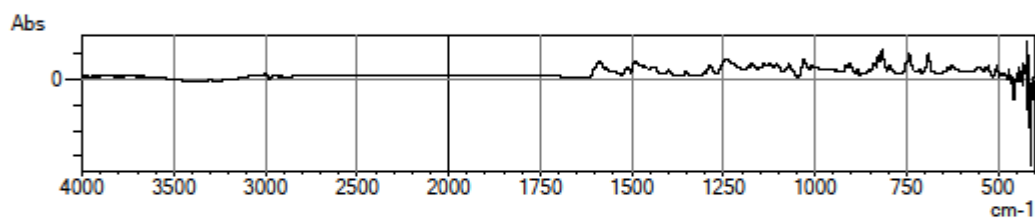


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	59.52	C20 H18 N2 O2	[M+H]+	319.1448	319.1441	0.7	2.19	61.35	13.0

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.ispd
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



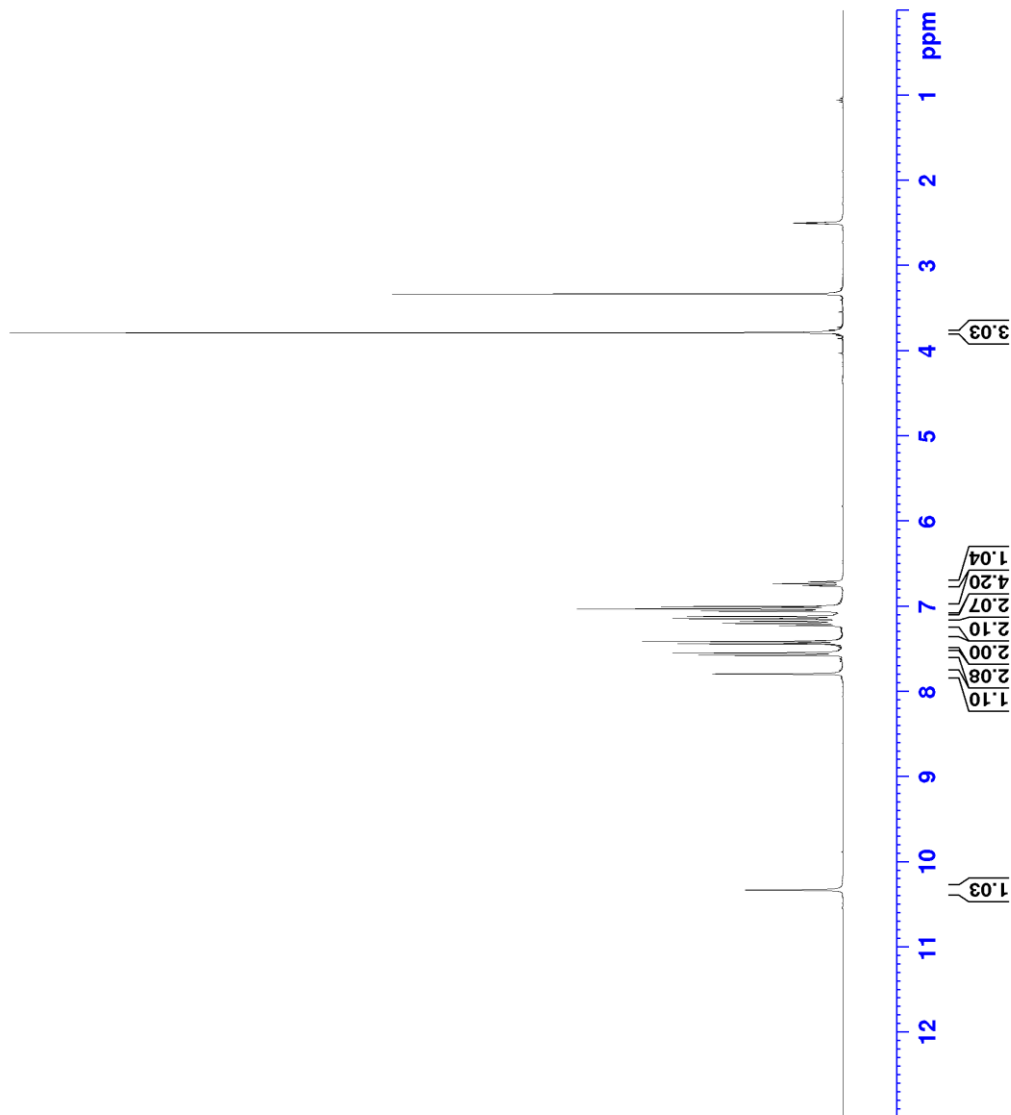
Current Data Parameters
NAME fa
EXPNO 464
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160531
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 0.378529 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 10.0000000 W

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

2.4938
2.4999
2.5060
3.3335
3.7875
6.7113
6.7354
6.7596
6.9927
7.0033
7.0106
7.0272
7.0435
7.0561
7.0598
7.1181
7.1462
7.1762
7.2006
7.2289
7.4123
7.4418
7.5466
7.5748
7.7953
10.3333



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



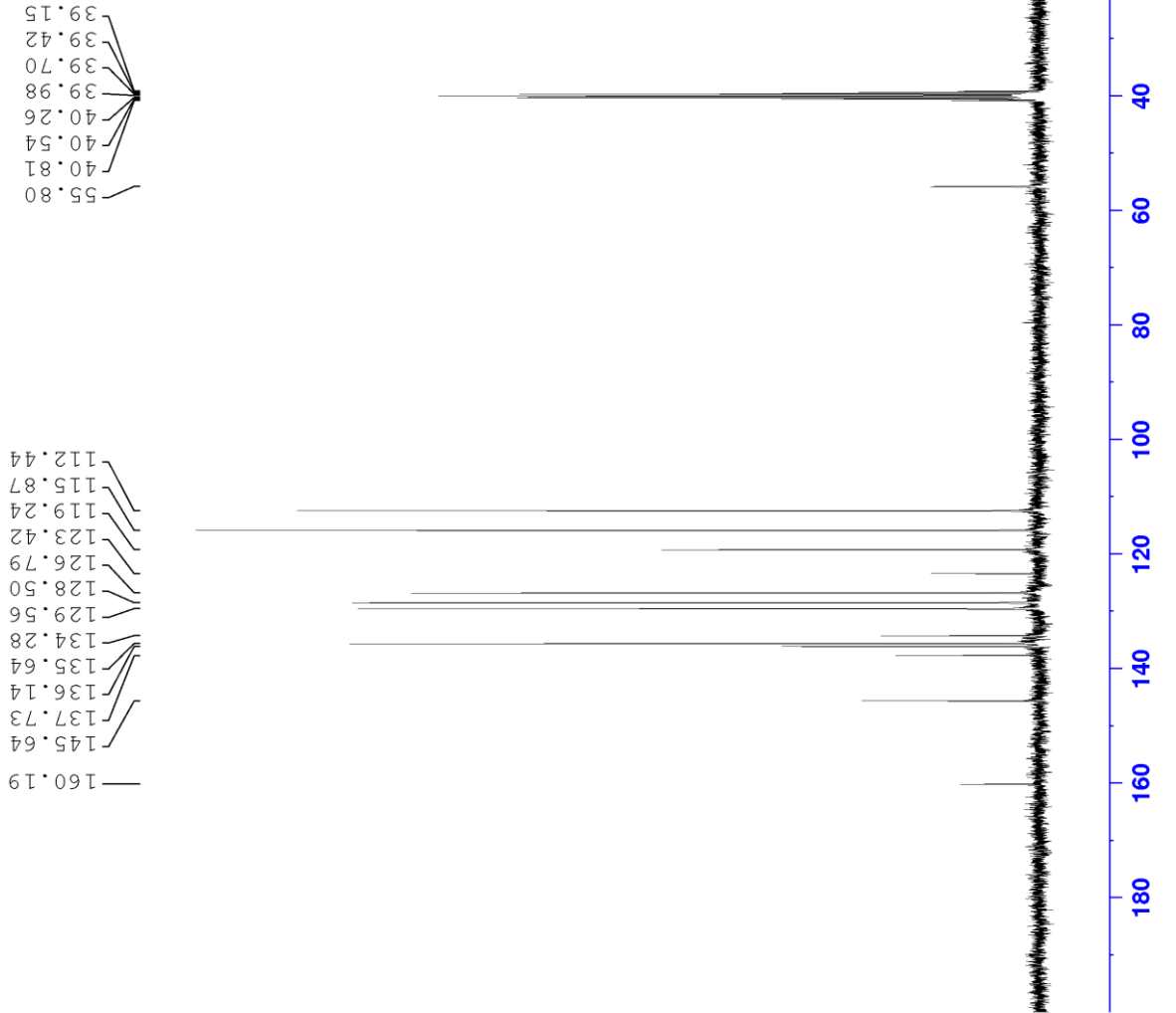
Current Data Parameters
NAME fa
EXPNO 465
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160531
Time 21.48
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 1.0000000 sec
D11 0.0300000 sec
D31 0.0001500 sec
D32 0.8999998 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 15.0000000 W

==== CHANNEL f2 =====
SFO2 300.1812007 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 10.0000000 W
PLW12 0.20863899 W
PLW13 0.10495000 W

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



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

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

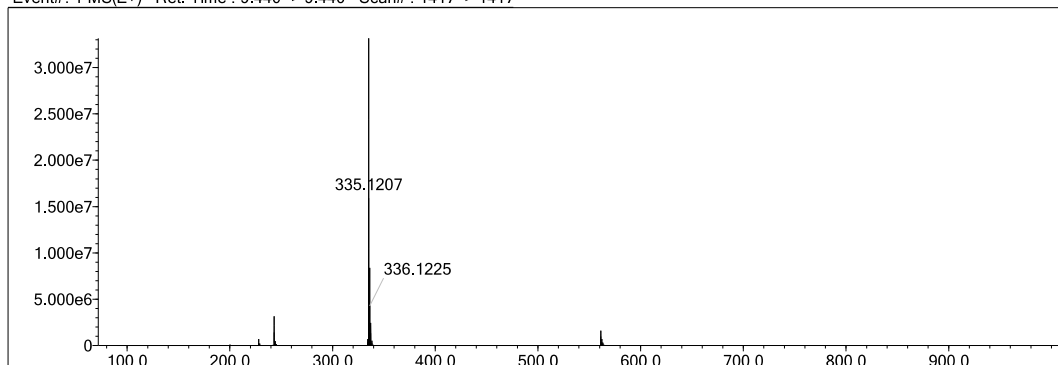
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	50	O	2	0	6	Cl	1	0	0	H
C	4	0	50	F	1	0	0	Br	1	0	0	
N	3	0	4	S	2	0	1	Pd	2	0	0	

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

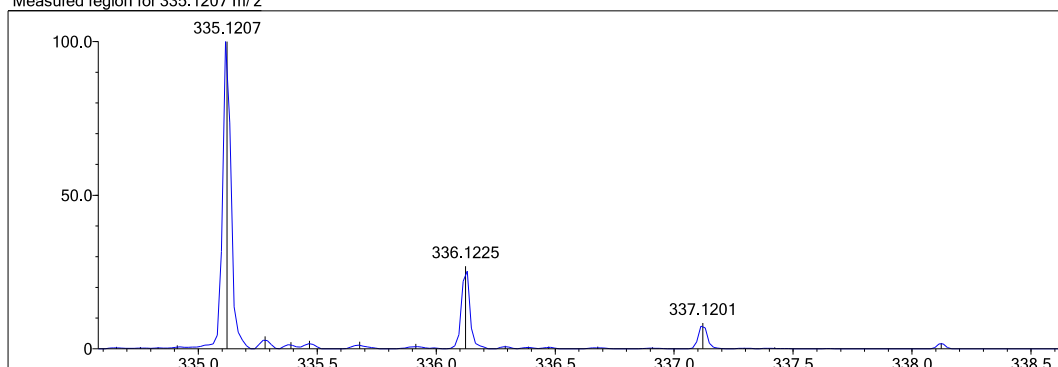
DBE Range: 10.0 - 20.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

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

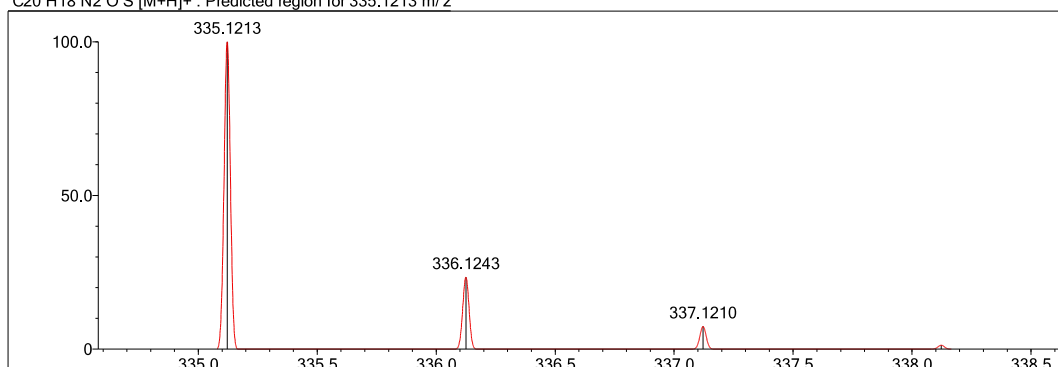
Event#: 1 MS(E+) Ret. Time : 9.440 -> 9.440 Scan#: 1417 -> 1417



Measured region for 335.1207 m/z



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

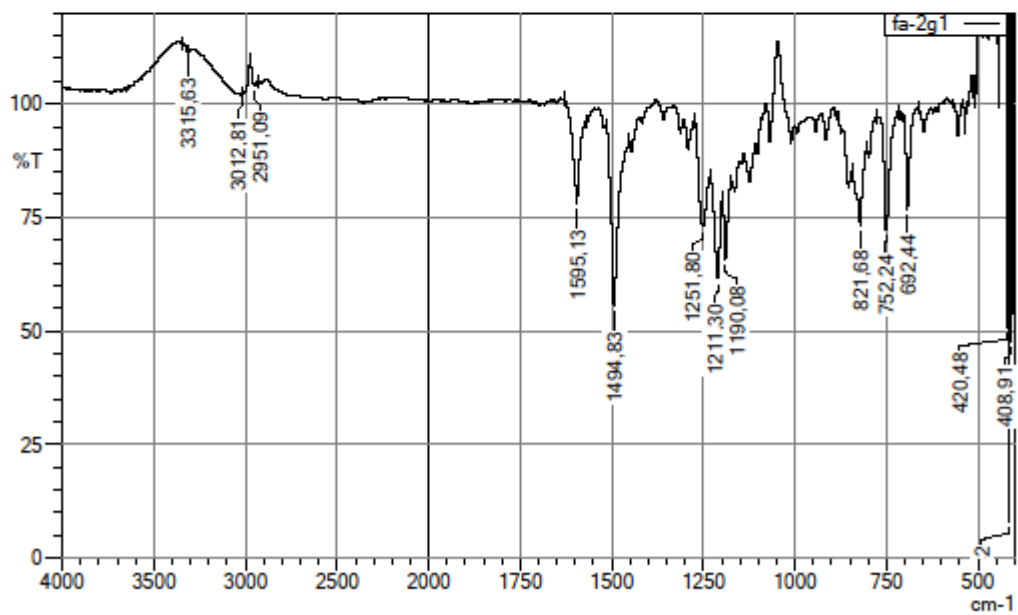
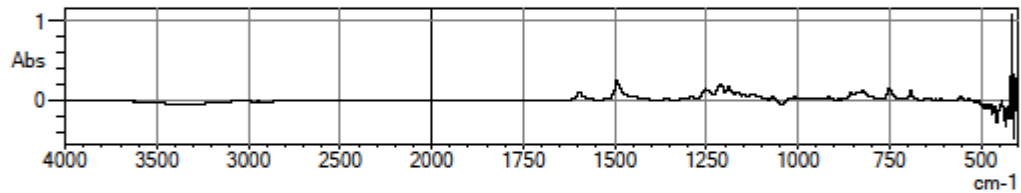


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	77.61	C20 H18 N2 O S	[M+H] ⁺	335.1207	335.1213	-0.6	-1.79	79.17	13.0

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\faifa-2g1.jspd
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

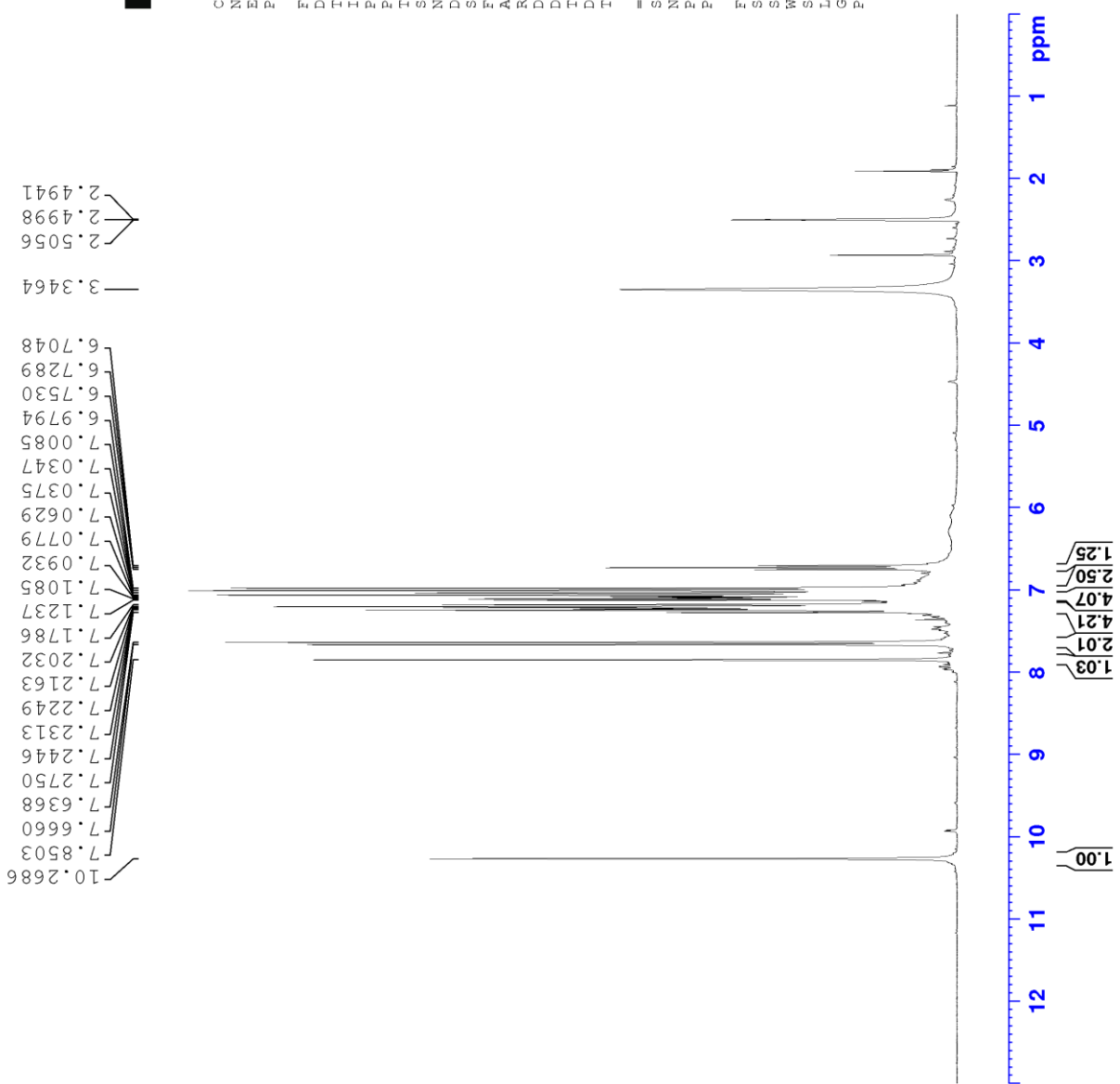


Current Data Parameters
NAME fa
EXPNO 466
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160531
Time 22.48
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 1.342173 sec
RG 12.5432
DW 81.920 usec
DE 6.50 usec
TE 298.0 K
D1 3.00000000 sec
TD0 1

==== CHANNEL f1 =====
SF01 300.1618537 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



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



Current Data Parameters
NAME Ia
EXPNO 467
PROCNO 1

F2 - Acquisition Parameters

Date_ 20160531
Time 22.50
INSTRUM FOURIER300
PROBHD 5 mm DUL 13C-1
PULPROG zgpg
TD 32768
SOLVENT DMSO
NS 2048
DS 4
SWH 24414.063 Hz
FIDRES 0.745056 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 0.00003990 sec
L4 23
L5 26
L6 26
P32 90.00 usec
TDO 1

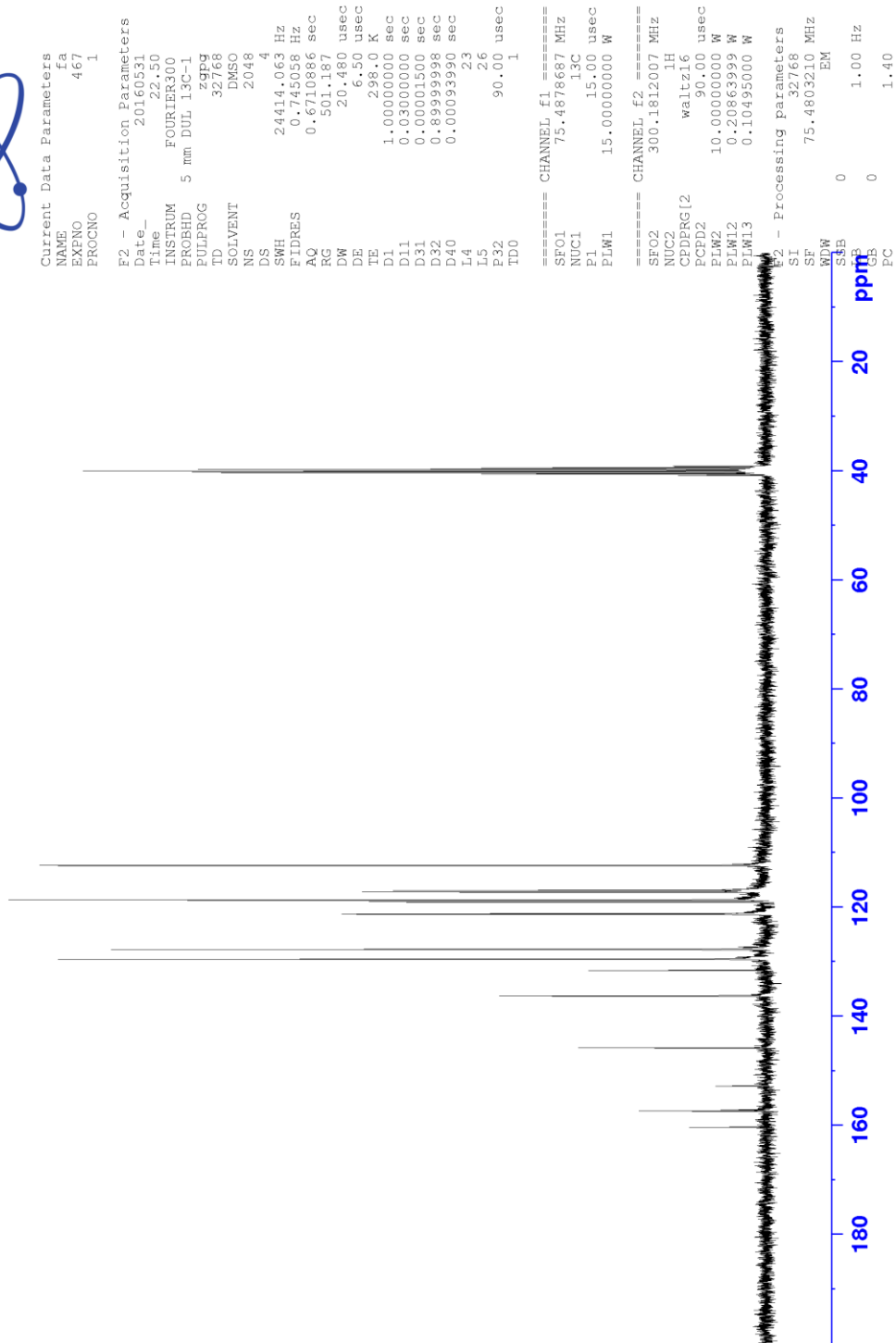
==== CHANNEL f1 =====
SFO1 75.4878687 MHz
NUC1 13C
P1 15.00 usec
PLW1 15.00000000 W

==== 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
GB 0
PC 1.40

40.81
40.53
40.25
39.97
39.70
39.42
39.14

160.37
157.42
157.19
152.82
145.82
136.30
131.62
129.55
127.76
121.34
121.22
119.05
118.70
117.25
116.94
112.36



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

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

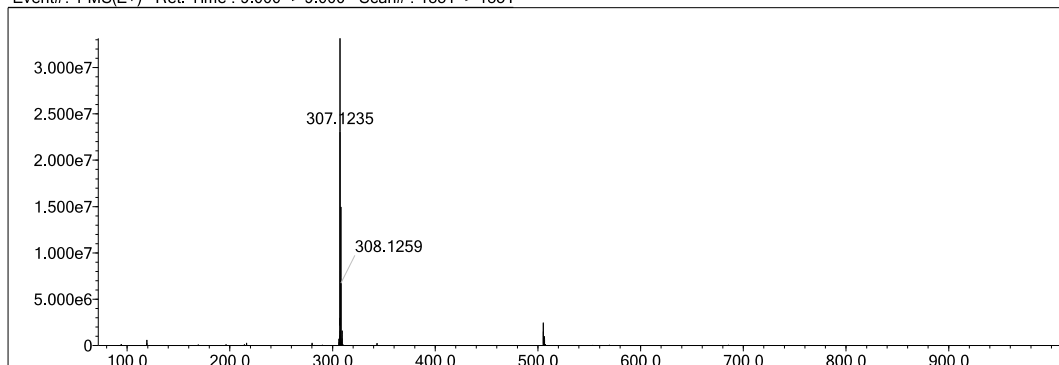
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	50	O	2	0	6	Cl	1	0	0	H
C	4	0	50	F	1	1	1	Br	1	0	0	
N	3	0	4	S	2	0	1	Pd	2	0	0	

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

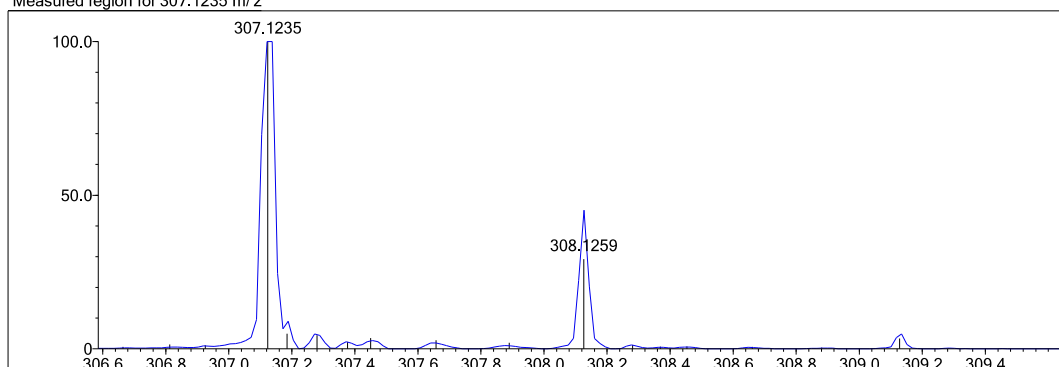
DBE Range: 10.0 - 20.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

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

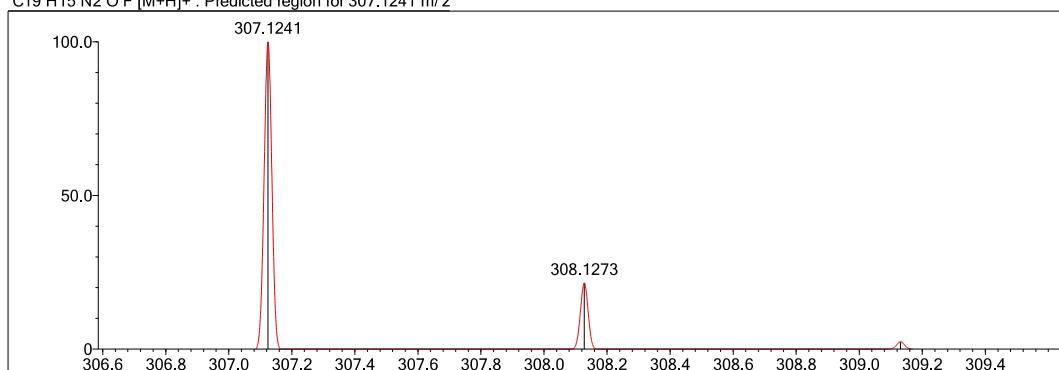
Event#: 1 MS(E+) Ret. Time : 9.000 -> 9.000 Scan#: 1351 -> 1351



Measured region for 307.1235 m/z



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

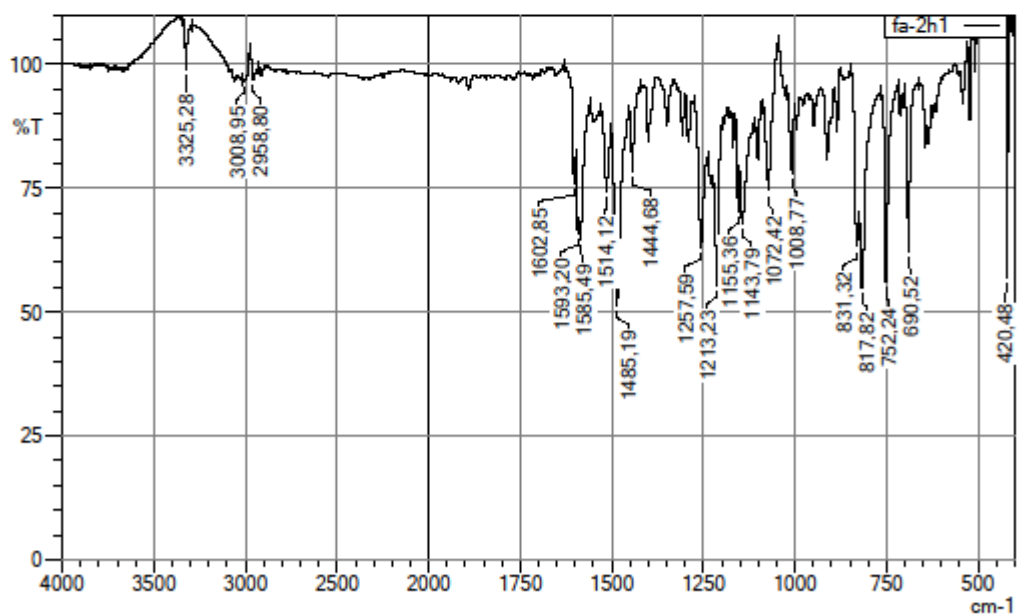
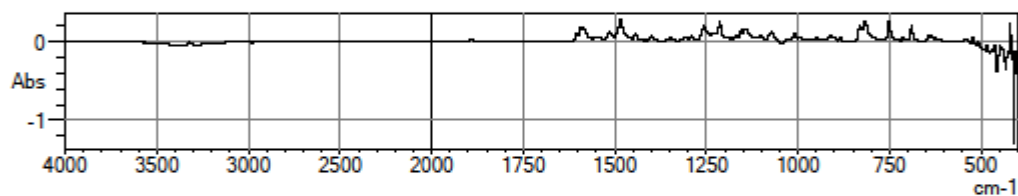


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	59.86	C19 H15 N2 O F	[M+H] ⁺	307.1235	307.1241	-0.6	-1.95	61.32	13.0

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\faifa-2h1.jspd
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

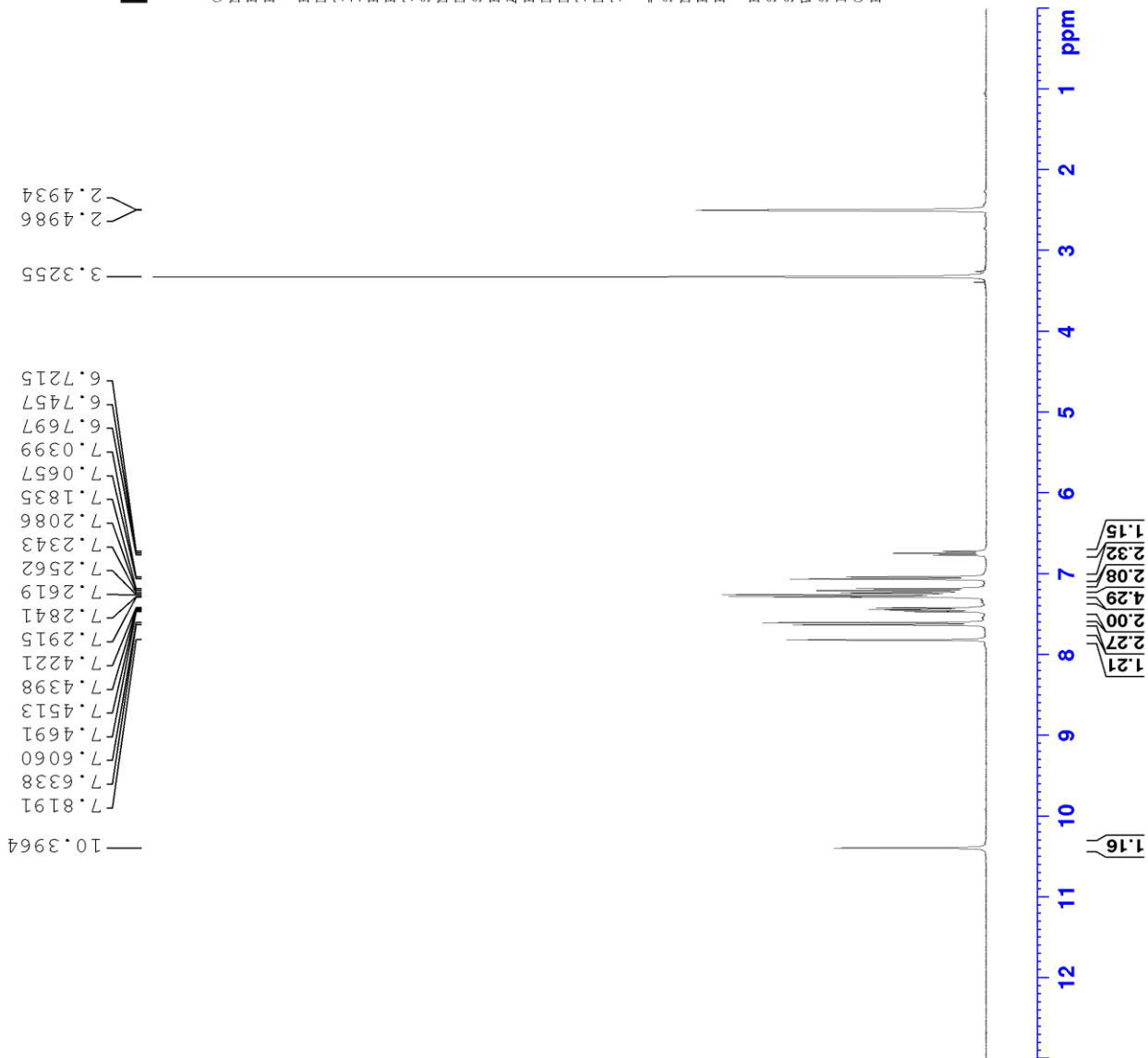


Current Data Parameters
NAME fa
EXPNO 468
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160531
Time 23.50
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 1.342173 sec
RG 43.5994
DW 81.920 usec
DE 6.50 usec
TE 297.9 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



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



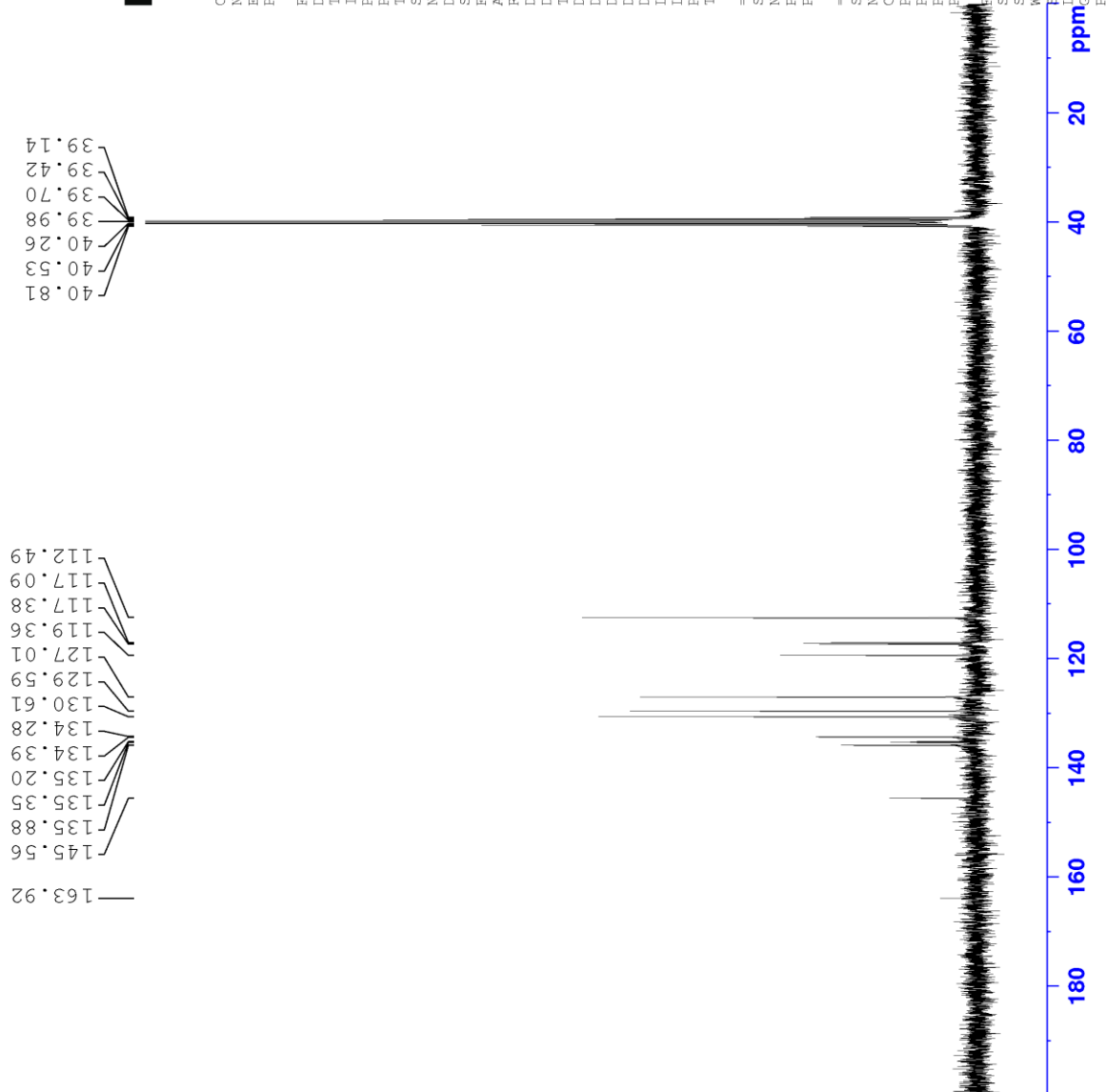
Current Data Parameters
NAME fa
EXPNO 469
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160531
Time 23.52
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
DM 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 0.00099990 sec
L4 23
L5 26
P32 90.00 usec
TD0 1

==== CHANNEL f1 =====
SF01 75.4878687 MHz
NUC1 13C
P1 15.00 usec
PLW1 15.0000000 W

==== CHANNEL f2 =====
SF02 300.1812007 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLM2 10.0000000 W
PLM12 0.20863999 W
PLM13 0.10495000 W

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



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

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

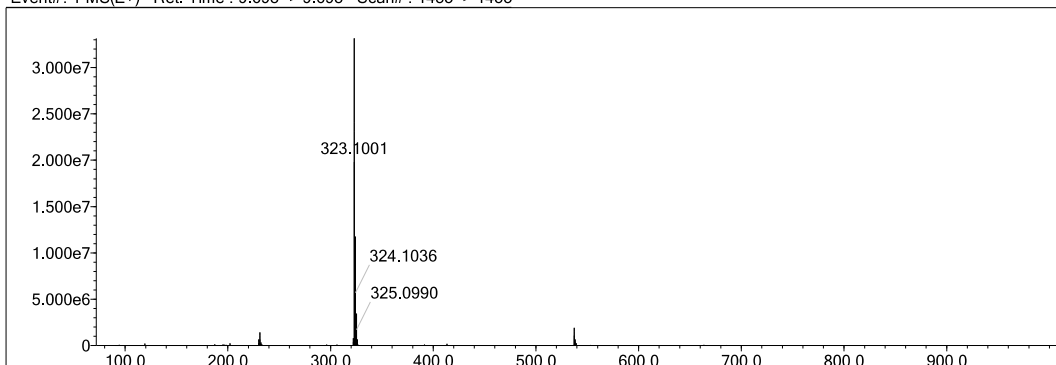
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	50	O	2	0	6	Cl	1	0	0	H
C	4	0	50	F	1	1	1	Br	1	0	0	
N	3	0	4	S	2	0	1	Pd	2	0	0	

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

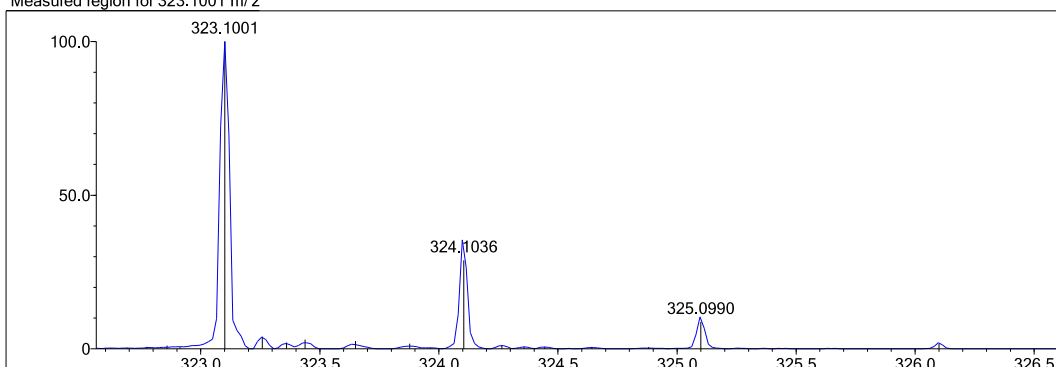
DBE Range: 10.0 - 20.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

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

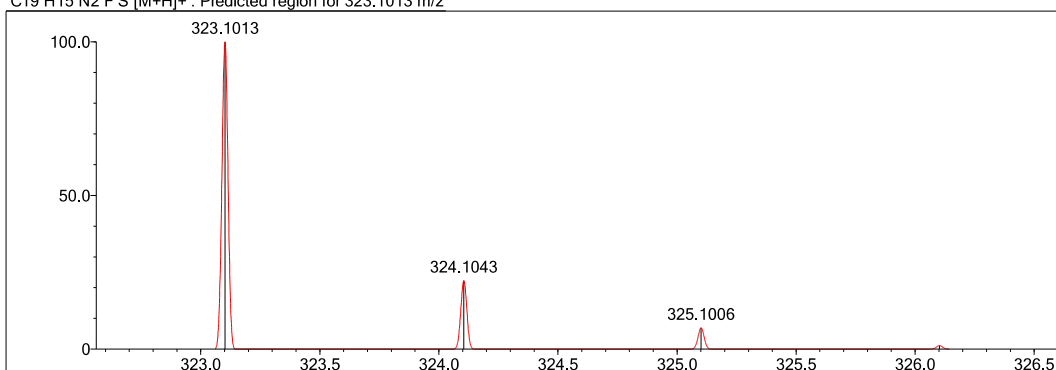
Event#: 1 MS(E+) Ret. Time : 9.693 -> 9.693 Scan#: 1455 -> 1455



Measured region for 323.1001 m/z



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

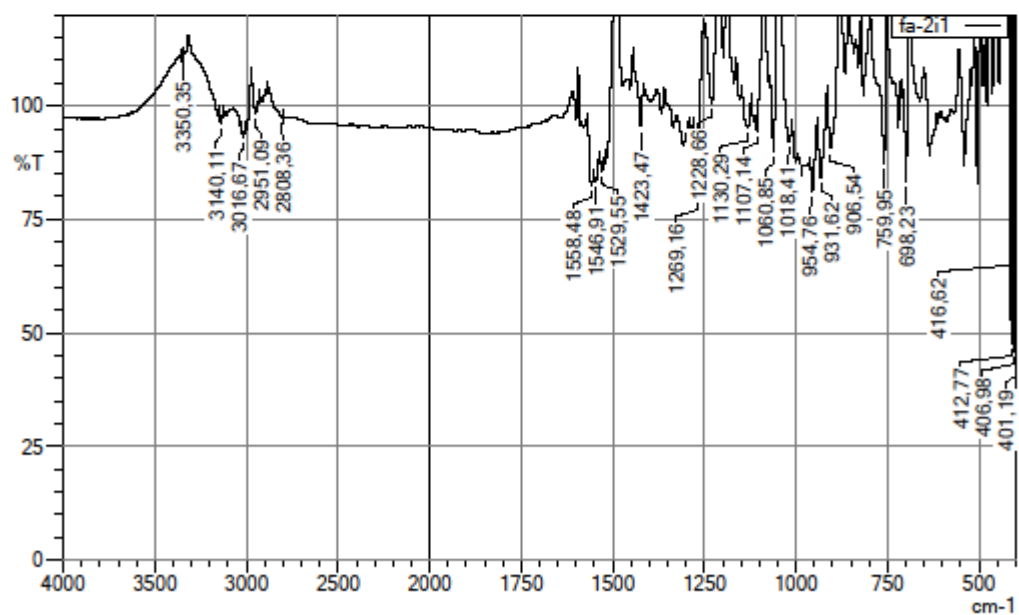
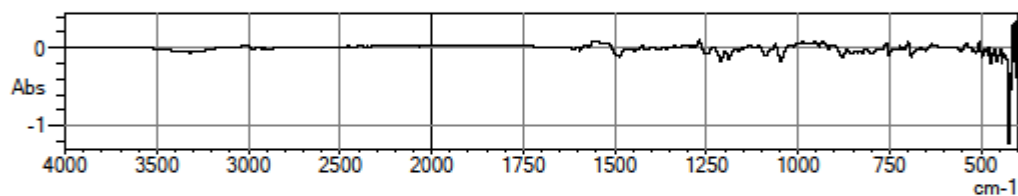


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	73.78	C19 H15 N2 F S	[M+H] ⁺	323.1001	323.1013	-1.2	-3.71	79.14	13.0

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-2i1.ispd
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



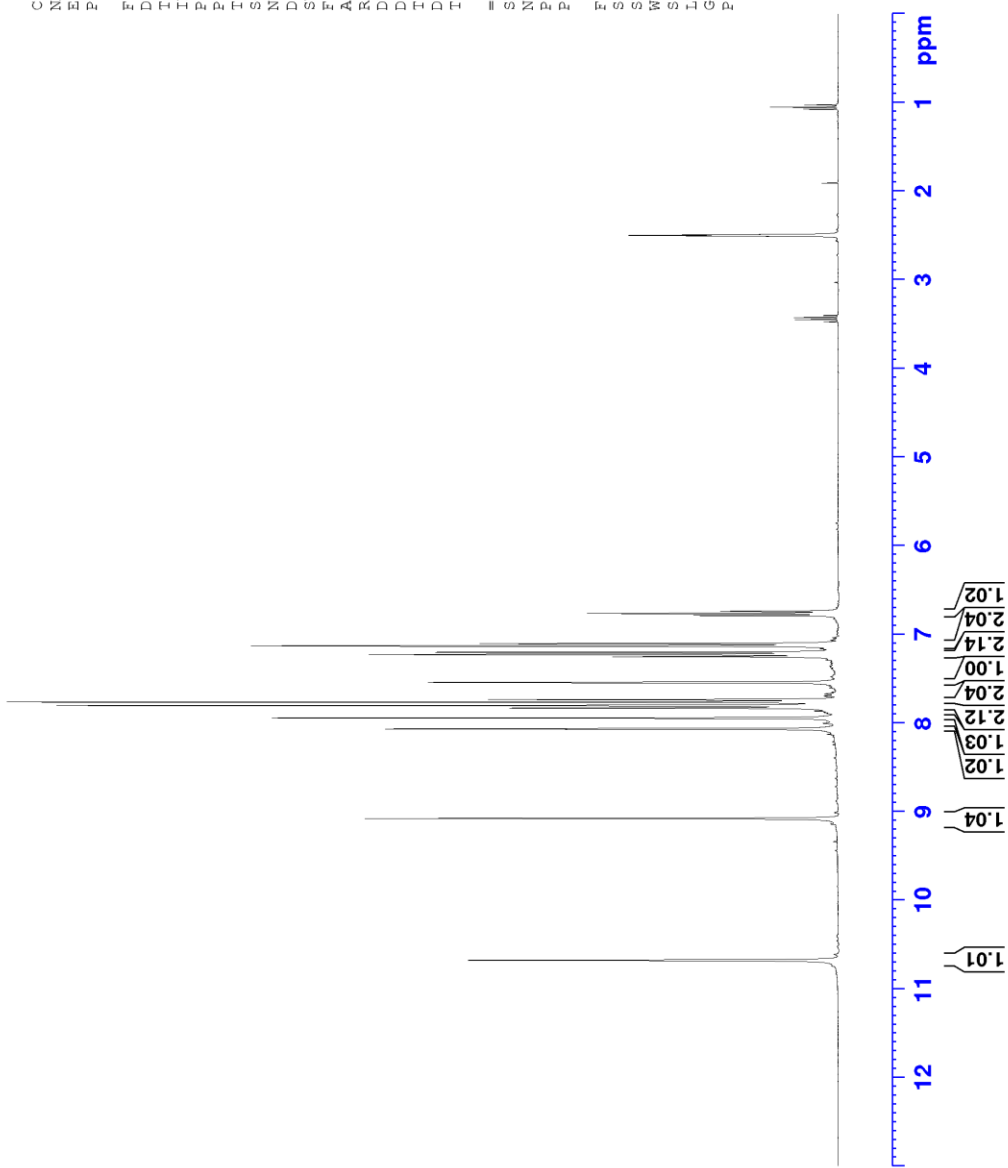
Current Data Parameters
NAME fa
EXPNO 470
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160601
Time 0.52
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 1.342173 sec
RG 11.1916
DW 81.920 usec
DE 6.50 usec
IE 298.0 K
D1 3.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 300.1616537 MHz
NUC1 1H
P1 13.00 usec
PLW1 10.00000000 W

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

10.6793
9.0800
8.0681
7.9457
7.8338
7.8046
7.7656
7.7364
7.5439
7.2552
7.2274
7.2031
7.1314
7.1064
6.7890
6.7651
6.7411
2.5113
2.5055
2.4995
2.4936
2.4880



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



Current Data Parameters
NAME fa
EXPNO 471
PROCNO 1

F2 - Acquisition Parameters

Date_ 20160601
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 1.0000000 sec
D11 0.0300000 sec
D31 0.0001500 sec
D32 0.8999998 sec
D40 0.0003990 sec
L4 23
L5 26
P32 90.00 usec
TDO 1

==== CHANNEL f1 =====
SF01 75.4878687 MHz
NUC1 13C
P1 15.00 usec
PLW1 15.0000000 W

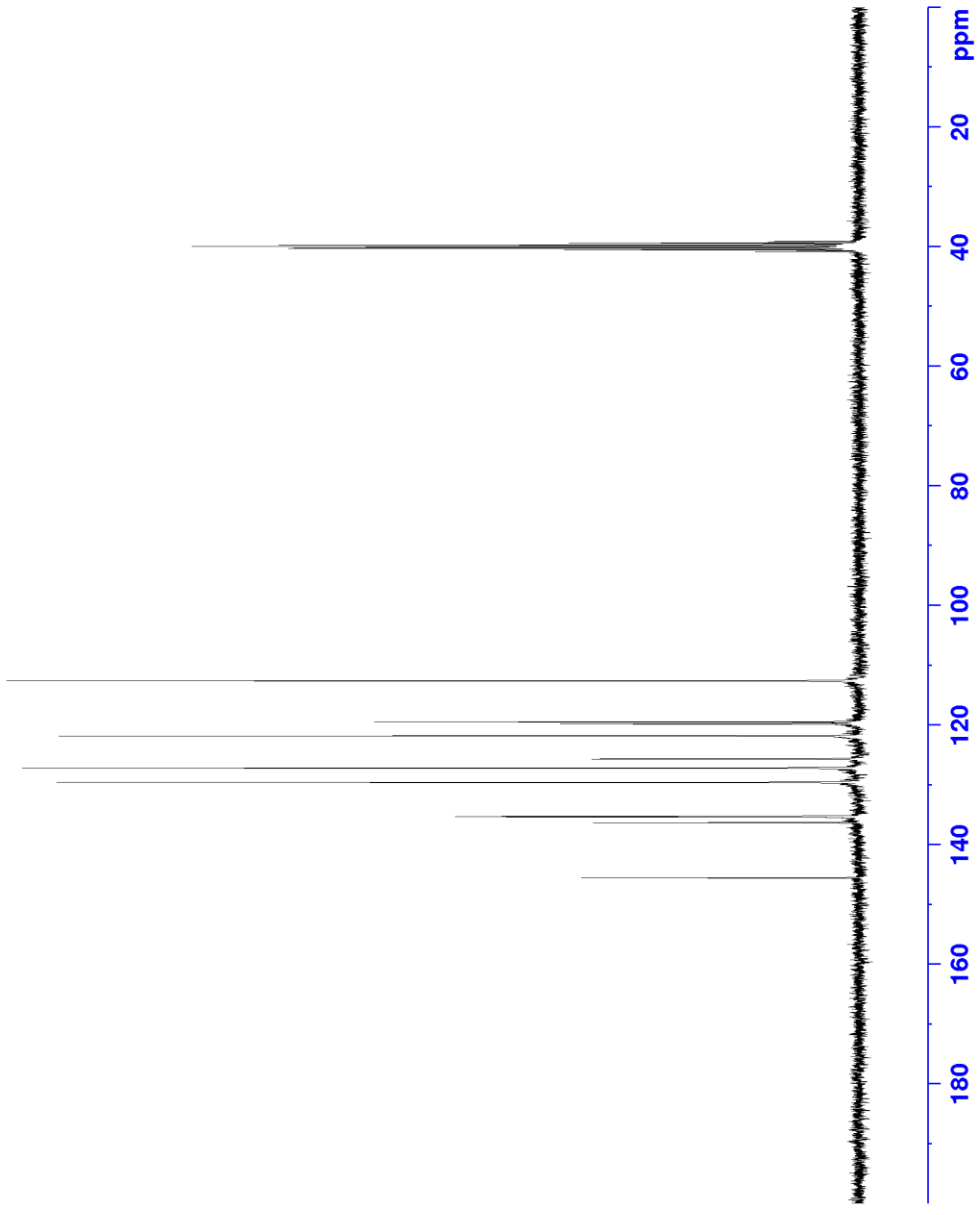
==== CHANNEL f2 =====
SF02 300.1812007 MHz
NUC2 1H
PCPRG12 waltz16
PCPD2 90.00 usec
PLW2 10.0000000 W
PLW12 0.20863999 W
PLW13 0.10495000 W

F2 - Processing parameters

SI 32768
SF 75.4803210 MHz
WDW EM
SSB 0
IB 0
GB 0
FC 1.40

40.81
40.54
40.26
39.98
39.70
39.42
39.15

145.55
136.33
135.38
135.33
135.26
129.59
127.19
125.67
121.84
119.80
119.48
112.61



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

Data File: C:\LabSolutions\Data\Analiz\derya\FA-9_9.Icd

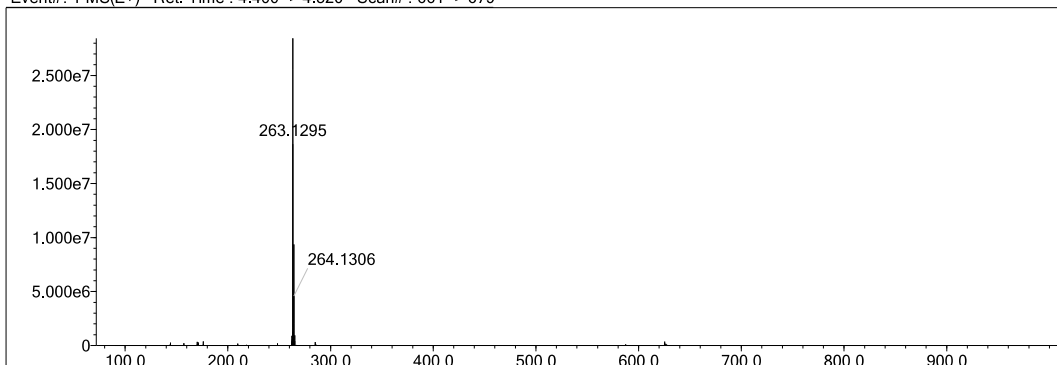
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	50	O	2	0	6	Cl	1	0	0	H
C	4	0	50	F	1	0	1	Br	1	0	0	
N	3	0	5	S	2	0	1	Pd	2	0	0	

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

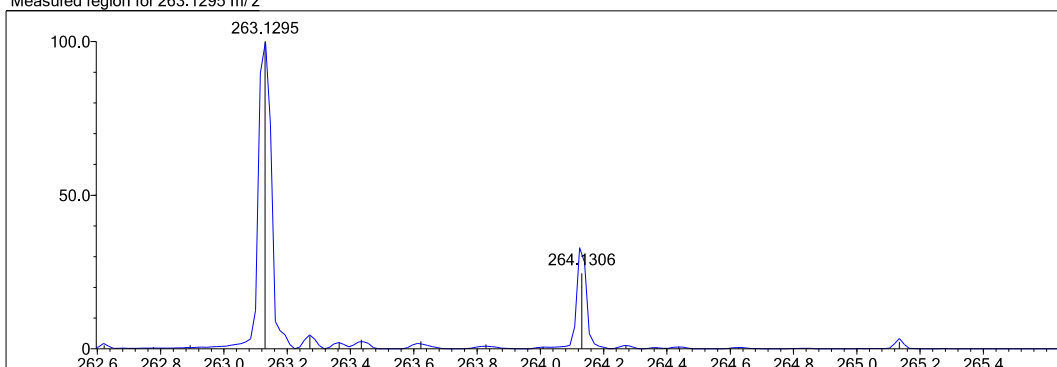
DBE Range: 10.0 - 20.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

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

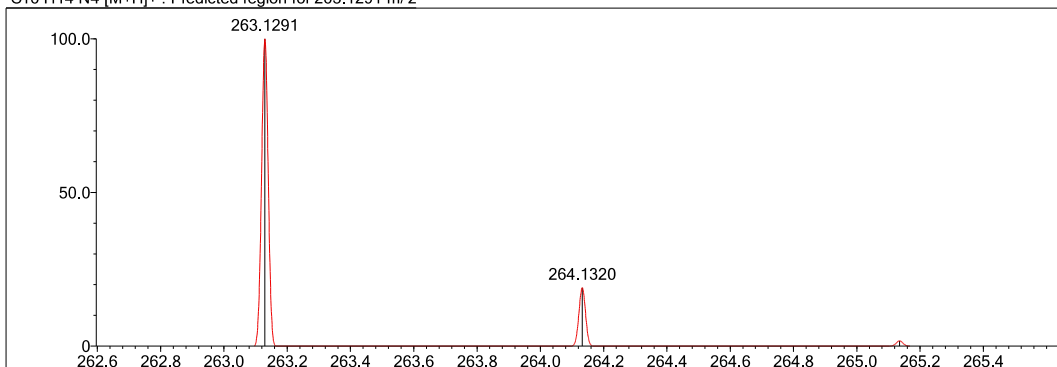
Event#: 1 MS(E+) Ret. Time : 4.400 -> 4.520 Scan# : 661 -> 679



Measured region for 263.1295 m/z



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

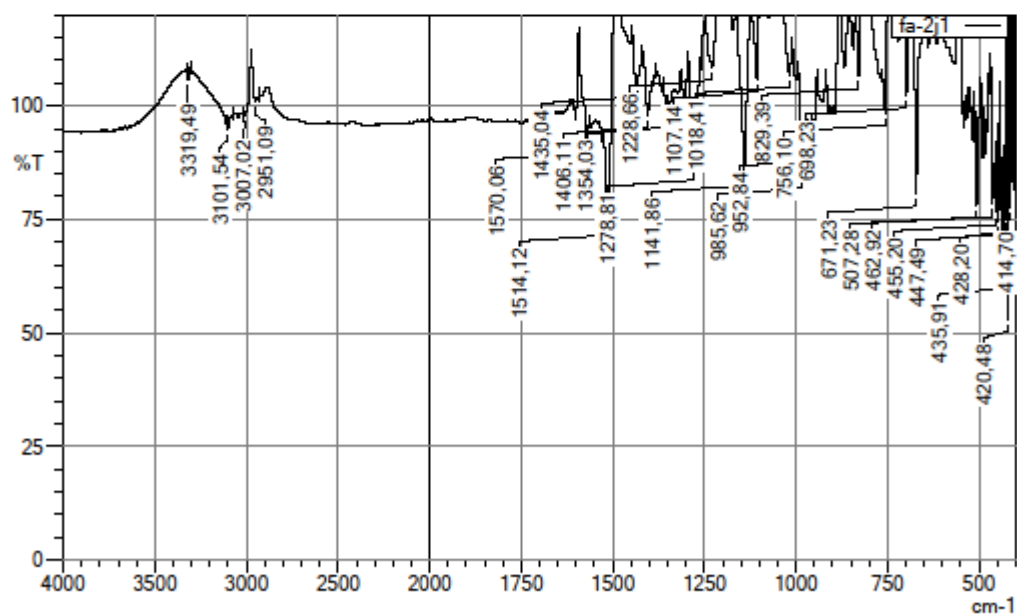
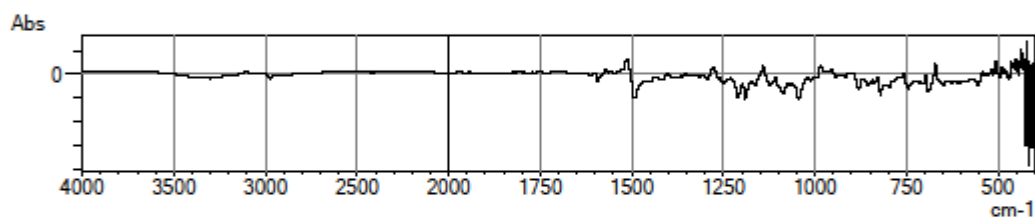


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	74.65	C16 H14 N4	[M+H]+	263.1295	263.1291	0.4	1.52	75.64	12.0

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\faifa-2\1.ispd
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

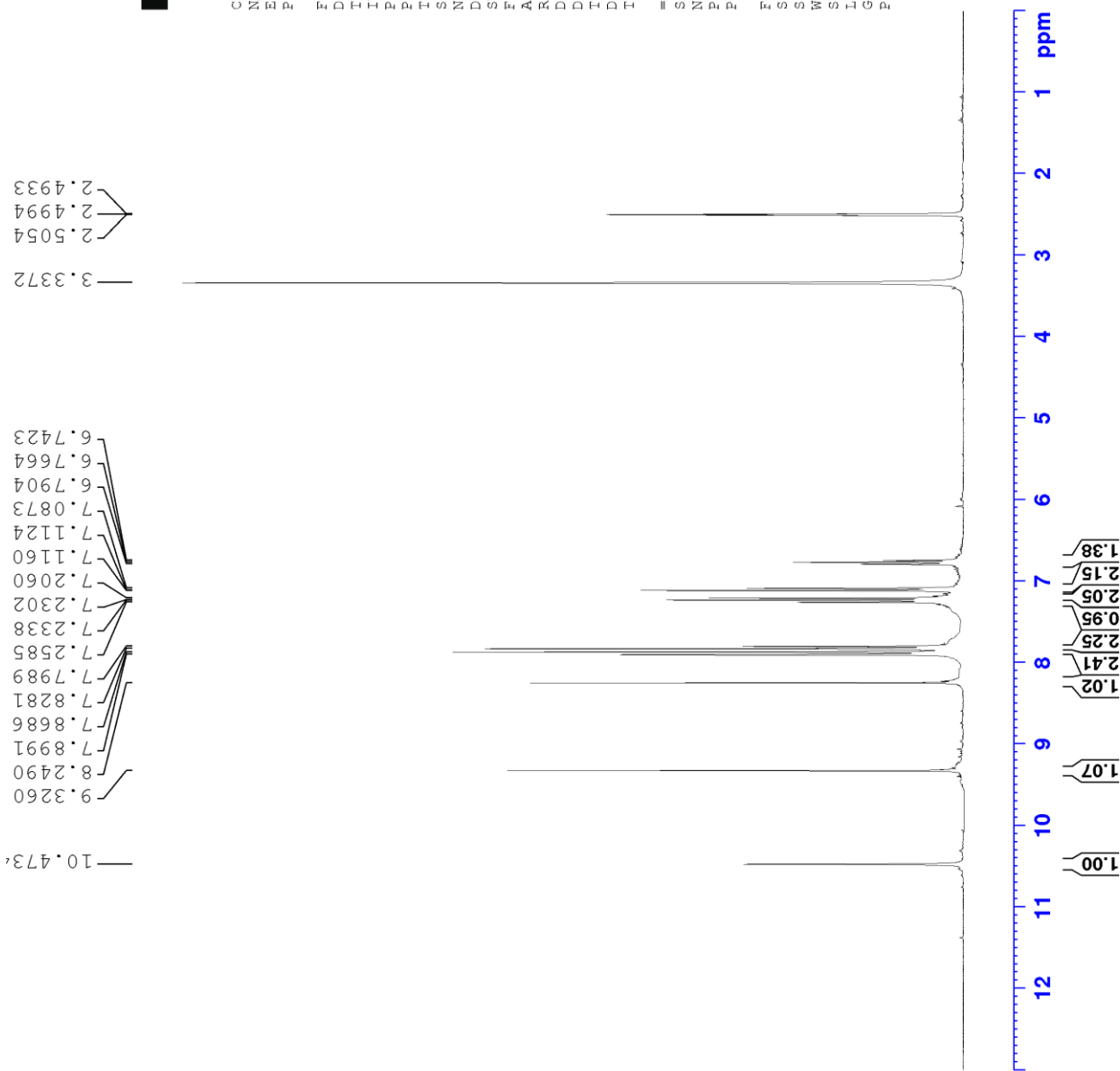


Current Data Parameters
NAME fa
EXPNO 472
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160601
Time 1.54
INSTRUM FOURIER300
PROBHD 5 mm DUL 13C-1
PULPROG zgpg
ID 16384
SOLVENT DMSO
NS 16
DS 0
SWH 6103.516 Hz
FIDRES 0.372529 Hz
AQ 1.3421773 sec
RG 20.8341
DW 81.920 usec
DE 6.50 usec
TE 298.2 K
D1 3.0000000 sec
TD0 1

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

F2 - Processing parameters
SI 63536
SF 300.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

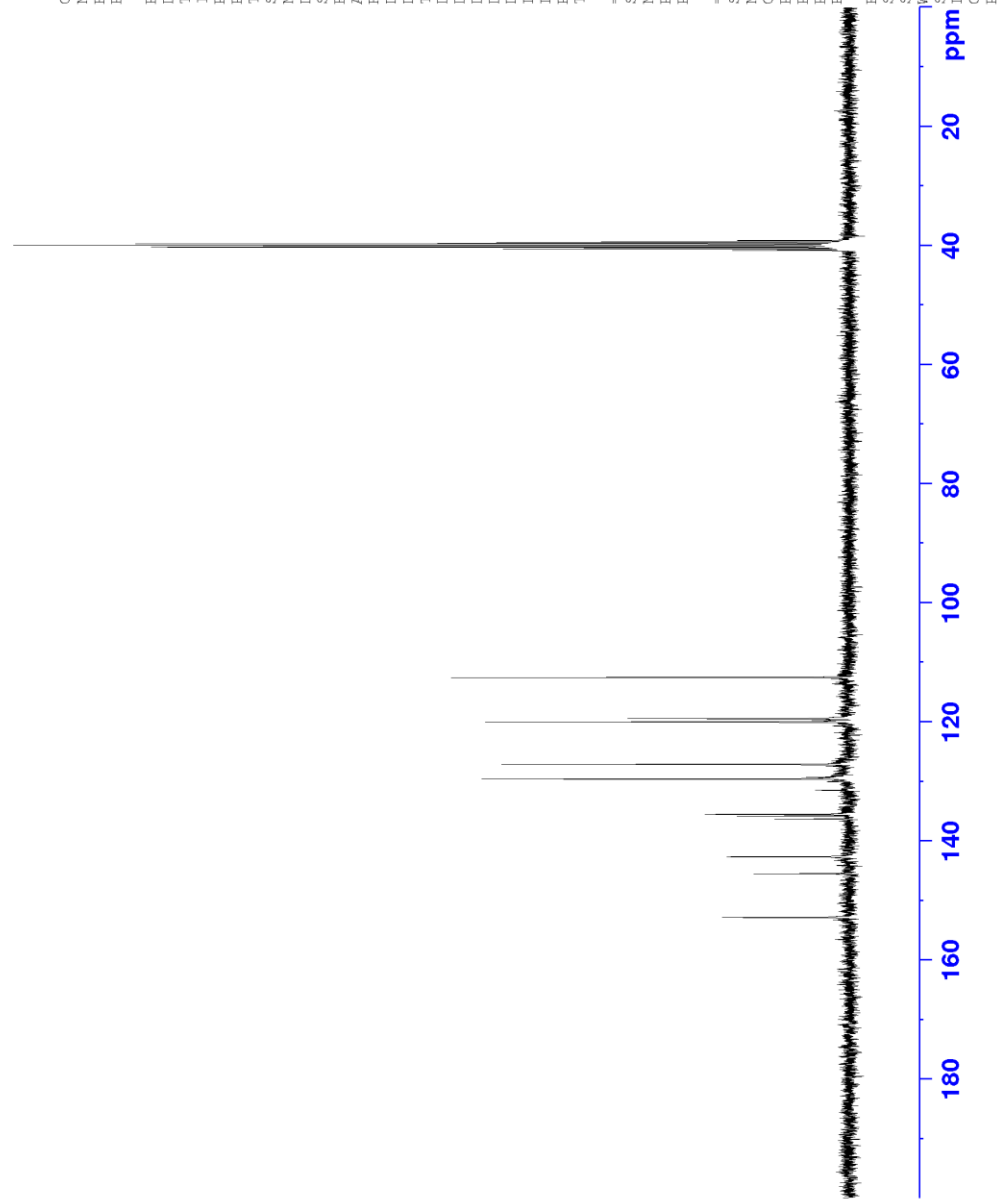


Spectra 38. ¹H NMR spectra of the compound 2j



40.81
40.53
40.25
39.98
39.70
39.42
39.14

152.87
145.55
142.67
136.35
135.82
135.55
129.61
127.17
120.05
119.45
112.56



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 20.460 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 0.00003990 sec
L4 23
L5 26
P32 90.00 usec
TD0 1

==== CHANNEL f1 =====
SF01 75.4878687 MHz
NUC1 13C
P1 15.00 usec
PLW1 15.00000000 W

==== CHANNEL f2 =====
SF02 300.1812007 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 10.00000000 W
PLW12 0.20863939 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

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

Data File: C:\LabSolutions\Data\Analiz\dera\FA-10_10.lcd

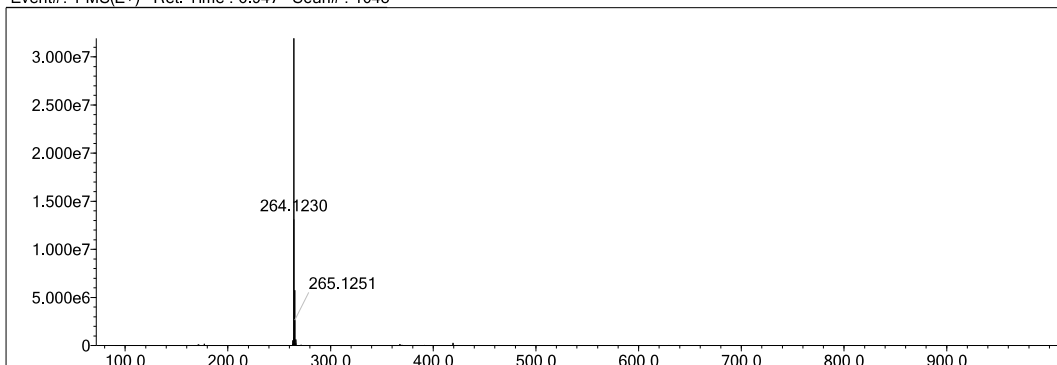
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	50	O	2	0	6	Cl	1	0	0	H
C	4	0	50	F	1	0	1	Br	1	0	0	
N	3	0	5	S	2	0	1	Pd	2	0	0	

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

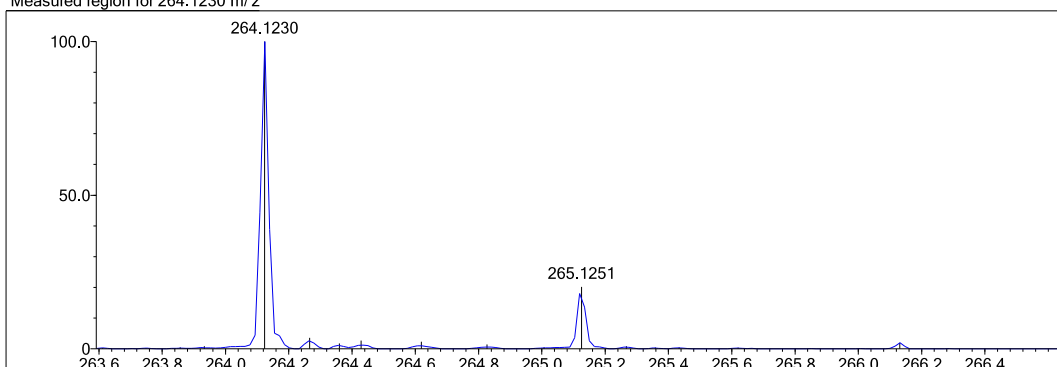
DBE Range: 10.0 - 20.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

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

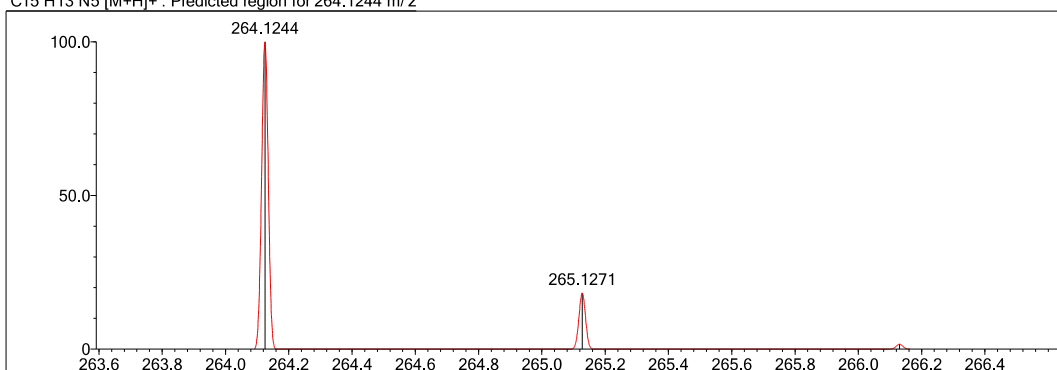
Event#: 1 MS(E+) Ret. Time : 6.947 Scan#: 1043



Measured region for 264.1230 m/z



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

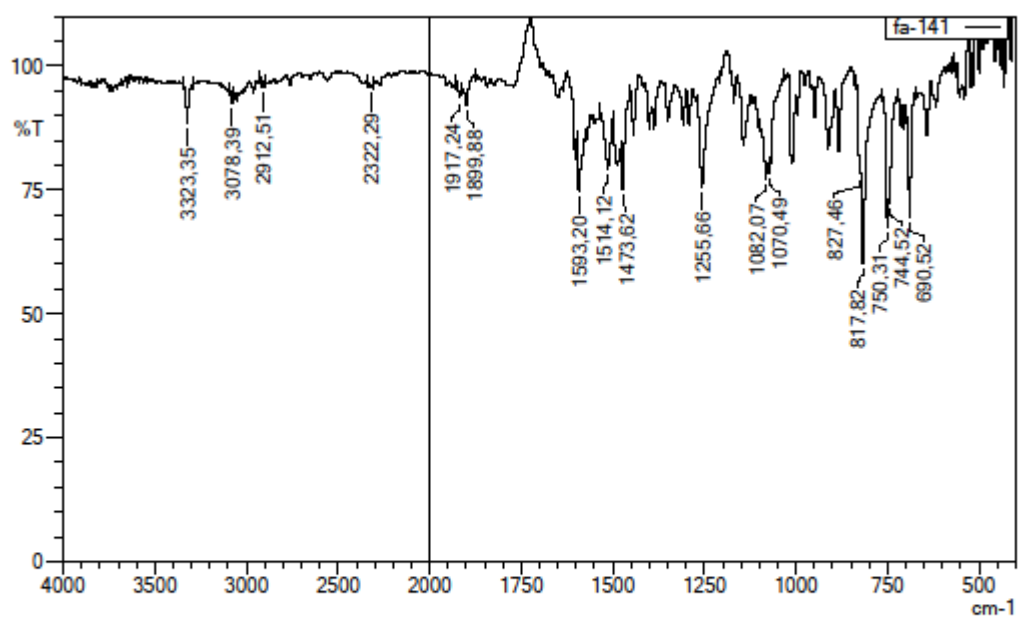
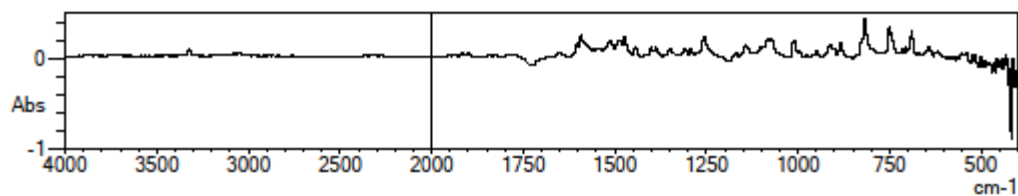


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	82.79	C15 H13 N5	[M+H]+	264.1230	264.1244	-1.4	-5.30	95.17	12.0

Spectra 40. HRMS spectra of the compound 2j

DOPNALAB

Item	Value
Acquired Date&Time	7.08.2017 10:39:00
Acquired by	System Administrator
Filename	C:\Users\dopnalab\Desktop\derya\fa-141.ispd
Spectrum name	fa-141
Sample name	fa-141
Sample ID	
Option	
Comment	
No. of Scans	10
Resolution	4 (cm-1)
Apodization	Happ-Genzel



Spectra 41. IR spectra of the compound 2k

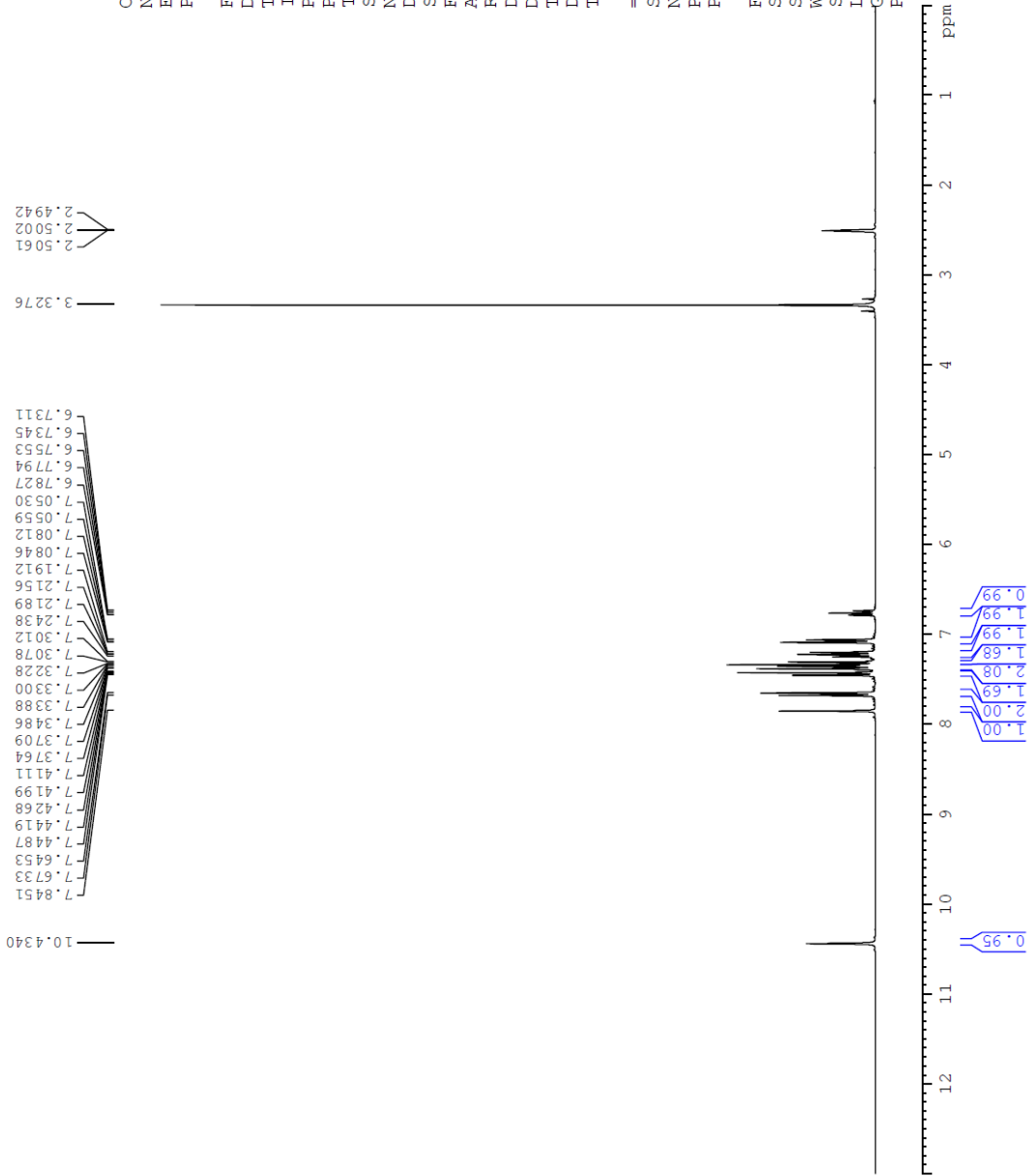


Current Data Parameters
NAME FA-14
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170804
Time 12.31
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 20.9771
DW 81.920 usec
DE 6.50 usec
TE 299.9 K
D1 3.0000000 sec
TD0 1

==== CHANNEL f1 =====
SF01 300.1818537 MHz
NUC1 1H
P1 13.00 usec
PLW1 10.0000000 W

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



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



Current Data Parameters
NAME FA-14
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170804
Time 12.33
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 300.1 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
F32 90.00 usec
TD0 1

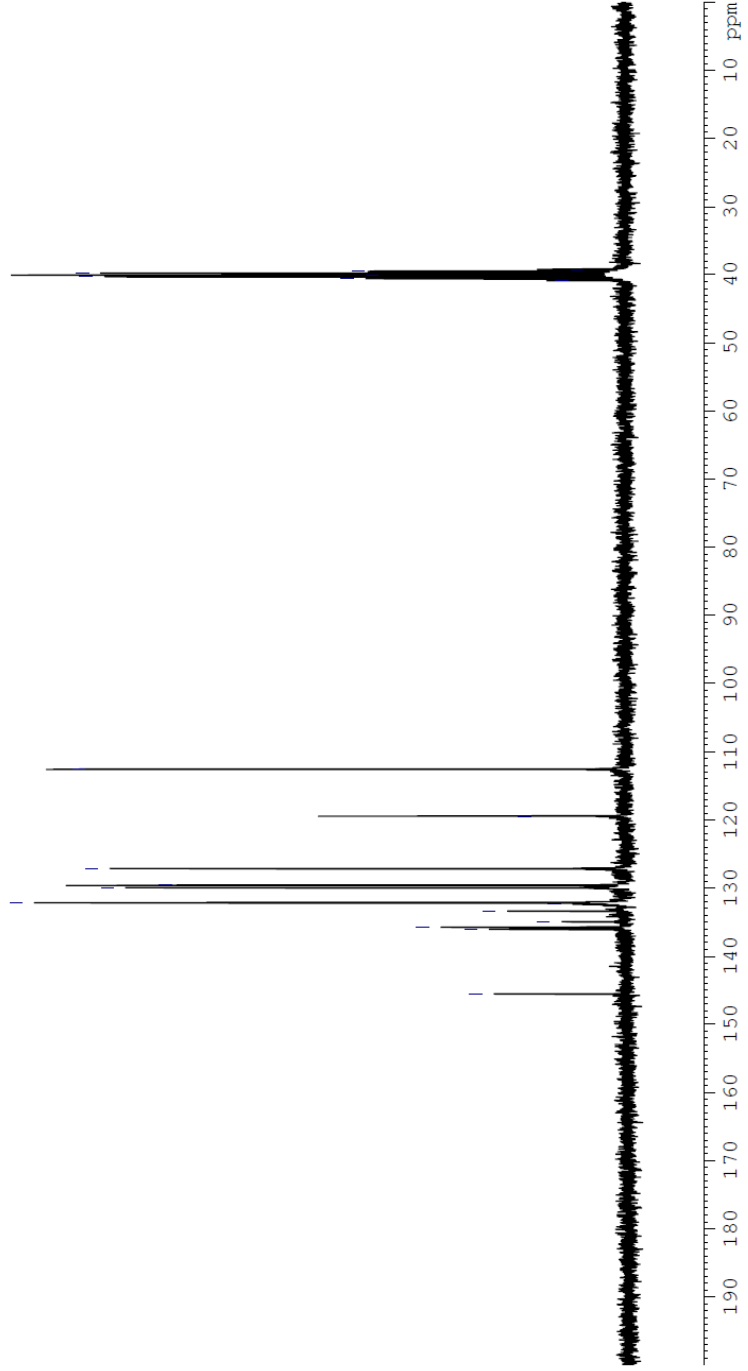
==== CHANNEL f1 =====
SF01 75.4878687 MHz
NUC1 13C
P1 15.00 usec
PLW1 15.00000000 W

==== CHANNEL f2 =====
SF02 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
EM
WDW 0
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

40.84
40.56
40.28
40.00
39.73
39.45
39.17

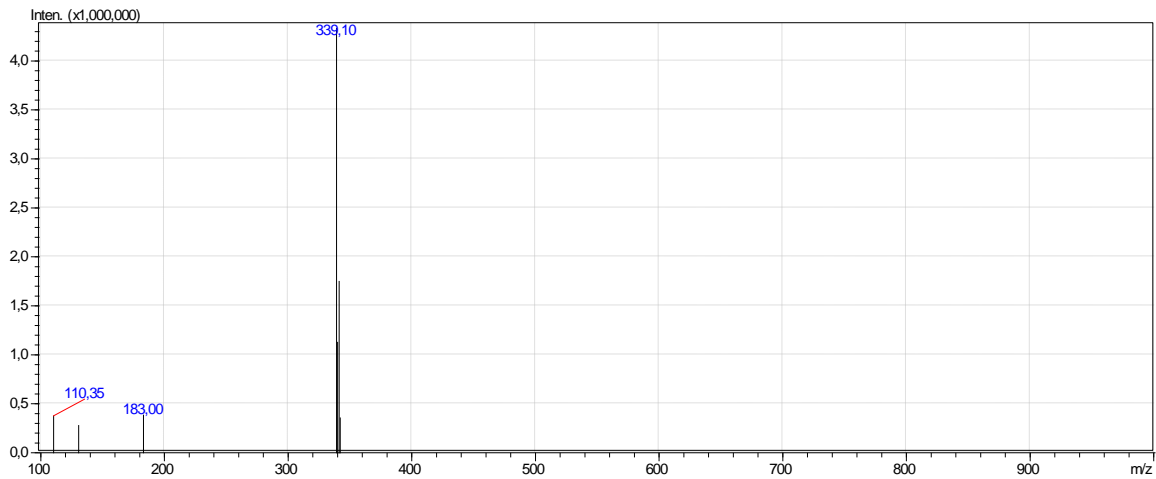
149.53
136.07
135.76
134.94
133.38
132.40
132.18
132.12
129.96
129.59
127.13
119.44
112.54



Spectra 43. ¹³C 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
Date Acquired : 04.08.2017 14:52:32
Date Processed : 04.08.2017 14:54:35
Sample Type : Unknown
Acquired by : System Administrator
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)

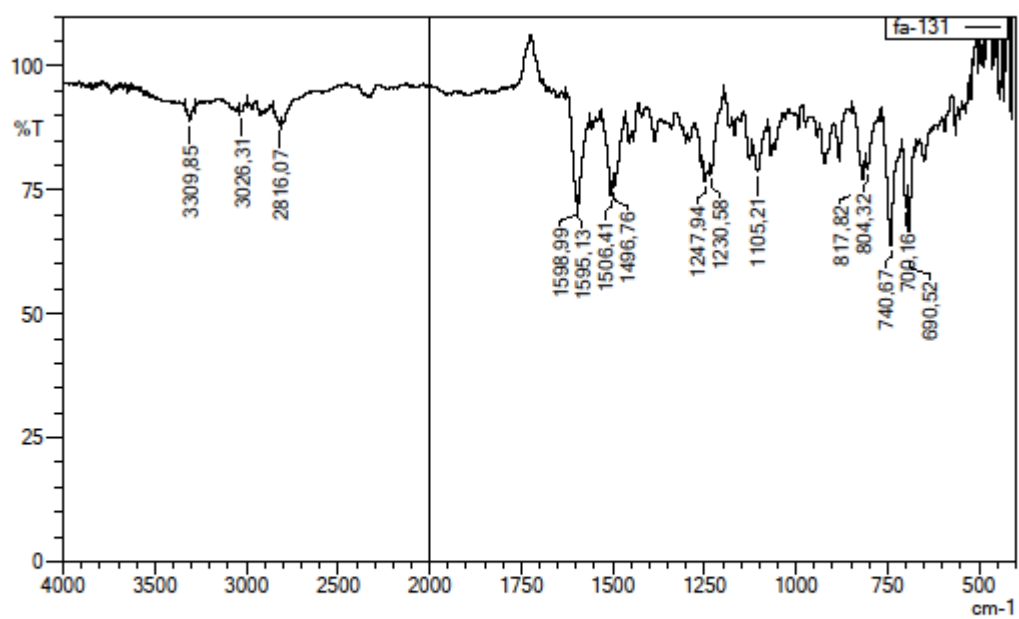
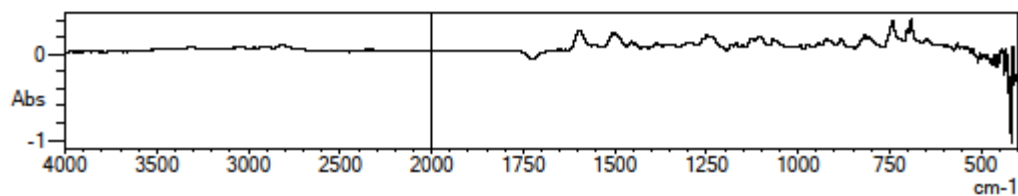
m/z	Absolute Intensity	Relative Intensity
110,35	377521	8,71
130,70	279346	6,44
183,00	385160	8,88
339,10	4335027	100,00
340,10	1128654	26,04
341,20	1751529	40,40
342,15	357781	8,25

Event 1

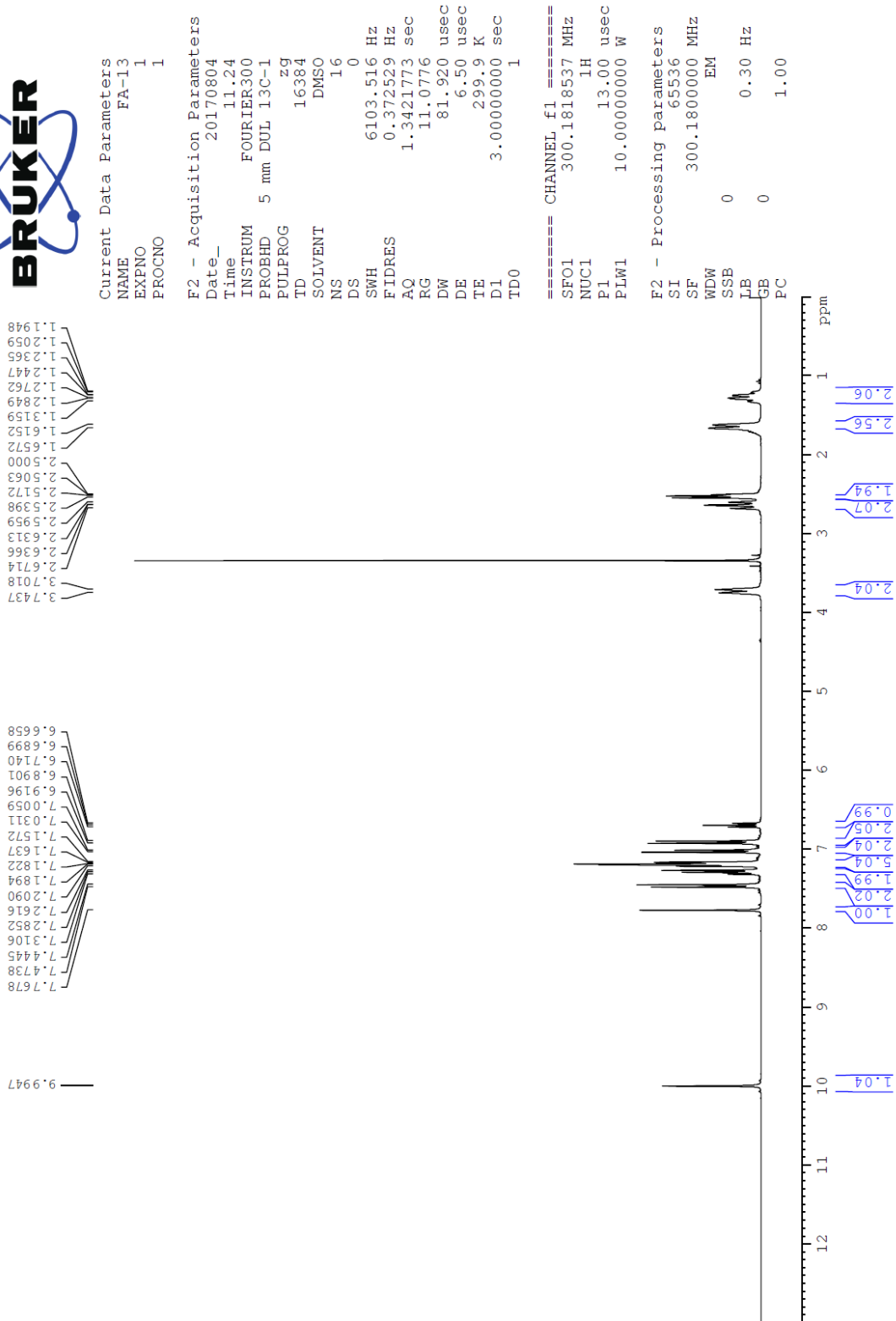
Spectra 44. LCMSMS spectra of the compound 2k

DOPNALAB

Item	Value
Acquired Date&Time	7.08.2017 10:36:28
Acquired by	System Administrator
Filename	C:\Users\dopnalab\Desktop\derya\fa-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. ^1H NMR spectra of the compound 21



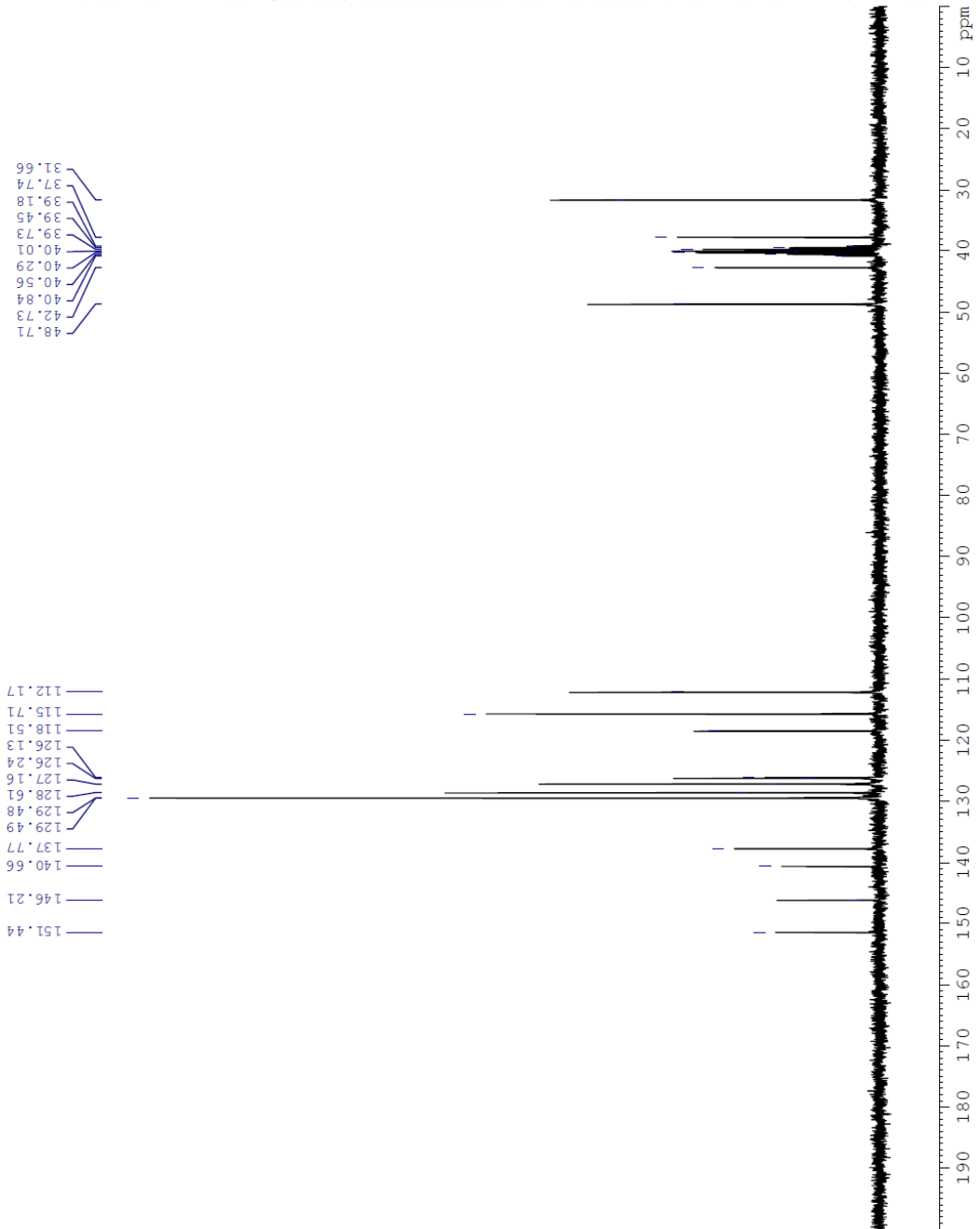
Current Data Parameters
NAME FA-13
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170804
Time 11.31
INSTRUM FOURIER300
PROBHD 5 mm DUL 13C-1
PULPROG zgpg
TD 32768
SOLVENT DMSO
NS 2048
DS 4
SWH 24414.063 Hz
FIDRES 0.745038 Hz
AQ 0.6710886 sec
RG 501.187
DW 20.480 usec
DE 6.50 usec
TE 299.7 K
D1 1.00000000 sec
D11 0.03000000 sec
D31 0.00001500 sec
D32 0.89999998 sec
D40 0.00009390 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
CFDPRG[2] waitz16
PCPD2 90.00 usec
PLW2 10.00000000 W
PLW12 0.20863999 W
PLW13 0.10495000 W

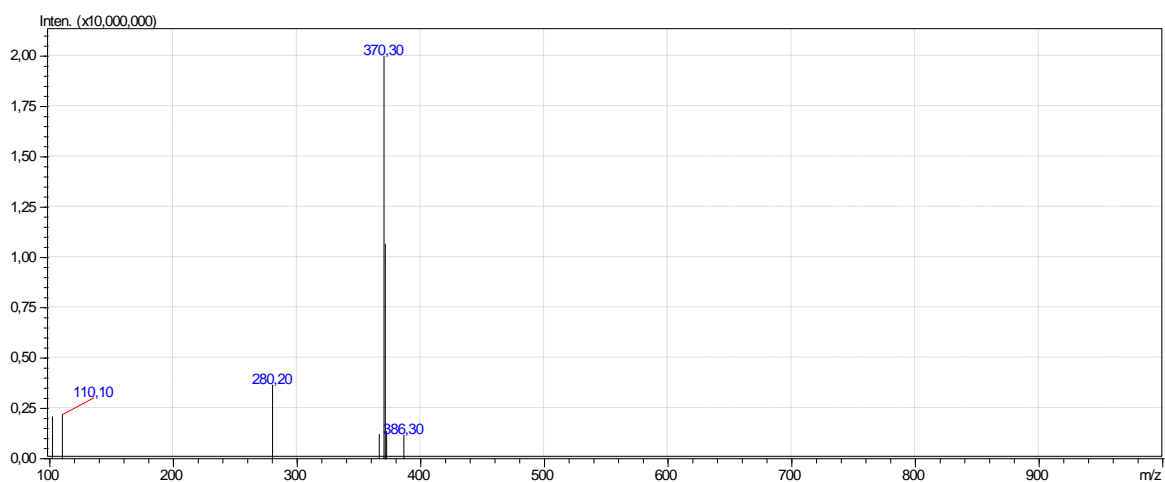
F2 - Processing Parameters
SI 32768
SF 75.4803210 MHz
WDW EM
SSB 0
GB 0
PC 1.40



Spectra 47. ¹³C NMR spectra of the compound 21

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
Date Acquired : 04.08.2017 14:49:53
Date Processed : 04.08.2017 14:51:56
Sample Type : Unknown
Acquired by : System Administrator
Processed by : System Administrator



[MS Spectrum]

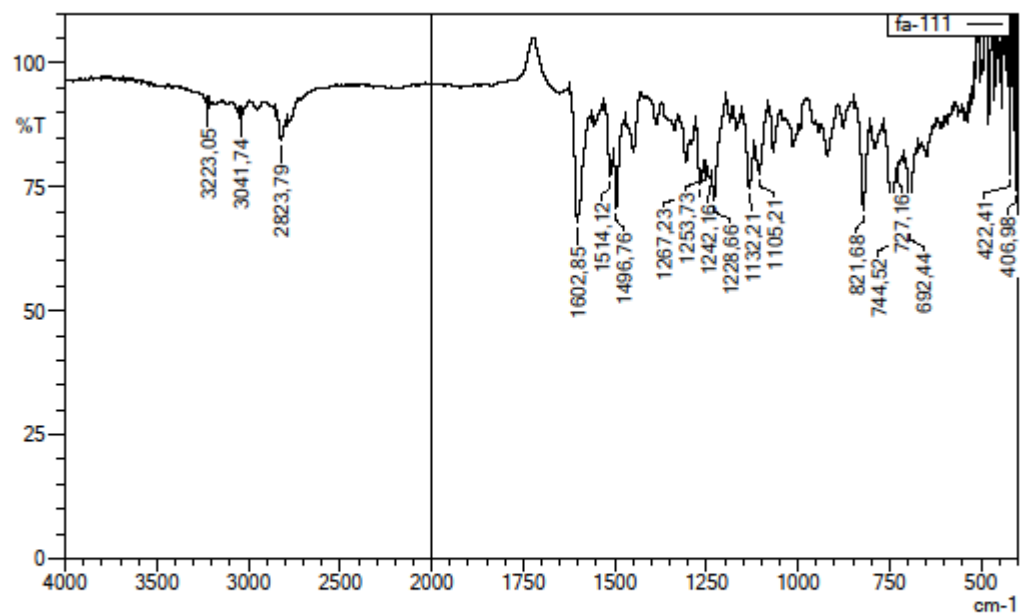
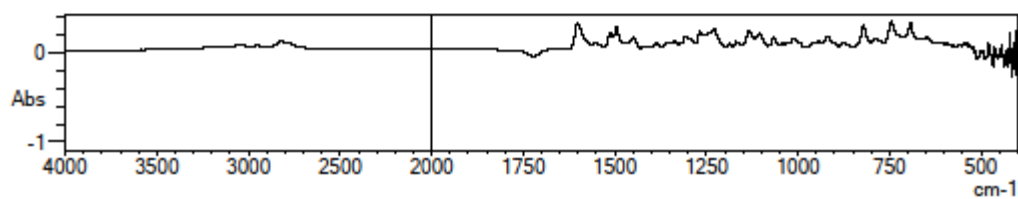
of Peaks : 8
Raw Spectrum : [1,590],(scan:[95])
Background : No Background Spectrum
Base Peak : m/z 370,30 (Inten : 20.000.000)

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	

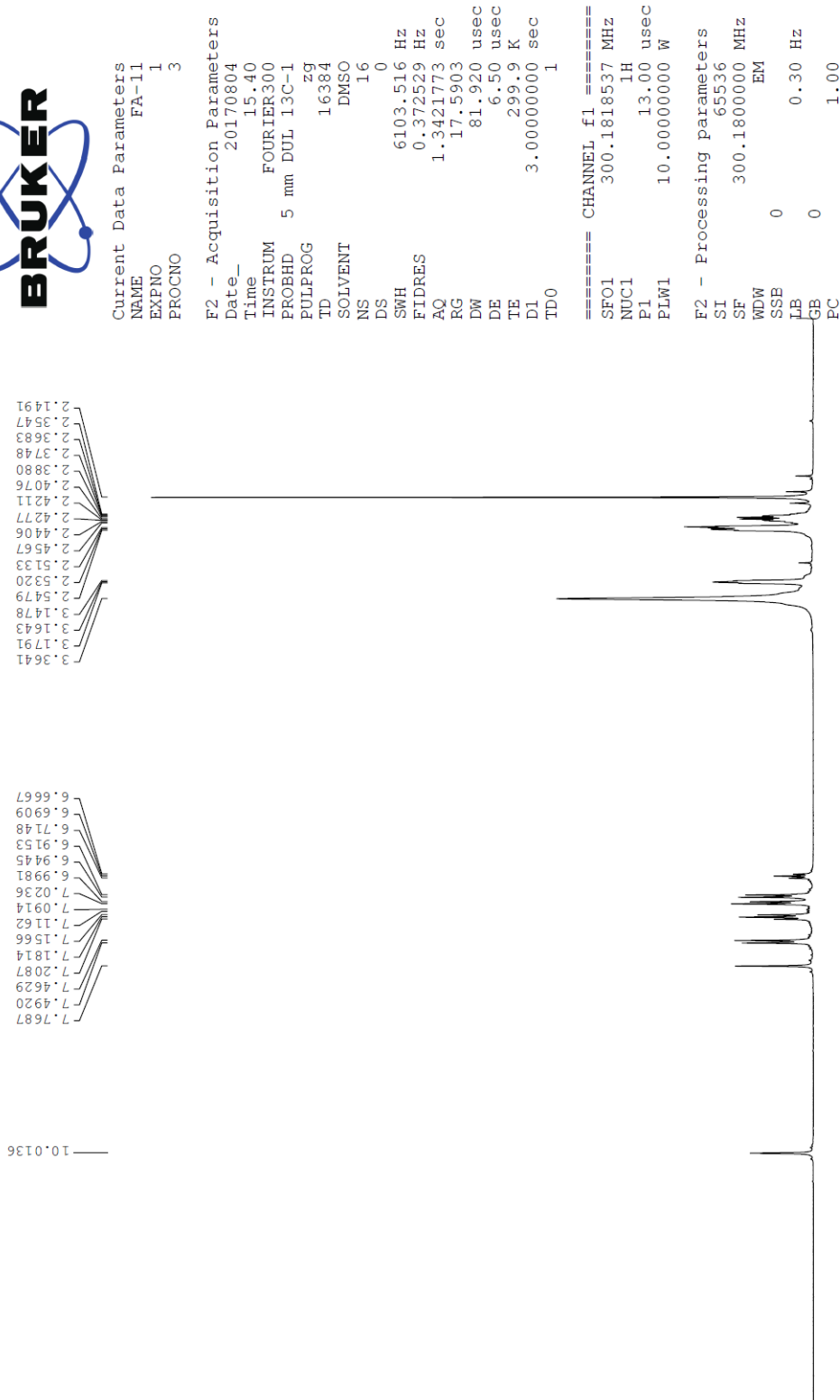
Spectra 48. LCMSMS spectra of the compound 21

DOPNALAB

Item	Value
Acquired Date&Time	7.08.2017 10:28:53
Acquired by	System Administrator
Filename	C:\Users\dopnalabi\Desktop\derya\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. ¹H NMR spectra of the compound 2m



```

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
F32          90.00 usec
TD0          1

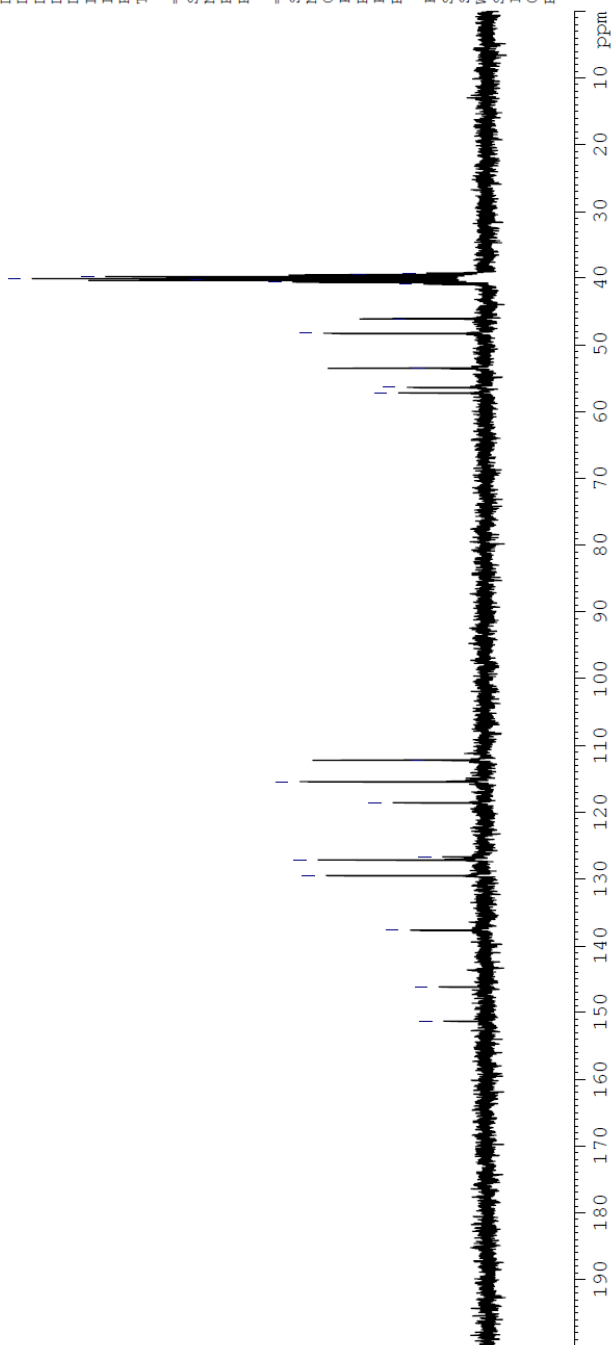
===== CHANNEL f1 =====
SFO1         75.4878687 MHz
NUC1         13C
P1           15.00 usec
PLW1        15.00000000 W

===== CHANNEL f2 =====
SFO2         300.1812007 MHz
NUC2         1H
CPDPRG2      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           0
GB           0
PC           1.40
  
```

39.19
 39.47
 39.74
 40.02
 40.30
 40.58
 40.86
 46.04
 48.24
 53.47
 56.34
 57.15

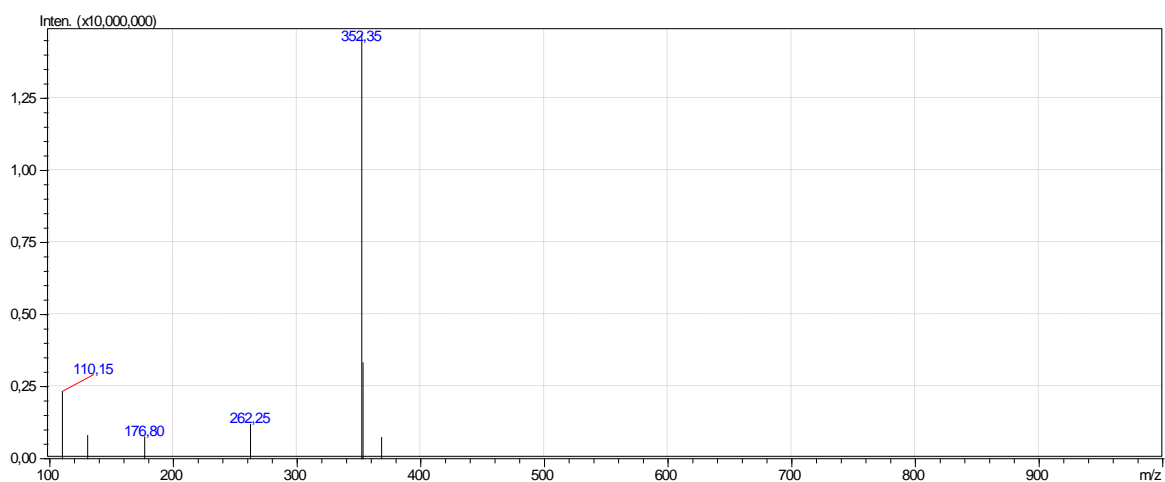
112.19
 115.41
 118.57
 126.65
 127.12
 129.50
 137.68
 146.18
 151.29



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

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
Date Acquired : 04.08.2017 14:44:33
Date Processed : 04.08.2017 14:46:36
Sample Type : Unknown
Acquired by : System Administrator
Processed by : System Administrator



[MS Spectrum]

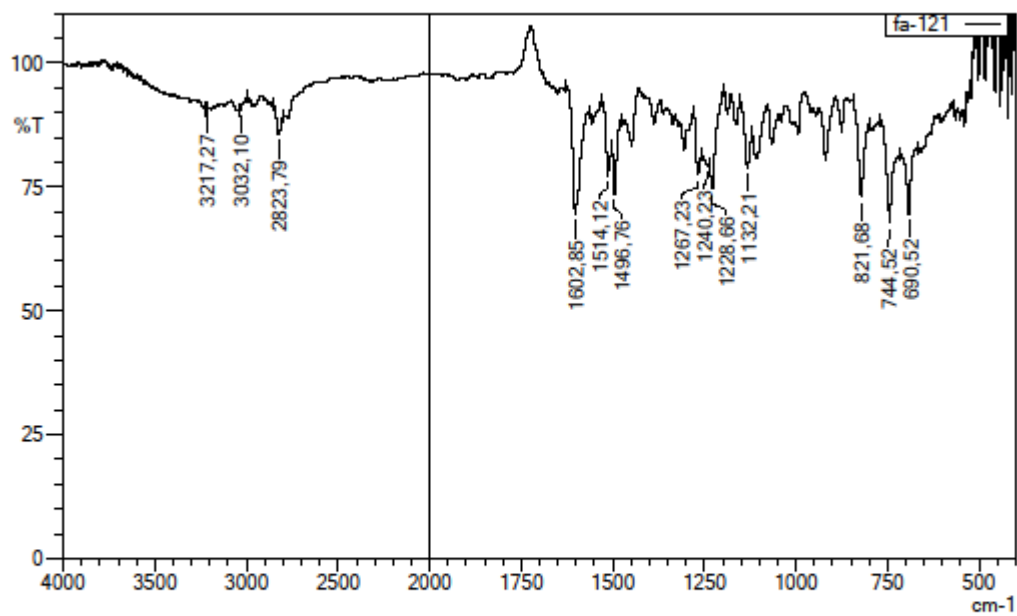
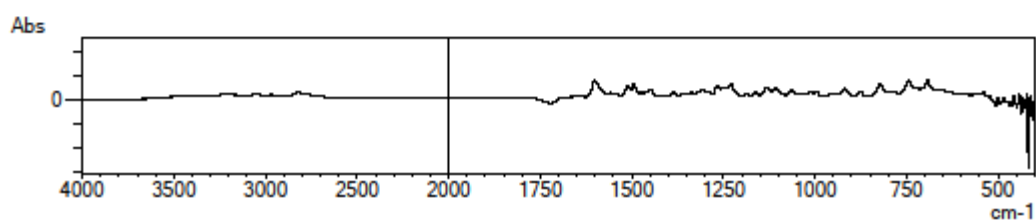
of Peaks 7
Raw Spectrum [1,624->1,759],(scan:[97->105])
Background [0,101->0,271],(scan:[7->17])
Base Peak m/z 352,35 (Inten :

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	

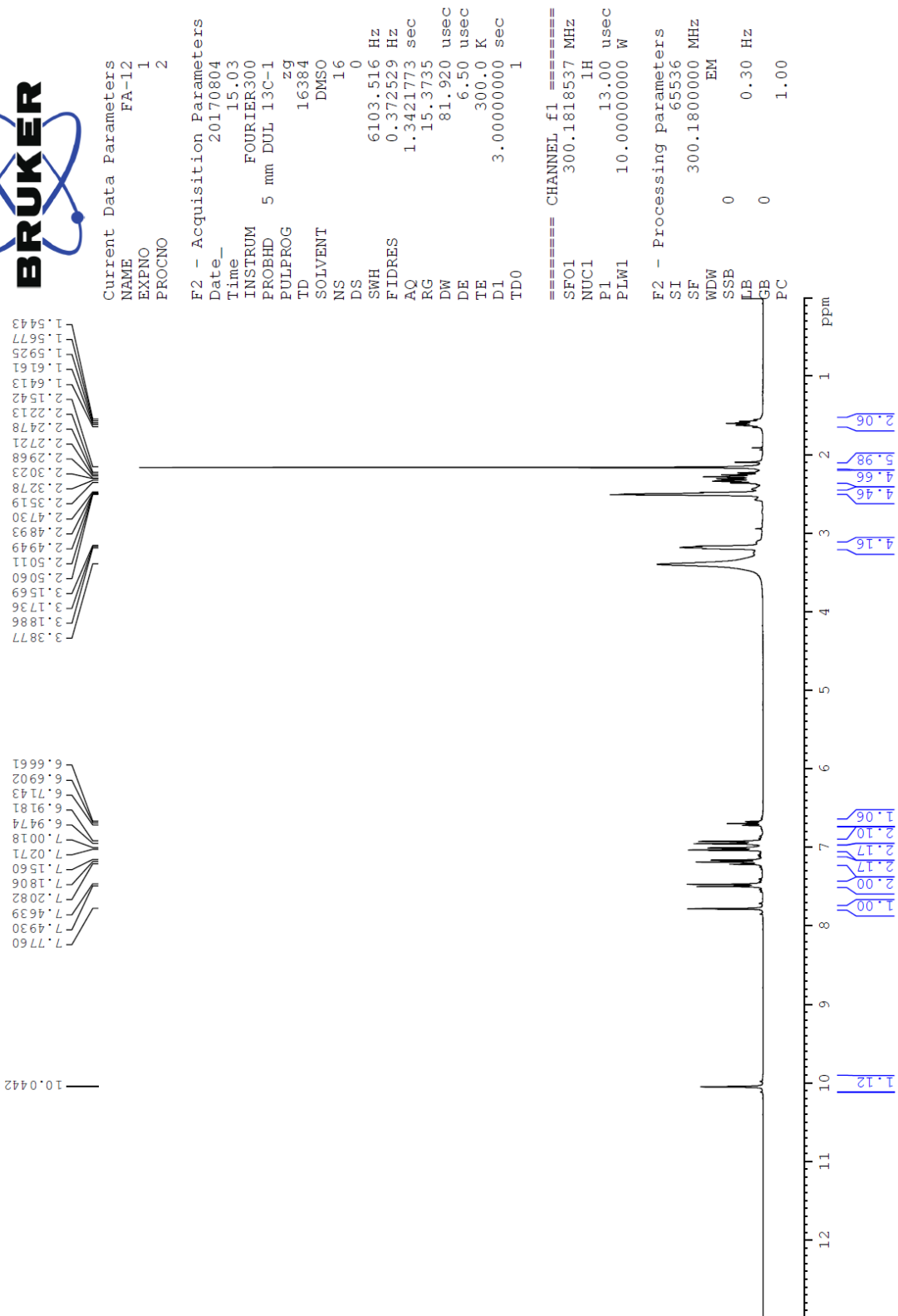
Spectra 52. LCMSMS spectra of the compound 2m

DOPNALAB

Item	Value
Acquired Date&Time	7.08.2017 10:33:21
Acquired by	System Administrator
Filename	C:\Users\dopnalabi\Desktop\derya\faifa-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. ¹H NMR spectra of the compound 2n



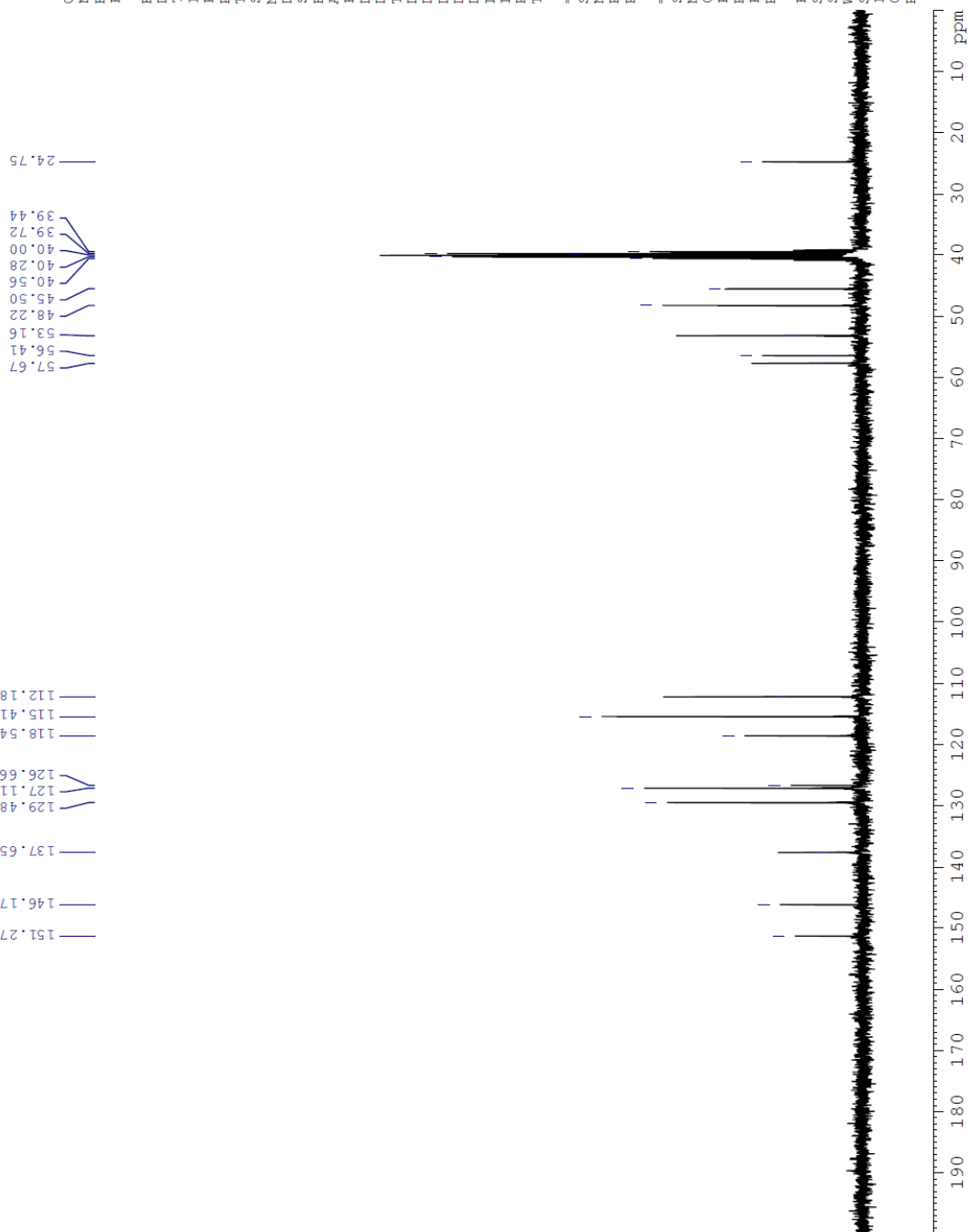
Current Data Parameters
NAME FA-12
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170804
Time_ 15.06
INSTRUM FOURIER300
PROBHD 5 mm DUL 13C-1
PULPROG zgpg
TD 32768
SOLVENT DMSO
NS 1075
DS 4
SWH 24414.063 Hz
FIDRES 0.745058 Hz
AQ 0.6710886 sec
RG 501.187
DM 20.480 usec
DE 6.50 usec
TE 299.9 K
D1 1.00000000 sec
D11 0.03000000 sec
D31 0.00001500 sec
D32 0.89999998 sec
D40 0.000093990 sec
L4 23
L5 26
F32 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
CFDPERG2 waltz16
PCPD2 90.00 usec
PLW2 10.00000000 W
PLW12 0.20863999 W
PLW13 0.10495000 W

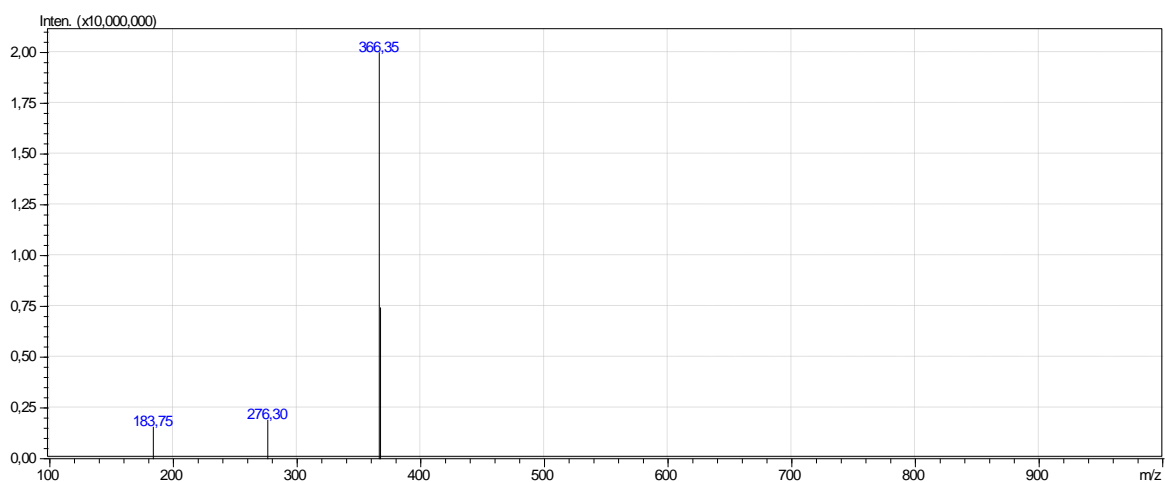
F2 - Processing parameters
SI 32768
SF 75.4803210 MHz
WDW EM
SSB 0
GB 0
FC 1.40



Spectra 55. ¹³C 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
Date Acquired : 04.08.2017 14:47:13
Date Processed : 04.08.2017 14:49:17
Sample Type : Unknown
Acquired by : System Administrator
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