SUPPORTING INFORMATION

SYNTHESIS AND AChE INHIBITORY ACTIVITY OF NEW BENZIMIDAZOLE DERIVATIVES

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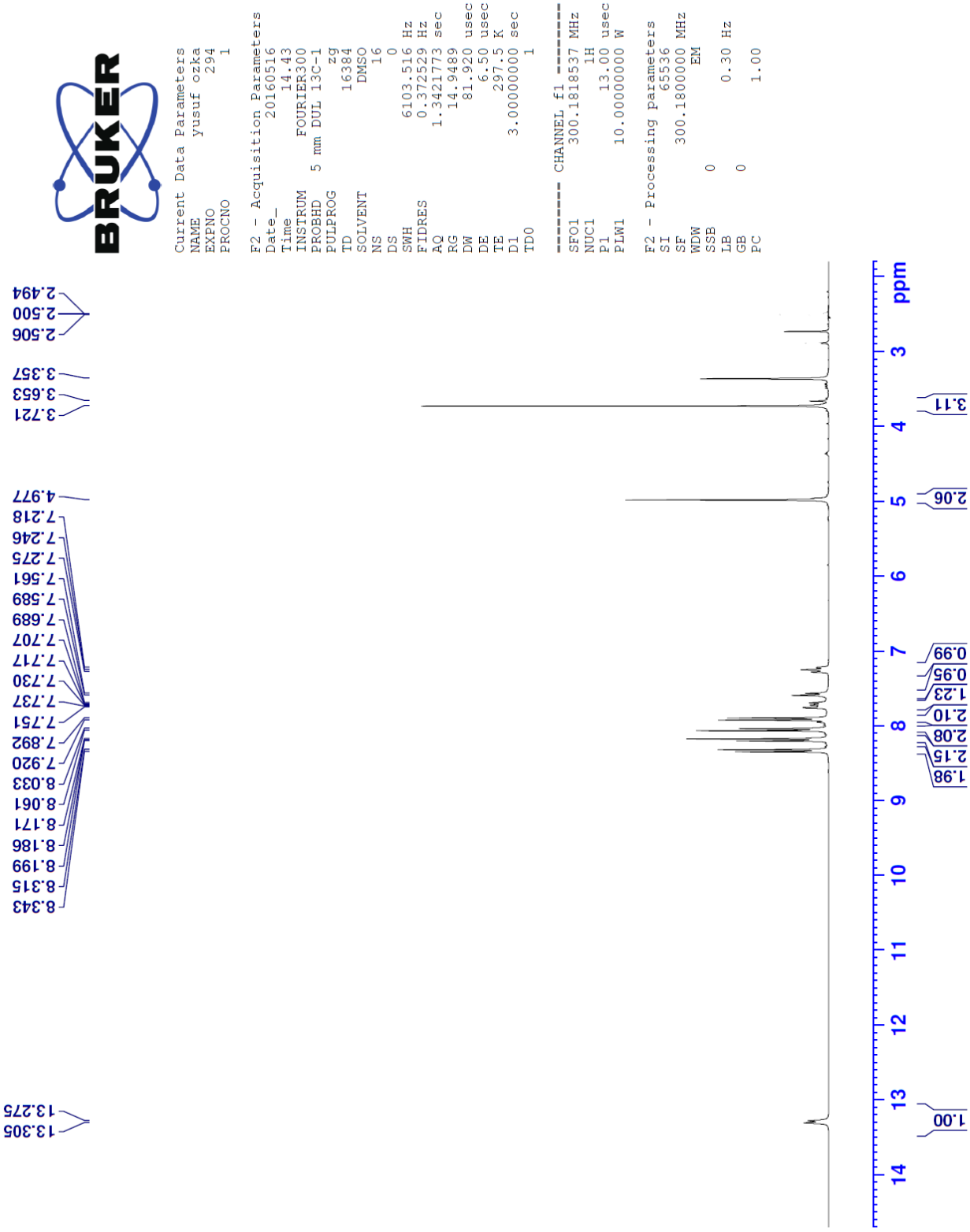
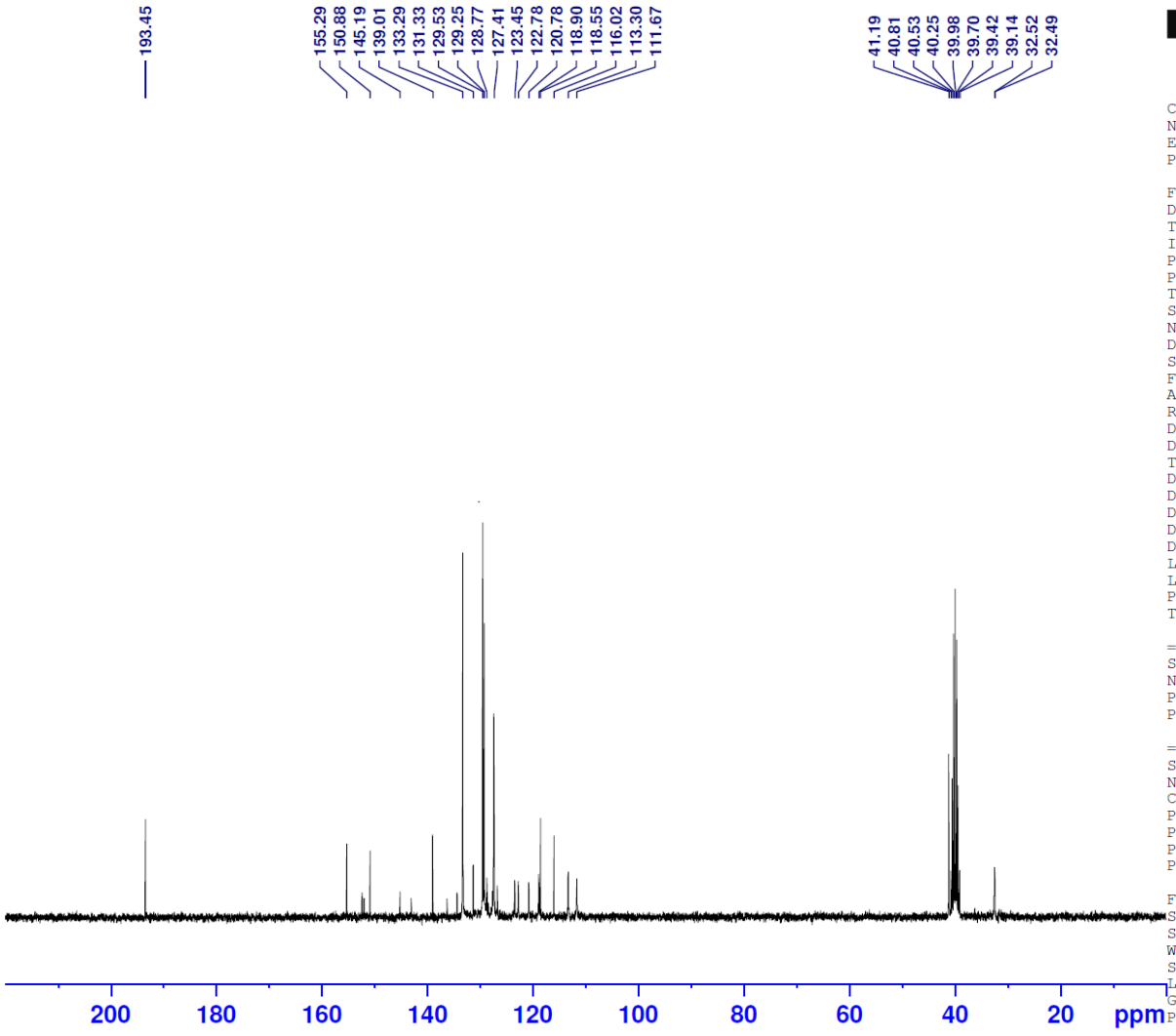
2-(4-(4-Methyl-5-(2-(4-cyanophenyl)-2-oxo-ethylthio)-4H-1,2,4-triazol-3yl)-phenyl)-5(6)-chloro-1H-benzoimidazole (3a)



13C, TU-22, DMSO, 298K



Current Data Parameters
NAME yusuf ozka
EXPNO 295
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160516
Time 14.45
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 297.9 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

Data File: C:\LabSolutions\Data\Analiz\uac\TU-22_34.lcd

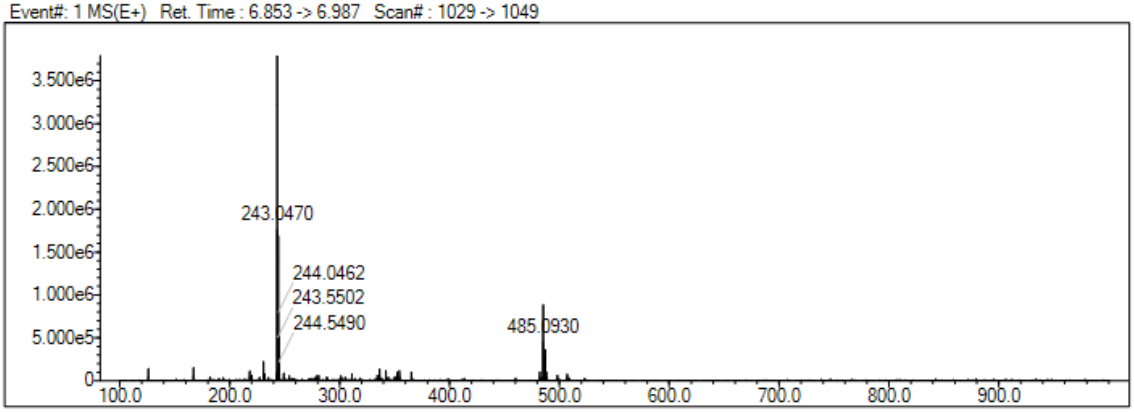
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	9	40	O	2	1	2	S	2	0	2	Ru	2	0	0	H
C	4	11	35	F	1	0	0	Cl	1	0	1	I	3	0	0	
N	3	0	6	P	3	0	0	Br	1	0	1					

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

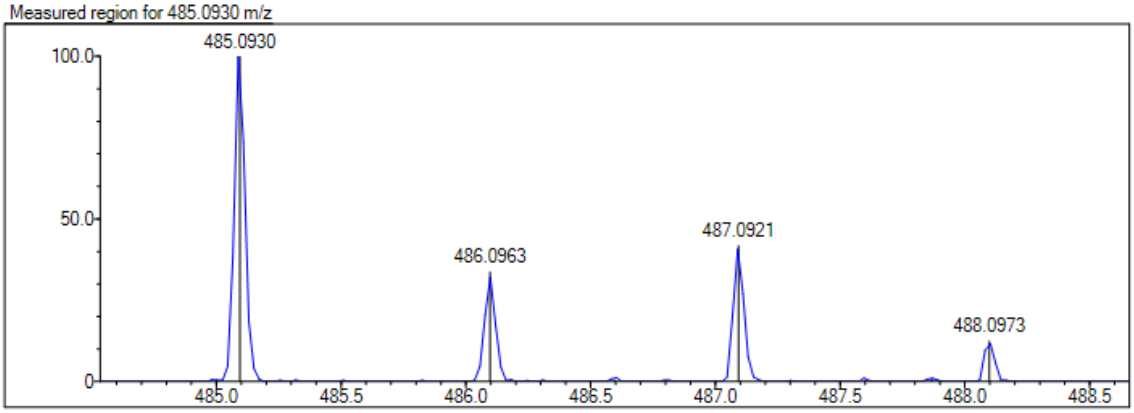
DBE Range: 17.0 - 20.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

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

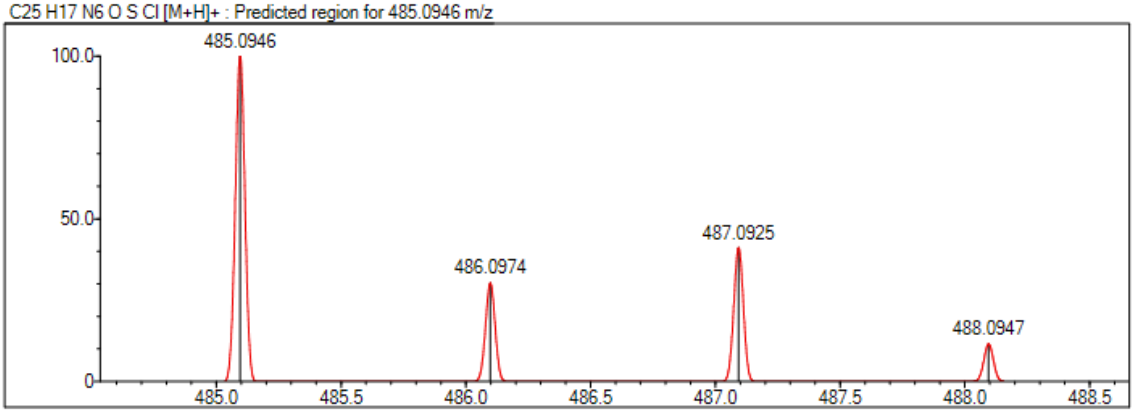
Event#: 1 MS(E+) Ret. Time : 6.853 -> 6.987 Scan# : 1029 -> 1049



Measured region for 485.0930 m/z

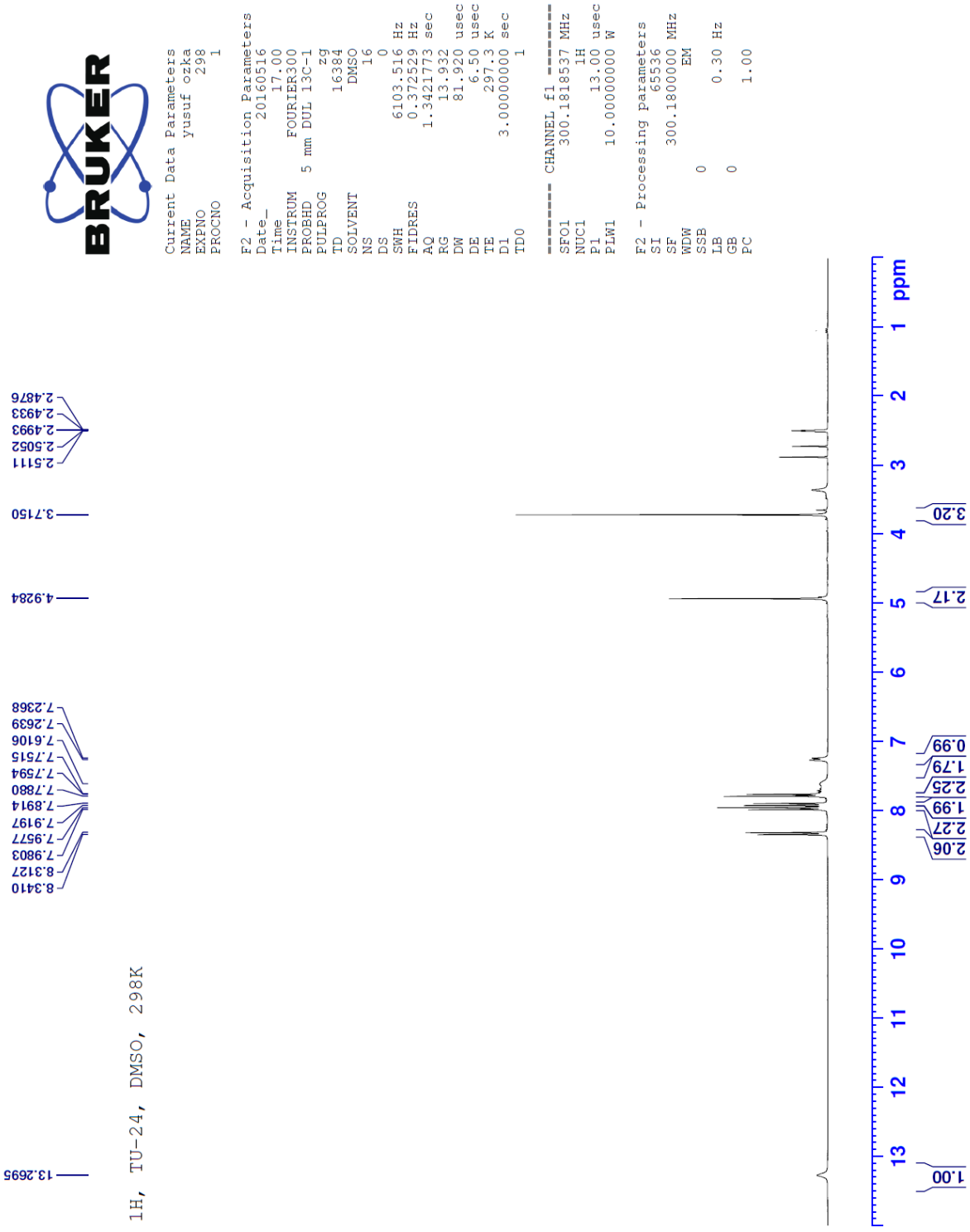


C25 H17 N6 O S Cl [M+H]+ : Predicted region for 485.0946 m/z

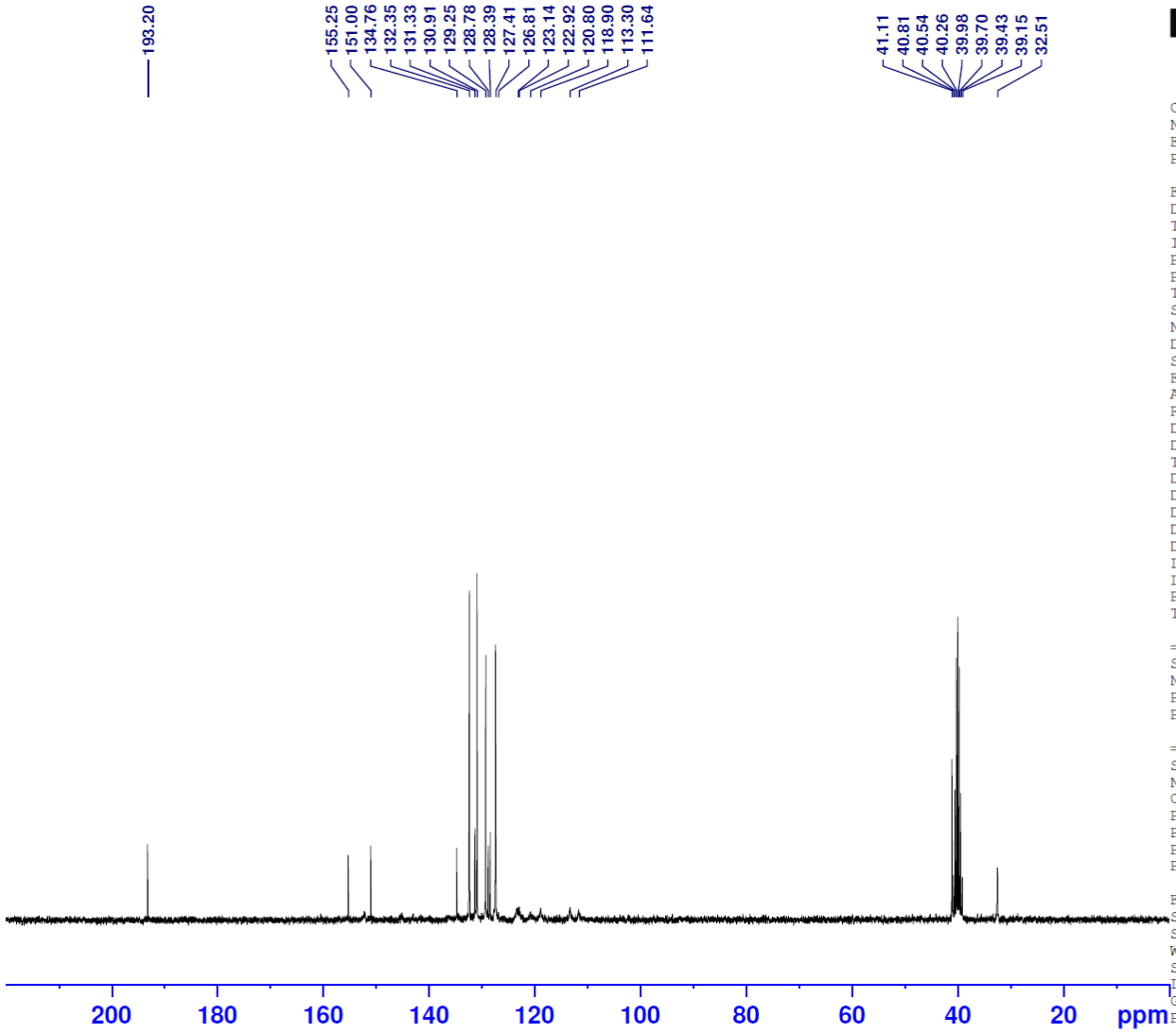


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	72.38	C25 H17 N6 O S Cl	[M+H]+	485.0930	485.0946	-1.6	-3.30	76.80	20.0

2-(4-(4-Methyl-5-(2-(4-bromophenyl)-2-oxo-ethylthio)-4H-1,2,4-triazol-3yl)-phenyl)-5(6)-chloro-1H-benzimidazole (3b)



13C, TU-24, DMSO, 298K



Current Data Parameters
NAME yusuf ozka
EXPNO 299
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160516
Time 17.01
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

Data File: C:\LabSolutions\Data\Analiz\uac\TU-24_36.lcd

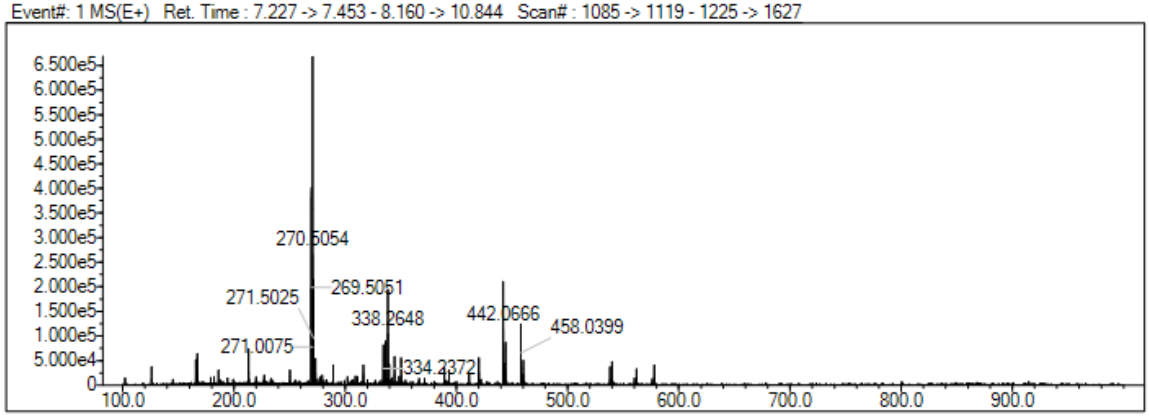
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	9	40	O	2	1	2	S	2	0	2	Ru	2	0	0	H
C	4	11	35	F	1	0	0	Cl	1	0	1	I	3	0	0	
N	3	0	6	P	3	0	0	Br	1	0	1					

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

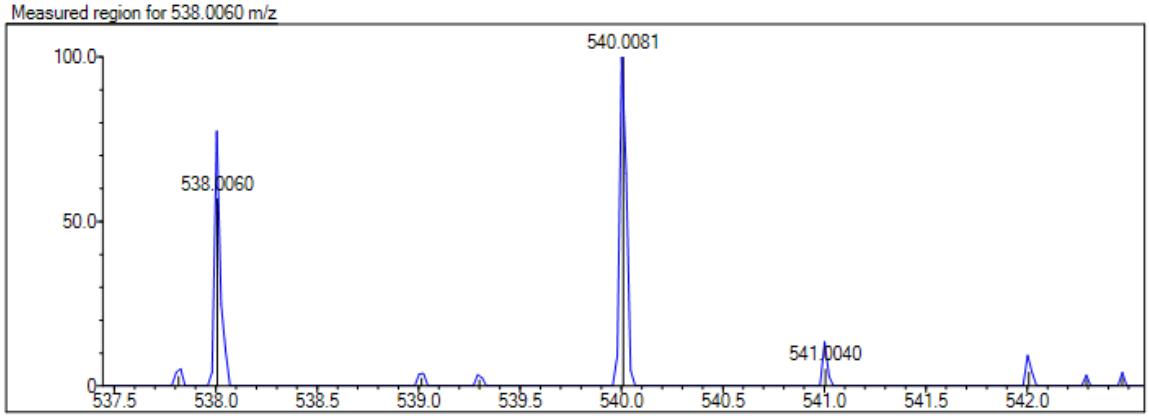
DBE Range: 17.0 - 20.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

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

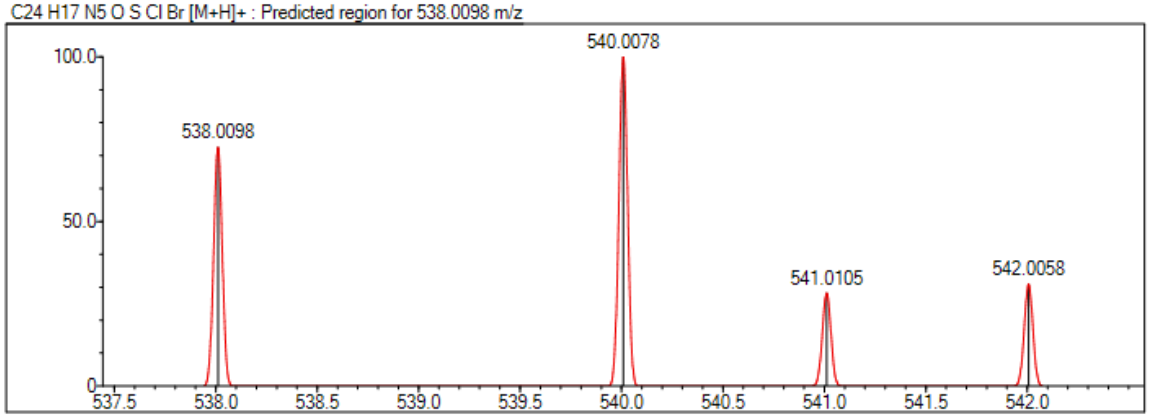
Event#: 1 MS(E+) Ret. Time : 7.227 -> 7.453 - 8.160 -> 10.844 Scan# : 1085 -> 1119 - 1225 -> 1627



Measured region for 538.0060 m/z

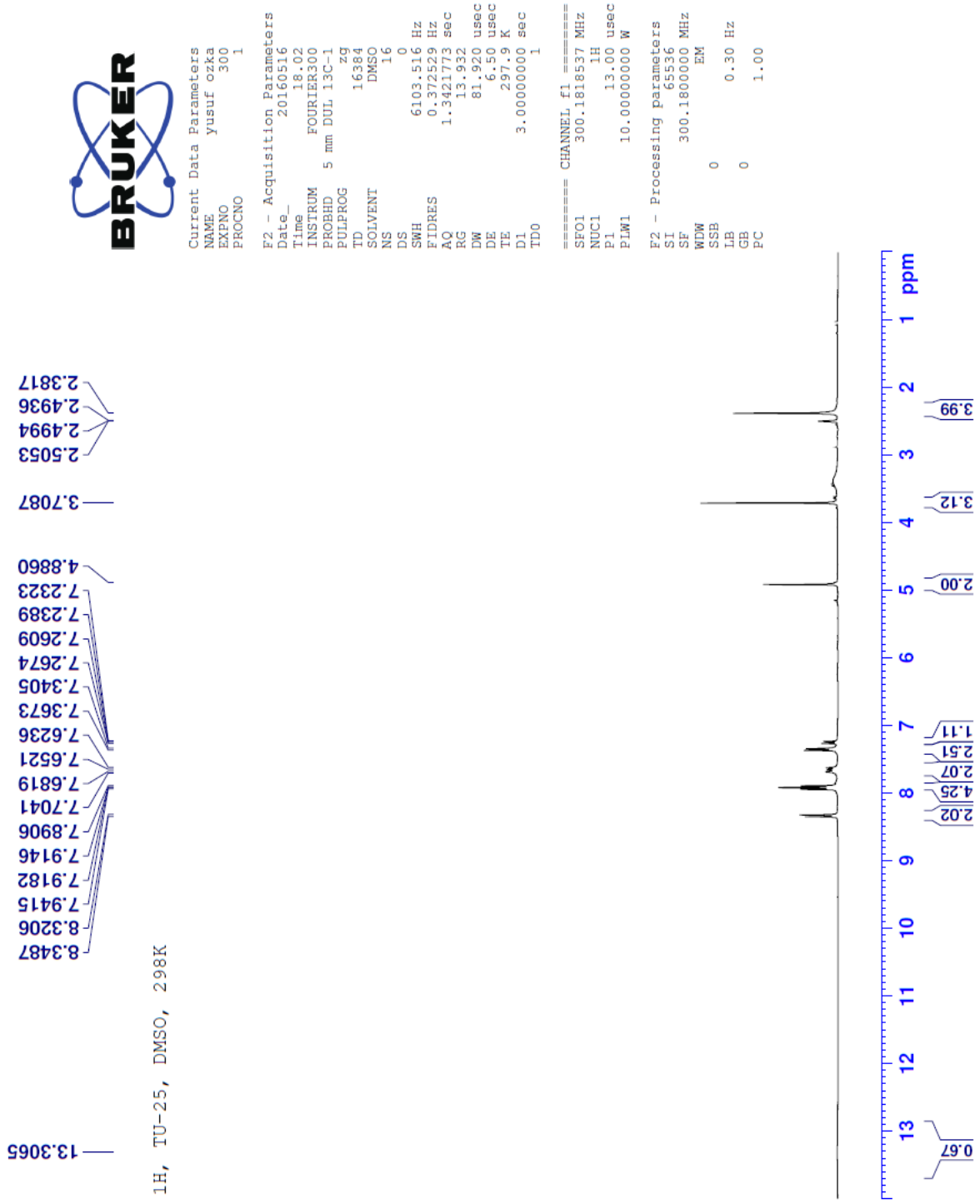


C24 H17 N5 O S Cl Br [M+H]+ : Predicted region for 538.0098 m/z

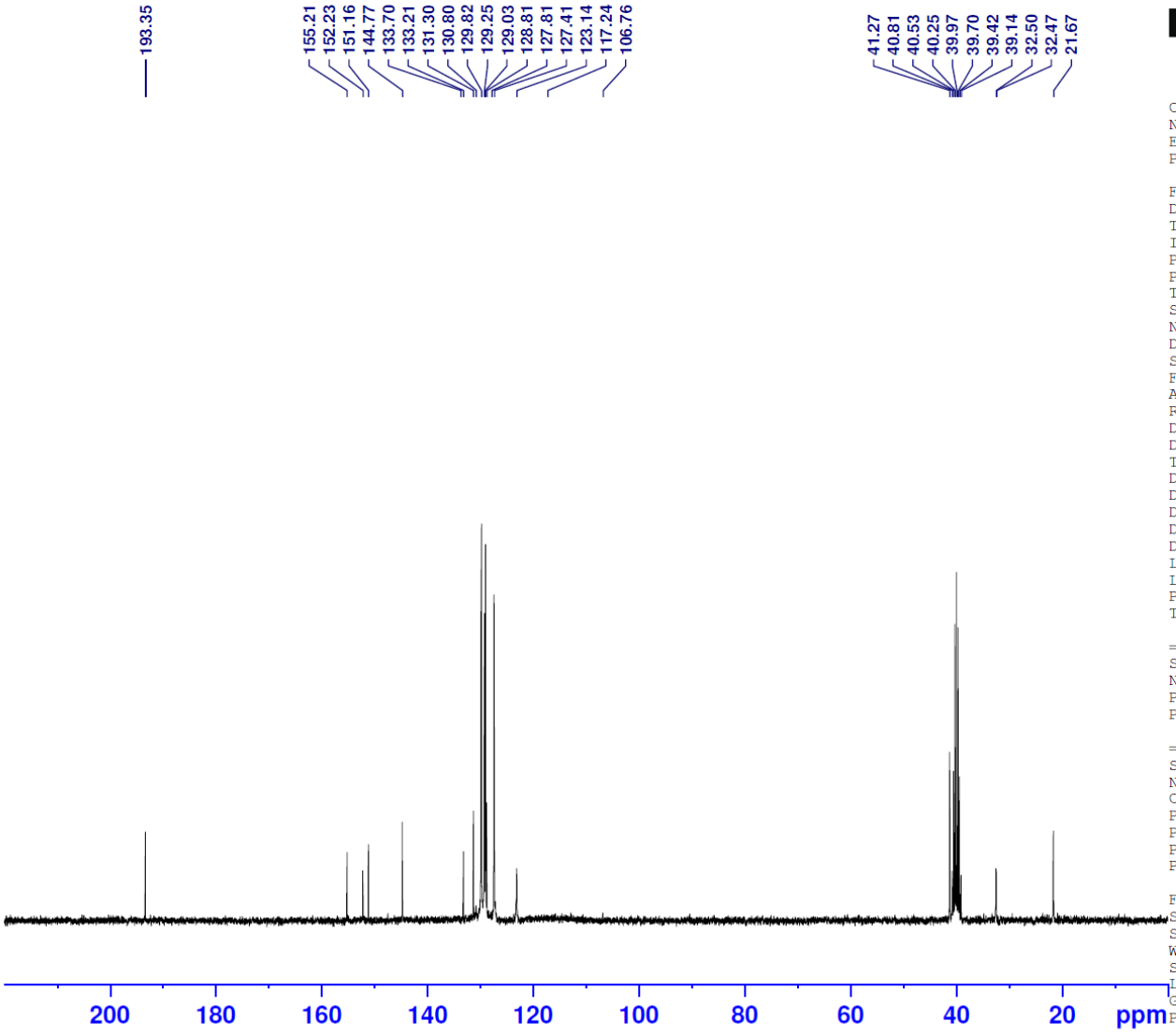


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	22.67	C24 H17 N5 O S Cl Br	[M+H]+	538.0060	538.0098	-3.8	-7.06	32.66	18.0

2-(4-(4-Methyl-5-(2-(4-methylphenyl)-2-oxo-ethylthio)-4H-1,2,4-triazol-3yl)-phenyl)-5(6)-chloro-1H-benzimidazole (3c)



13C, TU-25, DMSO, 298K



BRUKER

```
Current Data Parameters
NAME          yusuf ozka
EXPNO                301
PROCNO                 1

F2 - Acquisition Parameters
Date_           20160516
Time               18.04
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                297.9 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
```

Data File: C:\LabSolutions\Data\Analiz\uac\TU-25_37.lcd

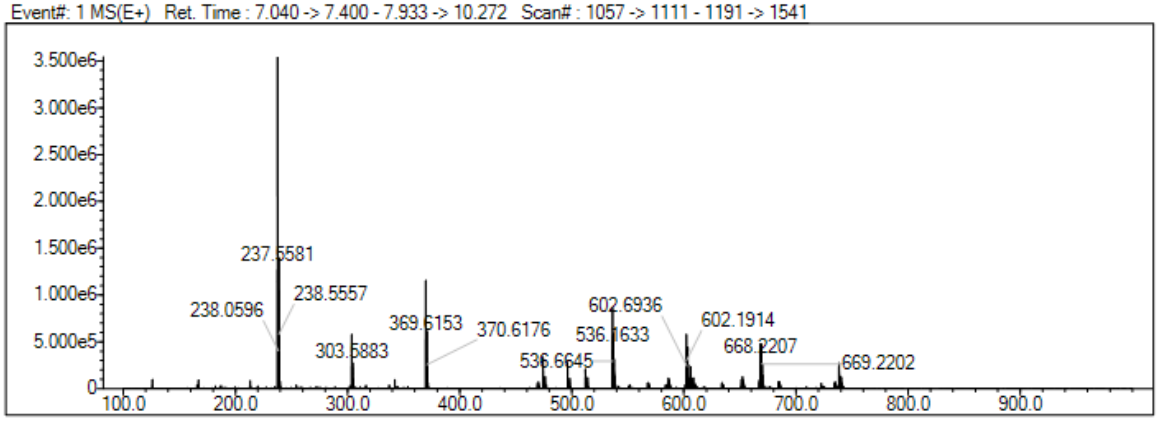
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	9	40	O	2	1	2	S	2	0	2	Ru	2	0	0	H
C	4	11	35	F	1	0	0	Cl	1	0	1	I	3	0	0	
N	3	0	6	P	3	0	0	Br	1	0	1					

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

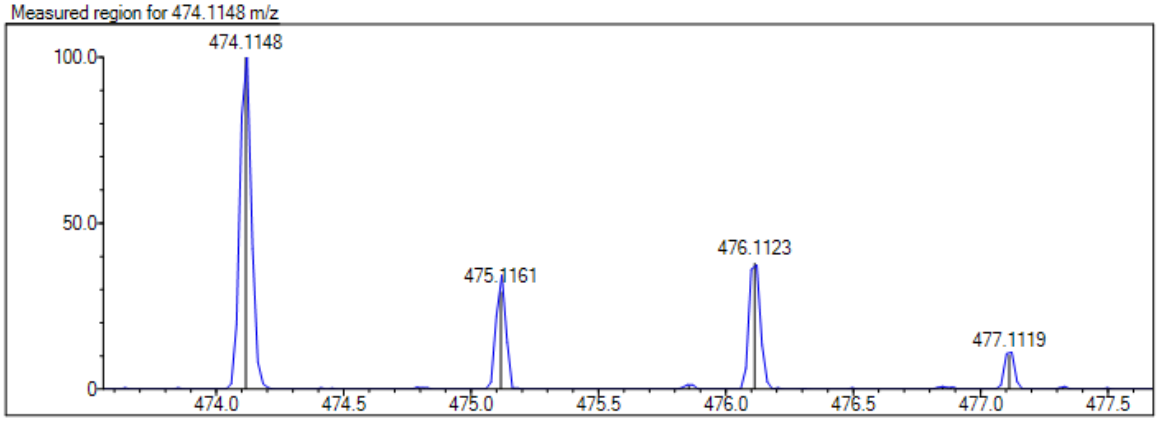
DBE Range: 17.0 - 20.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

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

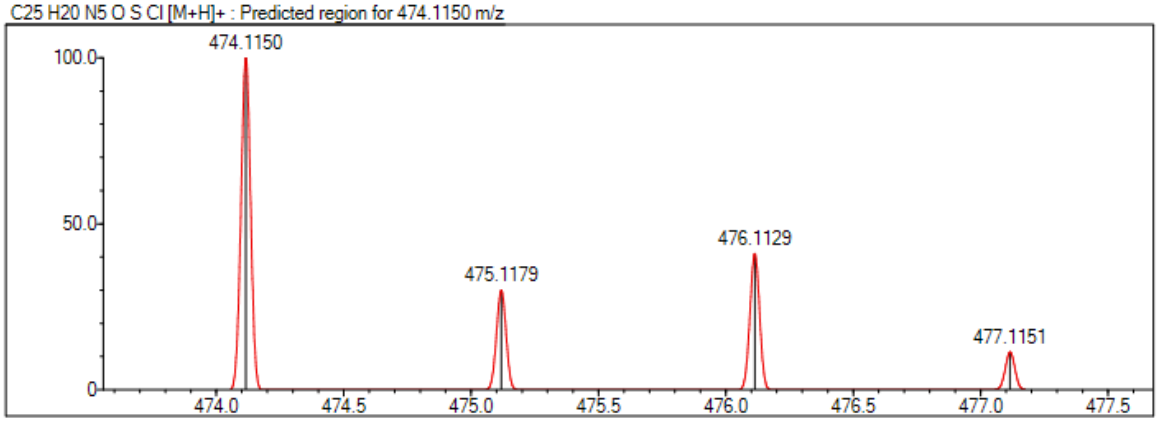
Event#: 1 MS(E+) Ret. Time : 7.040 -> 7.400 - 7.933 -> 10.272 Scan# : 1057 -> 1111 - 1191 -> 1541



Measured region for 474.1148 m/z

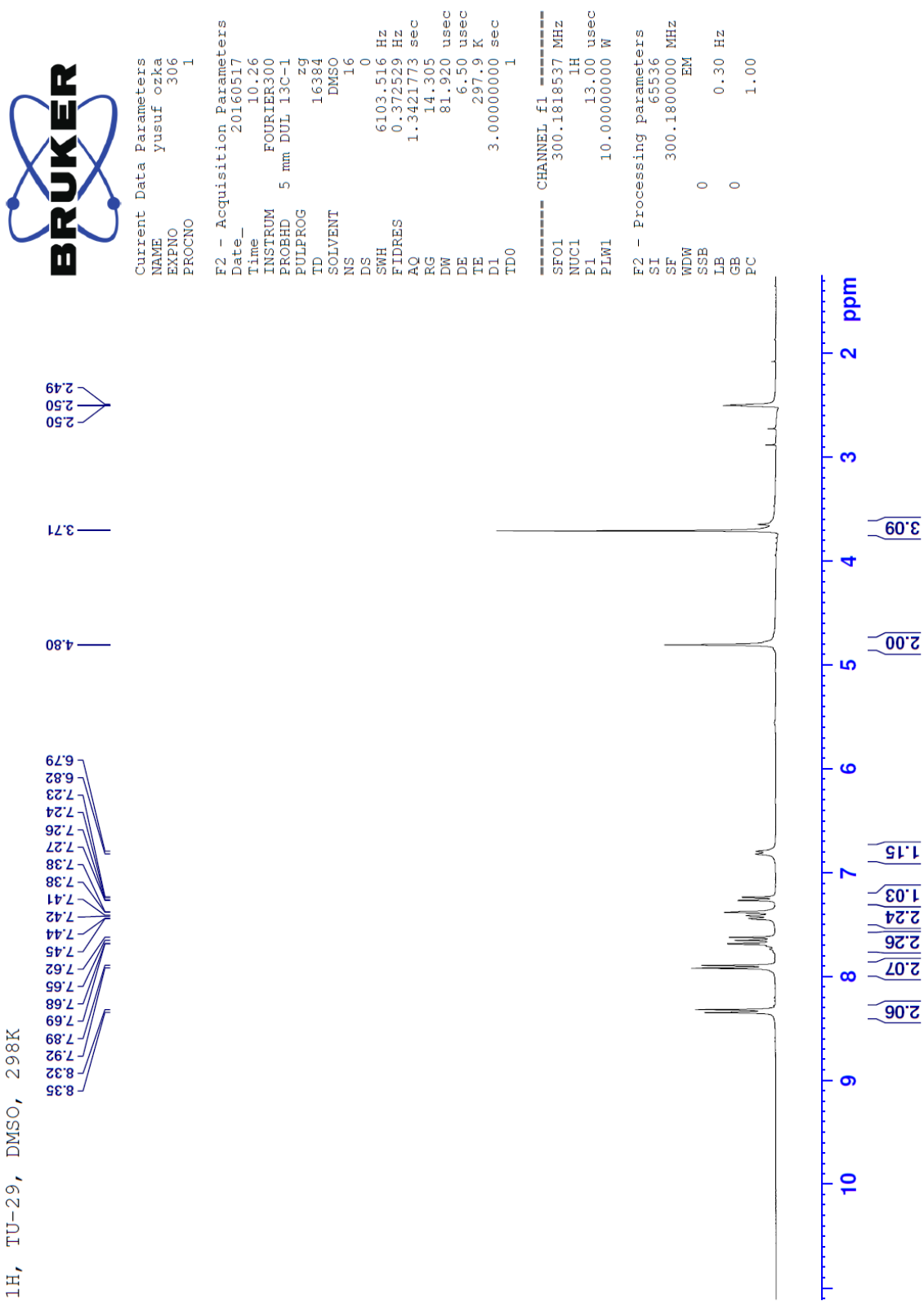


C25 H20 N5 O S Cl [M+H]+ : Predicted region for 474.1150 m/z

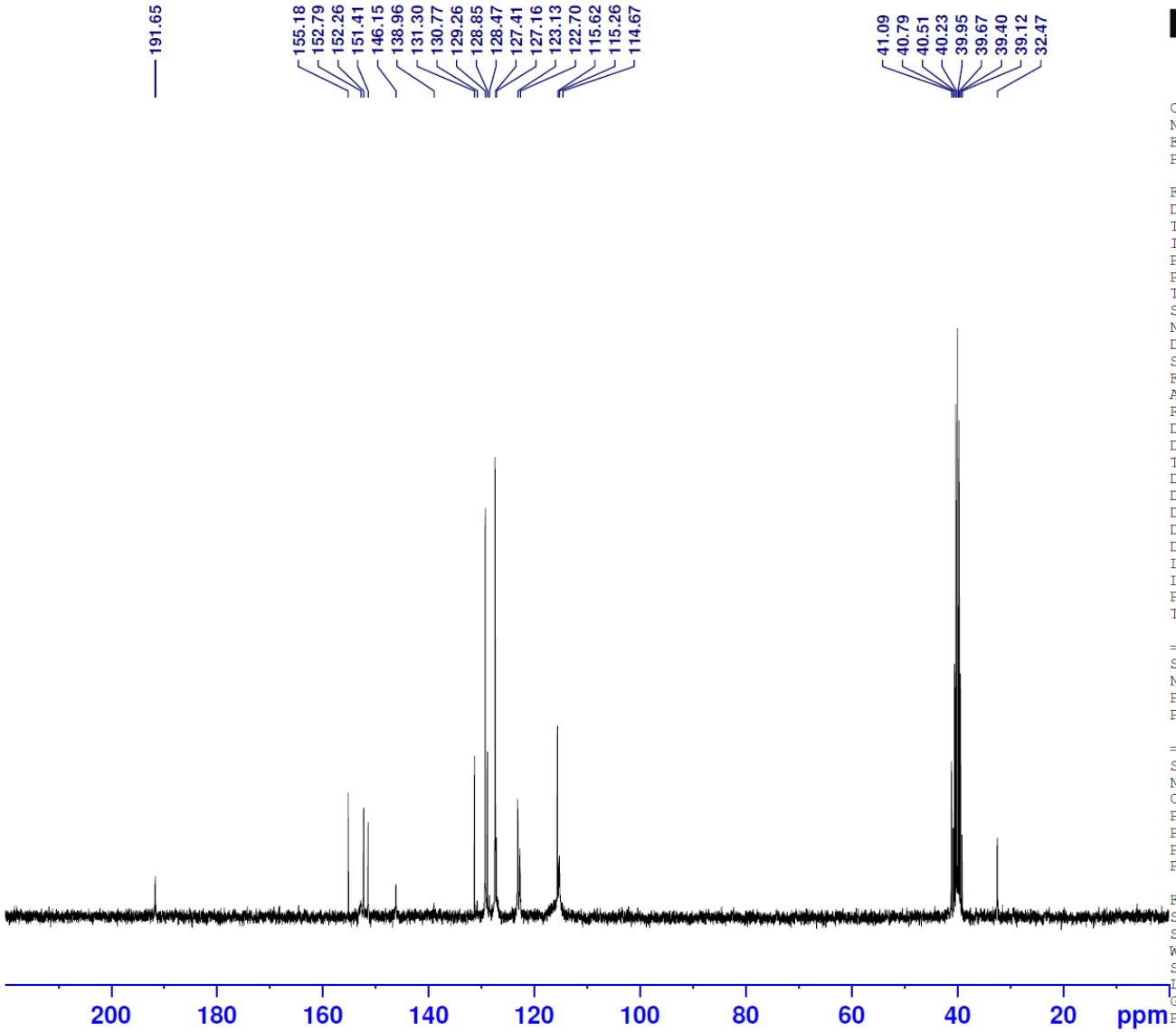


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	88.86	C25 H20 N5 O S Cl	[M+H]+	474.1148	474.1150	-0.2	-0.42	88.86	18.0

2-(4-(4-Methyl-5-(2-(3,4-dihydroxyphenyl)-2-oxo-ethylthio)-4H-1,2,4-triazol-3yl)-phenyl)-5(6)-chloro-1H- benzimidazole (3d)



13C, TU-29, DMSO, 298K




```
Current Data Parameters
NAME          yusuf ozka
EXPNO                307
PROCNO                 1

F2 - Acquisition Parameters
Date_           20160517
Time               10.28
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
```

Data File: C:\LabSolutions\Data\Analiz\uac\TU-29_42.lcd

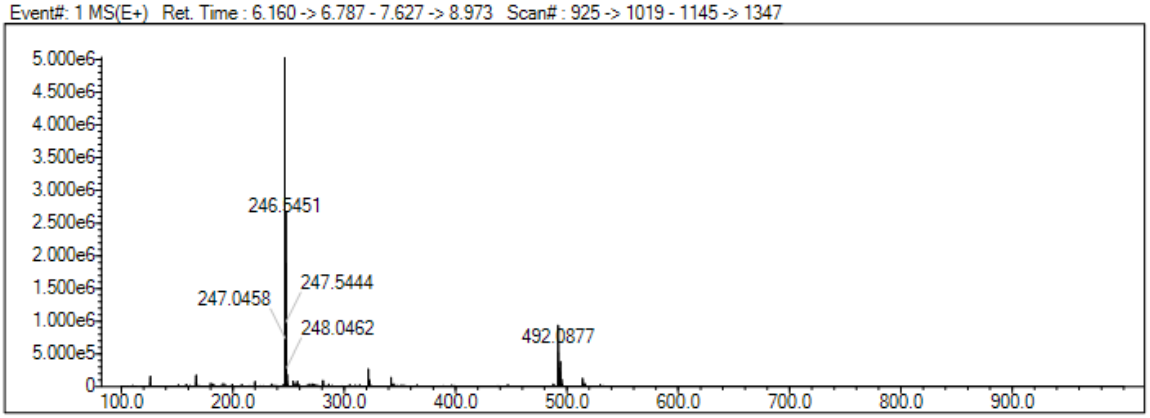
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	9	40	O	2	3	3	S	2	0	2	Ru	2	0	0	H
C	4	11	35	F	1	0	0	Cl	1	0	1	I	3	0	0	
N	3	0	6	P	3	0	0	Br	1	0	1					

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

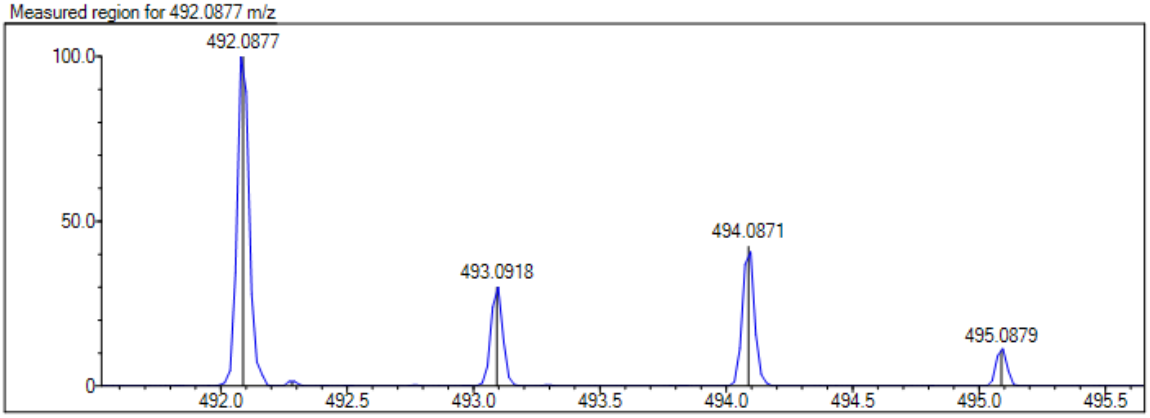
DBE Range: 17.0 - 20.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

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

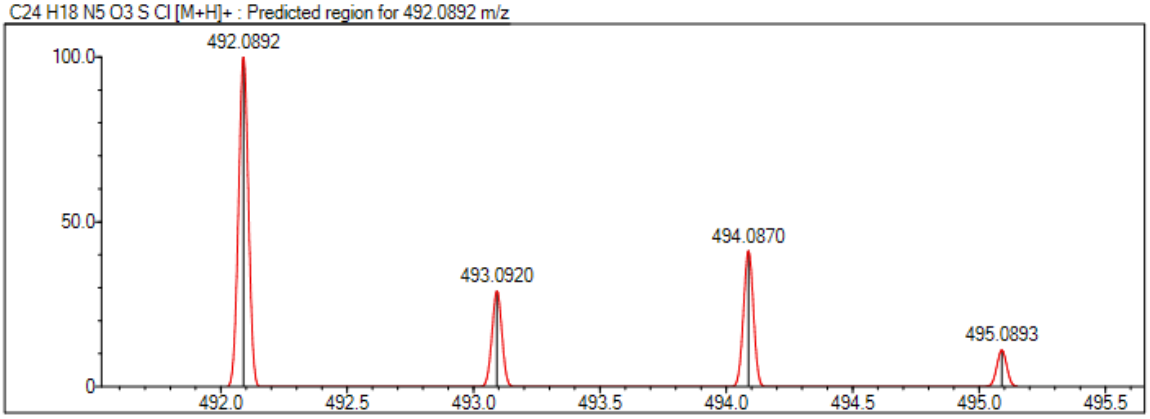
Event#: 1 MS(E+) Ret. Time : 6.160 -> 6.787 - 7.627 -> 8.973 Scan# : 925 -> 1019 - 1145 -> 1347



Measured region for 492.0877 m/z

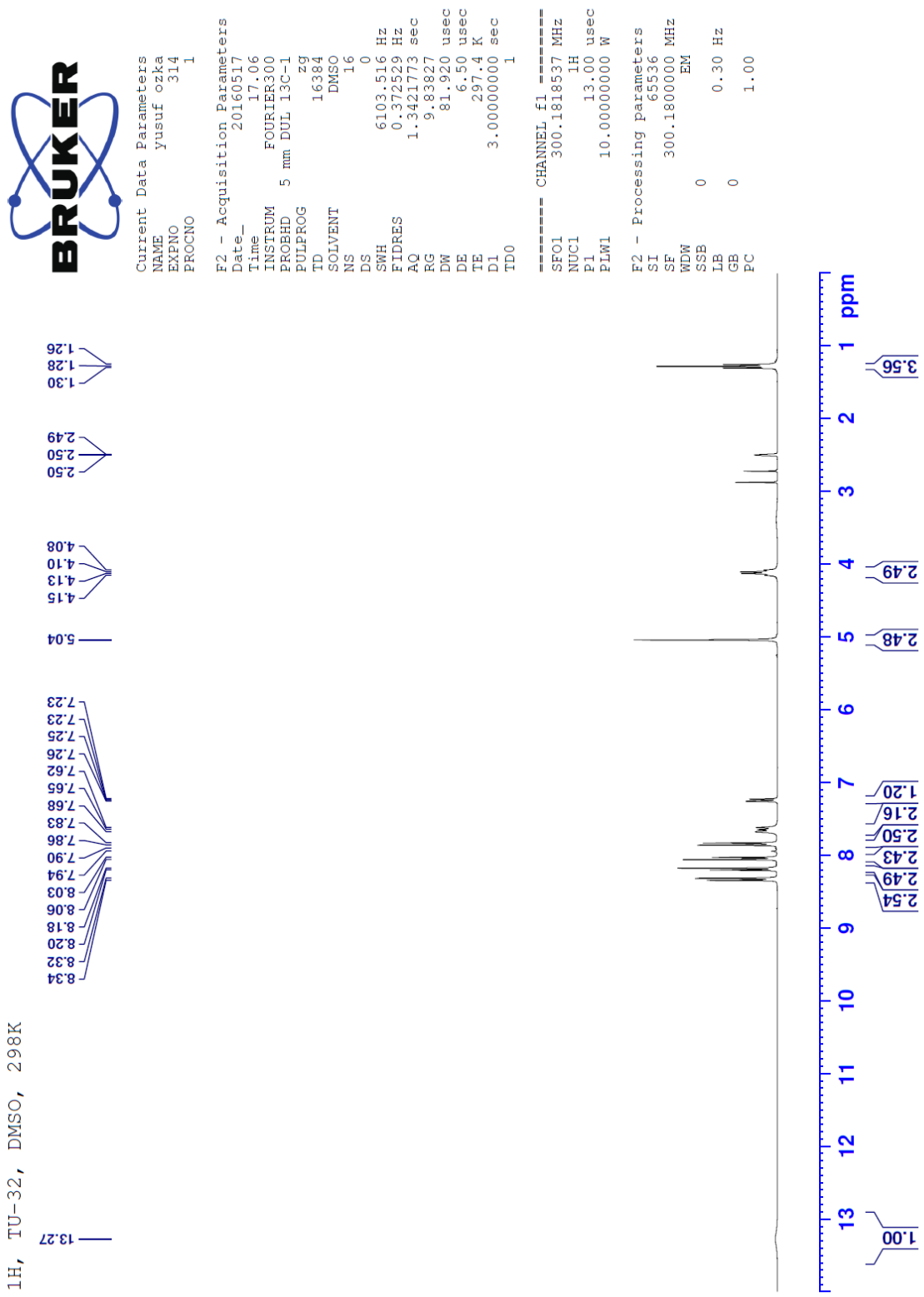


C24 H18 N5 O3 S Cl [M+H]+ : Predicted region for 492.0892 m/z

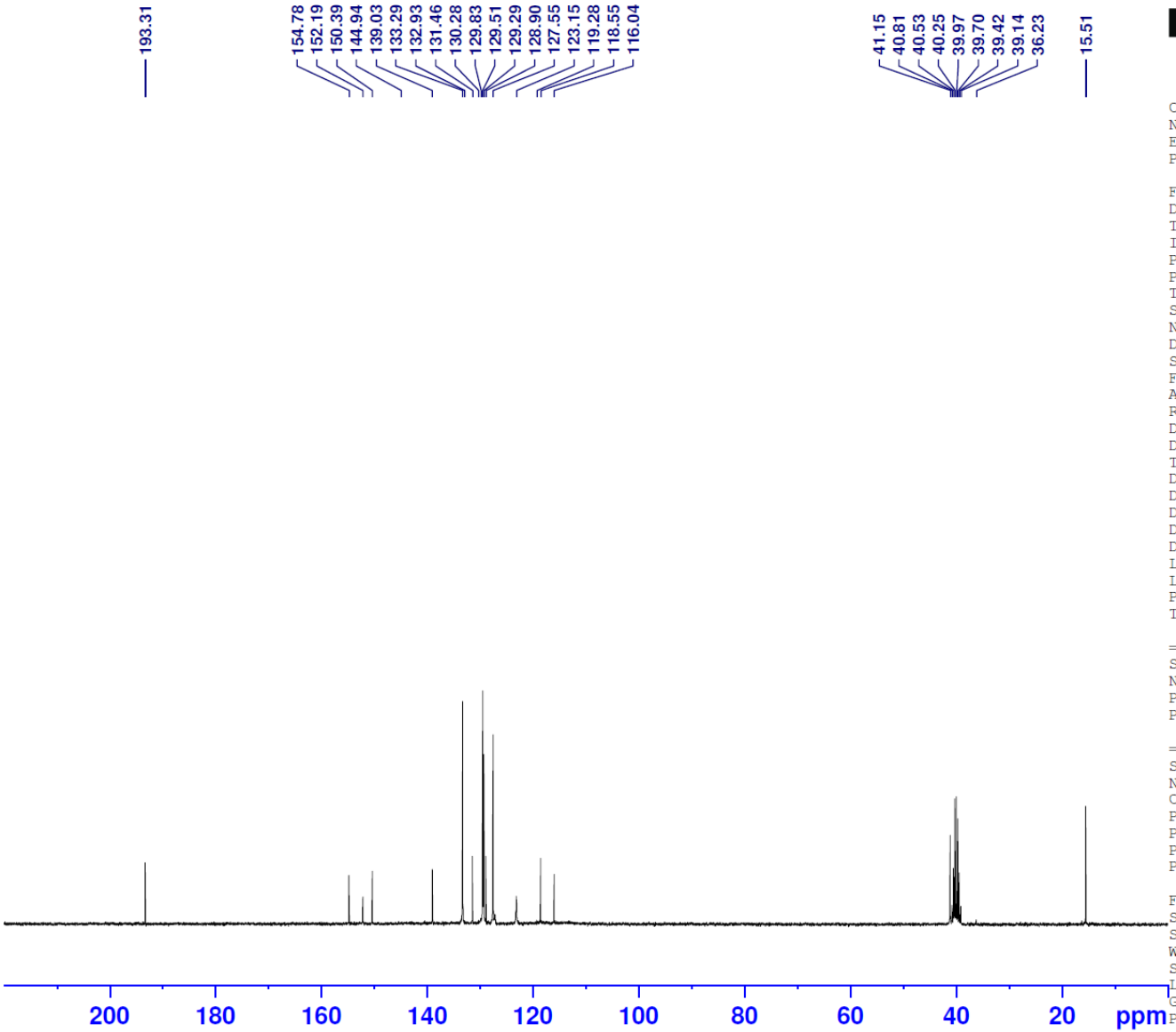


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	88.95	C24 H18 N5 O3 S Cl	[M+H]+	492.0877	492.0892	-1.5	-3.05	93.75	18.0

2-(4-(4-Ethyl-5-(2-(4-cyanophenyl)-2-oxo-ethylthio)-4H-1,2,4-triazol-3yl)-phenyl)-5(6)-chloro-1H-benzoimidazole (3e)



13C, TU-32, DMSO, 298K



Current Data Parameters

NAME	yusuf ozka
EXPNO	315
PROCNO	1

F2 - Acquisition Parameters

Date_	20160517
Time	17.08
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	297.9 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

Data File: C:\LabSolutions\Data\Analiz\uac\TU-32_46.lcd

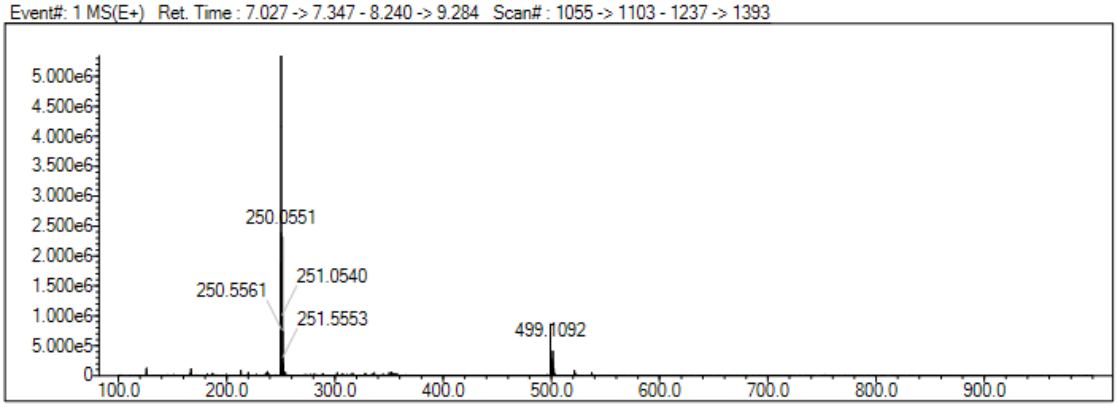
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	9	40	O	2	1	1	S	2	0	2	Ru	2	0	0	H
C	4	11	26	F	1	0	0	Cl	1	0	1	I	3	0	0	
N	3	0	6	P	3	0	0	Br	1	0	1					

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

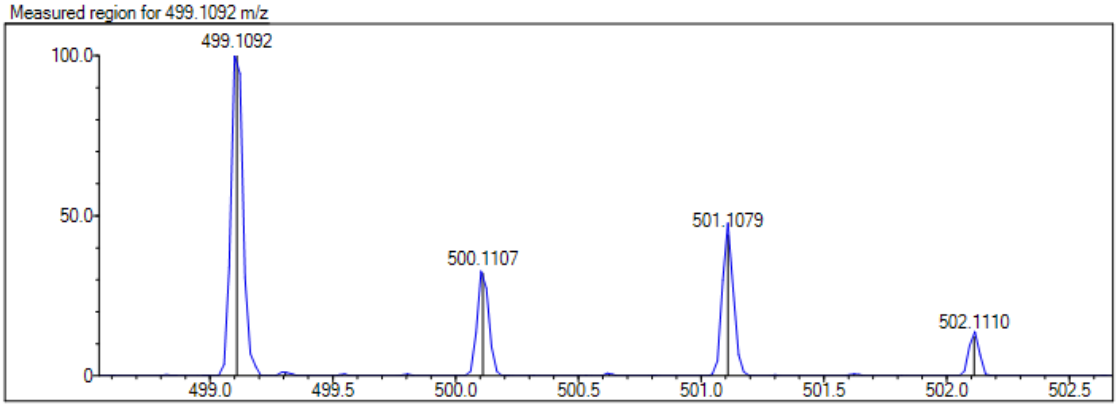
DBE Range: 17.0 - 20.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

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

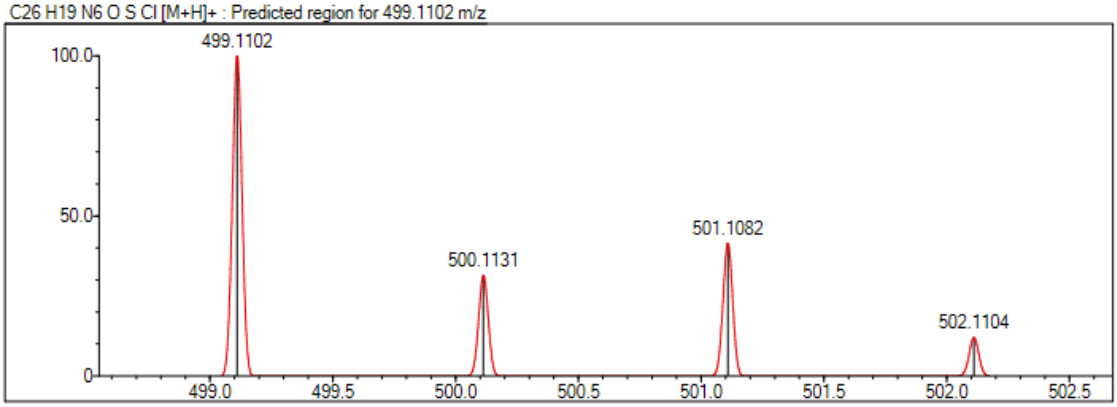
Event#: 1 MS(E+) Ret. Time : 7.027 -> 7.347 - 8.240 -> 9.284 Scan# : 1055 -> 1103 - 1237 -> 1393



Measured region for 499.1092 m/z

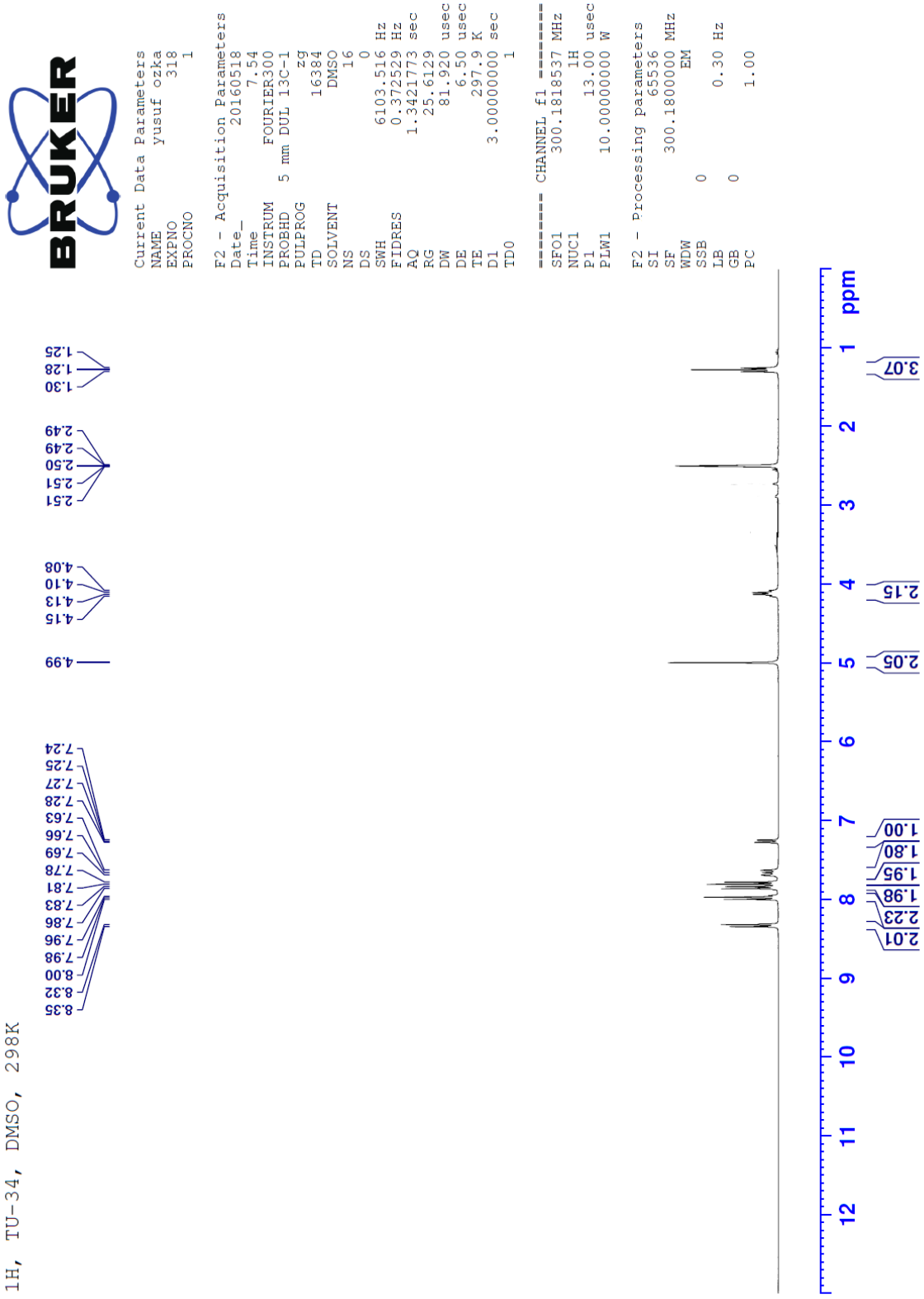


C26 H19 N6 O S Cl [M+H]+ : Predicted region for 499.1102 m/z

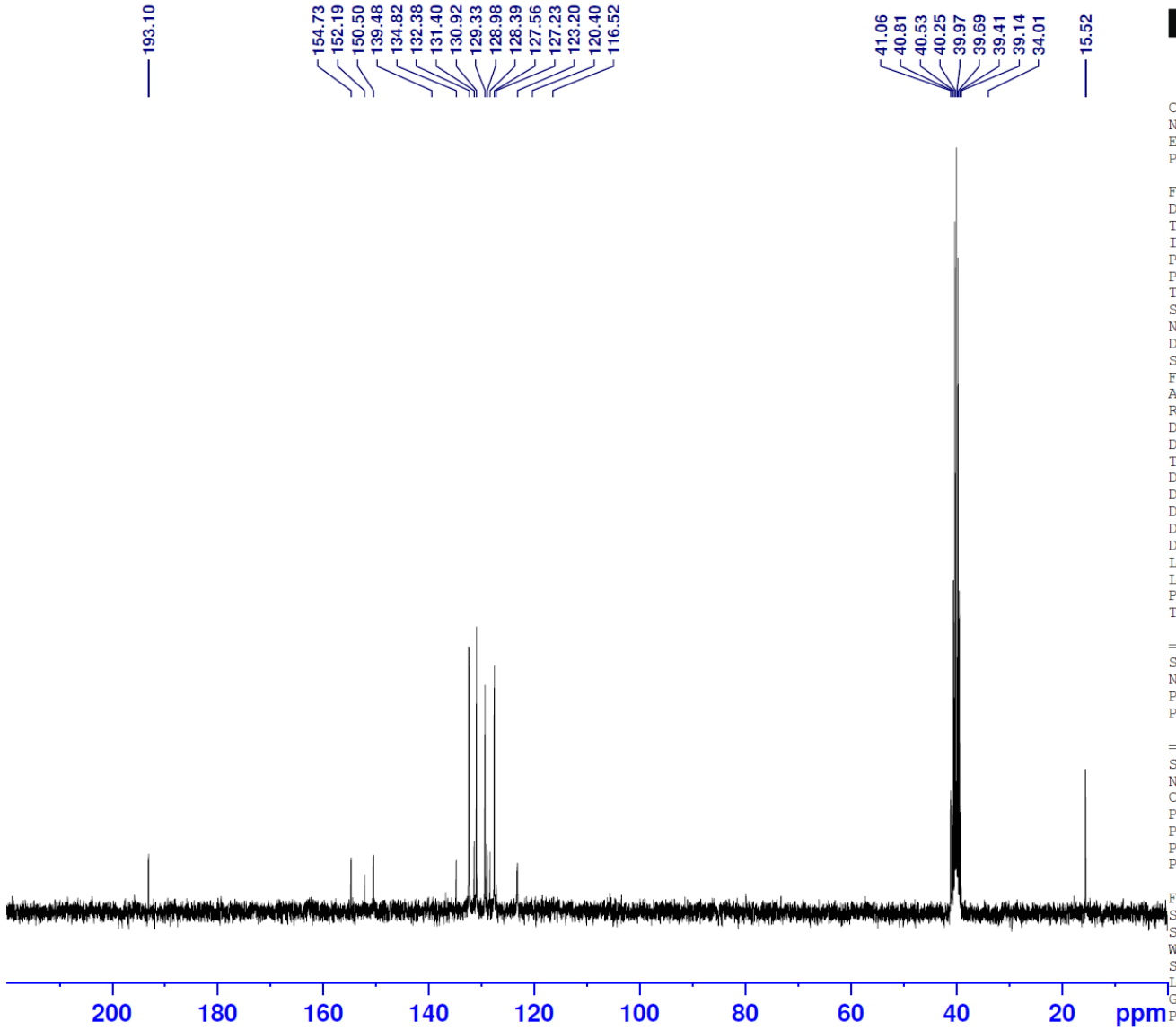


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	86.52	C26 H19 N6 O S Cl	[M+H]+	499.1092	499.1102	-1.0	-2.00	88.74	20.0

2-(4-(4-Ethyl-5-(2-(4-bromophenyl)-2-oxo-ethylthio)-4H-1,2,4-triazol-3yl)-phenyl)-5(6)-chloro-1H-benzimidazole (3f)



13C, TU-34, DMSO, 298K



BRUKER

```
Current Data Parameters
NAME          yusuf ozka
EXPNO                319
PROCNO                 1

F2 - Acquisition Parameters
Date_           20160518
Time                7.56
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
```

Data File: C:\LabSolutions\Data\Analiz\uac\TU-34_48.lcd

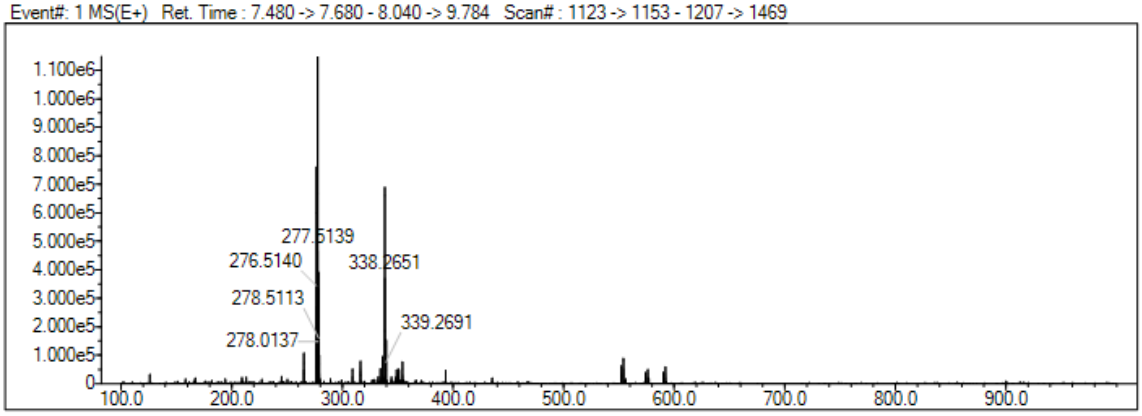
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	9	40	O	2	1	1	S	2	0	2	Ru	2	0	0	H
C	4	11	26	F	1	0	0	Cl	1	0	1	I	3	0	0	
N	3	0	6	P	3	0	0	Br	1	0	1					

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

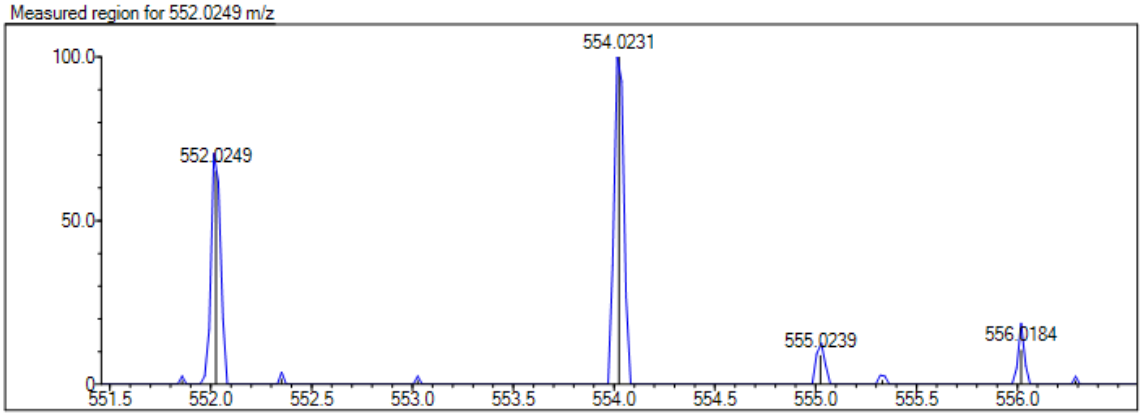
DBE Range: 17.0 - 20.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

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

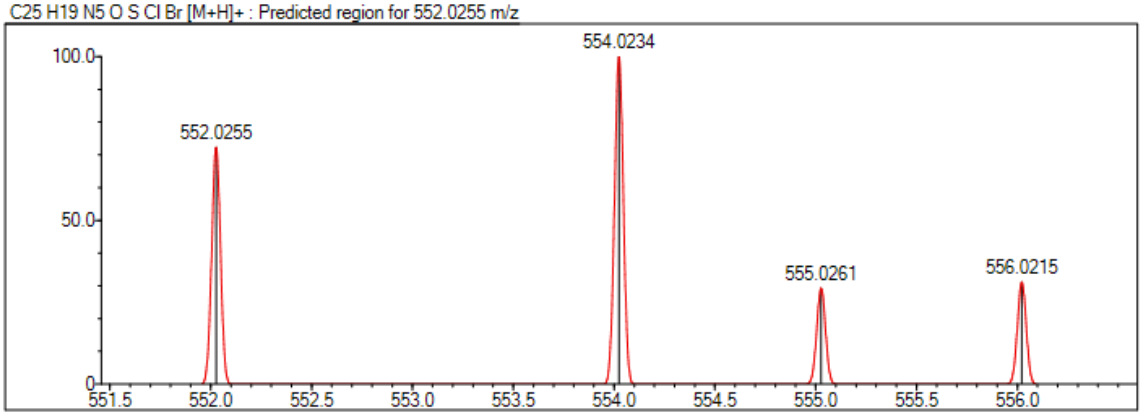
Event#: 1 MS(E+) Ret. Time : 7.480 -> 7.680 - 8.040 -> 9.784 Scan# : 1123 -> 1153 - 1207 -> 1469



Measured region for 552.0249 m/z

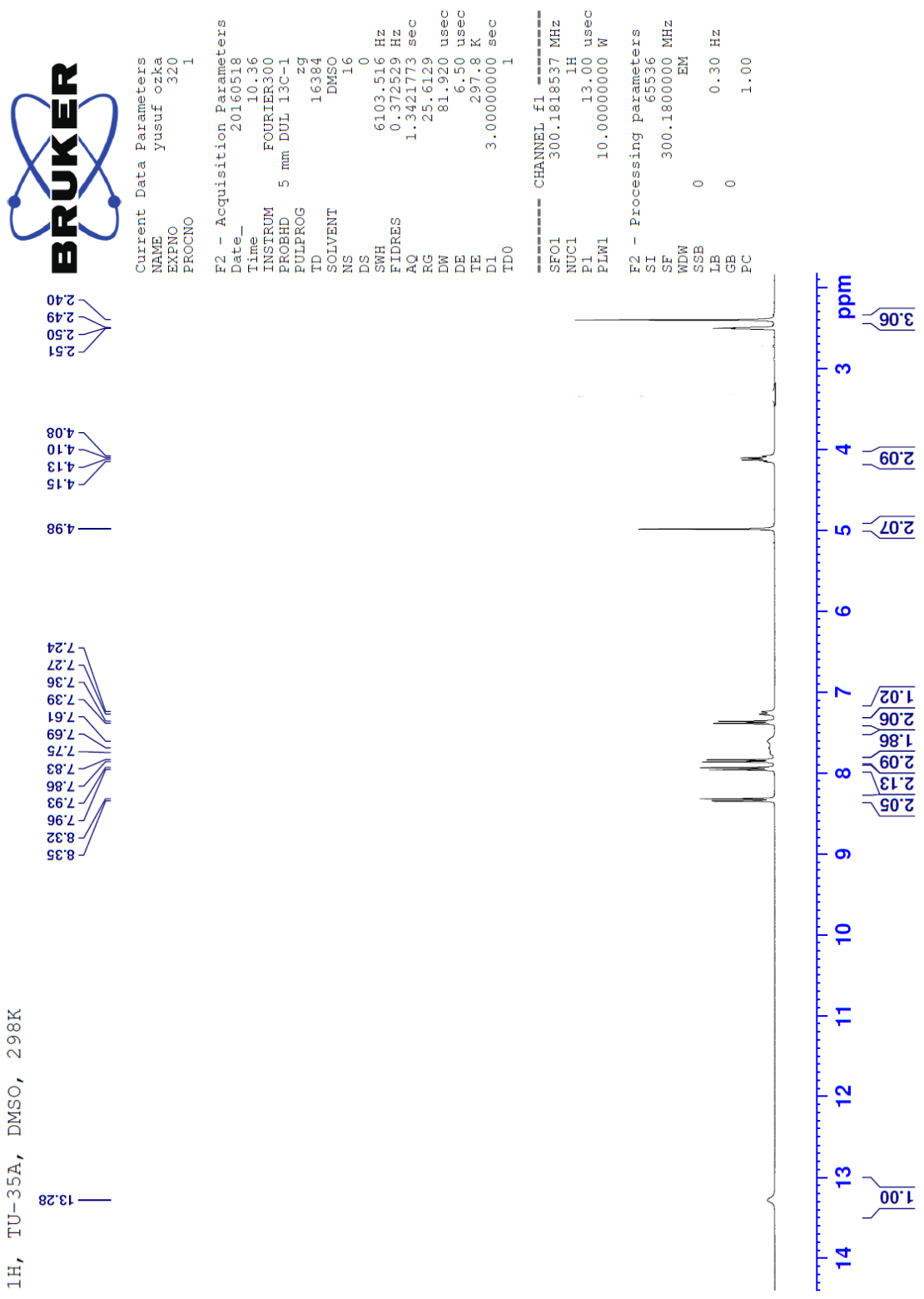


C25 H19 N5 O S Cl Br [M+H]+ : Predicted region for 552.0255 m/z

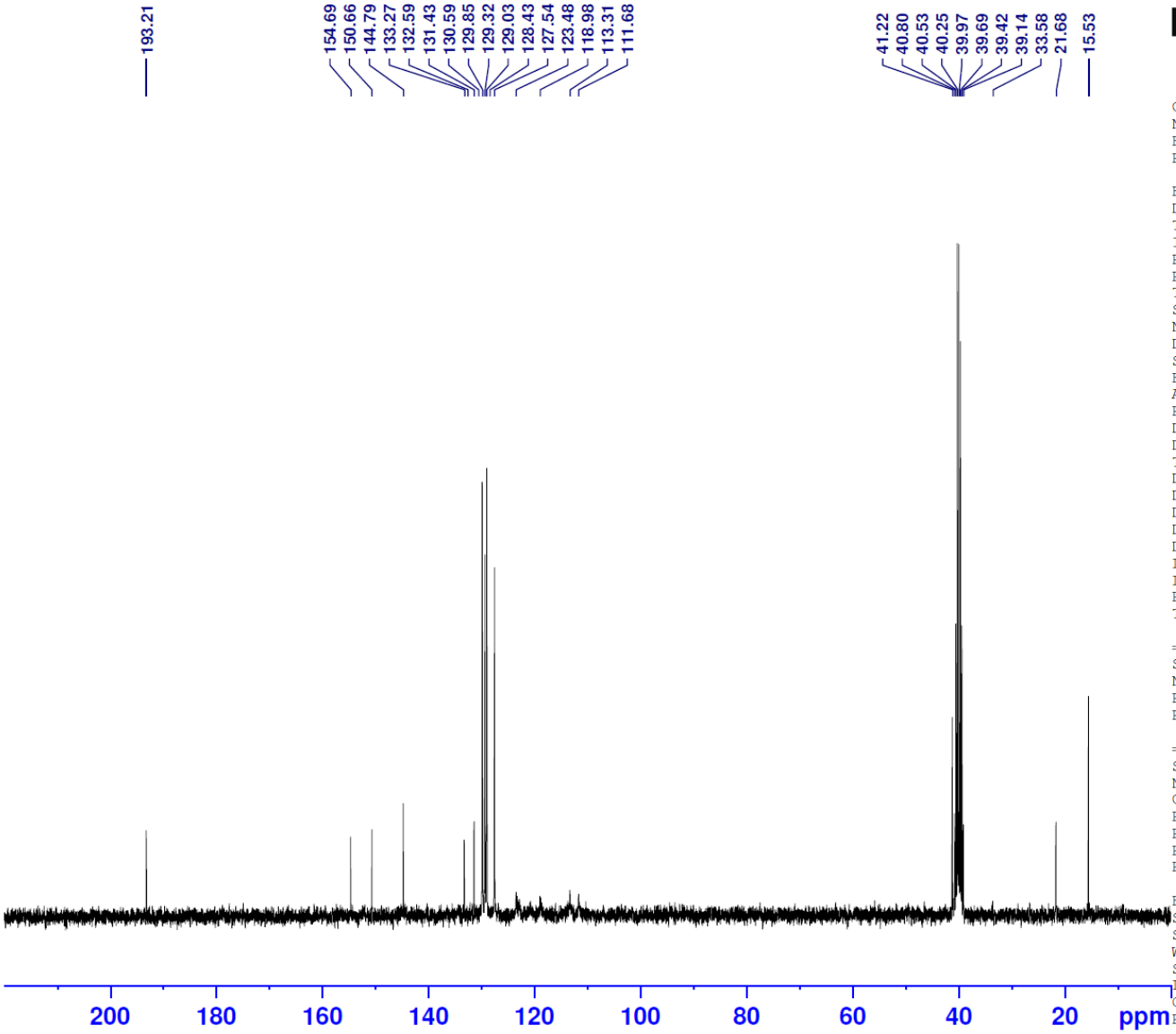


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	54.11	C25 H19 N5 O S Cl Br	[M+H]+	552.0249	552.0255	-0.6	-1.09	54.23	18.0

2-(4-(4-Ethyl-5-(2-(4-methylphenyl)-2-oxo-ethylthio)-4H-1,2,4-triazol-3yl)-phenyl)-5(6)-chloro-1H-benzimidazole (3g)



13C, TU-35A, DMSO, 298K



BRUKER

```
Current Data Parameters
NAME          yusuf ozka
EXPNO                321
PROCNO                 1

F2 - Acquisition Parameters
Date_           20160518
Time               10.38
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               297.9 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
```

Data File: C:\LabSolutions\Data\Analiz\uac\TU-35A_49.lcd

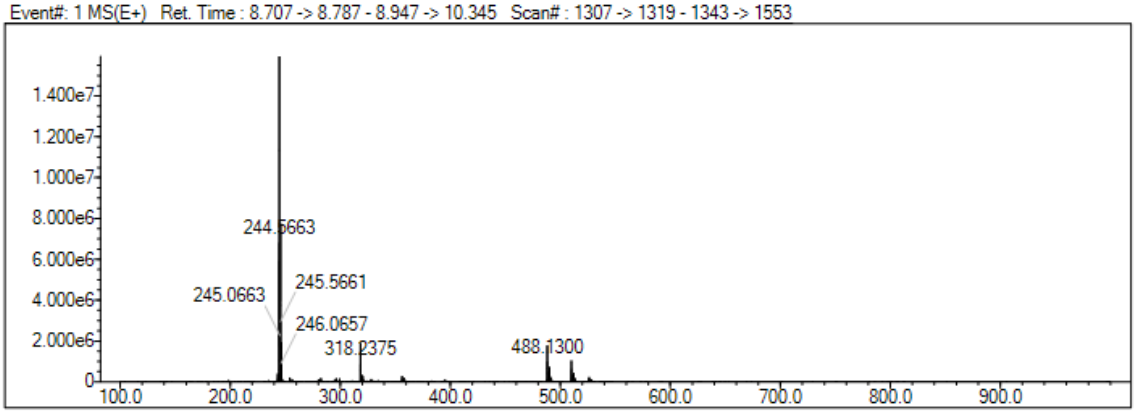
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	9	40	O	2	1	1	S	2	0	2	Ru	2	0	0	H
C	4	11	26	F	1	0	0	Cl	1	0	1	I	3	0	0	
N	3	0	6	P	3	0	0	Br	1	0	1					

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

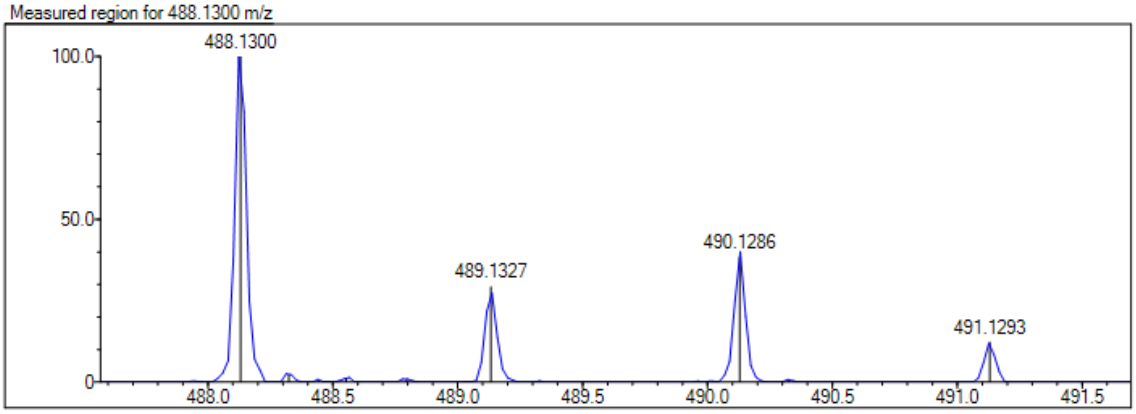
DBE Range: 17.0 - 20.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

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

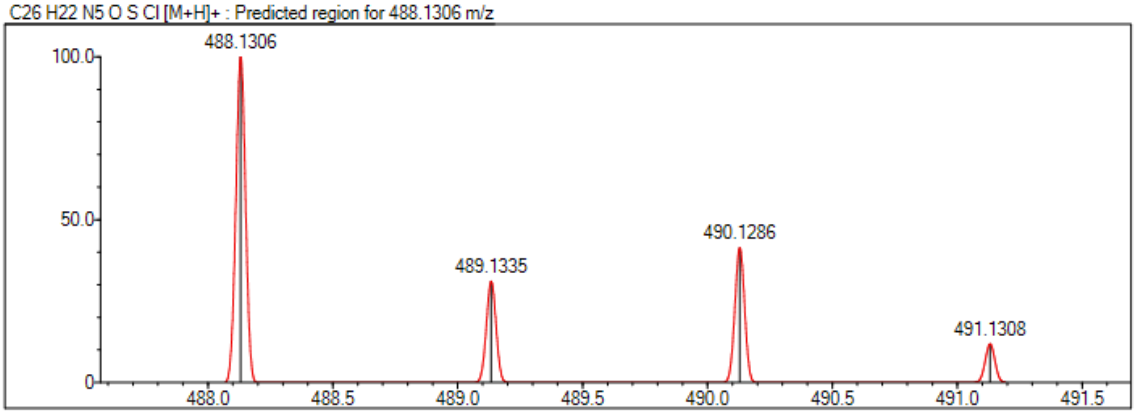
Event#: 1 MS(E+) Ret. Time : 8.707 -> 8.787 - 8.947 -> 10.345 Scan# : 1307 -> 1319 - 1343 -> 1553



Measured region for 488.1300 m/z

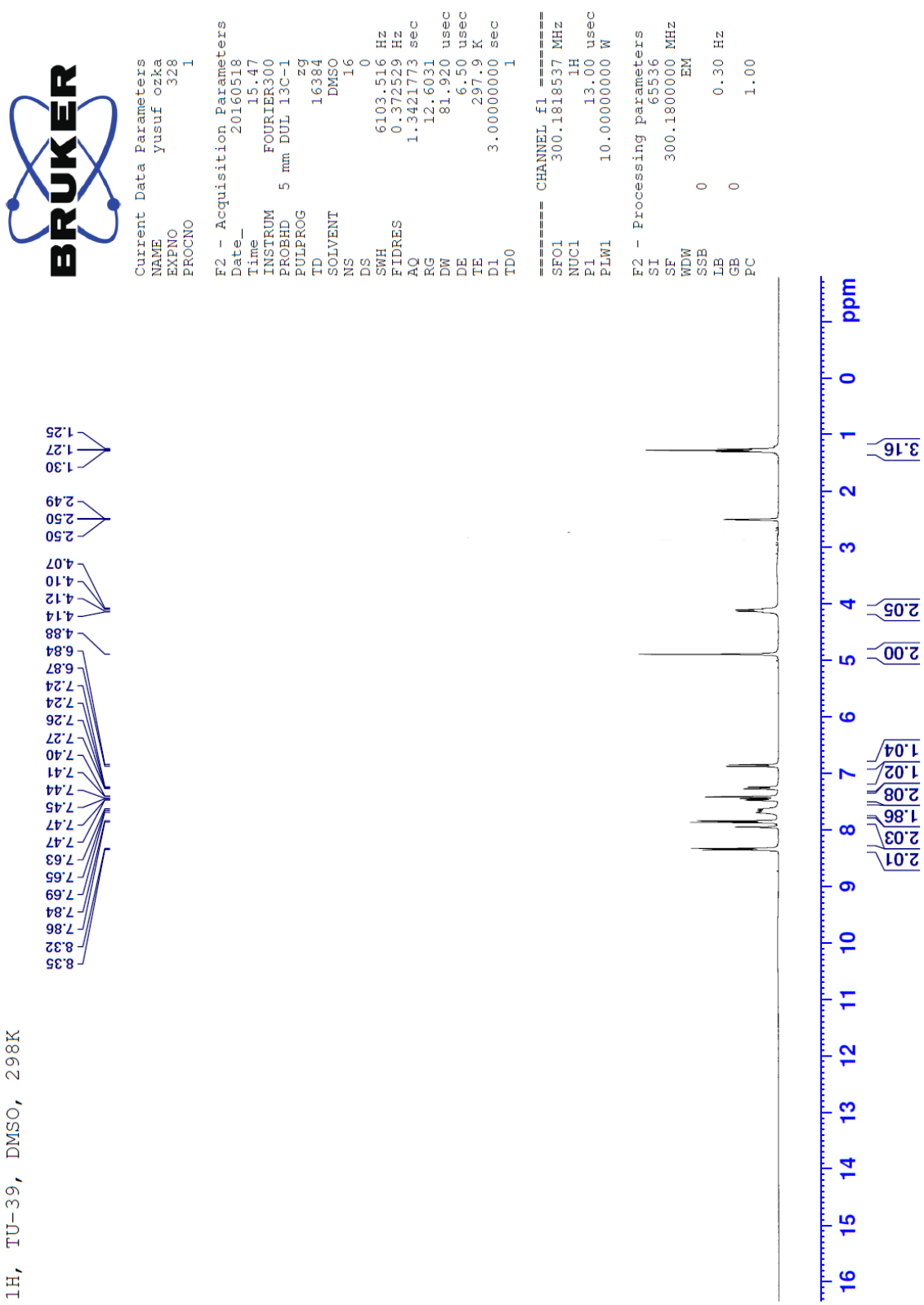


C26 H22 N5 O S Cl [M+H]+ : Predicted region for 488.1306 m/z

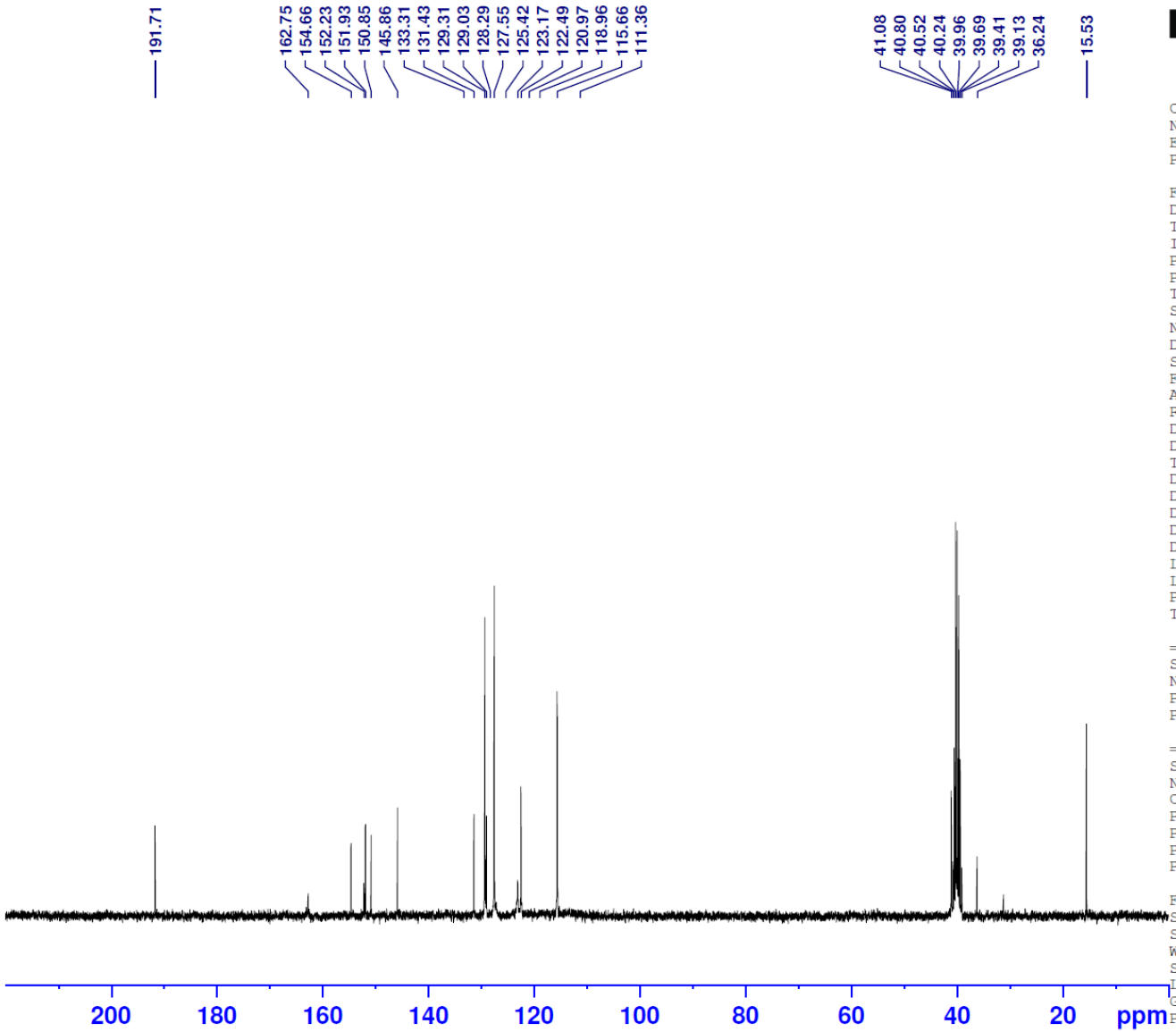


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	84.40	C26 H22 N5 O S Cl	[M+H]+	488.1300	488.1306	-0.6	-1.23	84.89	18.0

2-(4-(4-Ethyl-5-(2-(3,4-dihydroxyphenyl)-2-oxo-ethylthio)-4H-1,2,4-triazol-3yl)-phenyl)-5(6)-chloro-1H- benzimidazole (3h)



13C, TU-39, DMSO, 298K



BRUKER

```
Current Data Parameters
NAME          yusuf ozka
EXPNO                329
PROCNO                 1

F2 - Acquisition Parameters
Date_           20160518
Time               15.49
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                297.9 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
```

Data File: C:\LabSolutions\Data\Analiz\uac\TU-39_56.lcd

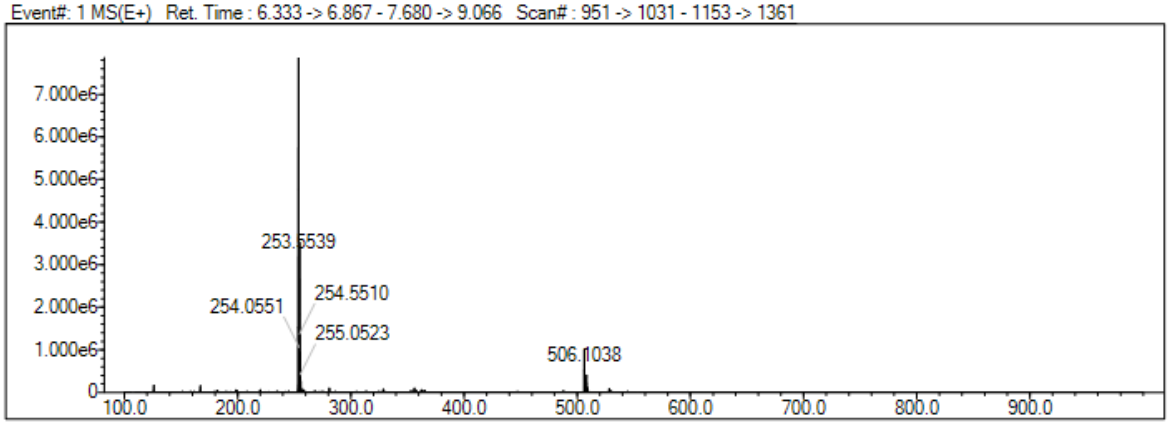
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	9	40	O	2	1	3	S	2	0	2	Ru	2	0	0	H
C	4	11	26	F	1	0	0	Cl	1	0	1	I	3	0	0	
N	3	0	6	P	3	0	0	Br	1	0	1					

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

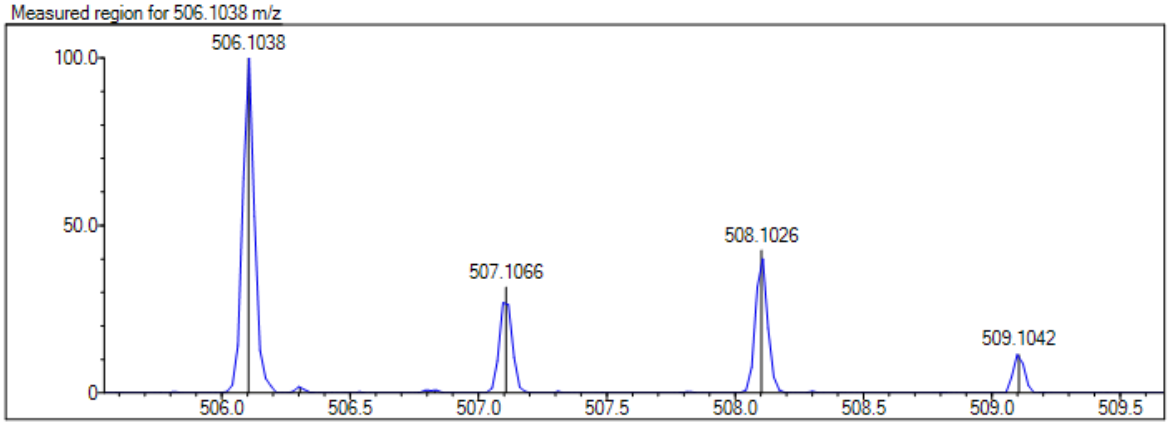
DBE Range: 17.0 - 20.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

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

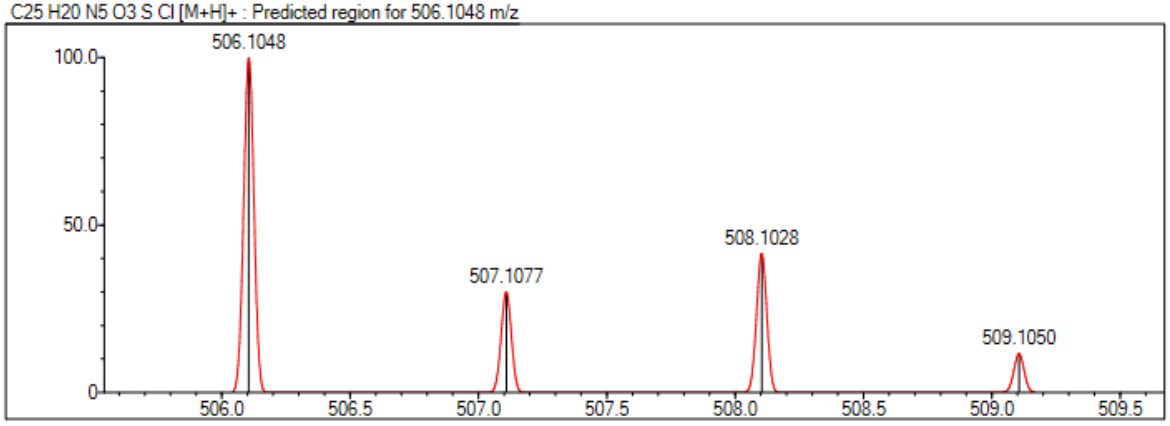
Event#: 1 MS(E+) Ret. Time : 6.333 -> 6.867 - 7.680 -> 9.066 Scan# : 951 -> 1031 - 1153 -> 1361



Measured region for 506.1038 m/z

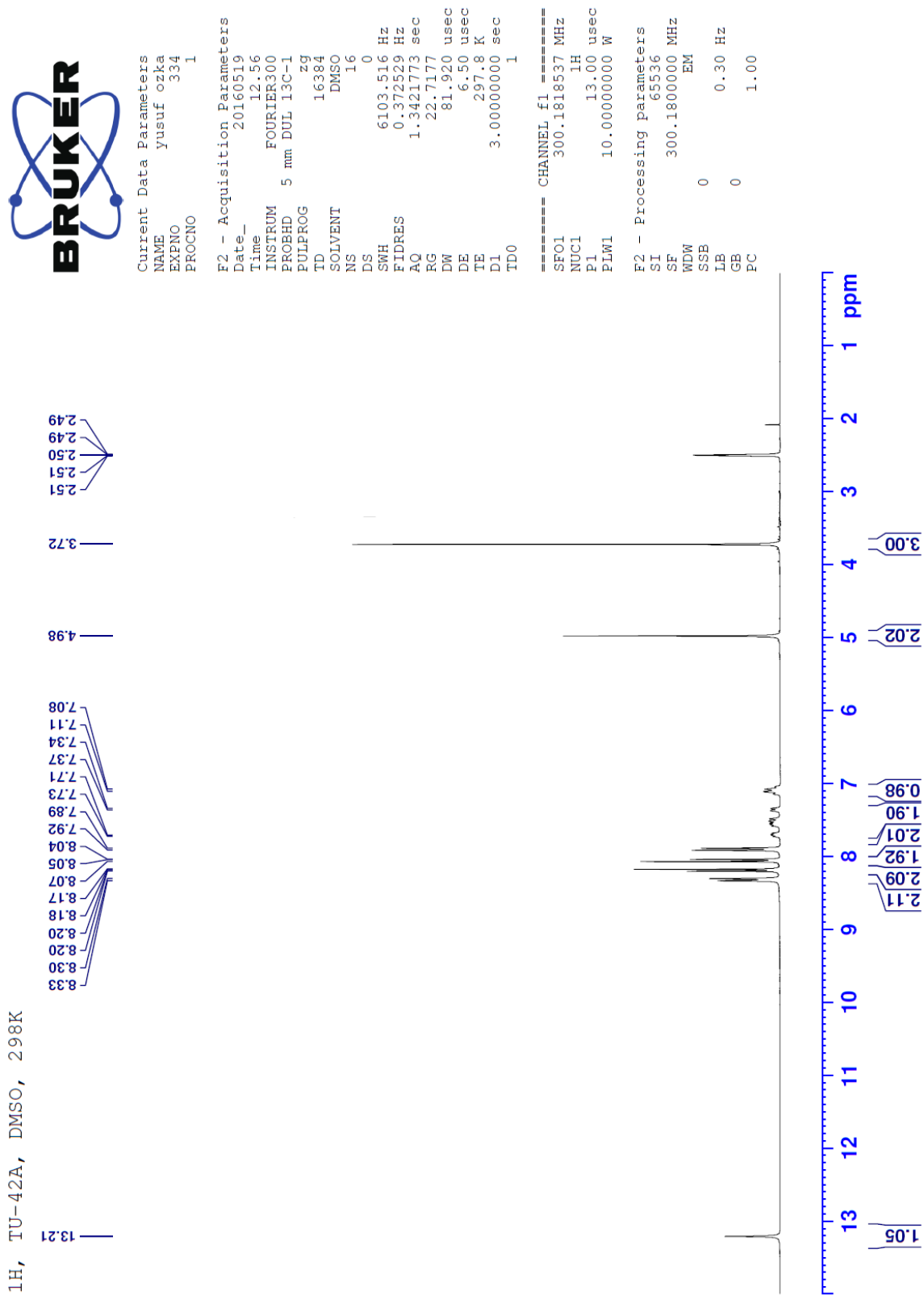


C25 H20 N5 O3 S Cl [M+H]+ : Predicted region for 506.1048 m/z

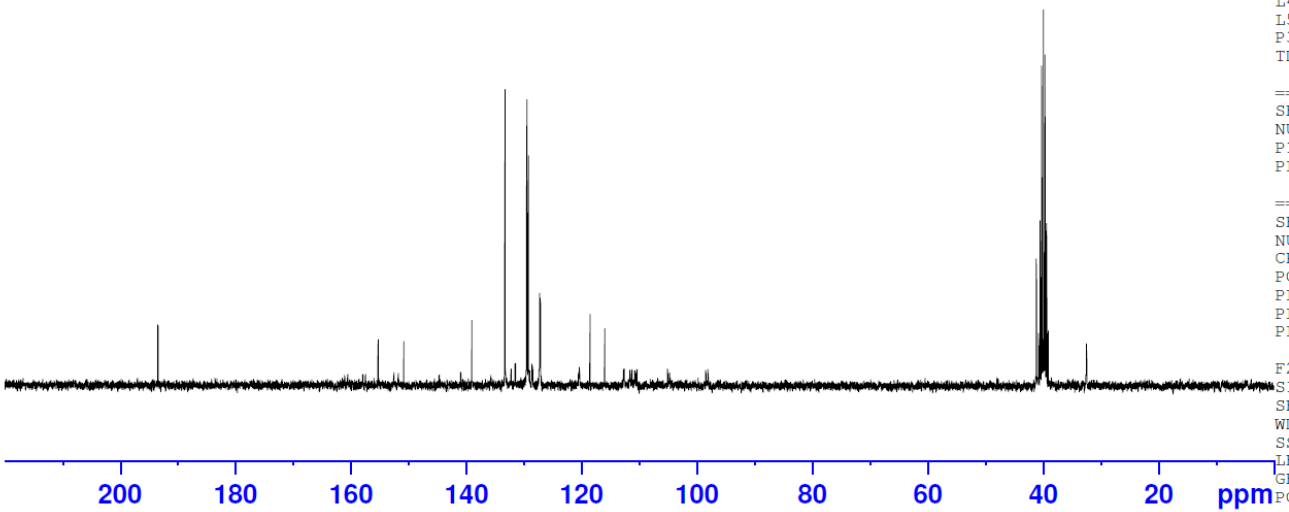


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	93.72	C25 H20 N5 O3 S Cl	[M+H]+	506.1038	506.1048	-1.0	-1.98	96.08	18.0

2-(4-(4-Methyl-5-(2-(4-cyanophenyl)-2-oxo-ethylthio)-4H-1,2,4-triazol-3yl)-phenyl)-5(6)-fluoro-1H-benzoimidazole (3i)



13C, TU-42A, DMSO, 298K



Current Data Parameters
NAME yusuf ozka
EXPNO 335
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160519
Time 12.58
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

Data File: C:\LabSolutions\Data\Analiz\uac\TU-42A_59.lcd

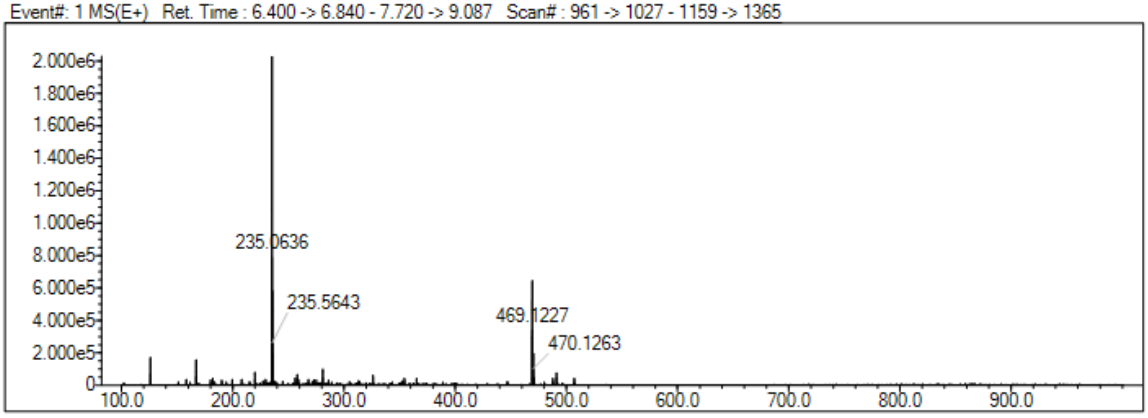
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	9	40	O	2	1	3	S	2	0	2	Ru	2	0	0	H
C	4	11	26	F	1	0	1	Cl	1	0	1	I	3	0	0	
N	3	0	6	P	3	0	0	Br	1	0	1					

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

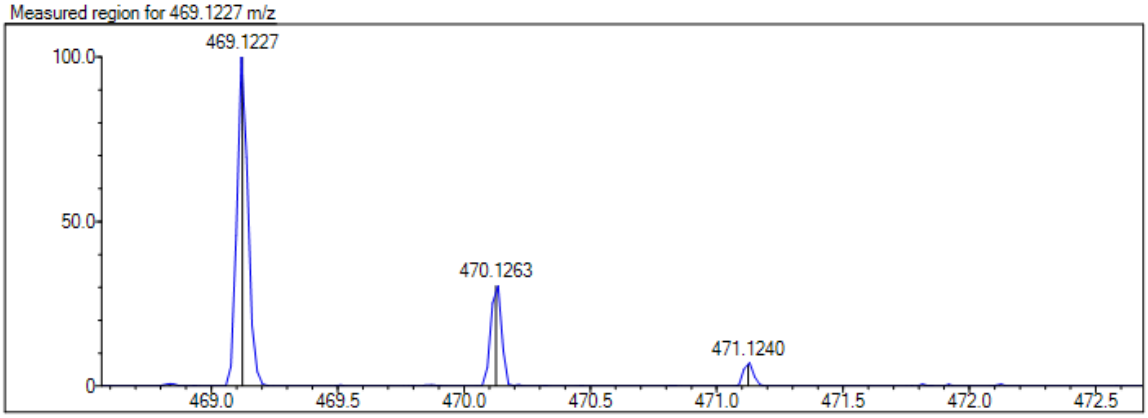
DBE Range: 17.0 - 20.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

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

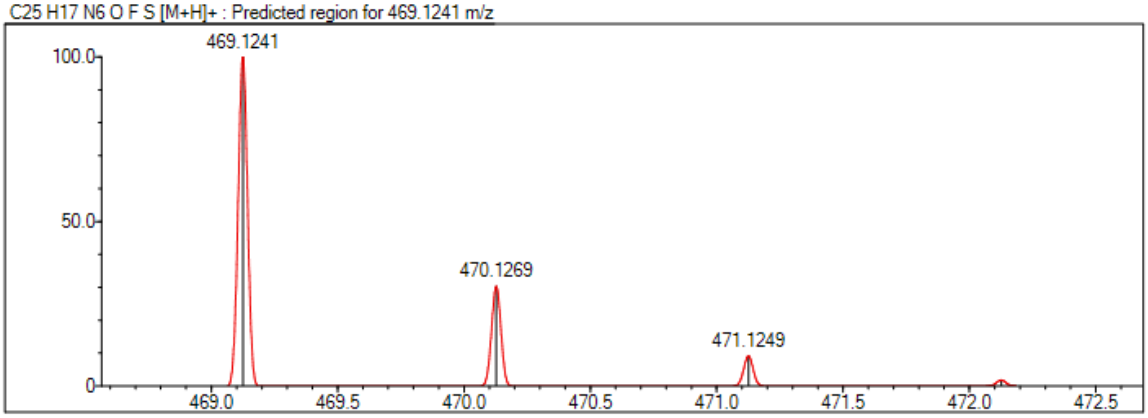
Event#: 1 MS(E+) Ret. Time : 6.400 -> 6.840 - 7.720 -> 9.087 Scan# : 961 -> 1027 - 1159 -> 1365



Measured region for 469.1227 m/z

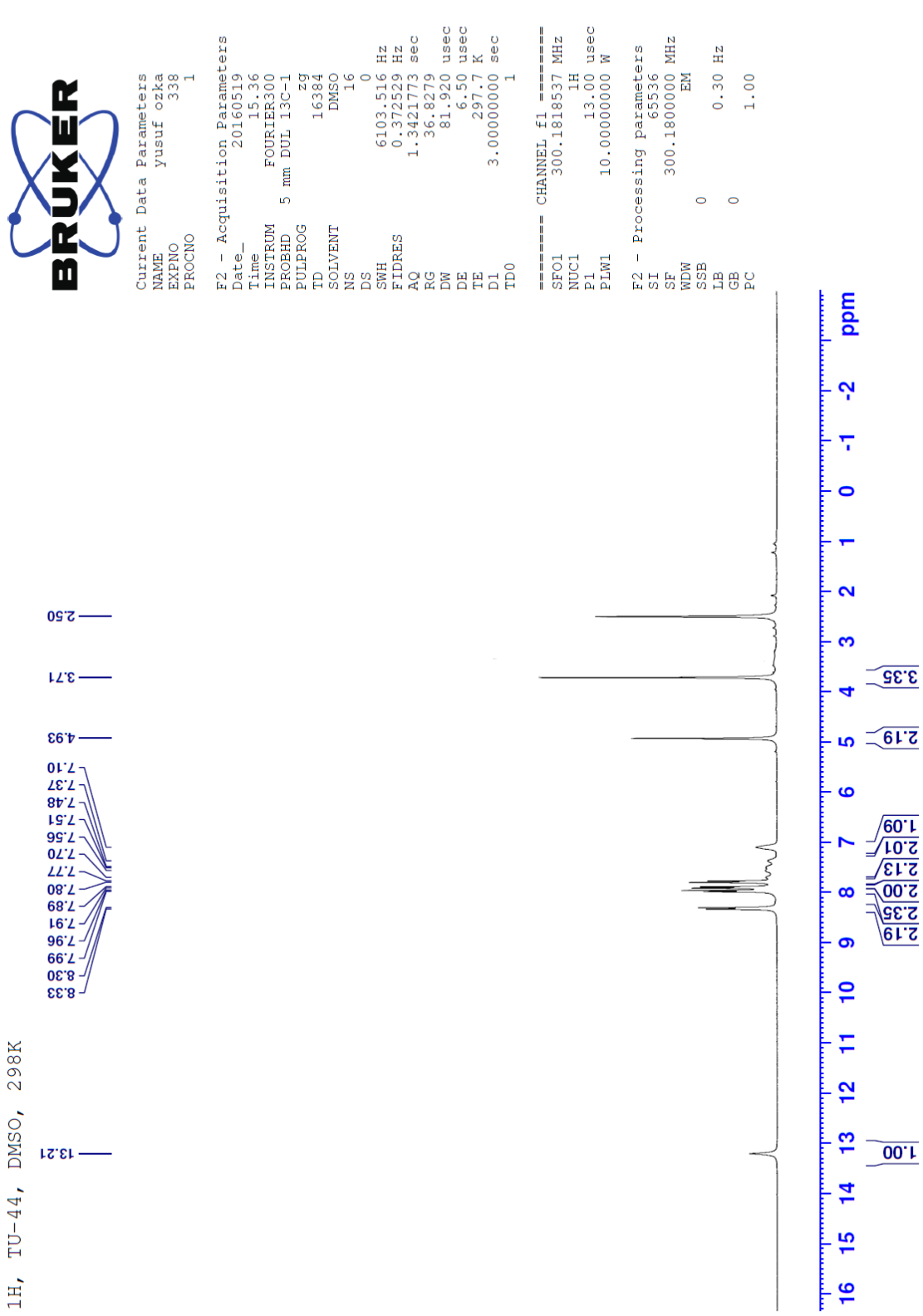


C25 H17 N6 O F S [M+H]+ : Predicted region for 469.1241 m/z

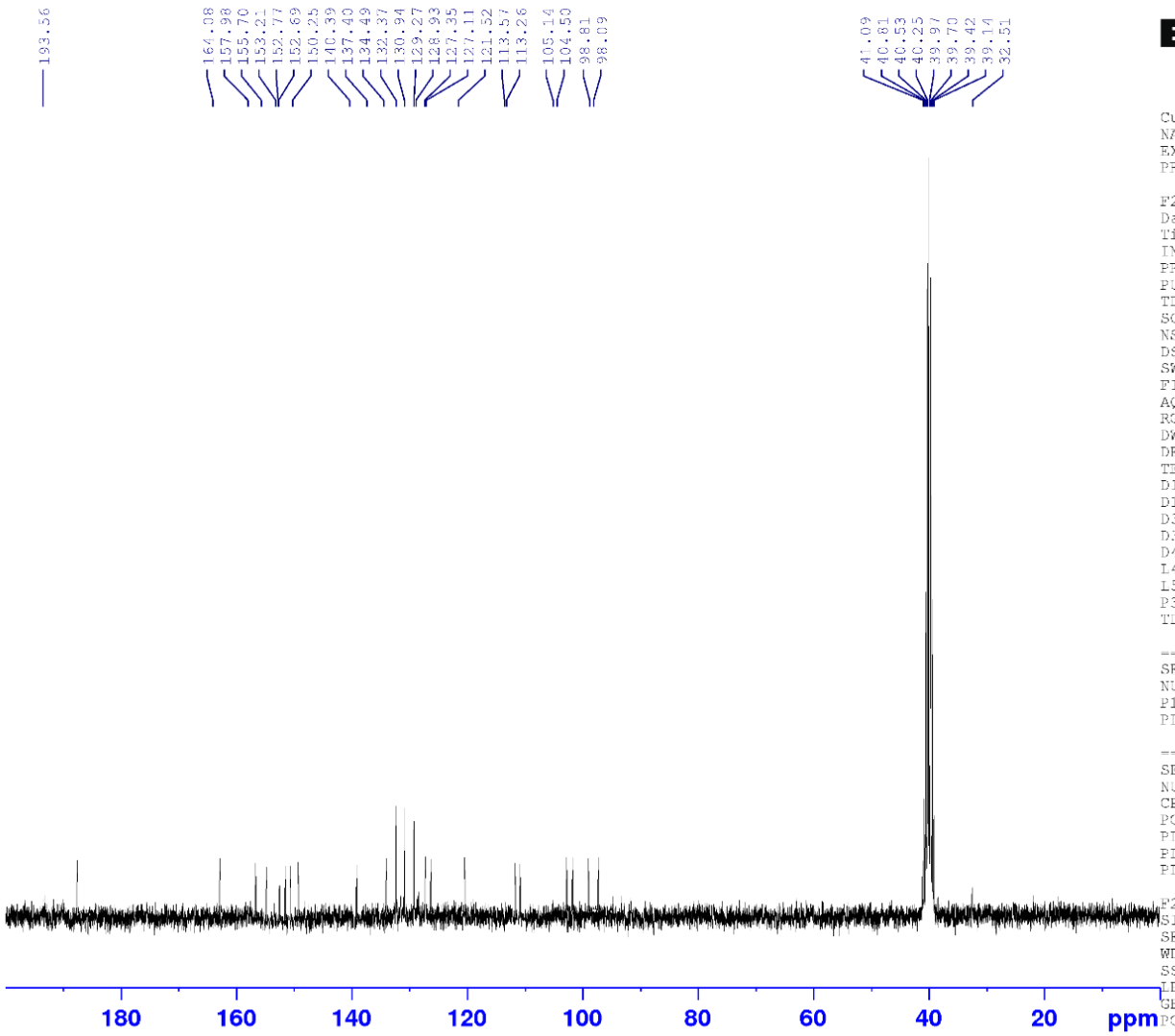


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	73.31	C25 H17 N6 O F S	[M+H]+	469.1227	469.1241	-1.4	-2.98	77.13	20.0

2-(4-(4-Methyl-5-(2-(4-bromophenyl)-2-oxo-ethylthio)-4H-1,2,4-triazol-3yl)-phenyl)-5(6)-fluoro-1H-benzimidazole (3j)



13C, TU-44, DMSO, 298K



Current Data Parameters
NAME Yusuf Ozkay
EXPNO 339
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160519
Time 15.38
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

Data File: C:\LabSolutions\Data\Analiz\uac\TU-44A_62.lcd

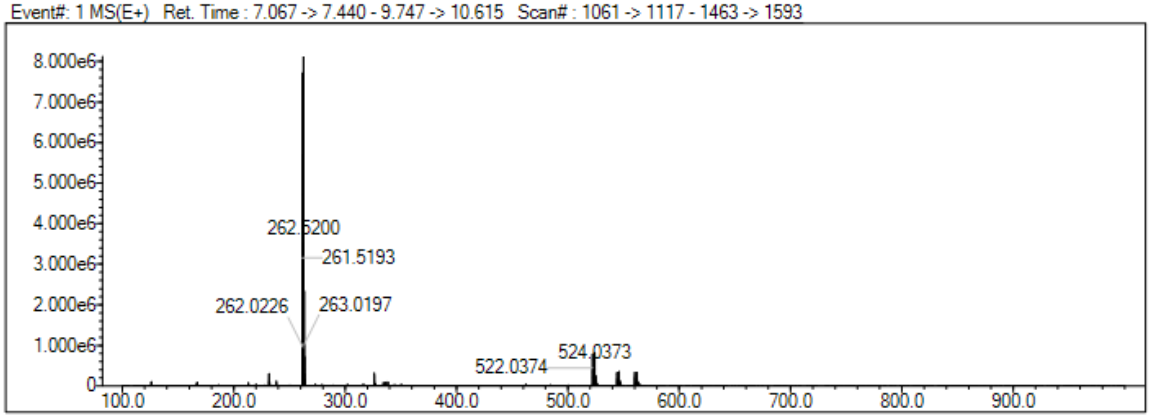
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	9	40	O	2	1	3	S	2	0	2	Ru	2	0	0	H
C	4	11	26	F	1	0	1	Cl	1	0	0	I	3	0	0	
N	3	0	6	P	3	0	0	Br	1	0	1					

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

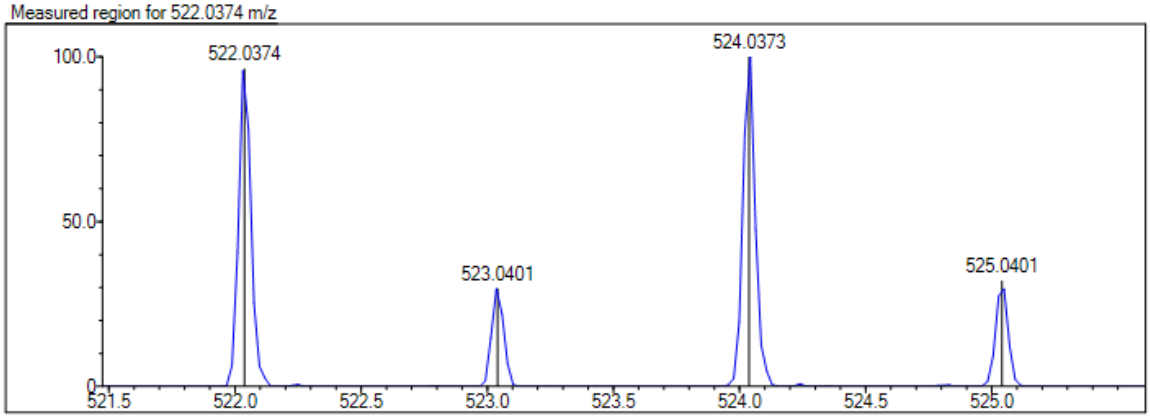
DBE Range: 17.0 - 20.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

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

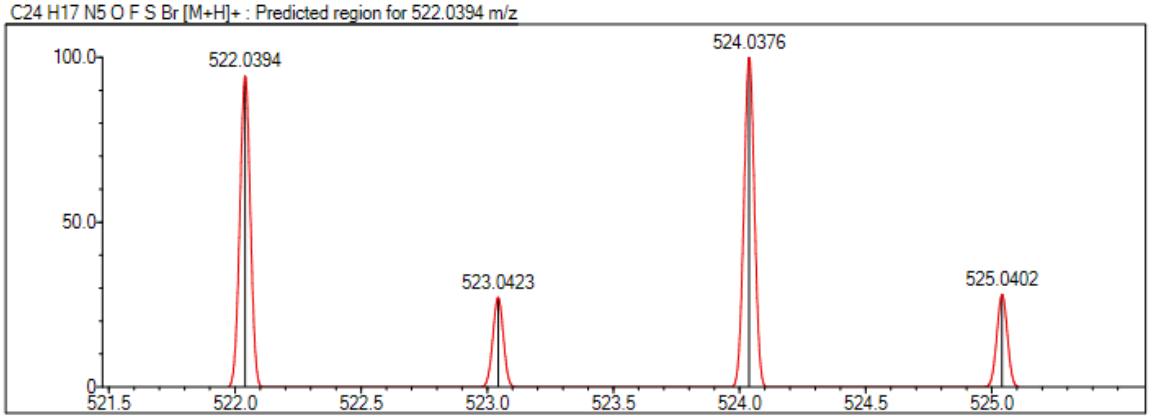
Event#: 1 MS(E+) Ret. Time : 7.067 -> 7.440 - 9.747 -> 10.615 Scan# : 1061 -> 1117 - 1463 -> 1593



Measured region for 522.0374 m/z

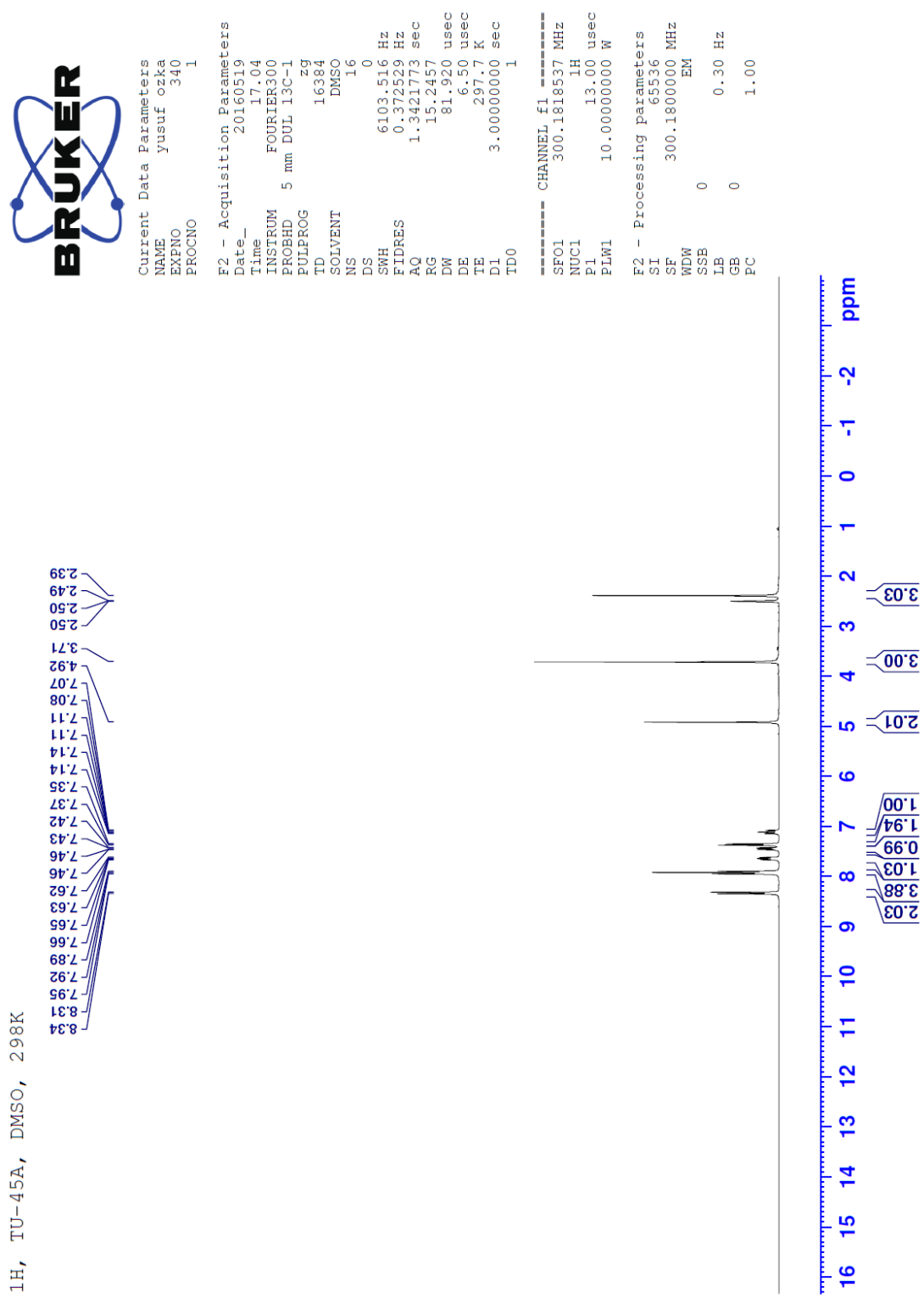


C24 H17 N5 O F S Br [M+H]+ : Predicted region for 522.0394 m/z

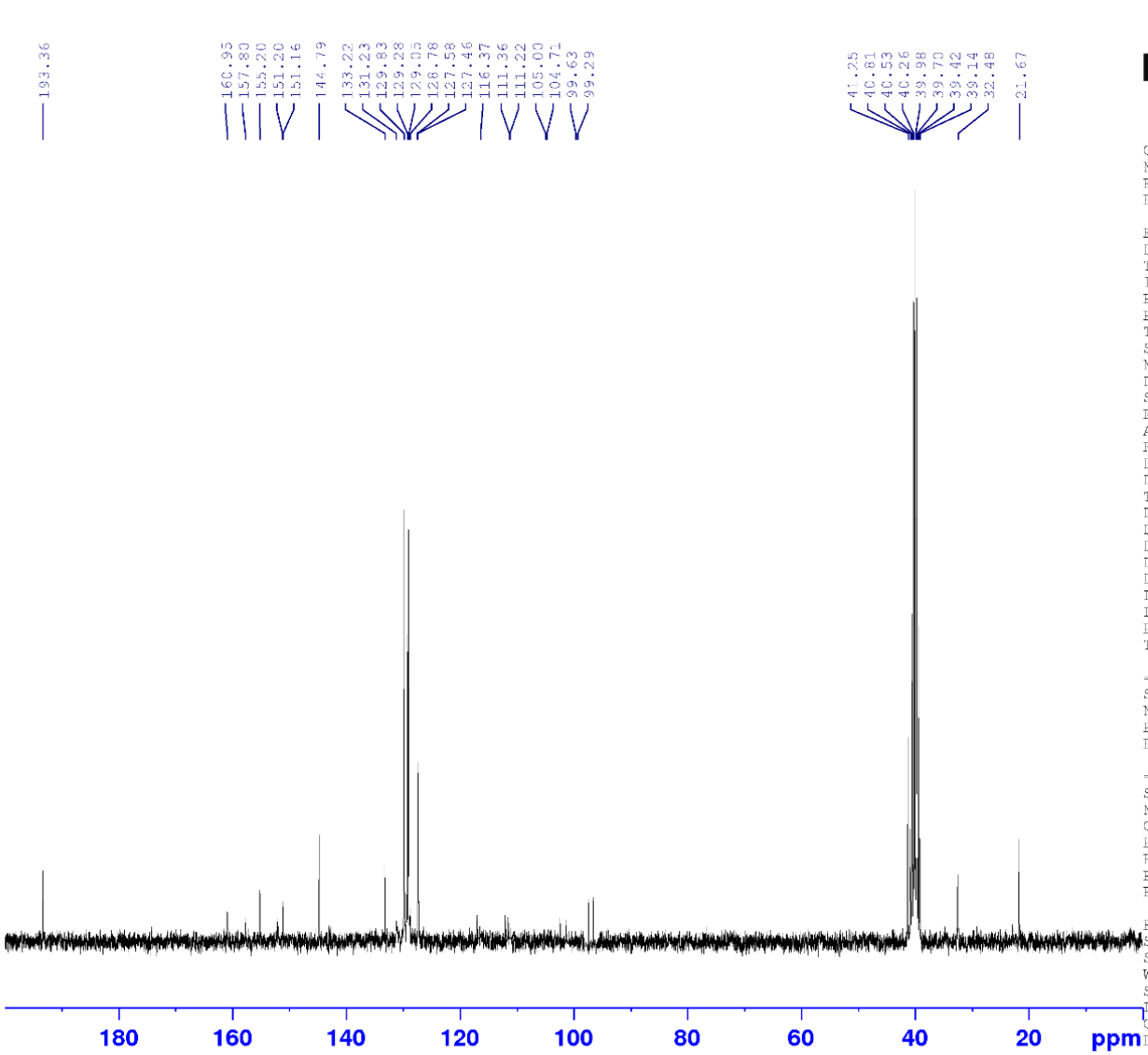


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	82.13	C24 H17 N5 O F S Br	[M+H]+	522.0374	522.0394	-2.0	-3.83	88.38	18.0

2-(4-(4-Methyl-5-(2-(4-methylphenyl)-2-oxo-ethylthio)-4H-1,2,4-triazol-3yl)-phenyl)-5(6)-fluoro-1H-benzimidazole (3k)



13C, TU-45A, DMSO, 298K



BRUKER

```
Current Data Parameters
NAME          Yusuf Ozkay
EXPNO                 341
PROCNO                  1

F2 - Acquisition Parameters
Date_          20160519
Time              17.05
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                297.8 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
```

Data File: C:\LabSolutions\Data\Analiz\uac\TU-45A_64.lcd

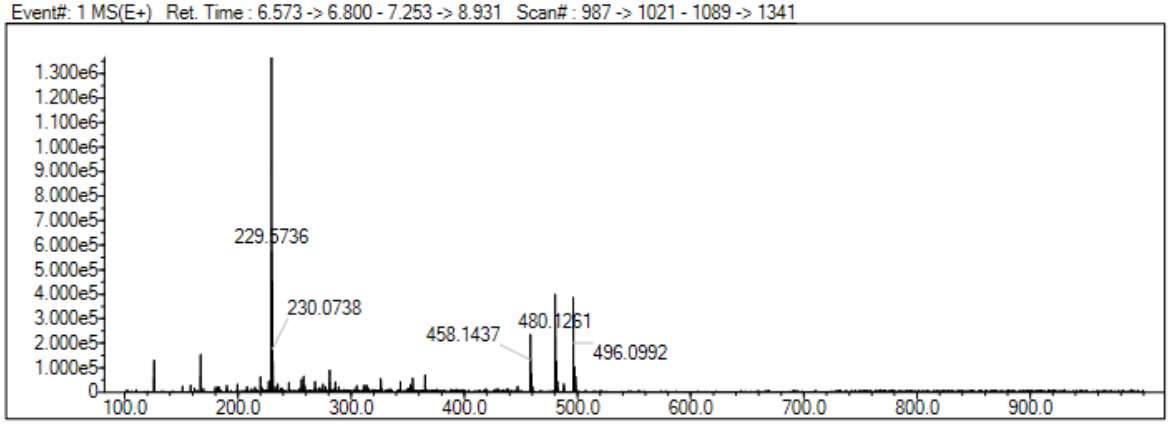
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	9	40	O	2	1	3	S	2	0	2	Ru	2	0	0	H
C	4	11	26	F	1	0	1	Cl	1	0	0	I	3	0	0	
N	3	0	6	P	3	0	0	Br	1	0	1					

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

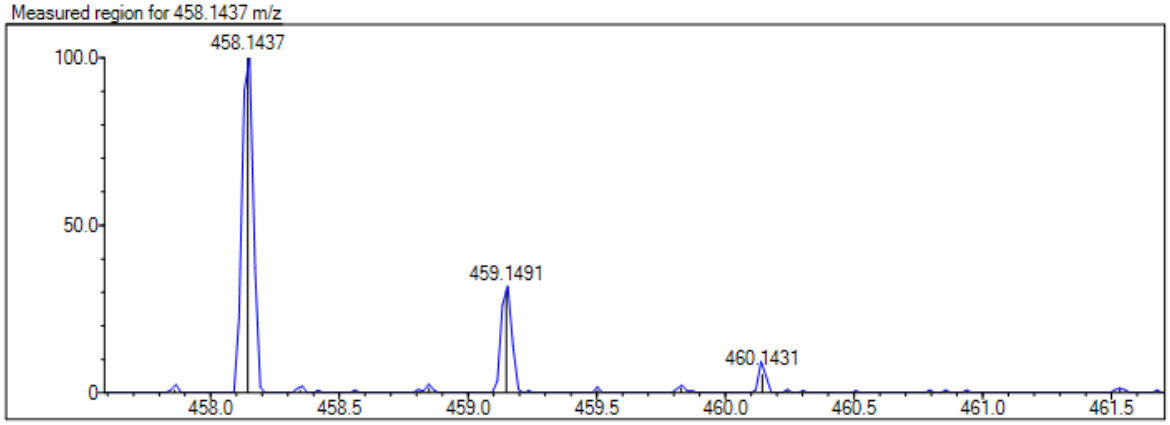
DBE Range: 17.0 - 20.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

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

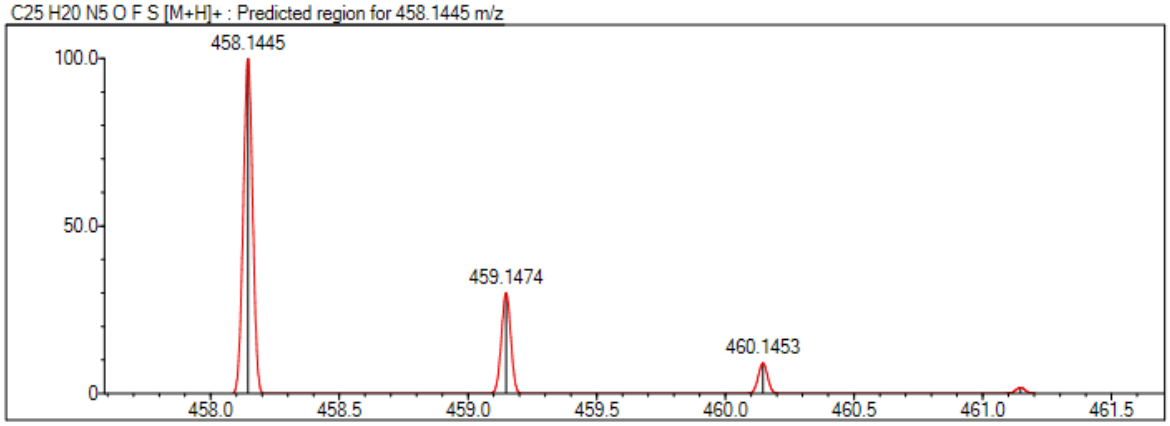
Event#: 1 MS(E+) Ret. Time : 6.573 -> 6.800 - 7.253 -> 8.931 Scan# : 987 -> 1021 - 1089 -> 1341



Measured region for 458.1437 m/z

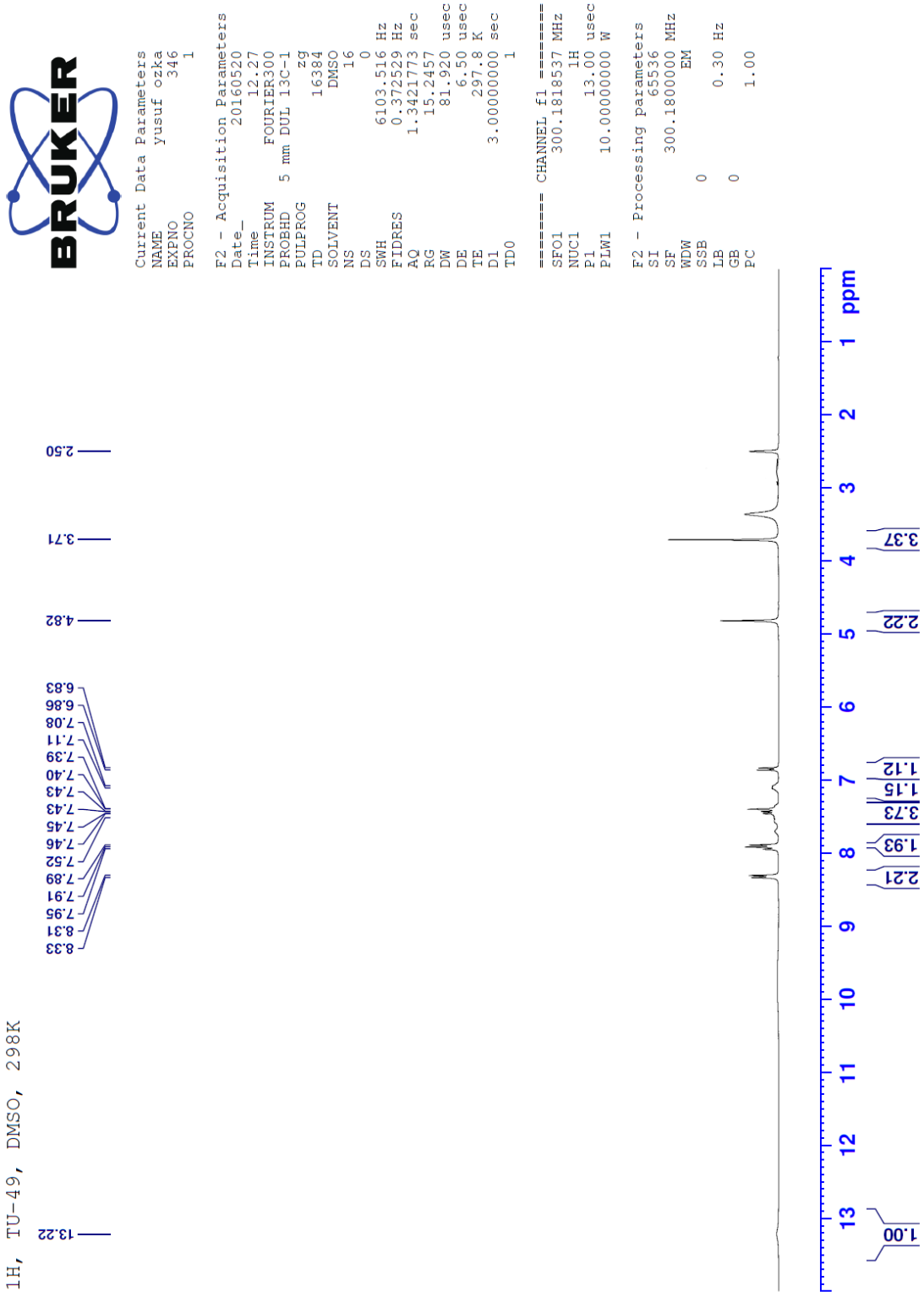


C25 H20 N5 O F S [M+H]+ : Predicted region for 458.1445 m/z

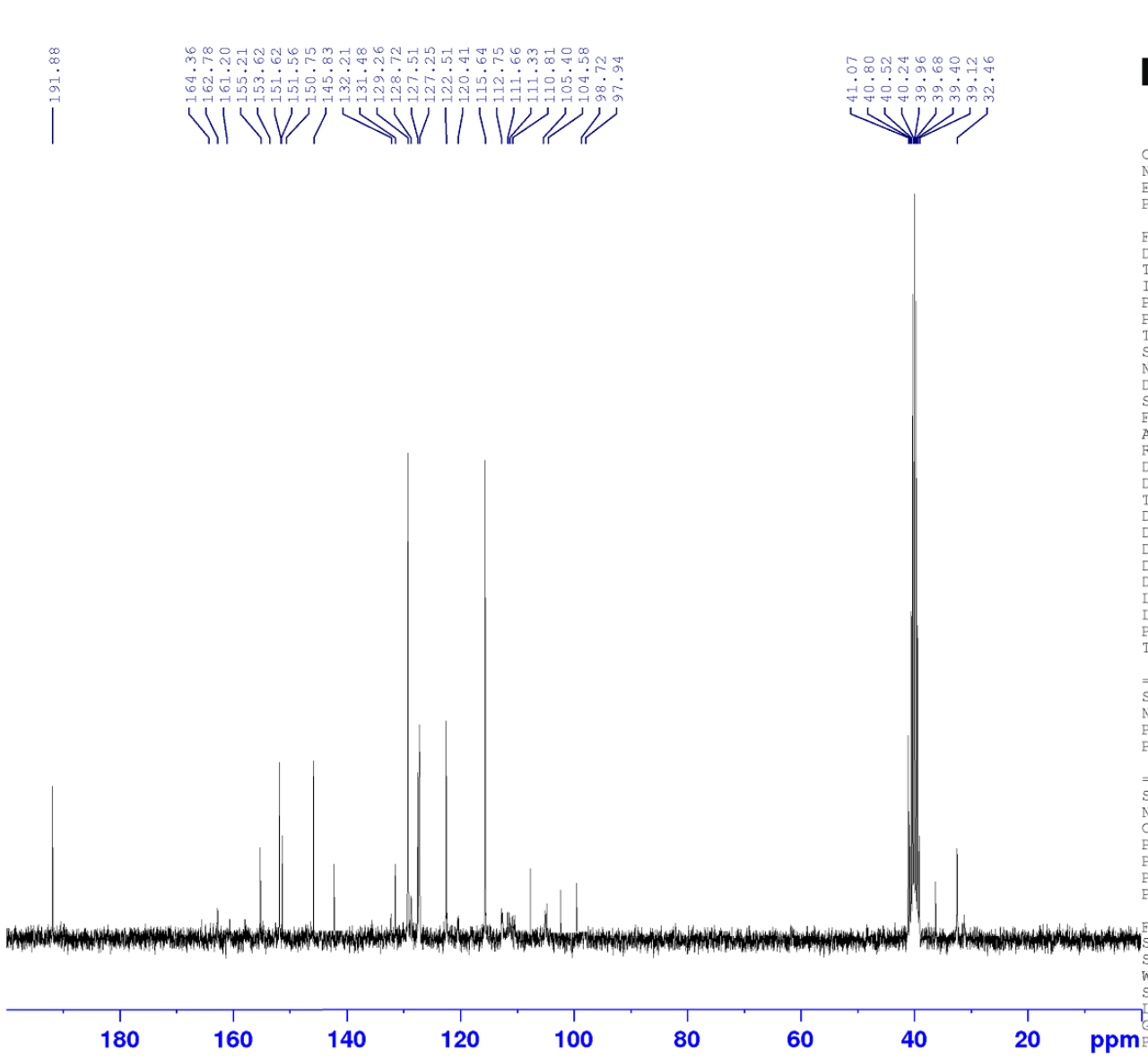


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	87.11	C25 H20 N5 O F S	[M+H]+	458.1437	458.1445	-0.8	-1.75	88.77	18.0

2-(4-(4-Methyl-5-(2-(3,4-dihydroxyphenyl)-2-oxo-ethylthio)-4H-1,2,4-triazol-3yl)-phenyl)-5(6)-fluoro-1H- benzimidazole (3l)



13C, TU-49, DMSO, 298K



Current Data Parameters
NAME Yusuf Ozkay
EXPNO 347
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160520
Time 12.29
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 297.9 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

Data File: C:\LabSolutions\Data\Analiz\uac\TU-49_70.lcd

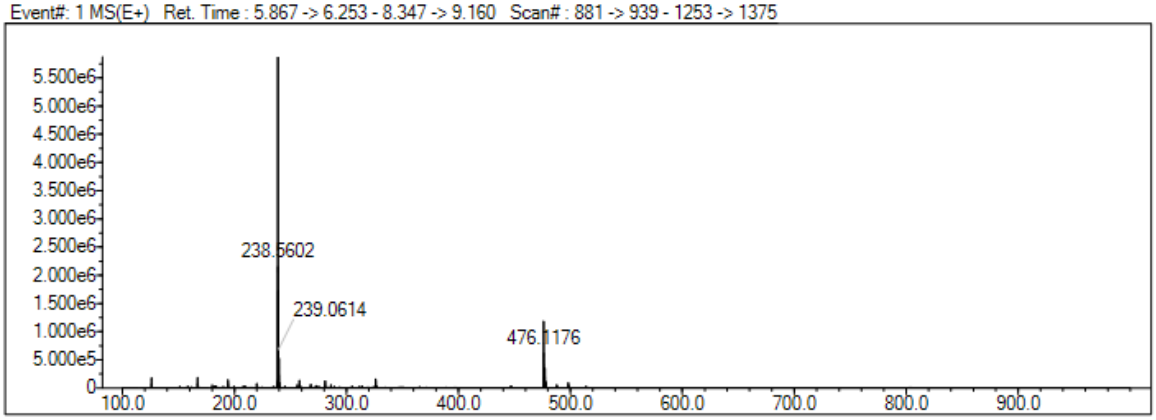
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	9	40	O	2	1	3	S	2	0	2	Ru	2	0	0	H
C	4	11	26	F	1	0	1	Cl	1	0	0	I	3	0	0	
N	3	0	6	P	3	0	0	Br	1	0	1					

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

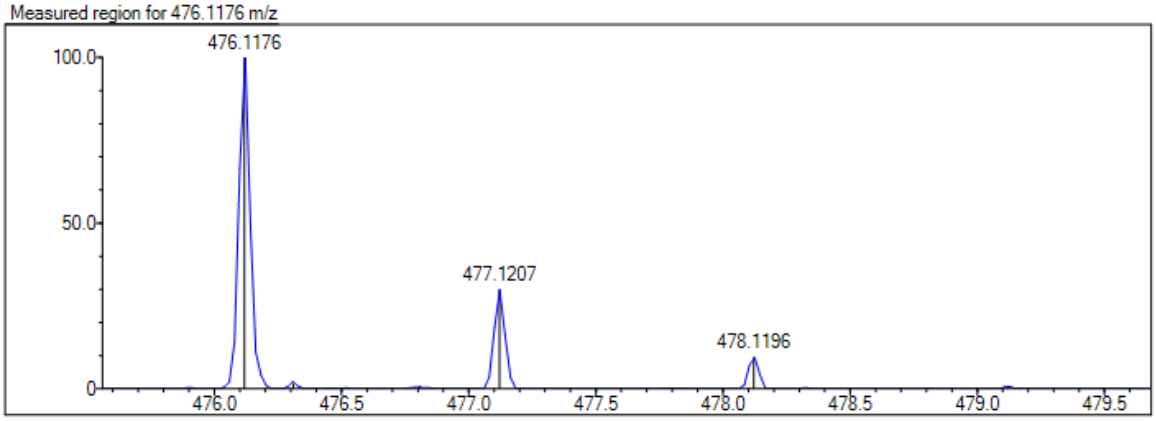
DBE Range: 17.0 - 20.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

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

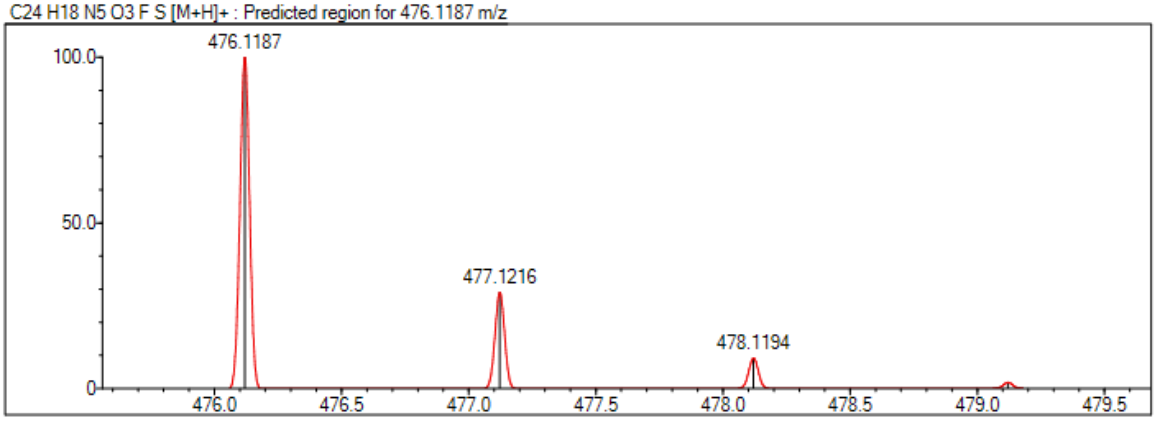
Event#: 1 MS(E+) Ret. Time : 5.867 -> 6.253 - 8.347 -> 9.160 Scan# : 881 -> 939 - 1253 -> 1375



Measured region for 476.1176 m/z

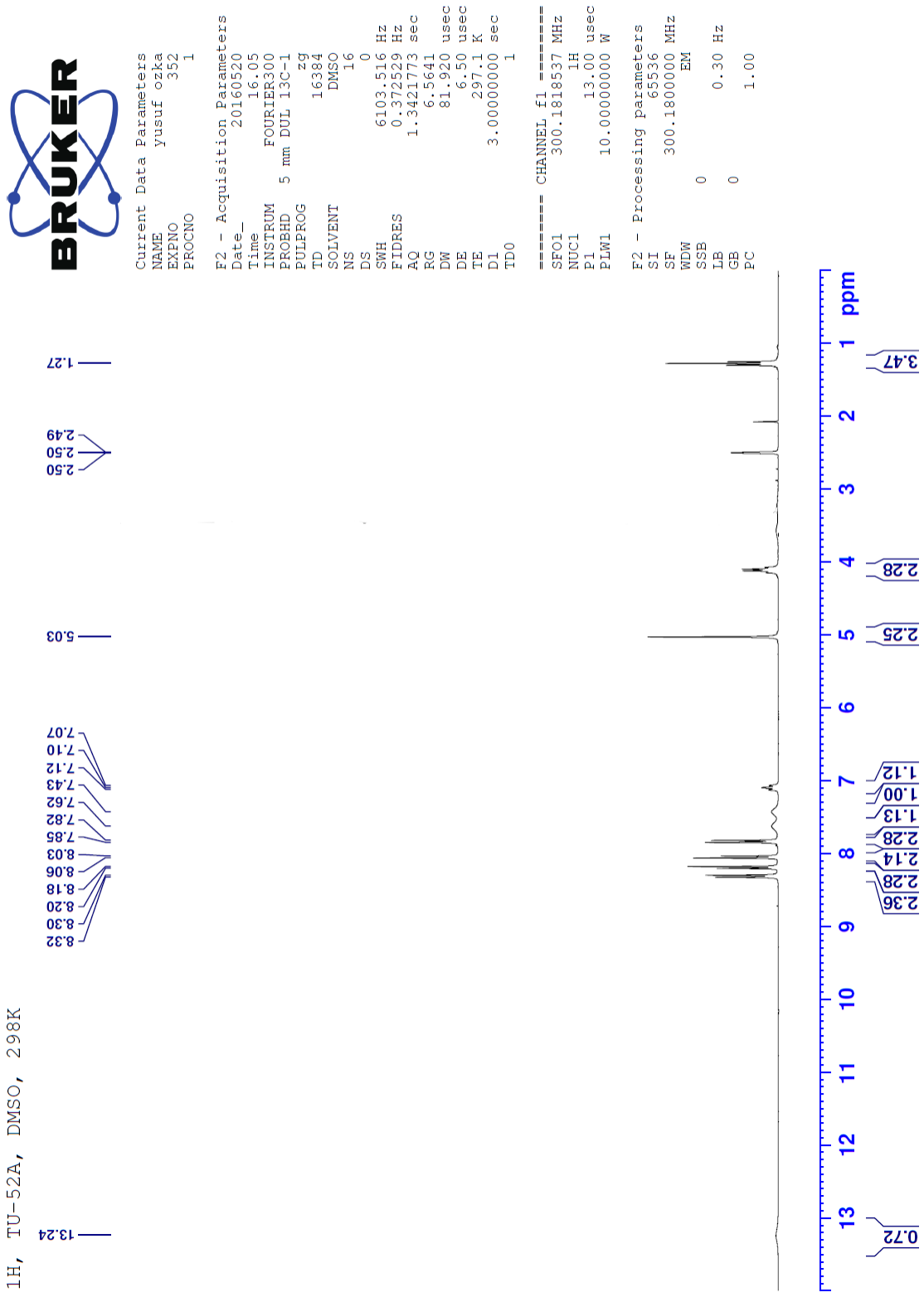


C24 H18 N5 O3 F S [M+H]+ : Predicted region for 476.1187 m/z

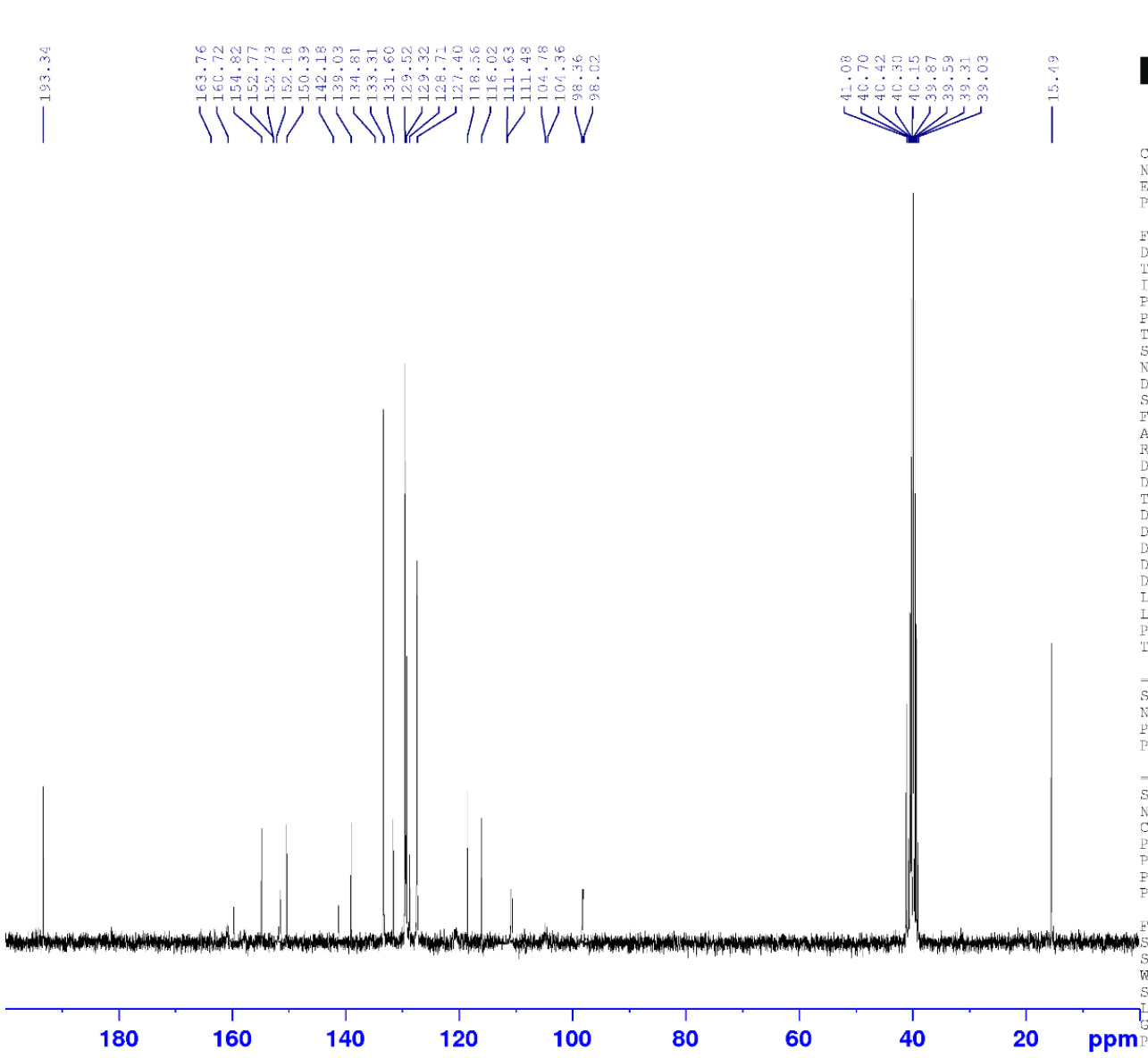


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	95.49	C24 H18 N5 O3 F S	[M+H]+	476.1176	476.1187	-1.1	-2.31	98.72	18.0

2-(4-(4-Ethyl-5-(2-(4-cyanophenyl)-2-oxo-ethylthio)-4H-1,2,4-triazol-3yl)-phenyl)-5(6)-fluoro-1H-benzoimidazole (3m)



13C, TU-52A, DMSO, 298K



BRUKER

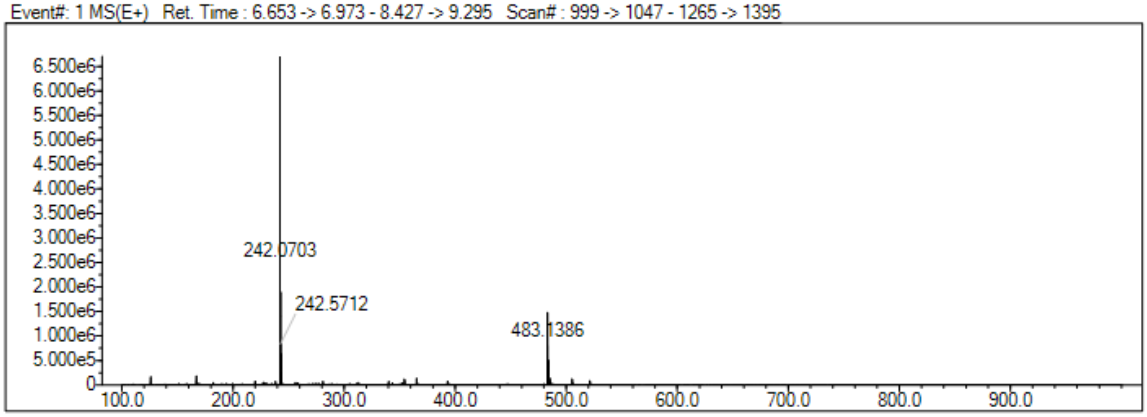
```
Current Data Parameters
NAME          Yusuf Ozkay
EXPNO                 353
PROCNO                  1

F2 - Acquisition Parameters
Date_           20160520
Time               16.06
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               297.5 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
```

Data File: C:\LabSolutions\Data\Analiz\uac\TU-52A_73.lcd

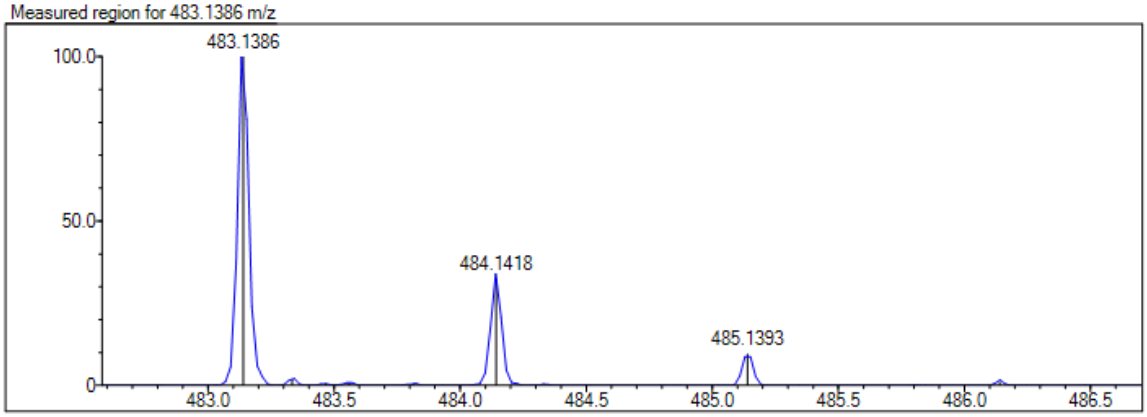
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	9	40	O	2	1	3	S	2	0	2	Ru	2	0	0	H
C	4	11	26	F	1	0	1	Cl	1	0	0	I	3	0	0	
N	3	0	6	P	3	0	0	Br	1	0	1					

Error Margin (ppm):	5	DBE Range:	17.0 - 20.0	Electron Ions:	both
HC Ratio:	unlimited	Apply N Rule:	yes	Use MSn Info:	no
Max Isotopes:	3	Isotope RI (%):	1.00	Isotope Res:	10000
MSn Iso RI (%):	10.00	MSn Logic Mode:	AND	Max Results:	500

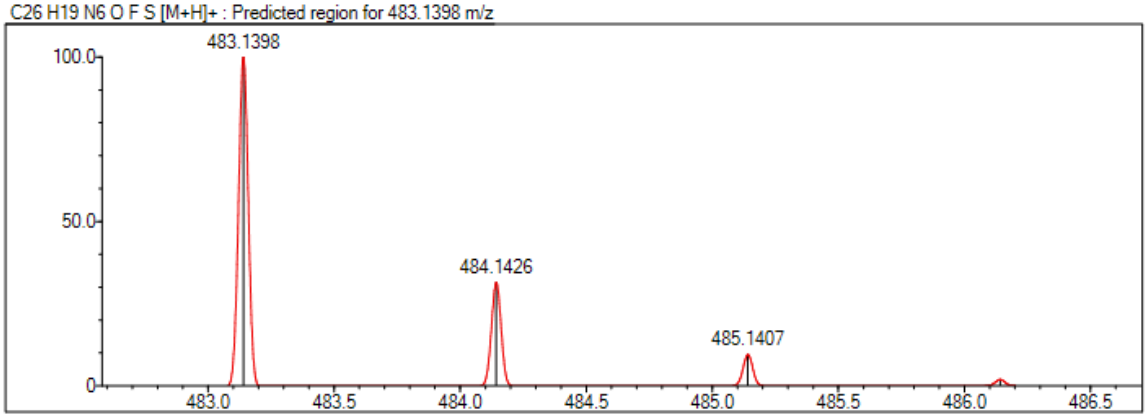
Event#: 1 MS(E+) Ret. Time : 6.653 -> 6.973 - 8.427 -> 9.295 Scan# : 999 -> 1047 - 1265 -> 1395



Measured region for 483.1386 m/z

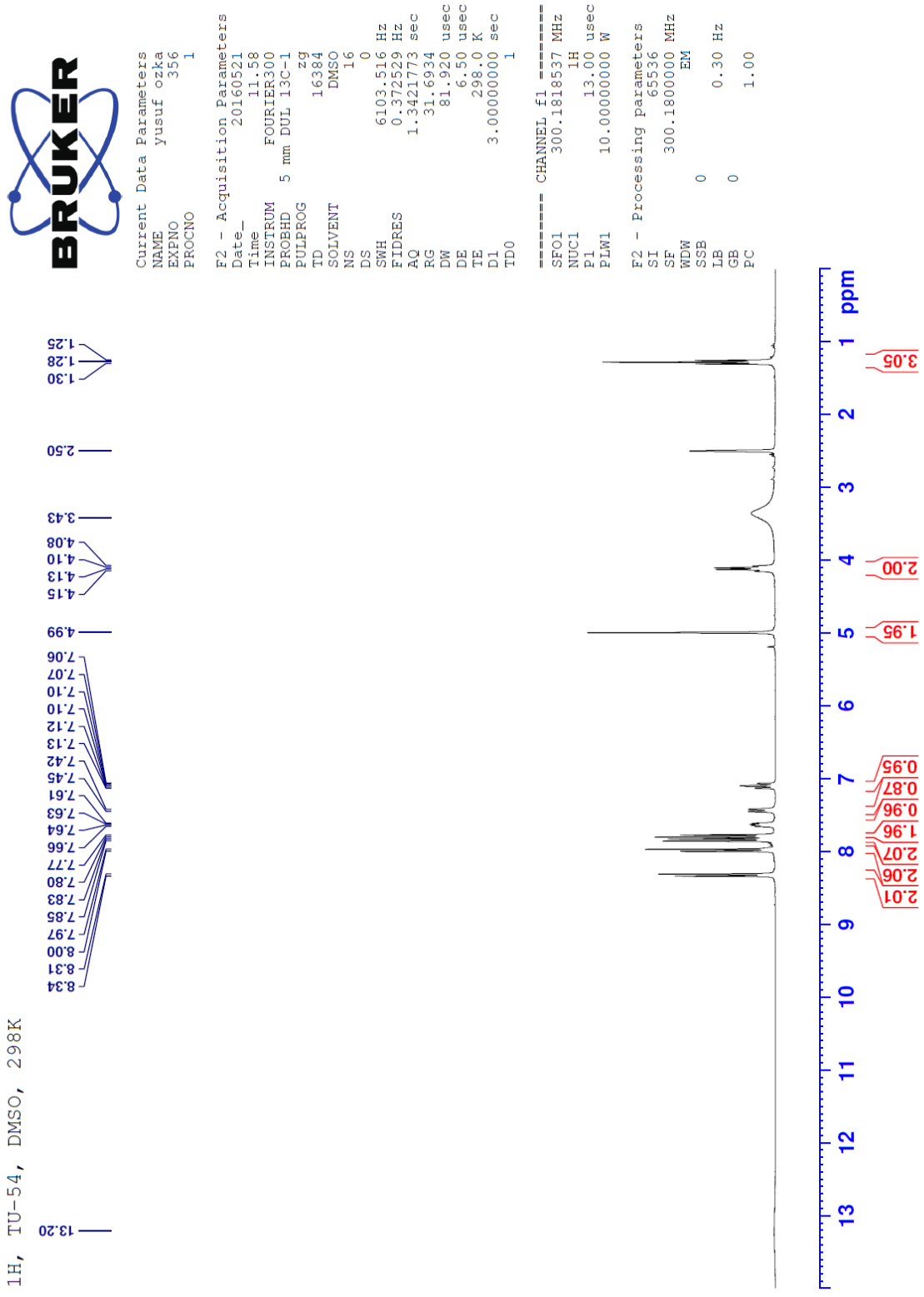


C26 H19 N6 O F S [M+H]+ : Predicted region for 483.1398 m/z

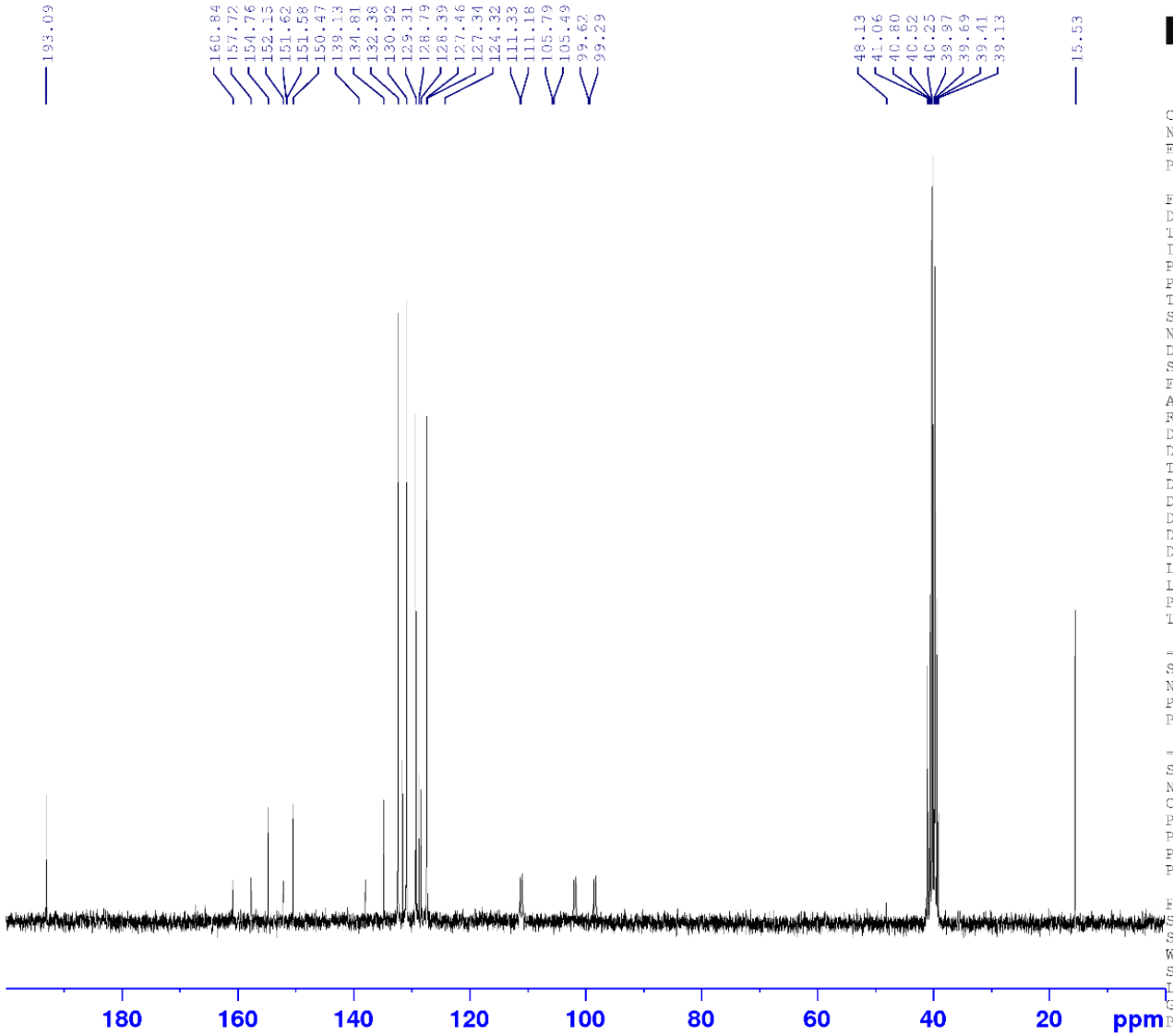


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	83.59	C26 H19 N6 O F S	[M+H]+	483.1386	483.1398	-1.2	-2.48	86.80	20.0

2-(4-(4-Ethyl-5-(2-(4-bromophenyl)-2-oxo-ethylthio)-4H-1,2,4-triazol-3yl)-phenyl)-5(6)-fluoro-1H-benzimidazole (3n)



13C, TU-54, DMSO, 298K



BRUKER

```
Current Data Parameters
NAME          Yusuf Ozkay
EXPNO                 357
PROCNO                  1

F2 - Acquisition Parameters
Date_            20160521
Time                12.00
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                297.3 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
```

Data File: C:\LabSolutions\Data\Analiz\uac\TU-54_76.lcd

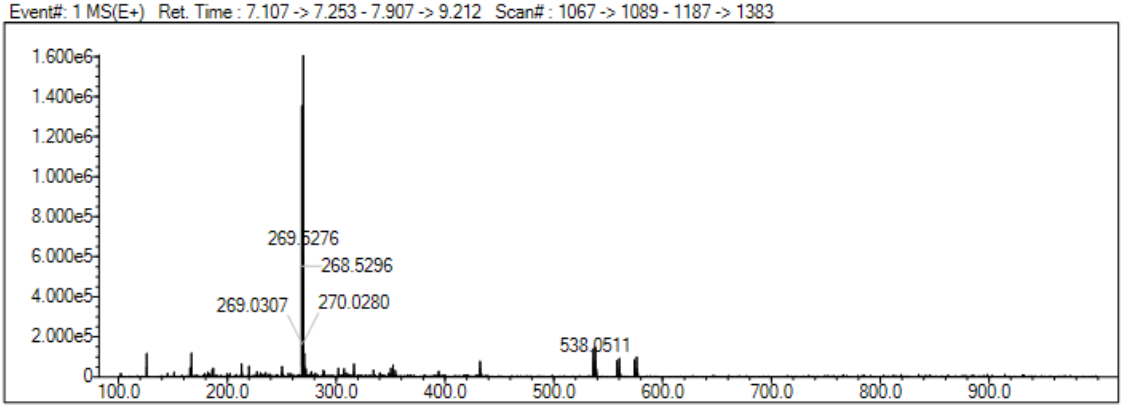
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	9	40	O	2	1	3	S	2	0	2	Ru	2	0	0	H
C	4	11	26	F	1	0	1	Cl	1	0	0	I	3	0	0	
N	3	0	6	P	3	0	0	Br	1	0	1					

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

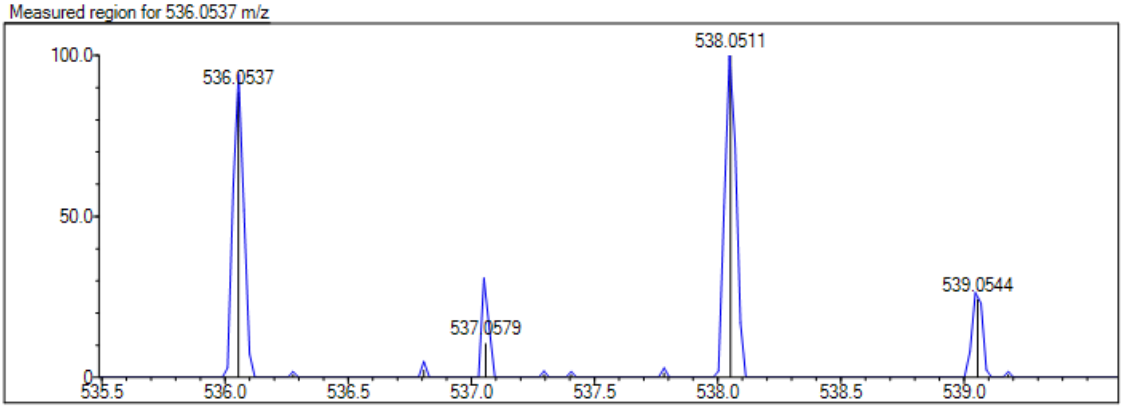
DBE Range: 17.0 - 20.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

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

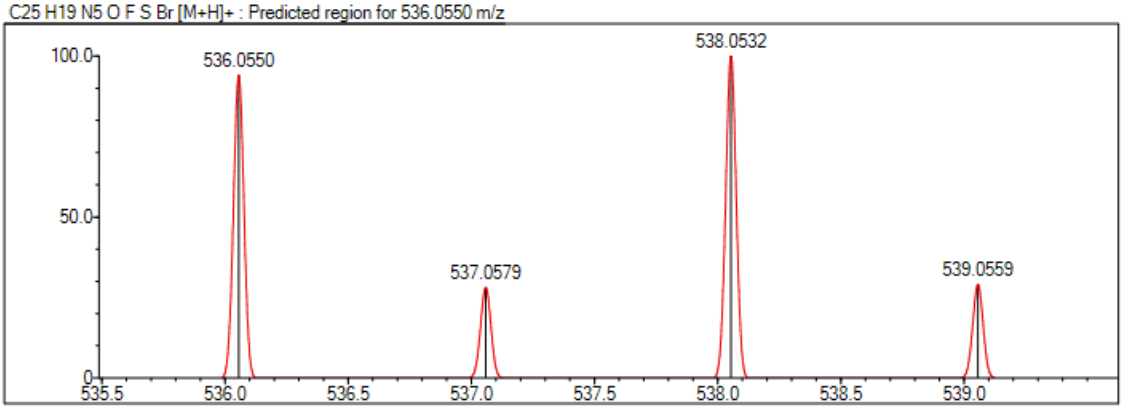
Event#: 1 MS(E+) Ret. Time : 7.107 -> 7.253 - 7.907 -> 9.212 Scan# : 1067 -> 1089 - 1187 -> 1383



Measured region for 536.0537 m/z

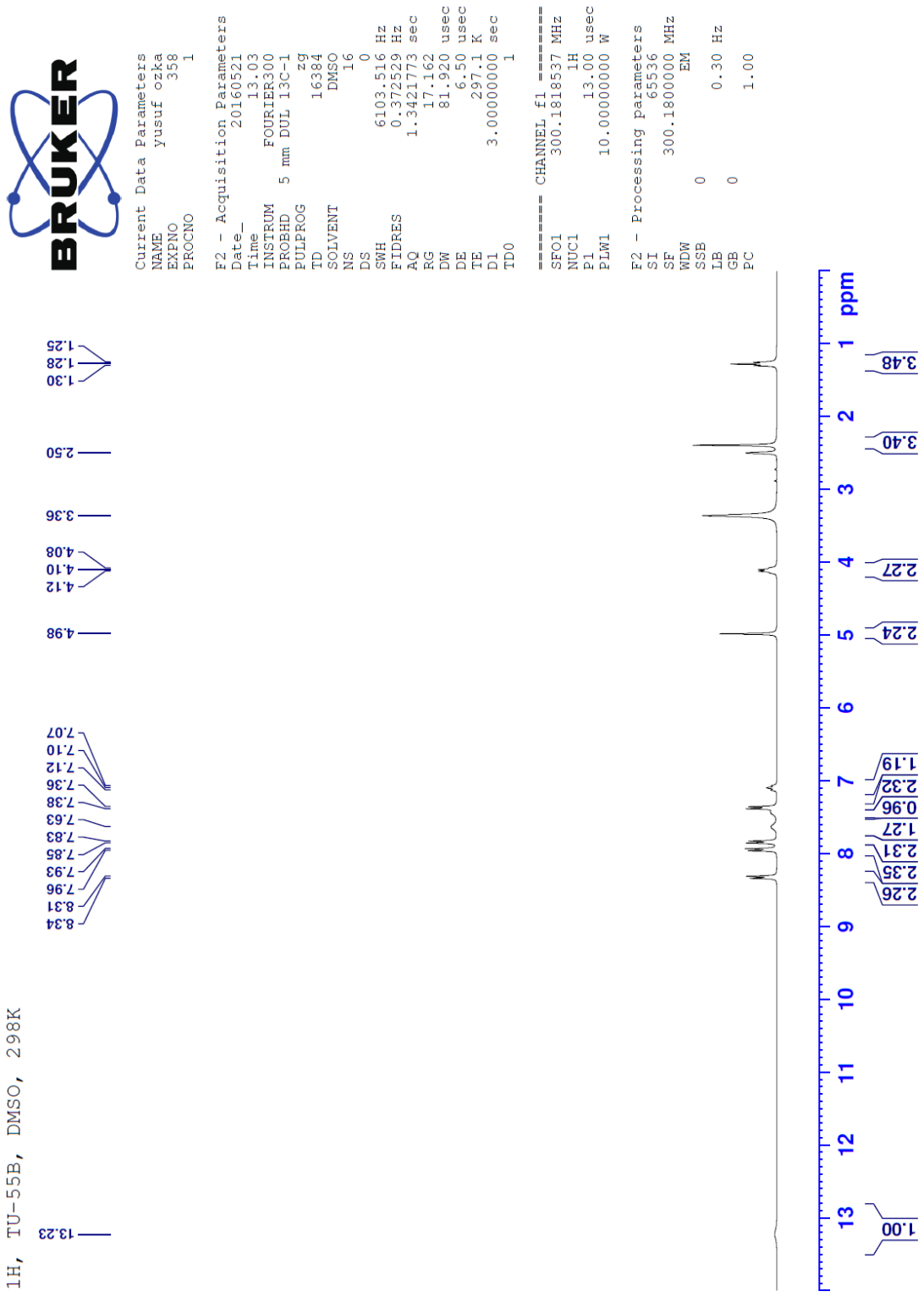


C25 H19 N5 O F S Br [M+H]+ : Predicted region for 536.0550 m/z

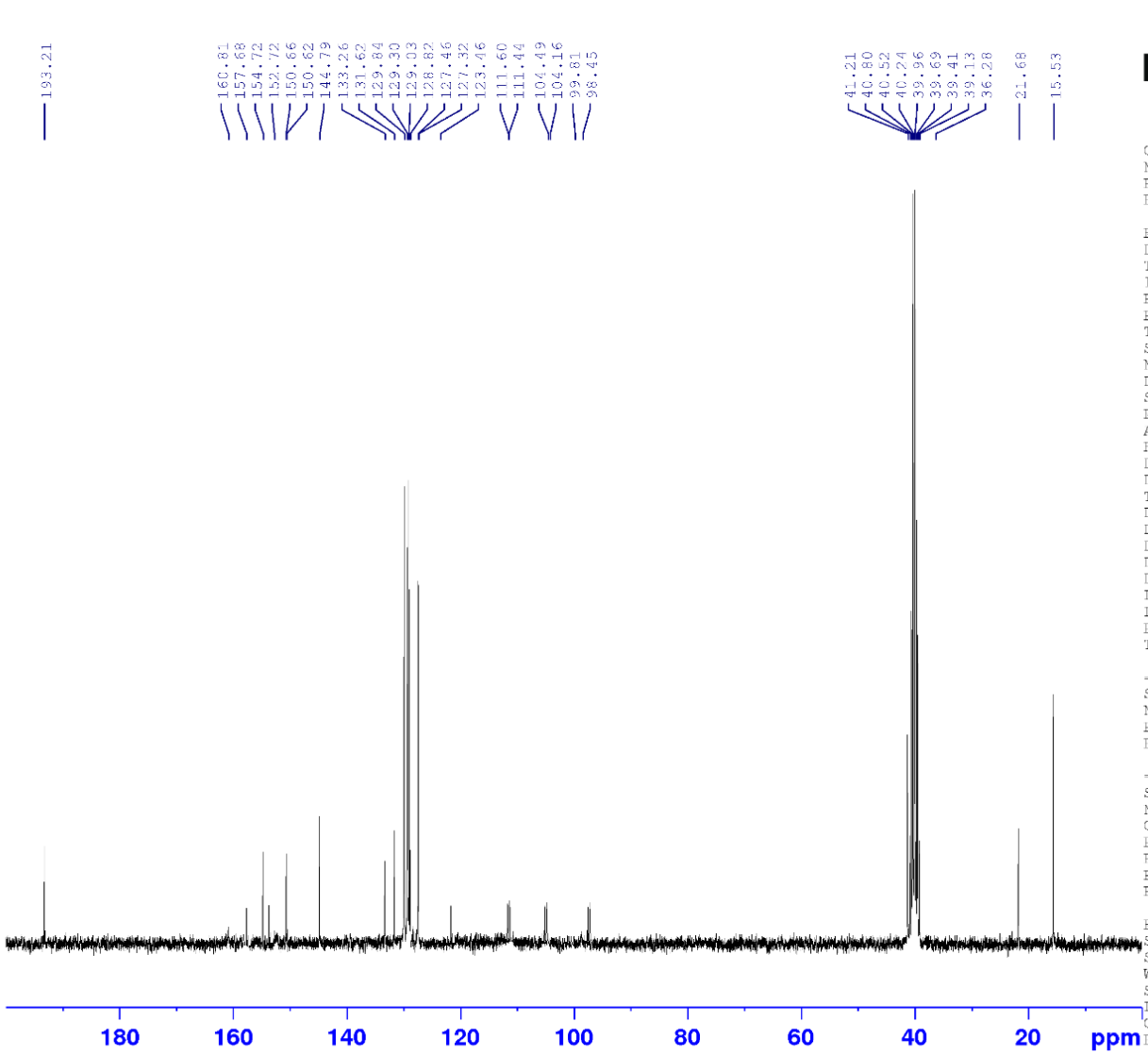


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	71.14	C25 H19 N5 O F S Br	[M+H]+	536.0537	536.0550	-1.3	-2.43	73.78	18.0

2-(4-(4-Ethyl-5-(2-(4-methylphenyl)-2-oxo-ethylthio)-4H-1,2,4-triazol-3yl)-phenyl)-5(6)-fluoro-1H-benzimidazole (3o)



13C, TU-55B, DMSO, 298K



BRUKER

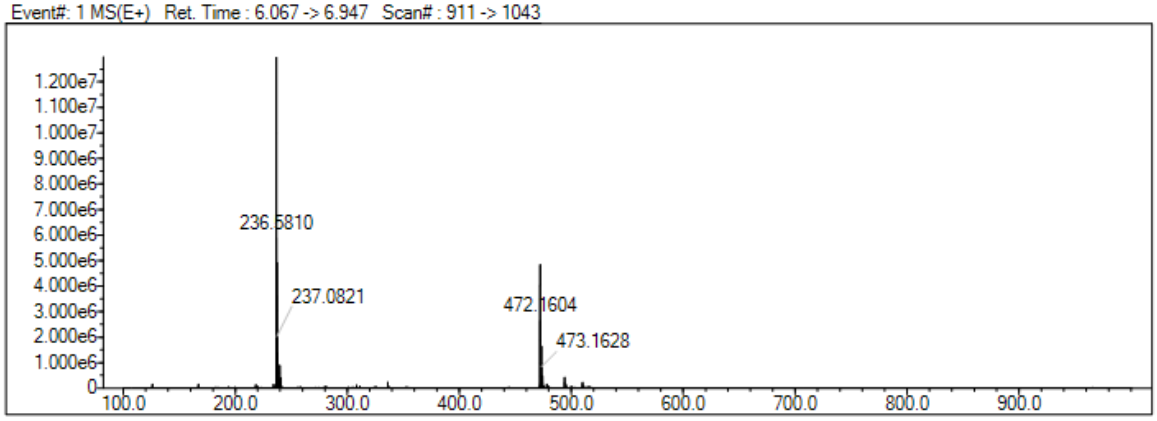
```
Current Data Parameters
NAME          Yusuf Ozkay
EXPNO                 359
PROCNO                  1

F2 - Acquisition Parameters
Date_           20160521
Time               13.05
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               297.6 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         300.1812067 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
```

Data File: C:\LabSolutions\Data\Analiz\uac\TU-73_11.lcd

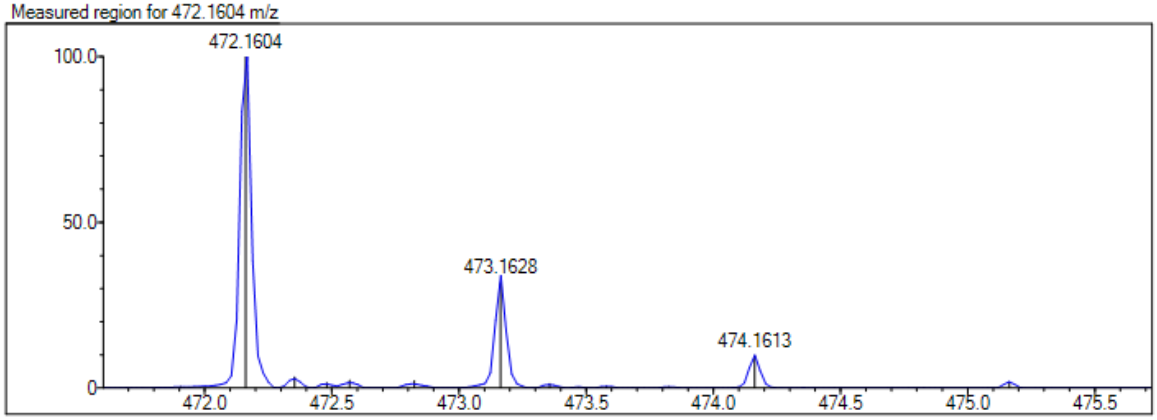
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	15	40	O	2	1	2	S	2	1	1	Ru	2	0	0	H
C	4	12	40	F	1	0	1	Cl	1	0	0	I	3	0	0	
N	3	1	6	P	3	0	0	Br	1	0	0					

Error Margin (ppm):	15	DBE Range:	5.0 - 25.0	Electron Ions:	both
HC Ratio:	unlimited	Apply N Rule:	yes	Use MSn Info:	no
Max Isotopes:	3	Isotope RI (%):	1.00	Isotope Res:	10000
MSn Iso RI (%):	10.00	MSn Logic Mode:	AND	Max Results:	500

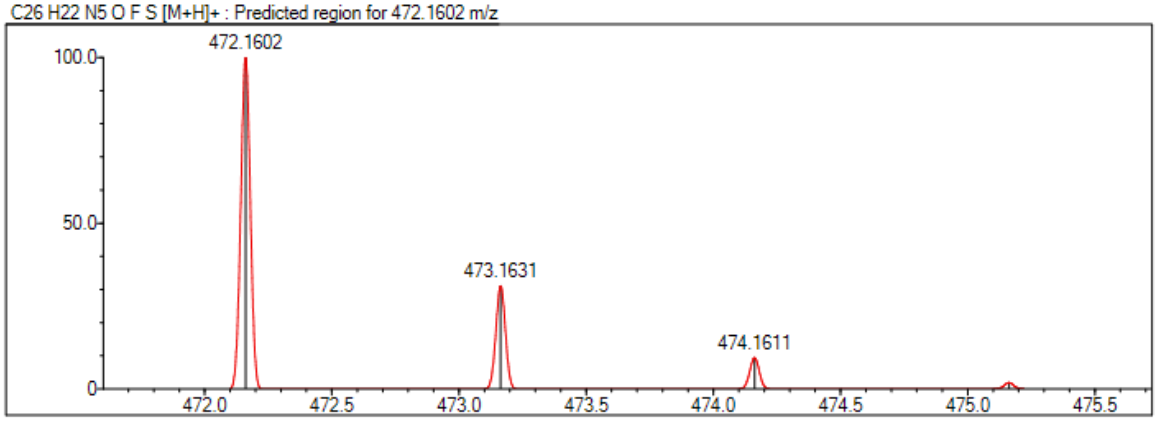
Event#: 1 MS(E+) Ret. Time : 6.067 -> 6.947 Scan# : 911 -> 1043



Measured region for 472.1604 m/z

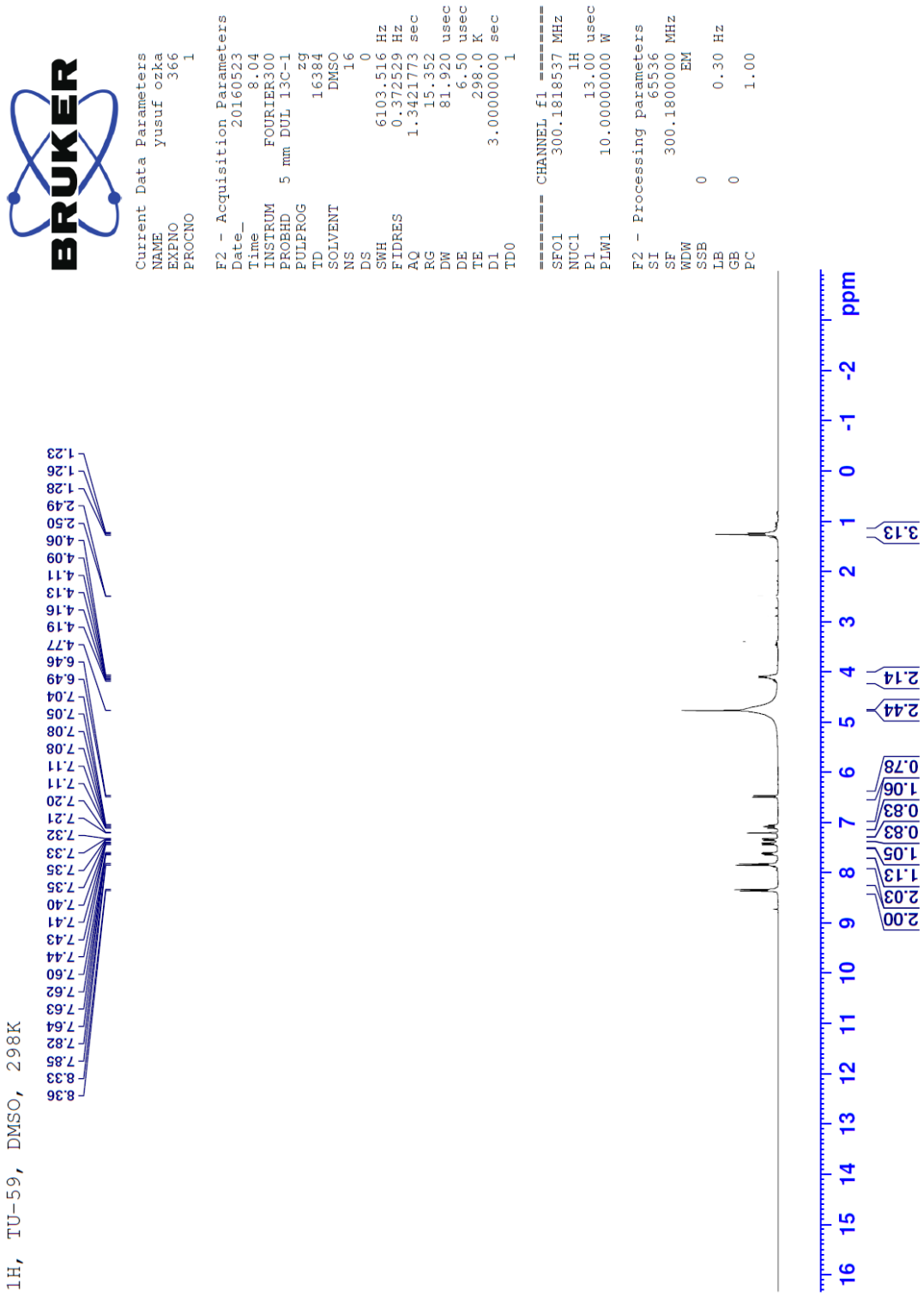


C26 H22 N5 O F S [M+H]+ : Predicted region for 472.1602 m/z

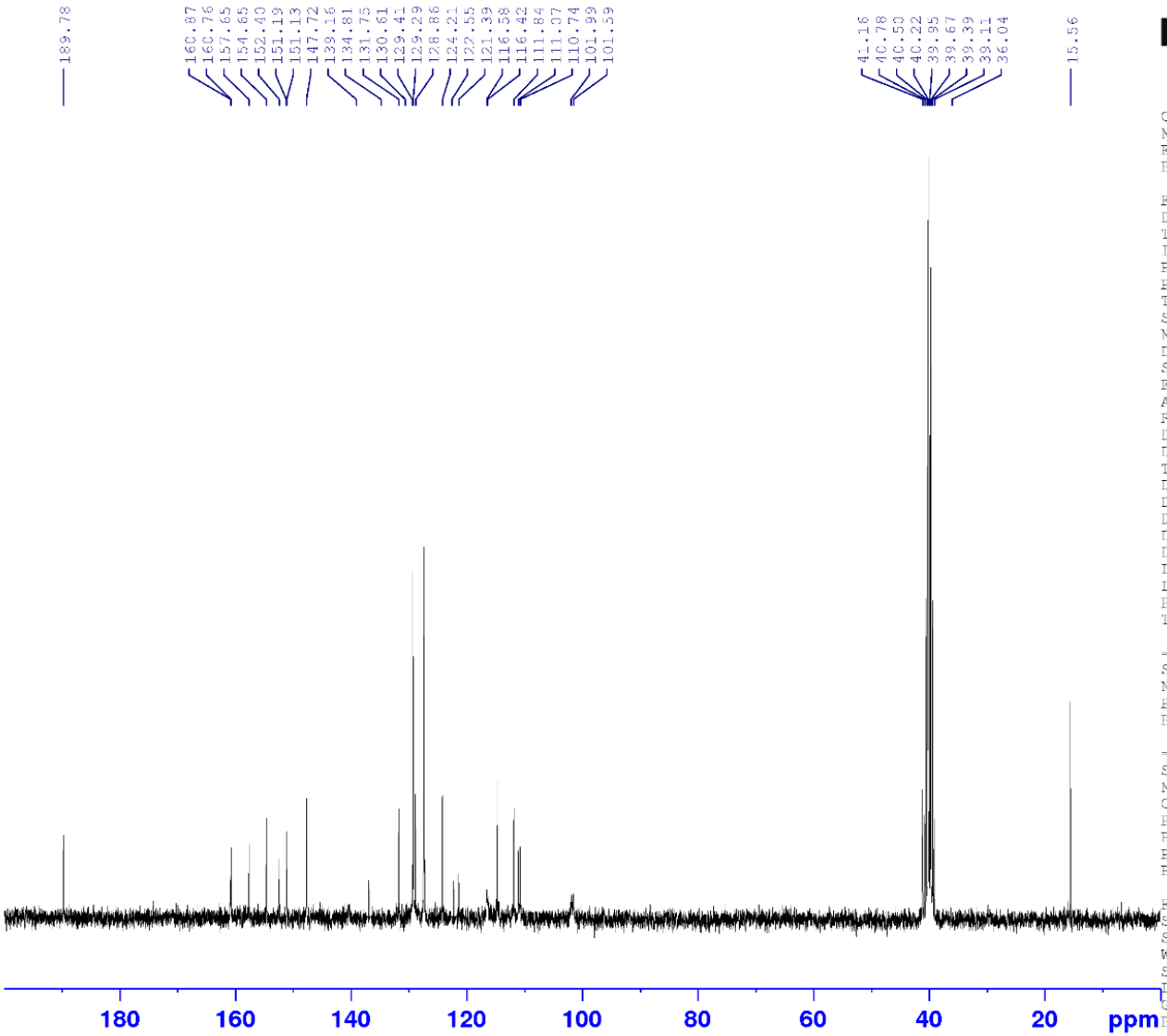


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	92.81	C26 H22 N5 O F S	[M+H]+	472.1604	472.1602	0.2	0.42	92.81	18.0

2-(4-(4-Ethyl-5-(2-(3,4-dihydroxyphenyl)-2-oxo-ethylthio)-4H-1,2,4-triazol-3yl)-phenyl)-5(6)-fluoro-1H- benzimidazole (3p)



13C, TU-59, DMSO, 298K



BRUKER

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Current Data Parameters
NAME          Yusuf Ozkay
EXPNO                 367
PROCNO                  1

F2 - Acquisition Parameters
Date_          20160523
Time               8.06
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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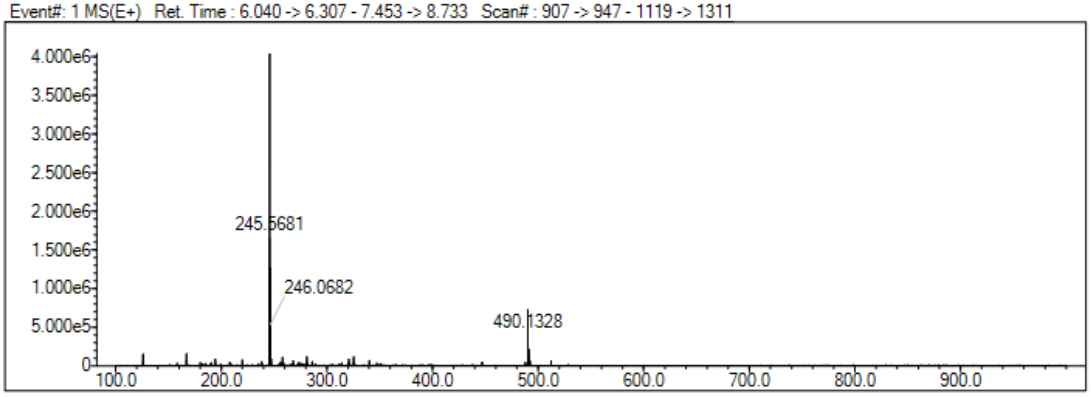
Data File: C:\LabSolutions\Data\Analiz\uac\TU-59_79.lcd

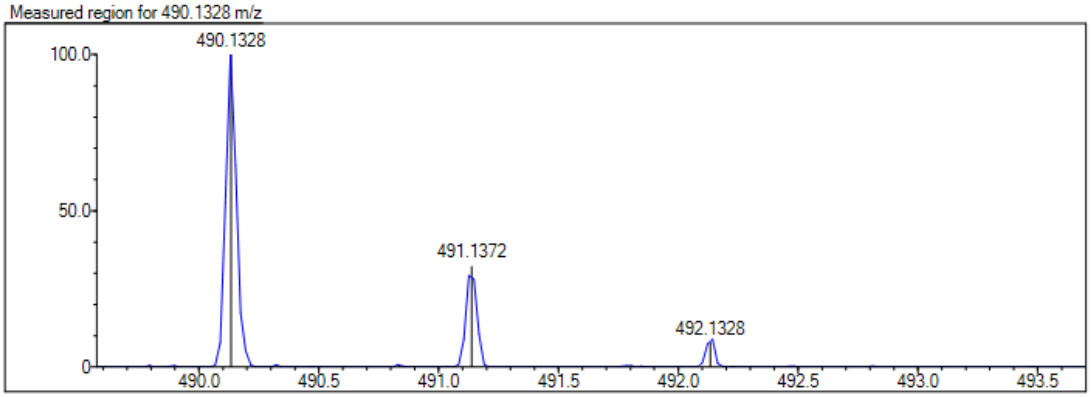
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	9	40	O	2	1	3	S	2	0	2	Ru	2	0	0	H
C	4	11	26	F	1	0	1	Cl	1	0	0	I	3	0	0	
N	3	0	6	P	3	0	0	Br	1	0	1					

Error Margin (ppm):	5	DBE Range:	17.0 - 20.0	Electron Ions:	both
HC Ratio:	unlimited	Apply N Rule:	yes	Use MSn Info:	no
Max Isotopes:	3	Isotope RI (%):	1.00	Isotope Res:	10000
MSn Iso RI (%):	10.00	MSn Logic Mode:	AND	Max Results:	500

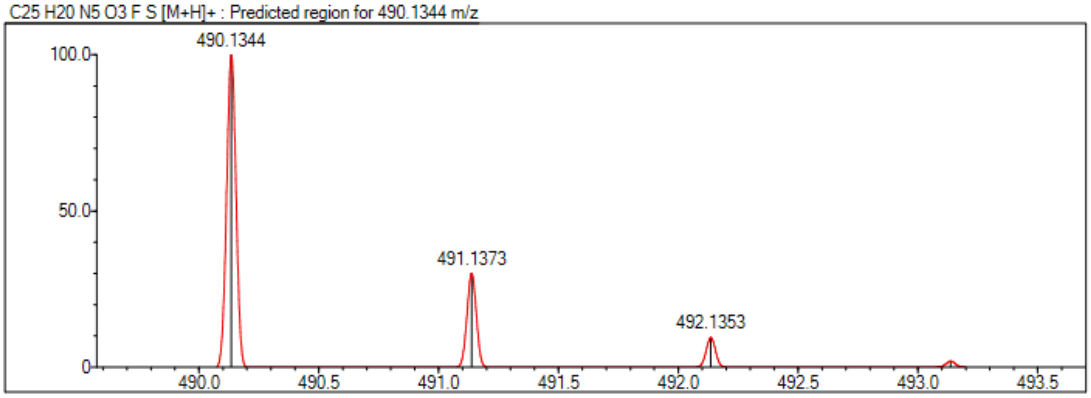
Event#: 1 MS(E+) Ret. Time : 6.040 -> 6.307 - 7.453 -> 8.733 Scan# : 907 -> 947 - 1119 -> 1311



Measured region for 490.1328 m/z



C25 H20 N5 O3 F S [M+H]+ : Predicted region for 490.1344 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	76.02	C25 H20 N5 O3 F S	[M+H]+	490.1328	490.1344	-1.6	-3.26	80.57	18.0

Structure of the synthesized compounds were elucidated by IR, ^{1}H NMR, ^{13}C NMR and HRMS analysis. In ^{1}H-NMR spectra, protons belonging to methylene bridge were recorded between 4.80 ppm and 2.64 ppm. Methyl protons in the methyl substituted derivatives (**5a-5d** and **5i-5l**) had singlet peak at 3.71 ppm or 3.72 ppm. Ethyl protons in the ethyl substituted derivatives (**5e-5h** and **5m-5p**) were observed as triplet and quartet peaks at 1.26 ppm- 1.28 ppm and 4.10 ppm- 4.12 ppm, respectively. Protons of aromatic rings were recorded between 6.81 ppm and 8.34 ppm and benzimidazole NH had singlet peak over 13.20 ppm. In ^{13}C-NMR, aliphatic carbons recorded between 15 ppm and 49 ppm and aromatic carbons gave peak from 97 ppm to 163 ppm. Carbonyl carbon were recorded around 190 ppm. Carbon-fluorine splitting in the fluorinated compounds were observed as expected. In high resolution mass spectrum, all masses were found as expected with maximum 5 ppm difference. In the mass spectrum, all masses were matched with the expected M+H values

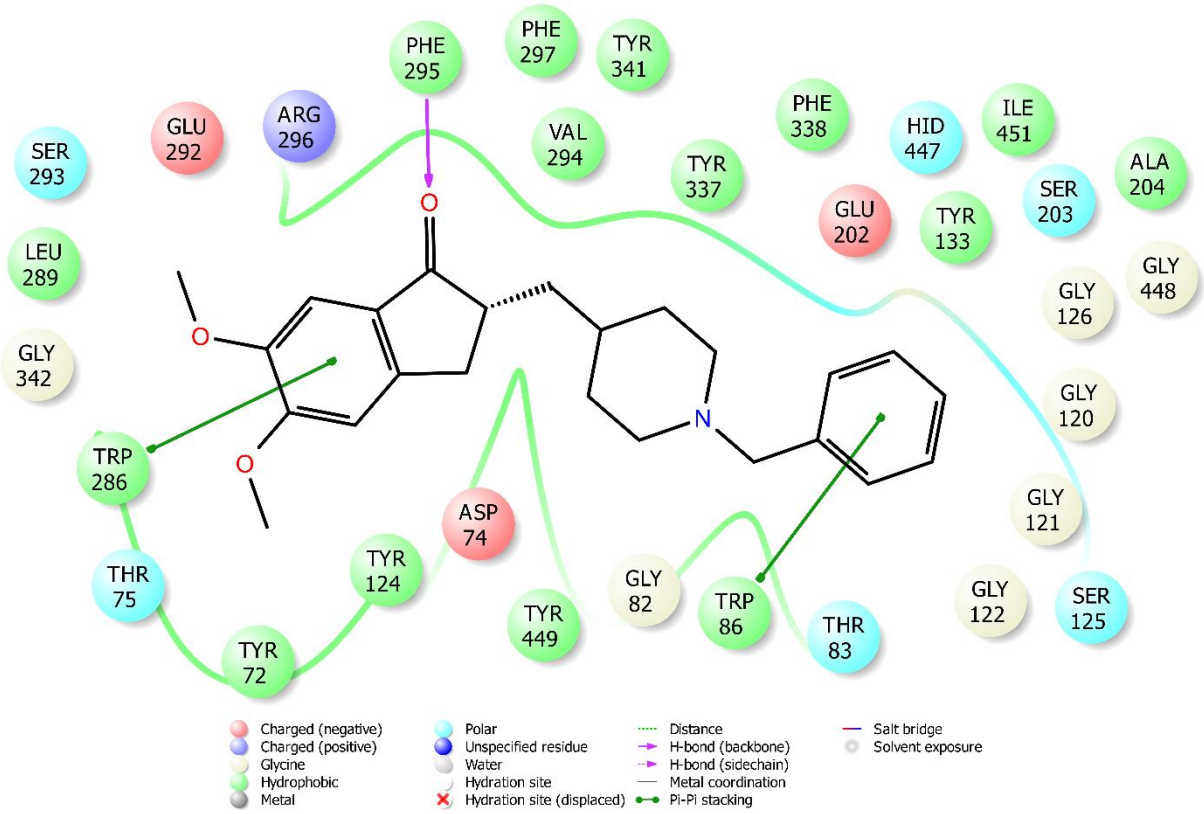


Figure S1. Two-dimensional interaction mode of donepezil in the enzyme active site of AChE.

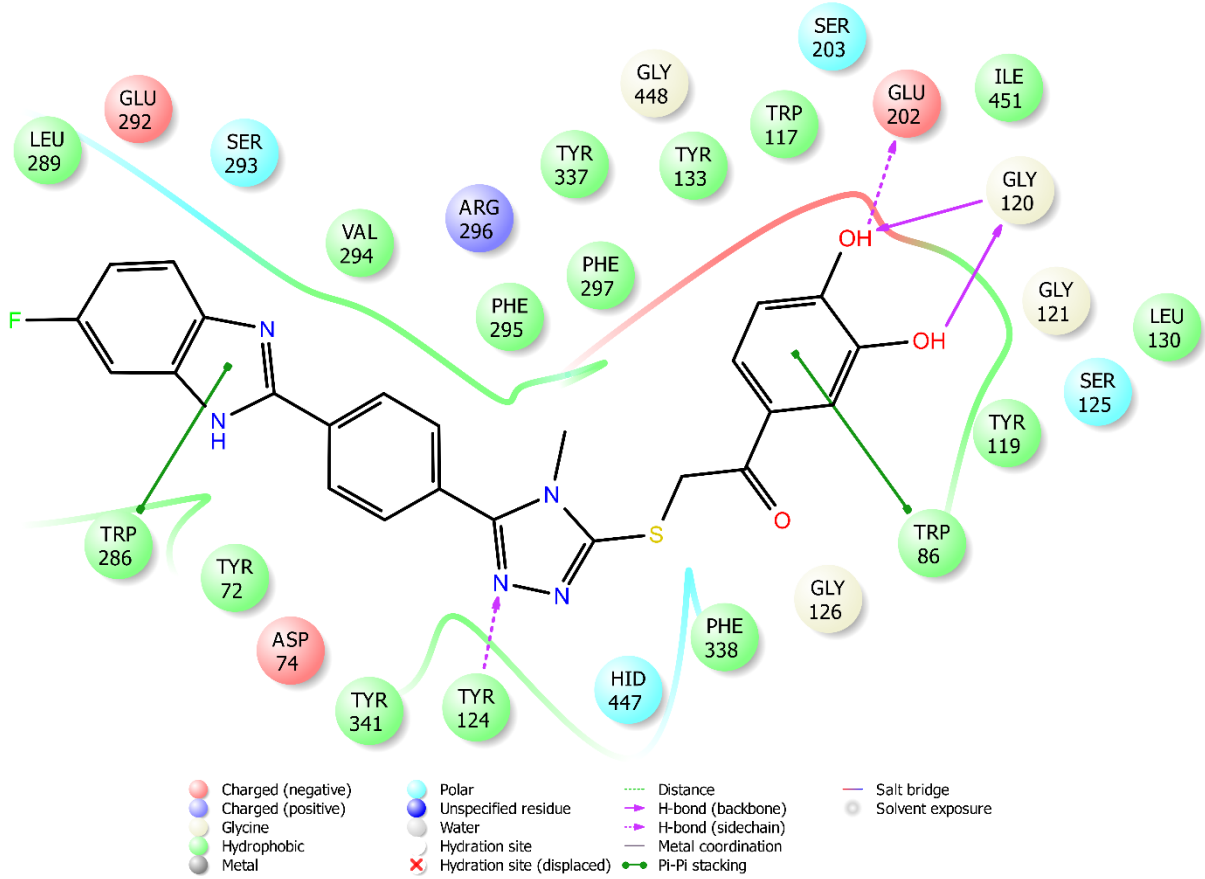


Figure S2. Two-dimensional interaction mode of compound **5l** in the enzyme active site of AChE.

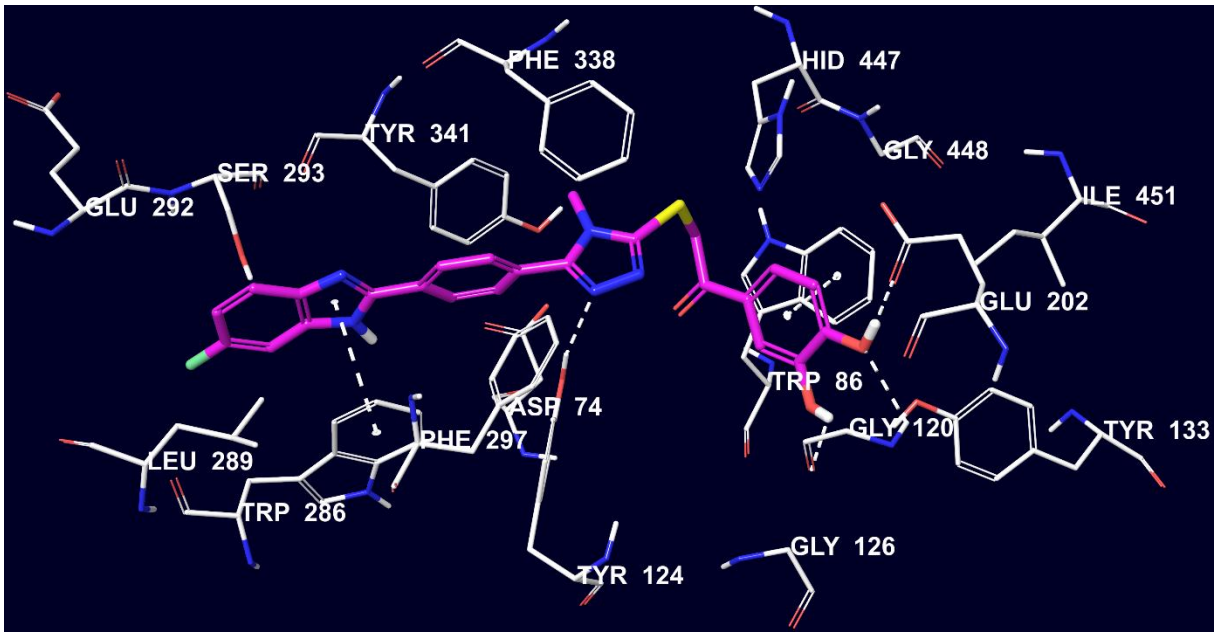


Figure S3. The interacting mode of compound **5l** in the active region of AChE. The inhibitor, colored with pink, and the important residues, colored with white, in the active site of the enzyme are presented by tube model.

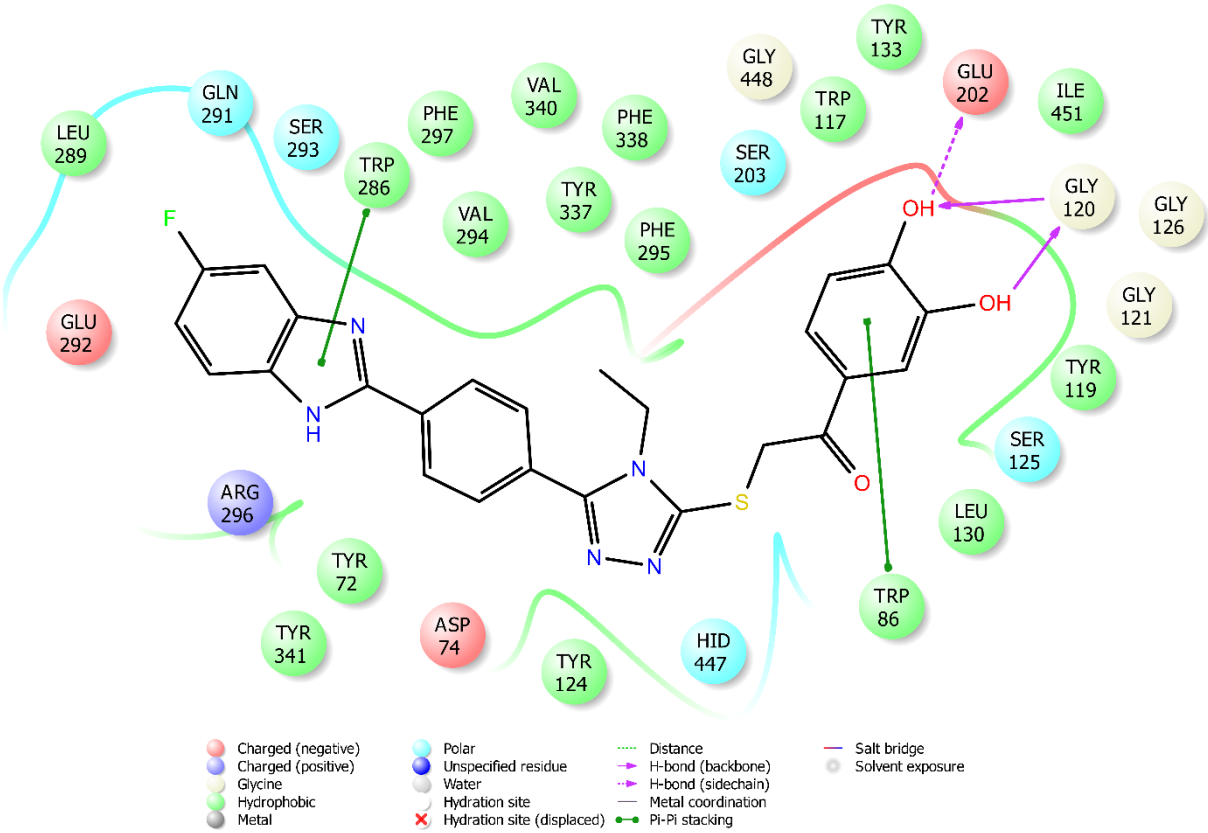


Figure S4. Two-dimensional interaction mode of compound **5p** in the enzyme active site of AChE.

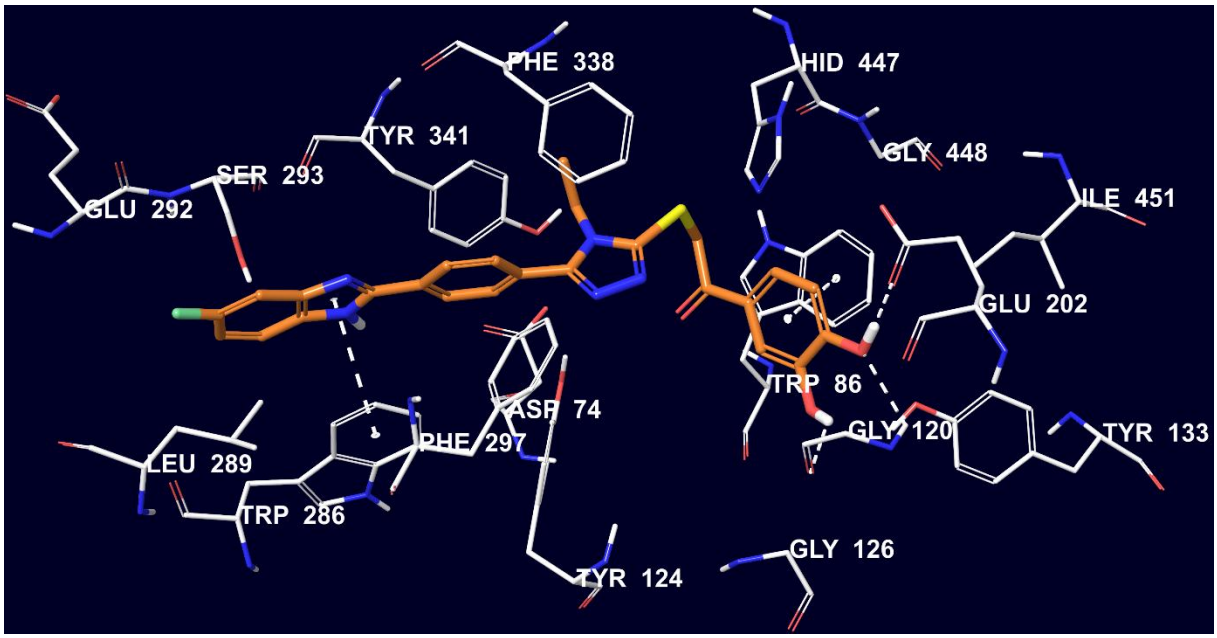


Figure S5. The interacting mode of compound **5p** in the active region of AChE. The inhibitor, colored with orange, and the important residues, colored with white, in the active site of the enzyme are presented by tube model.

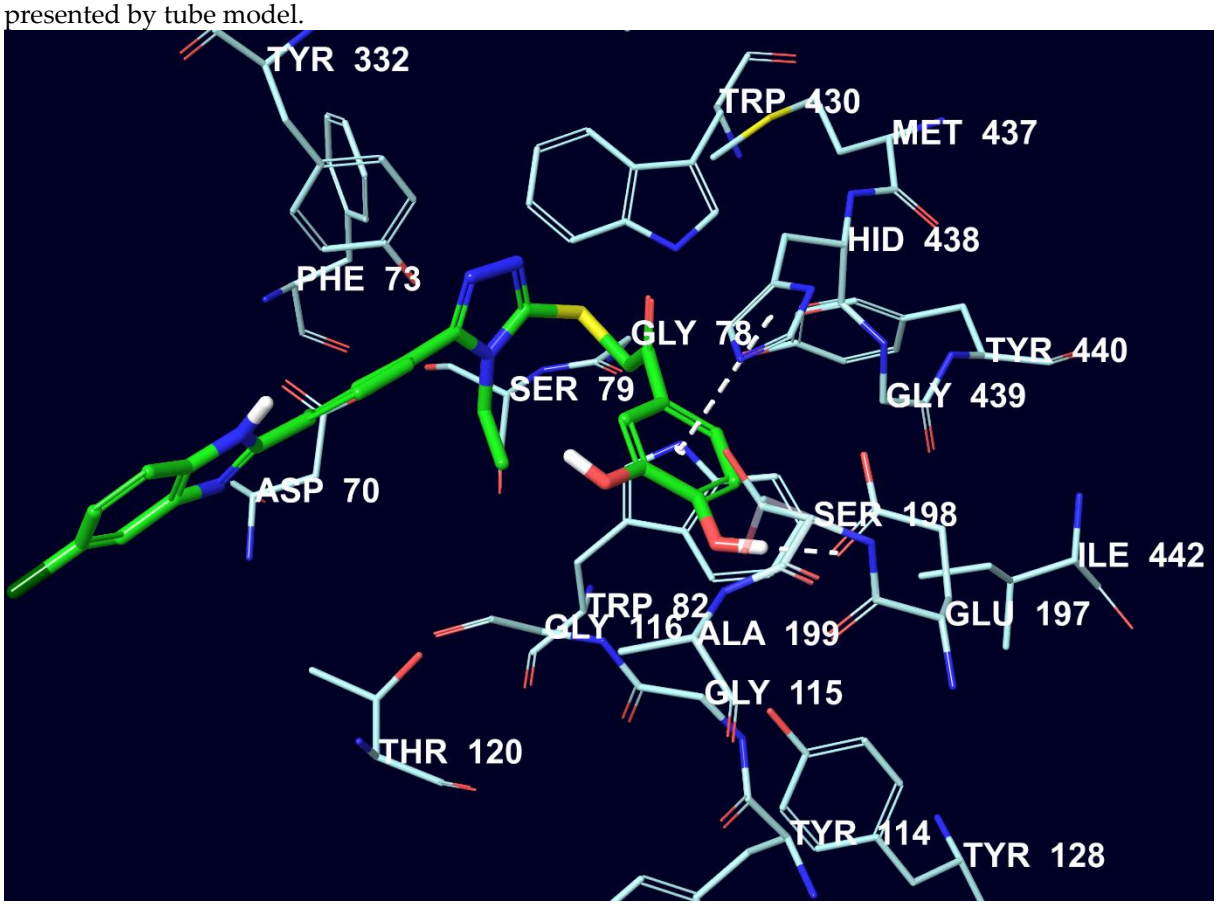


Figure S6. The interacting mode of compound **5h** in the active region of BChE. The inhibitor, colored with green, and the important residues, colored with turquoise, in the active site of the enzyme are presented by tube model.