Novel benzimidazole based compounds as antimicrobial: synthesis, molecular docking, molecular dynamics and *in silico* ADME profile studies

Elif Yeşilçayır[1], İsmail Çelik[2], Hasan Tahsin Şen[1,3], Suna Sibel Gürpınar[4], Müjde Eryılmaz[4], Gülgün Ayhan-Kılcıgil[1]*

[1]Ankara University, Faculty of Pharmacy, Department of Pharmaceutical Chemistry, Ankara, Turkey

[2]Erciyes University, Faculty of Pharmacy, Department of Pharmaceutical Chemistry, Kayseri, Turkey

[3]Lokman Hekim University, Faculty of Pharmacy, Department of Pharmaceutical Chemistry, Ankara, Turkey

[4]Ankara University, Faculty of Pharmacy, Department of Pharmaceutical Microbiology, Ankara, Turkey

^{1}H NMR, ^{13} C NMR and MS spectra of compounds 2 and 3

EG1

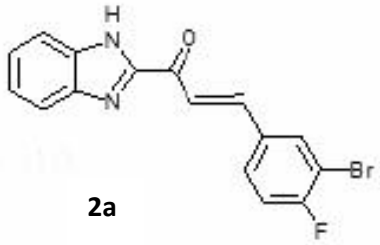
Sample Name:
EG1
Data Collected on:
mercury400-mercury400
Archive directory:
/home/vnmr1/vnmrsys/data
Sample directory:
EG1_20210427_01
FidFile: PROTON_03

Pulse Sequence: PROTON (s2pul)
Solvent: dmso
Data collected on: Apr 27 2021

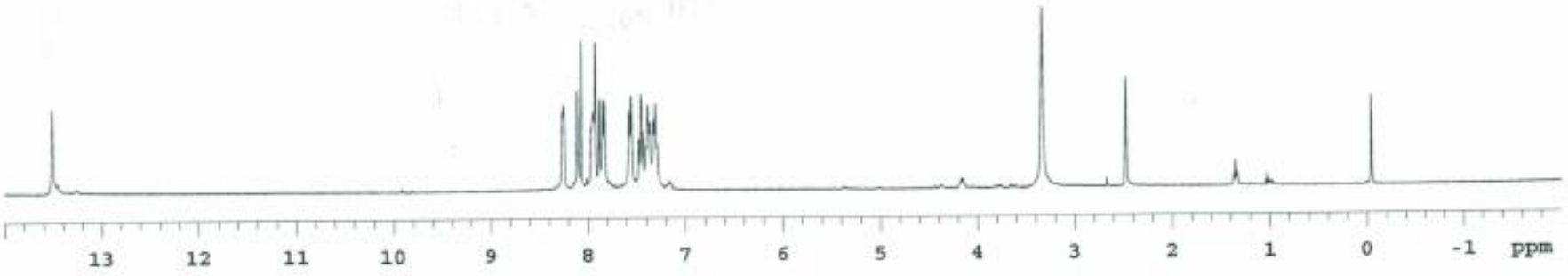
Temp. 25.0 C / 298.1 K
Operator: vnmr1

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.559 sec
Width 6402.0 Hz
16 repetitions
OBSERVE H1, 400.1759761 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 0 sec

Agilent Technologies



2a



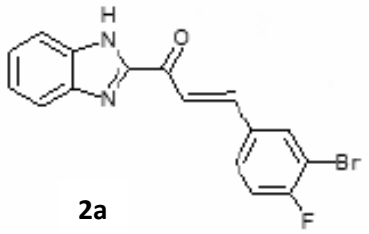
EG1

Sample Name:
EG1
Data Collected on:
mercury400-mercury400
Archive directory:
/home/vnmr1/vnmrsys/data
Sample directory:
EG1_20210427_01
FidFile: current

Pulse Sequence: CARBON (s2pul)
Solvent: dmso
Data collected on: Apr 27 2021

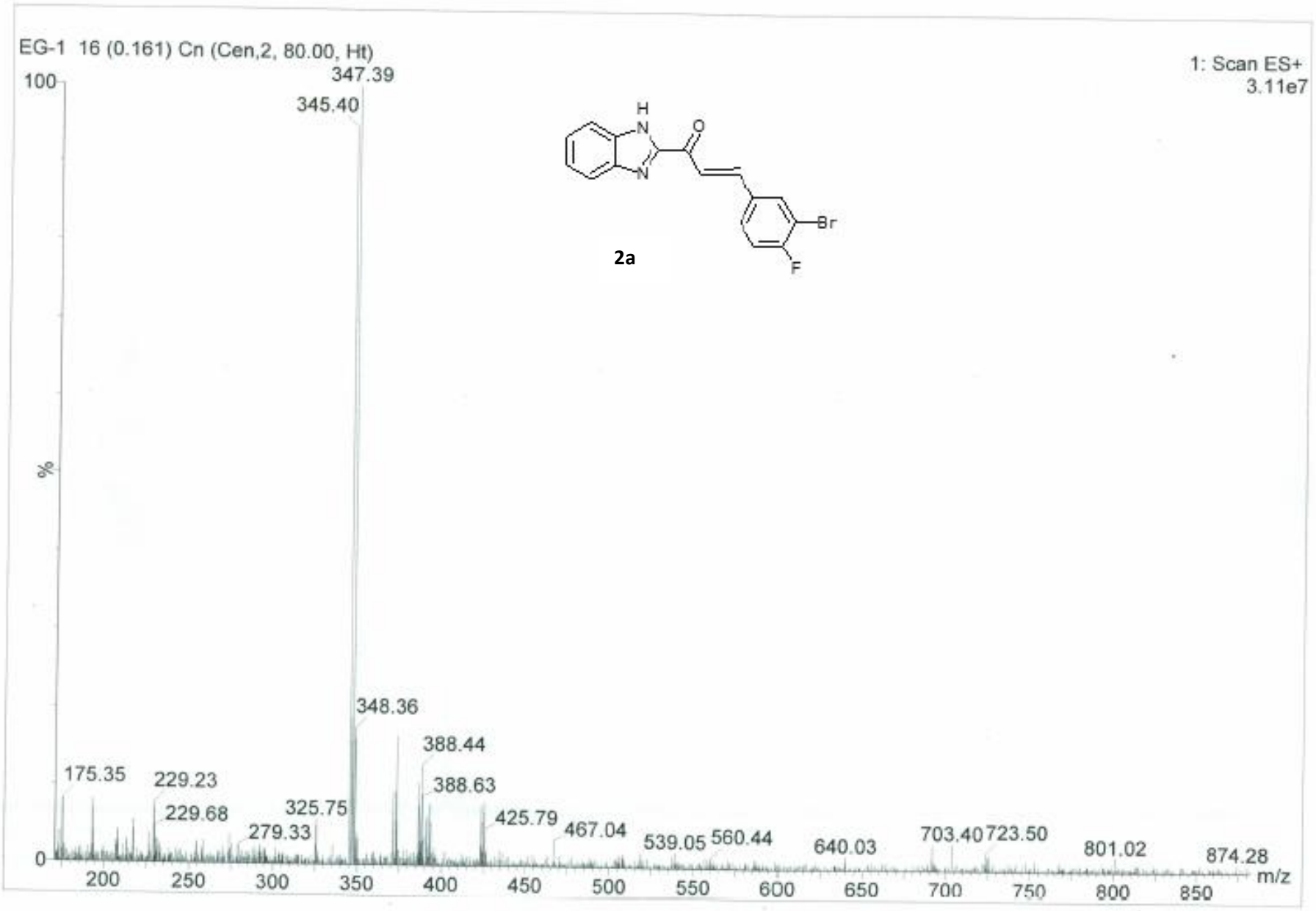
Temp. 25.0 C / 298.1 K
Operator: vnmr1

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.304 sec
Width 25125.6 Hz
256 repetitions
OBSERVE C13, 100.6243728 MHz
DECOUPLE H1, 400.1779555 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line Broadening 0.5 Hz
FT size 65536
Total time 40 min

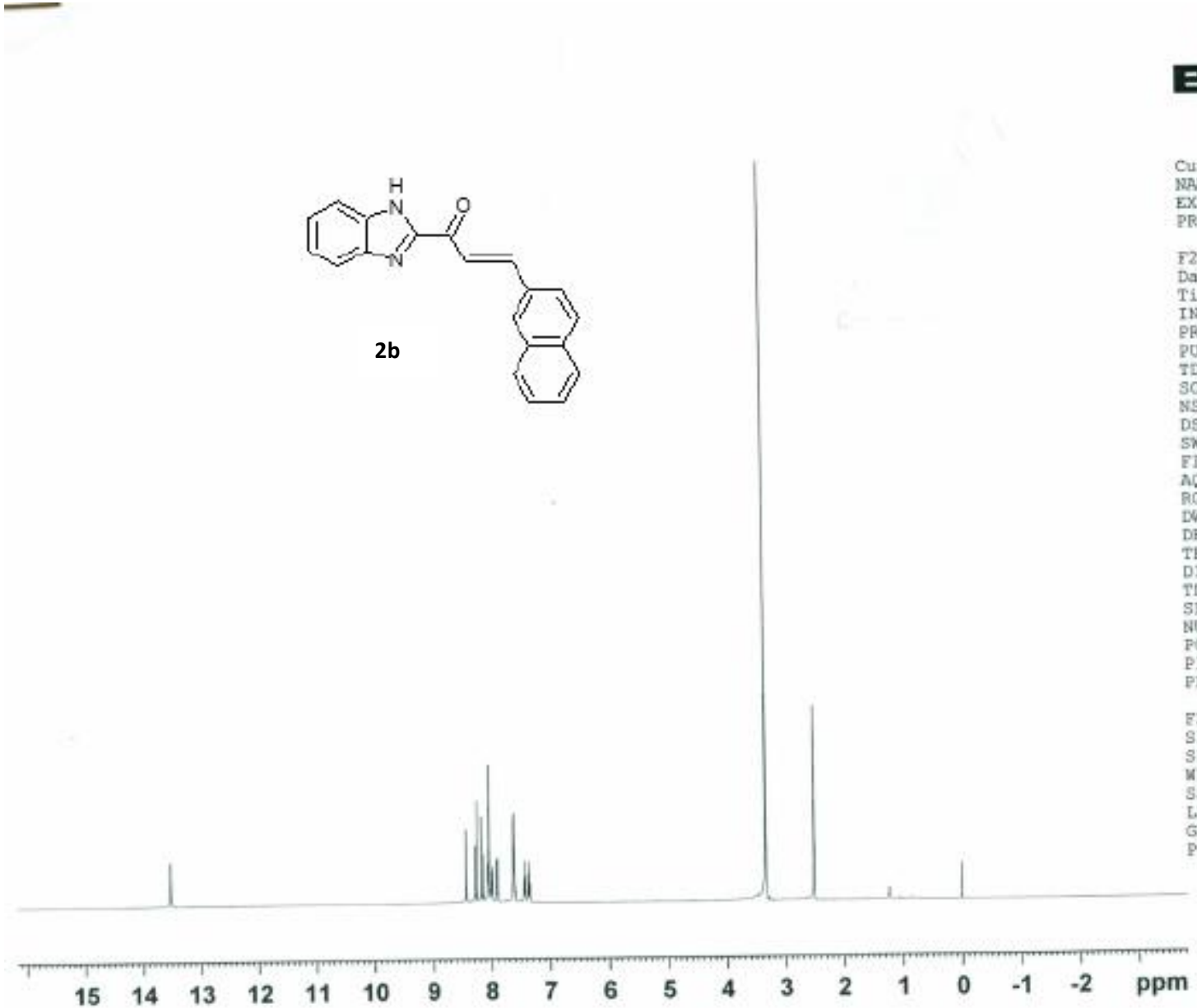


2a

Agilent Technologies

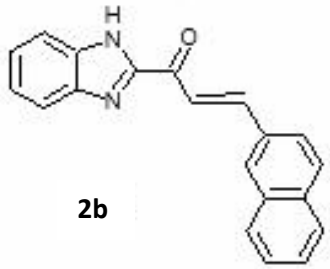

EG-1 16 (0.161) Cn (Cen,2, 80.00, Ht)
1: Scan ES+
3.11e7
100
%
0
347.39
345.40
348.36
388.44
388.63
175.35
229.23
229.68
325.75
279.33
425.79
467.04
539.05
560.44
640.03
703.40
723.50
801.02
874.28
200
250
300
350
400
450
500
550
600
650
700
750
800
850
m/z
H
N
N
O
Br
F

2a



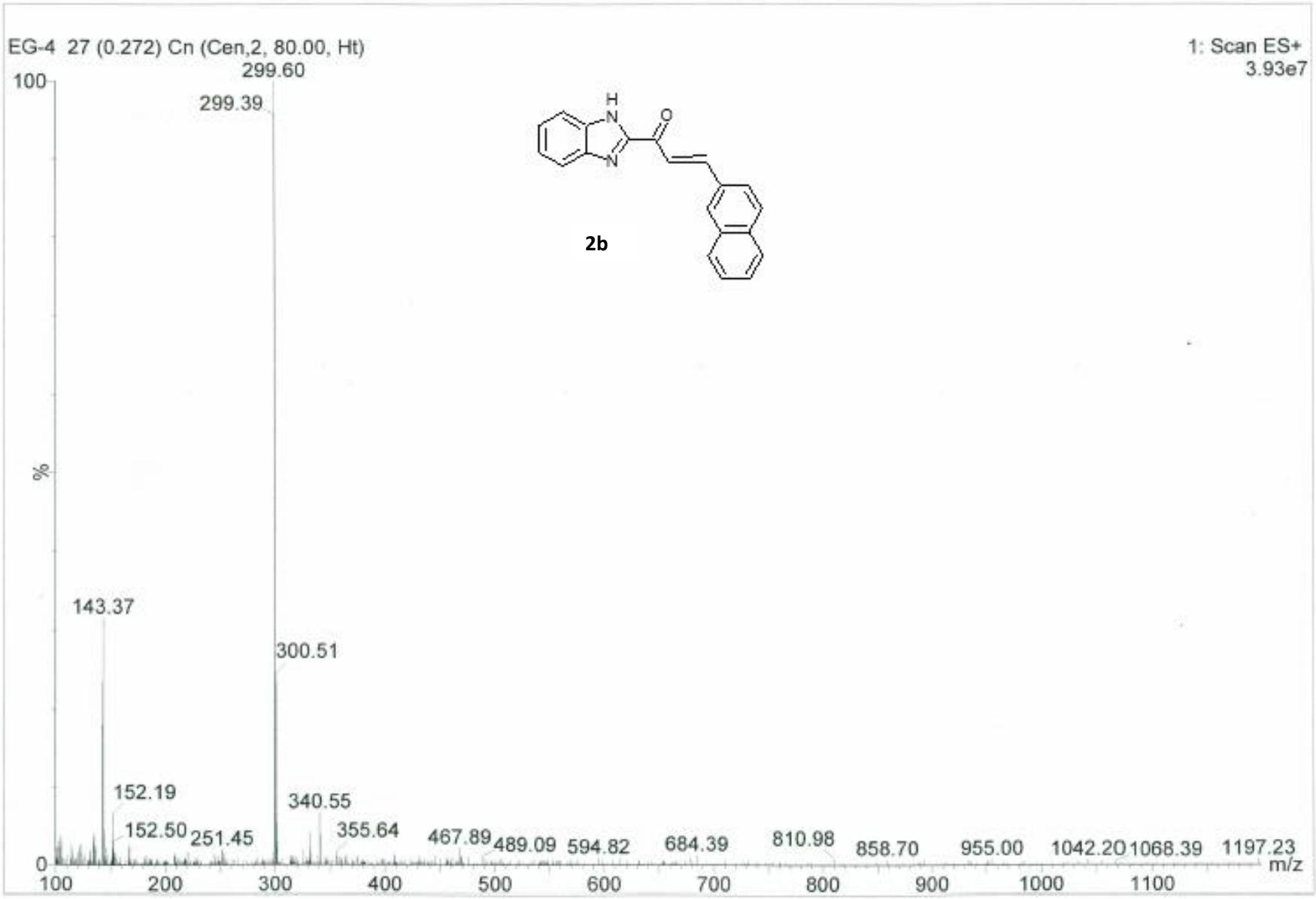
BRUKER

```
Current Data Parameters
NAME                  EG-4.2
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20210420
Time                  12.35 h
INSTRUM              Avance
PROBHD   Z151574_0038 (
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                        16
DS                         2
SWH               10000.000 Hz
FIDRES                0.305176 Hz
AQ                3.2767999 sec
RG                       101
DW                   50.000 usec
DE                   11.14 usec
TE                   297.4 K
D1               1.00000000 sec
TD0                        1
SFO1           500.1330883 MHz
NUC1                      1H
P0                   2.67 usec
P1                   8.00 usec
PLW1           24.04299927 W

F2 - Processing parameters
SI                    65536
SF             500.1300000 MHz
WDW                      EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
```

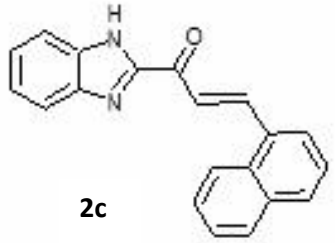


2b

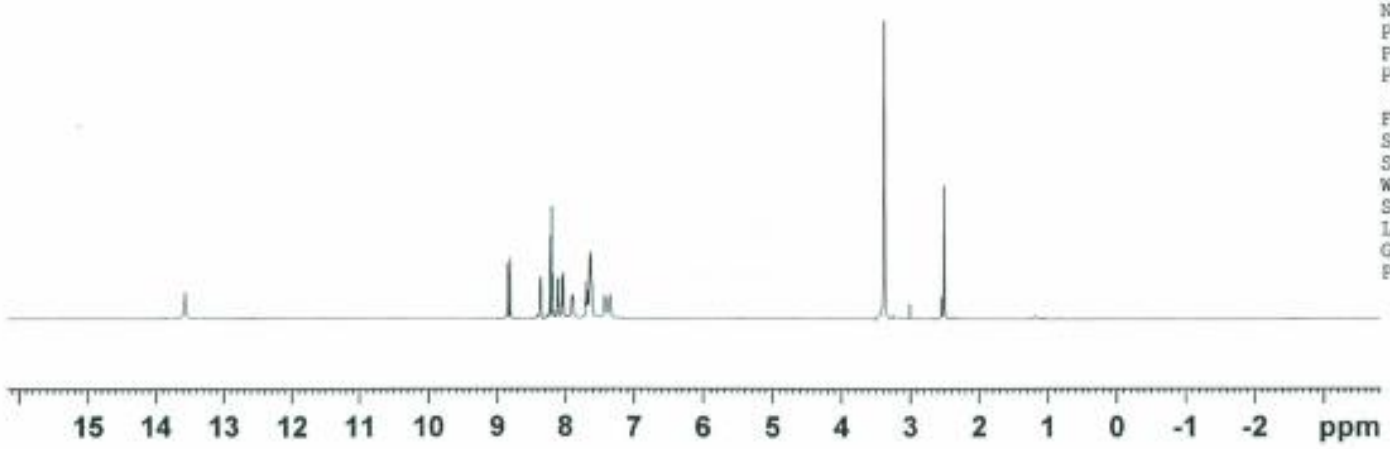

```
Current Data Parameters
NAME                  EG-4.2
EXPNO                      3
PROCNO                     1

F2 - Acquisition Parameters
Date_              20210429
Time                 16.08 h
INSTRUM              Avance
PROBHD    Z151574_0038 (
PULPROG              zgpg30
TD                    65536
SOLVENT                DMSO
NS                      3000
DS                         4
SWH               30120.482 Hz
FIDRES             0.919204 Hz
AQ                1.0878977 sec
RG                       101
DW                    16.600 usec
DE                     6.50 usec
TE                    298.8 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                        1
SFO1           125.7703643 MHz
NUC1                    13C
P0                     3.33 usec
P1                    10.00 usec
PLW1           85.18099976 W
SFO2           500.1320005 MHz
NUC2                    1H
CPDPRG[2             waltz65
PCPD2                 80.00 usec
PLW2           24.04299927 W
PLW12           0.24043000 W
PLW13           0.12093000 W

F2 - Processing parameters
SI                     32768
SF             125.7577885 MHz
WDW                       EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```


EG-4 27 (0.272) Cn (Cen,2, 80.00, Ht)
1: Scan ES+
3.93e7
100
%
0
299.60
299.39
143.37
300.51
152.19
152.50
251.45
340.55
355.64
467.89
489.09
594.82
684.39
810.98
858.70
955.00
1042.20
1068.39
1197.23
m/z
100
200
300
400
500
600
700
800
900
1000
1100
H
N
N
O

2b

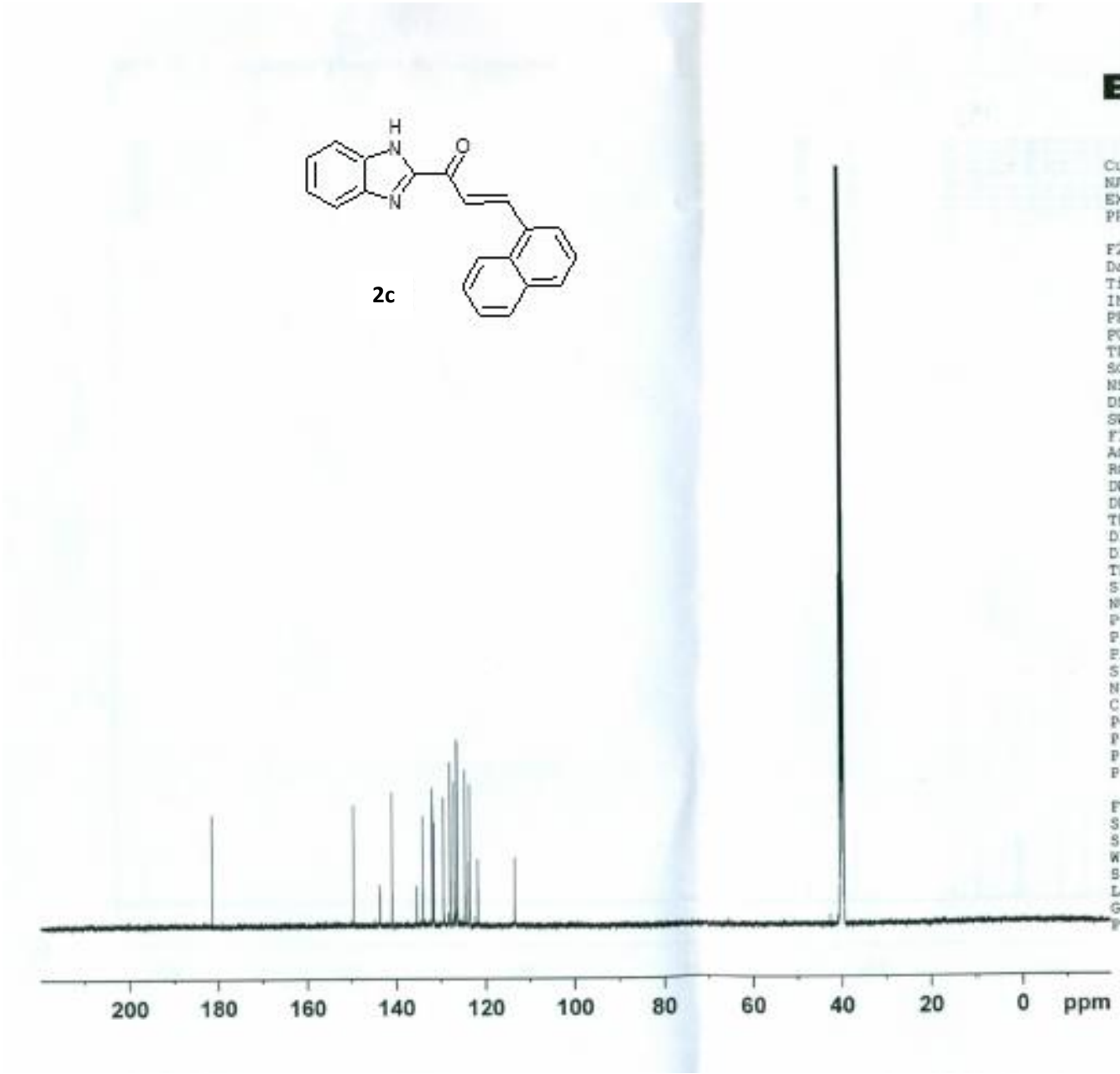


2c



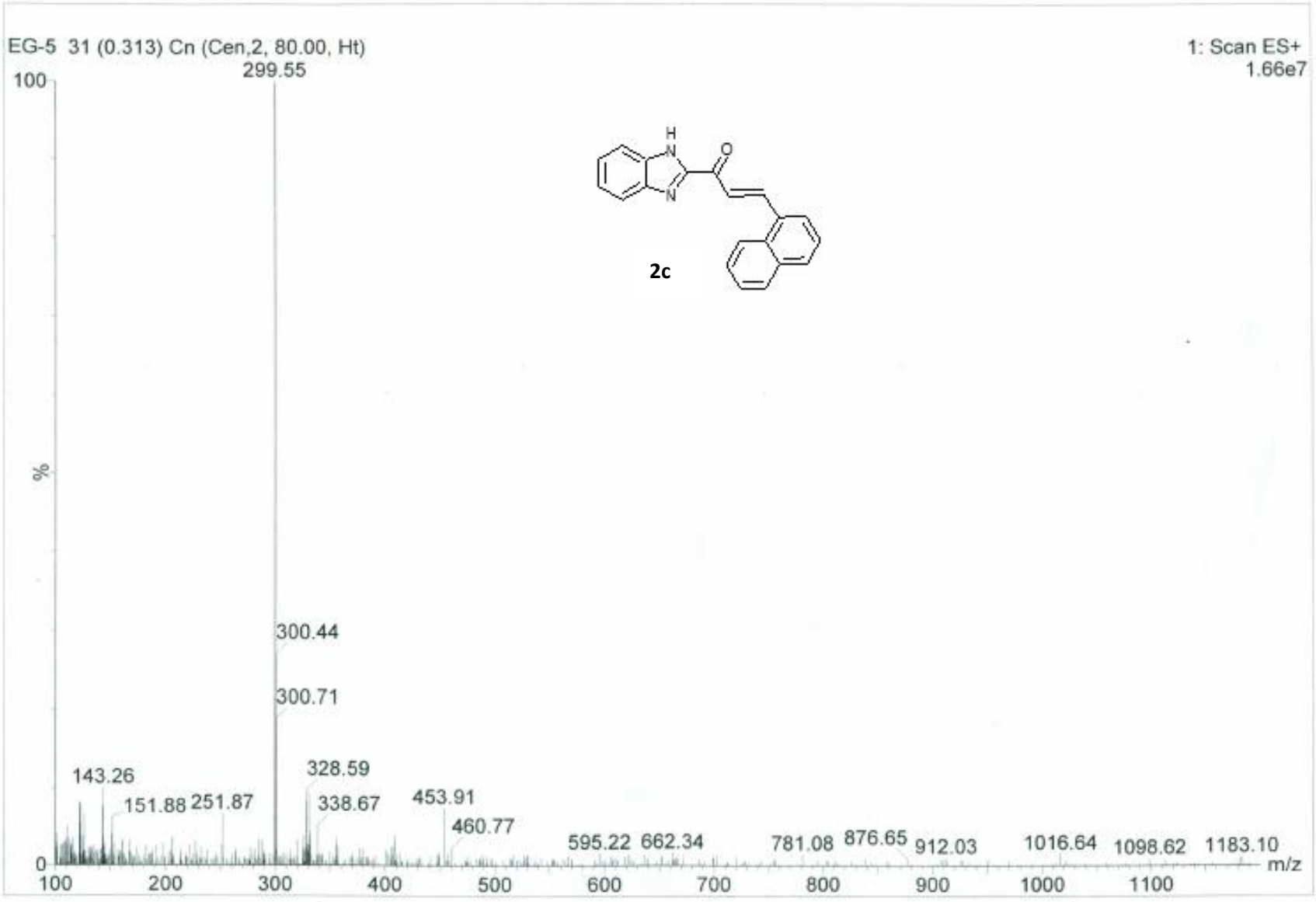
BRUKER

```
Current Data Parameters
NAME                  EG-5
EXPNO                    4
PROCNO                   1

F2 - Acquisition Parameters
Date_              20210811
Time                 16.25 h
INSTRUM              Avance
PROBHD   Z151574_0038 (
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                       16
DS                        2
SWH              10000.000 Hz
FIDRES               0.305176 Hz
AQ                3.2767999 sec
RG                       101
DW                    50.000 usec
DE                    11.14 usec
TE                    297.1 K
D1               1.00000000 sec
TD0                       1
SFO1           500.1330883 MHz
NUC1                     1H
P0                    2.67 usec
P1                    8.00 usec
PLW1          24.04299927 W

F2 - Processing parameters
SI                    65536
SF             500.1300000 MHz
WDW                      EM
SSB          0
LB                    0.30 Hz
GB           0
PC                    1.00
```



BRUKER

```
Current Data Parameters
NAME                  EG-5
EXPNO                    6
PROCNO                   1

F2 - Acquisition Parameters
Date_              20210812
Time                 10.15 h
INSTRUM              Avance
PROBHD    Z151574_0038 (
PULPROG              zgpg30
TD                    65536
SOLVENT                DMSO
NS                     1200
DS                        4
SWH               30120.482 Hz
FIDRES             0.919204 Hz
AQ                1.0878977 sec
RG                      101
DW                   16.600 usec
DE                    6.50 usec
TE                   298.2 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                       1
SFO1           125.7703643 MHz
NUC1                    13C
P0                    3.33 usec
P1                   10.00 usec
PLW1           85.18099976 W
SFO2           500.1320005 MHz
NUC2                    1H
CPDPRG[2             waltz65
PCPD2                80.00 usec
PLW2           24.04299927 W
PLW12           0.24043000 W
PLW13           0.12093000 W

F2 - Processing parameters
SI                    32768
SF             125.7577885 MHz
WDW                      EM
SSB          0
LB                    1.00 Hz
GB           0
PC                    1.40
```


EG-5 31 (0.313) Cn (Cen,2, 80.00, Ht)
1: Scan ES+
1.66e7
100
%
0
299.55
300.44
300.71
143.26
151.88
251.87
328.59
338.67
453.91
460.77
595.22
662.34
781.08
876.65
912.03
1016.64
1098.62
1183.10
m/z
100
200
300
400
500
600
700
800
900
1000
1100
H
N
N
O
2c

EG7

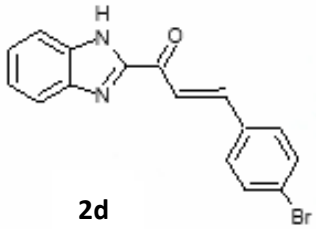
Sample Name:
EG7
Data Collected on:
mercury400-mercury400
Archive directory:
/home/vnmr1/vnmrsys/data
Sample directory:
EG7_20210427_01
FidFile: PROTON_02

Pulse Sequence: PROTON (s2pul)
Solvent: dmso
Data collected on: Apr 27 2021

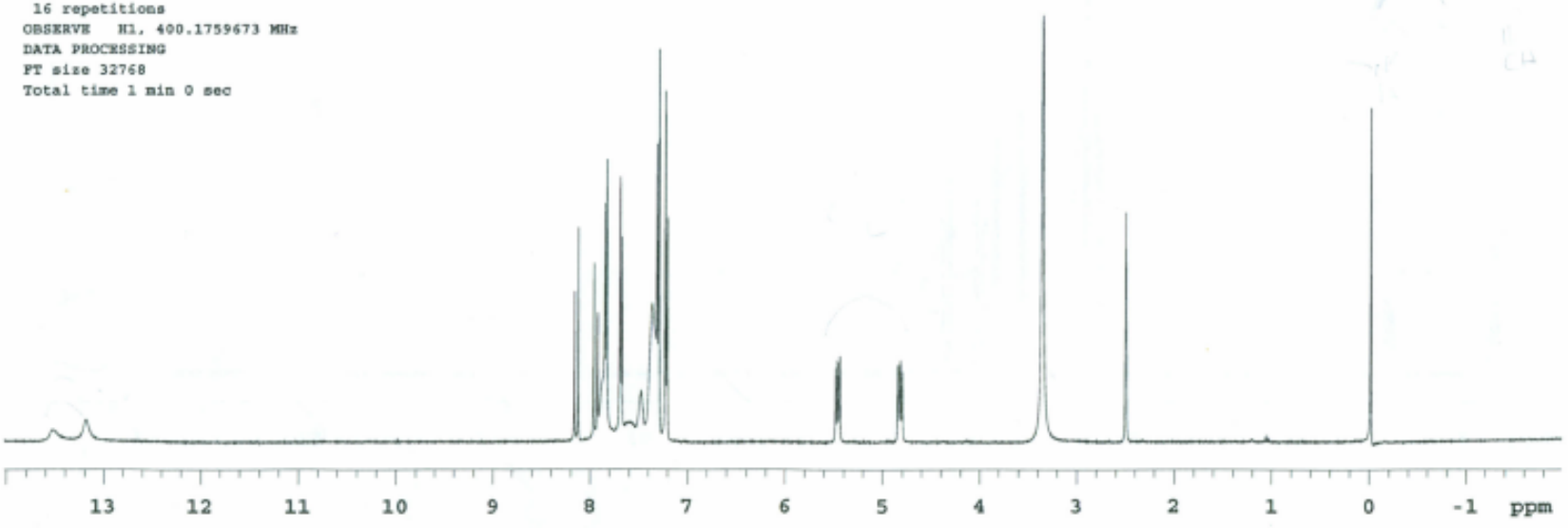
Temp. 25.0 C / 298.1 K
Operator: vnmr1

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.559 sec
Width 6402.0 Hz
16 repetitions
OBSERVE H1, 400.1759673 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 0 sec

Agilent Technologies



2d



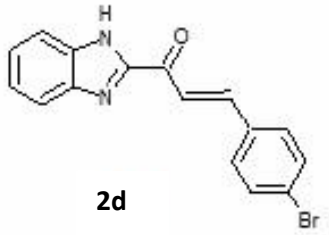
EG7

Sample Name:
EG7
Data Collected on:
mercury400-mercury400
Archive directory:
/home/vnmrl/vnmrsys/data
Sample directory:
EG7_20210427_01
PidFile: CARBON_01

Pulse Sequence: CARBON (s2pul)
Solvent: dmso
Data collected on: Apr 27 2021

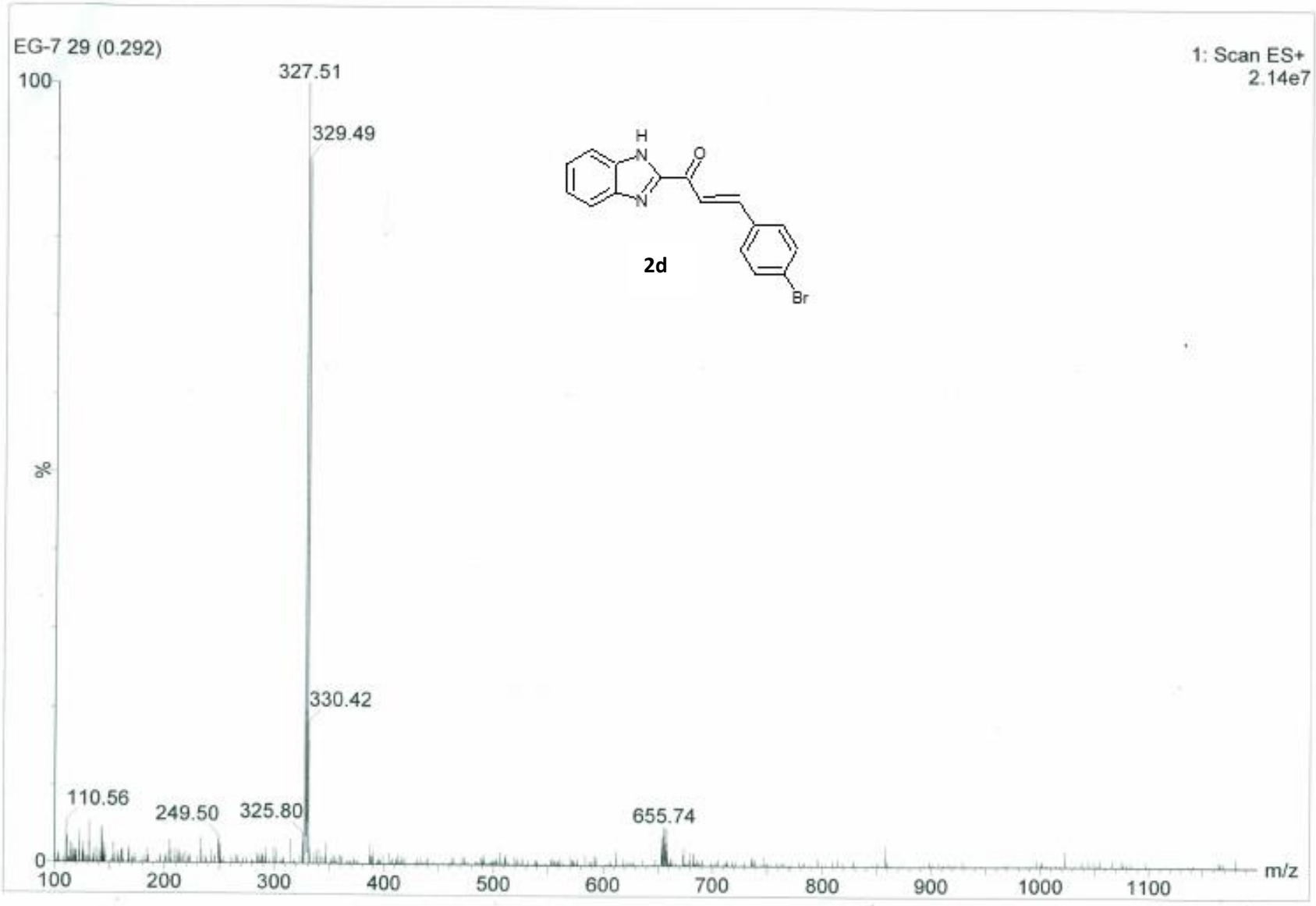
Temp. 25.0 C / 298.1 K
Operator: vnmrl

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.304 sec
Width 25125.6 Hz
1500 repetitions
OBSERVE C13, 100.6243735 MHz
DECOUPLE H1, 400.1779555 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 1 hr



2d

Agilent Technologies


EG-7 29 (0.292)
1: Scan ES+
2.14e7
100
%
0
327.51
329.49
330.42
110.56
249.50
325.80
655.74
100
200
300
400
500
600
700
800
900
1000
1100
m/z
H
N
N
O
Br

2d

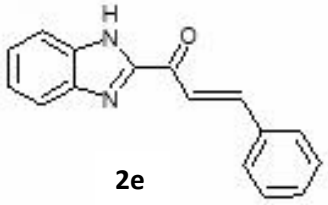
EG-8

Sample Name:
EG-8
Data Collected on:
mercury400-mercury400
Archive directory:
/home/vnmr1/vnmrsys/data
Sample directory:
EG-8_20210811_01
FidFile: CARBON_01

Pulse Sequence: CARBON (s2pul)
Solvent: dmso
Data collected on: Aug 11 2021

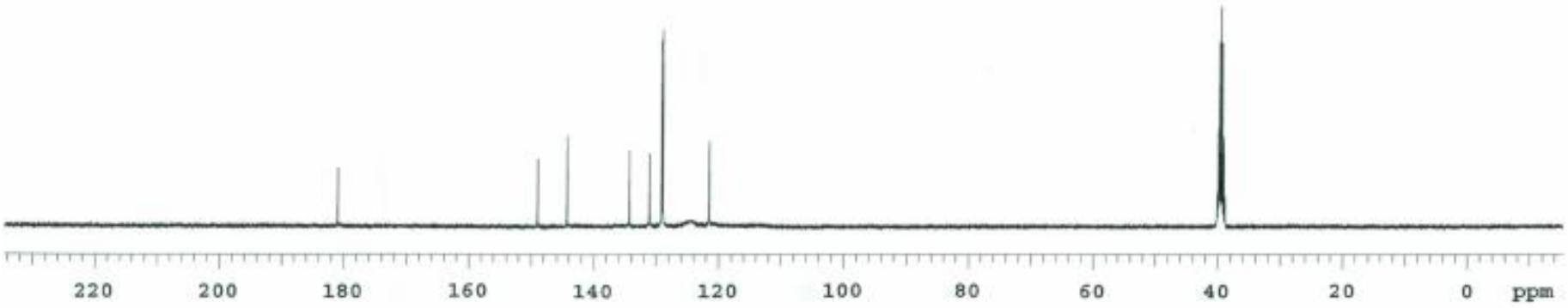
Temp. 25.0 C / 298.1 K
Operator: vnmr1

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.304 sec
Width 25125.6 Hz
1000 repetitions
OBSERVE C13, 100.6243743 MHz
DECOUPLE H1, 400.1779555 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 40 min



2e

Agilent Technologies



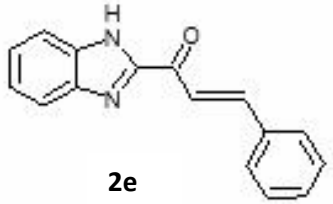
EG-8

Sample Name:
EG-8
Data Collected on:
mercury400-mercury400
Archive directory:
/home/vnmr1/vnmrsys/data
Sample directory:
EG-8_20210421_01
FidFile: PROTON_02

Pulse Sequence: PROTON (s2pul)
Solvent: dmso
Data collected on: Apr 21 2021

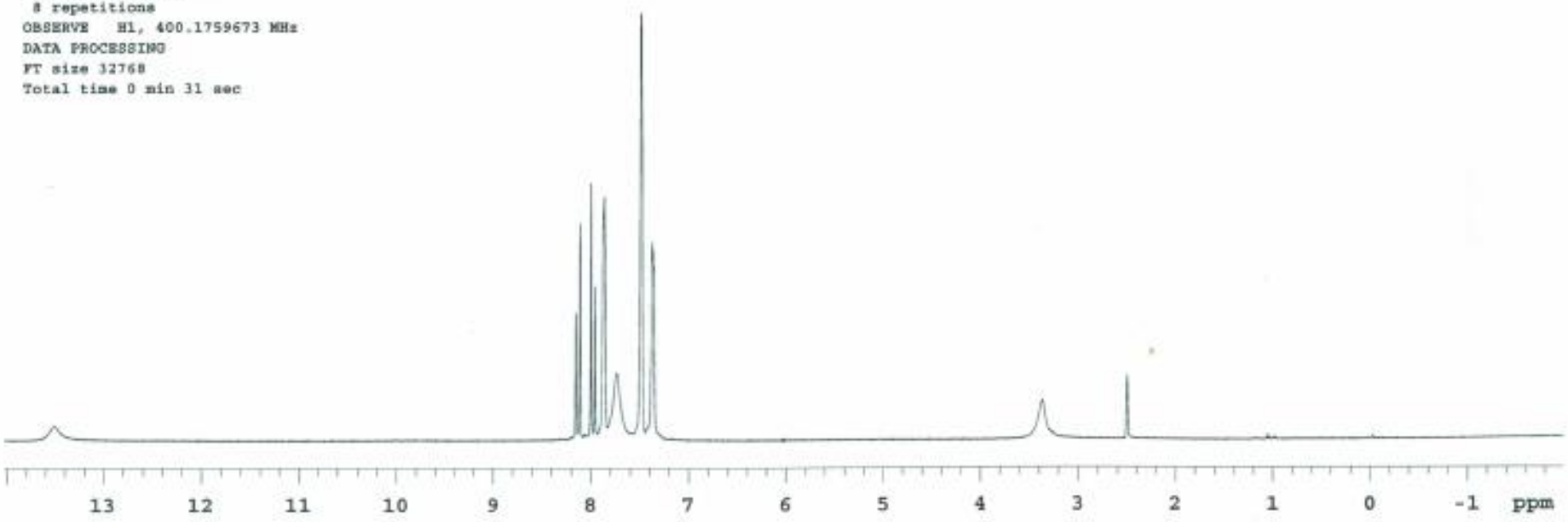
Temp. 25.0 C / 298.1 K
Operator: vnmr1

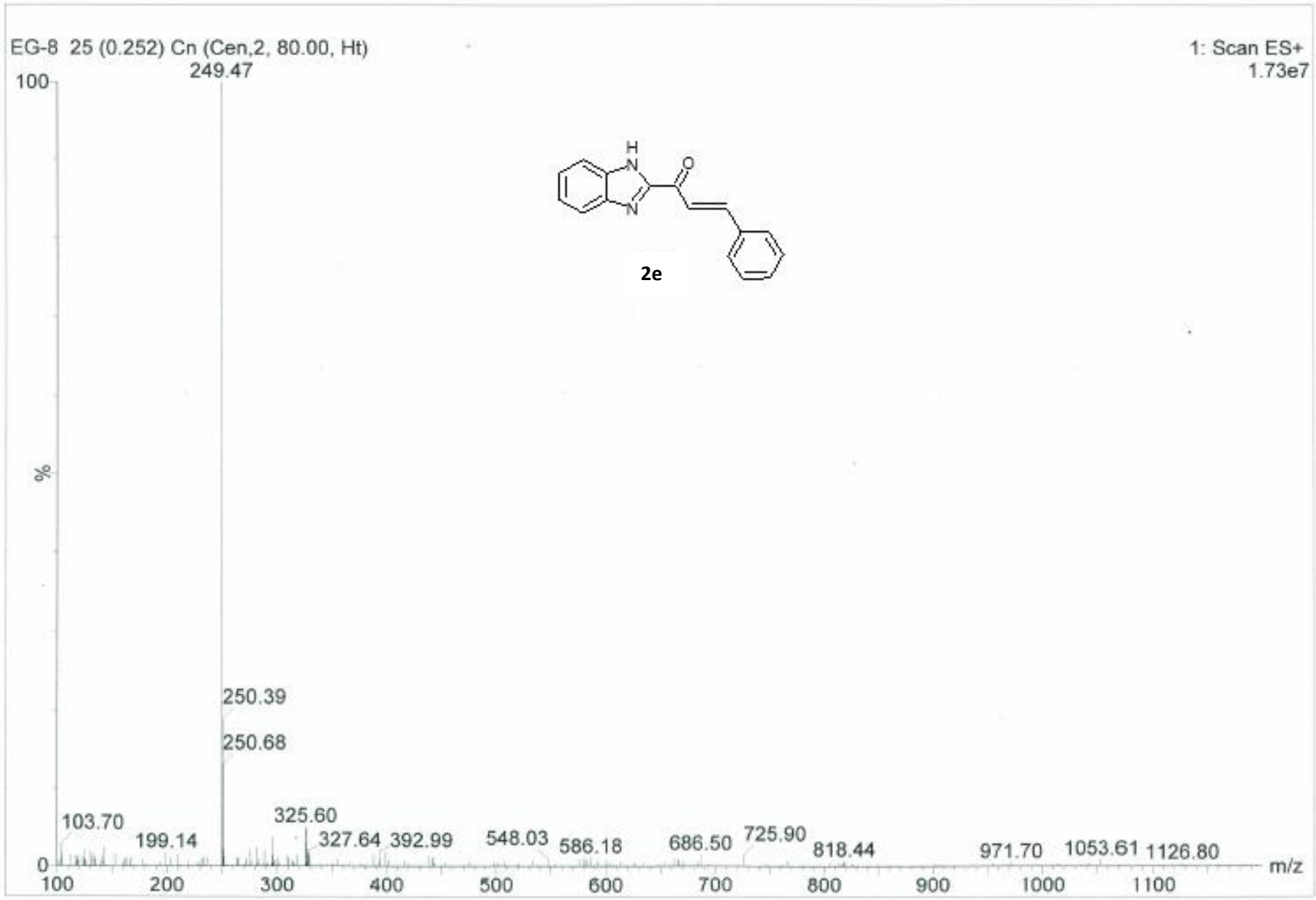
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.559 sec
Width 6402.0 Hz
8 repetitions
OBSERVE H1, 400.1759673 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 31 sec



2e

Agilent Technologies




EG-8 25 (0.252) Cn (Cen,2, 80.00, Ht)
1: Scan ES+
1.73e7
249.47
100
%
0
250.39
250.68
103.70
199.14
325.60
327.64
392.99
548.03
586.18
686.50
725.90
818.44
971.70
1053.61
1126.80
m/z
100
200
300
400
500
600
700
800
900
1000
1100

2e

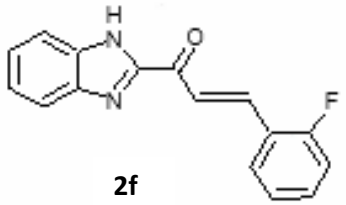
EG10

Sample Name:
EG10
Data Collected on:
mercury400-mercury400
Archive directory:
/home/vnmr1/vnmrsys/data
Sample directory:
EG10_20210421_01
FidFile: PROTON_04

Pulse Sequence: PROTON (s2pul)
Solvent: dmso
Data collected on: Apr 21 2021

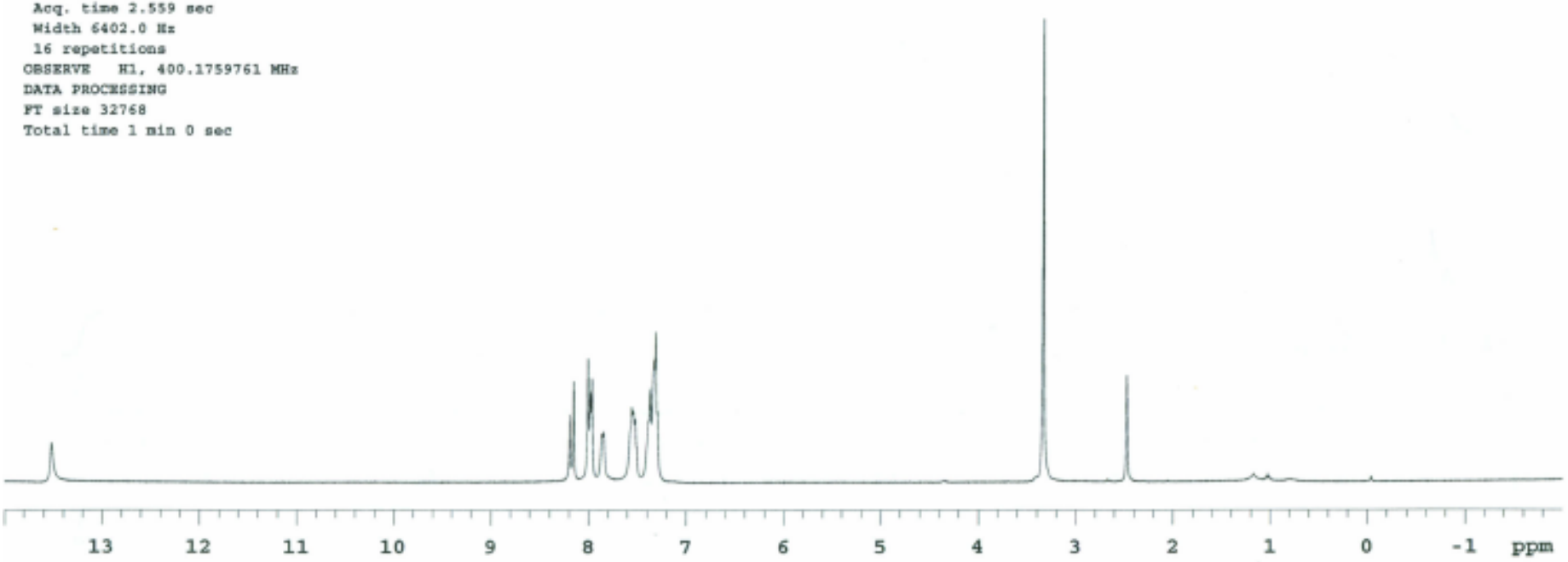
Temp. 25.0 C / 298.1 K
Operator: vnmr1

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.559 sec
Width 6402.0 Hz
16 repetitions
OBSERVE H1, 400.1759761 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 0 sec



2f

Agilent Technologies



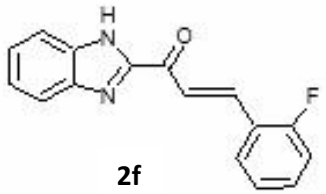
EG10

Sample Name:
EG10
Data Collected on:
mercury400-mercury400
Archive directory:
/home/vnmrl/vnmrsys/data
Sample directory:
EG10_20210421_01
FidFile: CARBON_01

Pulse Sequence: CARBON (s2pul)
Solvent: dmso
Data collected on: Apr 21 2021

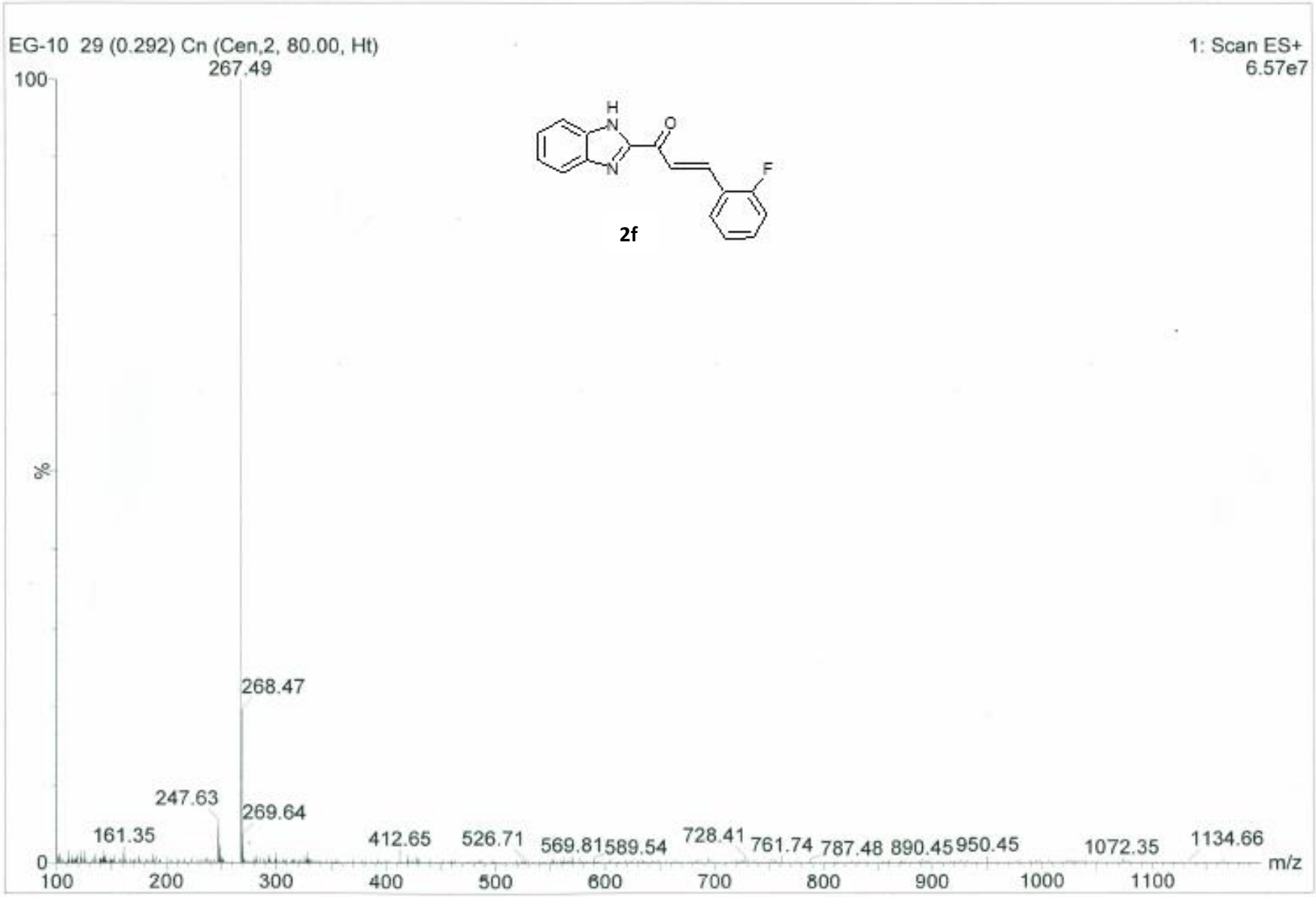
Temp. 25.0 C / 298.1 K
Operator: vnmrl

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.304 sec
Width 25125.6 Hz
1512 repetitions
OBSERVE C13, 100.6243292 MHz
DECOUPLE H1, 400.1779555 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 1 hr



2f

Agilent Technologies


EG-10 29 (0.292) Cn (Cen,2, 80.00, Ht)
1: Scan ES+
6.57e7
100
%
0
267.49
268.47
247.63
269.64
161.35
412.65
526.71
569.81
589.54
728.41
761.74
787.48
890.45
950.45
1072.35
1134.66
m/z
100
200
300
400
500
600
700
800
900
1000
1100
H
N
N
O
F

2f

EG11

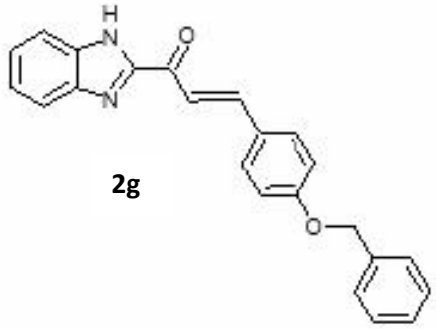
Sample Name:
EG11
Data Collected on:
mercury400-mercury400
Archive directory:
/home/vnmr1/vnmrsys/data
Sample directory:
EG11_20210427_01
FidFile: PROTON_02

Pulse Sequence: PROTON (s2pul)
Solvent: dmso
Data collected on: Apr 27 2021

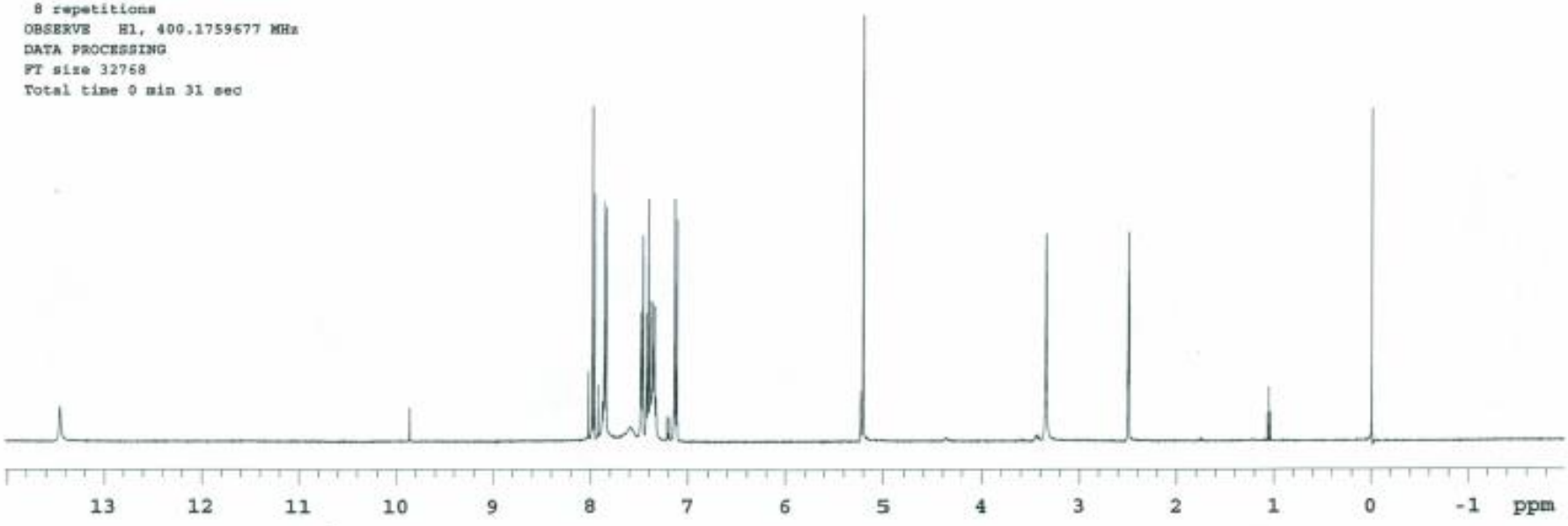
Temp. 25.0 C / 298.1 K
Operator: vnmr1

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.559 sec
Width 6402.0 Hz
8 repetitions
OBSERVE H1, 400.1759677 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 31 sec

Agilent Technologies



2g



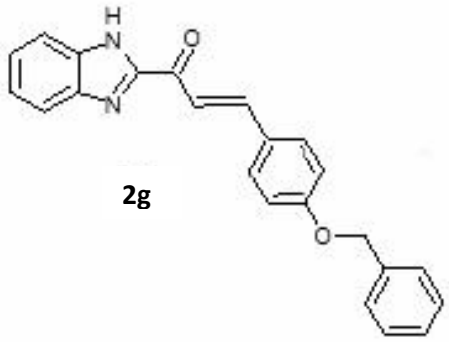
EG11

Sample Name:
EG11
Data Collected on:
mercury400-mercury400
Archive directory:
/home/vnmrl/vnmrsys/data
Sample directory:
EG11_20210427_01
FidFile: CARBON_01

Pulse Sequence: CARBON (s2pul)
Solvent: dmso
Data collected on: Apr 27 2021

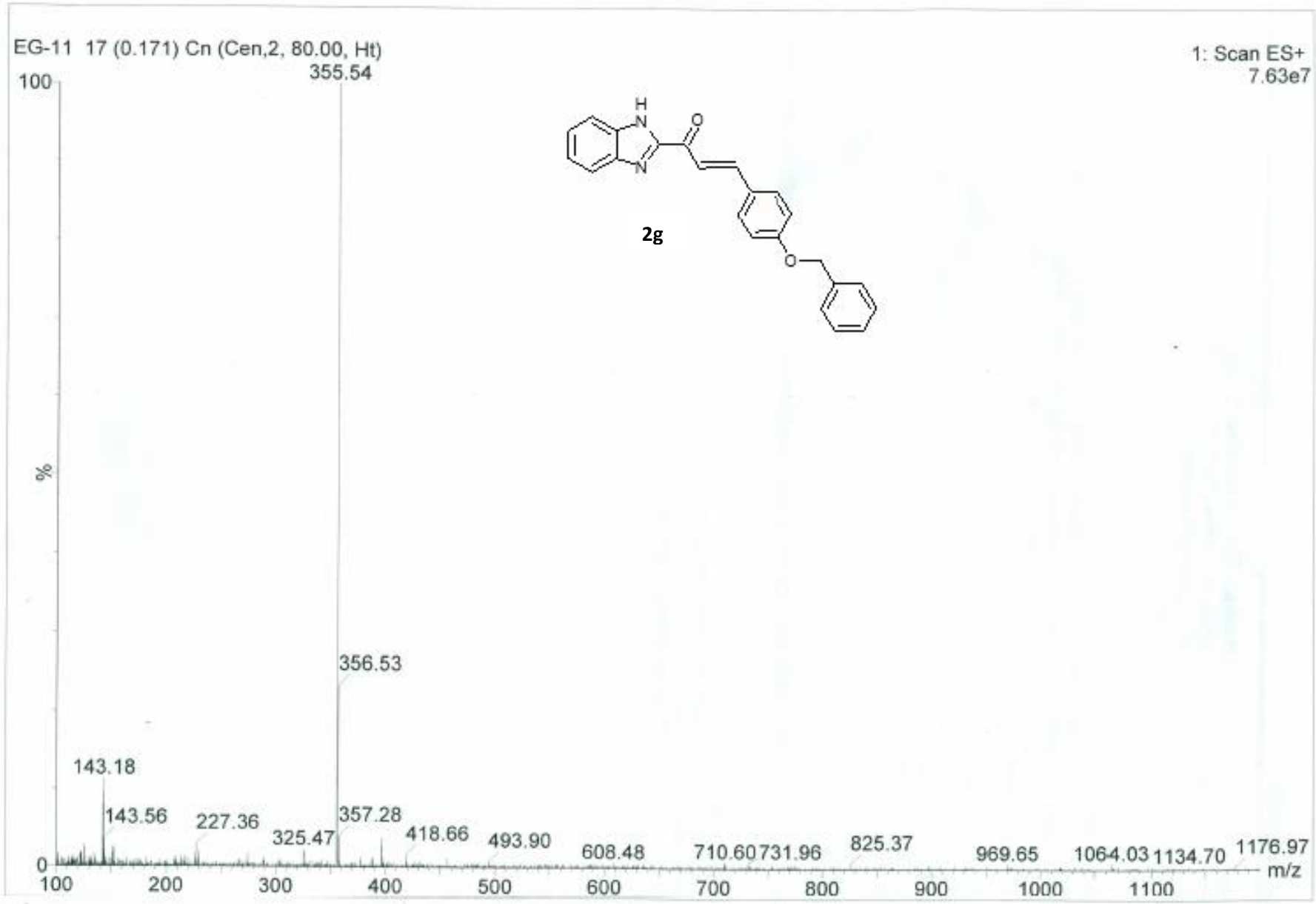
Temp. 25.0 C / 298.1 K
Operator: vnmrl

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.304 sec
Width 25125.6 Hz
2000 repetitions
OBSERVE C13, 100.6243743 MHz
DECOUPLE H1, 400.1779555 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 1 hr, 20 min



2g

Agilent Technologies


EG-11 17 (0.171) Cn (Cen,2, 80.00, Ht)
1: Scan ES+
7.63e7
100
%
0
355.54
356.53
143.18
143.56
227.36
325.47
357.28
418.66
493.90
608.48
710.60
731.96
825.37
969.65
1064.03
1134.70
1176.97
m/z
100
200
300
400
500
600
700
800
900
1000
1100
H
N
N
O
O

2g

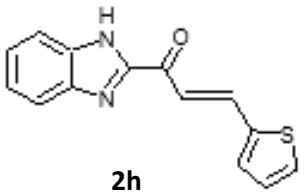
EG12a

Sample Name:
EG12a
Data Collected on:
mercury400-mercury400
Archive directory:
/home/vnmr1/vnmrsys/data
Sample directory:
EG12a_20210421_01
FidFile: PROTON_02

Pulse Sequence: PROTON (s2pul)
Solvent: dmso
Data collected on: Apr 21 2021

Temp. 25.0 C / 298.1 K
Operator: vnmr1

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.559 sec
Width 6402.0 Hz
8 repetitions
OBSERVE H1, 400.1759677 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 31 sec



2h

Agilent Technologies

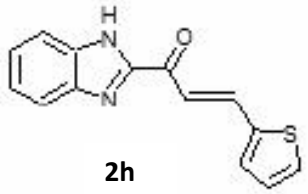
EG12a

Sample Name:
EG12a
Data Collected on:
mercury400-mercury400
Archive directory:
/home/vnmr1/vnmrsys/data
Sample directory:
EG12a_20210421_01
FidFile: CARBON_01

Pulse Sequence: CARBON (s2pul)
Solvent: dmso
Data collected on: Apr 21 2021

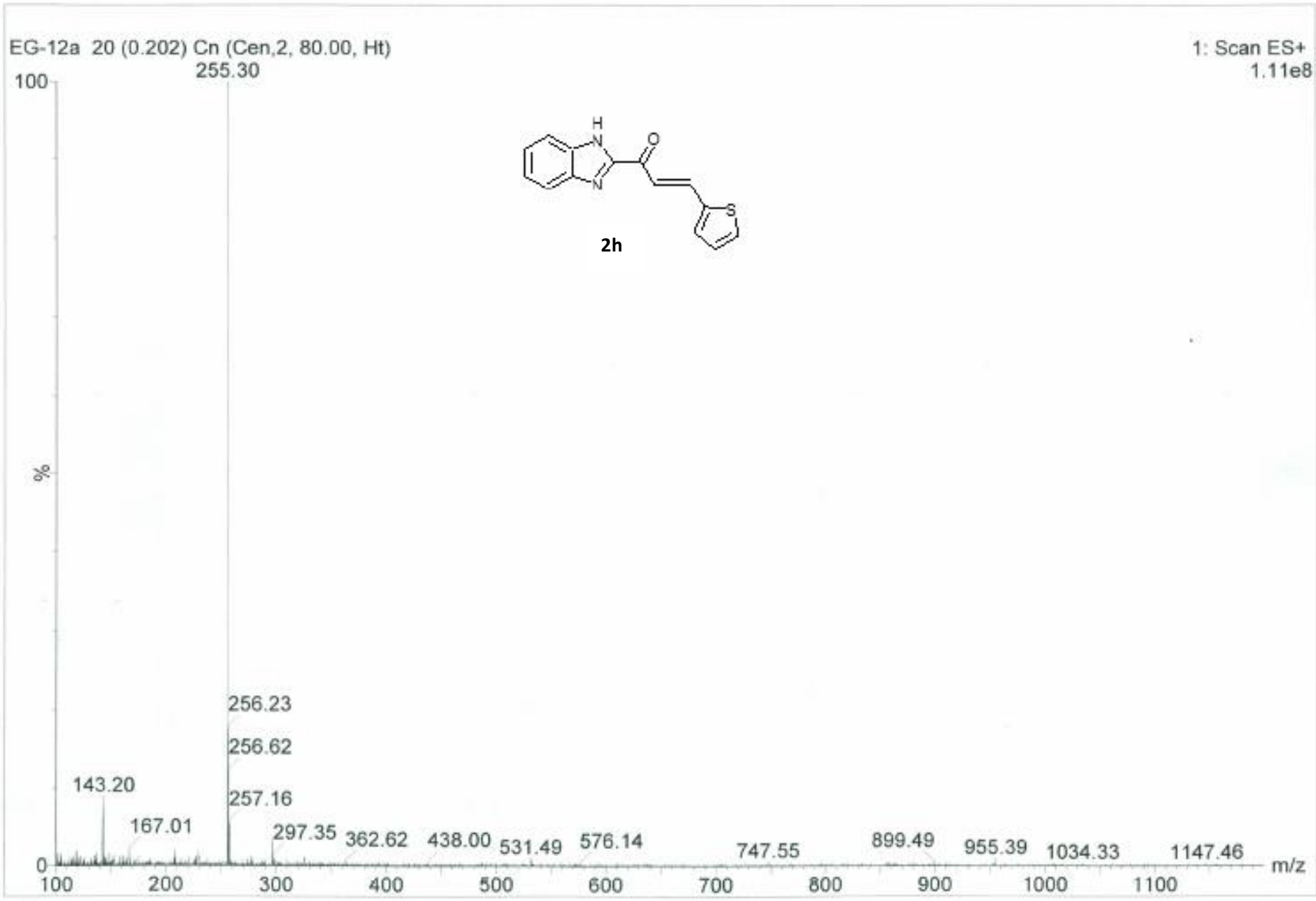
Temp. 25.0 C / 298.1 K
Operator: vnmr1

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.304 sec
Width 25125.6 Hz
2000 repetitions
OBSERVE C13, 100.6243735 MHz
DECOUPLE H1, 400.1779555 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 1 hr, 20 min

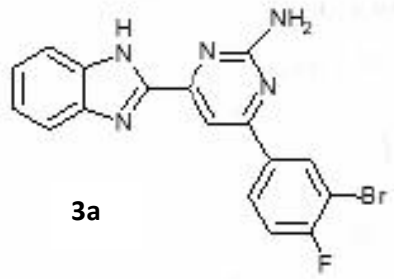


2h

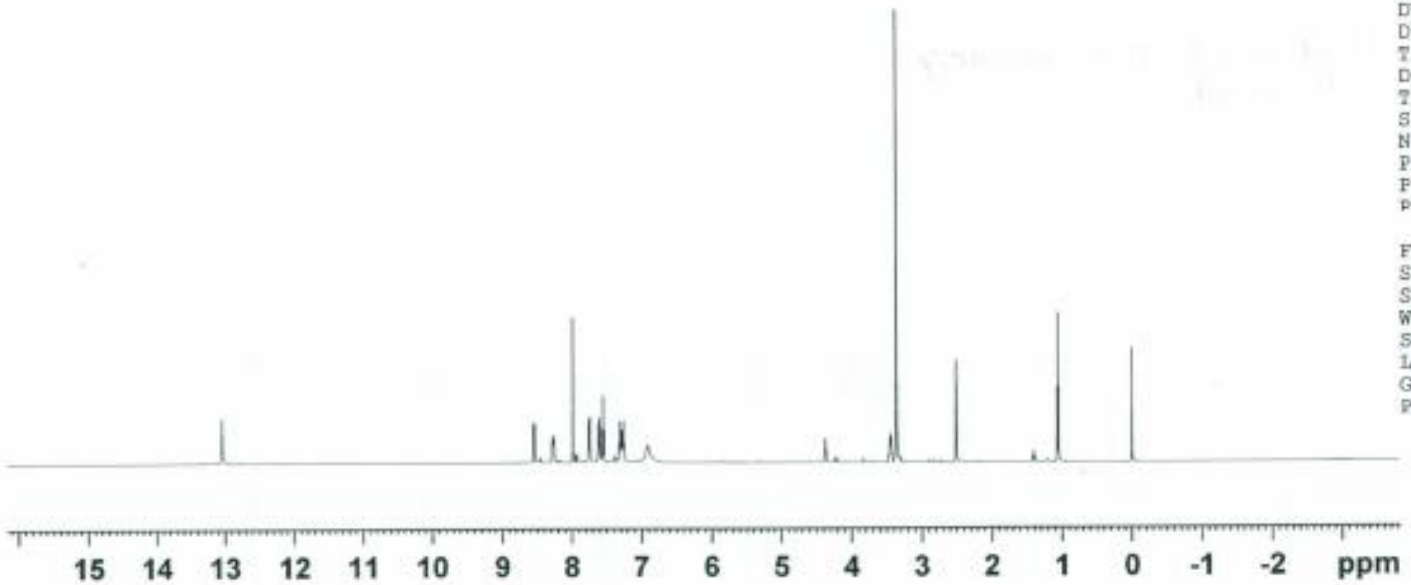
Agilent Technologies


EG-12a 20 (0.202) Cn (Cen,2, 80.00, Ht)
1: Scan ES+
1.11e8
255.30
100
%
0
256.23
256.62
143.20
257.16
167.01
297.35
362.62
438.00
531.49
576.14
747.55
899.49
955.39
1034.33
1147.46
m/z
100
200
300
400
500
600
700
800
900
1000
1100

2h

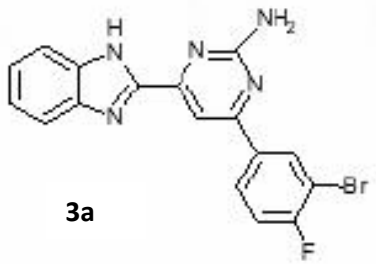


3a



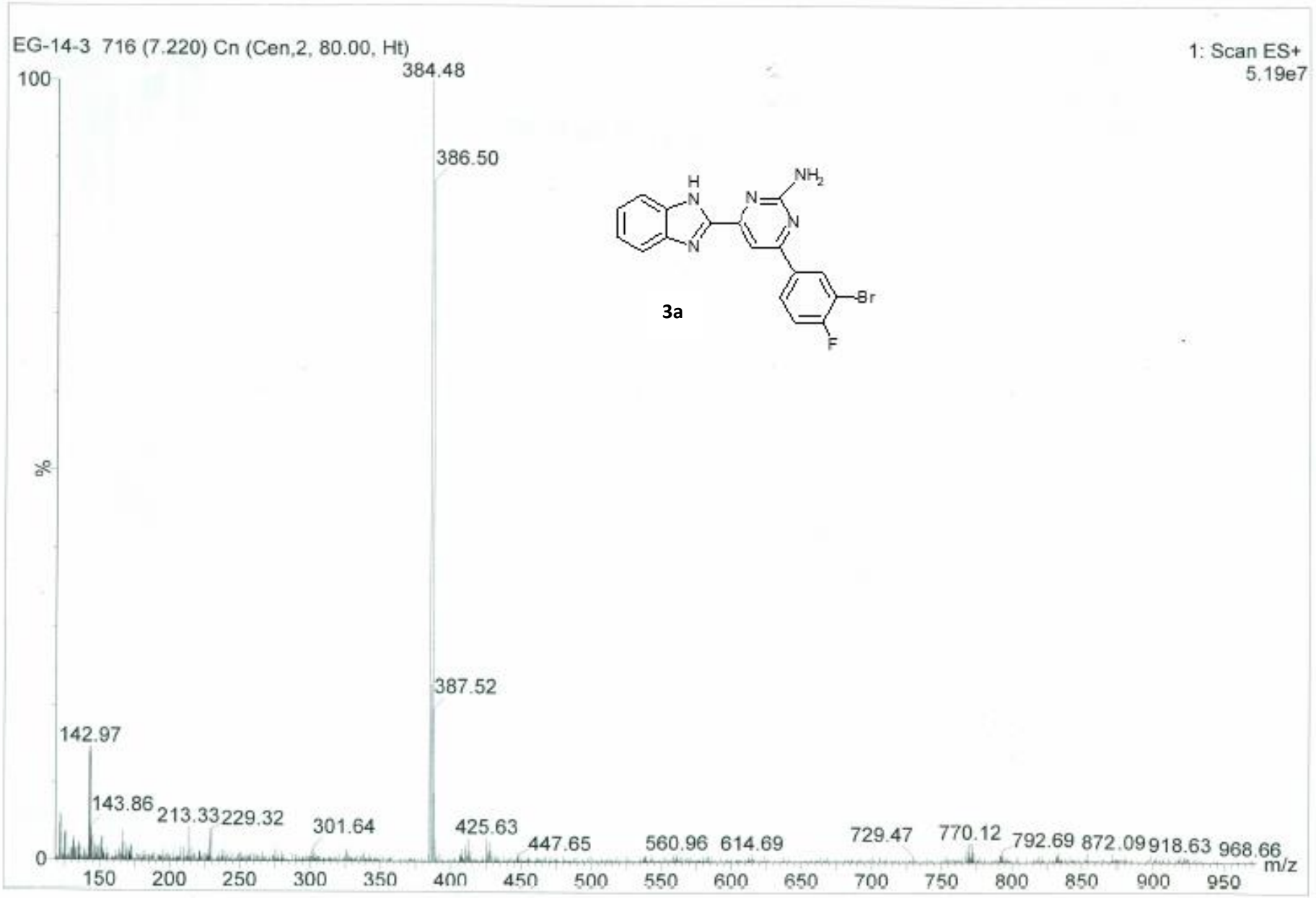
BRUKER

```
Current Data Parameters
NAME                  EG14(3)
EXPNO                       3
PROCNO                      1

F2 - Acquisition Parameters
Date_                20210402
Time                   11.27 h
INSTRUM                Avance
PROBHD    Z151574_0038 (
PULPROG                  zg30
TD                      65536
SOLVENT                  DMSO
NS                         16
DS                          2
SWH                10000.000 Hz
FIDRES             0.305176 Hz
AQ                 3.2767999 sec
RG                       101
DW                    50.000 usec
DE                    11.14 usec
TE                     295.6 K
D1                 1.00000000 sec
TD0                         1
SFO1            500.1330883 MHz
NUC1                       1H
P0                    2.67 usec
P1                    8.00 usec
PLW1           24.04299927 W

F2 - Processing parameters
SI                      65536
SF             500.1300000 MHz
WDW                        EM
SSB                 0
LB                     0.30 Hz
GB                  0
PC                     1.00
```

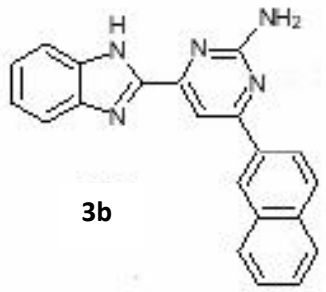


3a


```
Current Data Parameters
NAME                  EG14(3)
EXPNO                       6
PROCNO                      1

F2 - Acquisition Parameters
Date_              20210407
Time                  14.25 h
INSTRUM               Avance
PROBHD    Z151574_0038 (
PULPROG              zgpg30
TD                    65536
SOLVENT                DMSO
NS                     3000
DS                        4
SWH               30120.482 Hz
FIDRES             0.919204 Hz
AQ                 1.0878977 sec
RG                      101
DW                   16.600 usec
DE                    6.50 usec
TE                   298.9 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                       1
SFO1           125.7703643 MHz
NUC1                    13C
P0                    3.33 usec
P1                   10.00 usec
PLW1           85.18099976 W
SFO2           500.1320005 MHz
NUC2                    1H
CPDPRG[2             waltz65
PCPD2                80.00 usec
PLW2           24.04299927 W
PLW12           0.24043000 W
PLW13           0.12093000 W

F2 - Processing parameters
SI                    32768
SF             125.7577885 MHz
WDW                      EM
SSB          0
LB                    1.00 Hz
GB           0
PC                    1.40
```

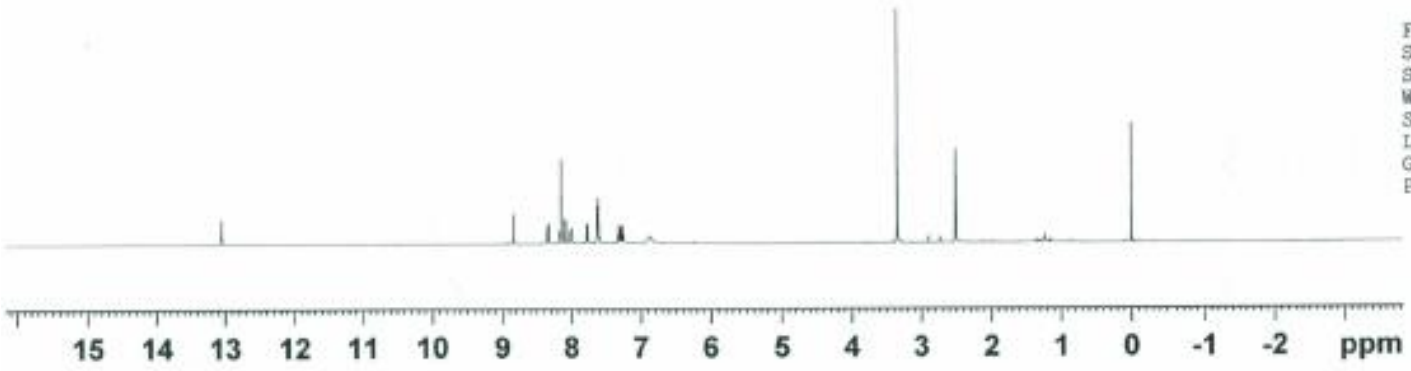

EG-14-3 716 (7.220) Cn (Cen,2, 80.00, Ht)
1: Scan ES+
5.19e7
100
%
0
384.48
386.50
387.52
142.97
143.86
213.33
229.32
301.64
425.63
447.65
560.96
614.69
729.47
770.12
792.69
872.09
918.63
968.66
m/z
150
200
250
300
350
400
450
500
550
600
650
700
750
800
850
900
950
H
N
N
N
NH2
Br
F

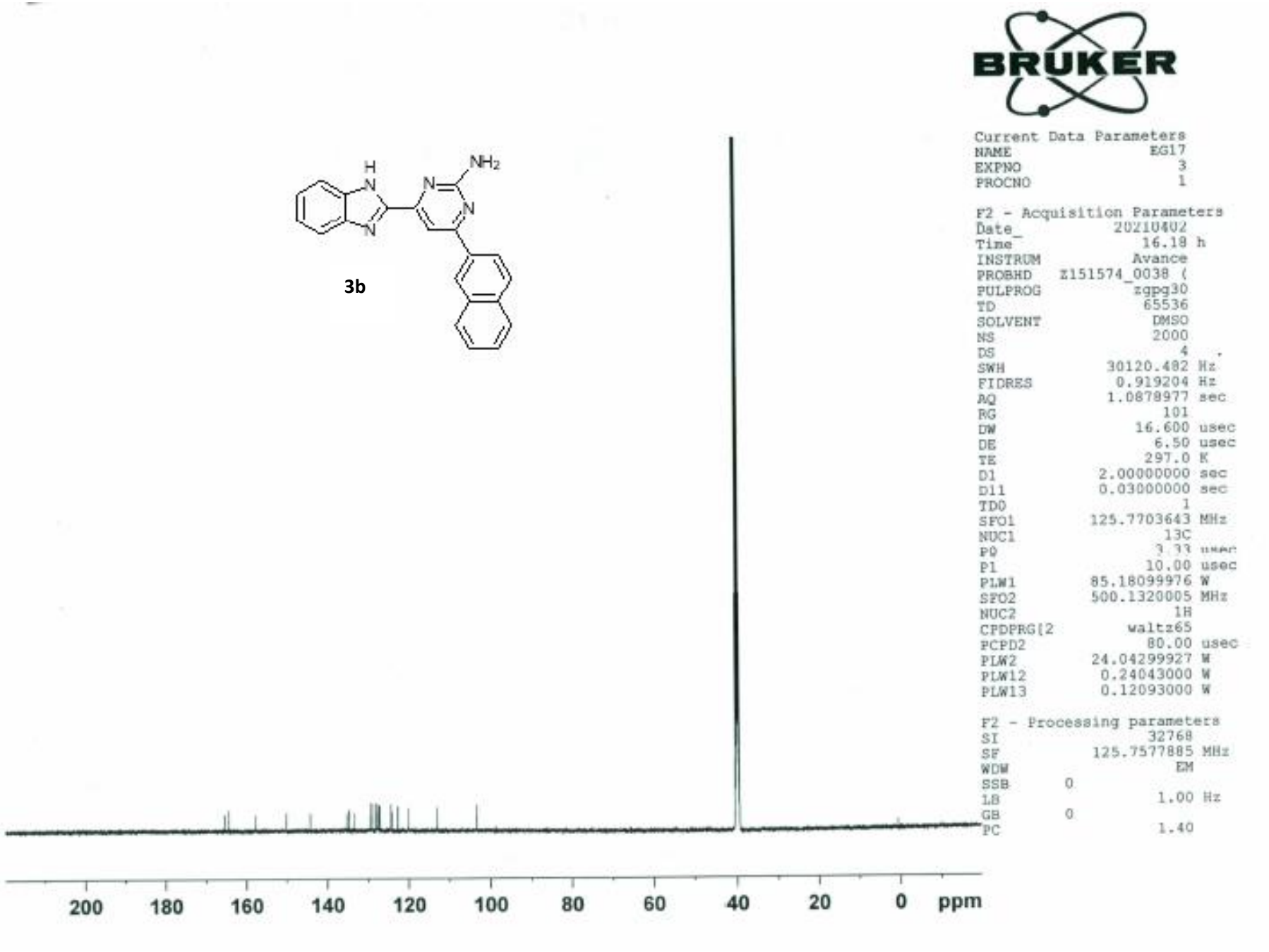
3a



3b

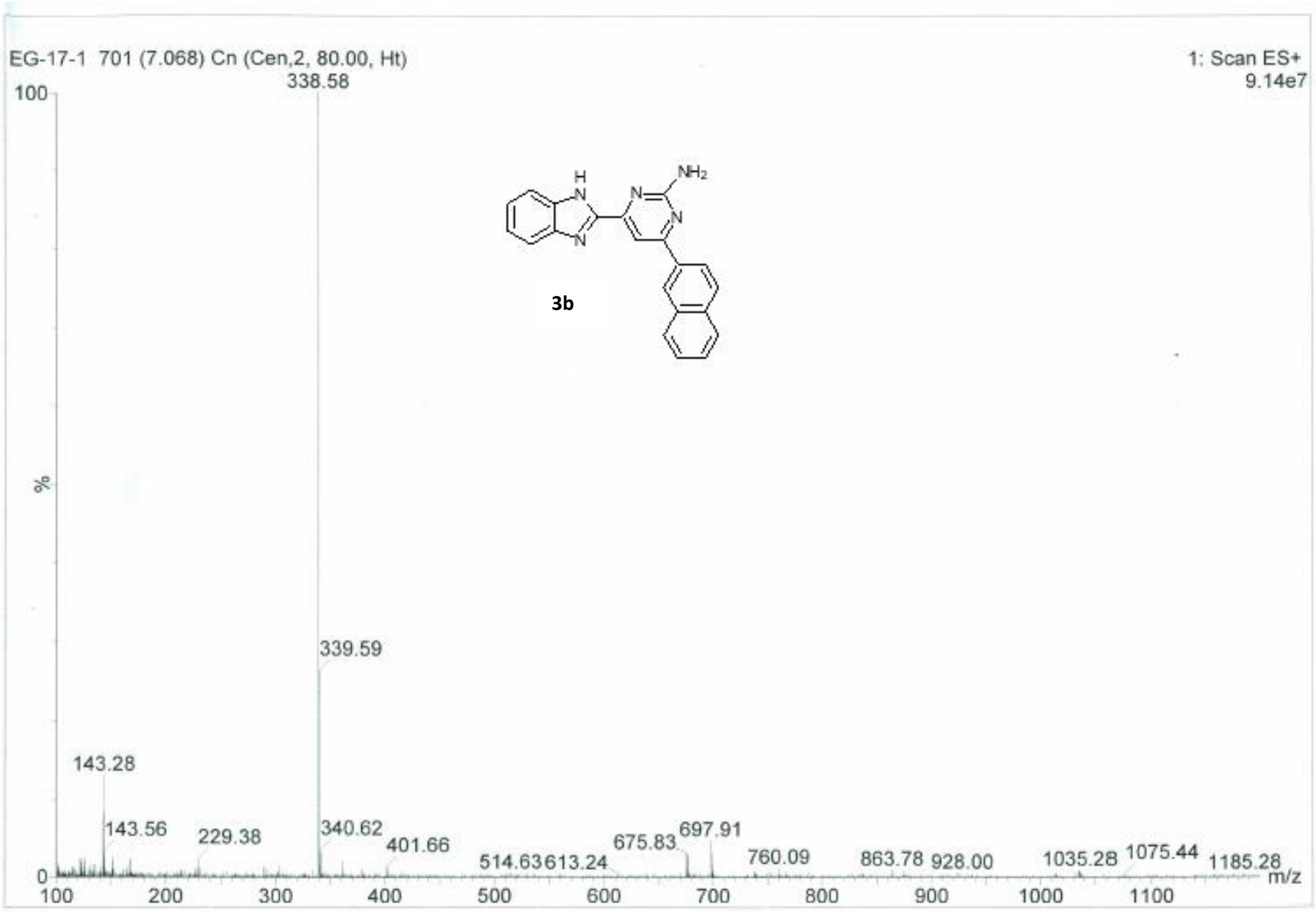
```
Current Data Parameters
NAME                  EG17
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_              20210402
Time                 10.12 h
INSTRUM              Avance
PROBHD   Z151574_0038 (
PULPROG               zg30
TD                   65536
SOLVENT               DMSO
NS                       16
DS                        2
SWH              10000.000 Hz
FIDRES               0.305176 Hz
AQ                3.2767999 sec
RG                      101
DW                   50.000 usec
DE                   11.14 usec
TE                   295.2 K
D1             1.00000000 sec
TD0                      1
SFO1          500.1330883 MHz
NUC1                    1H
P0                   2.67 usec
P1                   8.00 usec
PLW1          24.04299927 W

F2 - Processing parameters
SI                   65536
SF            500.1300000 MHz
WDW                     EM
SSB       0
LB                   0.30 Hz
GB        0
PC                   1.00
```



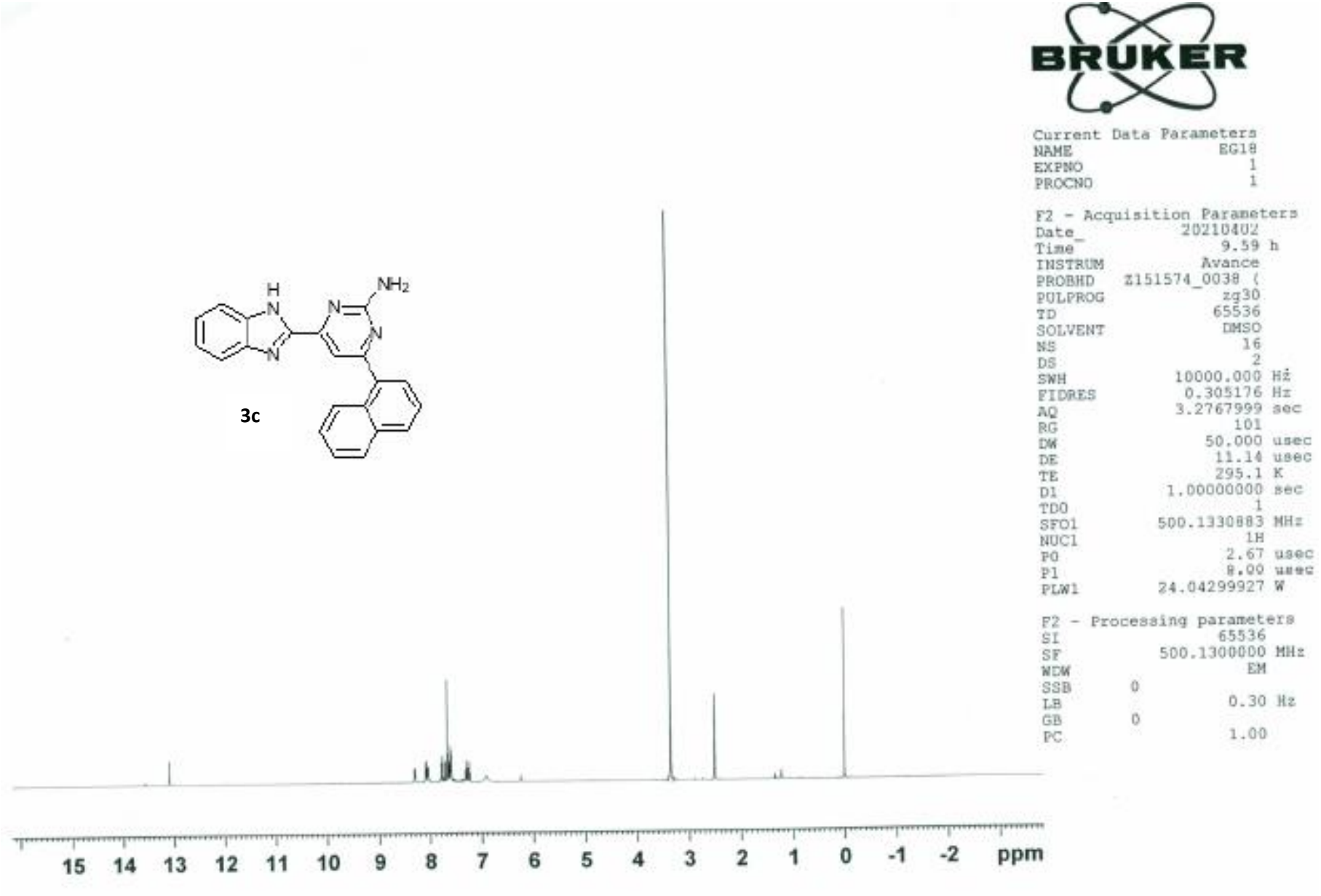


BRUKER

```
Current Data Parameters
NAME                  EG17
EXPNO                    3
PROCNO                   1

F2 - Acquisition Parameters
Date_              20210402
Time                 16.18 h
INSTRUM              Avance
PROBHD    Z151574_0038 (
PULPROG              zgpg30
TD                    65536
SOLVENT                DMSO
NS                     2000
DS                        4
SWH               30120.482 Hz
FIDRES             0.919204 Hz
AQ                 1.0878977 sec
RG                       101
DW                    16.600 usec
DE                     6.50 usec
TE                    297.0 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                       1
SFO1           125.7703643 MHz
NUC1                    13C
P0                    3.33 usec
P1                   10.00 usec
PLW1           85.18099976 W
SFO2           500.1320005 MHz
NUC2                    1H
CPDPRG[2             waltz65
PCPD2                80.00 usec
PLW2           24.04299927 W
PLW12           0.24043000 W
PLW13           0.12093000 W

F2 - Processing parameters
SI                     32768
SF             125.7577885 MHz
WDW                       EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```


EG-17-1 701 (7.068) Cn (Cen,2, 80.00, Ht)
1: Scan ES+
9.14e7
100
%
0
338.58
339.59
143.28
143.56
229.38
340.62
401.66
514.63
613.24
675.83
697.91
760.09
863.78
928.00
1035.28
1075.44
1185.28
m/z
100
200
300
400
500
600
700
800
900
1000
1100
H
N
N
N
N
NH2

3b



BRUKER

Current Data Parameters

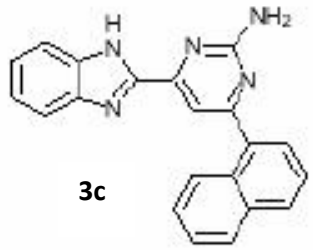
NAME	EG18
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20210402
Time	9.59 h
INSTRUM	Avance
PROBHD	Z151574_0038 (
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	16
DS	2
SWH	10000.000 Hz
FIDRES	0.305176 Hz
AQ	3.2767999 sec
RG	101
DW	50.000 usec
DE	11.14 usec
TE	295.1 K
D1	1.00000000 sec
TD0	1
SFO1	500.1330883 MHz
NUC1	1H
P0	2.67 usec
P1	8.00 usec
PLW1	24.04299927 W

F2 - Processing parameters

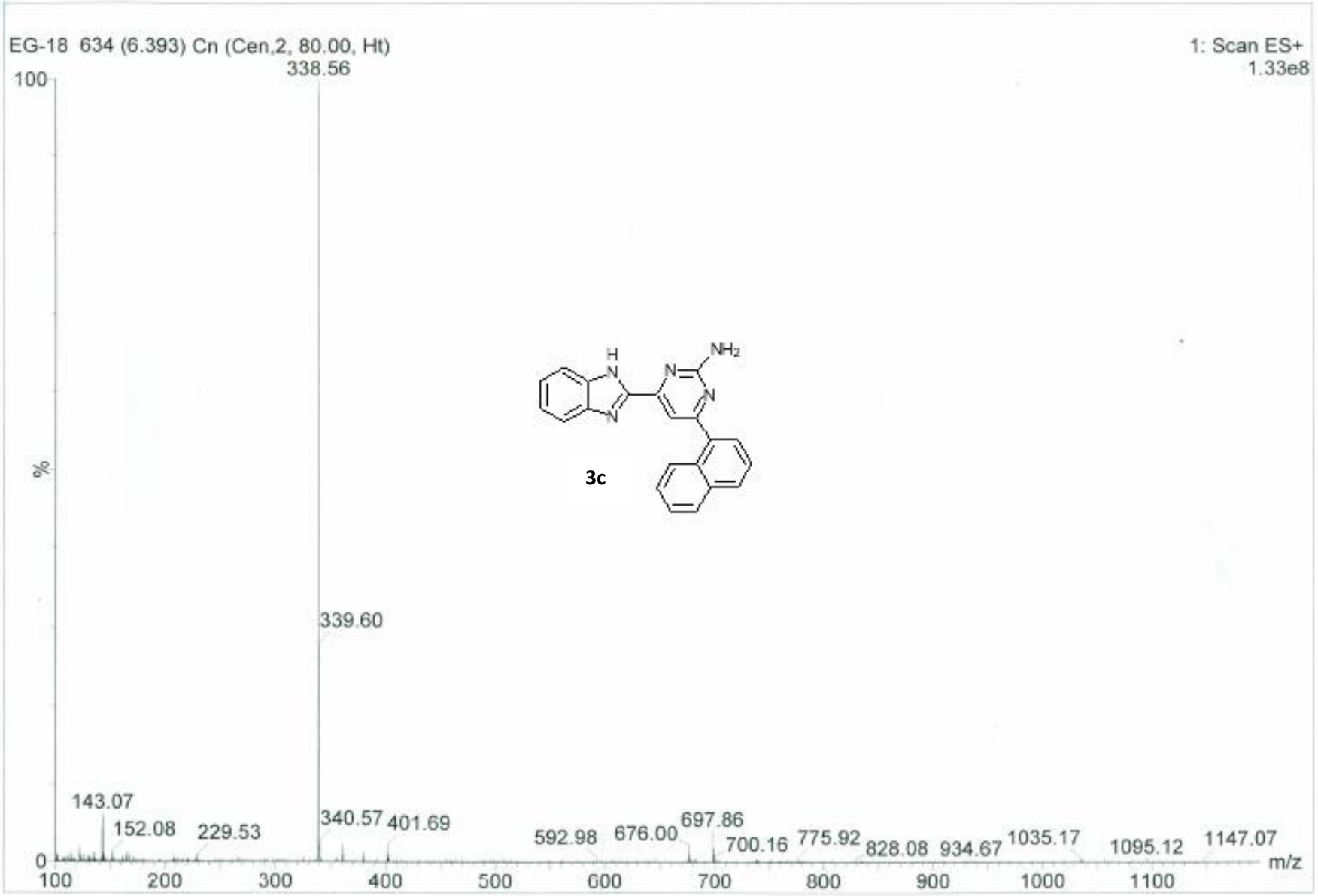
SI	65536
SF	500.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



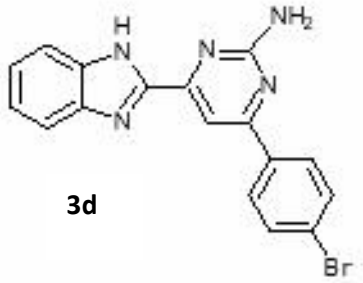
3c

BRUKER

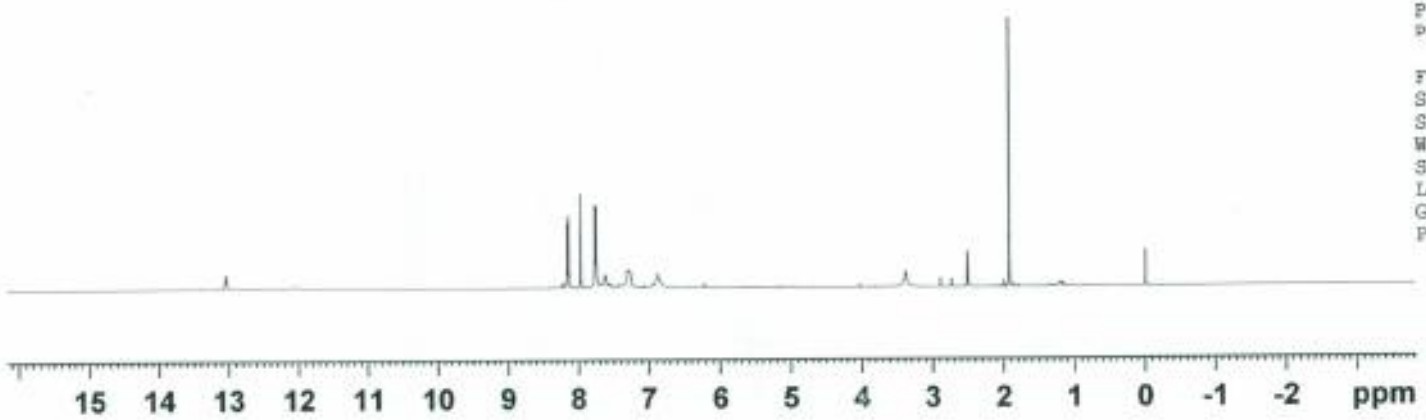
```
Current Data Parameters
NAME                  EG18
EXPNO                    3
PROCNO                   1

F2 - Acquisition Parameters
Date_              20210406
Time                 13.23 h
INSTRUM              Avance
PROBHD    Z151574_0038 (
PULPROG              zgpg30
TD                    65536
SOLVENT                DMSO
NS                      3000
DS                         4
SWH              30120.482 Hz
FIDRES            0.919204 Hz
AQ                1.0878977 sec
RG                      101
DW                   16.600 usec
DE                    6.50 usec
TE                   299.3 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                        1
SFO1          125.7703643 MHz
NUC1                    13C
P0                    3.33 usec
P1                   10.00 usec
PLW1          85.18099976 W
SFO2          500.1320005 MHz
NUC2                    1H
CPDPRG[2             waltz65
PCPD2                80.00 usec
PLW2          24.04299927 W
PLW12          0.24043000 W
PLW13          0.12093000 W

F2 - Processing parameters
SI                     32768
SF            125.7577885 MHz
WDW                       EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```


EG-18 634 (6.393) Cn (Cen,2, 80.00, Ht)
1: Scan ES+
1.33e8
100
%
0
338.56
339.60
143.07
152.08
229.53
340.57
401.69
592.98
676.00
697.86
700.16
775.92
828.08
934.67
1035.17
1095.12
1147.07
m/z
100
200
300
400
500
600
700
800
900
1000
1100
H
N
N
N
NH2

3c

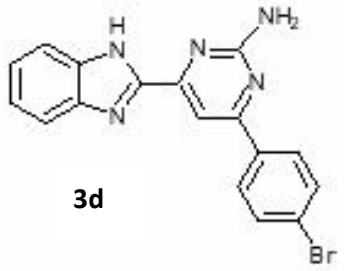


3d

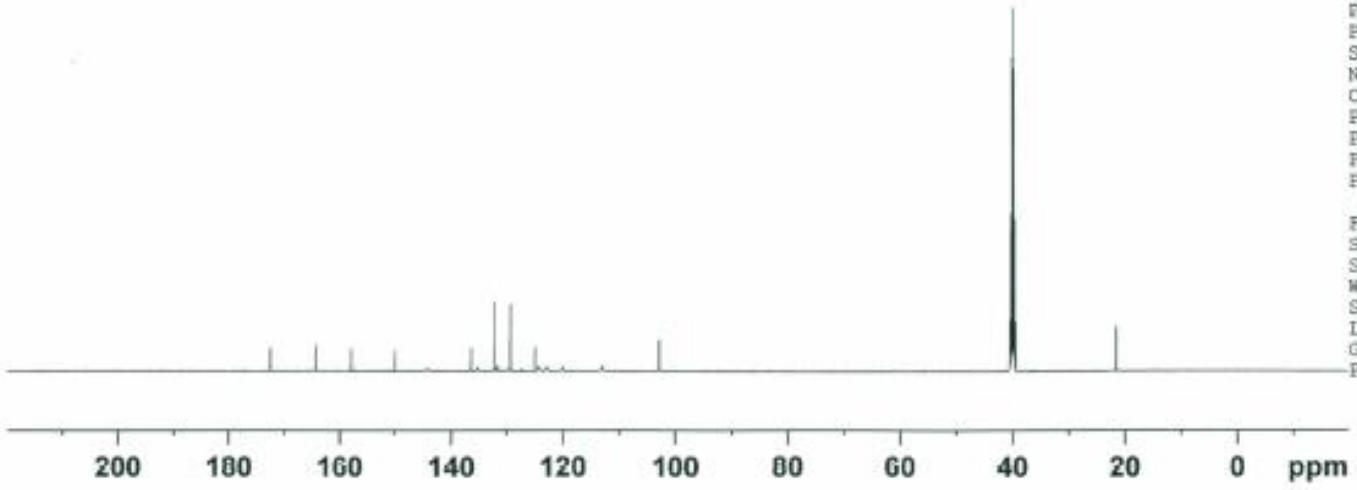


BRUKER

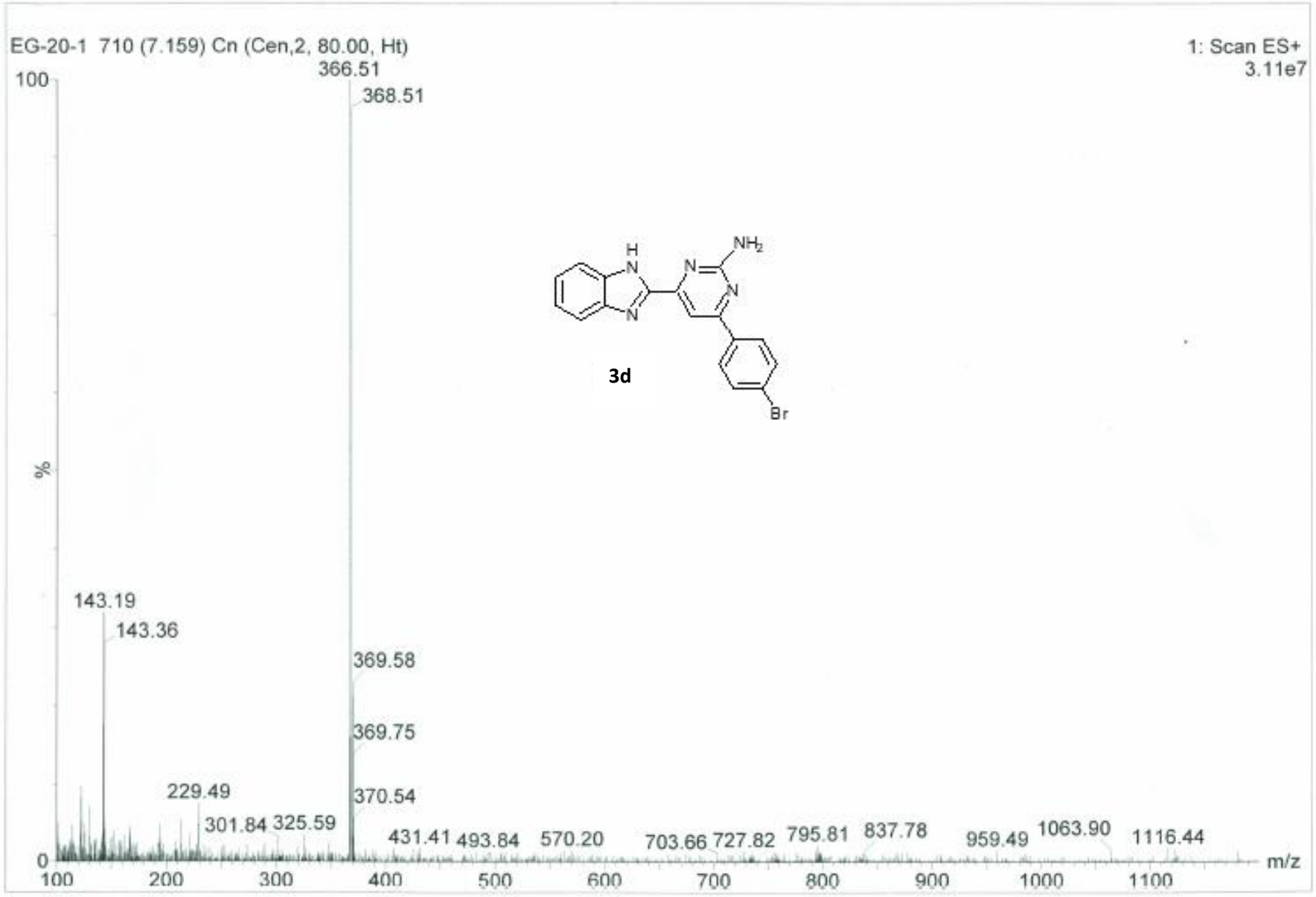
```
Current Data Parameters
NAME                  BG20(1)
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_              20210402
Time                  11.11 h
INSTRUM               Avance
PROBHD    Z151574_0038 (
PULPROG                 zg30
TD                     65536
SOLVENT                 DMSO
NS                        16
DS                         2
SWH               10000.000 Hz
FIDRES            0.305176 Hz
AQ                3.2767999 sec
RG                       101
DW                  50.000 usec
DE                  11.14 usec
TE                  295.6 K
D1               1.00000000 sec
TD0                        1
SFO1           500.1330883 MHz
NUC1                      1H
P0                   2.67 usec
P1                   8.00 usec
PLW1           24.04299927 W

F2 - Processing parameters
SI                     65536
SF             500.1300000 MHz
WDW                       EM
SSB       0
LB                   0.30 Hz
GB        0
PC                    1.00
```



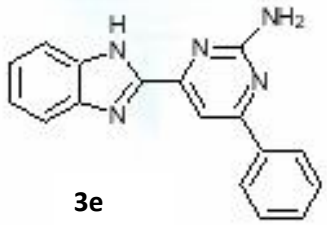
3d



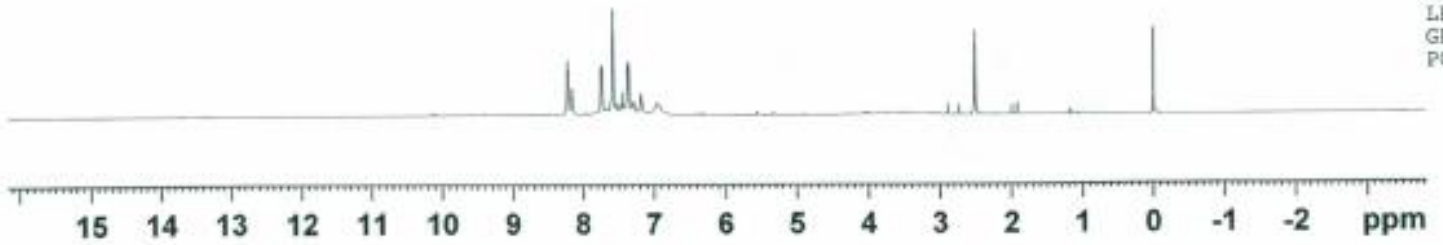

```
Current Data Parameters
NAME                  EG20(4)
EXPNO                       4
PROCNO                      1

F2 - Acquisition Parameters
Date_              20210407
Time                  11.34 h
INSTRUM              Avance
PROBHD    Z151574_0038 (
PULPROG             zgpg30
TD                   65536
SOLVENT               DMSO
NS                    1885
DS                       4
SWH              30120.482 Hz
FIDRES           0.919204 Hz
AQ               1.0878977 sec
RG                     101
DW                  16.600 usec
DE                   6.50 usec
TE                  299.9 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1           125.7703643 MHz
NUC1                  13C
P0                   3.33 usec
P1                  10.00 usec
PLW1           85.18099976 W
SFO2           500.1320005 MHz
NUC2                   1H
CPDPRG[2           waltz65
PCPD2                80.00 usec
PLW2           24.04299927 W
PLW12           0.24043000 W
PLW13           0.12093000 W

F2 - Processing parameters
SI                    32768
SF             125.7577885 MHz
WDW                     EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```


EG-20-1 710 (7.159) Cn (Cen,2, 80.00, Ht)
1: Scan ES+
3.11e7
100
%
0
366.51
368.51
143.19
143.36
369.58
369.75
229.49
370.54
301.84
325.59
431.41
493.84
570.20
703.66
727.82
795.81
837.78
959.49
1063.90
1116.44
m/z
100
200
300
400
500
600
700
800
900
1000
1100
H
N
N
N
N
NH2
Br

3d



3e



BRUKER

```
Current Data Parameters
NAME                  EG13
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date                20210402
Time                11.59 h
INSTRUM              Avance
PROBHD    Z151574_0038 (
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                       16
DS                        2
SWH              10000.000 Hz
FIDRES               0.305176 Hz
AQ                3.2767999 sec
RG                       101
DW                  50.000 usec
DE                  11.14 usec
TE                    295.7 K
D1              1.00000000 sec
TD0                      1
SFO1           500.1330883 MHz
NUC1                    1H
P0                   2.67 usec
P1                   8.00 usec
PLW1          24.04299927 W

F2 - Processing parameters
SI                    65536
SF           500.1300000 MHz
WDW                     EM
SSB       0
LB                   0.30 Hz
GB        0
PC                   1.00
```

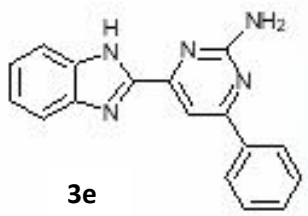
EG-13

Sample Name:
EG-13
Data Collected on:
mercury400-mercury400
Archive directory:
/home/vnmr1/vnmrsys/data
Sample directory:
EG-13_20210813_01
FidFile: CARBON_01

Pulse Sequence: CARBON (s2pul)
Solvent: dmso
Data collected on: Aug 13 2021

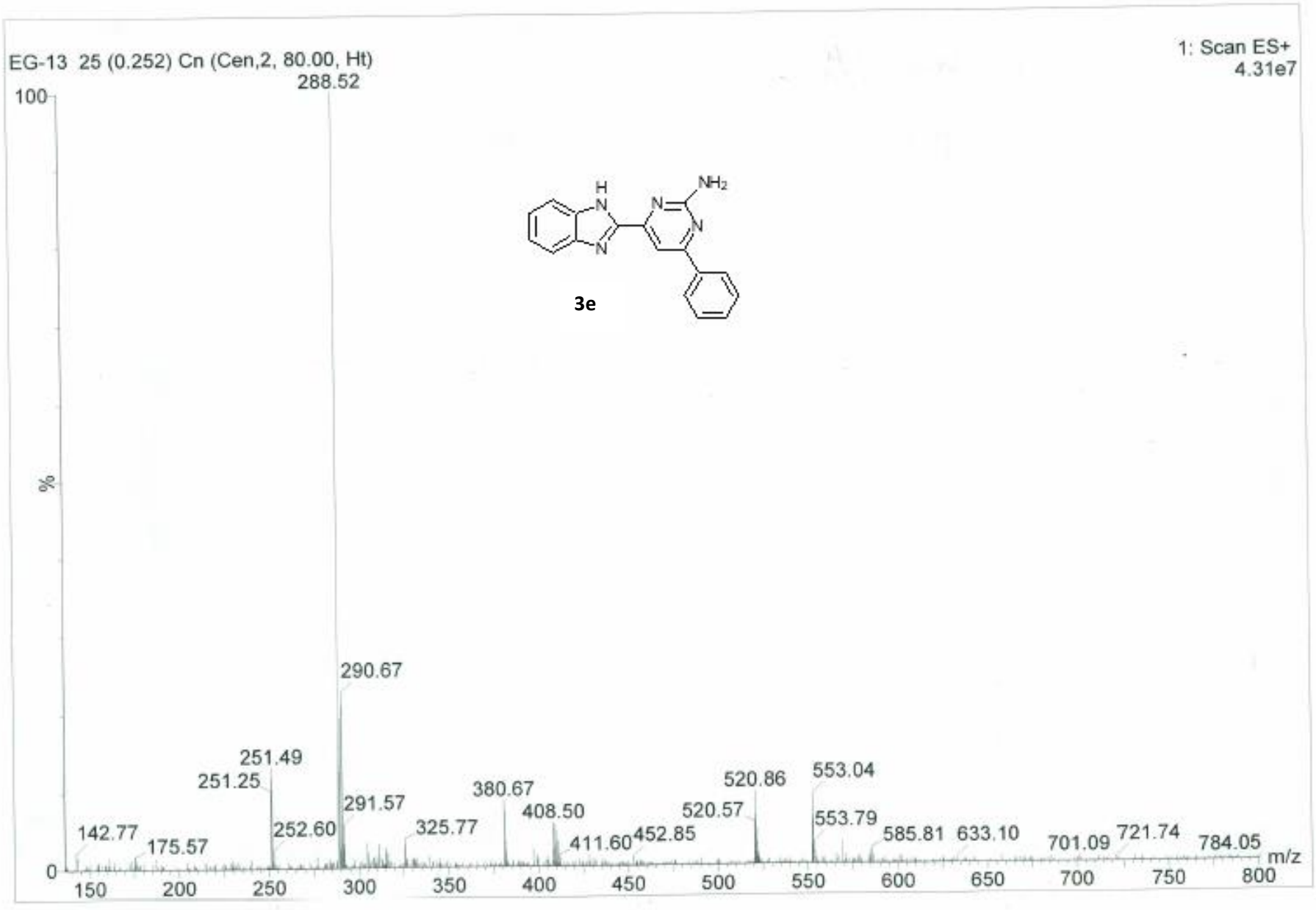
Temp. 25.0 C / 298.1 K
Operator: vnmr1

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.550 sec
Width 21141.6 Hz
5000 repetitions
OBSERVE C13, 100.6243292 MHz
DECOUPLE H1, 400.1779555 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 3 hr, 40 min

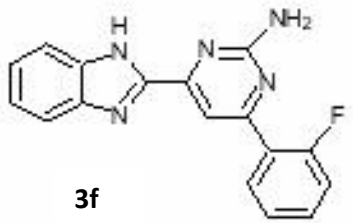


3e

Agilent Technologies

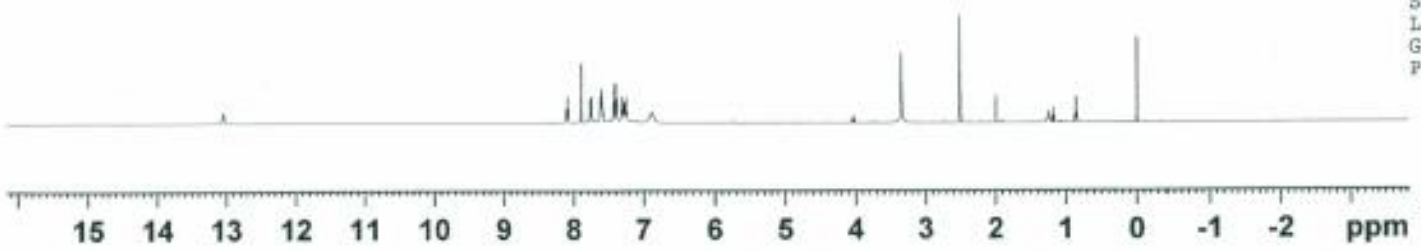

EG-13 25 (0.252) Cn (Cen,2, 80.00, Ht)
1: Scan ES+
4.31e7
100
%
0
288.52
290.67
251.49
251.25
291.57
380.67
408.50
520.86
553.04
520.57
553.79
142.77
175.57
252.60
325.77
411.60
452.85
585.81
633.10
701.09
721.74
784.05
m/z
150
200
250
300
350
400
450
500
550
600
650
700
750
800
H
N
N
N
NH2

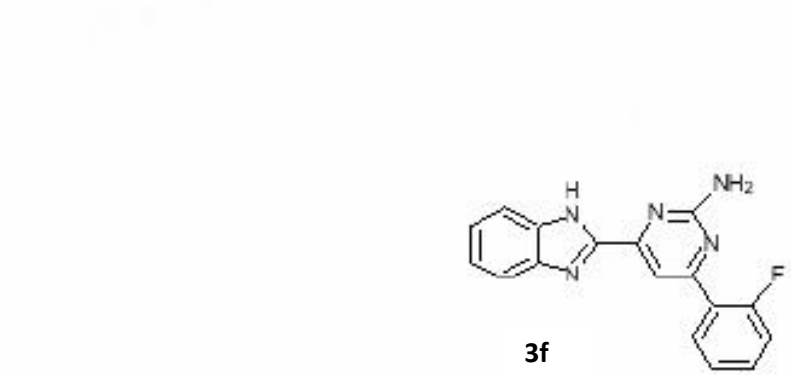
3e



3f

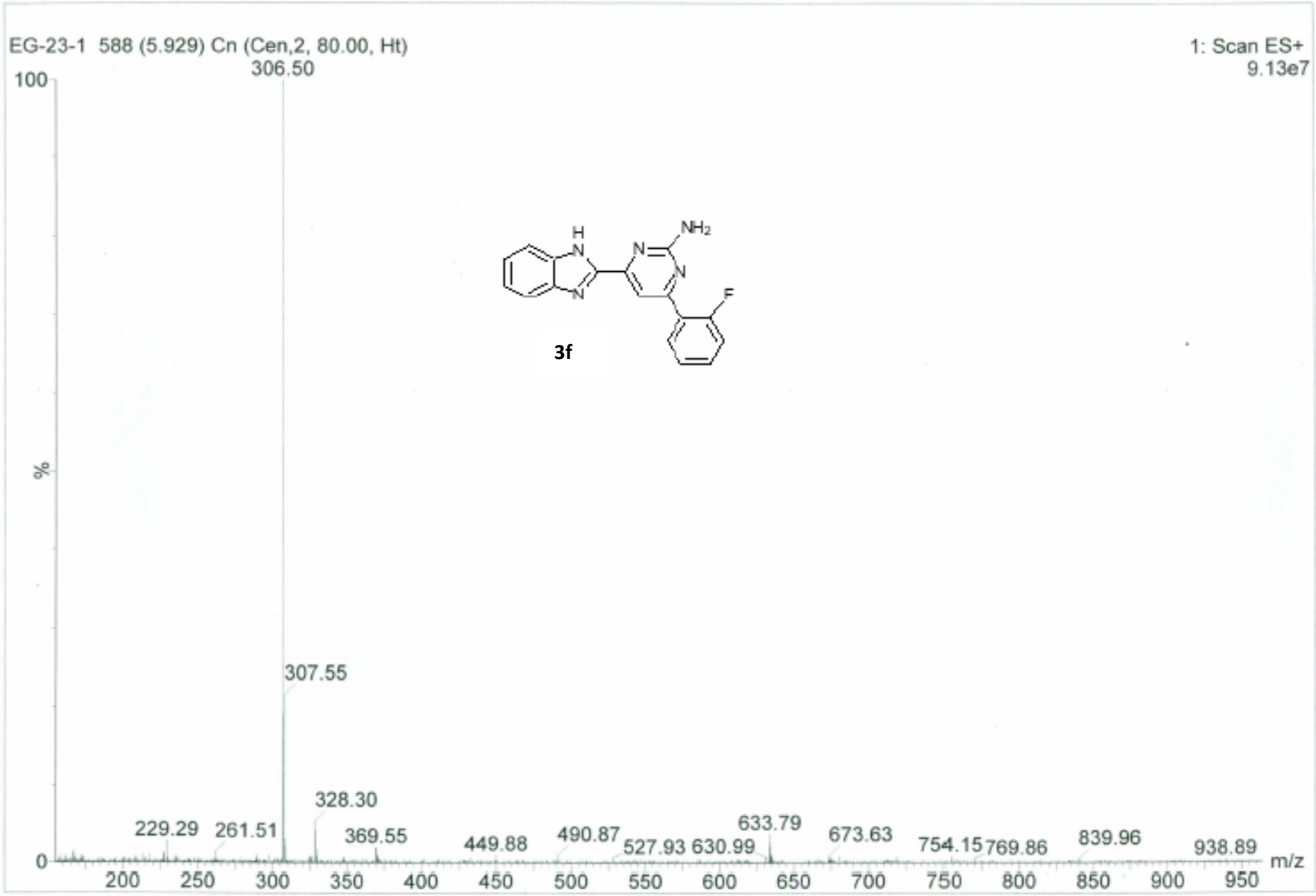
```
Current Data Parameters
NAME                  EG23
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_              20210402
Time_                11.40 h
INSTRUM              Avance
PROBHD   Z151574_0038 (
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                       16
DS                        2
SWH              10000.000 Hz
FIDRES               0.305176 Hz
AQ                3.2767999 sec
RG                       101
DW                  50.000 usec
DE                  11.14 usec
TE                   295.6 K
D1              1.00000000 sec
TD0                      1
SFO1           500.1330883 MHz
NUC1                    1H
P0                  2.67 usec
P1                  8.00 usec
PLW1           24.04299927 W

F2 - Processing parameters
SI                    65536
SF           500.1300000 MHz
WDW                     EM
SSB       0
LB                   0.30 Hz
GB        0
PC                   1.00
```



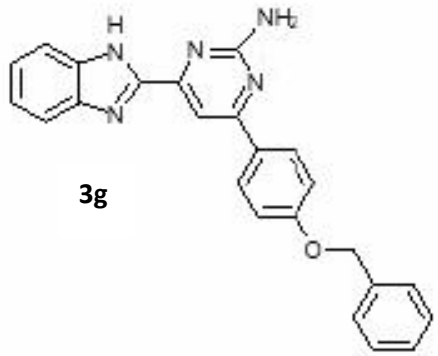


3f

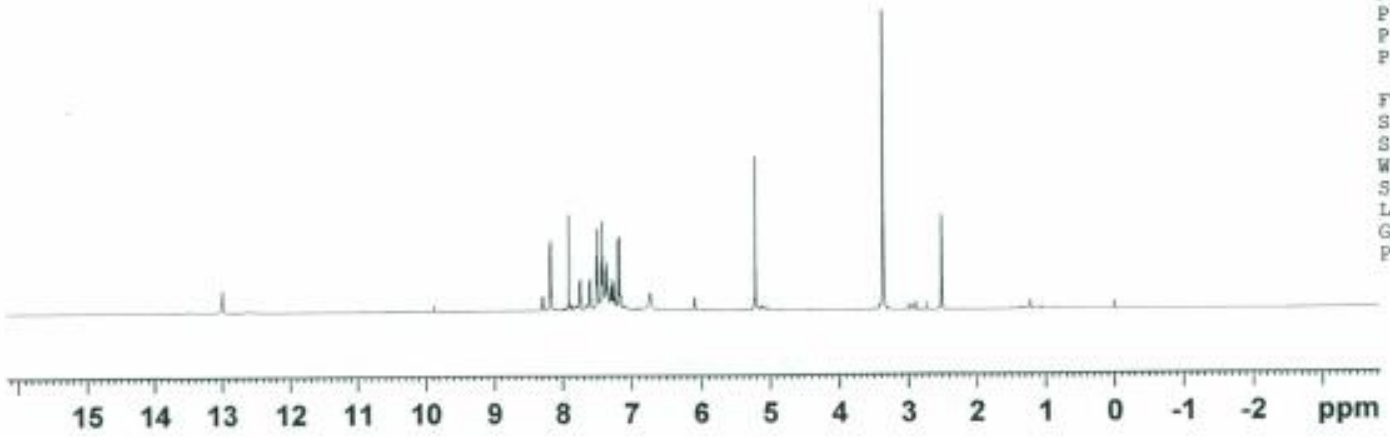

```
Current Data Parameters
NAME                  EG23
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_              20210406
Time                 16.41 h
INSTRUM              Avance
PROBHD    Z151574_0038 (
PULPROG              zgpg30
TD                    65536
SOLVENT                DMSO
NS                      2560
DS                         4
SWH                30120.482 Hz
FIDRES             0.919204 Hz
AQ                 1.0878977 sec
RG                       101
DW                    16.600 usec
DE                     6.50 usec
TE                    300.0 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                         1
SFO1           125.7703643 MHz
NUC1                     13C
P0                     3.33 usec
P1                    10.00 usec
PLW1           85.18099976 W
SFO2           500.1320005 MHz
NUC2                     1H
CPDPRG[2             waltz65
PCPD2                 80.00 usec
PLW2           24.04299927 W
PLW12           0.24043000 W
PLW13           0.12093000 W

F2 - Processing parameters
SI                       32768
SF             125.7577885 MHz
WDW                         EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```


EG-23-1 588 (5.929) Cn (Cen,2, 80.00, Ht)
1: Scan ES+
9.13e7
306.50
100
%
0
307.55
328.30
229.29
261.51
369.55
449.88
490.87
527.93
630.99
633.79
673.63
754.15
769.86
839.96
938.89
m/z
200
250
300
350
400
450
500
550
600
650
700
750
800
850
900
950
H
N
N
N
N
NH2
F

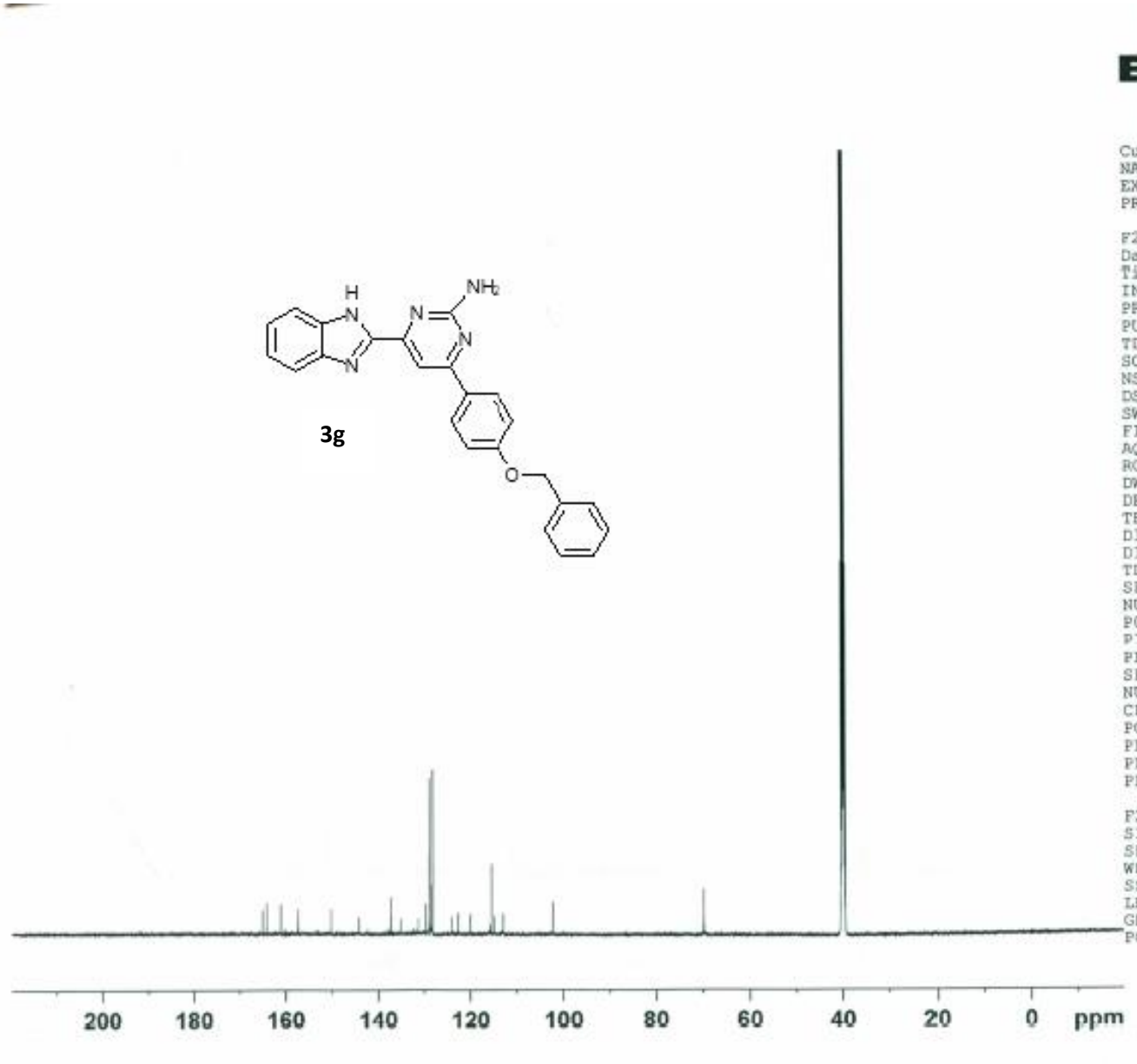
3f



3g

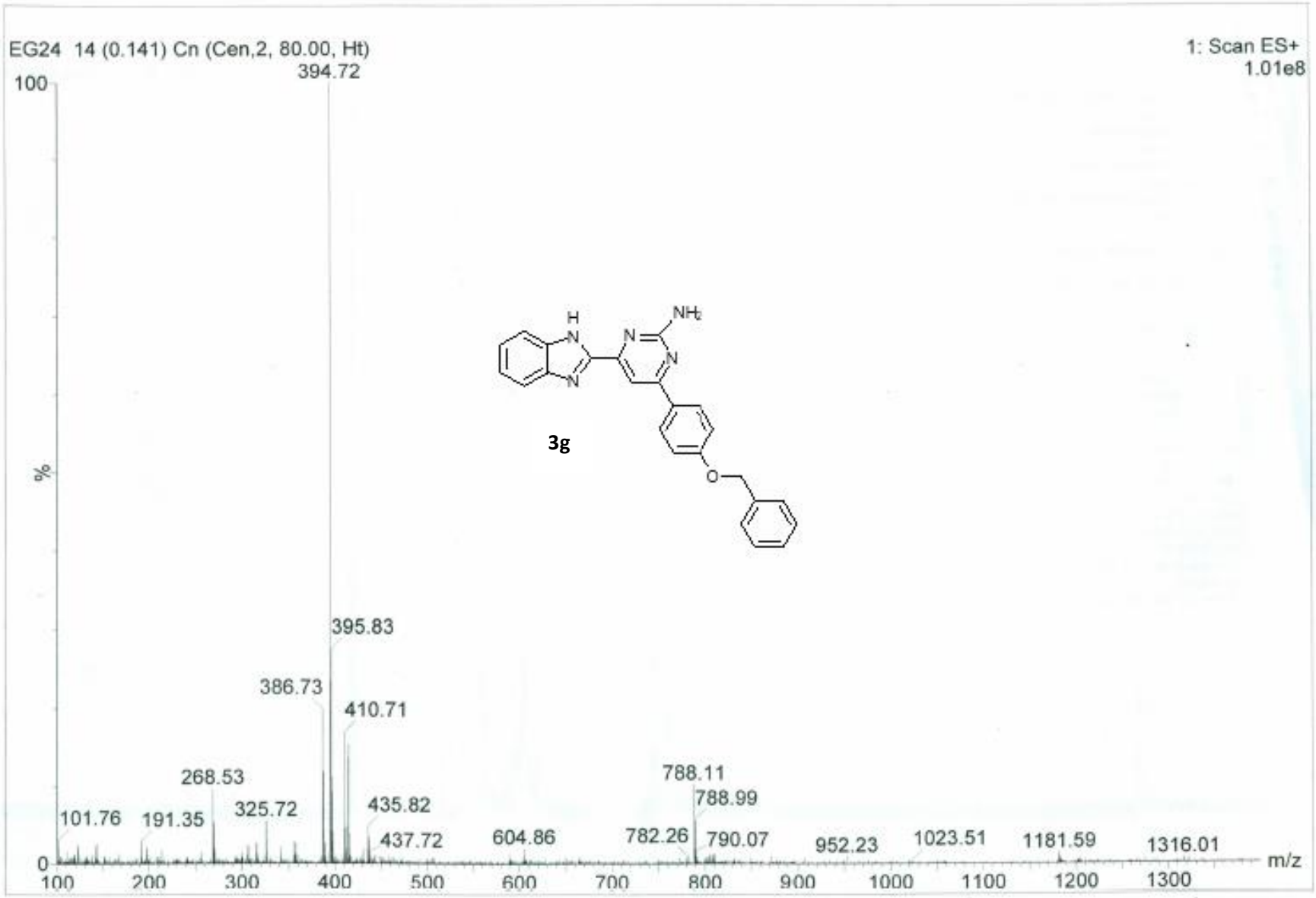



```
Current Data Parameters
NAME                  EG24
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_              20210402
Time                 10.49 h
INSTRUM              Avance
PROBHD   Z151574_0038 (
PULPROG               zg30
TD                   65536
SOLVENT               DMSO
NS                       16
DS                        2 .
SWH              10000.000 Hz
FIDRES               0.305176 Hz
AQ                3.2767999 sec
RG                       101
DW                    50.000 usec
DE                    11.14 usec
TE                    295.4 K
D1               1.00000000 sec
TD0                      1
SFO1           500.1330883 MHz
NUC1                    1H
P0                    2.67 usec
P1                    8.00 usec
PLW1           24.04299927 W

F2 - Processing parameters
SI                   65536
SF             500.1300000 MHz
WDW                     EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
```



BRUKER

```
Current Data Parameters
NAME                  EG24-2
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_                20210727
Time                   15.14 h
INSTRUM                Avance
PROBHD    Z151574_0038 (
PULPROG                zgpg30
TD                      65536
SOLVENT                  DMSO
NS                       4000
DS                          4
SWH                 30120.482 Hz
FIDRES               0.919204 Hz
AQ                   1.0878977 sec
RG                         101
DW                      16.600 usec
DE                       6.50 usec
TE                      298.5 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1
SFO1               125.7703643 MHz
NUC1                       13C
P0                       3.33 usec
P1                      10.00 usec
PLW1               85.18099976 W
SFO2               500.1320005 MHz
NUC2                       1H
CPDPRG[2                waltz65
PCPD2                   80.00 usec
PLW2               24.04299927 W
PLW12               0.24043000 W
PLW13               0.12093000 W

F2 - Processing parameters
SI                         32768
SF                 125.7577885 MHz
WDW                          EM
SSB                 0
LB                       1.00 Hz
GB                  0
PC                       1.40
```


EG24 14 (0.141) Cn (Cen,2, 80.00, Ht)
1: Scan ES+
1.01e8
100
%
0
394.72
395.83
386.73
410.71
268.53
325.72
101.76
191.35
435.82
437.72
604.86
788.11
788.99
782.26
790.07
952.23
1023.51
1181.59
1316.01
m/z
100
200
300
400
500
600
700
800
900
1000
1100
1200
1300
H
N
N
N
N
NH2
O

3g

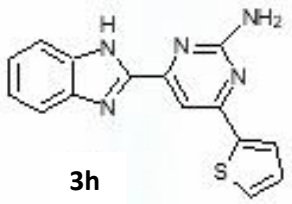
EG-26_2_

Sample Name:
EG-26_2_
Data Collected on:
mercury400-mercury400
Archive directory:
/home/vnmrl/vnmrsys/data
Sample directory:
EG-26_2__20210806_01
FidFile: PROTON_02

Pulse Sequence: PROTON (s2pul)
Solvent: dmso
Data collected on: Aug 6 2021

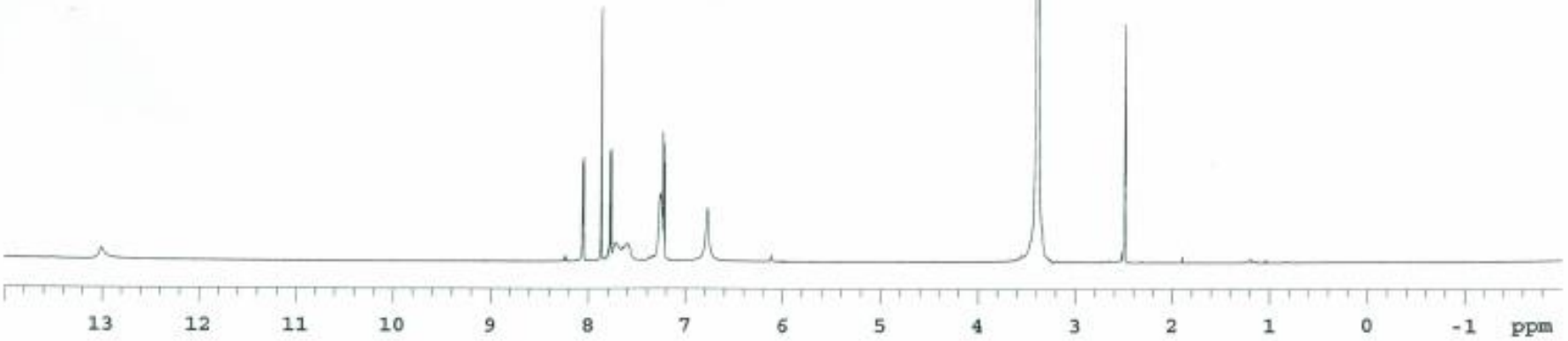
Temp. 25.0 C / 298.1 K
Operator: vnmrl

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.559 sec
Width 6402.0 Hz
32 repetitions
OBSERVE H1, 400.1759761 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 57 sec



3h

Agilent Technologies



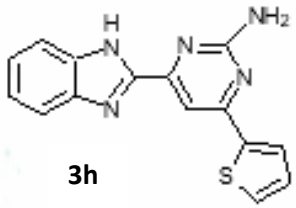
EG-16_2_

Sample Name:
EG-26_2_
Data Collected on:
nercury400-mercury400
Archive directory:
/home/vnmr1/vnmrs/s/data
Sample directory:
EG-26_2__20210806_01
FidFile: current

Pulse Sequence: CARBON (s2pul)
Solvent: dmso
Data collected on: Aug 6 2021

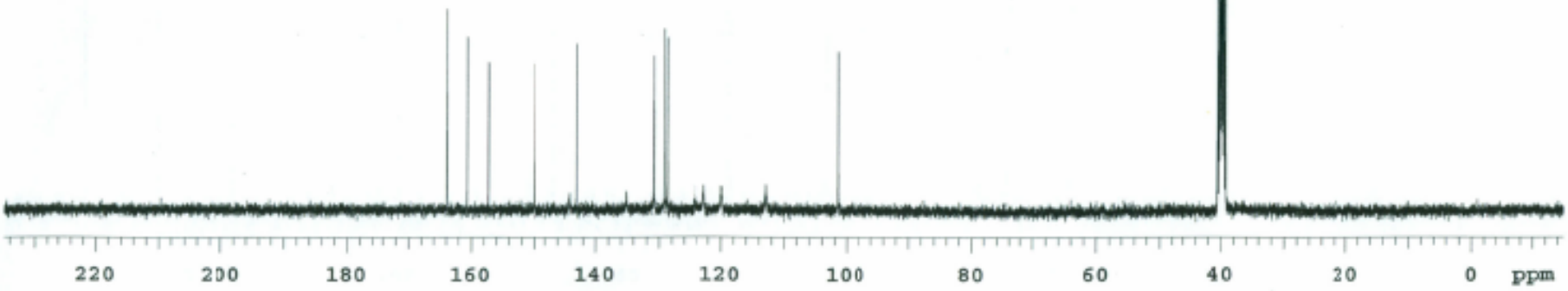
Temp. 25.0 C / 298.1 K
Operator: vnmr1

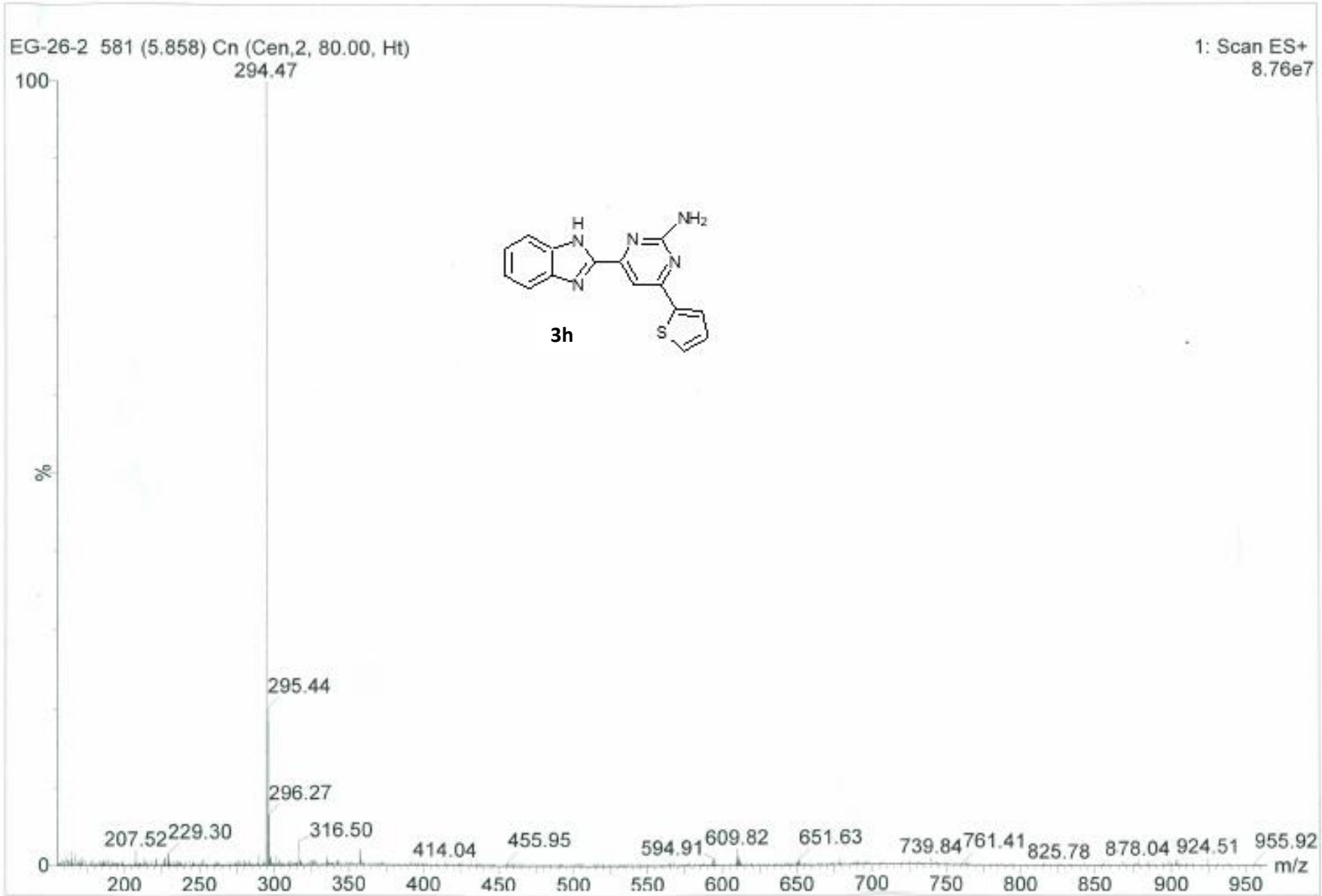
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.304 sec
Width 25125.6 Hz
4032 repetitions
OBSERVE C13, 100.6243292 MHz
DECOUPLE H1, 400.1779555 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 3 hr, 19 min



3h

Agilent Technologies




EG-26-2 581 (5.858) Cn (Cen,2, 80.00, Ht)
1: Scan ES+
8.76e7
294.47
100
%
0
295.44
296.27
207.52
229.30
316.50
414.04
455.95
594.91
609.82
651.63
739.84
761.41
825.78
878.04
924.51
955.92
m/z
200
250
300
350
400
450
500
550
600
650
700
750
800
850
900
950
H
N
N
N
NH2
N
S

3h