

Supporting Information

For

L-Proline catalyzed one-pot synthesis of polysubstituted pyridine system that incorporating benzothiazole moiety *via* sustainable sonochemical approach

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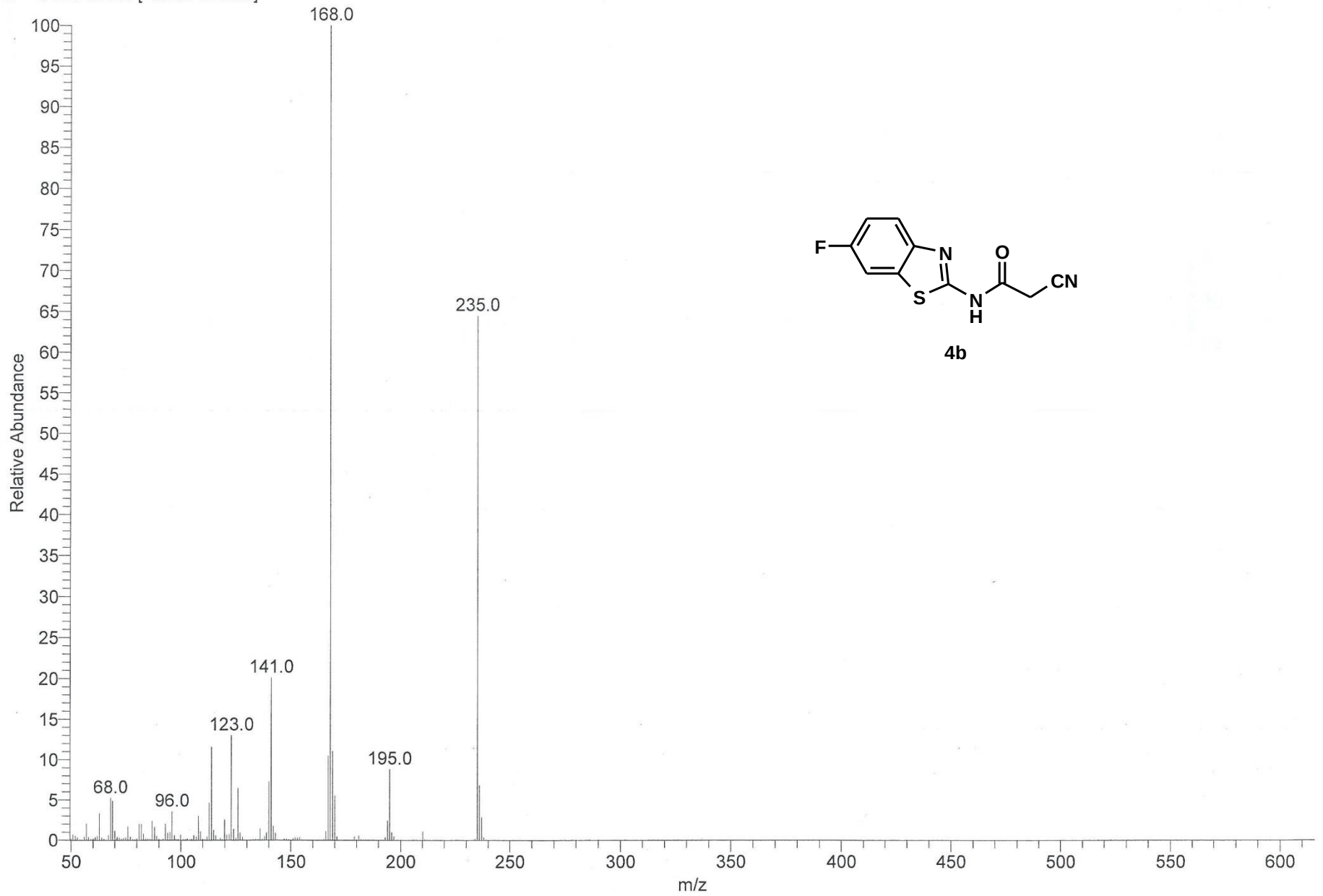
^c Chemistry Department, College of Science, Jouf University, P.O. Box 72341, Sakaka, Aljouf, Kingdom of Saudi Arabia.

Contents

Copies of ¹H, ¹³C NMR, MS, HRMS AND IR spectra of the reported compounds.

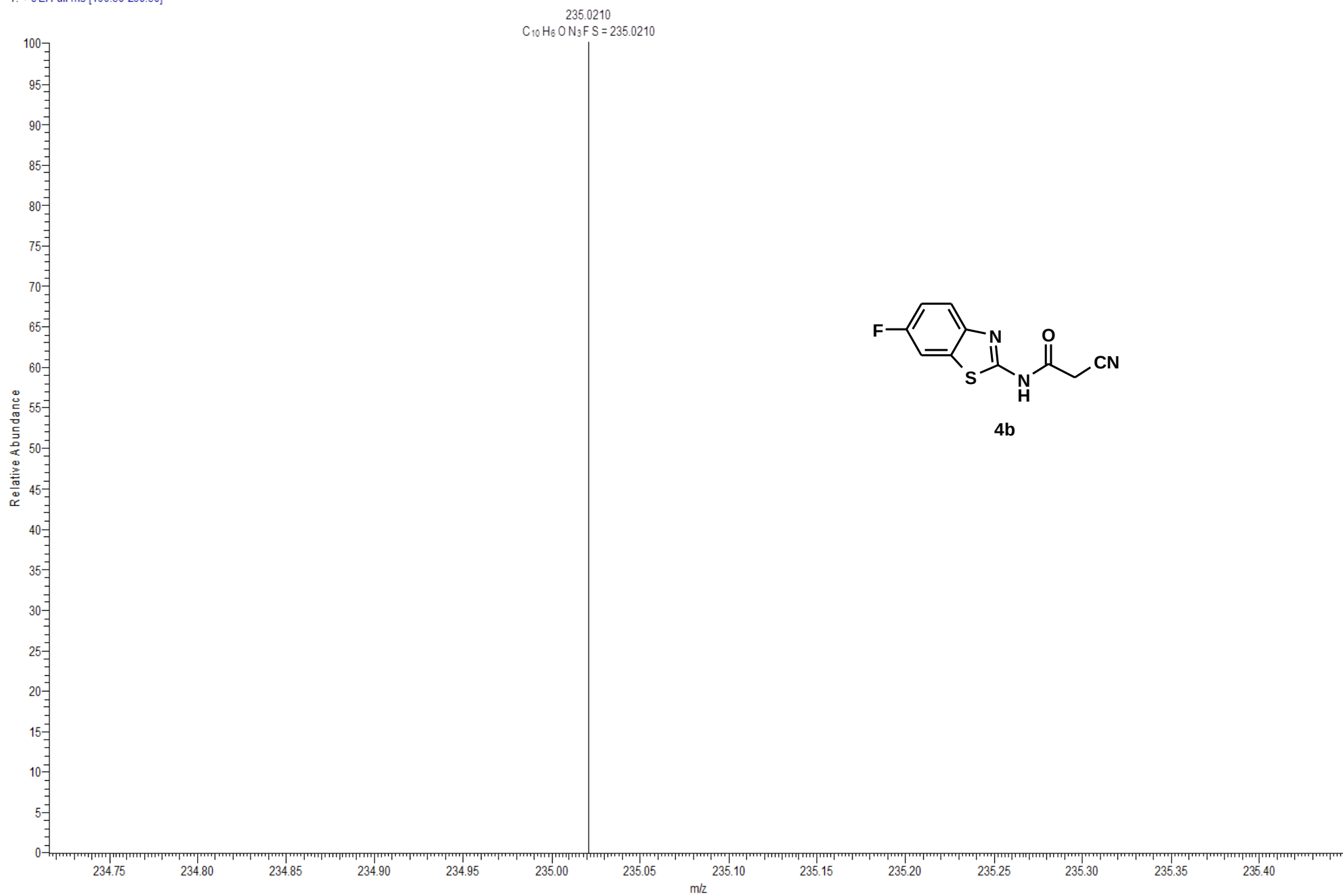
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Project No: GS01/03

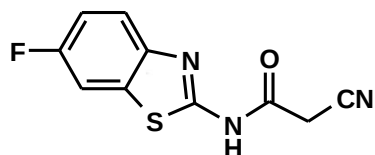
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T: + c EI Full ms [49.50-900.50]



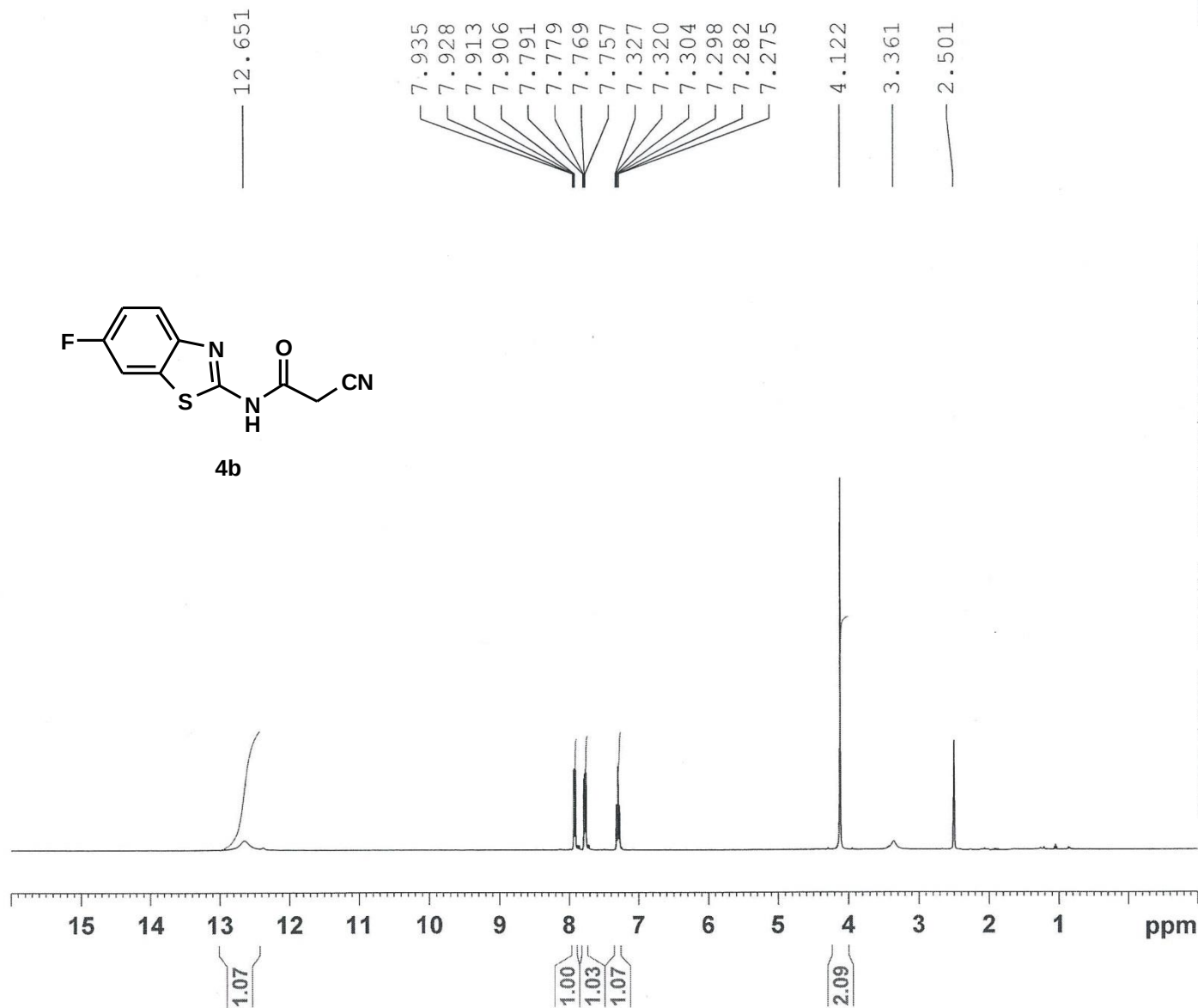
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T: + c EI Full ms [199.50-260.50]





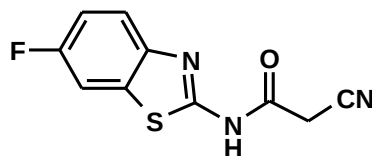
4b



INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 456.1
DW 60.400 usec
DE 6.00 usec
TE 673.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 9.00 usec
PL1 -4.50 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300027 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



4b

162.99
159.68
158.08
157.56
157.55
145.12
132.83
132.76
121.94
121.87
115.14
114.50
114.34
108.35
108.17

39.91
39.78
39.64
39.50
39.36
39.22
39.08
26.38

PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 150
DS 4
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9088159 sec
RG 203
DW 13.867 usec
DE 6.50 usec
TE 298.5 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

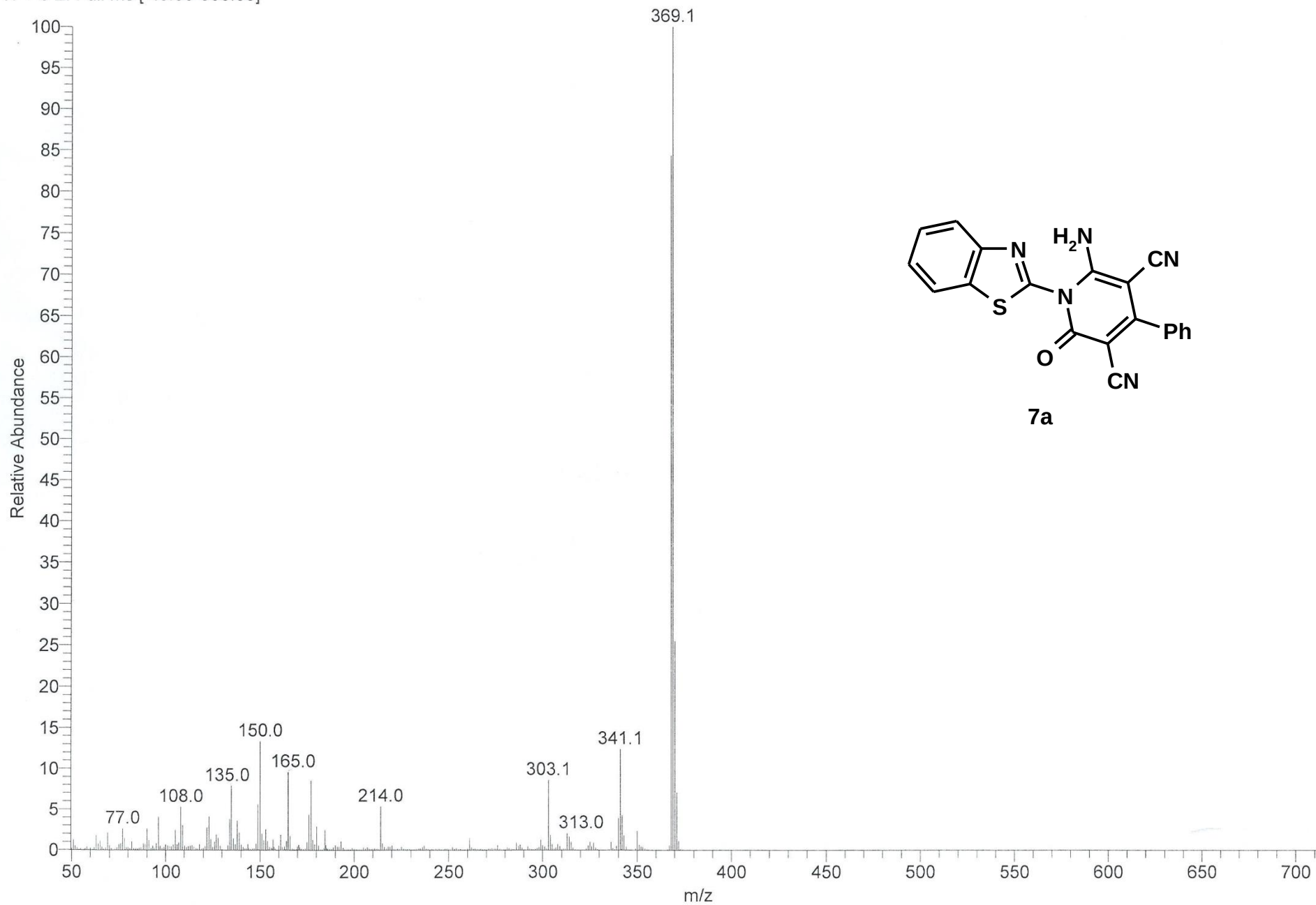
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PL13 15.00 dB
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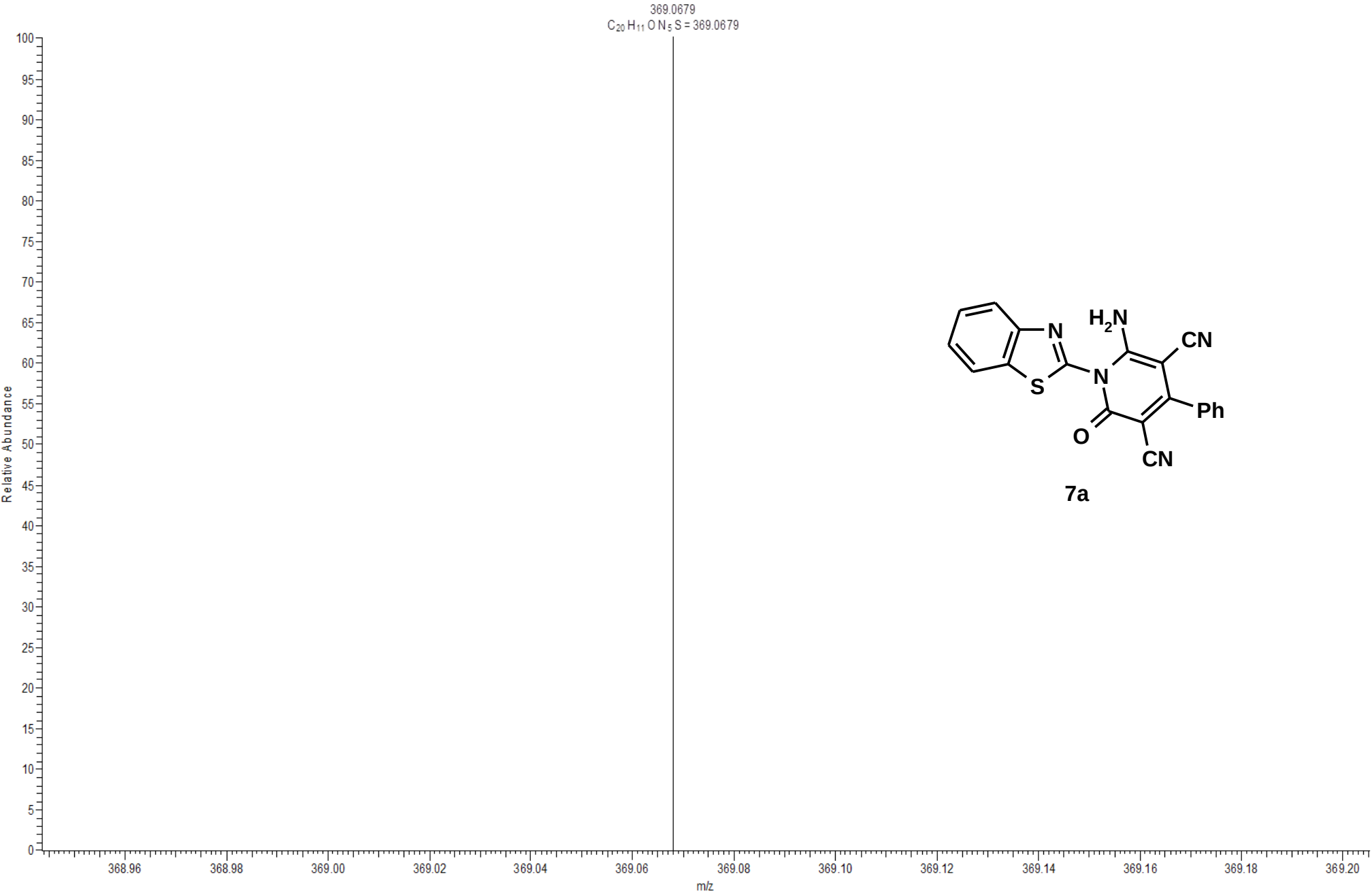
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GB 0
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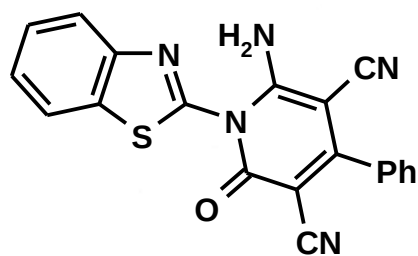
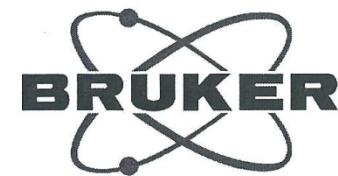
220 200 180 160 140 120 100 80 60 40 20 ppm

N #191 RT: 8.42 AV: 1 NL: 2.33E7
T: + c EI Full ms [49.50-900.50]



HRMS-BT4-mass1 #32 RT: 8.45 AV: 1 NL: 3.98E4
T: + c EI Full ms [339.50-400.50]





7a

8.711
8.219
8.206
8.132
8.118
7.650
7.638
7.626
7.594

3.085
2.501

INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 12335.526 Hz
FIDRES 0.188225 Hz
AQ 2.6563926 sec
RG 181
DW 40.533 usec
DE 20.00 usec
TE 358.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 600.1337060 MHz
NUC1 1H
P1 10.60 usec
PLW1 27.82500076 W

F2 - Processing parameters
SI 32768
SF 600.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

2.06
1.02
1.00
1.14
6.03

15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm

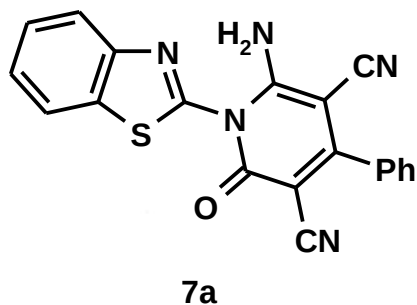


162.03
158.67
156.50
154.09
149.12
136.34
134.21
129.99
128.20
127.39
126.10
125.97
123.23
122.10
114.96
114.53

— 87.68

— 75.84

39.92
39.78
39.64
39.50
39.36
39.22
39.08

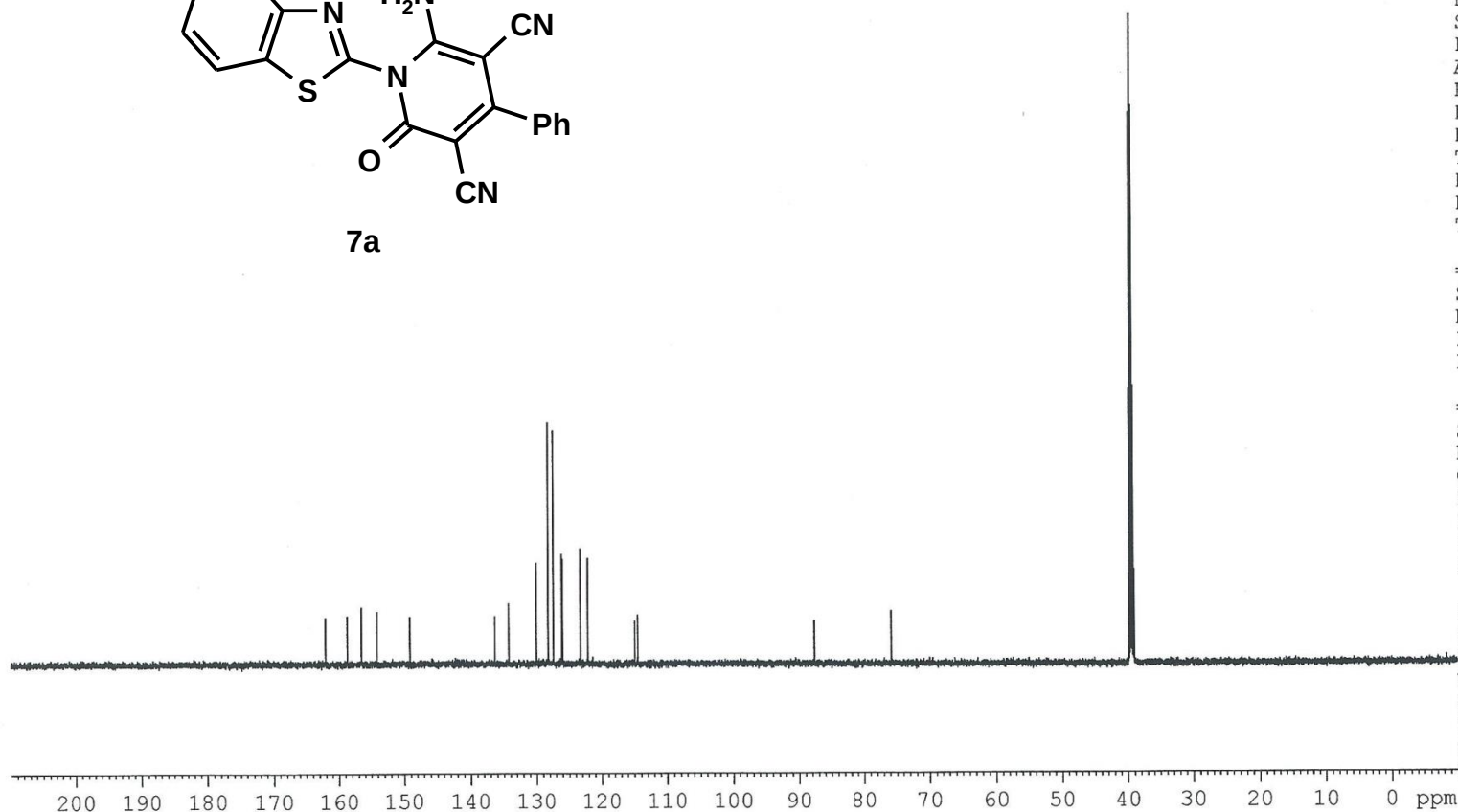


PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 84
DS 4
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 203
DW 13.867 usec
DE 50.00 usec
TE 358.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

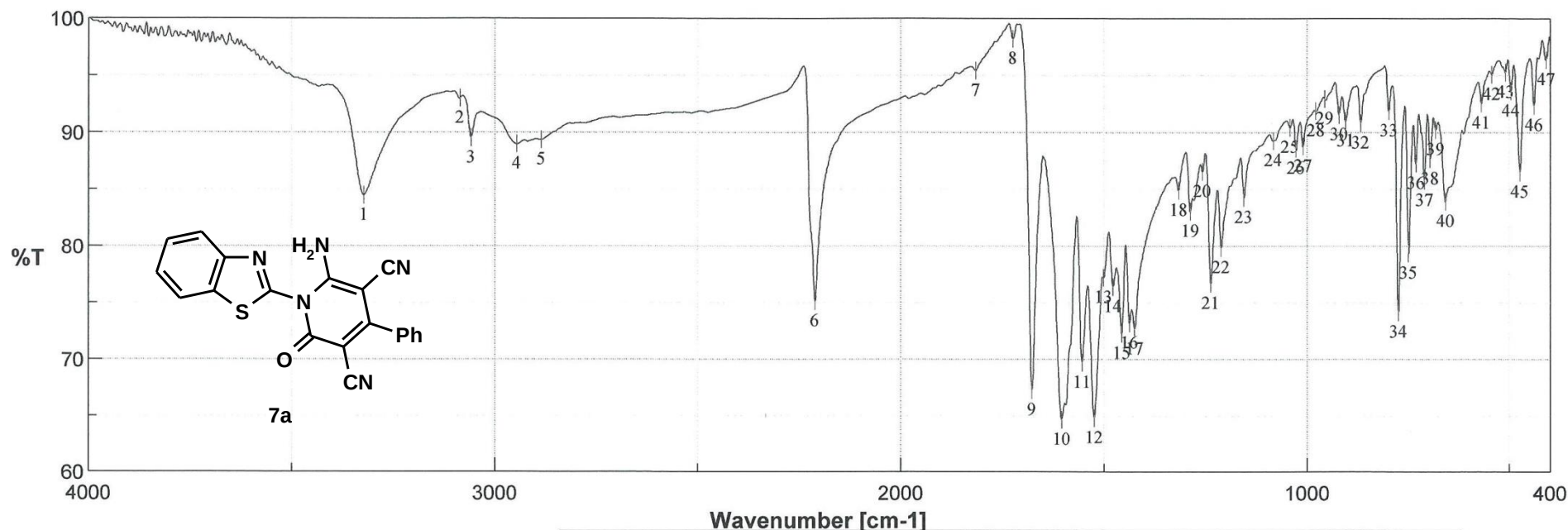
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NUC1 13C
P1 8.80 usec
PLW1 78.13500214 W

===== CHANNEL f2 =====
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 70.00 usec
PLW2 27.82500076 W
PLW12 0.63804001 W
PLW13 0.31264001 W

F2 - Processing parameters
SI 32768
SF 150.9029422 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



FT-IR Spectral Data



Wavenumber [cm-1]

Result of Peak Picking

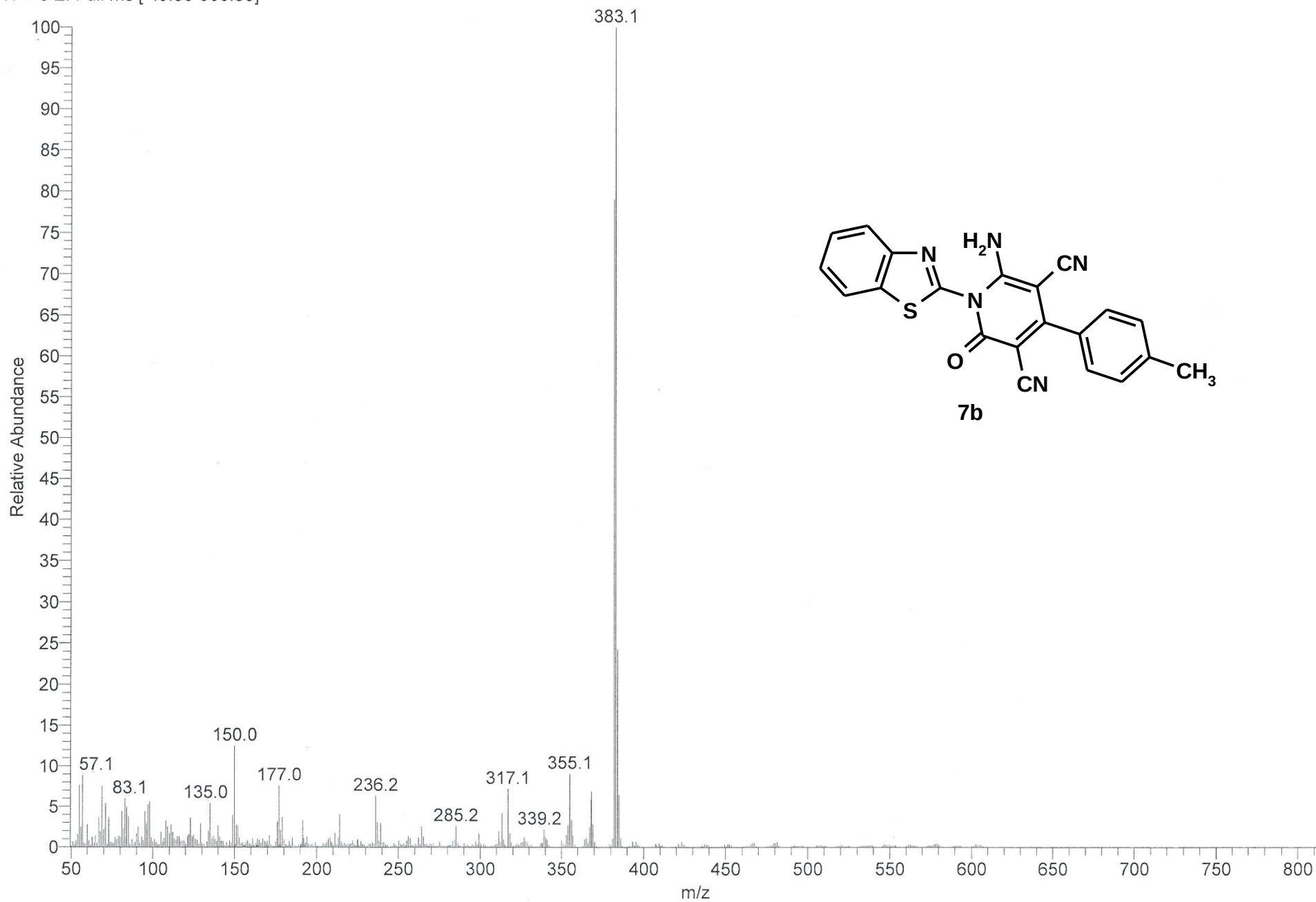
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1	3321.78	84.4246	2	3085.55	92.9391	3	3058.55	89.4821
4	2945.73	88.9266	5	2885.95	89.3316	6	2210.02	75.1057
7	1814.69	95.3699	8	1723.09	98.1812	9	1676.8	67.2494
10	1604.48	64.6244	11	1553.38	69.6791	12	1524.45	64.7336
13	1501.31	77.183	14	1477.21	76.3586	15	1455.99	72.216
16	1436.71	73.1706	17	1424.17	72.6385	18	1316.18	84.8761
19	1287.25	83.0173	20	1257.36	86.5206	21	1237.11	76.6728
22	1211.08	79.7967	23	1155.15	84.2081	24	1082.83	89.2273
25	1041.37	90.3895	26	1025.94	88.538	27	1008.59	88.7437
28	977.733	91.8317	29	955.555	92.9308	30	920.843	91.5232
31	904.451	90.9556	32	866.846	90.7785	33	798.385	91.8319
34	775.244	74.117	35	750.174	79.2979	36	731.853	87.2112
37	711.604	85.7197	38	697.141	87.6142	39	683.642	90.1744
40	659.536	83.8702	41	569.862	92.5097	42	543.828	95.0554
43	510.08	95.2518	44	496.58	93.5728	45	474.403	86.4624
46	439.69	92.343	47	409.799	96.3494			

[Measurement Information]

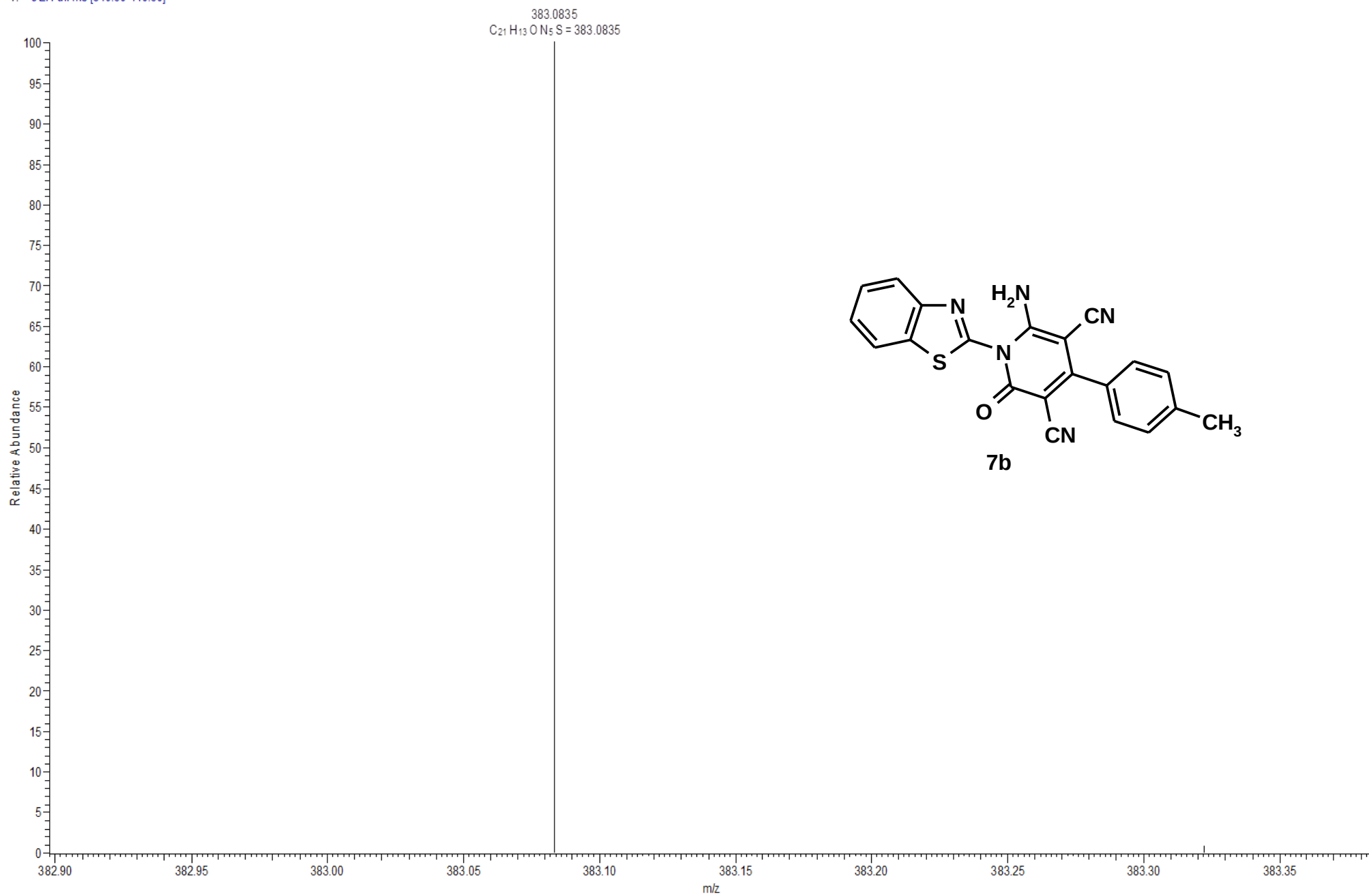
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Serial Number A009861024

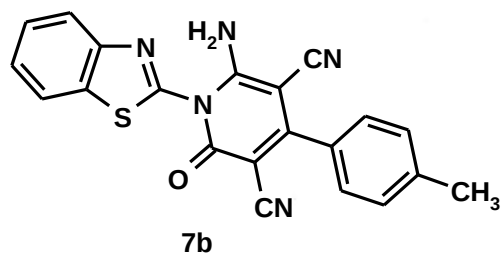
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Detector TGS
Accumulation Auto (37)
Resolution 4 cm⁻¹
Zero Filling On
Apodization Cosine
Gain Auto (4)
Aperture Auto (7.1 mm)
Scanning Speed Auto (2 mm/sec)
Filter Auto (10000 Hz)

BT9 #181 RT: 7.98 AV: 1 NL: 8.31E7
T: + c EI Full ms [49.50-900.50]



HRMS-BT9-mass1#14 RT: 8.94 AV: 1 NL: 8.89E4
T: + c EI Full ms [349.50-410.50]





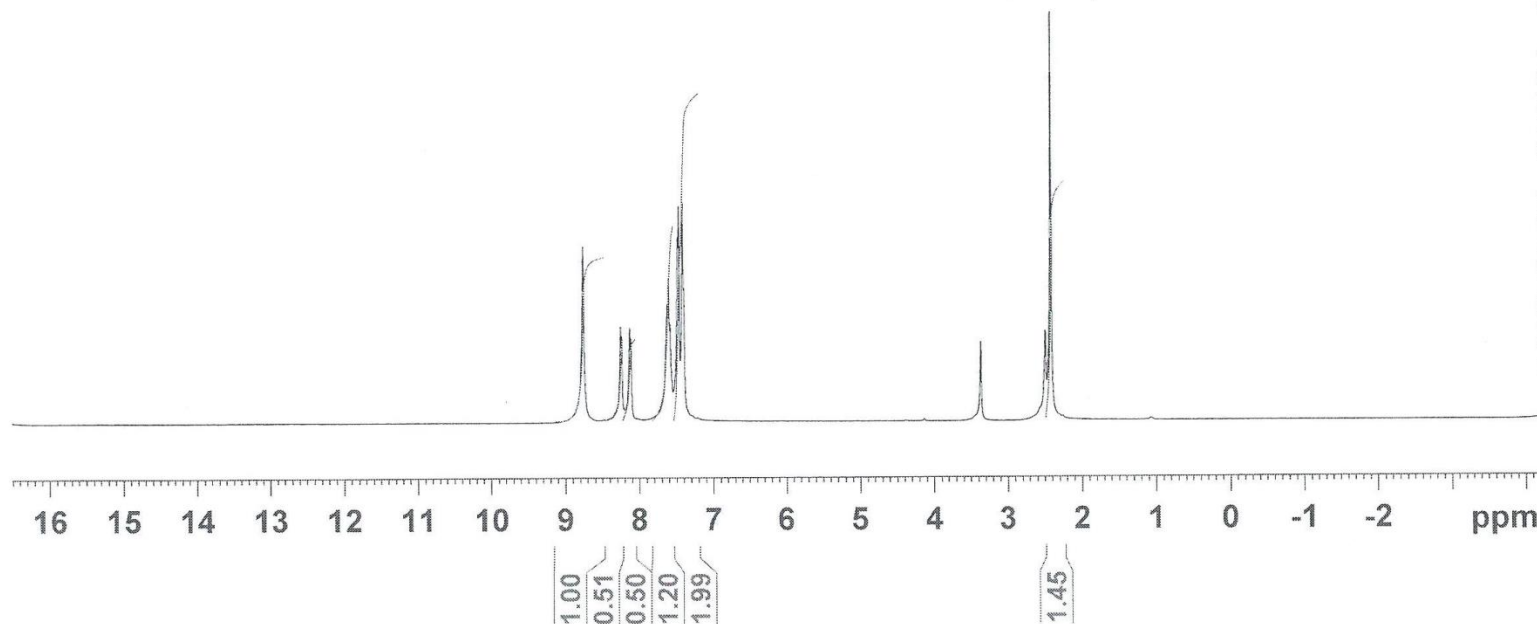
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8.117
7.629
7.610
7.590
7.488
7.470
7.418

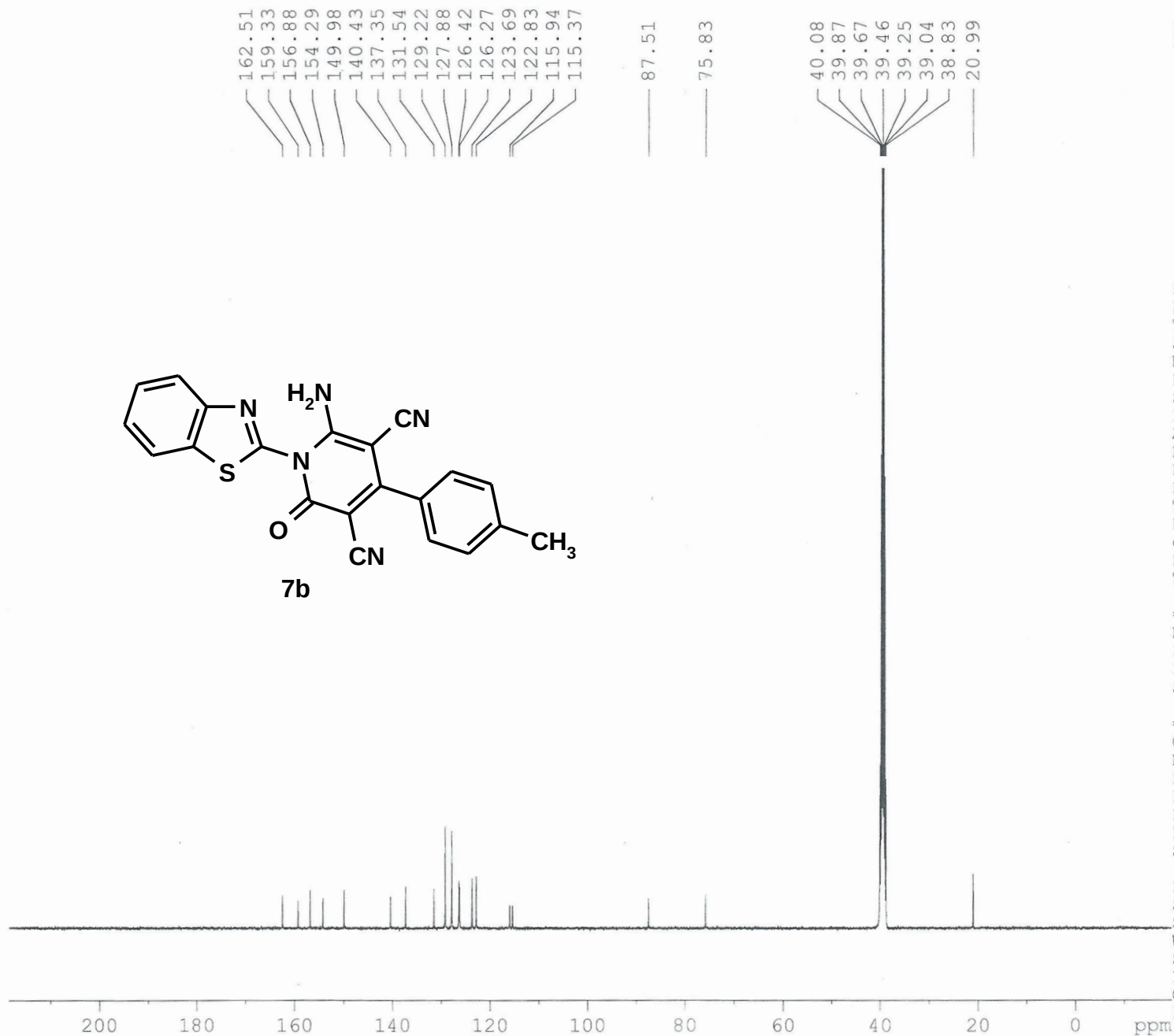
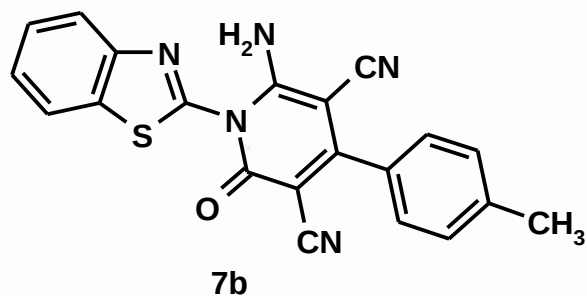
3.369
2.498
2.419

PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 181
DW 60.400 usec
DE 6.00 usec
TE 673.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 9.00 usec
PL1 -4.50 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300027 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





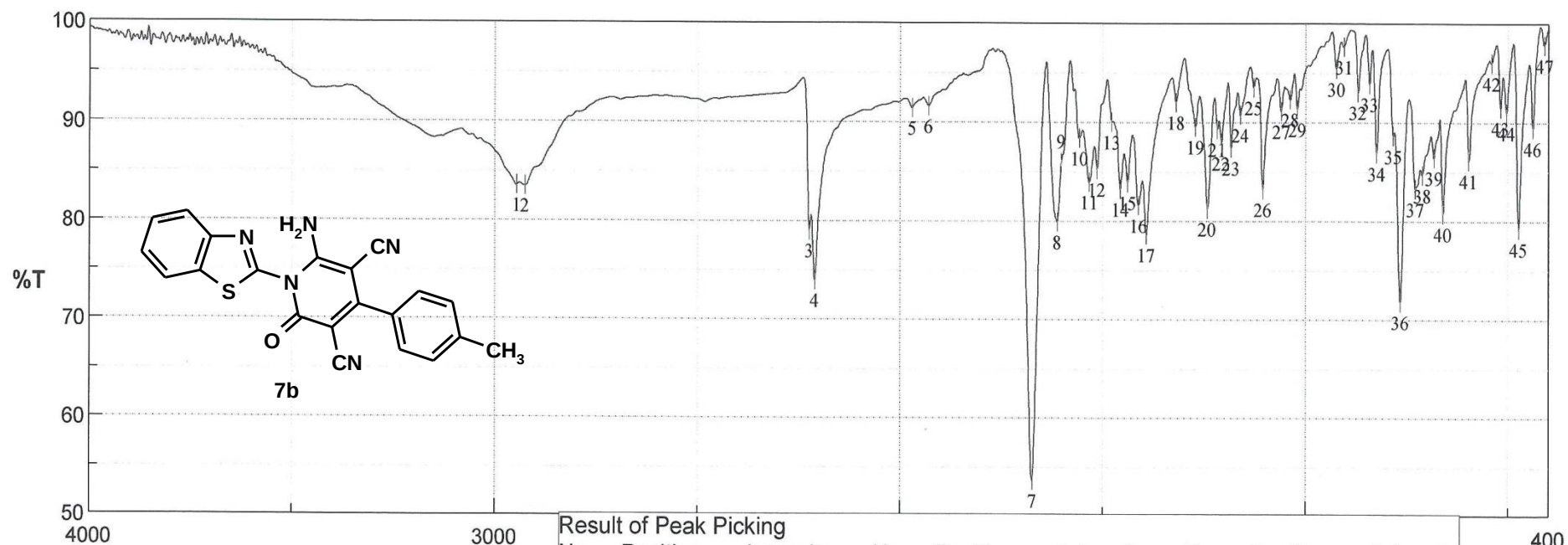
PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 10240
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 1290.2
 DW 20.850 usec
 DE 6.00 usec
 TE 673.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 7.20 usec
 PL1 -6.00 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -3.00 dB
 PL12 15.06 dB
 PL13 18.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
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 SF 100.6128193 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

FT-IR Spectral Data



Result of Peak Picking

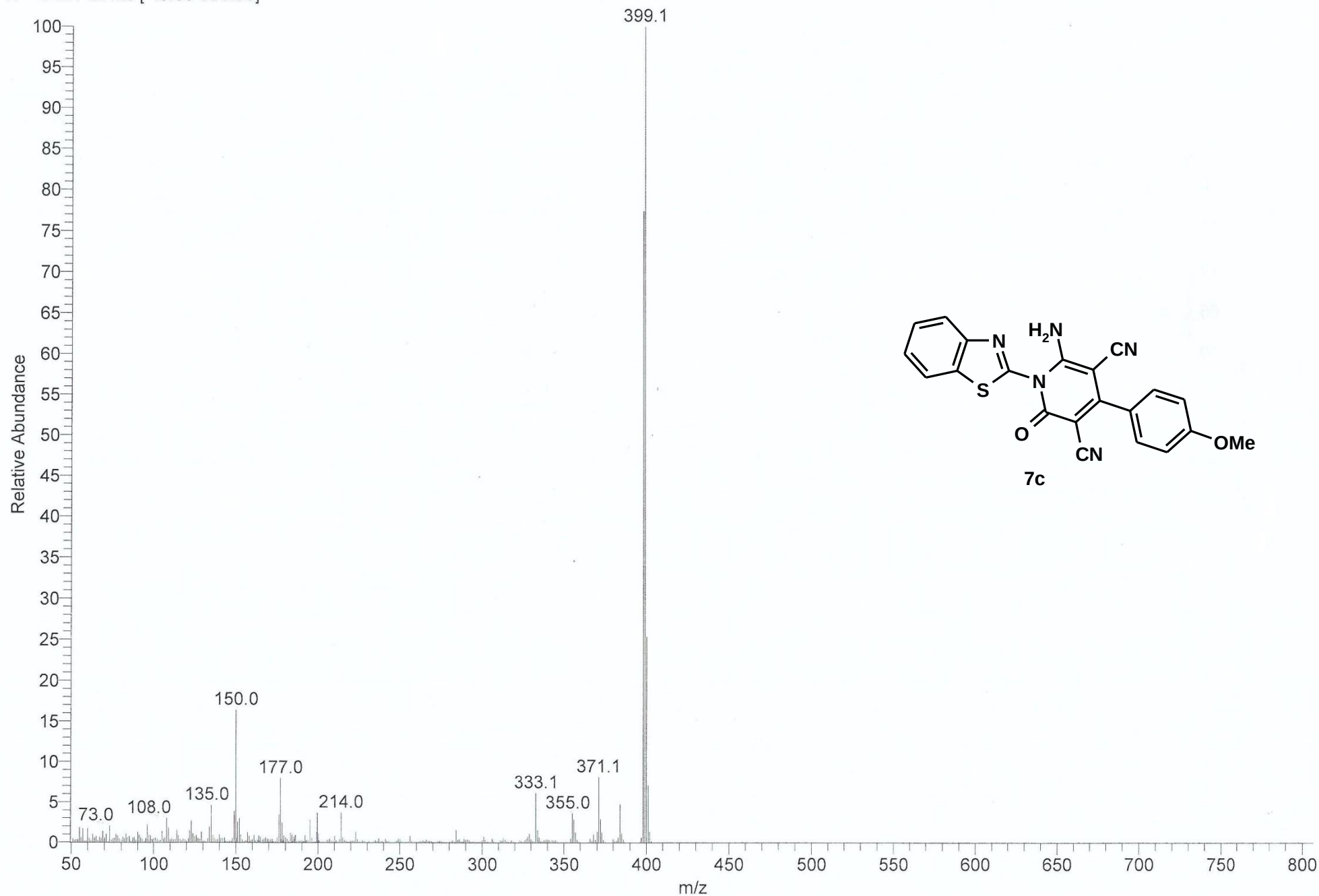
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4	2211.95	73.9108	5	1969.93	91.396	6	1928.47	91.5905
7	1673.91	53.584	8	1612.2	79.8246	9	1602.56	85.8862
10	1558.2	88.3237	11	1533.13	83.9102	12	1513.85	85.2145
13	1477.21	90.0083	14	1455.99	83.1789	15	1437.67	83.8592
16	1411.64	81.5313	17	1392.35	78.5568	18	1319.07	91.972
19	1270.86	89.4735	20	1241.93	81.1944	21	1217.83	89.2599
22	1208.18	87.8518	23	1184.08	87.3503	24	1160.94	90.7305
25	1128.15	93.5313	26	1105.01	83.2104	27	1059.69	91.0991
28	1037.52	92.265	29	1020.16	91.2782	30	923.736	95.4111
31	904.451	97.628	32	869.739	93.0336	33	841.776	93.8881
34	823.455	86.8062	35	782.958	88.6126	36	765.601	71.8052
37	728.961	83.2228	38	711.604	84.6657	39	682.677	86.3841
40	660.5	80.732	41	597.825	86.1341	42	541.899	95.974
43	519.722	91.4498	44	504.294	90.9809	45	474.403	79.1625
46	439.69	89.3712	47	409.799	97.8315			

[Measurement Information]

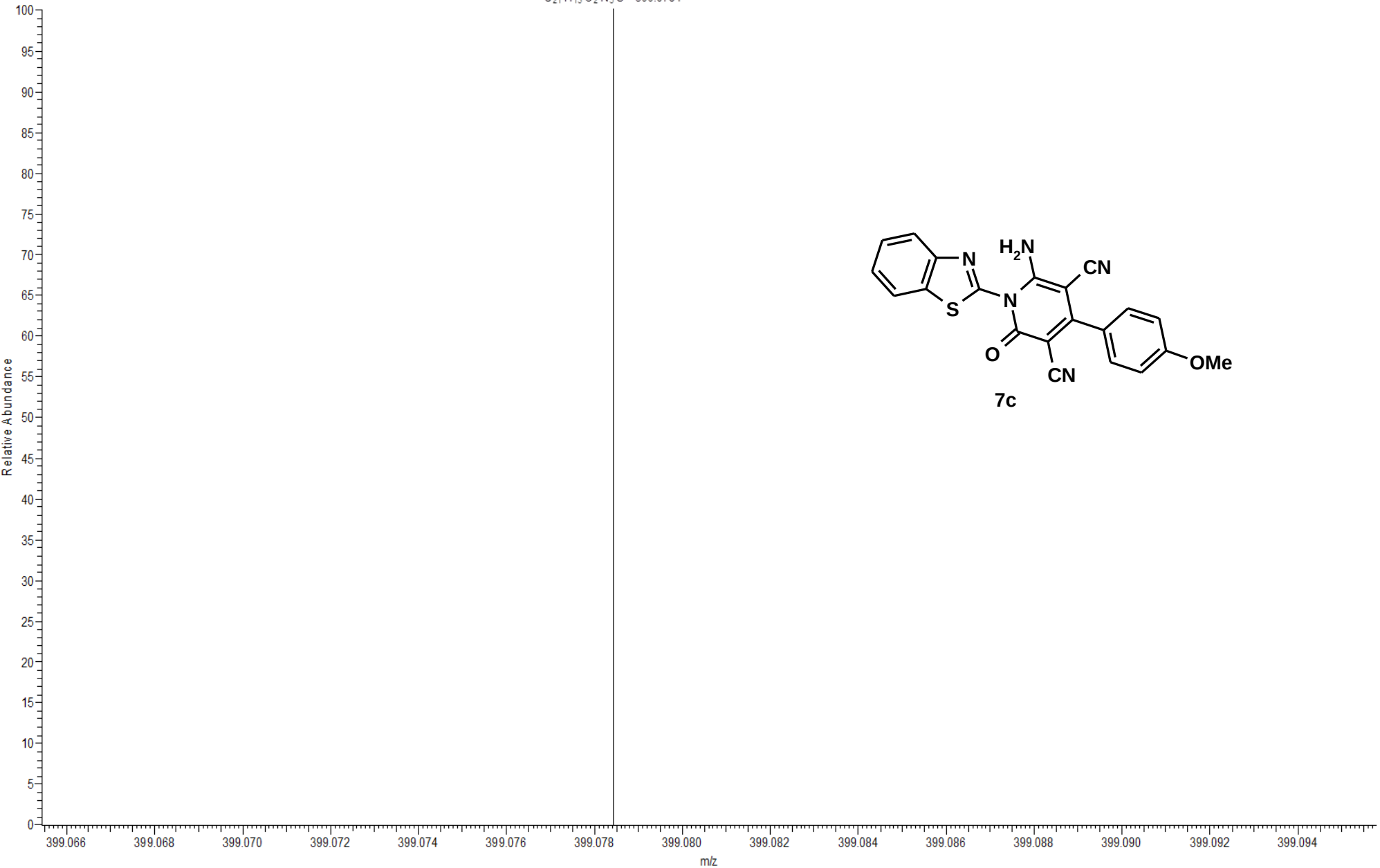
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Serial Number A009861024

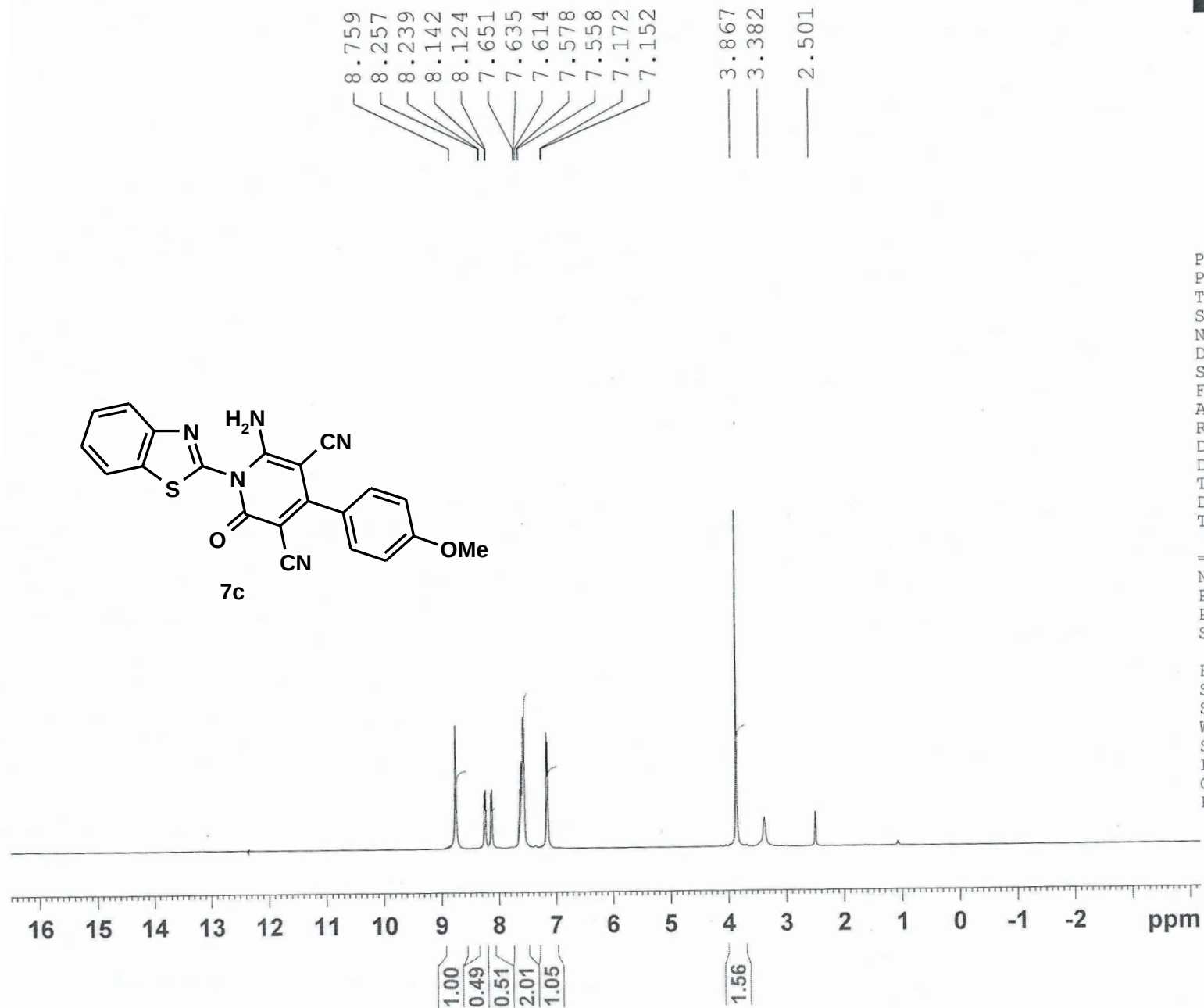
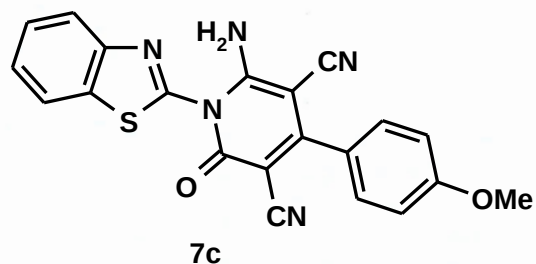
Light Source Standard
Detector TGS
Accumulation Auto (44)
Resolution 4 cm⁻¹
Zero Filling On
Apodization Cosine
Gain Auto (4)
Aperture Auto (7.1 mm)
Scanning Speed Auto (2 mm/sec)
Filter Auto (10000 Hz)

BT7C #204 RT: 9.00 AV: 1 NL: 9.82E7
T: + c EI Full ms [49.50-900.50]



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T: + c EI Full ms [359.50-420.50]

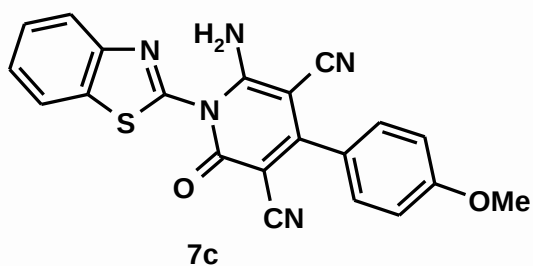




PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 181
DW 60.400 usec
DE 6.00 usec
TE 673.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 9.00 usec
PL1 -4.50 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300027 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



162.14
160.98
159.41
156.88
154.33
149.96
137.32
129.85
126.44
126.29
123.69
122.81
116.14
115.56
114.03

87.40

75.82

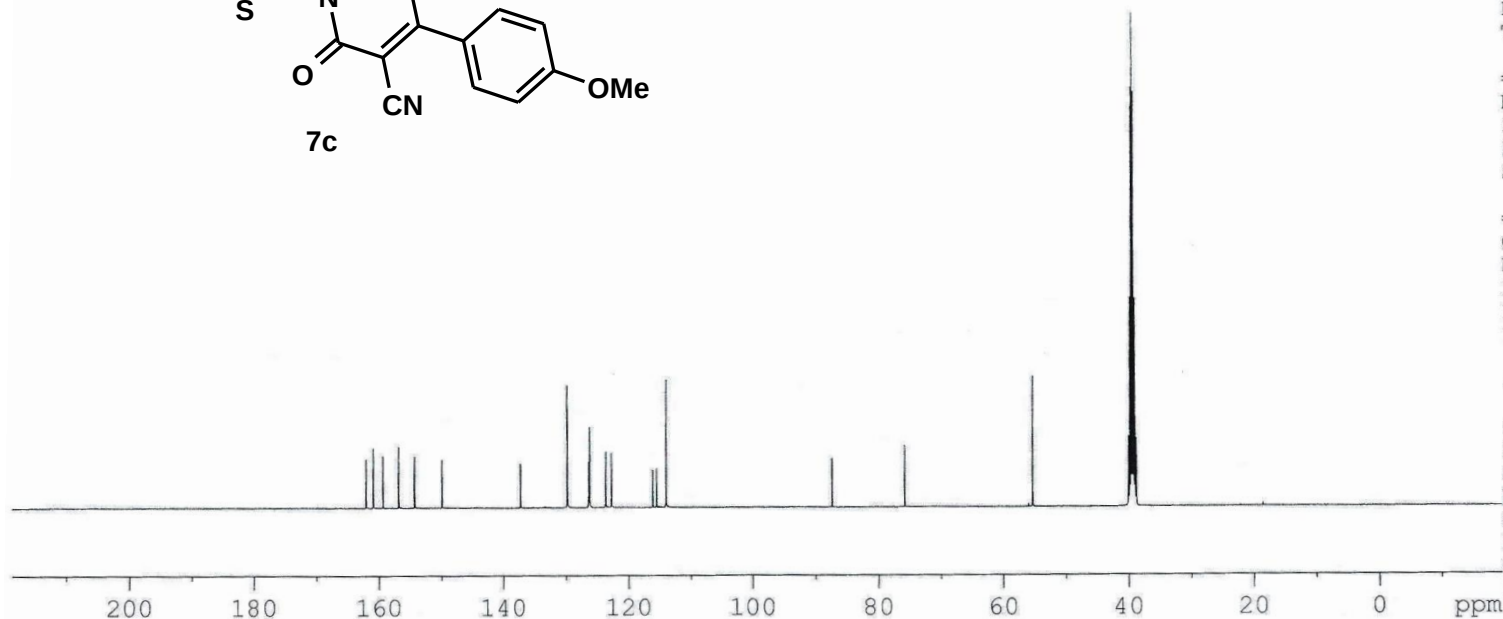
55.37
40.05
39.84
39.63
39.42
39.21
39.00
38.80

PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 10240
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 2298.8
DW 20.850 usec
DE 6.00 usec
TE 673.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

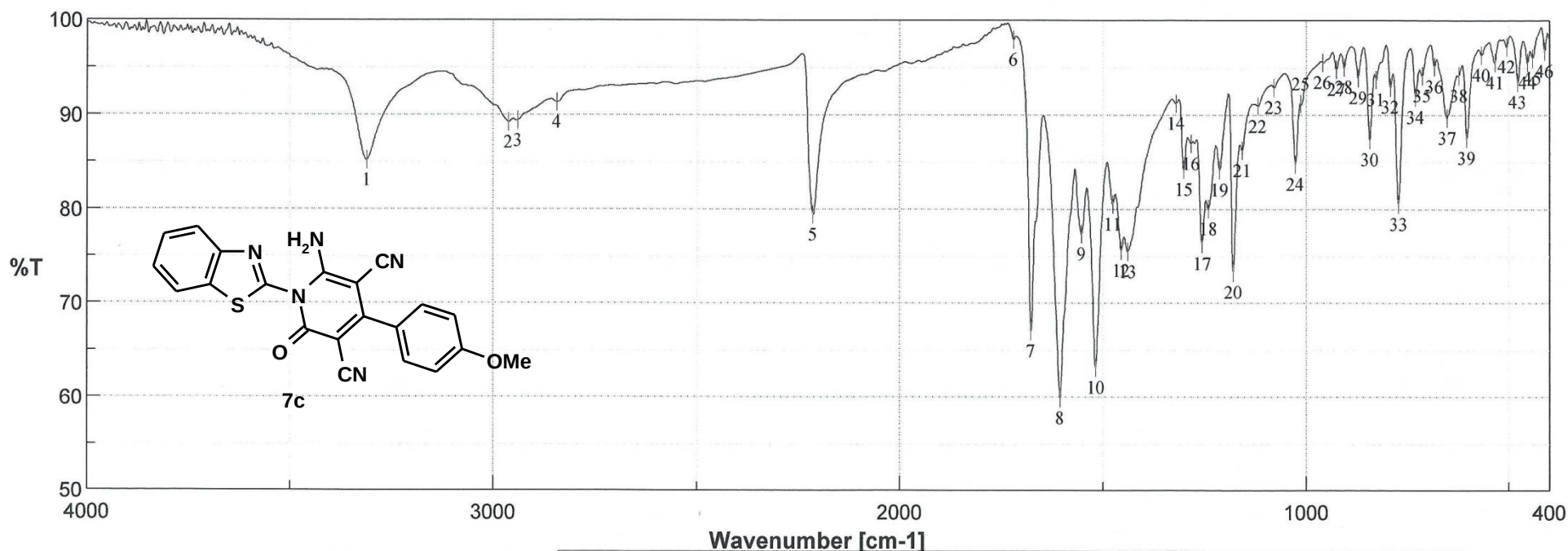
===== CHANNEL f1 =====
NUC1 13C
P1 7.20 usec
PL1 -6.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 15.06 dB
PL13 18.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6128193 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



FT-IR Spectral Data



[Measurement Information]

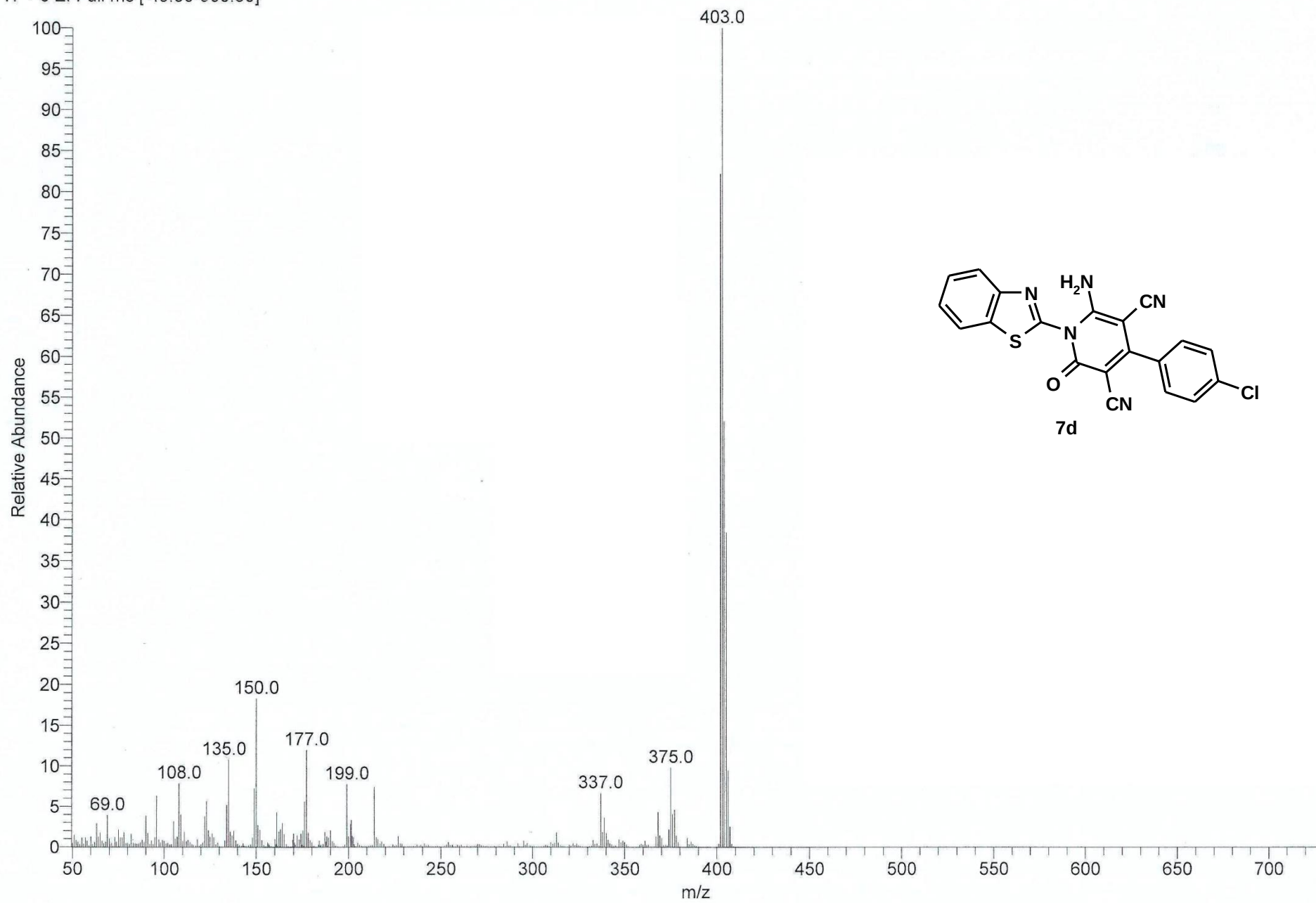
Model Name FT/IR-6300typeA
Serial Number A009861024

Light Source Standard
Detector TGS
Accumulation Auto (38)
Resolution 4 cm⁻¹
Zero Filling On
Apodization Cosine
Gain Auto (4)
Aperture Auto (7.1 mm)
Scanning Speed Auto (2 mm/sec)
Filter Auto (10000 Hz)

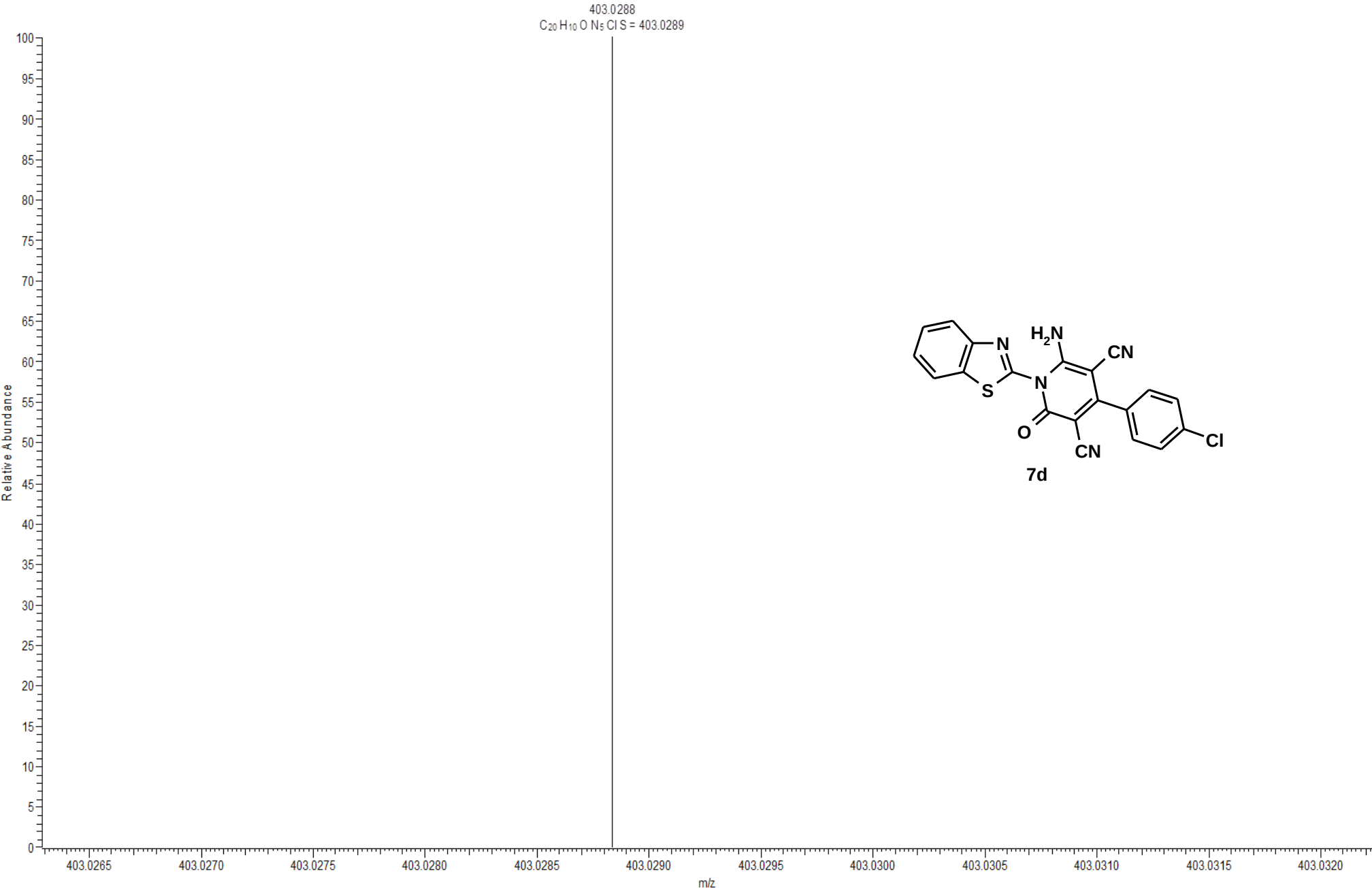
Result of Peak Picking

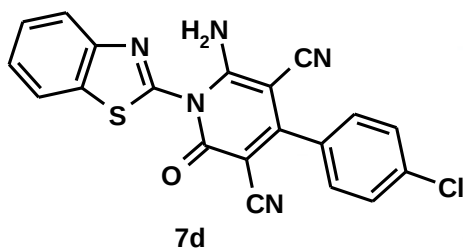
No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	3311.18	85.1406	2	2961.16	89.1617	3	2938.98	89.3424
4	2843.52	91.2853	5	2213.88	79.3401	6	1719.23	97.9193
7	1676.8	66.9811	8	1605.45	59.8333	9	1552.42	77.3147
10	1517.7	63.0808	11	1475.28	80.4812	12	1455.03	75.5402
13	1438.64	75.4488	14	1319.07	91.121	15	1299.79	84.1466
16	1281.47	86.8822	17	1255.43	76.2767	18	1240	79.9843
19	1212.04	84.1195	20	1179.26	73.2404	21	1157.08	86.1726
22	1118.51	90.8567	23	1078.98	92.8366	24	1025.94	84.7178
25	1012.45	91.1271	26	958.448	95.5223	27	924.7	94.7917
28	905.415	95.0187	29	870.703	93.8825	30	841.776	87.3125
31	826.348	93.6777	32	791.636	92.8904	33	771.387	80.4607
34	729.925	91.8153	35	714.497	94.1213	36	683.642	95.0776
37	652.786	89.6529	38	624.823	94.0864	39	604.574	87.5073
40	567.934	96.2865	41	535.15	95.4954	42	506.223	97.2312
43	478.26	93.4682	44	454.154	95.4829	45	441.619	96.006
46	411.728	96.7484						

B-T-Z #201 RT: 8.86 AV: 1 NL: 2.51E7
T: + c EI Full ms [49.50-900.50]



HRMS-BT5-mass1#62 RT: 2.56 AV: 1 NL: 2.41E3
T: + c EI Full ms [374.50-435.50]





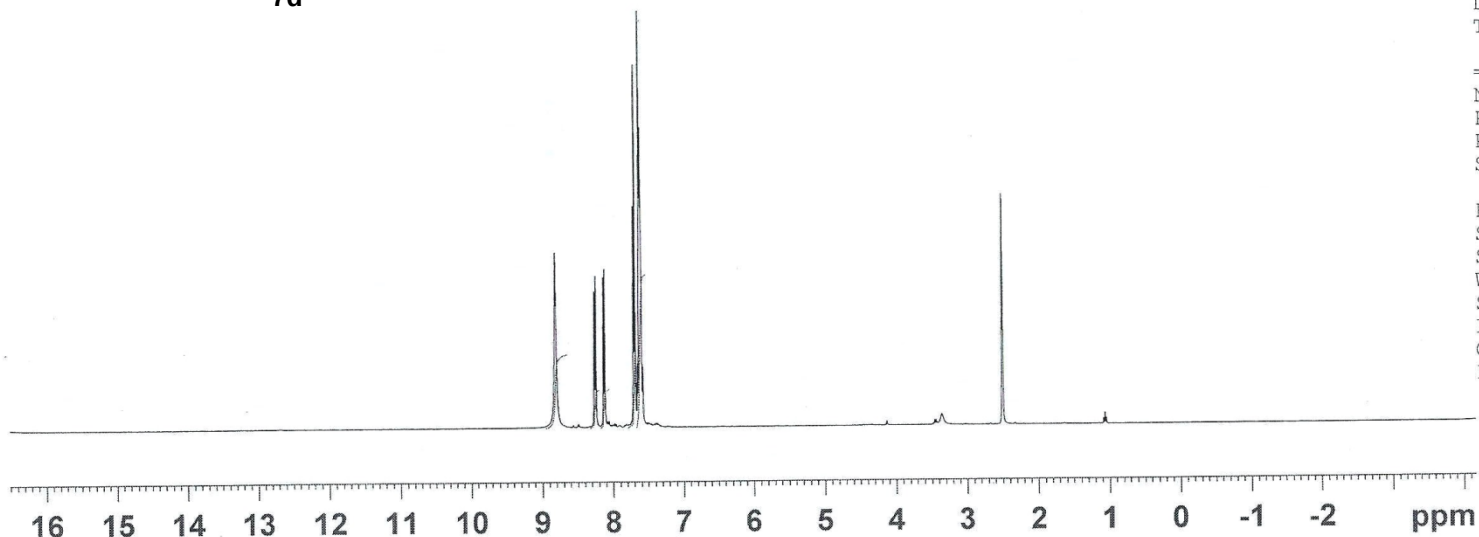
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7.713
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7.639
7.631
7.610
7.582

3.379
2.509

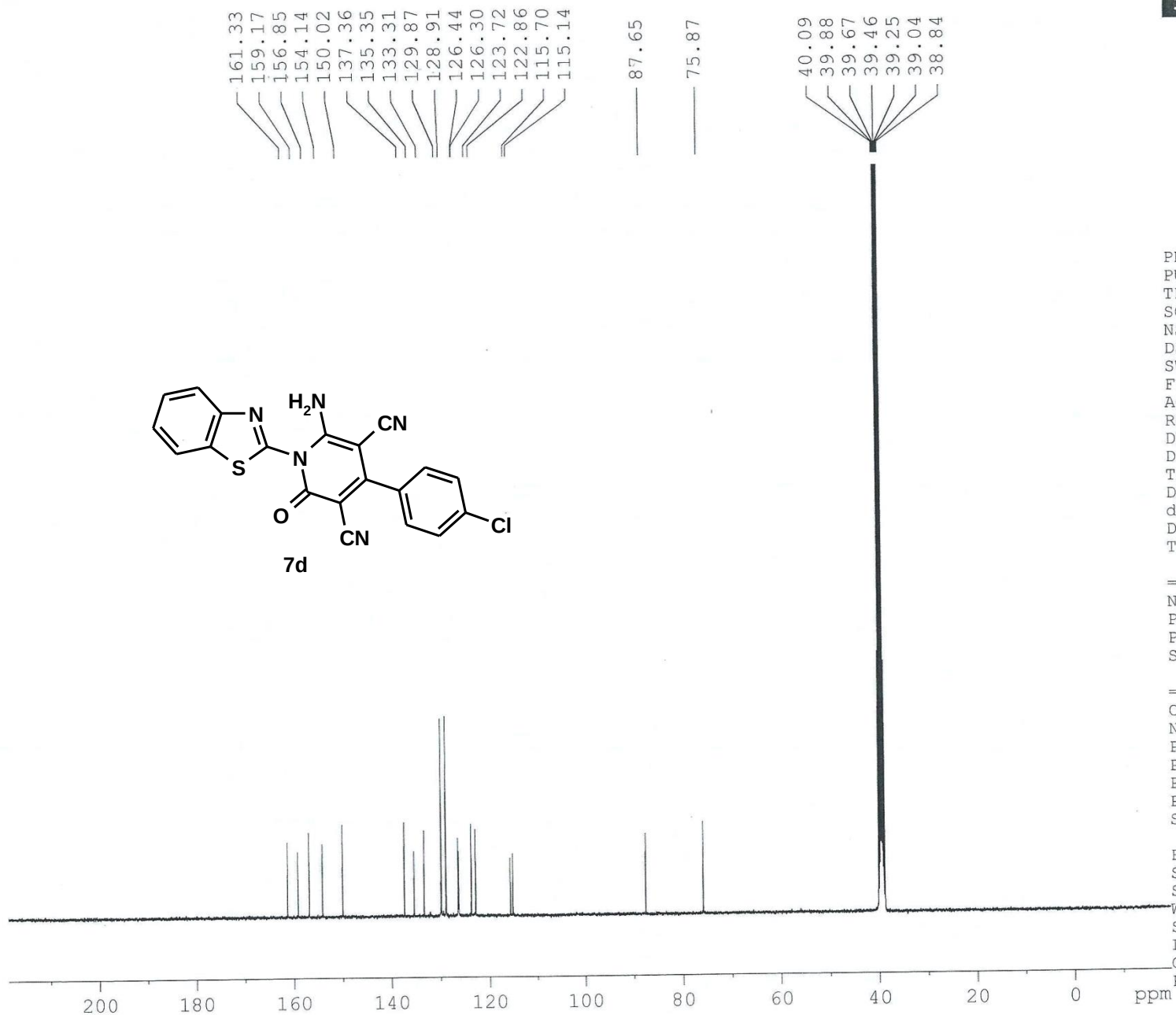
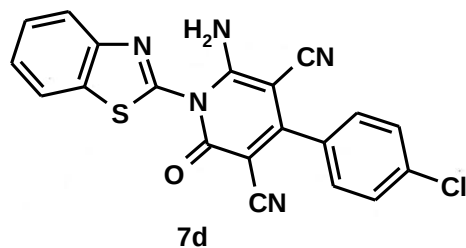
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 29
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 406.4
DW 60.400 usec
DE 6.00 usec
TE 673.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 9.00 usec
PL1 -4.50 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



1.96
1.00
1.04
2.04
4.07



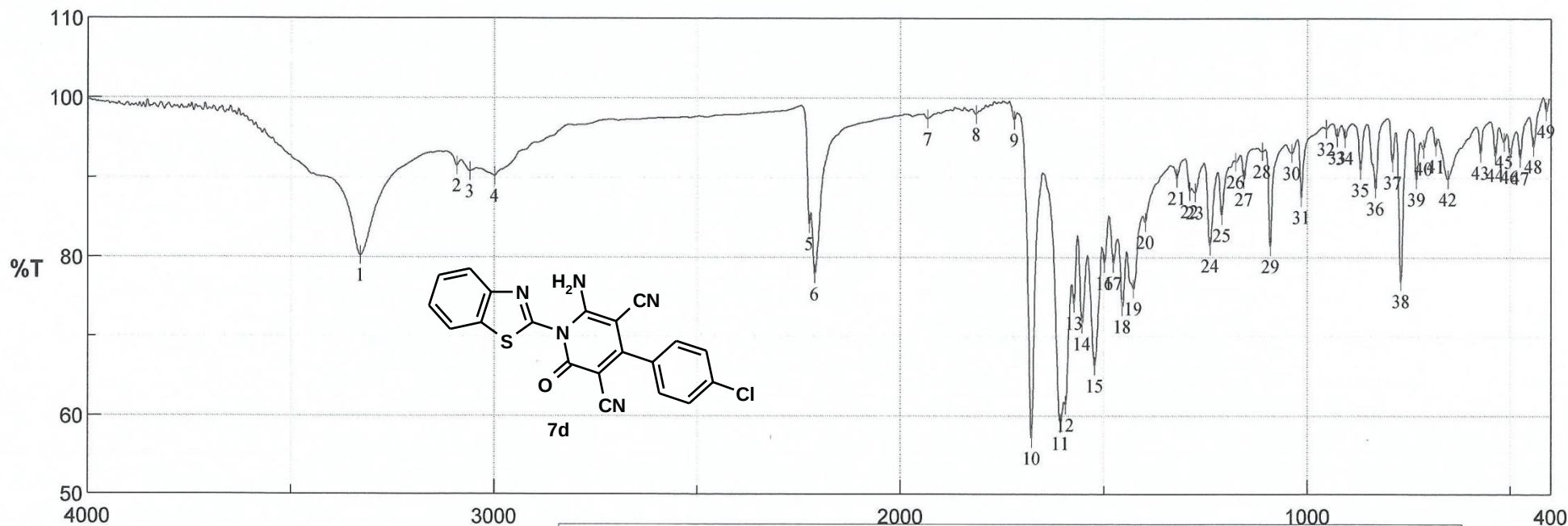
PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 10240
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 5160.6
 DW 20.850 usec
 DE 6.00 usec
 TE 673.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 7.20 usec
 PL1 -6.00 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -3.00 dB
 PL12 15.06 dB
 PL13 18.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6128193 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

FT-IR Spectral Data



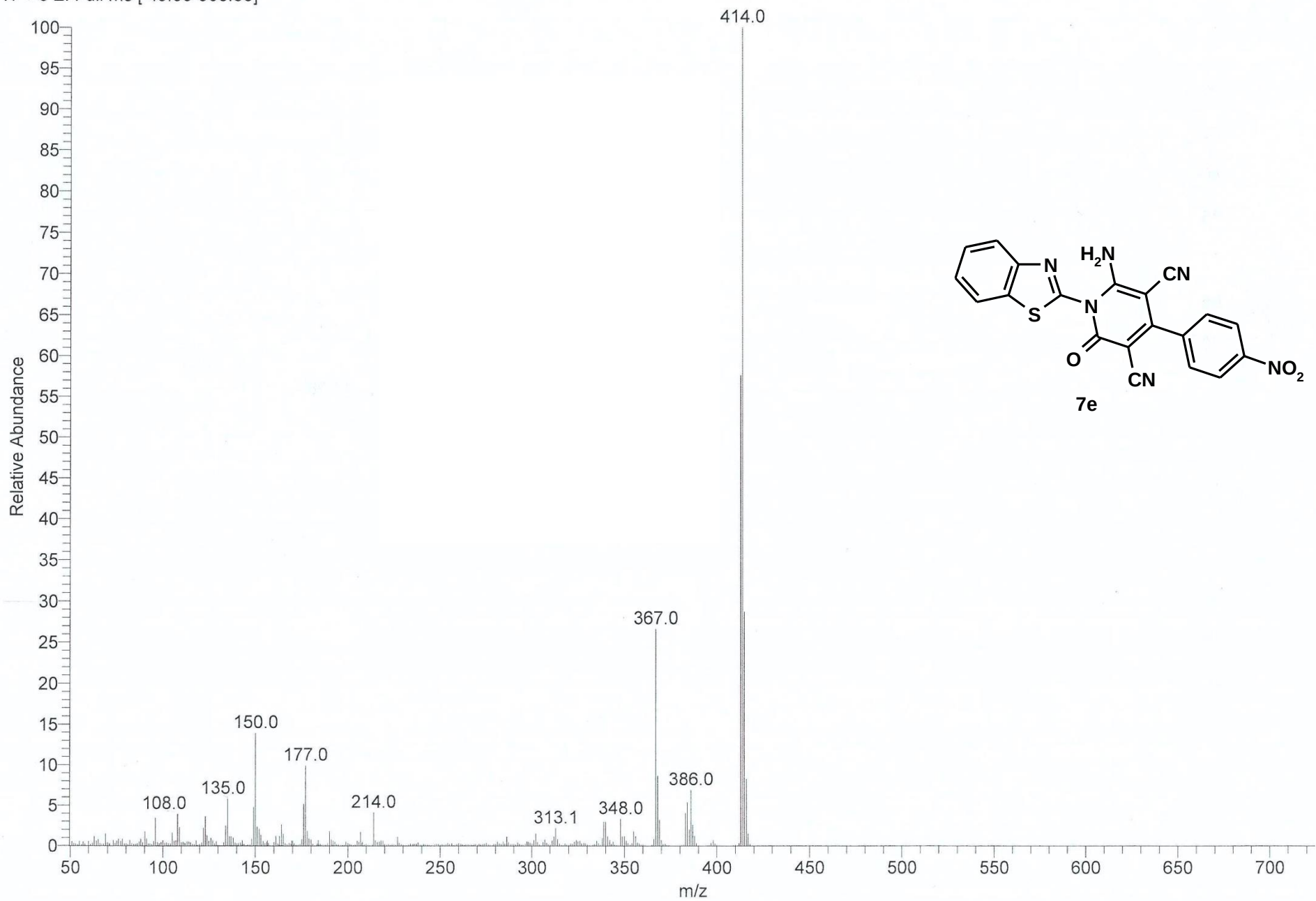
Result of Peak Picking								
No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	3328.53	80.1467	2	3091.33	91.4435	3	3059.51	90.6767
4	2998.77	90.1242	5	2223.52	84.1668	6	2210.02	77.8225
7	1933.29	97.3582	8	1813.72	97.9476	9	1719.23	97.1821
10	1677.77	57.0505	11	1606.41	58.9692	12	1594.84	61.3182
13	1572.66	74.1932	14	1553.38	71.5592	15	1522.52	66.2562
16	1498.42	79.2157	17	1476.24	79.1778	18	1454.06	73.7108
19	1427.07	75.9734	20	1398.14	84.3609	21	1320.04	89.915
22	1288.22	88.2399	23	1275.68	88.0791	24	1239.04	81.3646
25	1210.11	85.25	26	1175.4	91.9694	27	1155.15	89.7784
28	1110.8	93.2646	29	1090.55	81.3139	30	1037.52	93.0581
31	1014.37	87.5132	32	953.627	96.0816	33	925.664	95.0307
34	906.379	94.9183	35	868.774	90.9477	36	832.133	88.5633
37	790.671	91.9007	38	769.458	76.9239	39	731.853	89.7482
40	714.497	93.6262	41	684.606	93.9212	42	654.715	89.7829
43	573.719	93.0817	44	537.078	92.7805	45	515.865	94.5176
46	501.401	92.5939	47	476.331	92.4436	48	443.547	93.8999
49	411.728	98.3592						

[Measurement Information]

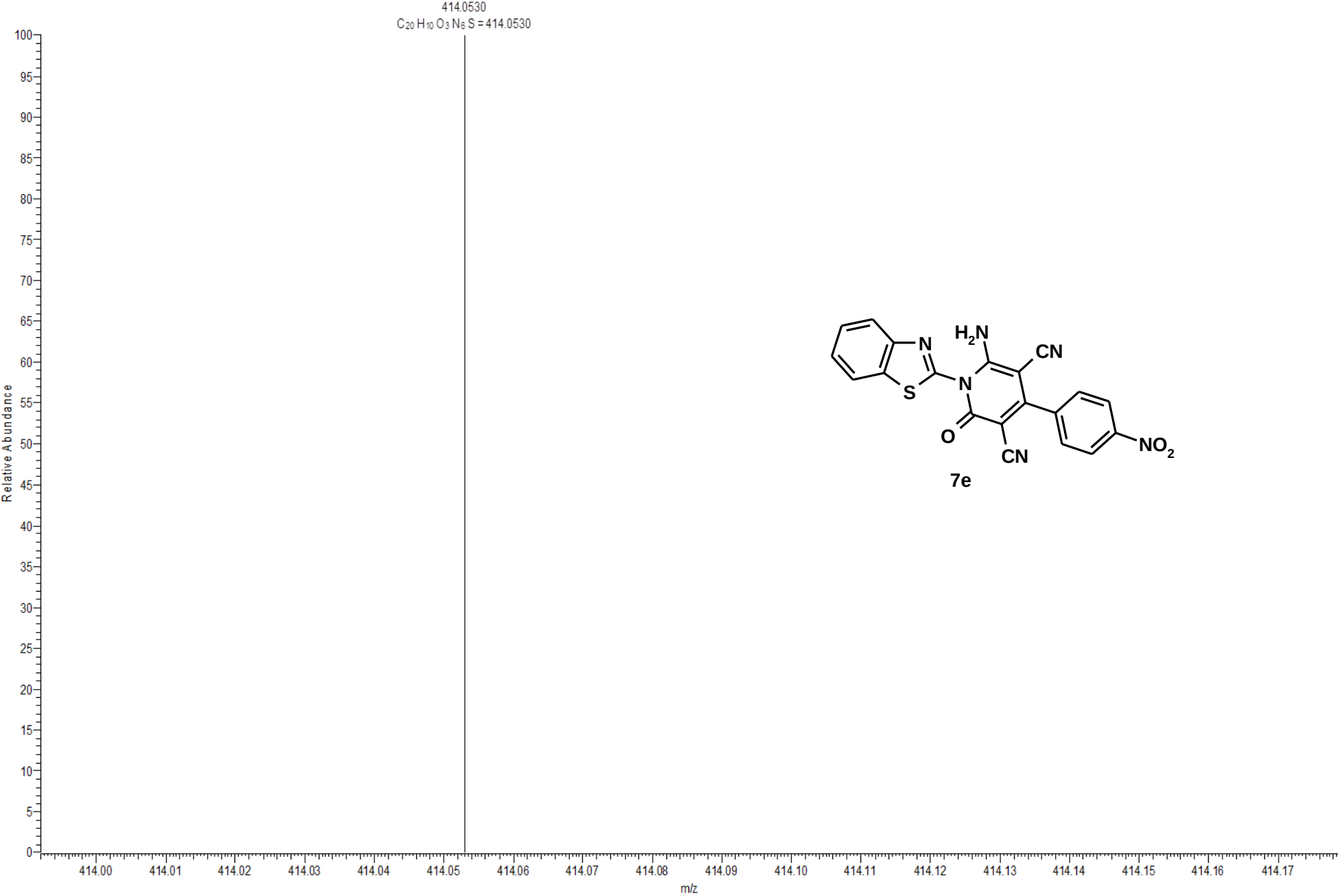
Model Name FT/IR-6300typeA
Serial Number A009861024

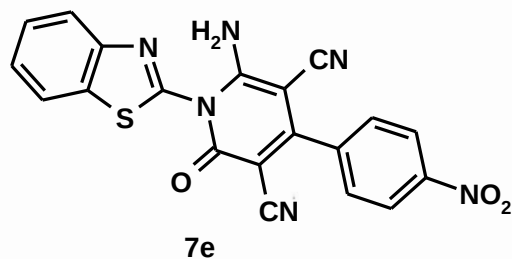
Light Source Standard
Detector TGS
Accumulation Auto (39)
Resolution 4 cm⁻¹
Zero Filling On
Apodization Cosine
Gain Auto (4)
Aperture Auto (7.1 mm)
Scanning Speed Auto (2 mm/sec)
Filter Auto (10000 Hz)

BT6 #231 RT: 10.19 AV: 1 NL: 1.17E8
T: + c EI Full ms [49.50-900.50]



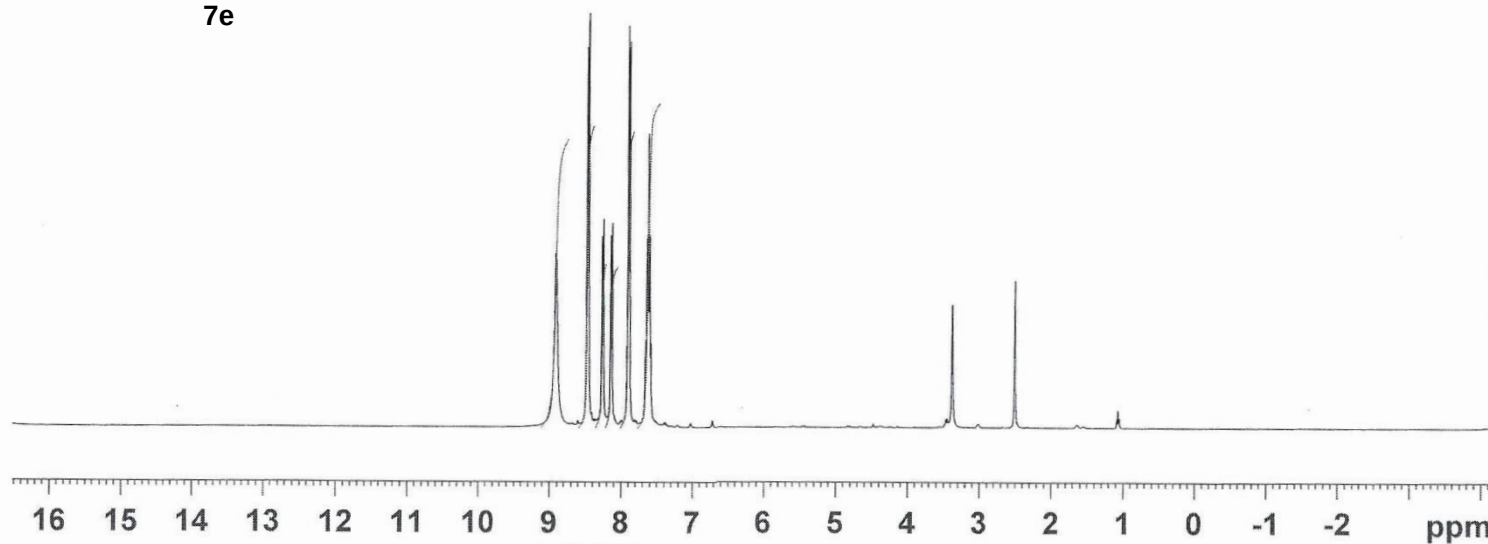
HRMS-BT6-mass1#69 RT: 9.40 AV: 1 NL: 7.91E4
T: + cEI Full ms [389.50-440.50]





8.917
8.484
8.463
8.416
8.274
8.256
8.153
8.134
7.911
7.891
7.666
7.648
7.628
7.608
7.591

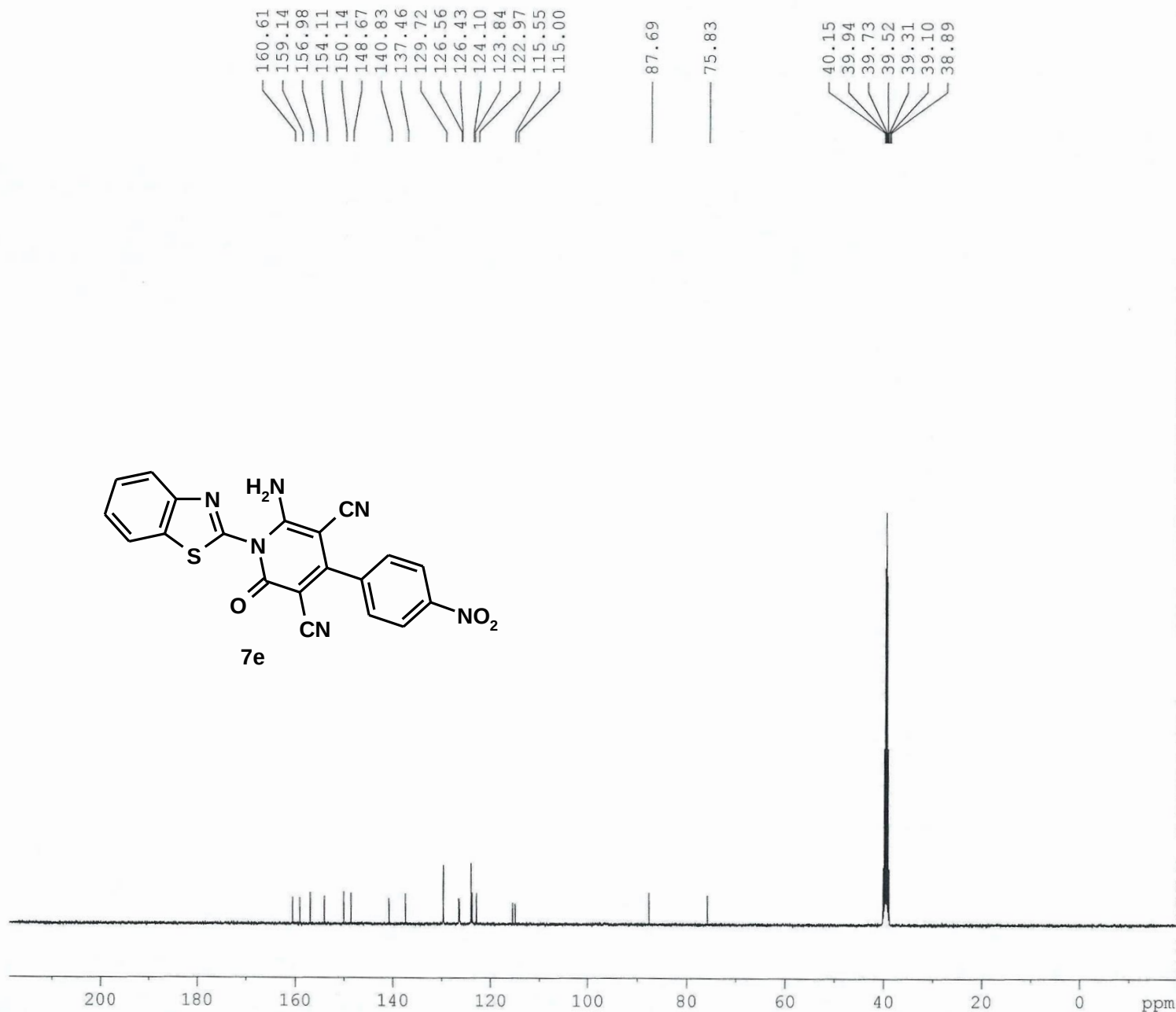
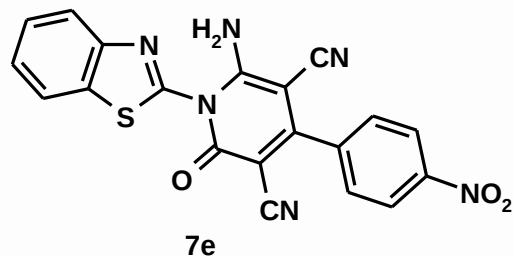
3.377
2.508



PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 9
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 181
DW 60.400 usec
DE 6.00 usec
TE 673.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 9.00 usec
PL1 -4.50 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



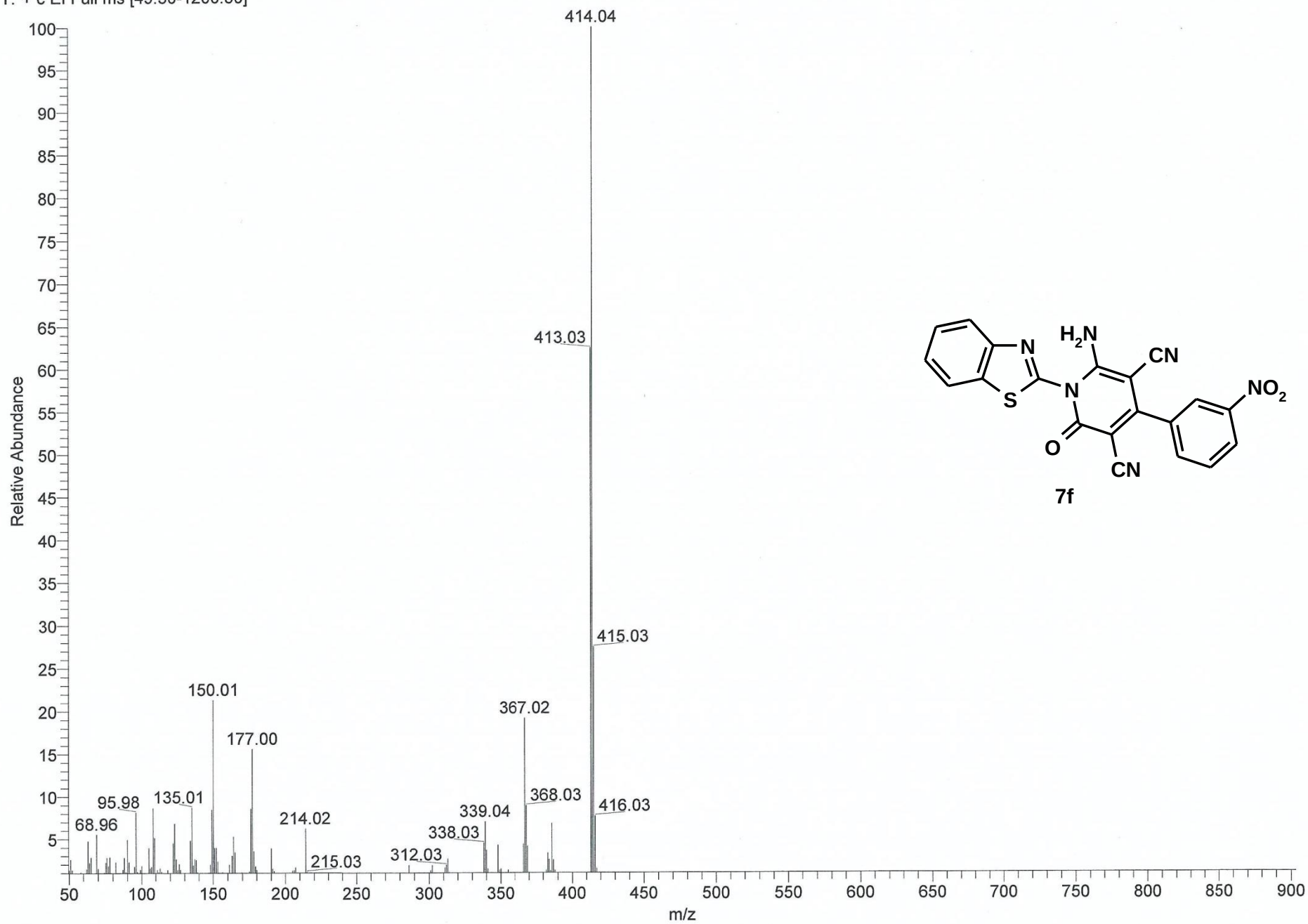
PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 609
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 5792.6
 DW 20.850 usec
 DE 6.00 usec
 TE 673.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 7.00 usec
 PL1 -6.00 dB
 SFO1 100.6228298 MHz

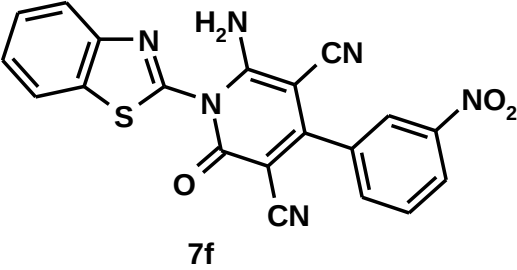
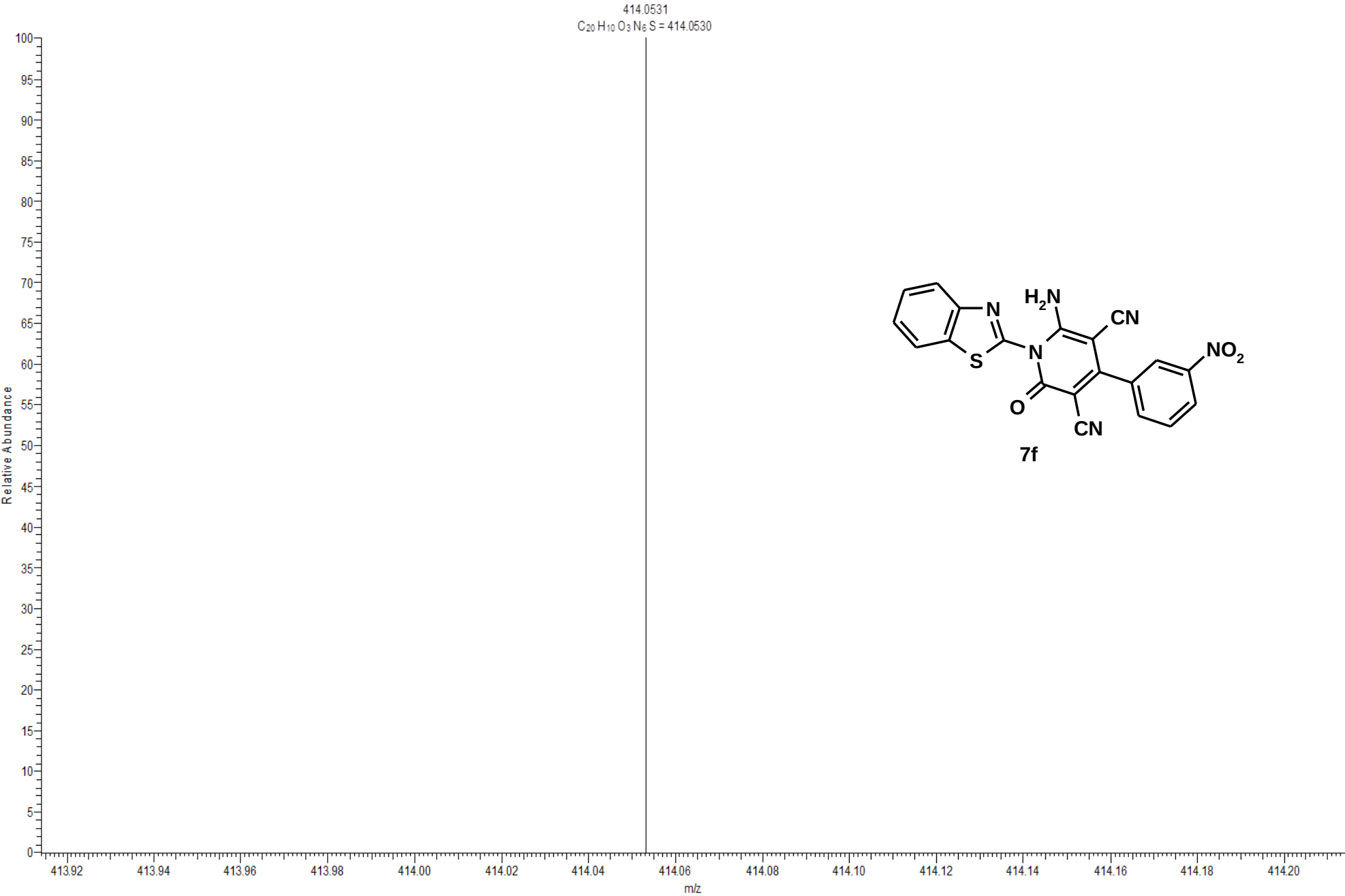
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -4.50 dB
 PL12 18.00 dB
 PL13 21.00 dB
 SFO2 400.1316005 MHz

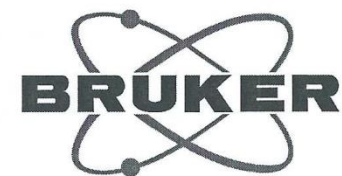
F2 - Processing parameters
 SI 32768
 SF 100.6128110 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

BT19 #302 RT: 14.59 AV: 1 NL: 2.42E7
T: + c EI Full ms [49.50-1200.50]



HRMS-BT19-cmass1#26 RT: 9.02 AV: 1 NL: 3.57E4
T: + c EI Full ms [389.50-440.50]

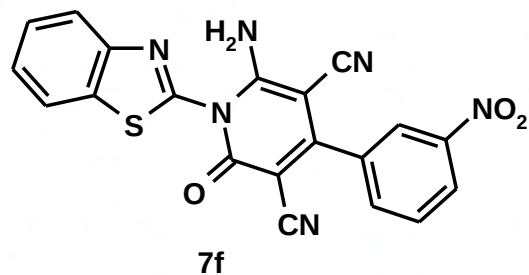




8.883
8.475
8.472
8.468
8.452
8.254
8.241
8.143
8.130
8.072
8.059
7.952
7.939
7.926
7.655
7.643
7.631
7.630
7.616
7.603
7.591

— 3.248

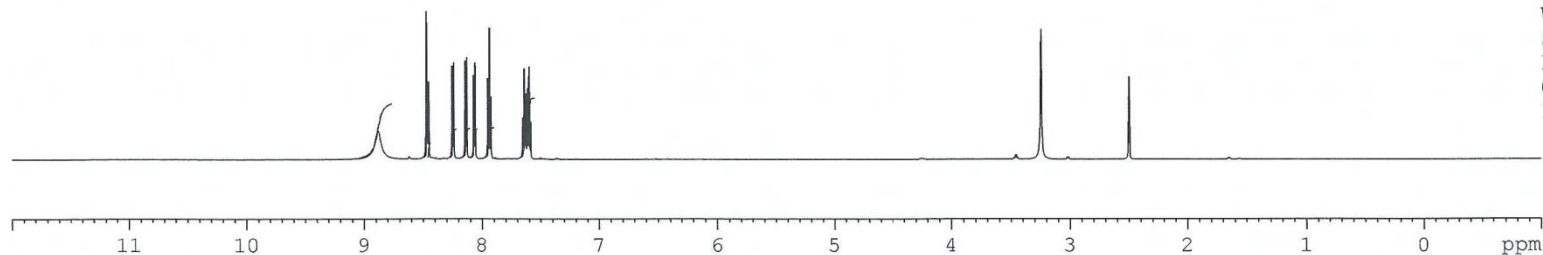
2.503
2.500
2.498



PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 2
SWH 12335.526 Hz
FIDRES 0.188225 Hz
AQ 2.6563926 sec
RG 203
DW 40.533 usec
DE 20.00 usec
TE 319.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 600.1337060 MHz
NUC1 1H
P1 10.60 usec
PLW1 27.82500076 W

F2 - Processing parameters
SI 32768
SF 600.1300003 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



1.89
1.32
0.51
1.00
1.03
1.01
1.05
2.08

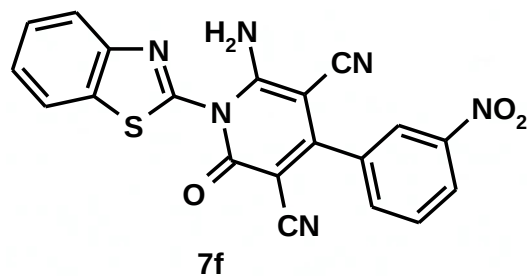


159.89
158.84
156.74
153.93
149.79
147.56
136.99
135.87
134.37
130.58
126.32
126.20
124.99
123.59
122.73
122.59
115.24
114.74

— 87.82

— 76.01

39.92
39.78
39.64
39.50
39.36
39.22
39.08

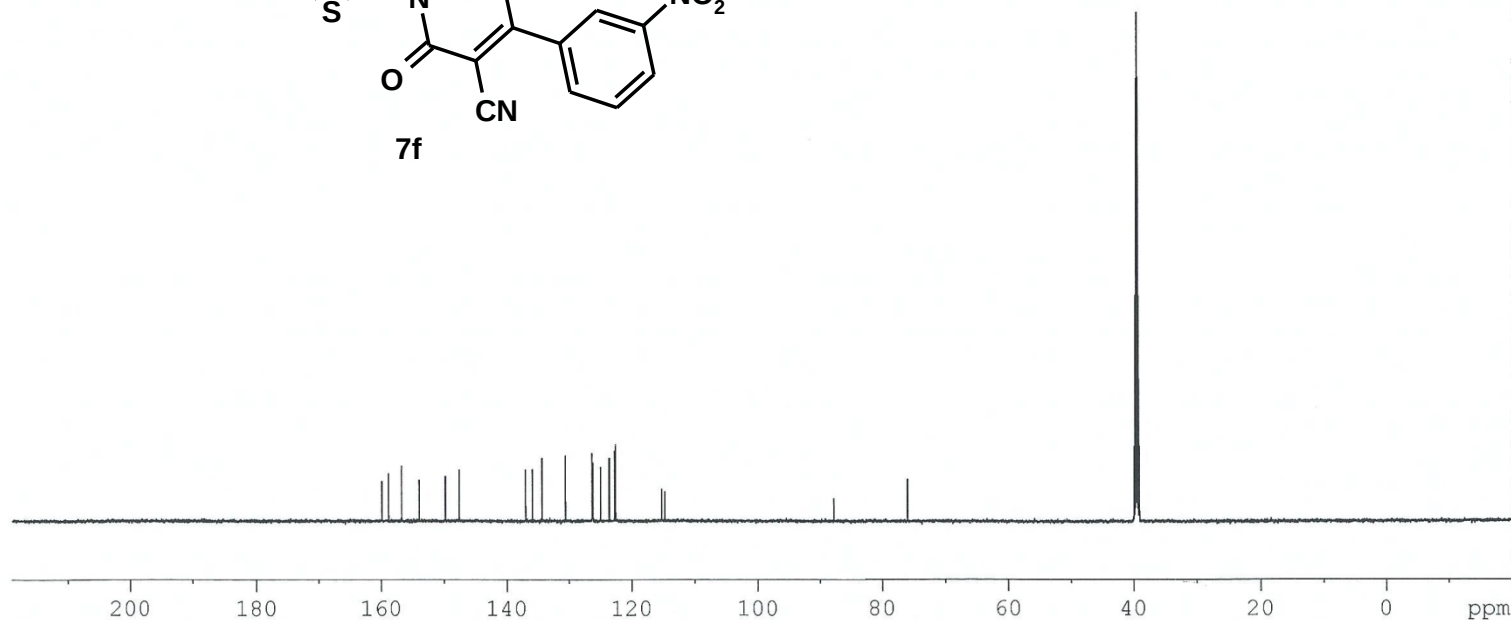


PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 302
DS 4
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 203
DW 13.867 usec
DE 50.00 usec
TE 320.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

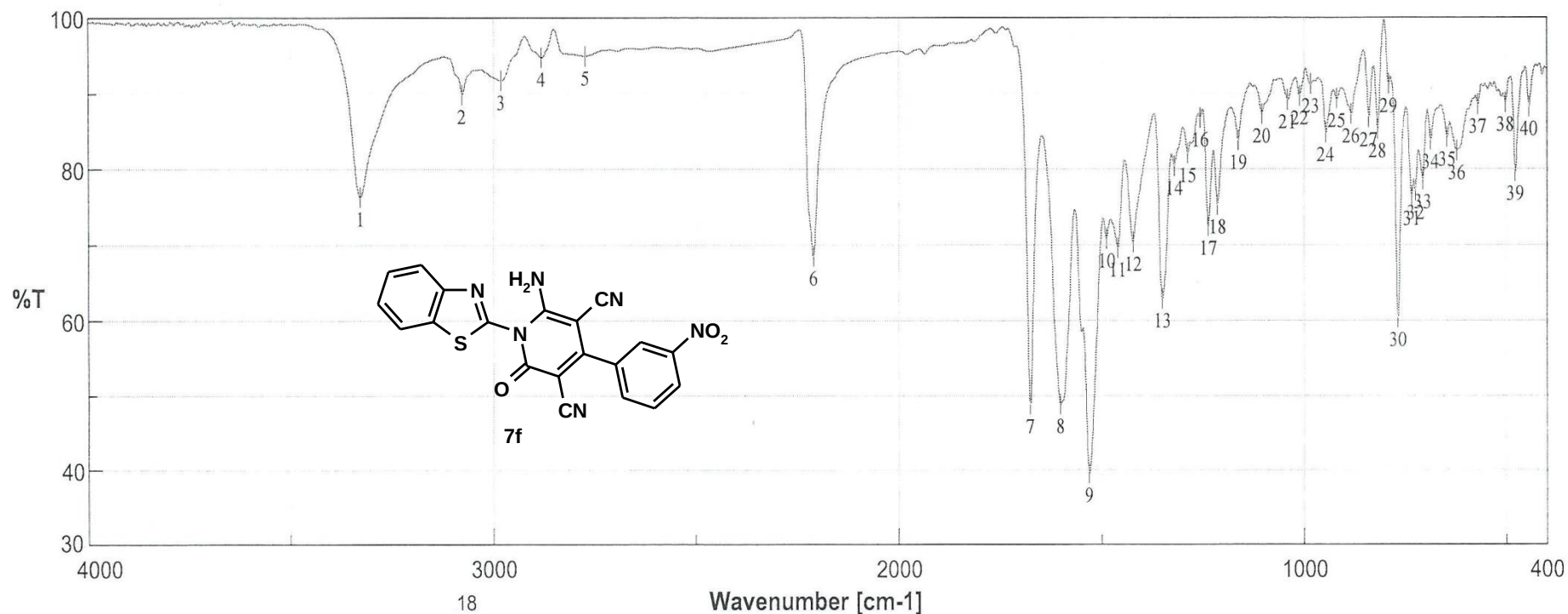
===== CHANNEL f1 =====
SFO1 150.9178979 MHz
NUC1 13C
P1 8.80 usec
PLW1 78.13500214 W

===== CHANNEL f2 =====
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 70.00 usec
PLW2 27.82500076 W
PLW12 0.63804001 W
PLW13 0.31264001 W

F2 - Processing parameters
SI 32768
SF 150.9029077 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



FT- IR Spectral Data



Result of Peak Picking

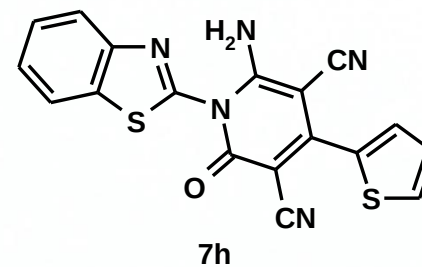
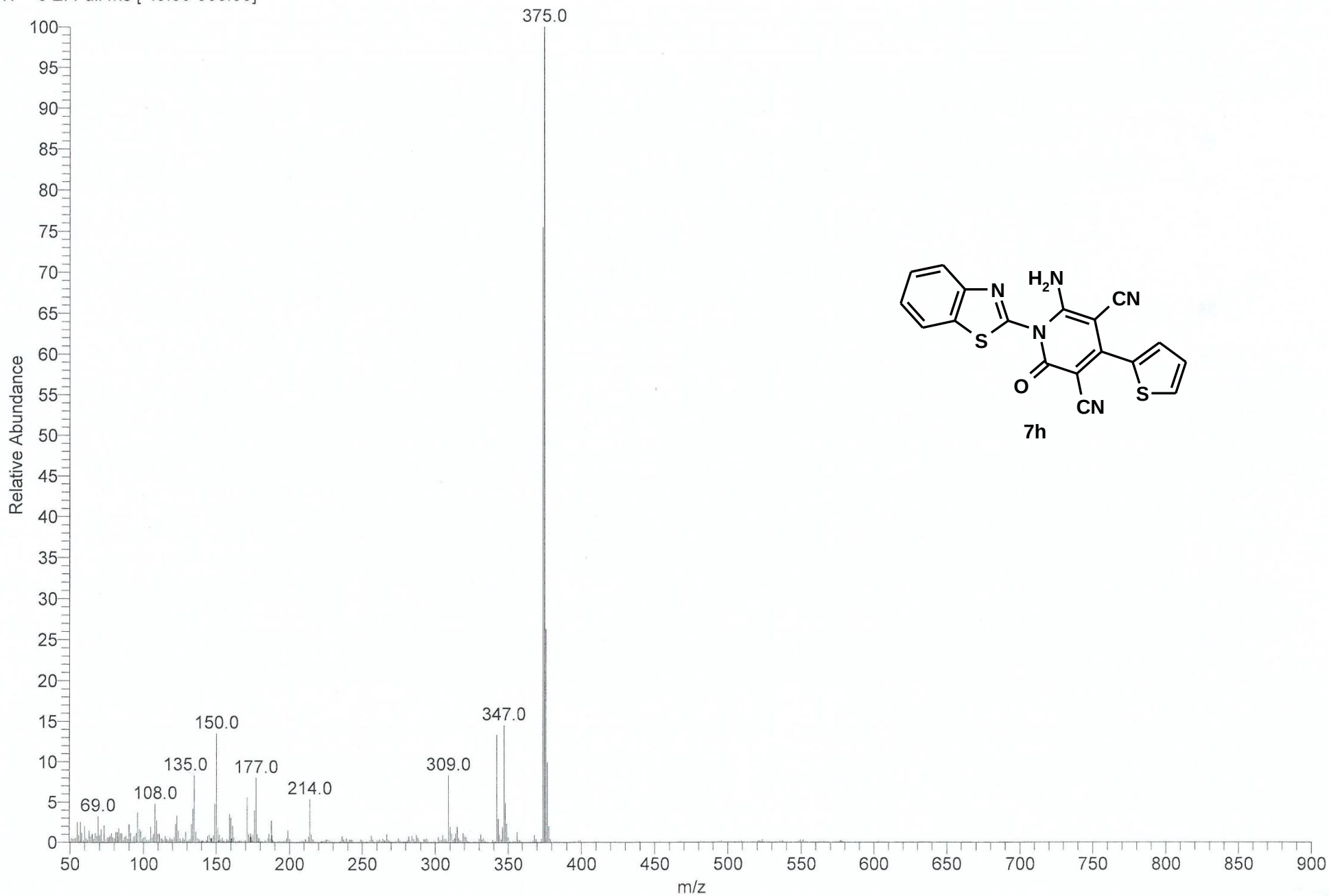
[Measurement Information]

Model Name FT/IR-6300typeA
Serial Number A009861024

Light Source Standard
Detector TGS
Accumulation 64
Resolution 4 cm-1
Zero Filling On
Apodization Cosine
Gain Auto (4)
Aperture Auto (7.1 mm)
Scanning Speed Auto (2 mm/sec)
Filter Auto (10000 Hz)

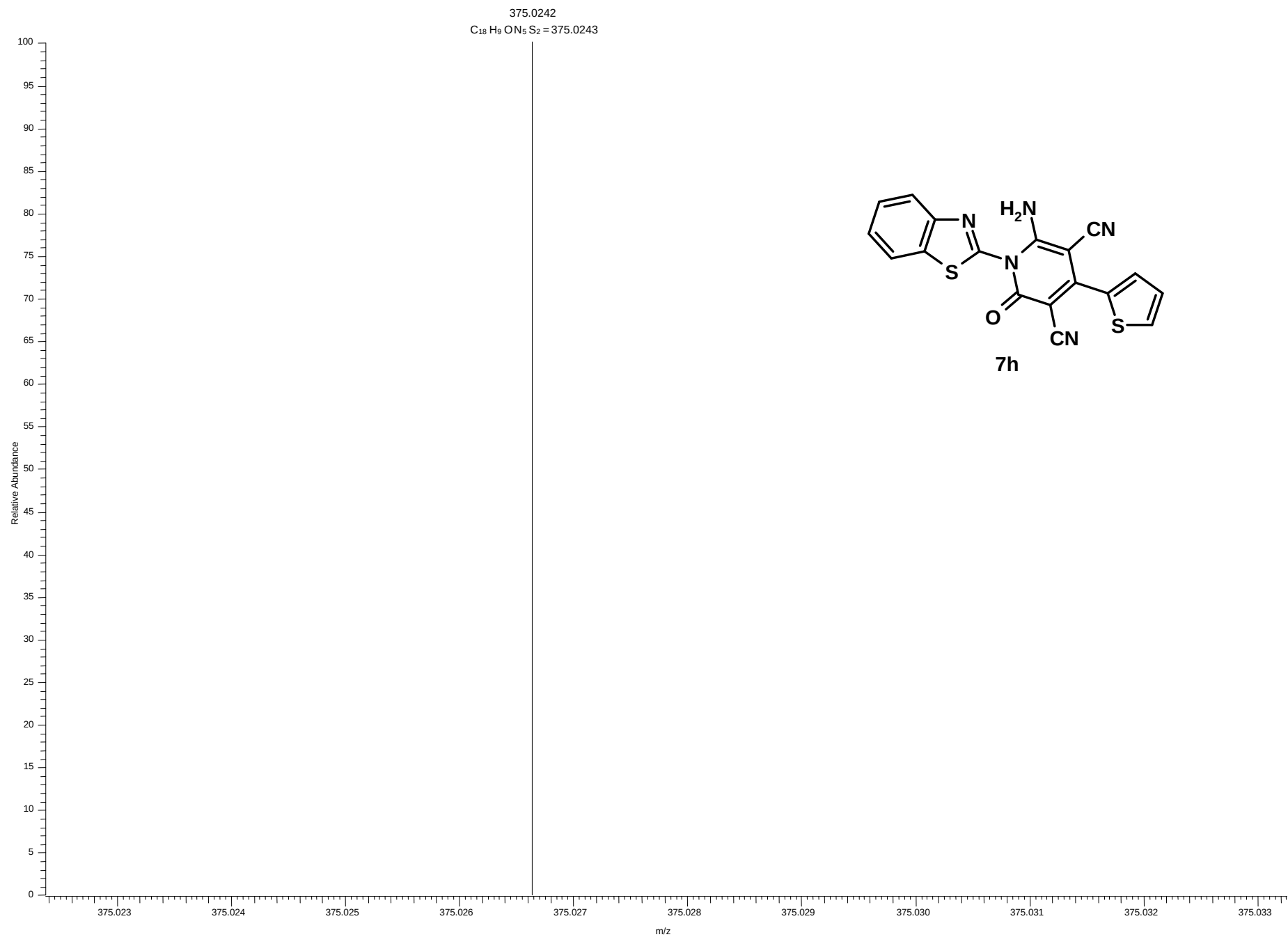
No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	3327.57	76.306	2	3076.87	89.827	3	2980.45	91.6381	4	2881.13	94.7149
5	2771.21	94.9059	6	2209.06	68.4596	7	1675.84	48.7953	8	1601.59	48.7854
9	1530.24	39.5468	10	1487.81	70.7738	11	1459.85	69.5807	12	1422.24	70.347
13	1349.93	62.8721	14	1320.04	80.4081	15	1287.25	82.1067	16	1256.4	86.7726
17	1237.11	72.5094	18	1213.97	75.3094	19	1162.87	83.737	20	1104.05	87.2901
21	1039.44	89.1589	22	1010.52	89.6655	23	982.554	91.2267	24	945.913	84.765
25	918.914	89.2569	26	883.238	87.2507	27	839.847	86.7821	28	818.634	85.31
29	791.636	91.2203	30	768.494	60.3639	31	734.746	76.3715	32	725.104	77.1455
33	707.747	78.5932	34	687.498	83.8329	35	647.001	84.1636	36	622.895	82.3764
37	570.826	88.4894	38	503.33	88.8116	39	478.26	79.6594	40	444.512	88.1732

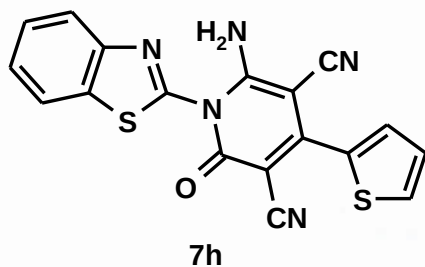
BT8C #185 RT: 8.16 AV: 1 NL: 7.20E7
T: + c EI Full ms [49.50-900.50]



HRMS-BT8-cmass1 #88 RT: 2.39 AV: 1 NL: 1.44E6

T: + c EI Full ms [374.50-420.50]





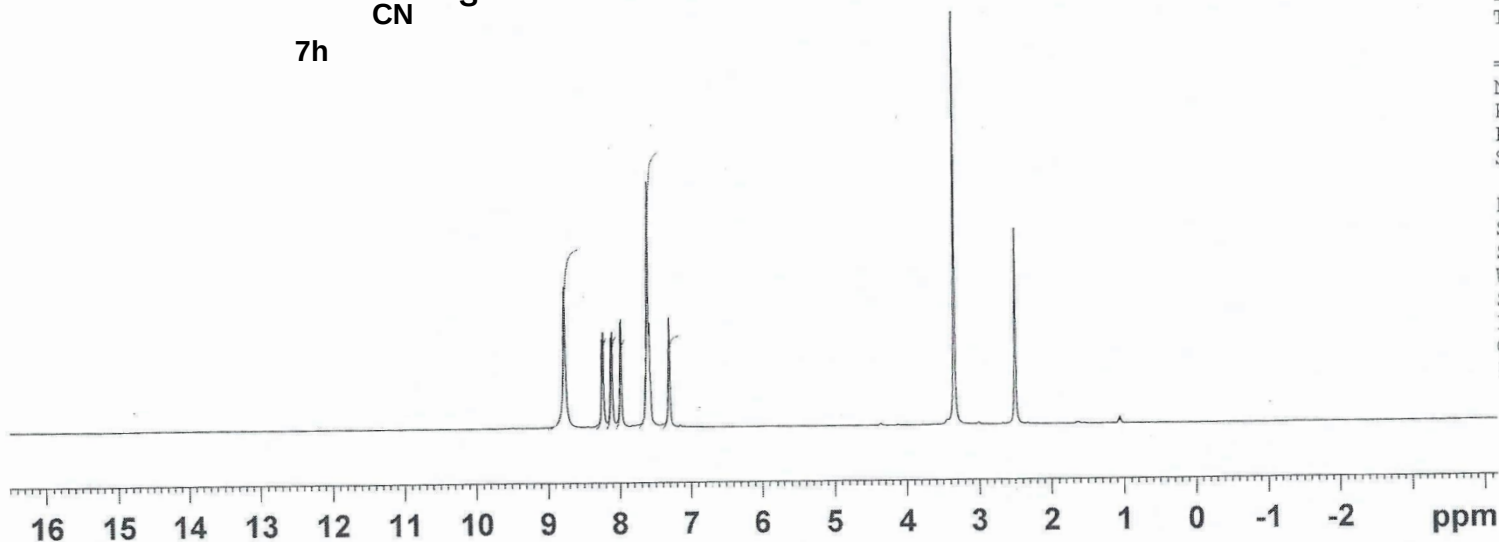
8.773
8.253
8.235
8.128
8.109
7.995
7.984
7.610
7.588
7.311

3.347
2.501

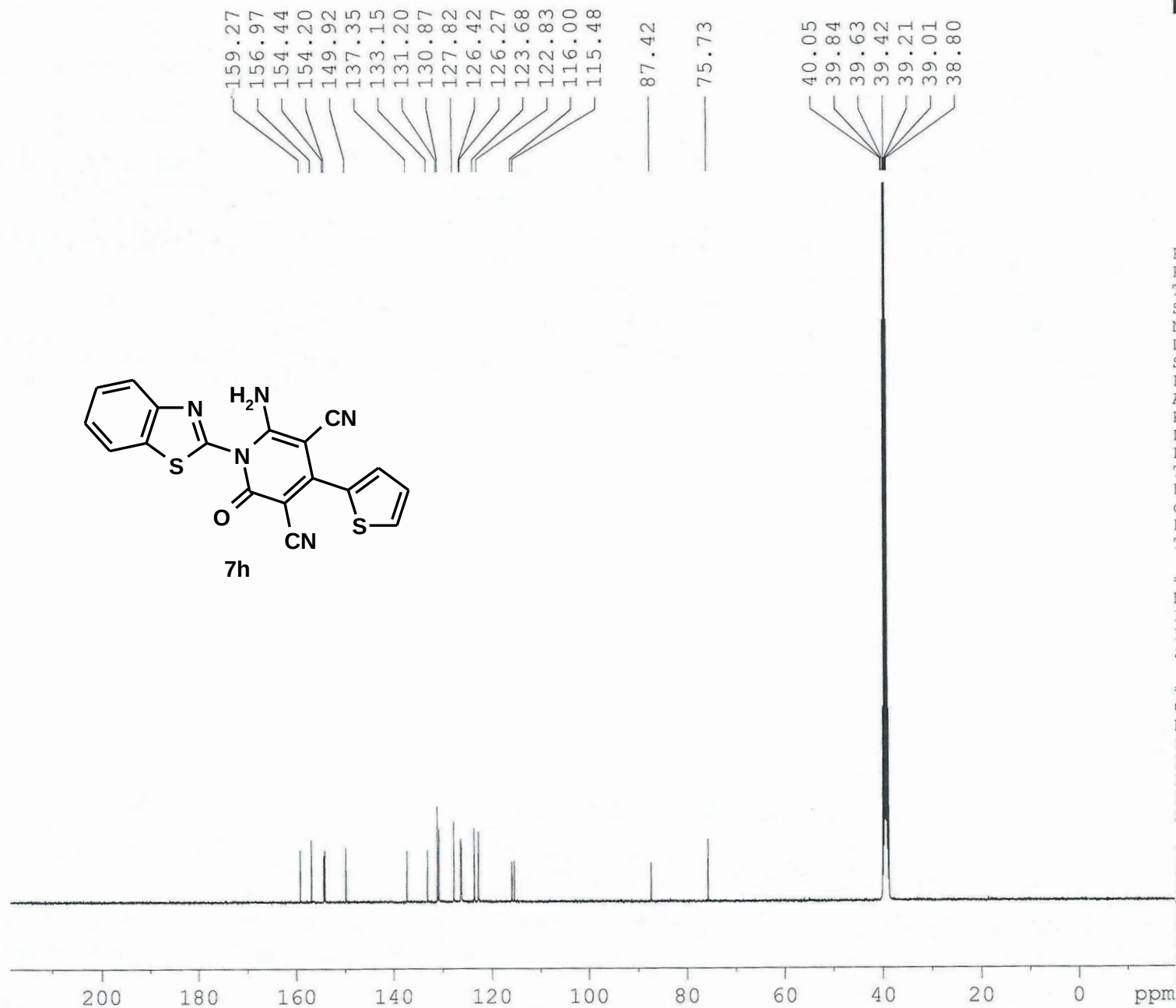
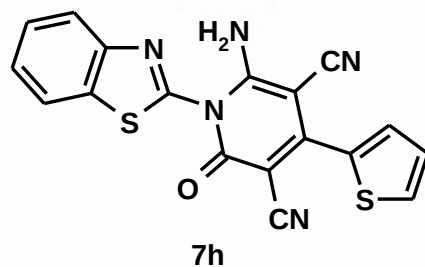
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 406.4
DW 60.400 usec
DE 6.00 usec
TE 673.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 9.00 usec
PL1 -4.50 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300027 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



1.00
0.51
0.52
0.50
1.53
0.52



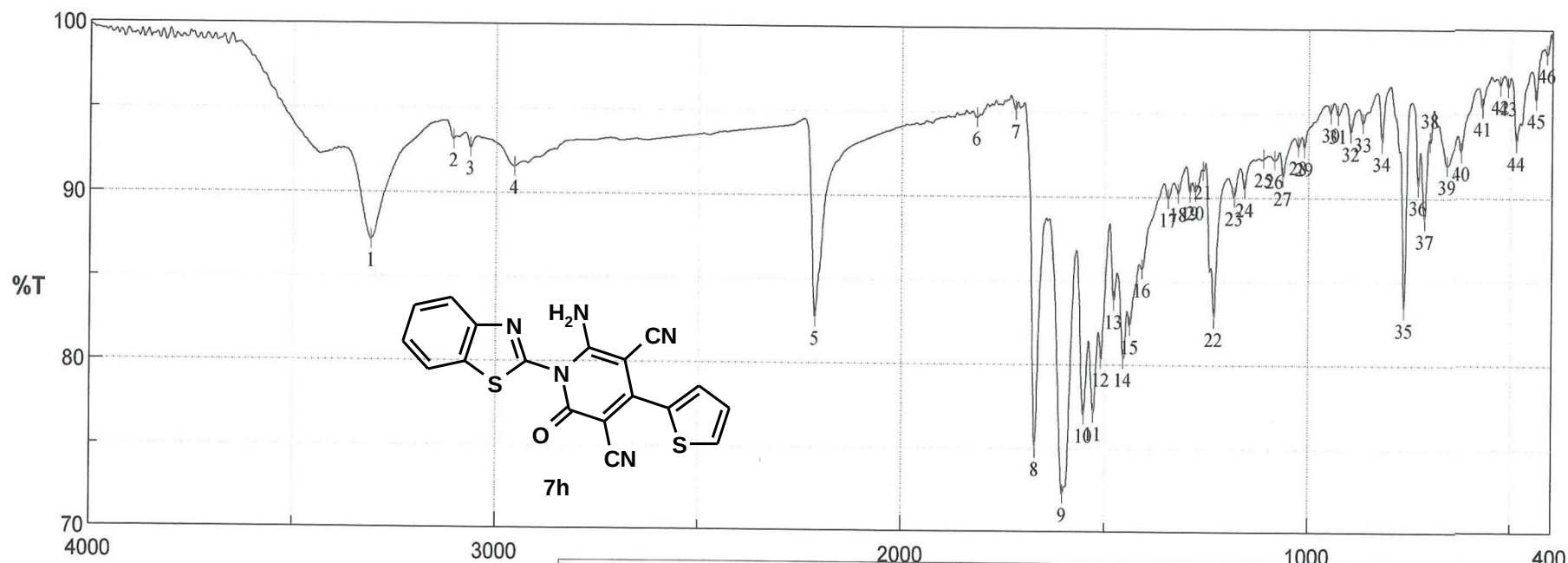
PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 10240
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 2896.3
 DW 20.850 usec
 DE 6.00 usec
 TE 673.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 7.20 usec
 PL1 -6.00 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -3.00 dB
 PL12 15.06 dB
 PL13 18.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6128193 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

FT-IR Spectral Data



Result of Peak Picking

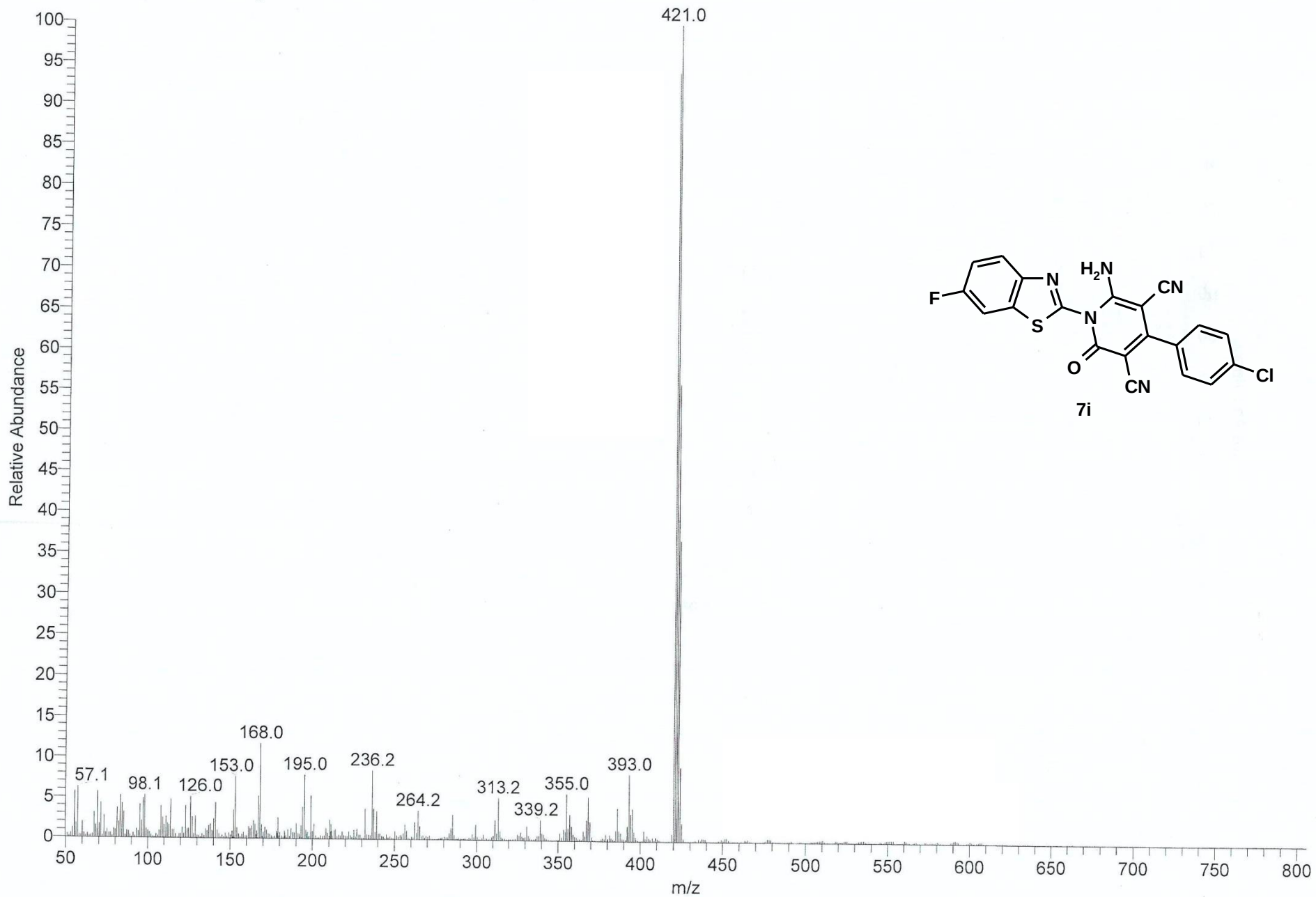
No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	3307.32	87.1509	2	3104.83	93.1245	3	3063.37	92.6288
4	2955.38	91.5276	5	2212.92	82.7104	6	1816.62	94.6338
7	1720.19	95.0994	8	1671.02	75.0037	9	1602.56	72.2649
10	1551.45	77.0018	11	1527.35	77.0982	12	1509.03	80.3446
13	1477.21	83.7957	14	1454.06	80.34	15	1438.64	82.2946
16	1407.78	85.6871	17	1345.11	89.8887	18	1320.04	90.2203
19	1291.11	90.2698	20	1278.57	90.3069	21	1258.32	91.5379
22	1231.33	82.7727	23	1183.11	89.9846	24	1157.08	90.5064
25	1110.8	92.273	26	1083.8	92.219	27	1062.59	91.2001
28	1024.98	93.0023	29	1009.55	92.955	30	944.949	94.9784
31	926.628	94.8912	32	895.773	93.8634	33	865.882	94.4207
34	819.598	93.2756	35	764.637	83.3508	36	729.925	90.667
37	714.497	88.6897	38	701.962	93.3549	39	659.536	91.9086
40	624.823	92.69	41	571.79	95.3478	42	527.436	96.6619
43	508.151	96.5661	44	487.902	93.292	45	439.69	95.8353
46	413.656	98.5292						

[Measurement Information]

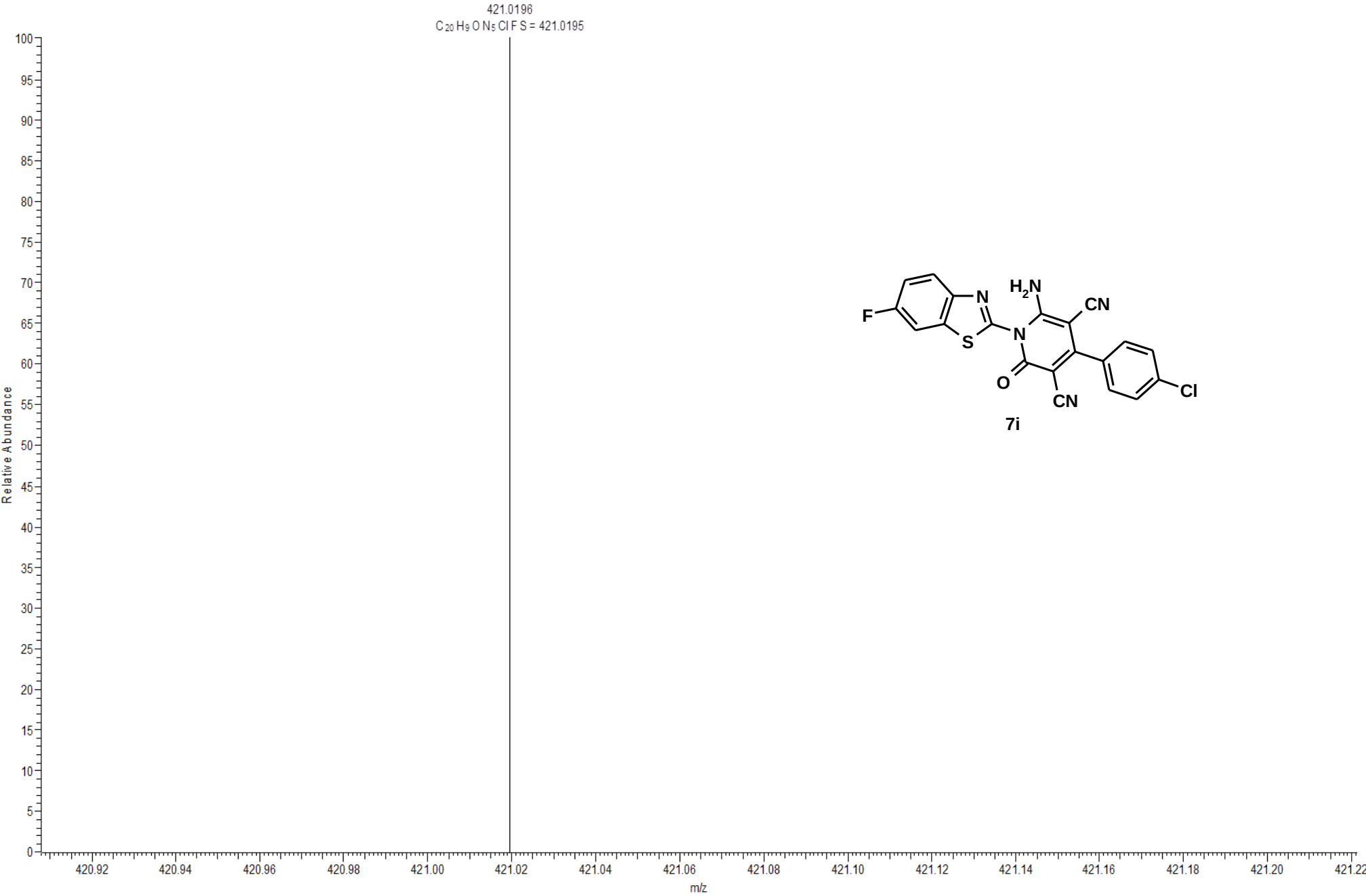
Model Name FT/IR-6300typeA
Serial Number A009861024

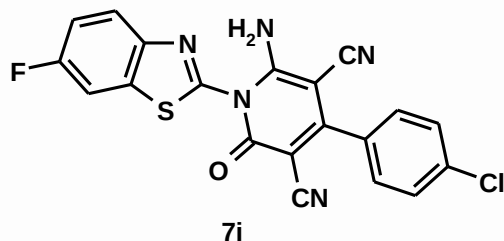
Light Source Standard
Detector TGS
Accumulation Auto (41)
Resolution 4 cm⁻¹
Zero Filling On
Apodization Cosine
Gain Auto (4)
Aperture Auto (7.1 mm)
Scanning Speed Auto (2 mm/sec)
Filter Auto (10000 Hz)

F4 #196 RT: 8.64 AV: 1 NL: 9.81E7
T: + c EI Full ms [49.50-900.50]



HRMS-F4-cmass1#14 RT: 0.87 AV: 1 NL: 1.26E6
T: + c EI Full ms [399.50-450.50]





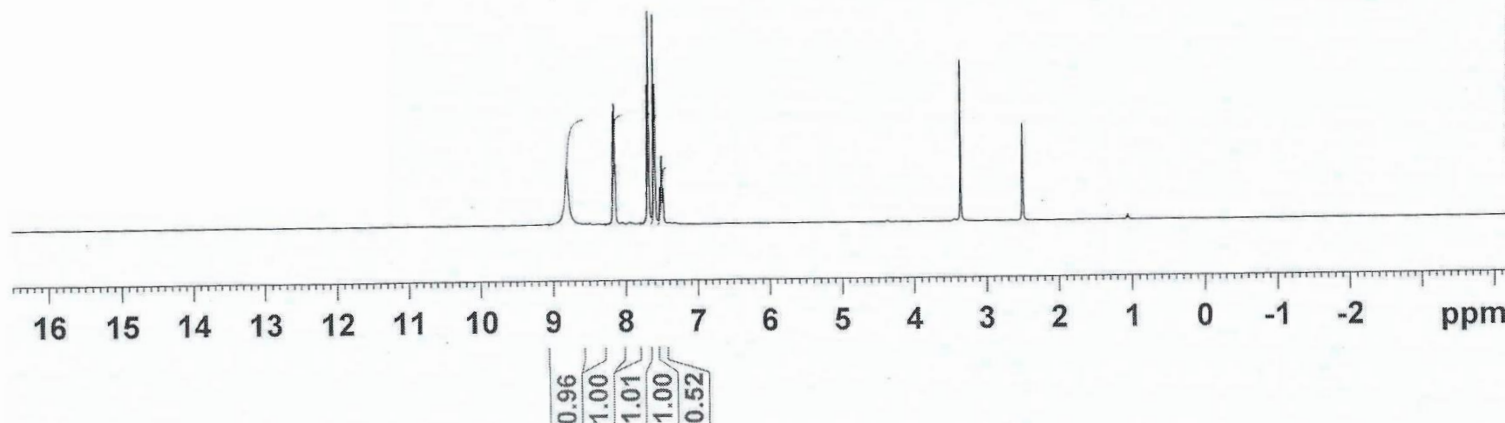
8.812
8.176
8.161
8.155
8.141
7.707
7.686
7.618
7.598
7.531
7.509
7.487

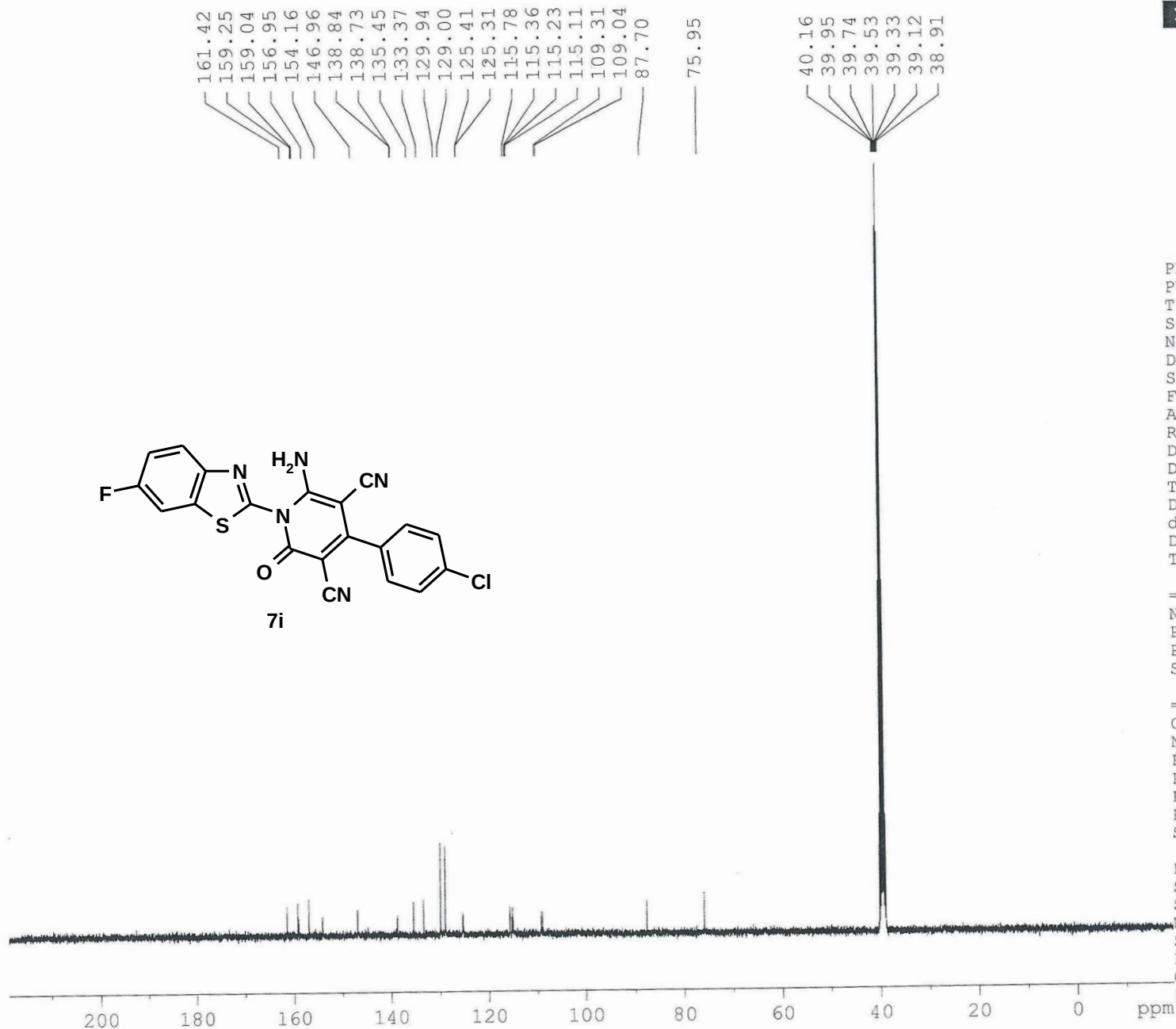
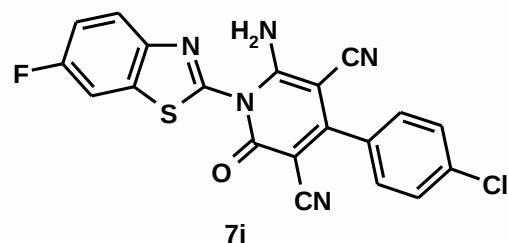
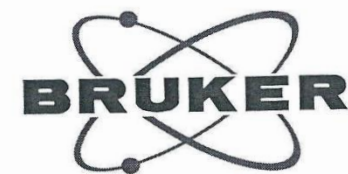
3.358
2.501

PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 322.5
DW 60.400 usec
DE 6.00 usec
TE 673.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 9.00 usec
PL1 -4.50 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300027 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





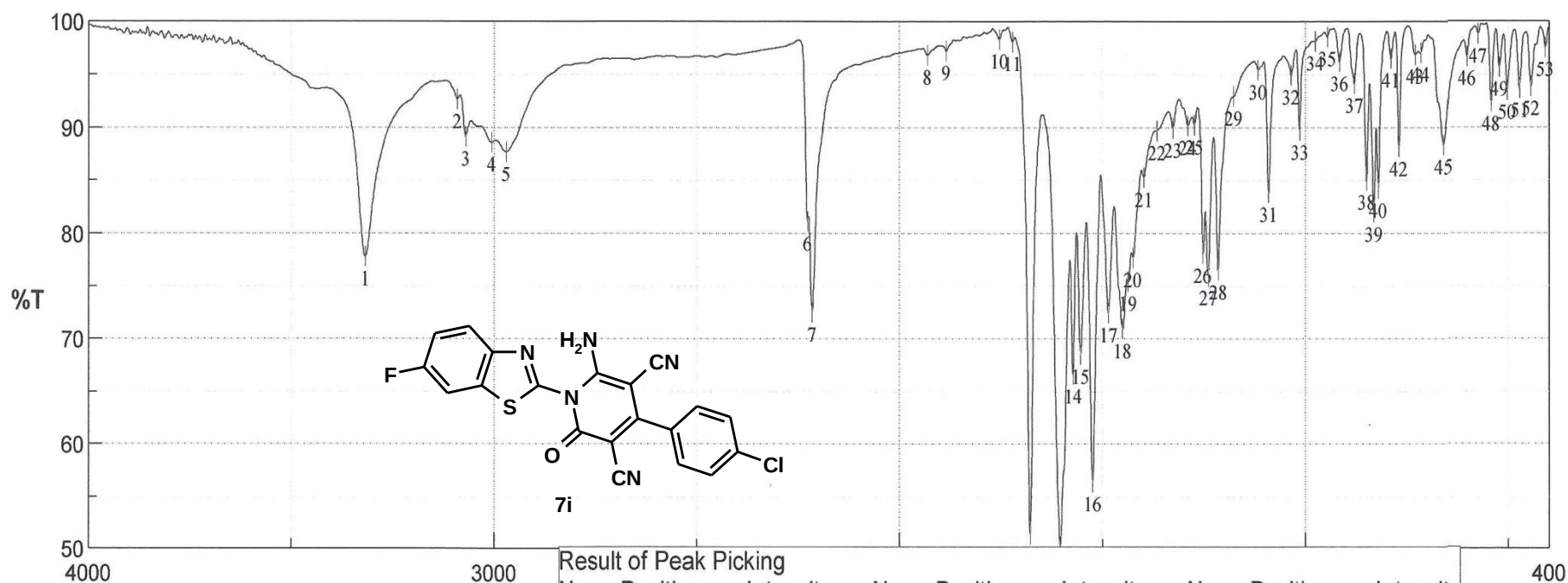
PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 481
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 5792.6
 DW 20.850 usec
 DE 6.00 usec
 TE 673.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 7.00 usec
 PL1 -6.00 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -4.50 dB
 PL12 18.00 dB
 PL13 21.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6128110 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

FT-IR Spectral Data

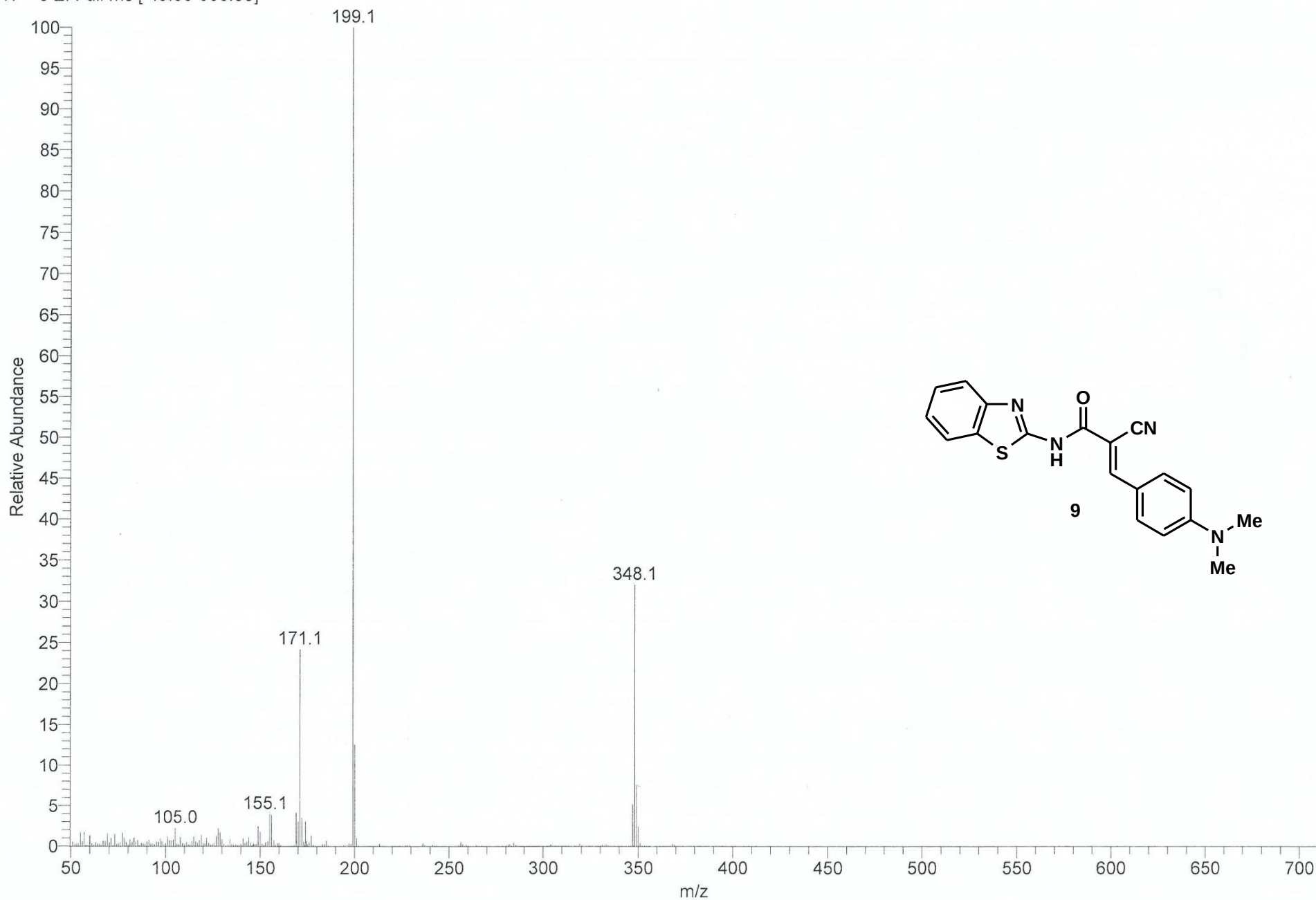


[Measurement Information]

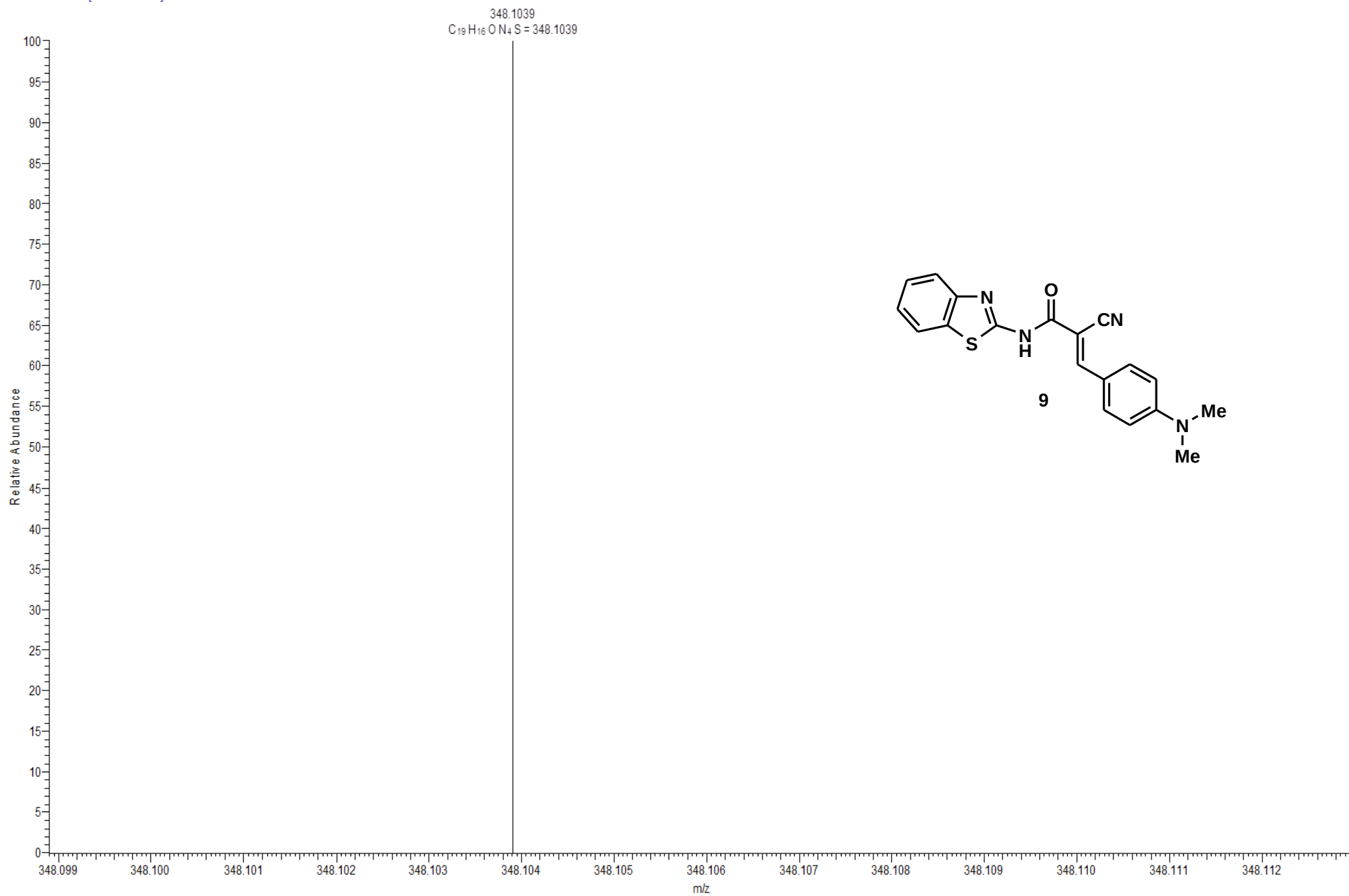
Model Name FT/IR-6300typeA
Serial Number A009861024

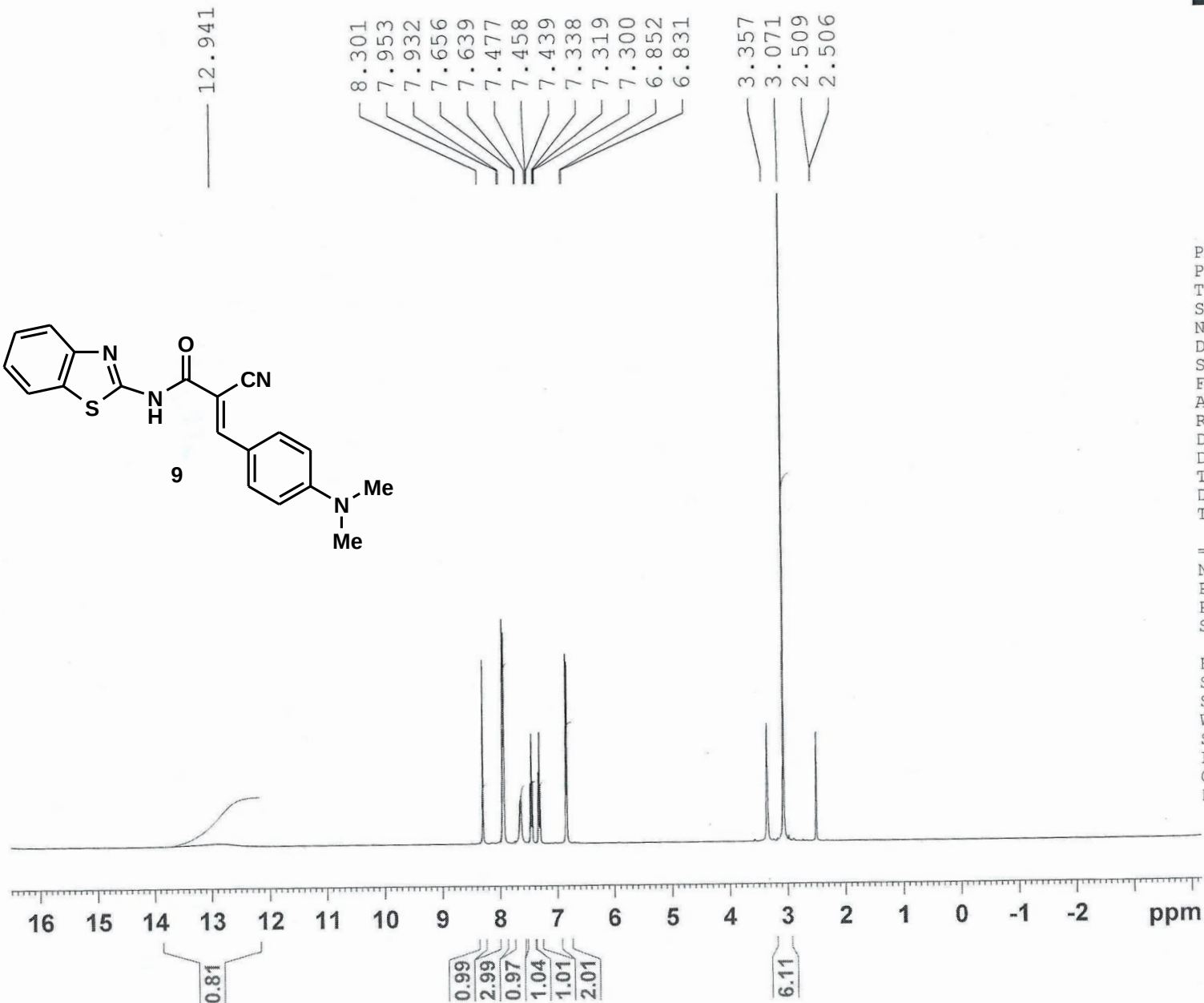
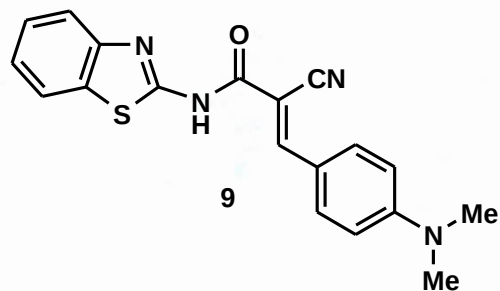
Light Source Standard
Detector TGS
Accumulation Auto (33)
Resolution 4 cm⁻¹
Zero Filling On
Apodization Cosine
Gain Auto (4)
Aperture Auto (7.1 mm)
Scanning Speed Auto (2 mm/sec)
Filter Auto (10000 Hz)

10 #164 RT: 7.22 AV: 1 NL: 5.26E7
T: + c EI Full ms [49.50-900.50]



HRMS-BT10-cmass1#19 RT: 6.68 AV: 1 NL: 4.21E4
T: + c EI Full ms [309.50-370.50]





PROBHD 5 mm DUL 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 13
 DS 2
 SWH 8278.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.9584243 sec
 RG 256
 DW 60.400 usec
 DE 6.00 usec
 TE 673.2 K
 D1 1.00000000 sec
 TD0 1

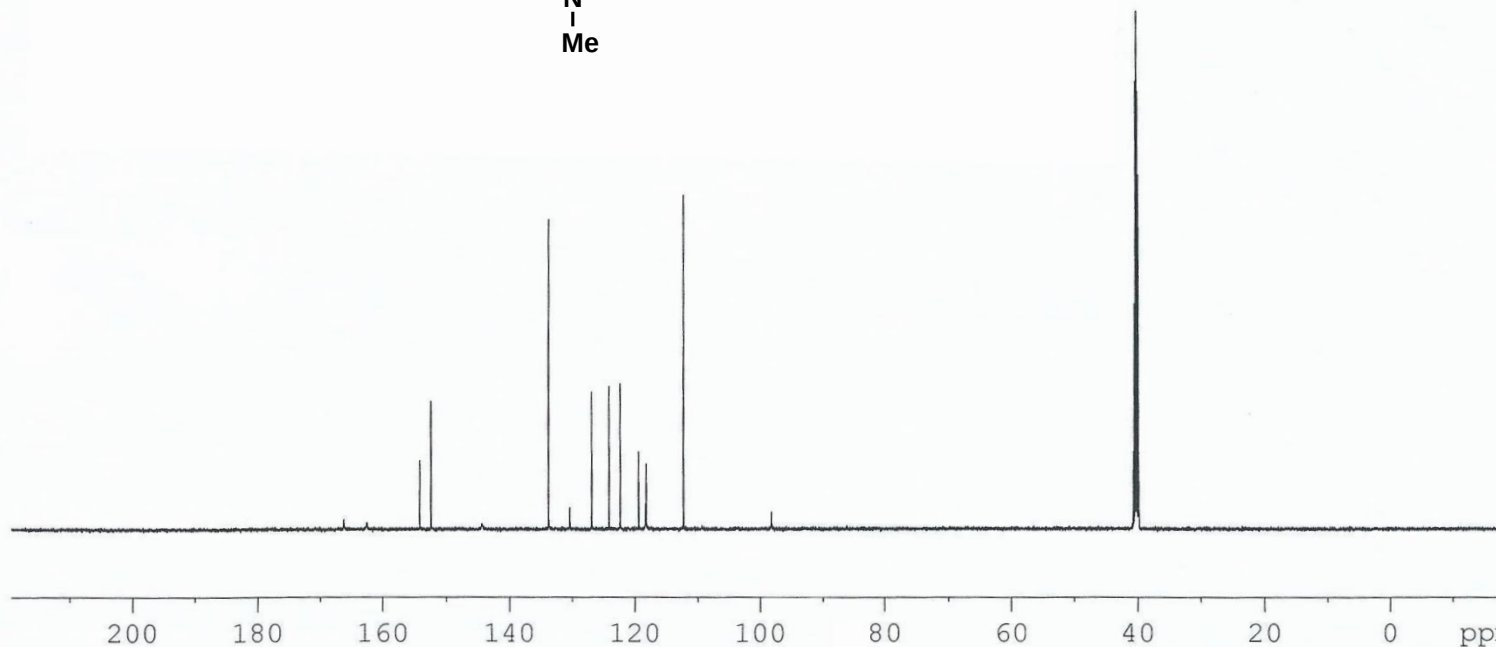
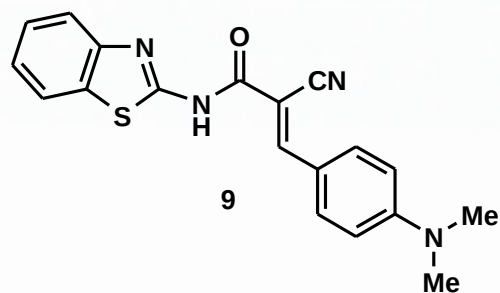
===== CHANNEL f1 =====
 NUC1 1H
 P1 9.00 usec
 PL1 -4.50 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



166.20
162.47
154.15
152.37
144.35
133.77
130.40
126.88
124.11
122.32
119.40
118.24
118.16
112.24
98.23

40.64
40.50
40.36
40.22
40.09
39.95
39.89
39.81



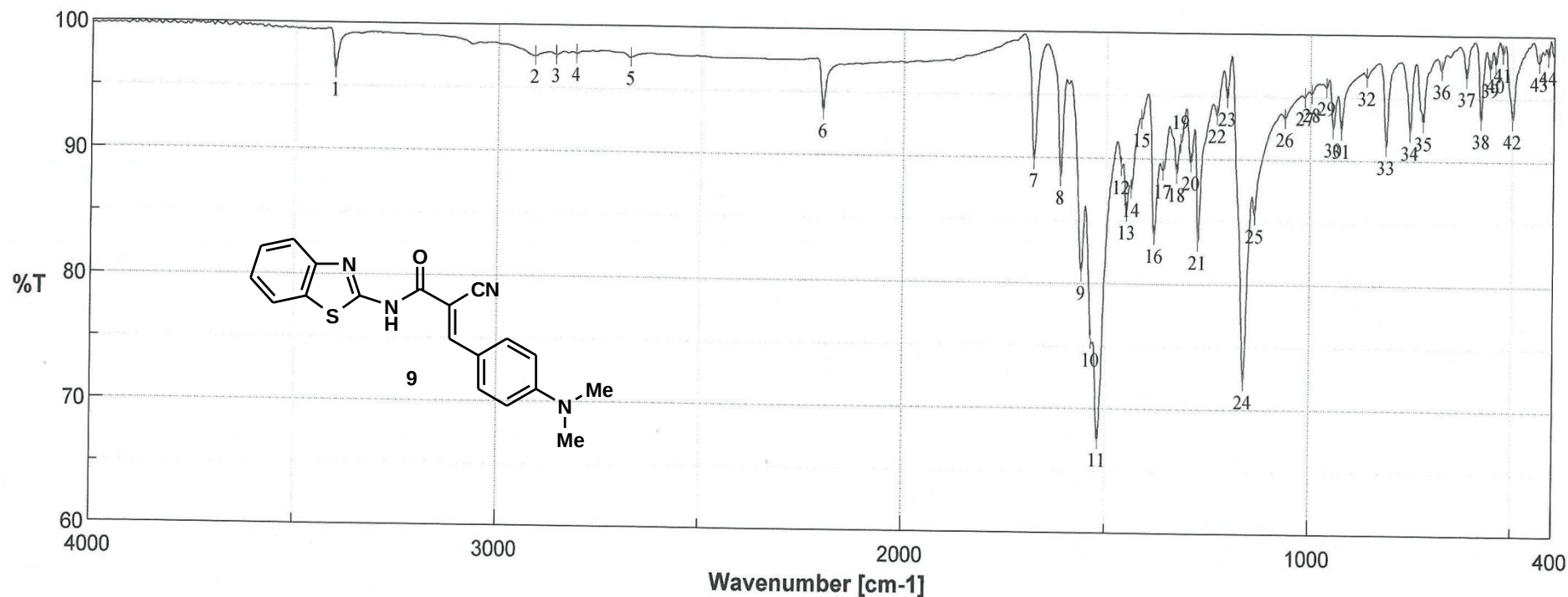
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1122
DS 4
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9088159 sec
RG 203
DW 13.867 usec
DE 6.50 usec
TE 368.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 7.30 usec
PL1 2.00 dB
SFO1 150.9178988 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz65
NUC2 1H
PCPD2 70.00 usec
PL12 12.00 dB
PL13 15.00 dB
PL2 -4.00 dB
SFO2 600.1324005 MHz

F2 - Processing parameters
SI 32768
SF 150.9028090 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

FT-IR Spectral Data



Result of Peak Picking

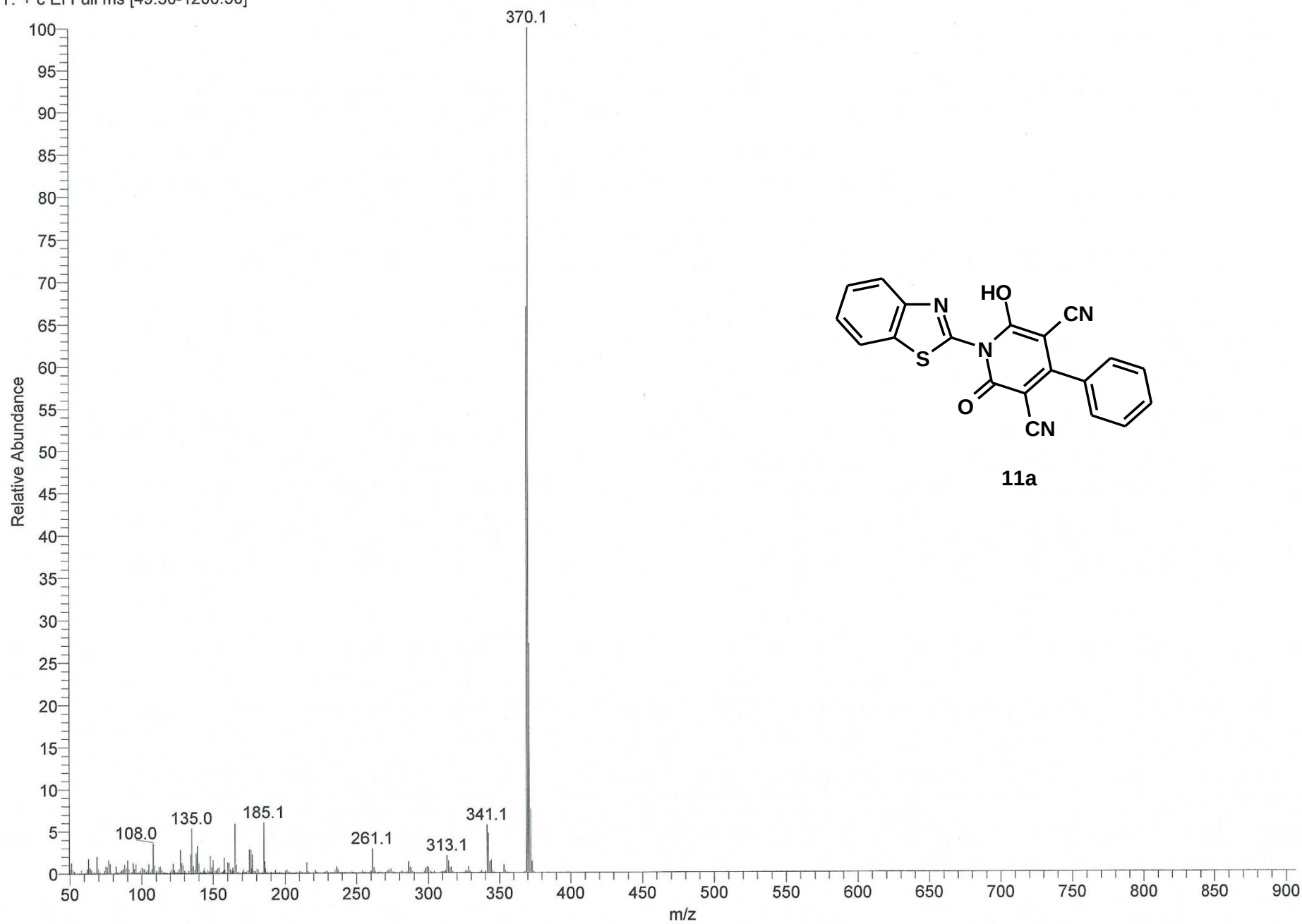
No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	3400.85	96.3199	2	2910.06	97.503	3	2858.95	97.6432
4	2807.85	97.7339	5	2672.86	97.4687	6	2198.45	93.5479
7	1678.73	89.7964	8	1613.16	88.4333	9	1561.09	80.8837
10	1536.02	75.5128	11	1518.67	67.5097	12	1463.71	89.3041
13	1451.17	85.7331	14	1439.6	87.5067	15	1415.49	93.11
16	1382.71	83.8744	17	1361.5	89.0174	18	1327.75	88.7835
19	1319.07	91.1912	20	1293.04	89.7009	21	1274.72	83.3812
22	1229.4	93.5076	23	1204.33	94.8423	24	1160.94	72.2998
25	1135.87	85.5456	26	1061.62	93.2673	27	1012.45	94.9567
28	996.053	95.2503	29	960.377	95.7597	30	943.02	92.4875
31	922.771	92.3986	32	860.096	96.6096	33	812.849	91.123
34	754.031	92.2733	35	722.211	93.0433	36	677.856	97.2373
37	616.145	96.6323	38	579.504	93.3086	39	557.327	97.3705
40	543.828	97.7724	41	526.471	98.6082	42	501.401	93.322
43	436.798	97.9184	44	414.62	98.4139			

[Measurement Information]

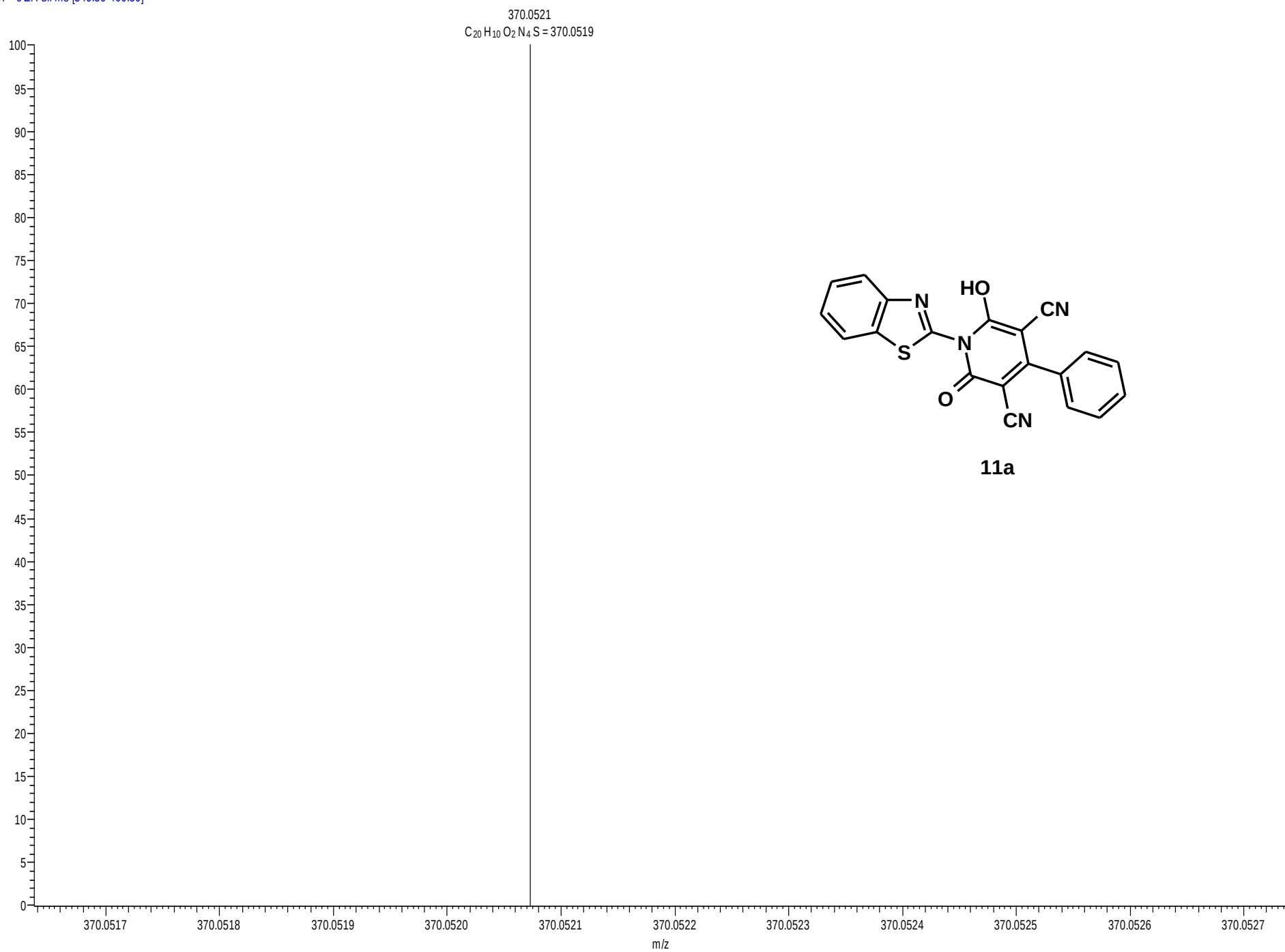
Model Name FT/IR-6300typeA
Serial Number A009861024

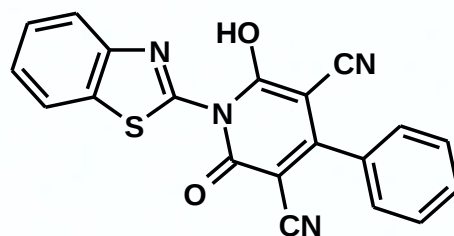
Light Source Standard
Detector TGS
Accumulation Auto (33)
Resolution 4 cm-1
Zero Filling On
Apodization Cosine
Gain Auto (4)
Aperture Auto (7.1 mm)
Scanning Speed Auto (2 mm/sec)
Filter Auto (10000 Hz)

Ph_180423122717 #259 RT: 12.50 AV: 1 NL: 1.60E7
T: + c EI Full ms [49.50-1200.50]

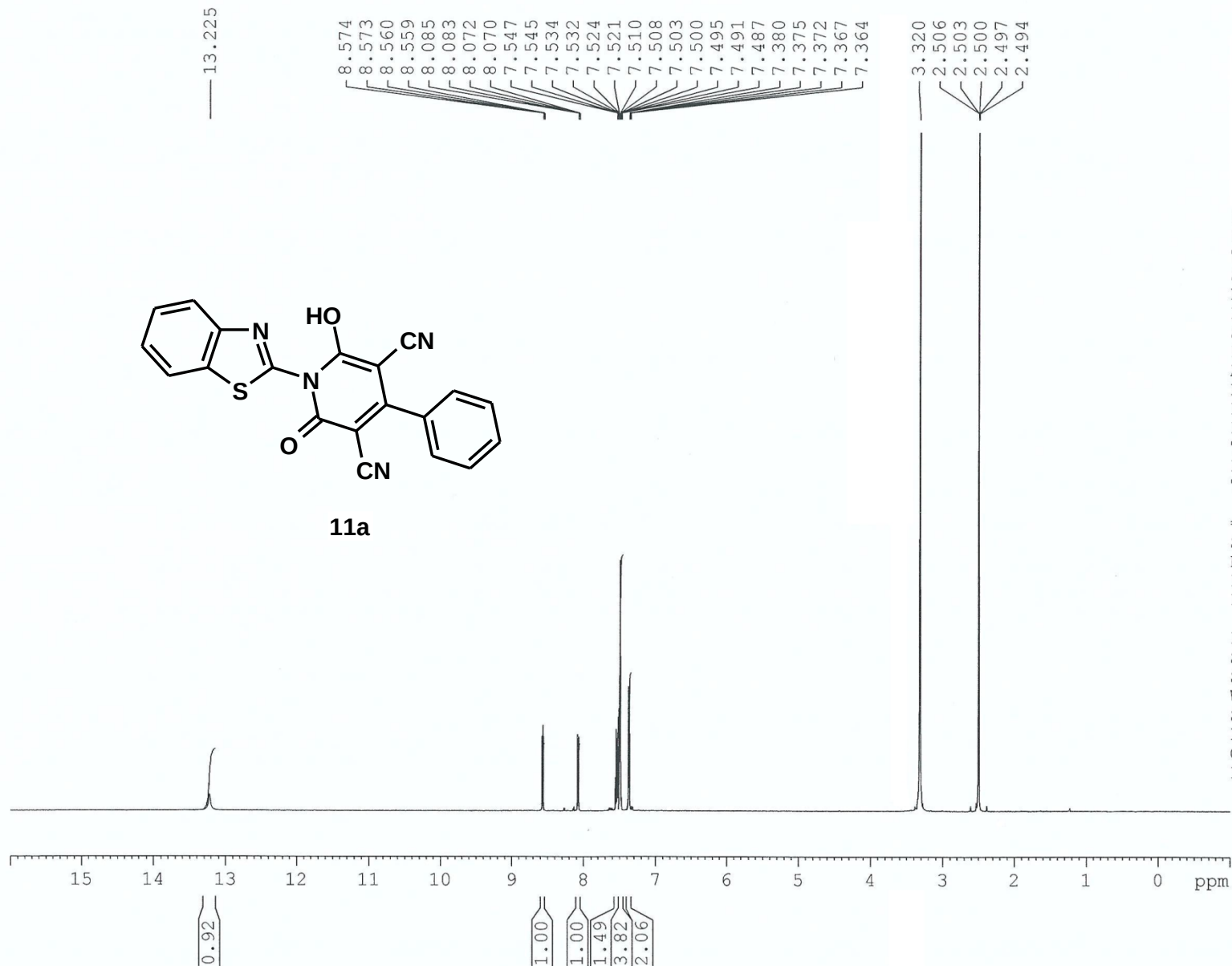


HRMS-BT16-cmass3 #233 RT: 8.06 AV: 1 NL: 7.70E4
T: + c EI Full ms [349.50-400.50]





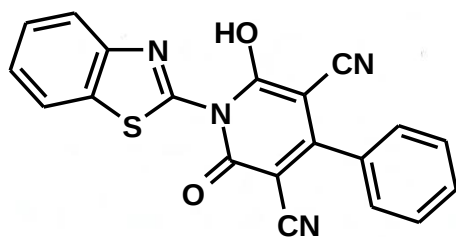
11a



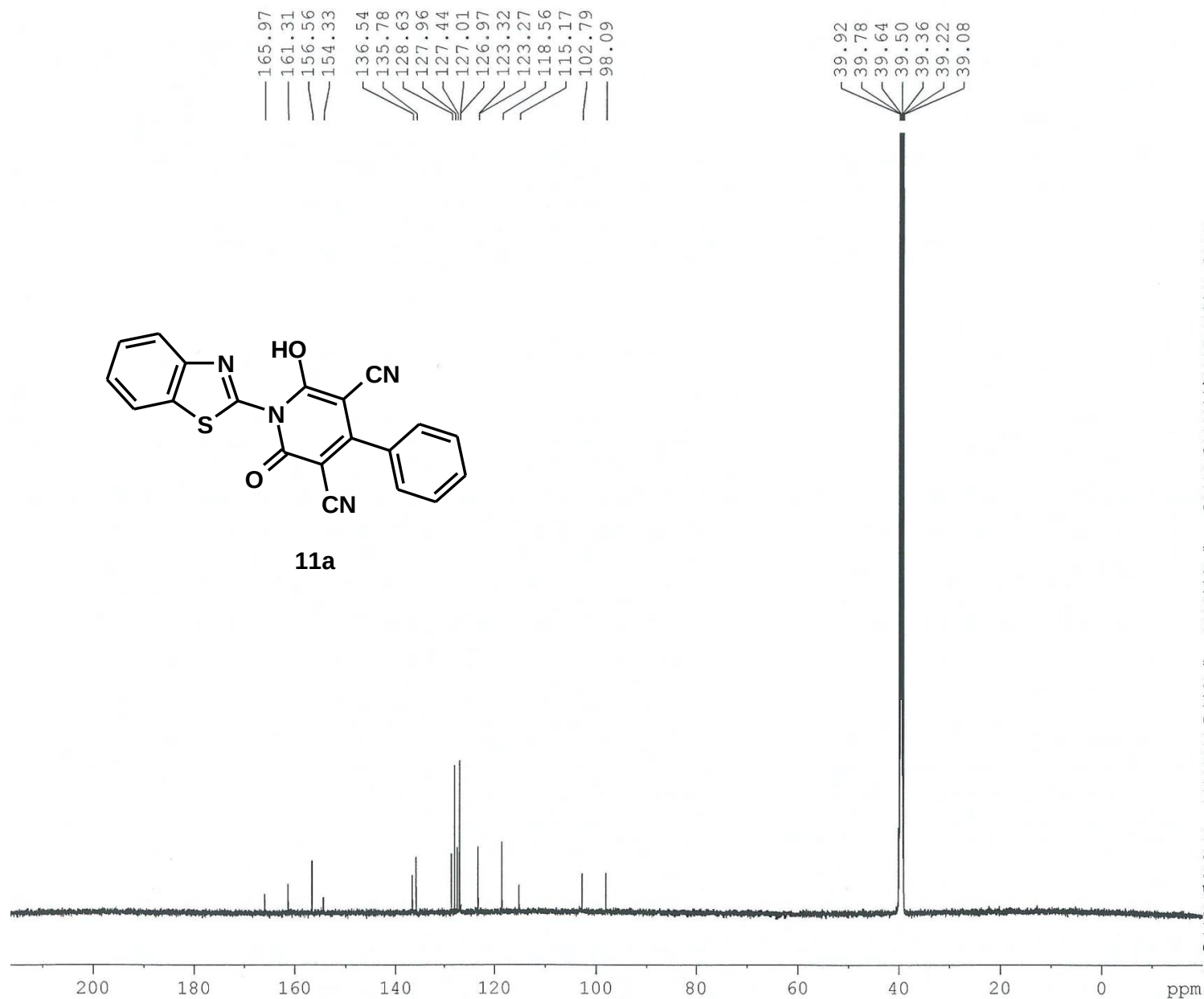
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 12335.526 Hz
FIDRES 0.188225 Hz
AQ 2.6563926 sec
RG 203
DW 40.533 usec
DE 20.00 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 600.1337060 MHz
NUC1 1H
P1 10.60 usec
PLW1 27.82500076 W

F2 - Processing parameters
SI 32768
SF 600.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



11a



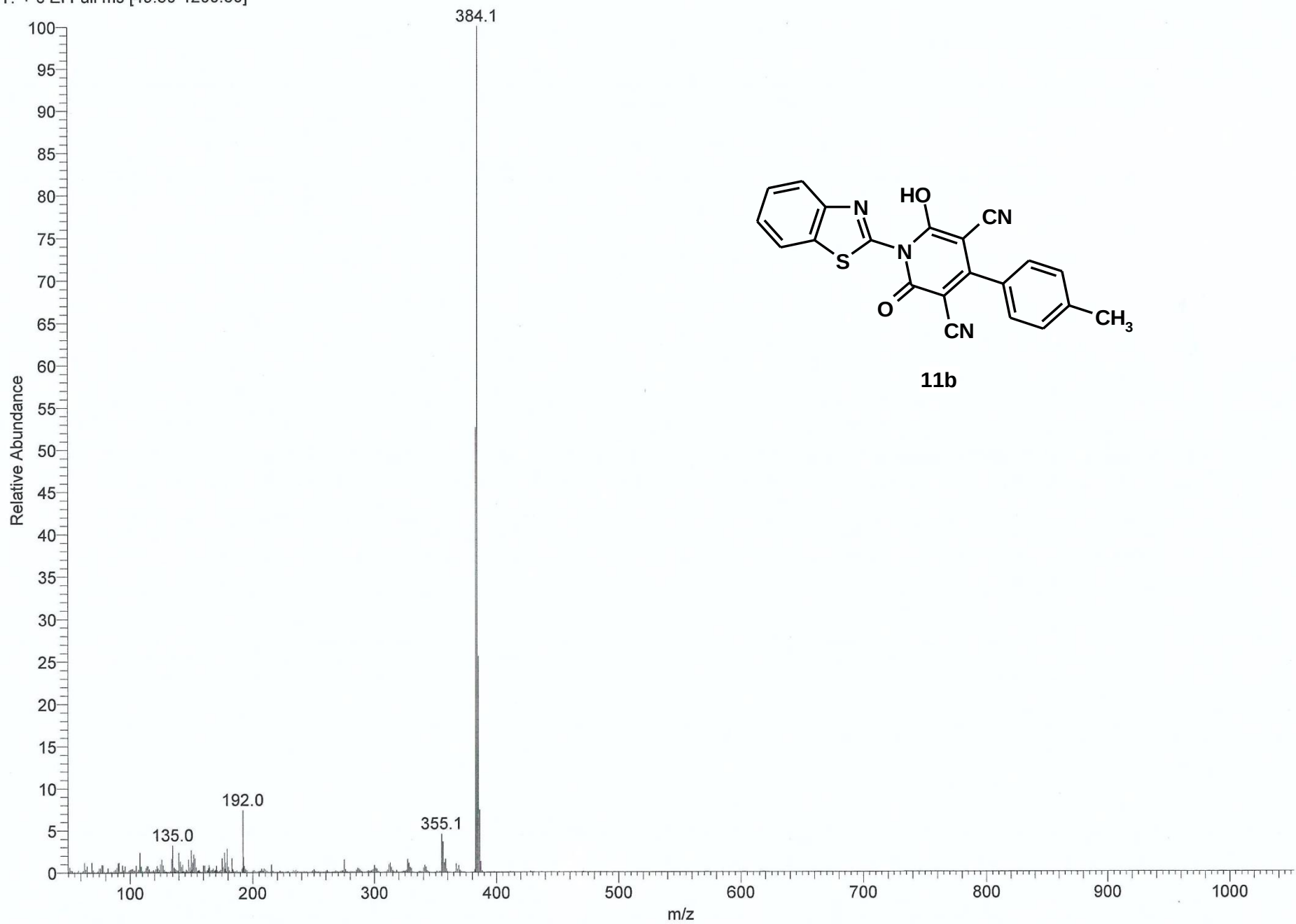
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 10240
DS 4
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 203
DW 13.867 usec
DE 50.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 150.9178979 MHz
NUC1 13C
P1 8.80 usec
PLW1 78.13500214 W

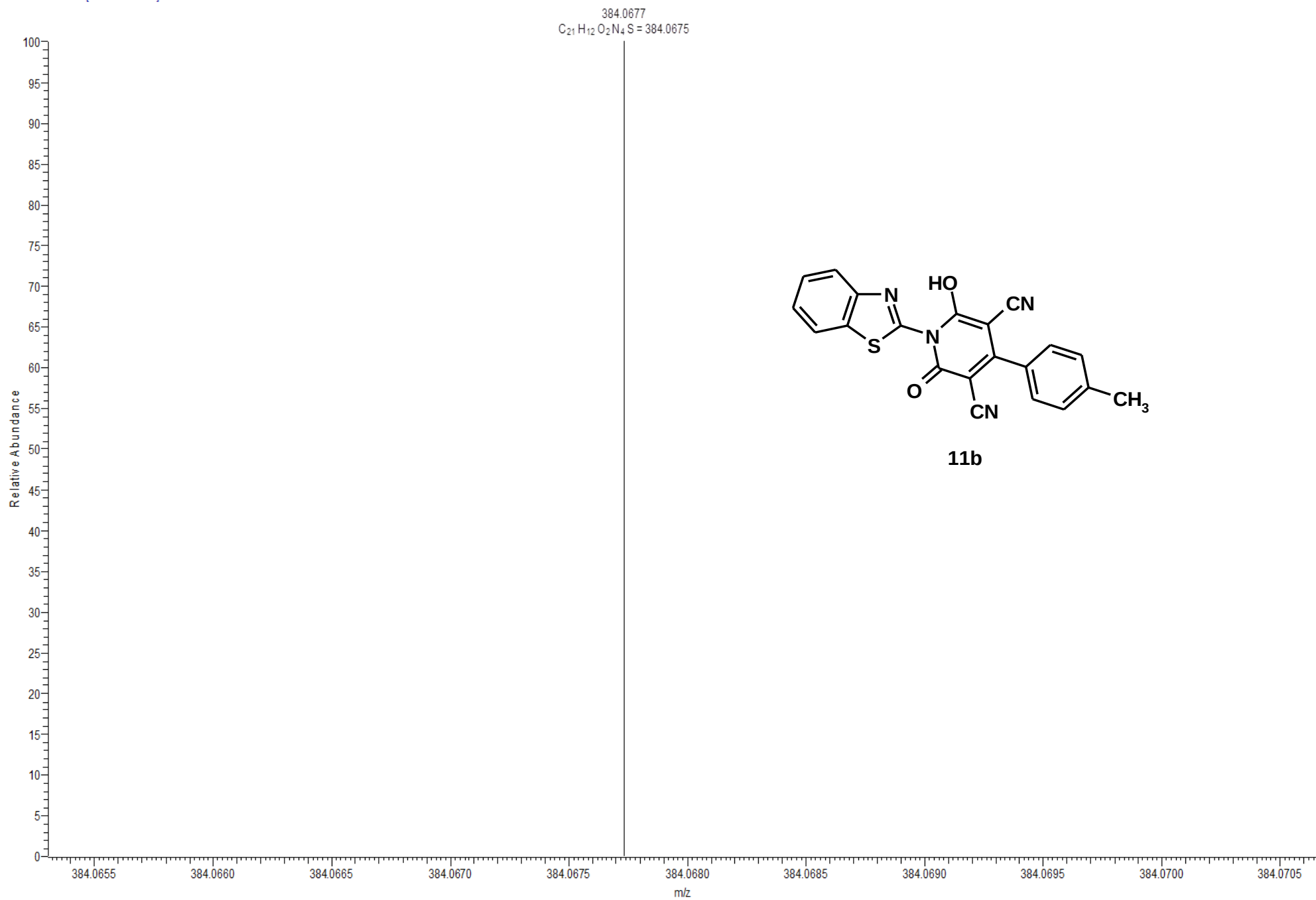
===== CHANNEL f2 =====
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 70.00 usec
PLW2 27.82500076 W
PLW12 0.63804001 W
PLW13 0.31264001 W

F2 - Processing parameters
SI 32768
SF 150.9028828 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

BT17CH3 #247 RT: 11.93 AV: 1 NL: 1.51E7
T: + c EI Full ms [49.50-1200.50]



HRMS-BT17-cmass2 #164 RT: 12.00 AV: 1 NL: 2.44E3
T: + c EI Full ms [359.50-410.50]

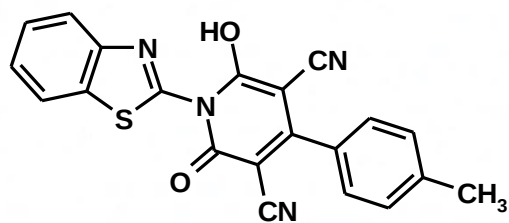




— 12.803

8.588
8.587
8.575
8.573
8.016
8.014
8.005
8.003
8.002
7.538
7.536
7.526
7.524
7.514
7.511
7.501
7.498
7.488
7.313
7.299
7.278
7.265

2.991
2.506
2.503
2.500
2.497
2.494
2.439

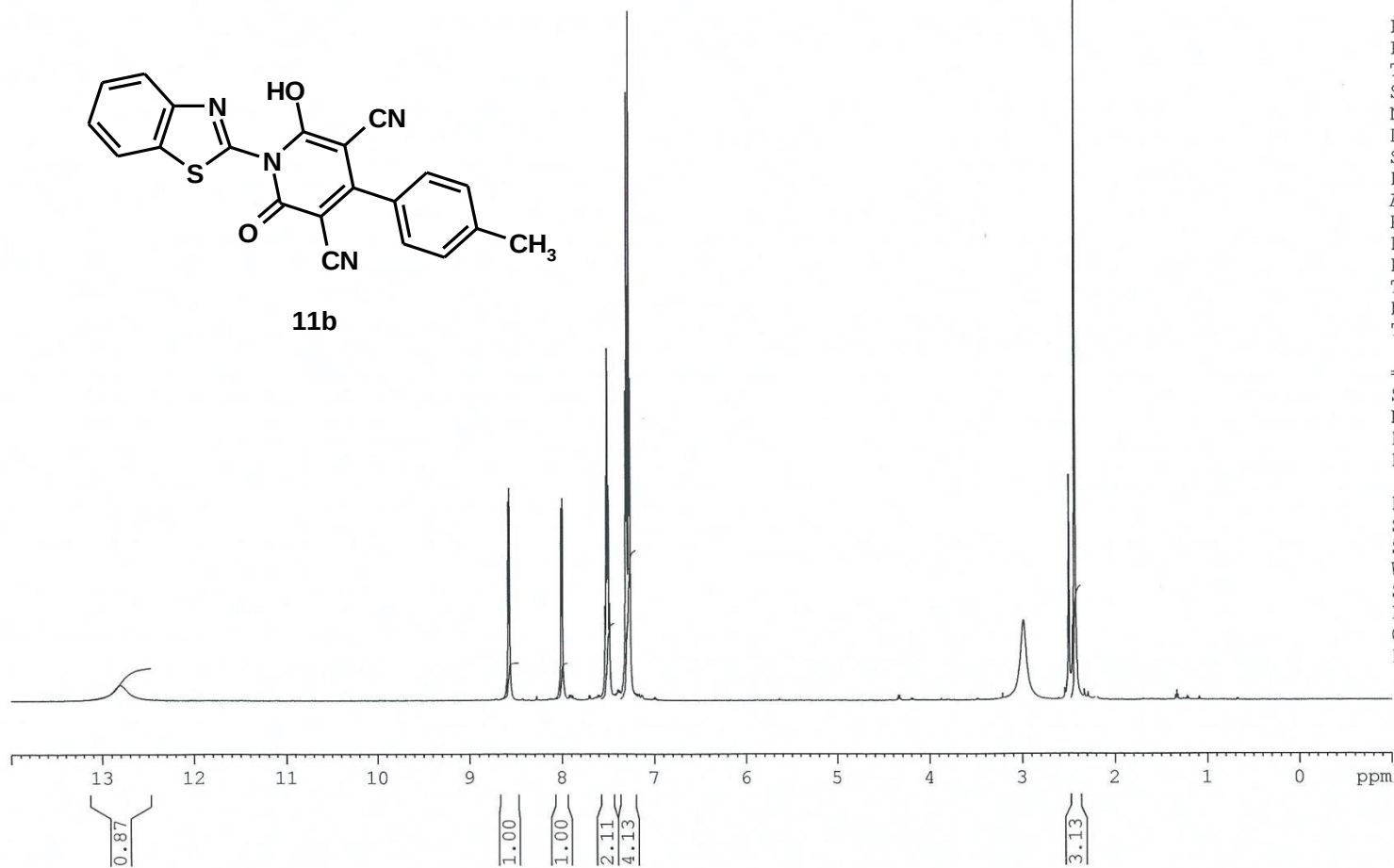


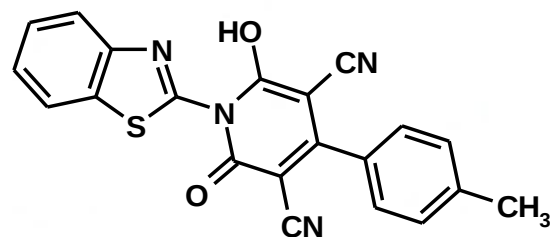
11b

PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 12335.526 Hz
FIDRES 0.188225 Hz
AQ 2.6563926 sec
RG 203
DW 40.533 usec
DE 20.00 usec
TE 368.2 K
D1 1.00000000 sec
TD0 1

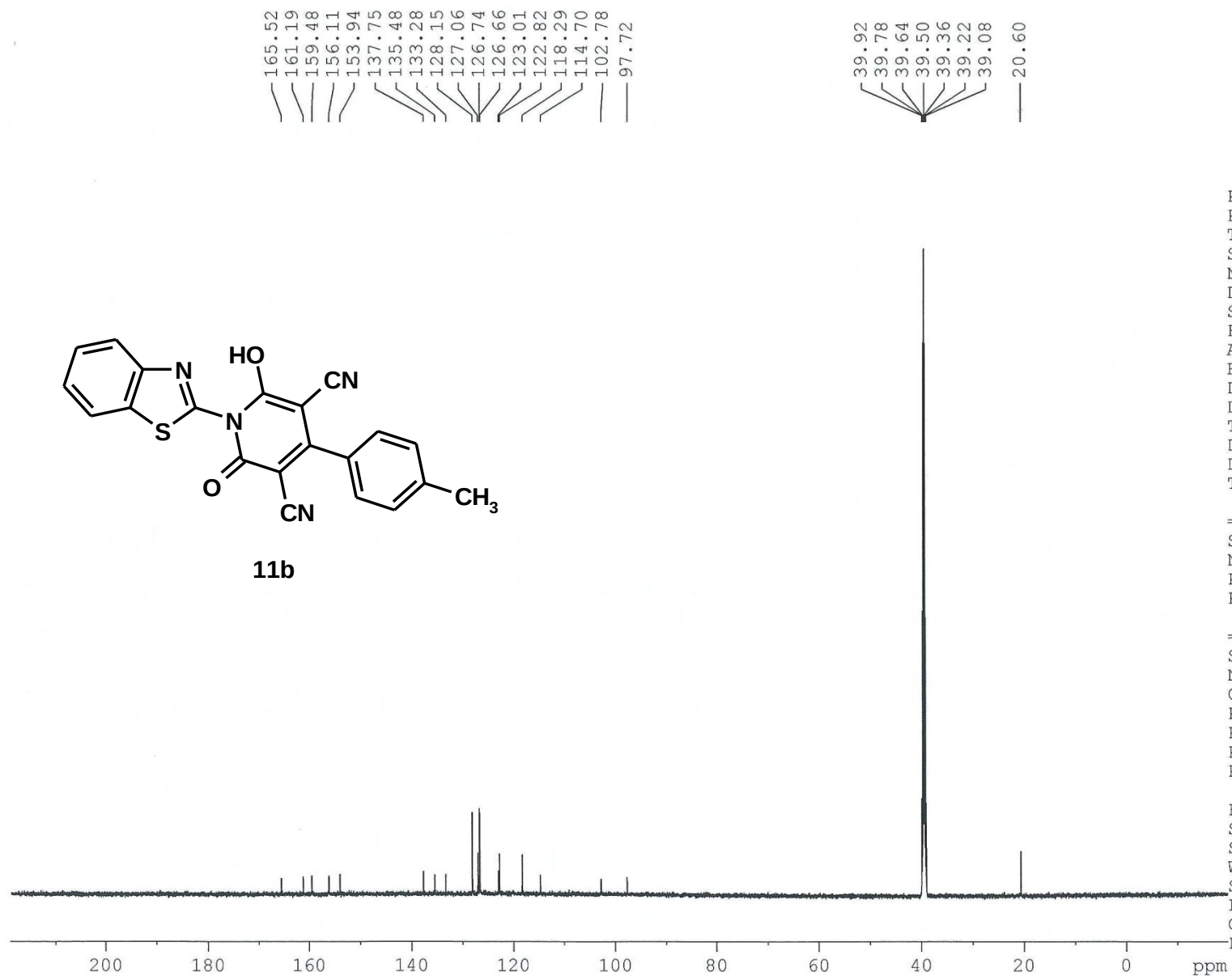
===== CHANNEL f1 =====
SFO1 600.1337060 MHz
NUC1 1H
P1 10.60 usec
PLW1 27.82500076 W

F2 - Processing parameters
SI 32768
SF 600.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





11b



```

PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1794
DS 4
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 203
DW 13.867 usec
DE 50.00 usec
TE 340.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
  
```

```

===== CHANNEL f1 =====
SFO1 150.9178979 MHz
NUC1 13C
P1 8.80 usec
PLW1 78.13500214 W
  
```

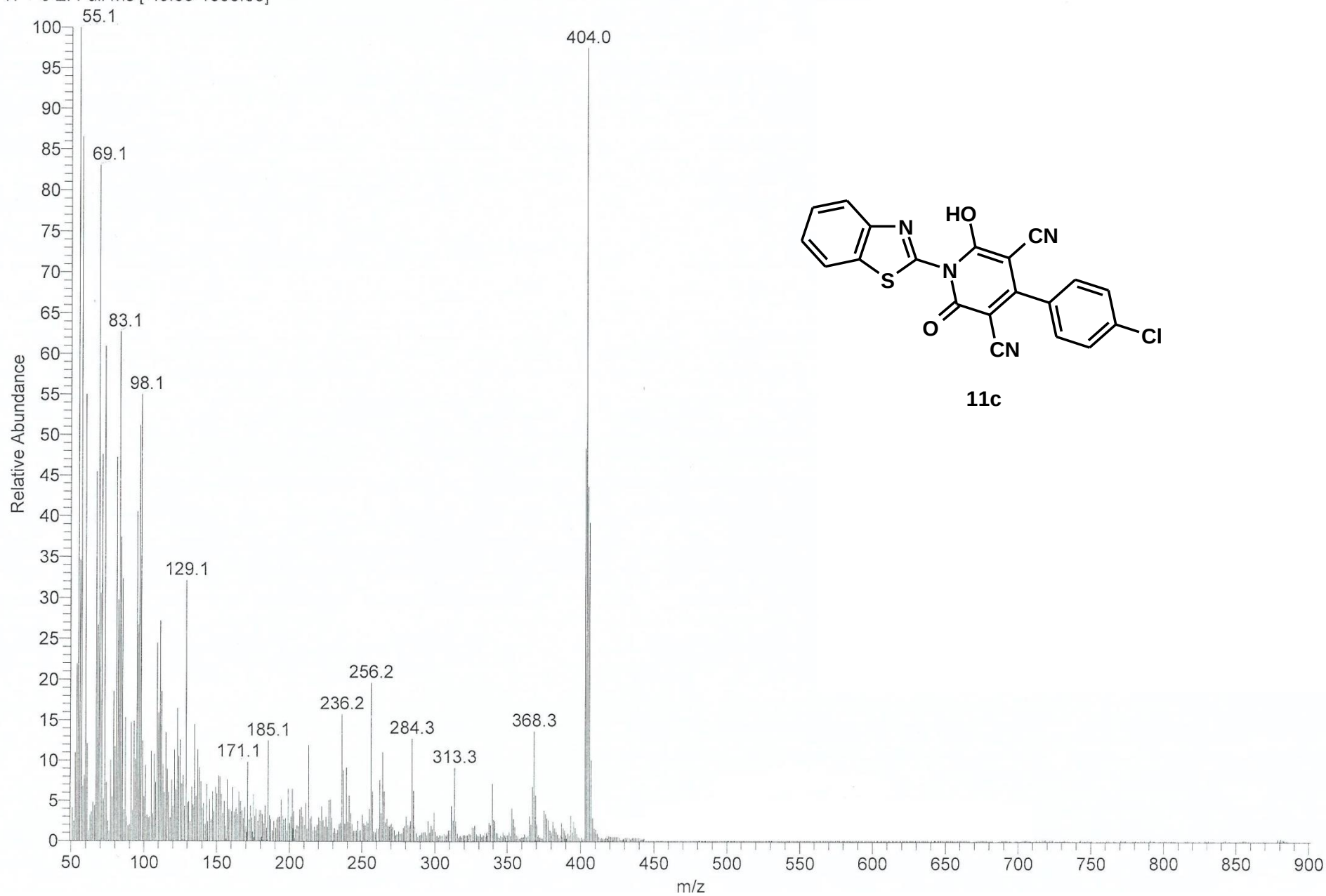
```

===== CHANNEL f2 =====
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 70.00 usec
PLW2 27.82500076 W
PLW12 0.63804001 W
PLW13 0.31264001 W
  
```

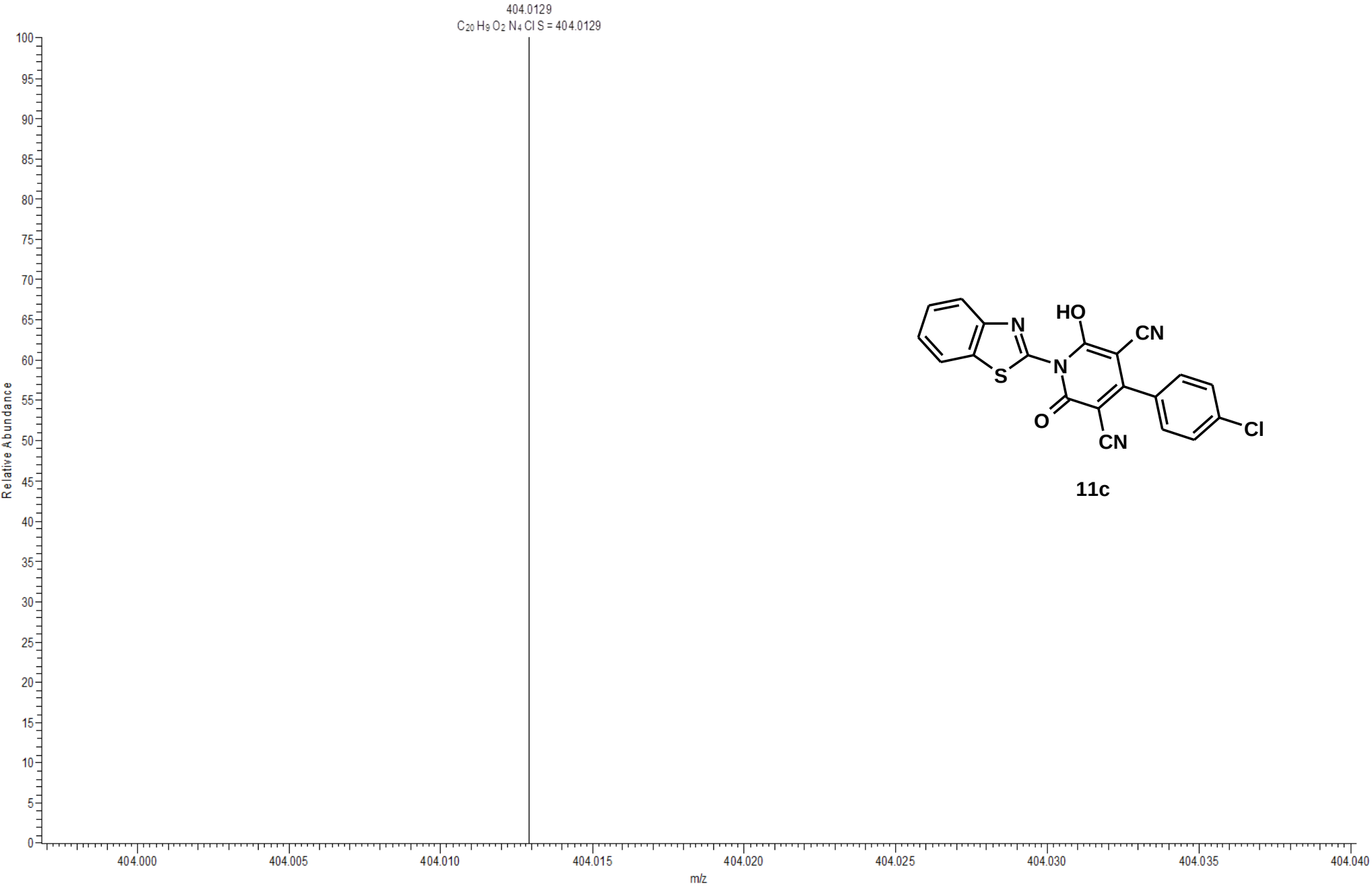
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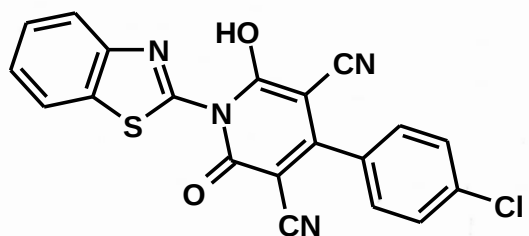
F2 - Processing parameters
SI 32768
SF 150.9029304 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
  
```

BTECA #180 RT: 7.93 AV: 1 NL: 2.32E6
T: + c EI Full ms [49.50-1000.50]

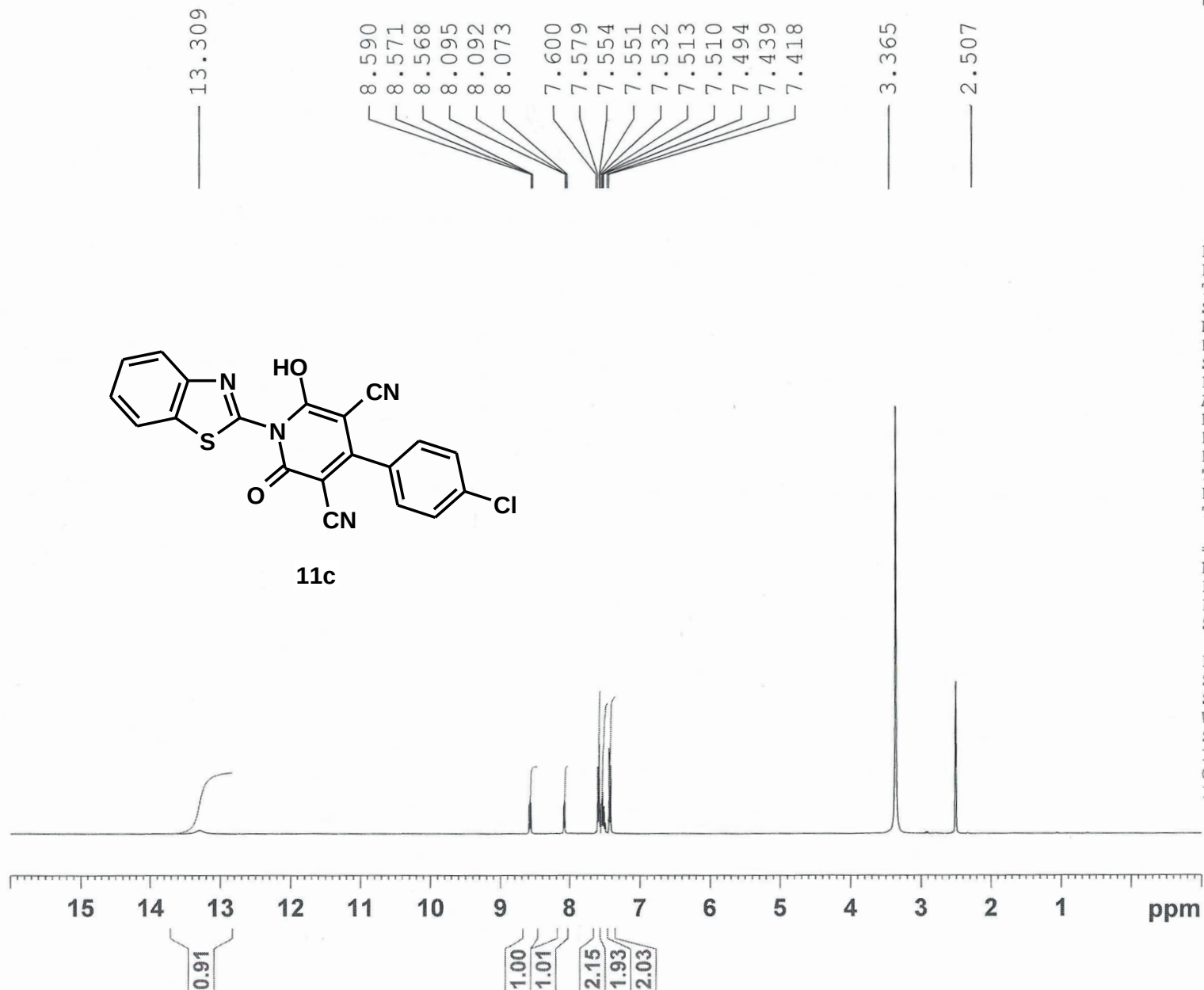


HRMS-BT14-cmass1#173 RT: 6.35 AV: 1 NL: 5.96E3
T: + c EI Full ms [374.50-435.50]





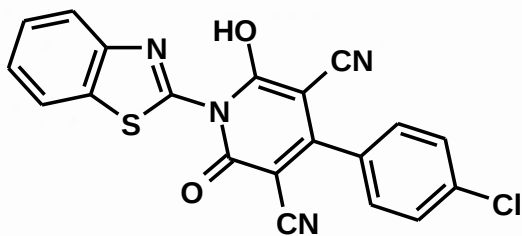
11c



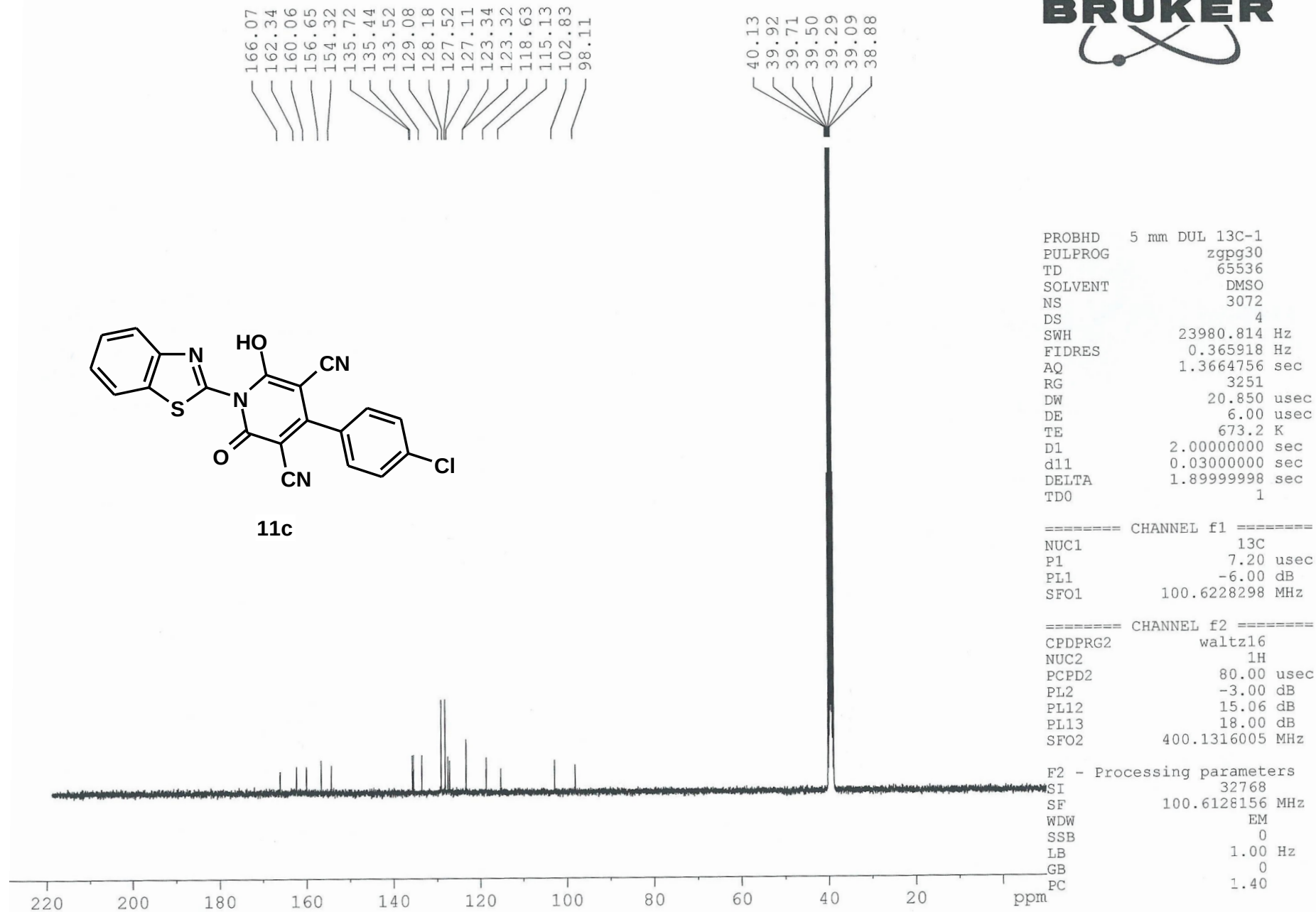
PROBHD 5 mm DUL 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 8278.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.9584243 sec
 RG 322.5
 DW 60.400 usec
 DE 6.00 usec
 TE 673.2 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.20 usec
 PL1 -3.00 dB
 SFO1 400.1324710 MHz

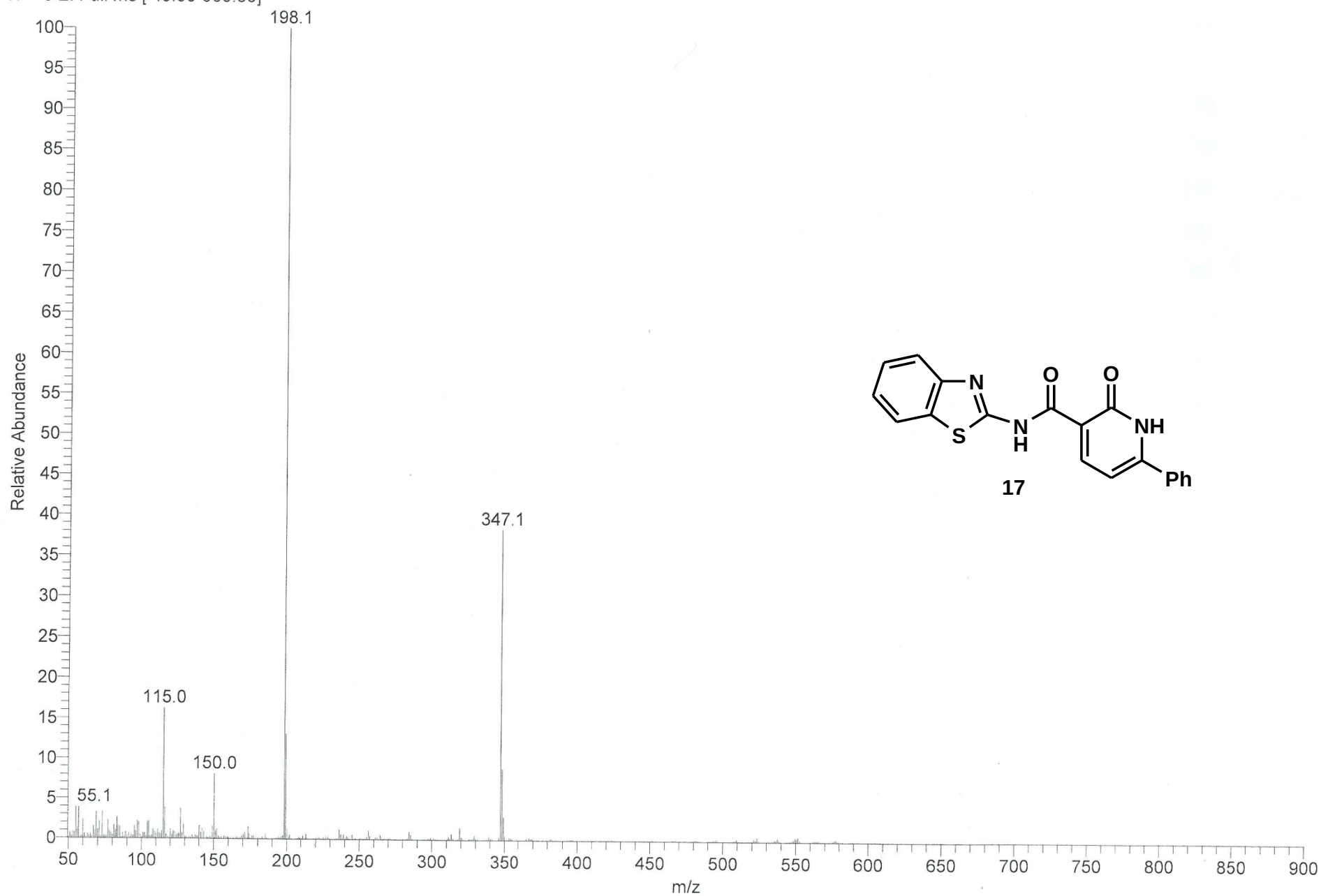
F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



11c



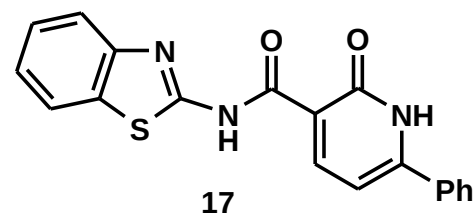
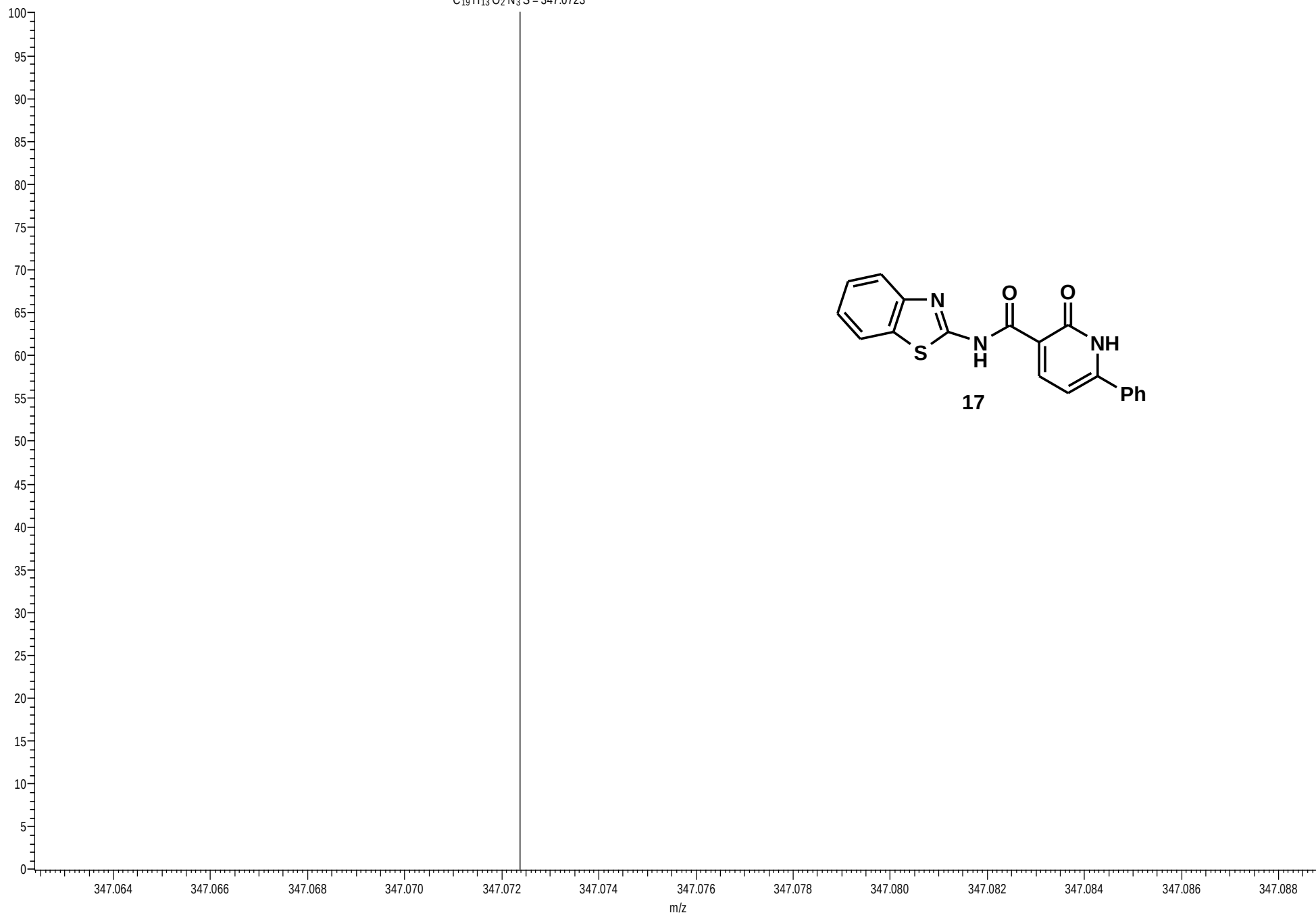
BT12CDMF #203 RT: 8.95 AV: 1 NL: 5.03E7
T: + c EI Full ms [49.50-900.50]

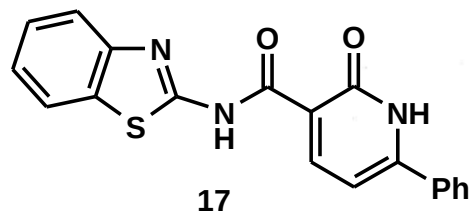


HRMS-BT12-cmass1 #323 RT: 17.01 AV: 1 NL: 1.75E6

T: + c EI Full ms [309.50-370.50]

347.0724
C₁₉H₁₃O₂N₃S = 347.0723





13.586
13.223

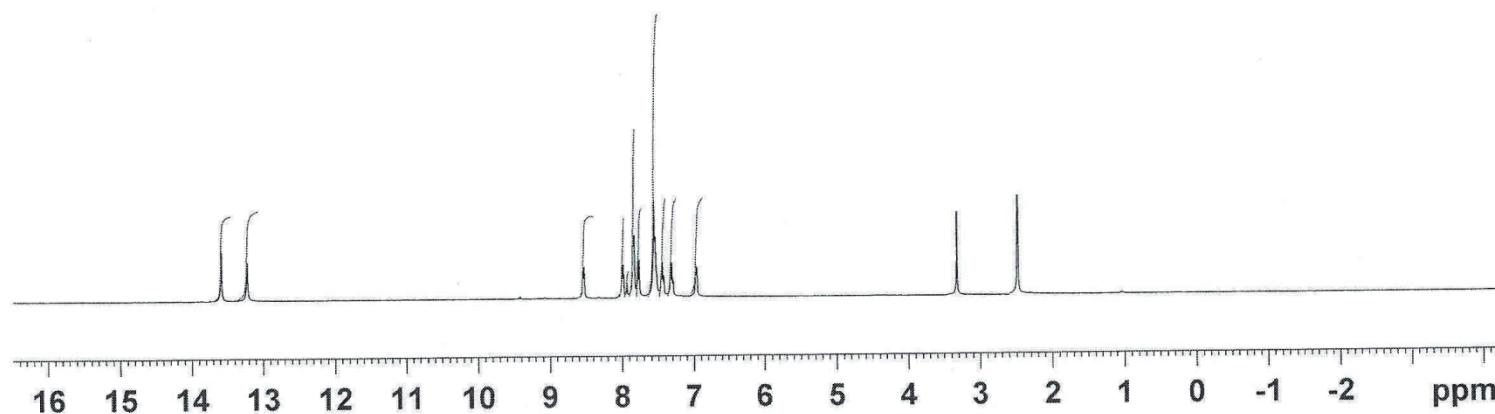
8.548
8.530
8.004
7.985
7.851
7.835
7.785
7.766
7.559
7.541
7.460
7.442
7.423
7.331
7.313
7.295
6.978
6.960
3.327

2.484

PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 362
DW 60.400 usec
DE 6.00 usec
TE 673.2 K
D1 1.00000000 sec
TD0 1

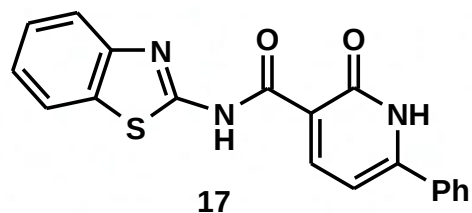
===== CHANNEL f1 =====
NUC1 1H
P1 9.00 usec
PL1 -4.50 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 0.01



1.04
1.10

1.00
1.01
2.10
1.11
3.50
1.23
1.23
1.22



PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 10240
DS 4
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 203
DW 13.867 usec
DE 50.00 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 150.9178979 MHz
NUC1 13C
P1 8.80 usec
PLW1 78.13500214 W

===== CHANNEL f2 =====
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 70.00 usec
PLW2 27.82500076 W
PLW12 0.63804001 W
PLW13 0.31264001 W

F2 - Processing parameters
SI 32768
SF 150.9028796 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40