Supporting Information

Efficient Cu-catalyzed intramolecular O-arylation for synthesis of benzoxazoles in water†

Yanling Tang, Minxin Li, Hui Gao, Gaoxiong Rao and Zewei Mao*

College of Pharmaceutical Science, Yunnan University of Chinese Medicine, Kunming 650500, P.R. China

1. Experimental section

1.1 General considerations

Starting materials were commercially available and analytically pure without purification. ^{1}H NMR and ^{13}C NMR spectras were recorded on a Bruker AV 400 spectrometer (Bruker Company, Germany), using TMS as standard. High-resolution mass spectra were performed on an ESI Q-TOF MS spectrometer (Micromass, England).

1.2 Synthesis of ligand **DPPAP**

To a stirred solution of 1-(2-aminoethyl)pyrrolidine (2.28 g, 20 mmol) and triethylamine (3.03 g, 30 mmol) in dry DCM (50 mL), acryloyl chloride (2.26 g, 25 mmol) was added and reaction mixture was stirred for 12 h at room temperature. After completion of the reaction as indicated by TLC, the reaction was quenched by the addition of 5% NaOH (20 mL) and was extracted with DCM (3×30 mL). The organic layer was washed by H_2O (3×30 mL), and dried using anhydrous Na_2SO_4, concentrated in vacuo. Then diphenylphosphine (4.65 g, 25 mmol), CH_3CN (50 mL) and TEAOH (25% wt, 0.2 mL) was add to the residue in sequence for 24 h. When the reaction was completed, the mixture was concentrated in vacuo to form crude amide. After that, amide was dissolved in dry THF (50 mL), and $LiAlH_4$ (1.52 g, 40 mmol) was added slowly. The reaction was carried out at 60 ^{o}C for 12 h. The crude product was dried and purified by column chromatography (DCM) to obtain ligand **DPPAP**. Pale green oil; ^{1}H NMR(400Hz, $CDCl_3$) δ:7.39-7.46(m, 5H), 7.28-7.32(m, 5H), 3.58(t, *J*=5.8Hz, 2H), 2.70-2.74(m, 3H), 2.61(t, *J*=6.0Hz, 2H), 2.48-2.53(m, 4H), 2.04-2.09(m, 2H), 1.72-1.76(m, 4H), 1.61-1.69(m, 2H); ^{13}C NMR(100MHz, $CDCl_3$) δ: 138.50, 138.37, 132.61, 132.43, 130.64, 130.55, 128.59, 128.47, 128.38, 128.27, 128.21, 55.31, 53.98, 50.67, 50.53, 47.78, 25.92, 25.76, 25.51, 25.40, 23.22; HRMS-ESI: *m/z* calcd for $C_{21}H_{30}N_2P$ $(M+H)^+$ 341.2141 found 341.2145.

1.3 General procedure for the synthesis of benzoxazoles (**2**)

To a stirred solution of the *o*-halobenzanilides **1** (1 mmol), $Cu(OAc)_2$ (9 mg, 0.05 mmol), Et_3N (202 mg, 2 mmol) and DPPAP (17 mg, 0.1 mmol) in water (3 mL) at 110 ^{o}C for 12 h. After cooled to room temperature, the reaction was extracted with EtOAc (3×5 mL). The organic layer was dried using anhydrous Na_2SO_4, concentrated in vacuo and purified by column chromatography to afford respective products.

Compound 2a: ^{1}H NMR (400MHz, $CDCl_3$) δ: 8.18-8.21(m, 2H), 7.72-7.74(m, 1H), 7.46-7.48(m, 1H), 7.40-7.43(m, 3H), 7.24-7.27(m, 2H); ^{13}C NMR (100MHz, $CDCl_3$) δ: 162.85, 150.64, 142.07, 131.31, 128.73, 127.50, 127.08, 124.94, 124.43, 119.92, 110.45; HRMS-ESI: *m/z* calcd for $C_{13}H_{10}NO$ $(M+H)^+$ 196.0757 found 196.0759.

Compound 2b:^{1}H NMR (400MHz, $CDCl_3$) δ: 8.11(d, *J*=8.2Hz, 2H), 7.73-7.75(m, 1H), 7.50-7.73(m, 1H), 7.25-7.30(m, 4H), 2.36(s, 3H); ^{13}C NMR (100MHz, $CDCl_3$) δ: 163.30, 150.74, 142.27, 142.00, 129.63, 127.62, 124.86, 124.48, 119.88, 110.50, 21.62; HRMS-ESI: *m/z* calcd for $C_{14}H_{12}NO(M+H)^+$ 210.0913 found 210.0910.

Compound 2c:^{1}H NMR (400MHz, $CDCl_3$) δ: 8.16(d, *J*=8.3Hz, 2H), 7.74-7.76(m, 1H), 7.52-7.74(m, 1H), 7.29-7.33(m, 4H), 2.72(q, *J*=7.6Hz, 2H), 1.27(t, *J*=7.6Hz, 3H); ^{13}C NMR (100MHz, $CDCl_3$) δ: 163.35, 150.78, 148.28, 142.30, 128.48, 127.76, 124.89, 124.70, 124.51, 119.91, 110.53, 28.98, 15.23; HRMS-ESI: *m/z* calcd for $C_{15}H_{14}NO(M+H)^+$ 224.1070 found 224.1069.

Compound 2d: ^{1}H NMR (400MHz, $CDCl_3$) δ: 8.20(d, *J*=8.6Hz, 2H), 7.72-7.75(m, 1H), 7.54-7.56(m, 1H), 7.30-7.35(m, 2H), 7.03(d, *J*=8.6Hz, 2H), 3.88(s, 3H); ^{13}C NMR (100MHz, $CDCl_3$) δ: 163.32, 162.48, 150.83, 142.44, 129.53, 124.72, 124.55, 119.86, 119.76, 114.50, 110.50, 55.57; HRMS-ESI: *m/z* calcd for $C_{14}H_{12}NO_2(M+H)^+$ 226.0863 found 226.0865.

Compound 2e: ^{1}H NMR (400MHz, $CDCl_3$) δ: 8.18(d, *J*=9.0Hz, 2H), 7.55-7.74(m, 1H), 7.52-7.54(m, 1H), 7.29-7.32(m, 2H), 7.00(d, *J*=9.0Hz, 2H), 4.11(q, *J*=7.0Hz, 2H), 1.45(t, *J*=7.0Hz, 3H); ^{13}C NMR (100MHz, $CDCl_3$) δ: 163.36, 161.87, 150.79, 142.44, 129.49, 124.65, 124.49, 119.71, 119.61, 114.92, 110.46, 63.81, 14.82; HRMS-ESI: *m/z* calcd for $C_{15}H_{14}NO_2(M+H)^+$ 240.1019 found 240.1018.

Compound 2f: ^{1}H NMR (400MHz, $CDCl_3$) δ: 8.17-8.21(dd, *J*=5.4Hz, 5.4Hz, 2H), 7.71-7.74(m, 1H), 7.49-7.52(m, 1H), 7.29-7.32(m, 2H), 7.17(t, *J*=8.7Hz, 2H); ^{13}C NMR (100MHz, $CDCl_3$) δ: 166.10, 163.59, 162.15, 150.82, 142.15, 129.89, 129.80, 125.15, 124.68, 123.58, 123.55, 120.05, 116.28, 116.06, 110.58; HRMS-ESI: *m/z* calcd for $C_{13}H_9FNO$ $(M+H)^+$ 241.0663 found 241.0661.

Compound 2h: ^{1}H NMR (400MHz, $CDCl_3$) δ: 8.18(d, *J*=8.7Hz, 2H), 7.75-7.77(m, 1H), 7.55-7.57(m, 1H), 7.49(d, *J*=8.8Hz, 1H), 7.33-7.37(m, 2H); ^{13}C NMR (100MHz, $CDCl_3$) δ: 162.19, 150.92, 142.18, 137.90, 129.40, 128.98, 125.84, 125.47, 124.87, 120.24, 110.74; HRMS-ESI: *m/z* calcd for $C_{13}H_9ClNO$ $(M+H)^+$ 230.0367 found 230.0366.

Compound 2i: ^{1}H NMR (400MHz, $CDCl_3$) δ: 8.14-8.16(dd, *J*=2.1Hz, 2.2Hz, 1H), 7.84-7.86(m, 1H), 7.62-7.63(m, 1H), 7.56-7.61(dd, *J*=11.4Hz, 6.3Hz, 1H), 7.47(d, *J*=1.9Hz, 1H), 7.45(d, *J*=2.0Hz, 1H), 7.43(d, *J*=2.1Hz, 1H), 7.38-7.42(m, 1H); ^{13}C NMR (100MHz, $CDCl_3$) δ: 161.11, 150.75, 141.85, 133.65, 132.03, 131.97, 131.52, 127.05, 126.44, 125.70, 124.78, 120.65, 110.87; HRMS-ESI: *m/z* calcd for $C_{13}H_9ClNO$ $(M+H)^+$ 230.0367 found 230.0366.

Compound 2j: ^{1}H NMR (400MHz, $CDCl_3$) δ: 8.15(s, 2H), 7.80(d, *J*=9.1Hz, 1H), 7.61(d, *J*=2.6Hz, 1H), 7.51(s, 1H), 7.41(t, *J*=3.7Hz, 2H); ^{13}C NMR (100MHz, $CDCl_3$) δ: 151.32, 141.93, 135.98, 131.40, 126.12, 126.01, 125.20, 120.61, 110.97; HRMS-ESI: *m/z* calcd for $C_{13}H_8Cl_{12}NO$ $(M+H)^+$ 263.9977 found 263.9975.

Compound 2k: ^{1}H NMR(400Hz, $CDCl_3$) δ: 8.09(d, *J*=8.7Hz, 2H), 7.74-7.76(m, 1H), 7.64(d, *J*=8.6Hz, 2H), 7.53-7.56(m, 1H), 7.33-7.35(m, 2H); ^{13}C NMR(100MHz, $CDCl_3$) δ: 162.22, 150.87, 142.15, 132.33, 129.10, 126.33, 126.23, 126.23, 125.48, 124.86, 120.24, 110.73; HRMS-ESI: *m/z* calcd for $C_{13}H_9BrNO(M+H)^+$ 273.9862 found 273.9862.

Compound 2l: ^{1}H NMR(400Hz, $CDCl_3$) δ: 8.26(d, *J*=8.1Hz, 2H), 7.69-7.71(m, 1H), 7.68(d, *J*=8.9Hz, 2H), 7.48-7.50(m, 1H), 7.27-7.30(m, 2H); ^{13}C NMR(100MHz, $CDCl_3$) δ: 161.58, 150.99,

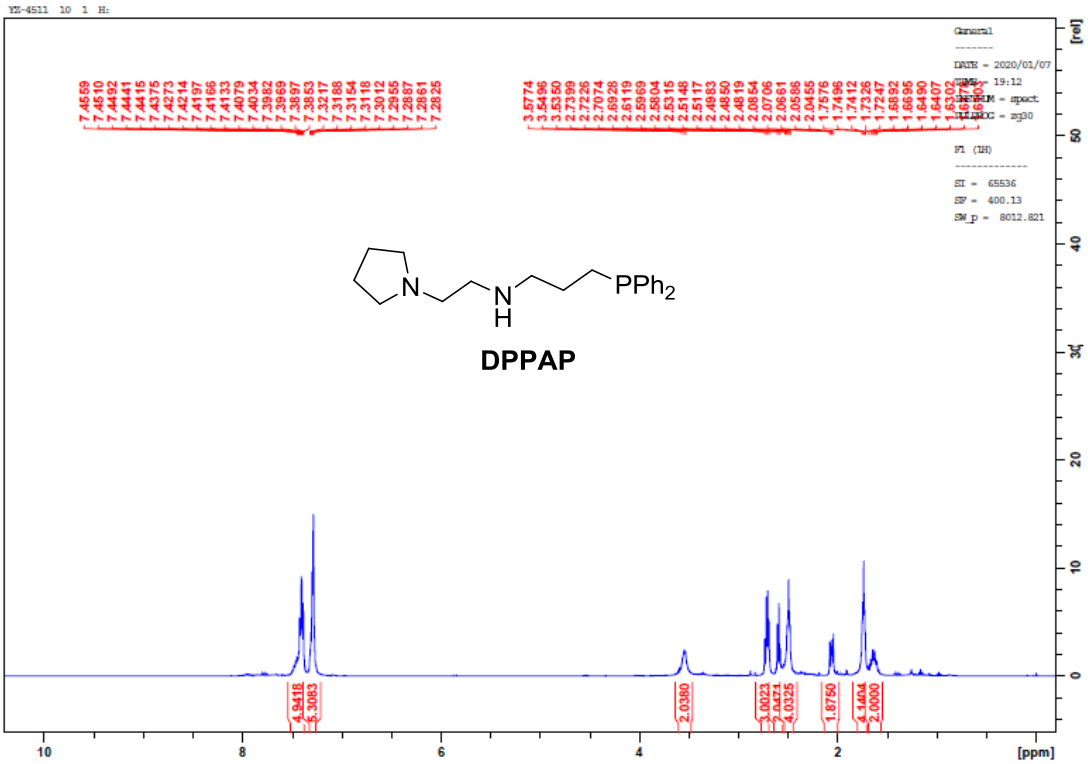
142.05, 127.97, 126.04, 126.01, 125.92, 125.06, 120.54, 110.91; HRMS-ESI: *m/z* calcd for $C_{14}H_9F_3NO(M+H)^+$ 264.0631 found 264.0632.

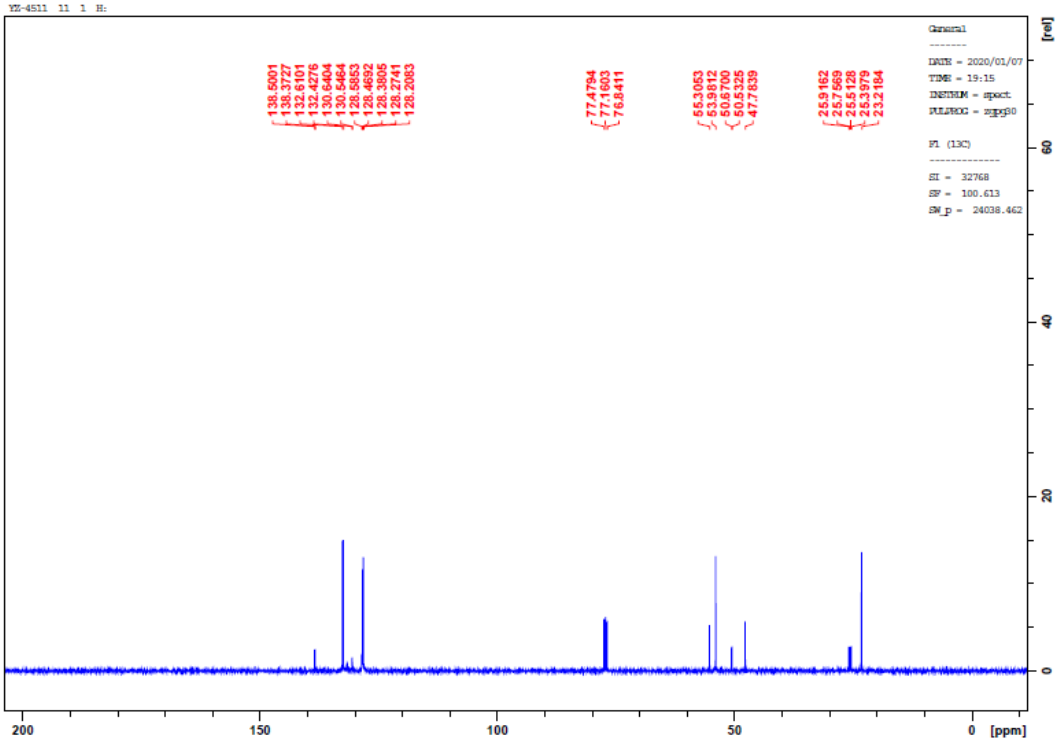
Compound 2m: ^{1}H NMR(400Hz, $CDCl_3$) δ: 8.44(s, 1H), 8.34(d, *J*=7.8Hz, 1H), 7.68-7.71(m, 2H), 7.58(d, *J*=7.8Hz, 1H), 7.50-7.54(m, 1H), 7.28-7.31(m, 2H); ^{13}C NMR(100MHz, $CDCl_3$) δ: 161.62, 150.96, 142.02, 130.74, 129.66, 128.20, 128.05, 128.02, 125.85, 125.05, 124.65, 124.61, 120.46, 110.90; HRMS-ESI: *m/z* calcd for $C_{14}H_9F_3NO(M+H)^+$ 264.0631 found 264.0631.

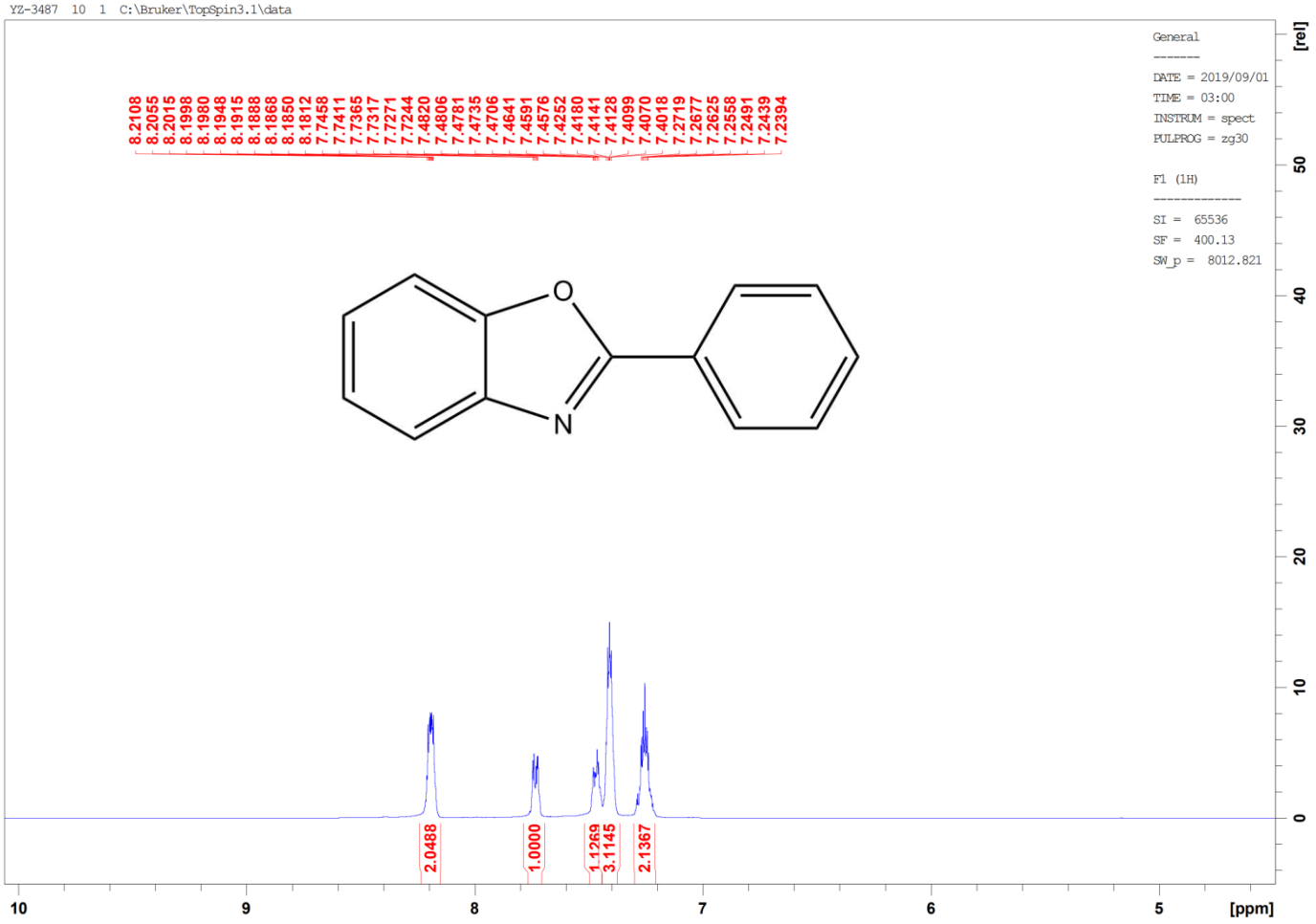
Compound 2n: ^{1}H NMR(400Hz, $CDCl_3$) δ: 8.16(d, *J*=7.2Hz, 1H), 7.83-7.89(m, 2H), 7.62-7.72(m, 3H), 7.40-7.42(m, 2H); ^{13}C NMR(100MHz, $CDCl_3$) δ: 161.30, 151.38, 141.78, 139.13, 132.37, 132.05, 131.17, 127.26, 127.20, 125.83, 124.90, 120.70, 111.05; HRMS-ESI: *m/z* calcd for $C_{14}H_9F_3NO(M+H)^+$ 264.0631 found 264.0628.

Compound 2o: ^{1}H NMR(400Hz, $CDCl_3$) δ: 8.75(s, 1H), 8.31(d, *J*=8.6Hz, 1H), 7.94-7.97(dd, *J*=5.2Hz, 7.1Hz, 2H), 7.87(d, *J*=7.3Hz, 1H), 7.79-7.81(m, 1H), 7.57-7.79(m, 1H), 7.53-7.56(m, 2H), 7.34-7.37(m, 2H); ^{13}C NMR(100MHz, $CDCl_3$) δ: 163.33, 151.01, 142.37, 134.88, 133.11, 129.07, 128.89, 128.27, 128.03, 127.91, 127.01, 125.29, 124.76, 124.54, 124.09, 120.16, 110.71; HRMS-ESI: *m/z* calcd for $C_{17}H_{12}NO(M+H)^+$ 246.0913 found 246.091.

2. NMR spectra



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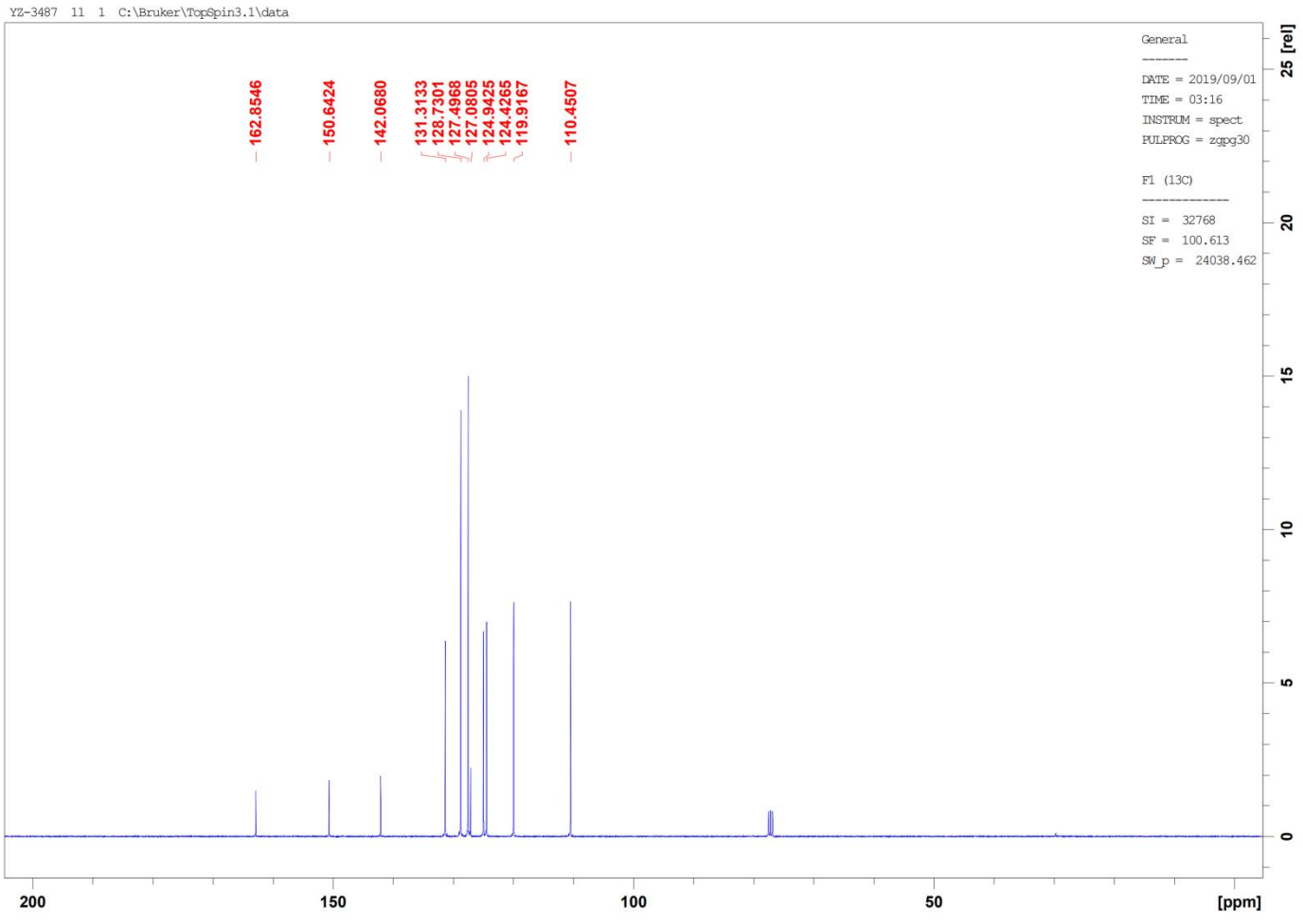
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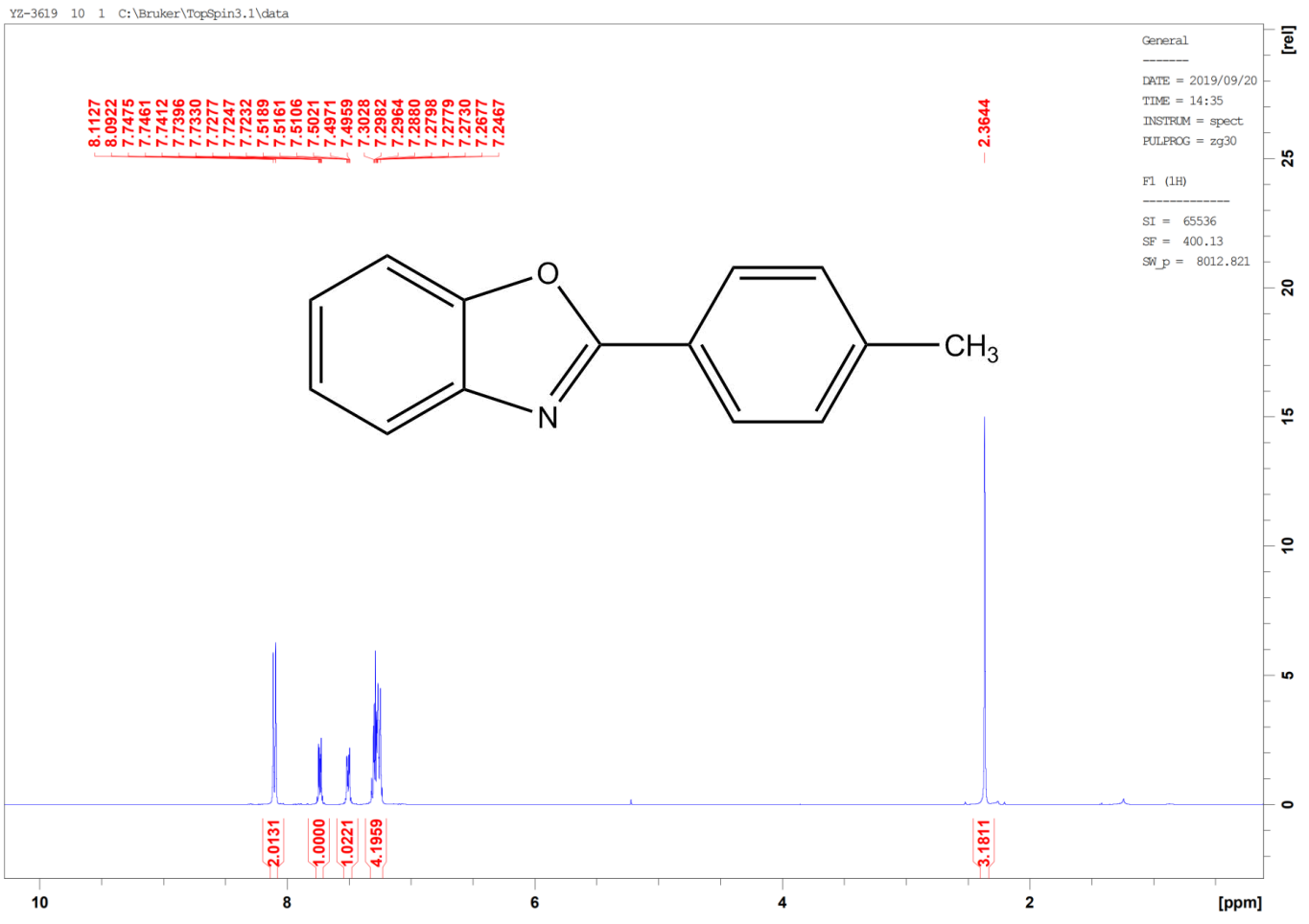
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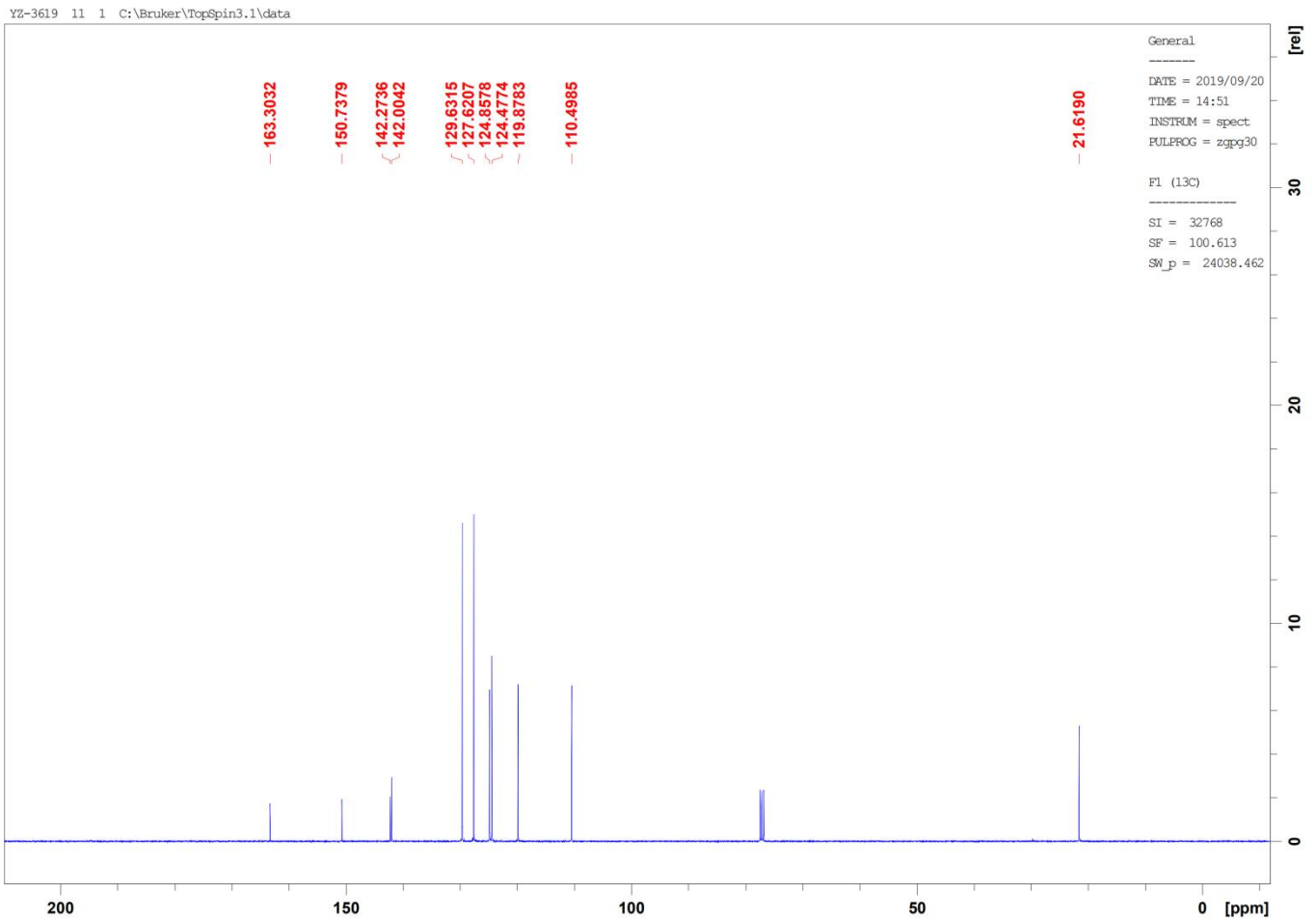
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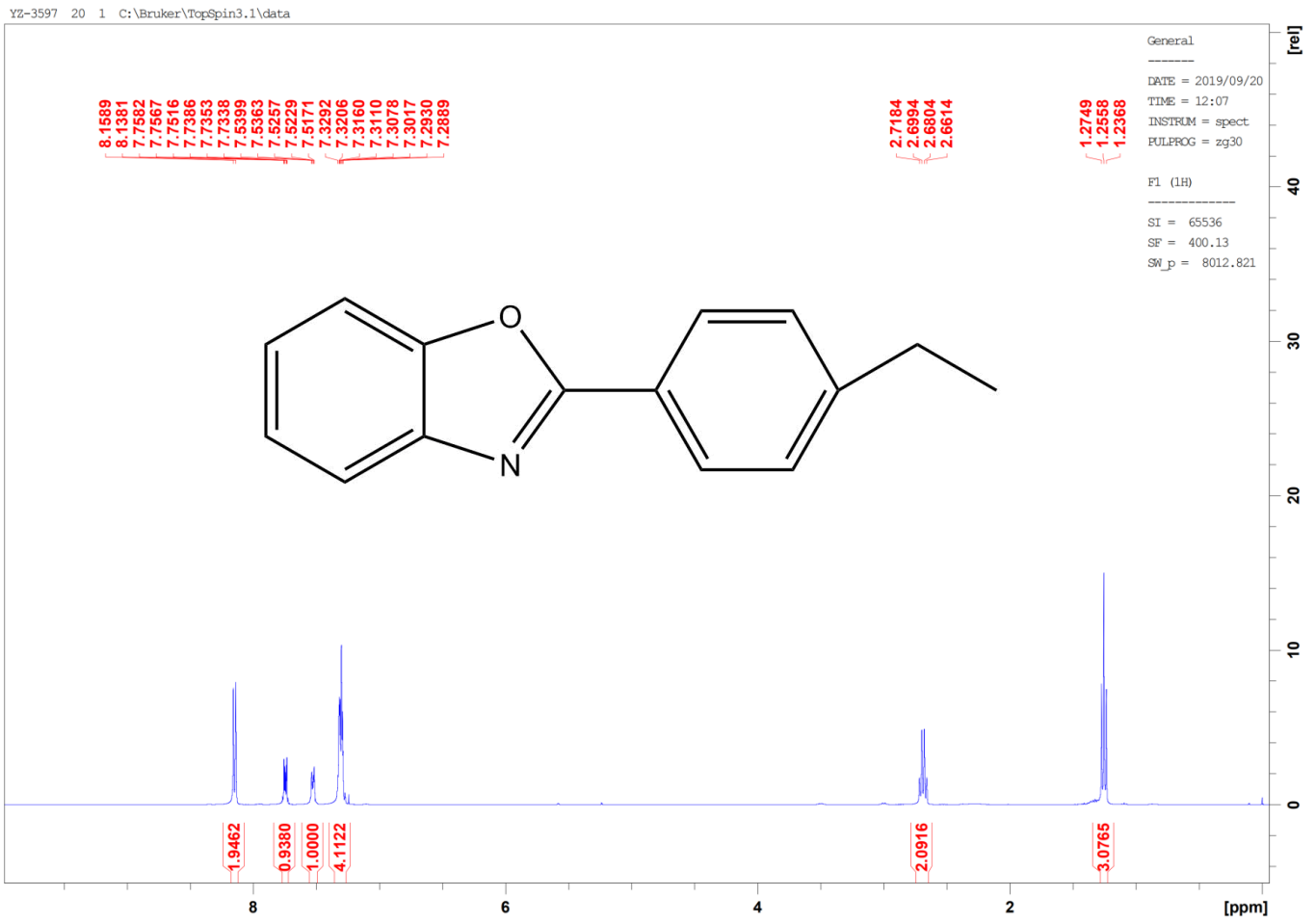
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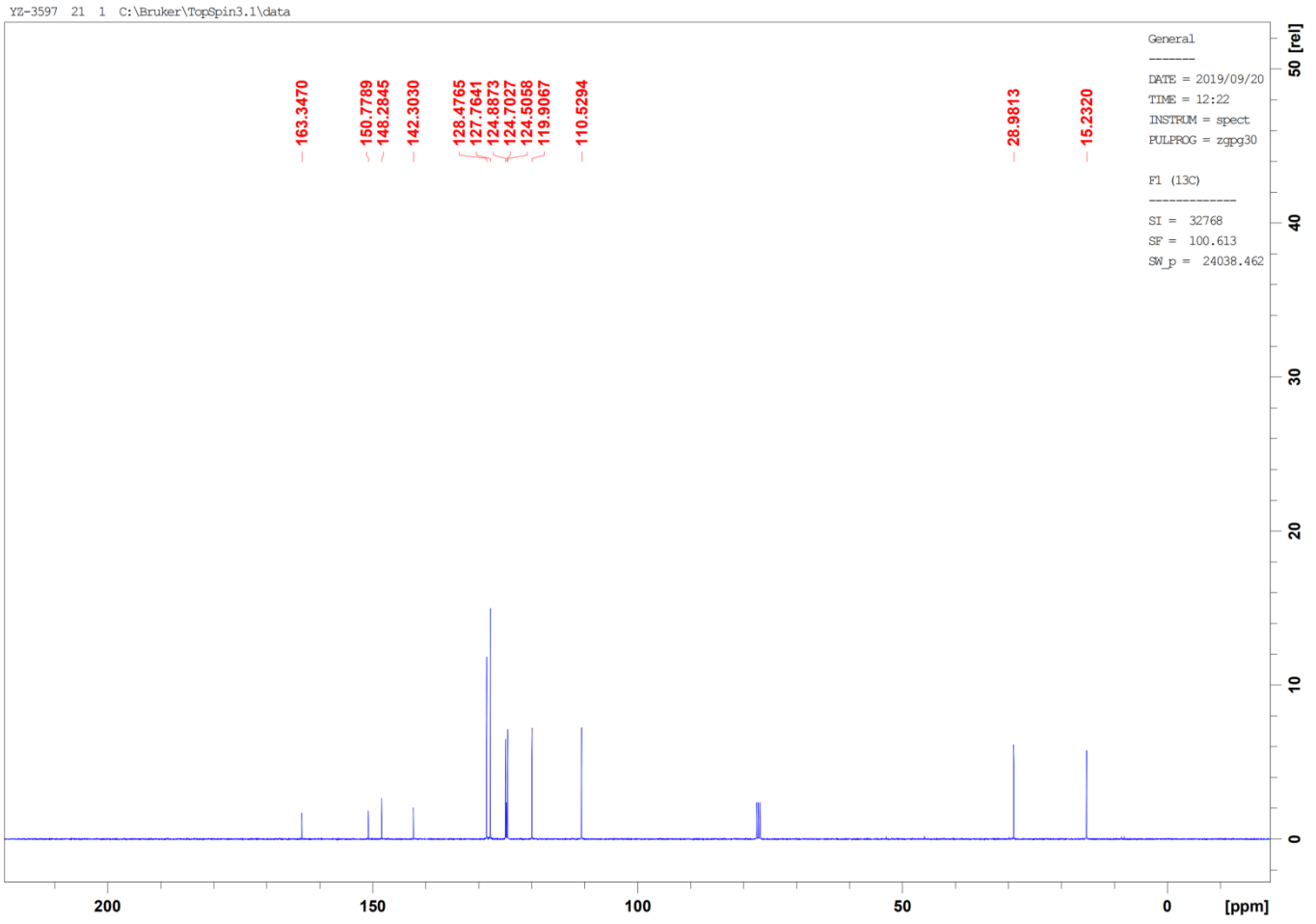
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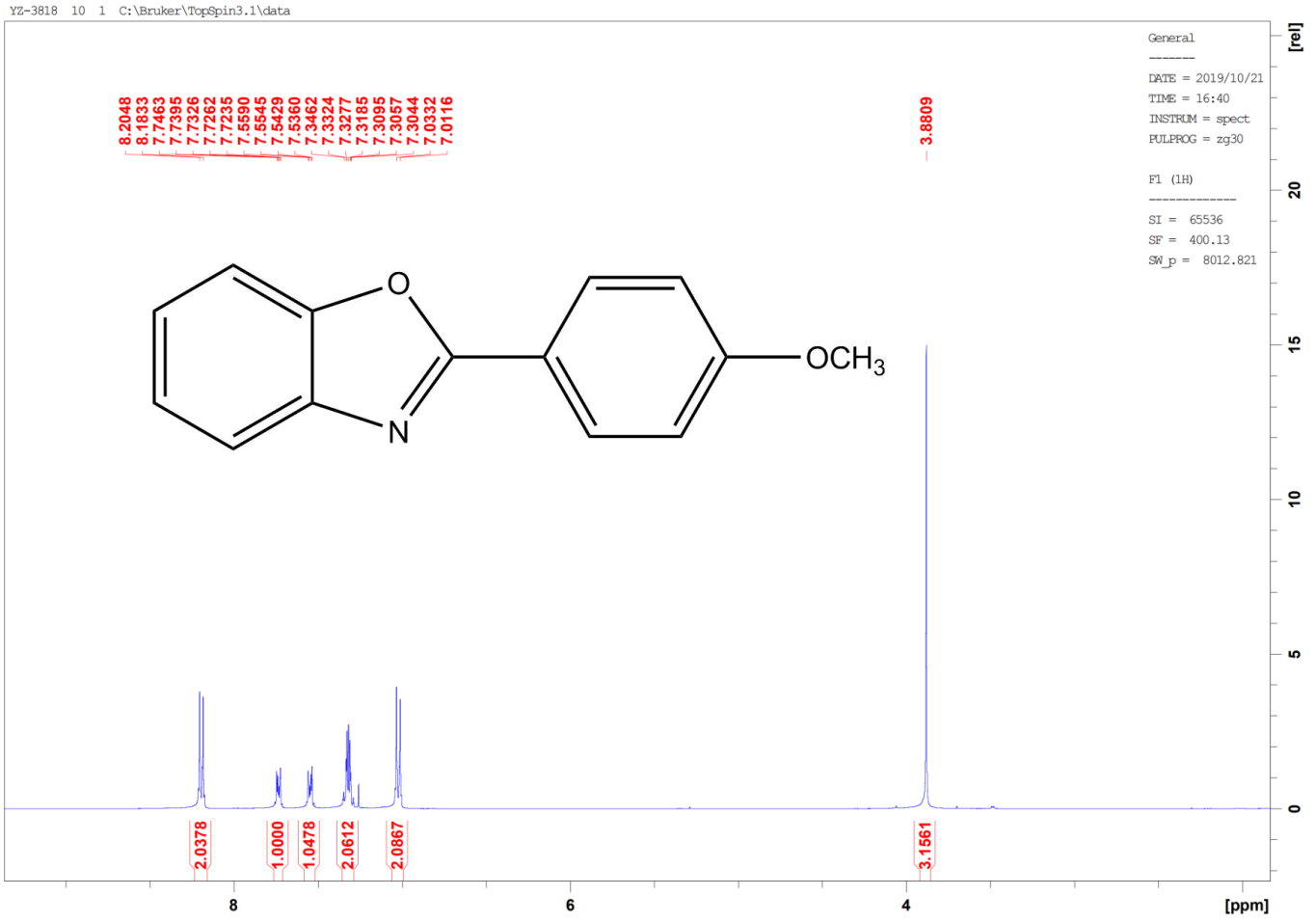
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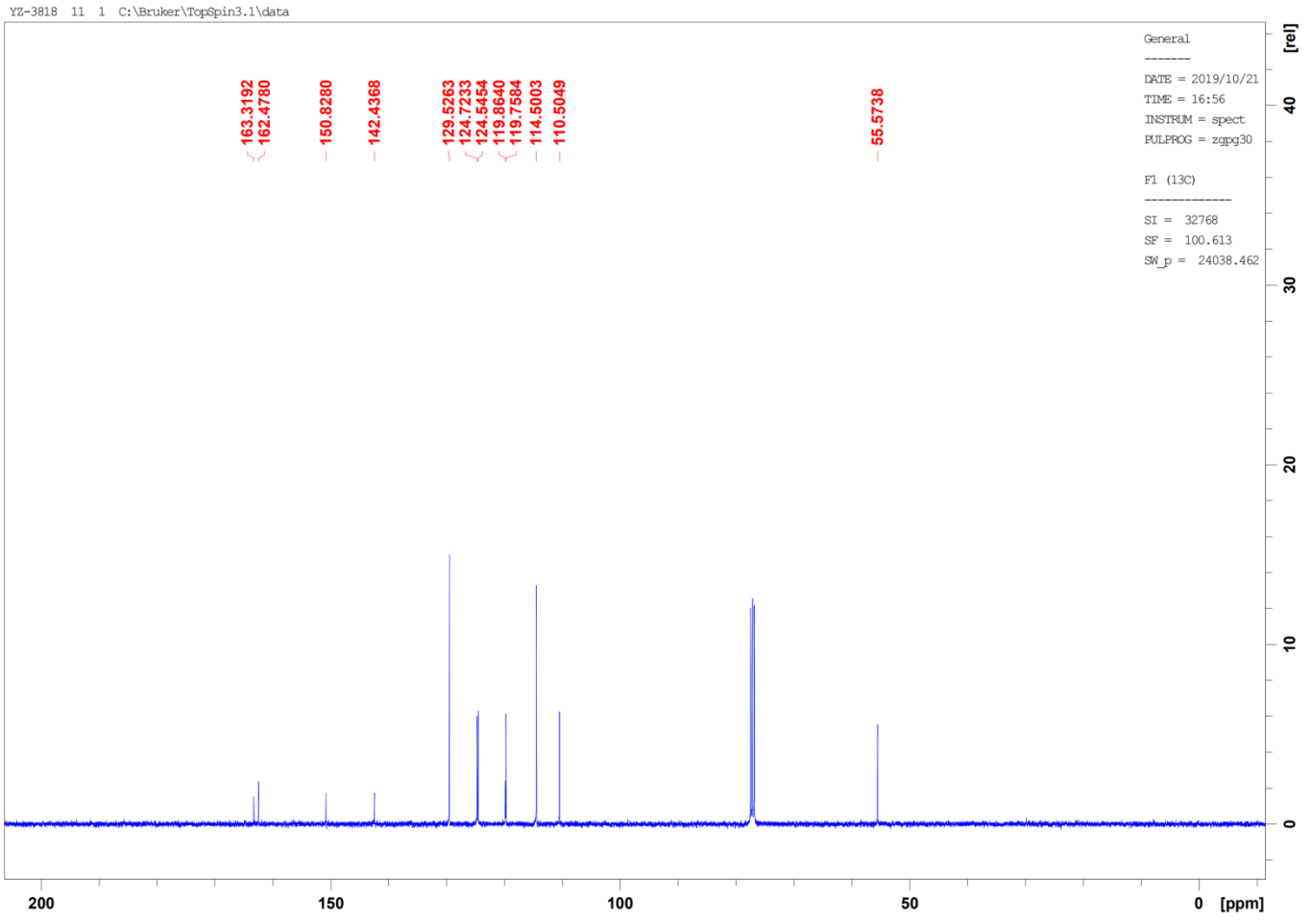
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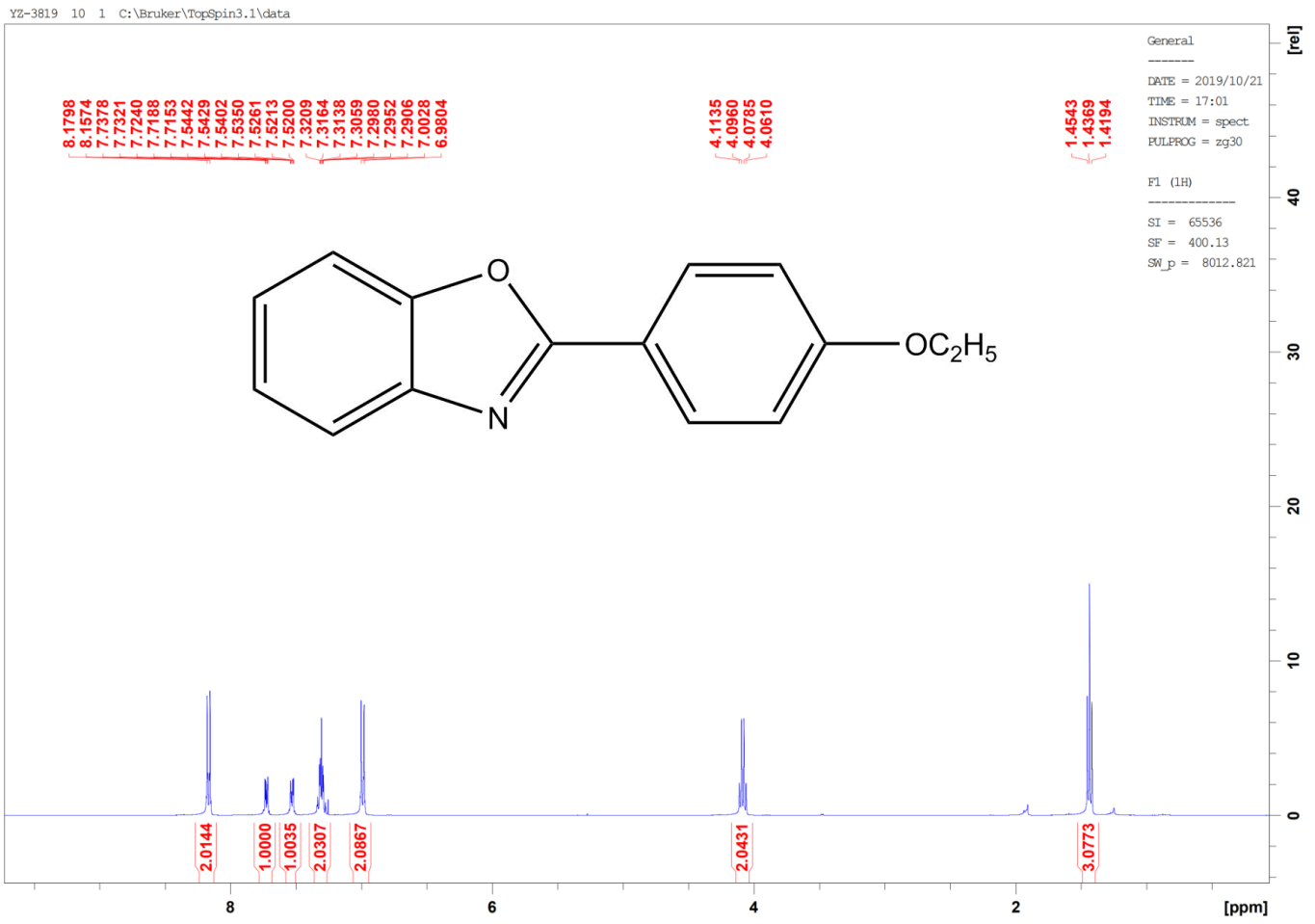
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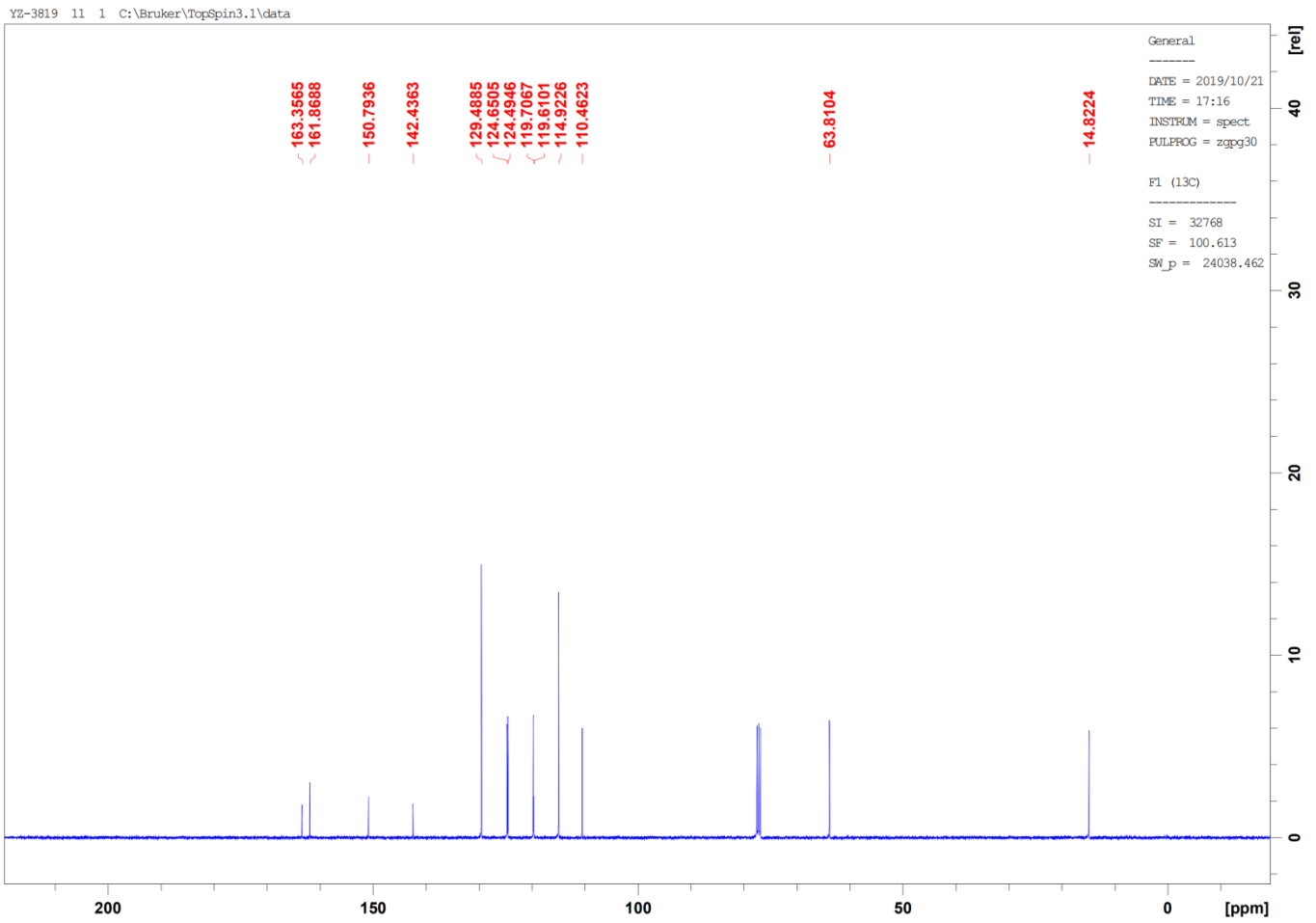
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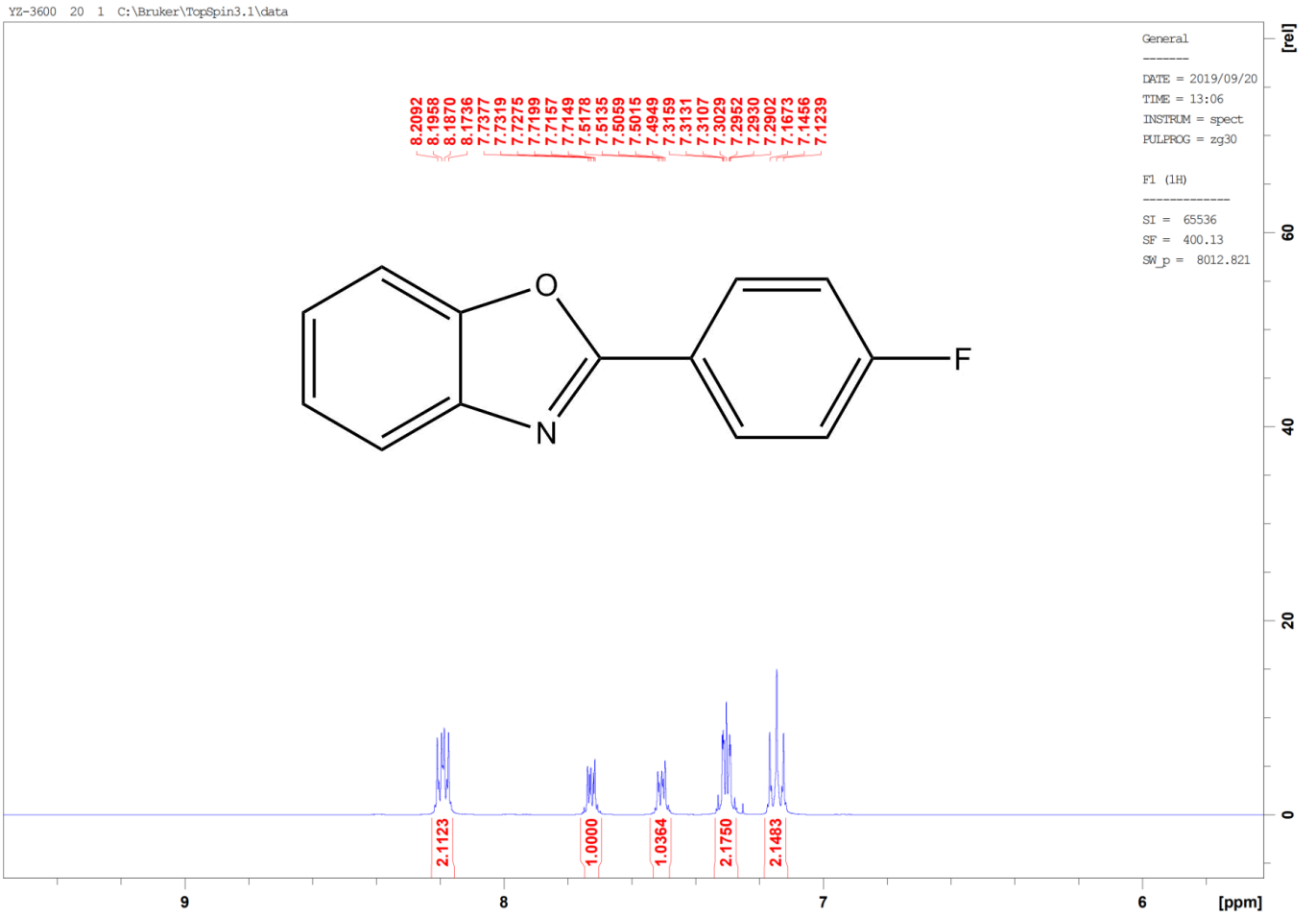
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7.7149
7.5178
7.5135
7.5059
7.5015
7.4949
7.3159
7.3131
7.3107
7.3029
7.2952
7.2930
7.2902
7.1673
7.1456
7.1239
O
N
F
General
DATE = 2019/09/20
TIME = 13:06
INSTRUM = spect
PULPROG = zg30
F1 (1H)
SI = 65536
SF = 400.13
SW_p = 8012.821
2.1123
1.0000
1.0364
2.1750
2.1483
9
8
7
6
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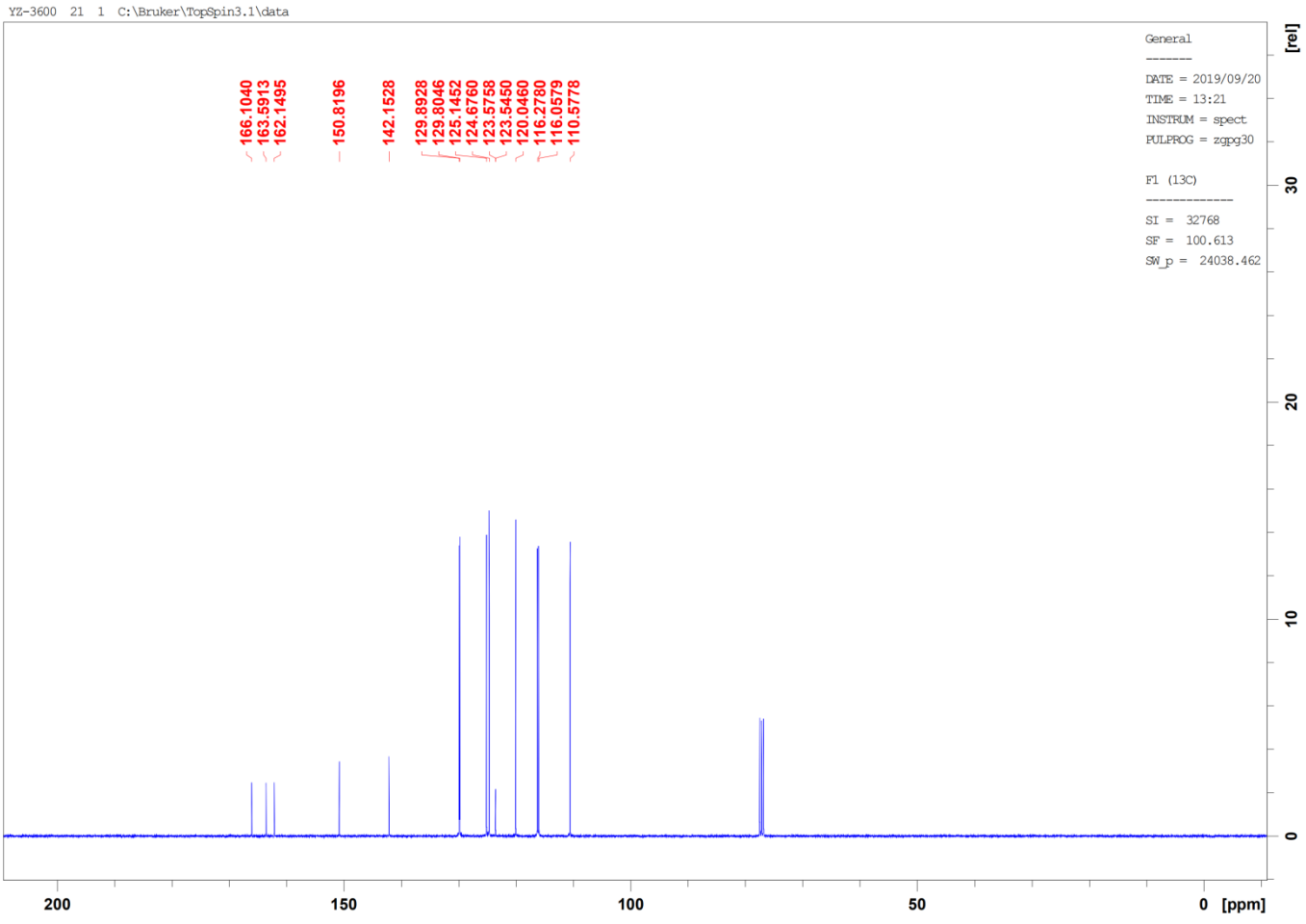
60
40
20
0


YZ-3600 21 1 C:\Bruker\TopSpin3.1\data
166.1040
163.5913
162.1495
150.8196
142.1528
129.8928
129.8046
125.1452
124.6760
123.5758
123.5450
120.0460
116.2780
116.0579
110.5778
General
DATE = 2019/09/20
TIME = 13:21
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 100.613
SW_p = 24038.462
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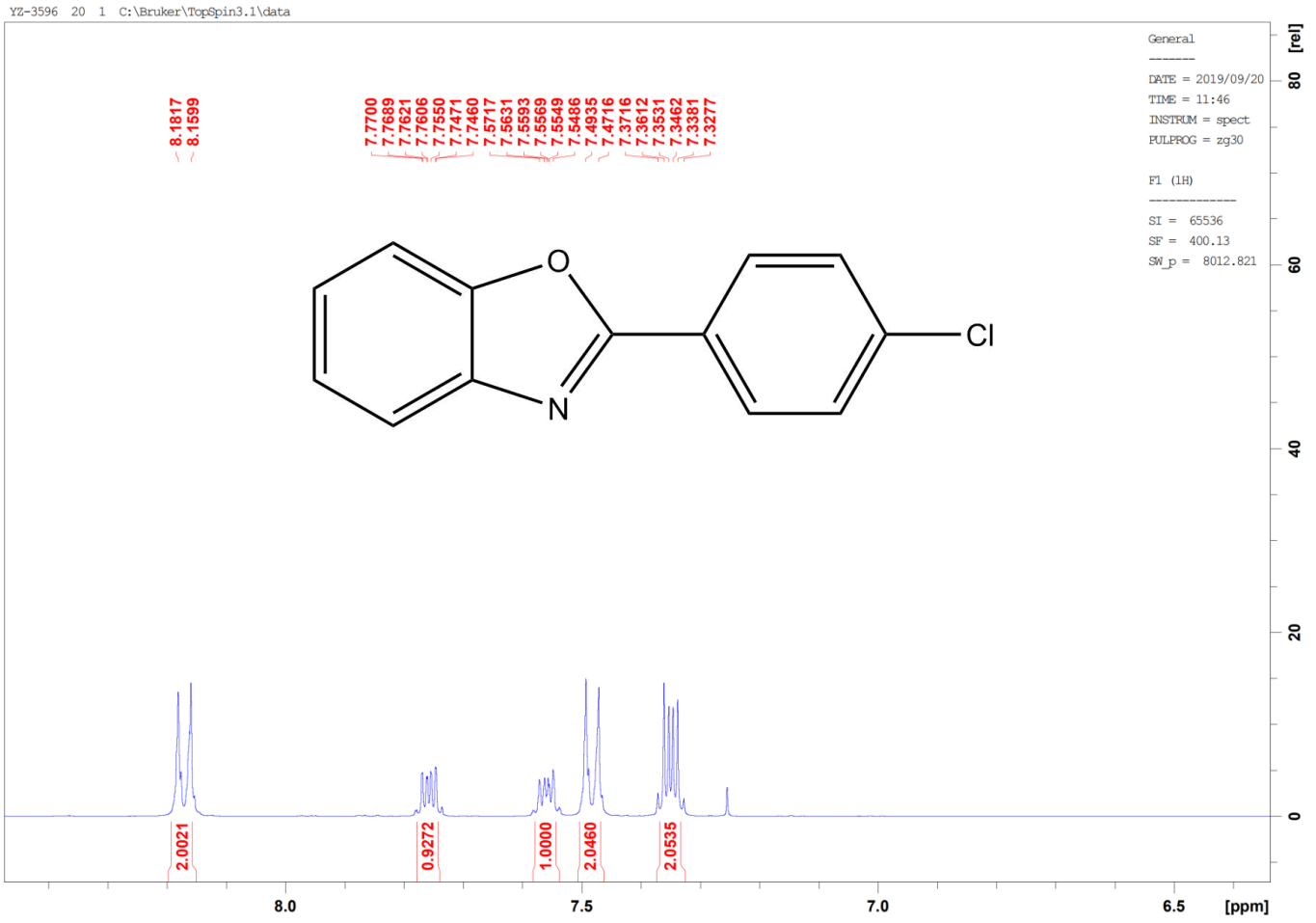
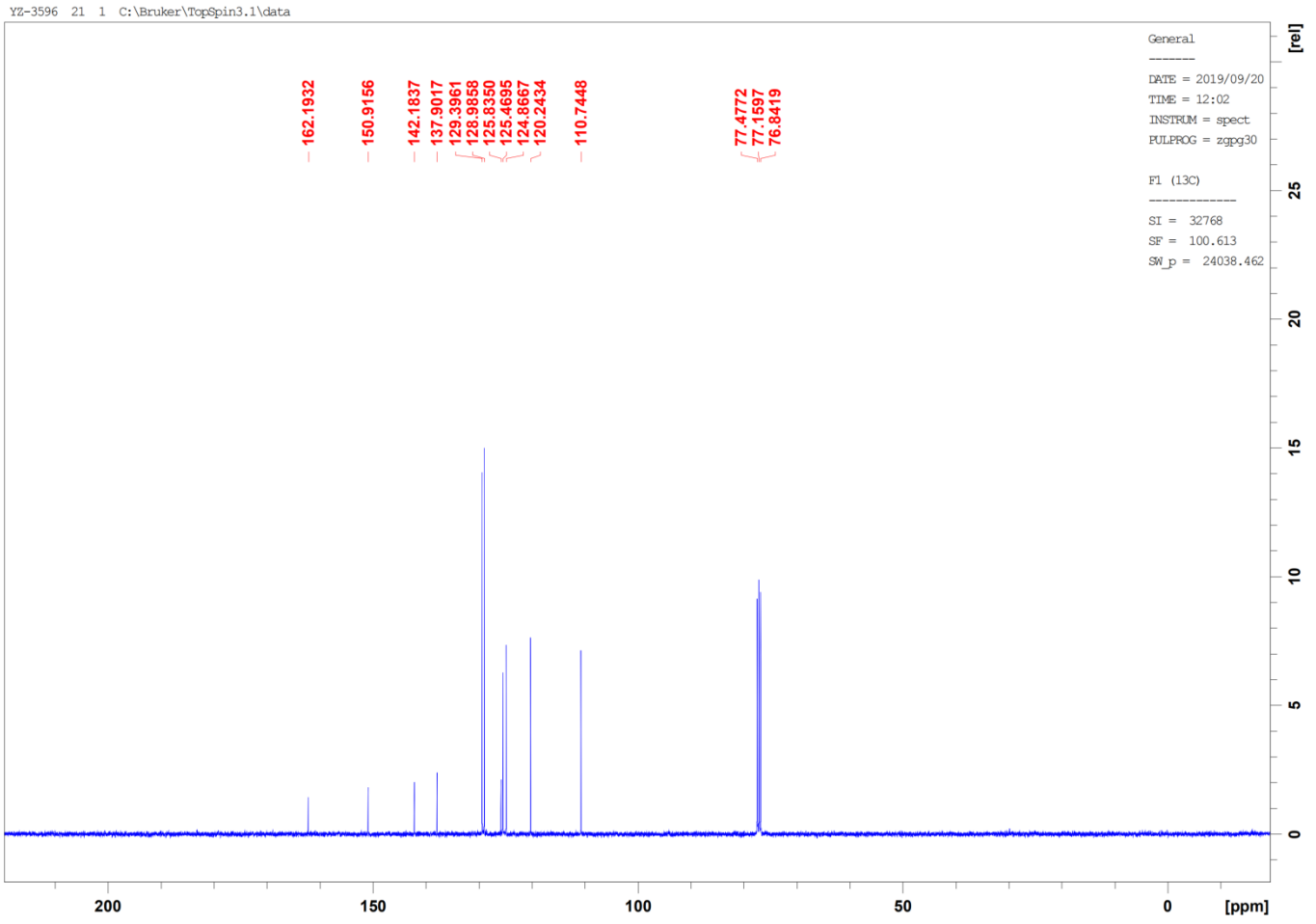
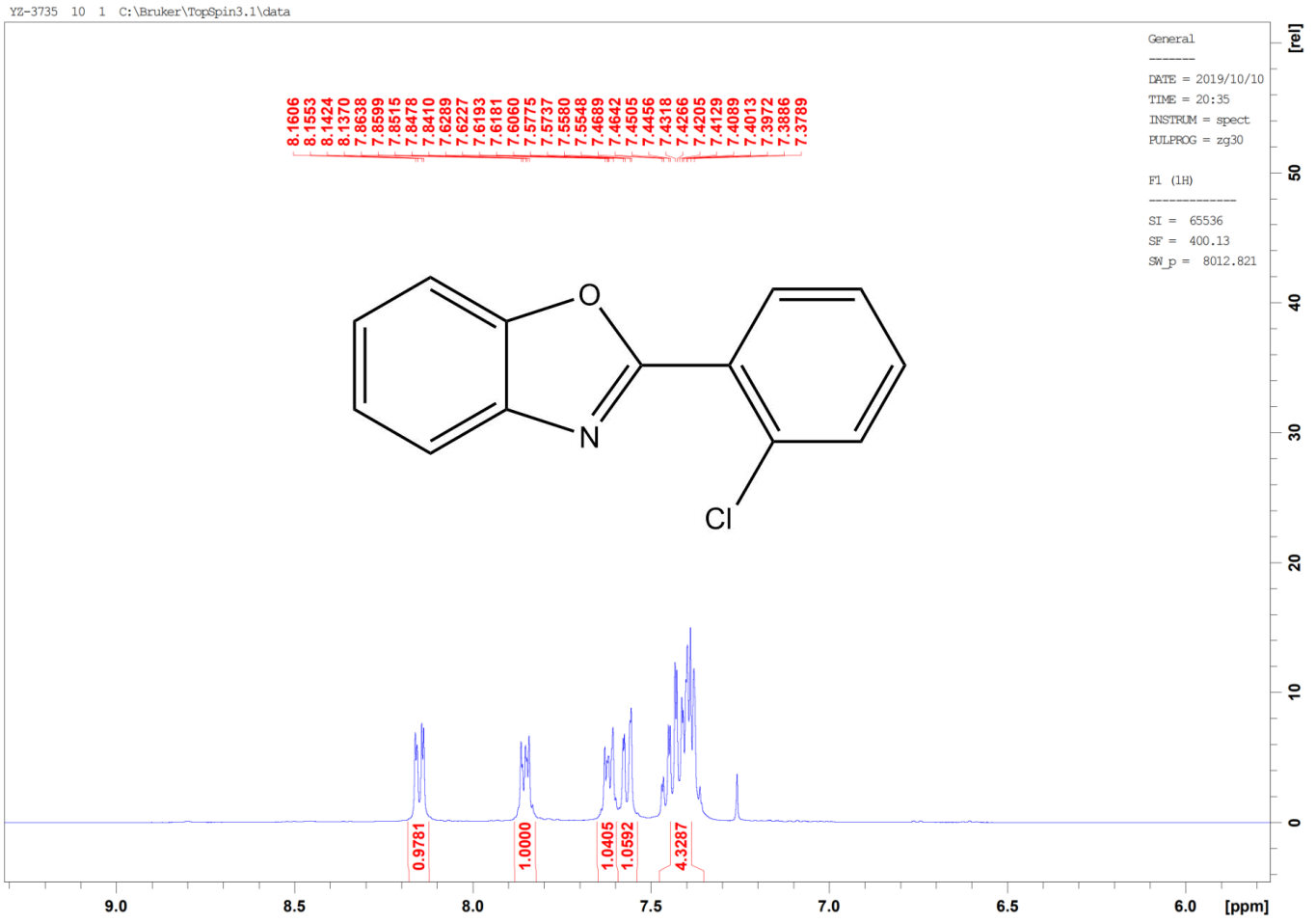
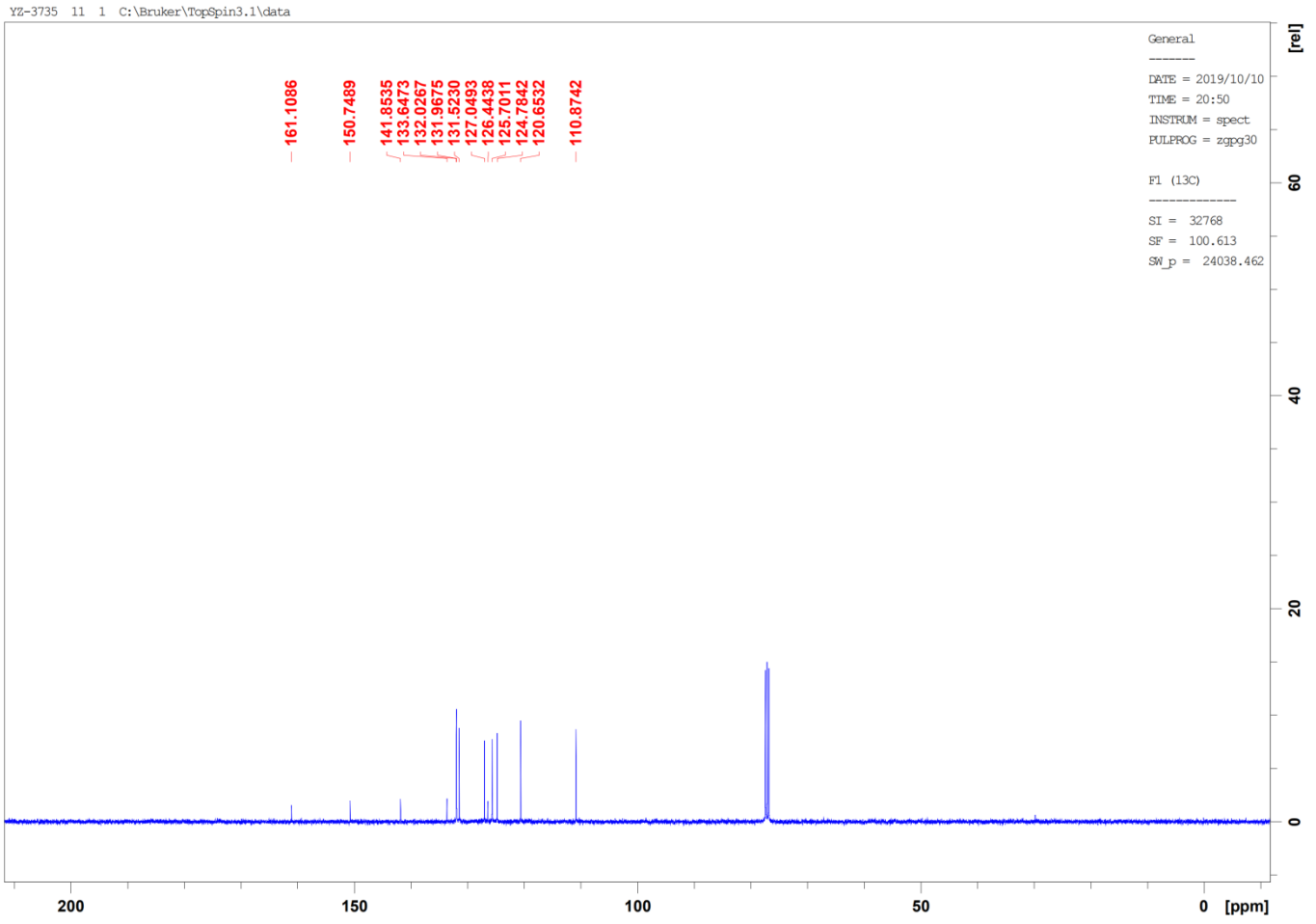
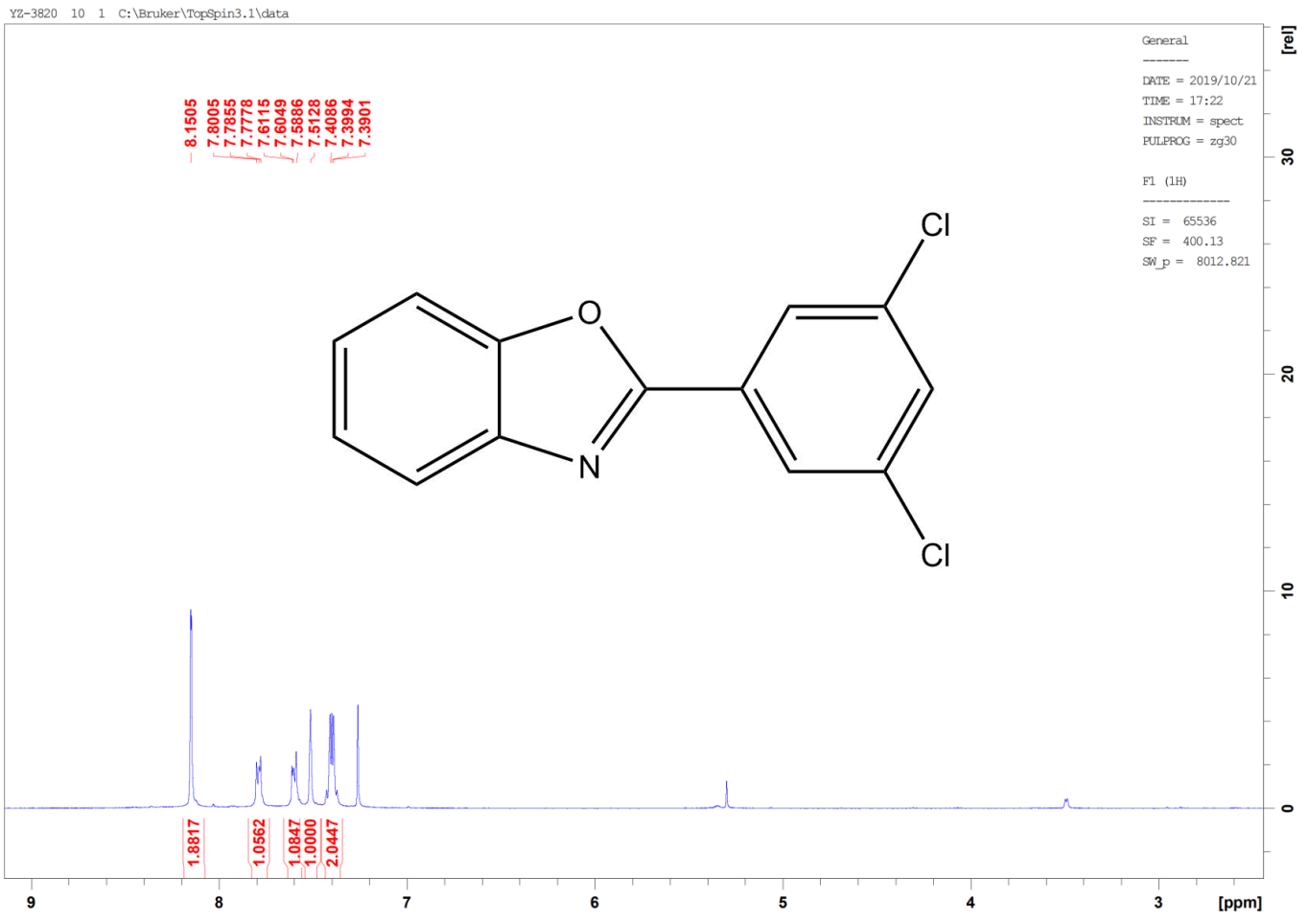
150
100
50
0 [ppm]
[rel]
30
20
10
0

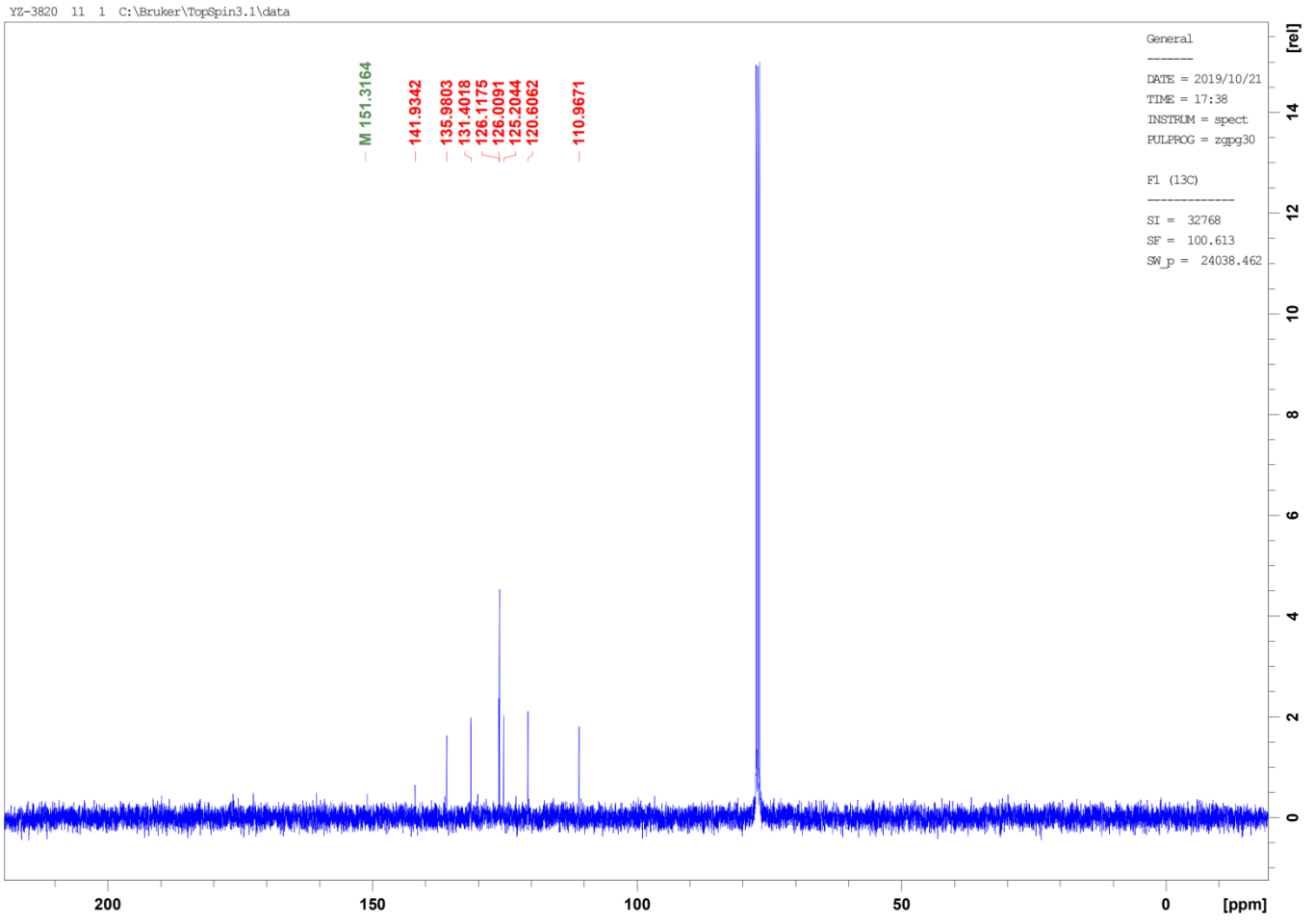

YZ-3596 20 1 C:\Bruker\TopSpin3.1\data
8.1817
8.1599
7.7700
7.7689
7.7621
7.7606
7.7550
7.7471
7.7460
7.5717
7.5631
7.5593
7.5569
7.5549
7.5486
7.4935
7.4716
7.3716
7.3612
7.3531
7.3462
7.3381
7.3277
O
N
Cl
General
DATE = 2019/09/20
TIME = 11:46
INSTRUM = spect
PULPROG = zg30
F1 (1H)
SI = 65536
SF = 400.13
SW_p = 8012.821
2.0021
0.9272
1.0000
2.0460
2.0535
8.0
7.5
7.0
6.5
[ppm]
[rel]

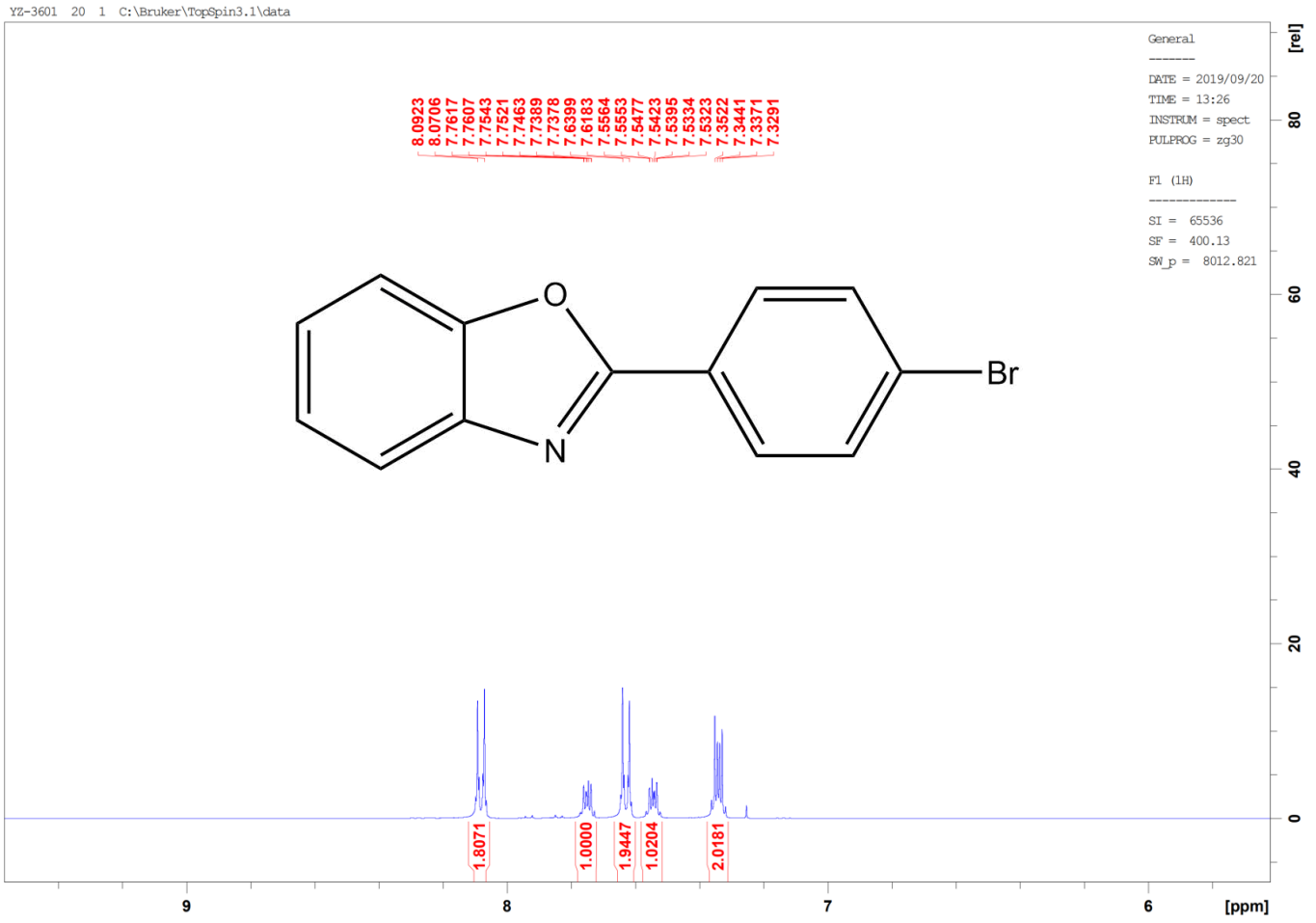

YZ-3596 21 1 C:\Bruker\TopSpin3.1\data
162.1932
150.9156
142.1837
137.9017
129.3961
128.9858
125.8350
125.4695
124.8667
120.2434
110.7448
77.4772
77.1597
76.8419
General
DATE = 2019/09/20
TIME = 12:02
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 100.613
SW_p = 24038.462
200
150
100
50
0
[ppm]
[rel]

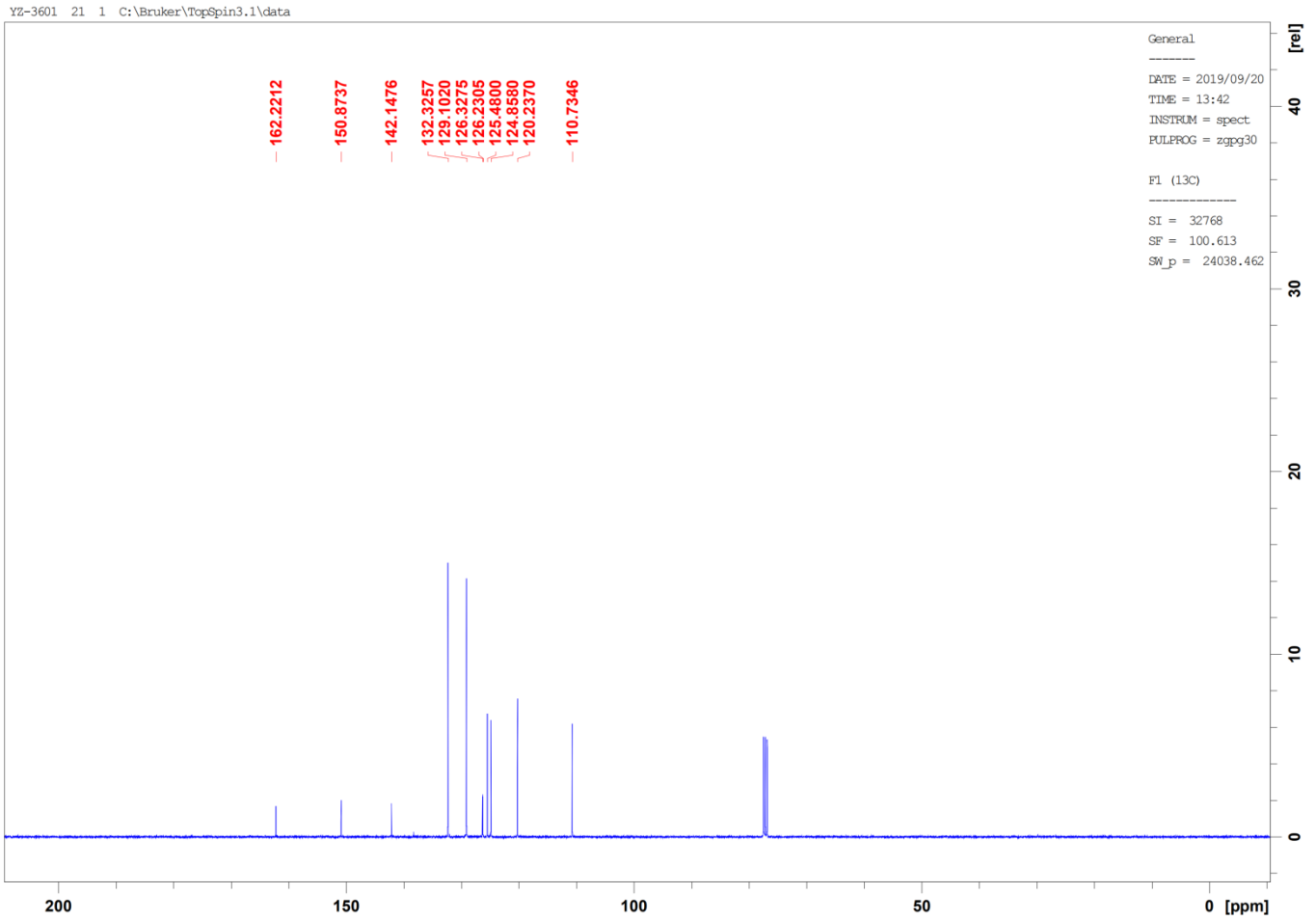

YZ-3735 10 1 C:\Bruker\TopSpin3.1\data
8.1606
8.1553
8.1424
8.1370
7.8638
7.8599
7.8515
7.8478
7.8410
7.6289
7.6227
7.6193
7.6181
7.6060
7.5775
7.5737
7.5580
7.5548
7.4689
7.4642
7.4505
7.4456
7.4318
7.4266
7.4205
7.4129
7.4089
7.4013
7.3972
7.3886
7.3789
O
N
Cl
General
DATE = 2019/10/10
TIME = 20:35
INSTRUM = spect
PULPROG = zg30
F1 (1H)
SI = 65536
SF = 400.13
SW_p = 8012.821
0.9781
1.0000
1.0405
1.0592
4.3287
9.0
8.5
8.0
7.5
7.0
6.5
6.0
[ppm]
[rel]


YZ-3735 11 1 C:\Bruker\TopSpin3.1\data
161.1086
150.7489
141.8535
133.6473
132.0267
131.9675
131.5230
127.0493
126.4438
125.7011
124.7842
120.6532
110.8742
General
DATE = 2019/10/10
TIME = 20:50
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 100.613
SW_p = 24038.462
200
150
100
50
0
[ppm]
[rel]


YZ-3820 10 1 C:\Bruker\TopSpin3.1\data
8.1505
7.8005
7.7855
7.7778
7.6115
7.6049
7.5886
7.5128
7.4086
7.3994
7.3901
General
DATE = 2019/10/21
TIME = 17:22
INSTRUM = spect
PULPROG = zg30
F1 (1H)
SI = 65536
SF = 400.13
SW_p = 8012.821
Cl
O
N
Cl
1.8817
1.0562
1.0847
1.0000
2.0447
[rel]
[ppm]


YZ-3820 11 1 C:\Bruker\TopSpin3.1\data
M 151.3164
141.9342
135.9803
131.4018
126.1175
126.0091
125.2044
120.6062
110.9671
General
DATE = 2019/10/21
TIME = 17:38
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 100.613
SW_p = 24038.462
[rel]
[ppm]


YZ-3601 20 1 C:\Bruker\TopSpin3.1\data
8.0923
8.0706
7.7617
7.7607
7.7543
7.7521
7.7463
7.7389
7.7378
7.6399
7.6183
7.5564
7.5553
7.5477
7.5423
7.5395
7.5334
7.5323
7.3522
7.3441
7.3371
7.3291
O
N
Br
1.8071
1.0000
1.9447
1.0204
2.0181
General
DATE = 2019/09/20
TIME = 13:26
INSTRUM = spect
PULPROG = zg30
F1 (1H)
SI = 65536
SF = 400.13
SW_p = 8012.821
[rel]
[ppm]


YZ-3601 21 1 C:\Bruker\TopSpin3.1\data
162.2212
150.8737
142.1476
132.3257
129.1020
126.3275
126.2305
125.4800
124.8580
120.2370
110.7346
General
DATE = 2019/09/20
TIME = 13:42
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 100.613
SW_p = 24038.462
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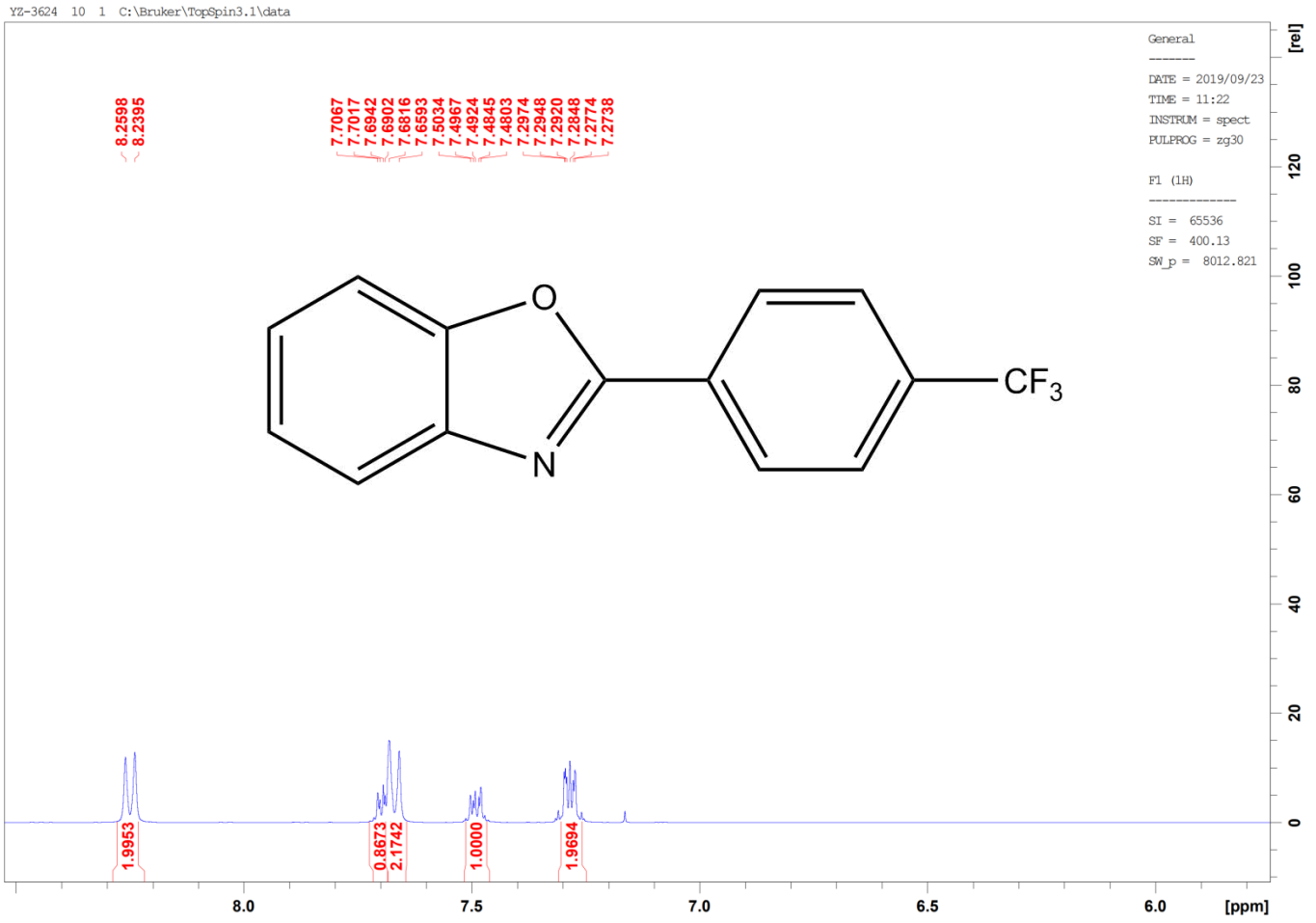
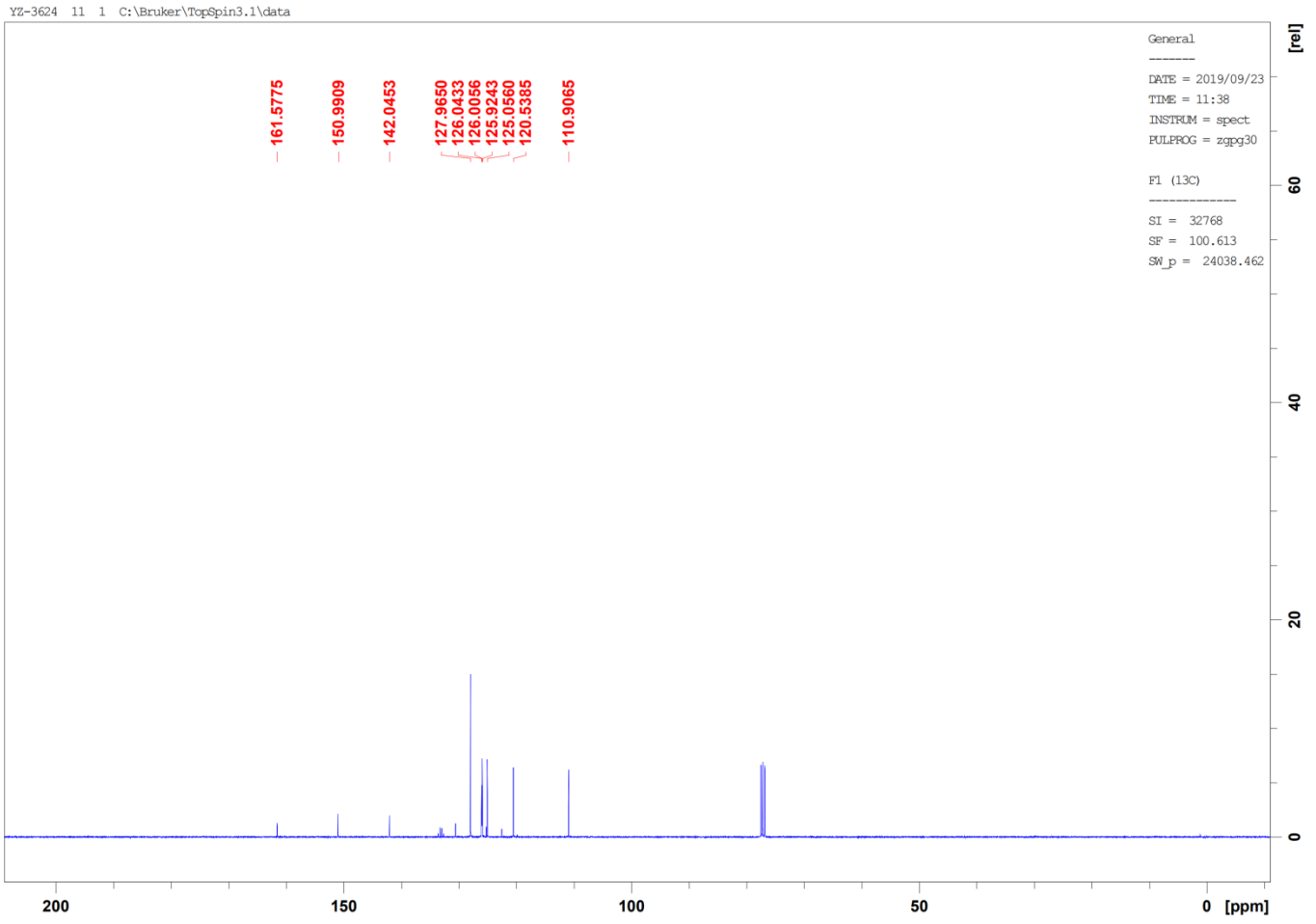
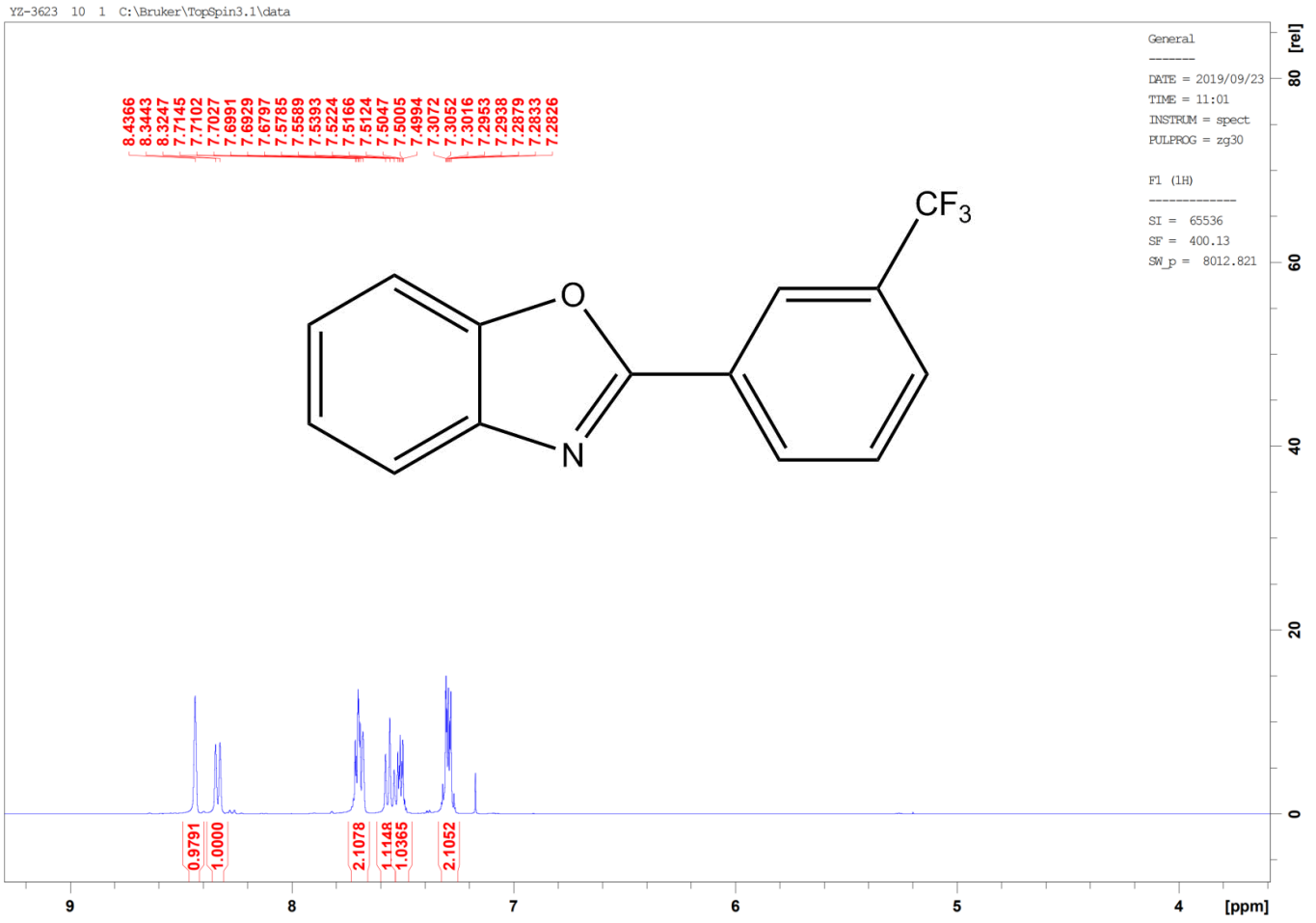
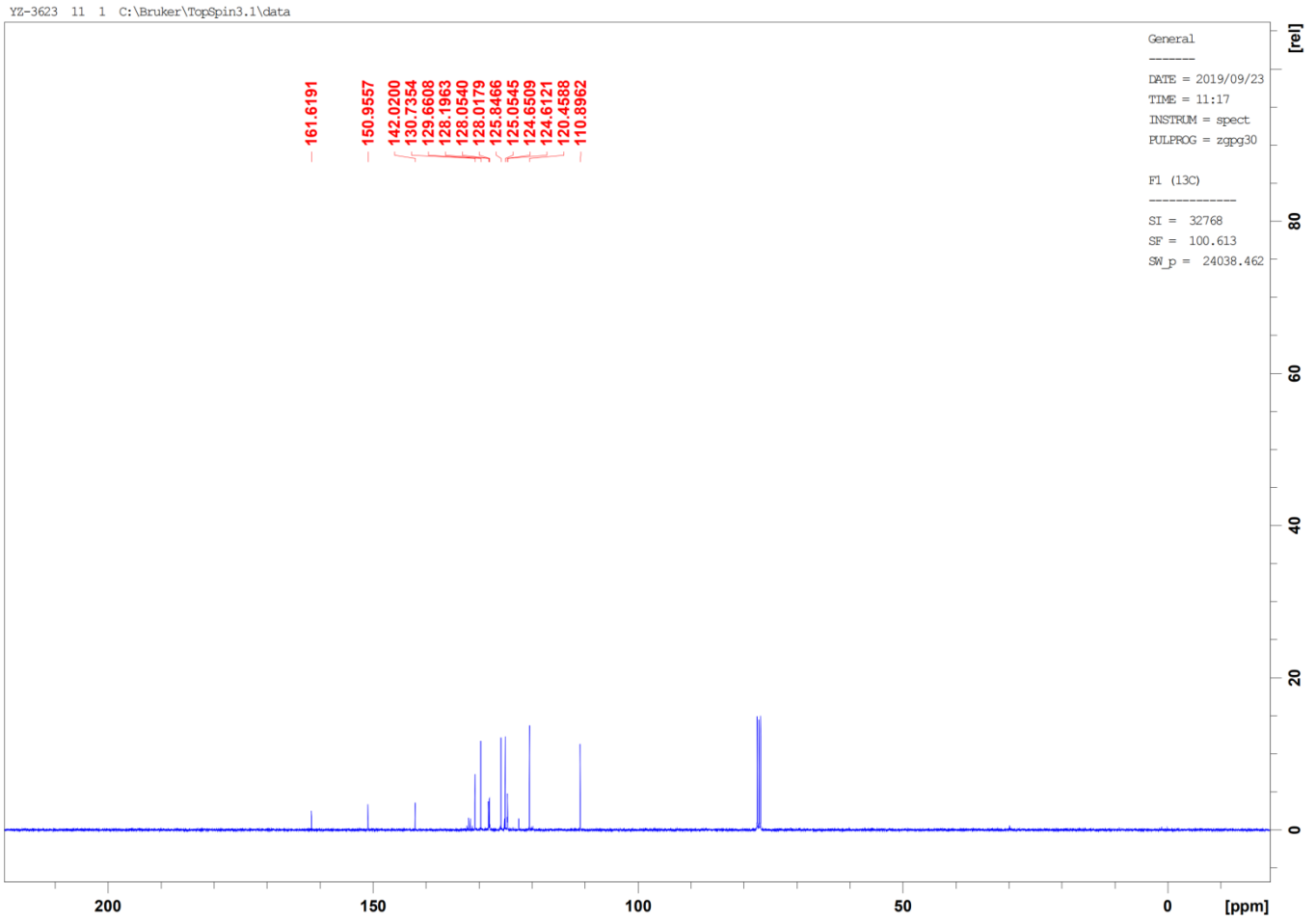
[ppm]


YZ-3624 10 1 C:\Bruker\TopSpin3.1\data
8.2598
8.2395
7.7067
7.7017
7.6942
7.6902
7.6816
7.6593
7.5034
7.4967
7.4924
7.4845
7.4803
7.2974
7.2948
7.2920
7.2848
7.2774
7.2738
O
N
CF3
1.9953
0.8673
2.1742
1.0000
1.9694
8.0
7.5
7.0
6.5
6.0
[ppm]
[rel]
General
DATE = 2019/09/23
TIME = 11:22
INSTRUM = spect
PULPROG = zg30
F1 (1H)
SI = 65536
SF = 400.13
SW_p = 8012.821


YZ-3624 11 1 C:\Bruker\TopSpin3.1\data
161.5775
150.9909
142.0453
127.9650
126.0433
126.0056
125.9243
125.0560
120.5385
110.9065
200
150
100
50
0
[ppm]
[rel]
General
DATE = 2019/09/23
TIME = 11:38
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 100.613
SW_p = 24038.462


YZ-3623 10 1 C:\Bruker\TopSpin3.1\data
8.4366
8.3443
8.3247
7.7145
7.7102
7.7027
7.6991
7.6929
7.6797
7.5785
7.5589
7.5393
7.5224
7.5166
7.5124
7.5047
7.5005
7.4994
7.3072
7.3052
7.3016
7.2953
7.2938
7.2879
7.2833
7.2826
CF3
O
N
0.9791
1.0000
2.1078
1.1148
1.0365
2.1052
General
DATE = 2019/09/23
TIME = 11:01
INSTRUM = spect
PULPROG = zg30
F1 (1H)
SI = 65536
SF = 400.13
SW_p = 8012.821
[rel]
[ppm]


YZ-3623 11 1 C:\Bruker\TopSpin3.1\data
161.6191
150.9557
142.0200
130.7354
129.6608
128.1963
128.0540
128.0179
125.8466
125.0545
124.6509
124.6121
120.4588
110.8962
General
DATE = 2019/09/23
TIME = 11:17
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 100.613
SW_p = 24038.462
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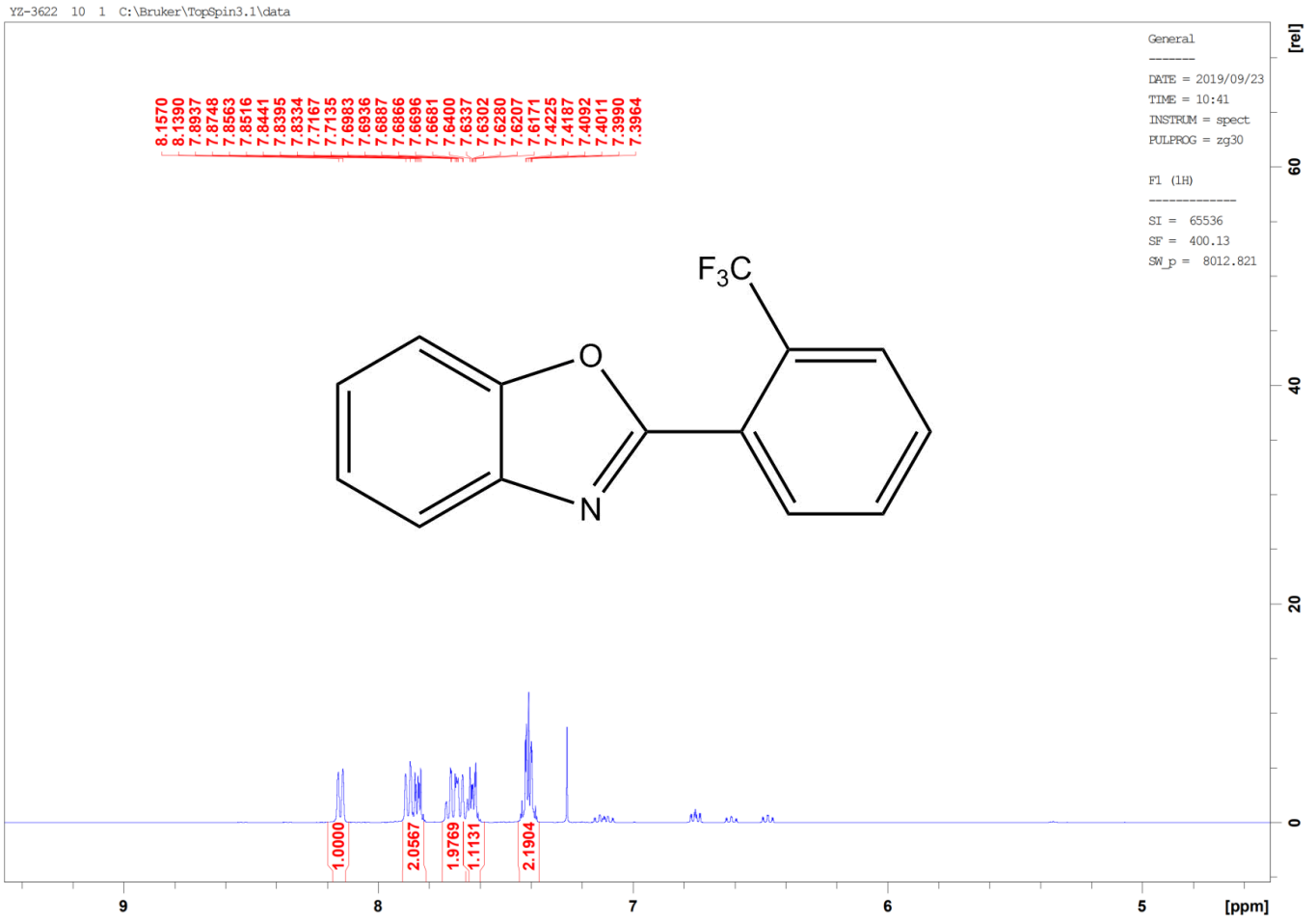
YZ-3622 10 1 C:\Bruker\TopSpin3.1\data
8.1570
8.1390
7.8937
7.8748
7.8563
7.8516
7.8441
7.8395
7.8334
7.7167
7.7135
7.6983
7.6936
7.6887
7.6866
7.6696
7.6681
7.6400
7.6337
7.6302
7.6280
7.6207
7.6171
7.4225
7.4187
7.4092
7.4011
7.3990
7.3964
F3C
O
N
General
DATE = 2019/09/23
TIME = 10:41
INSTRUM = spect
PULPROG = zg30
F1 (1H)
SI = 65536
SF = 400.13
SW_p = 8012.821
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2.0567
1.9769
1.1131
2.1904
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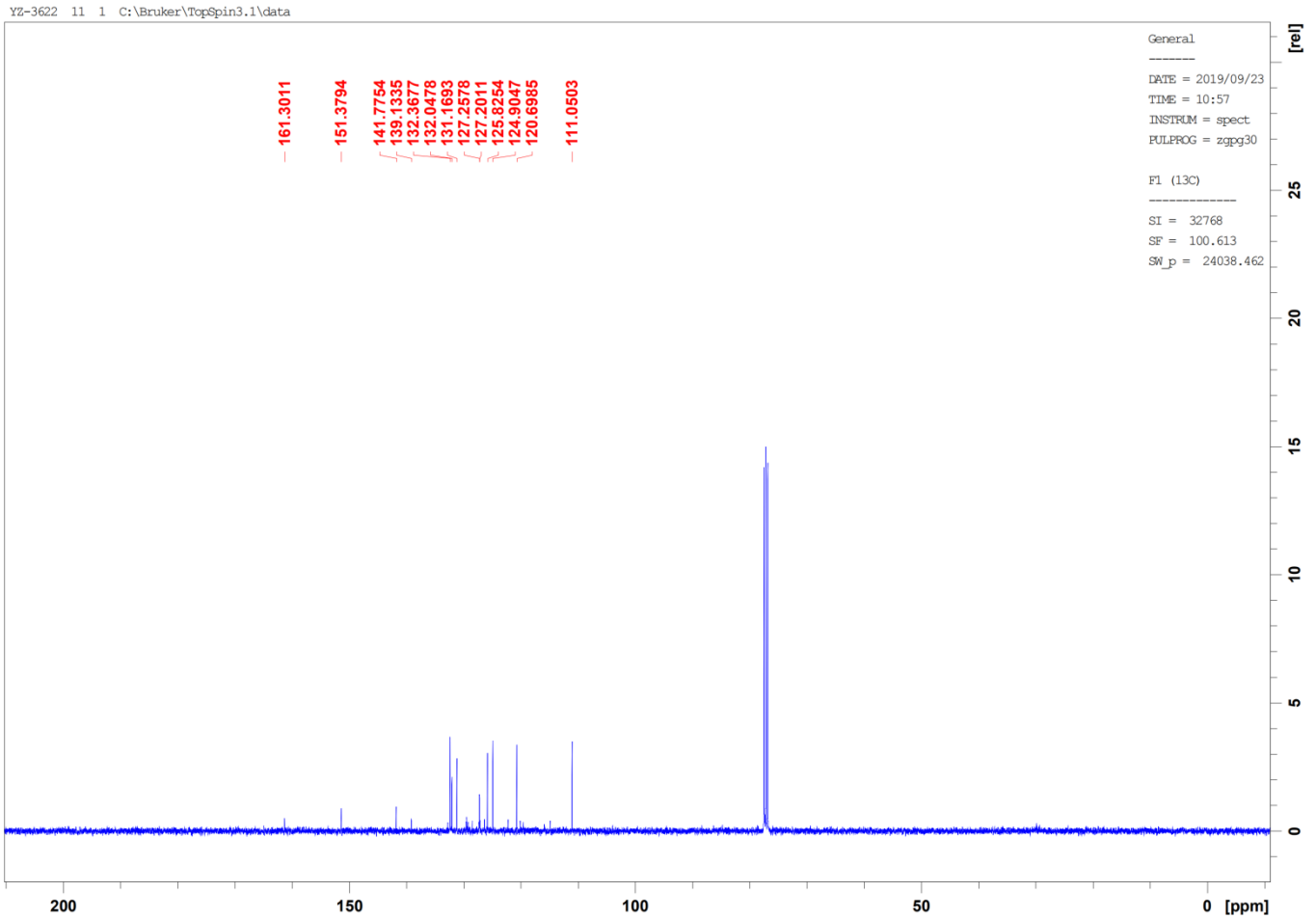
YZ-3622 11 1 C:\Bruker\TopSpin3.1\data
161.3011
151.3794
141.7754
139.1335
132.3677
132.0478
131.1693
127.2578
127.2011
125.8254
124.9047
120.6985
111.0503
General
DATE = 2019/09/23
TIME = 10:57
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 100.613
SW_p = 24038.462
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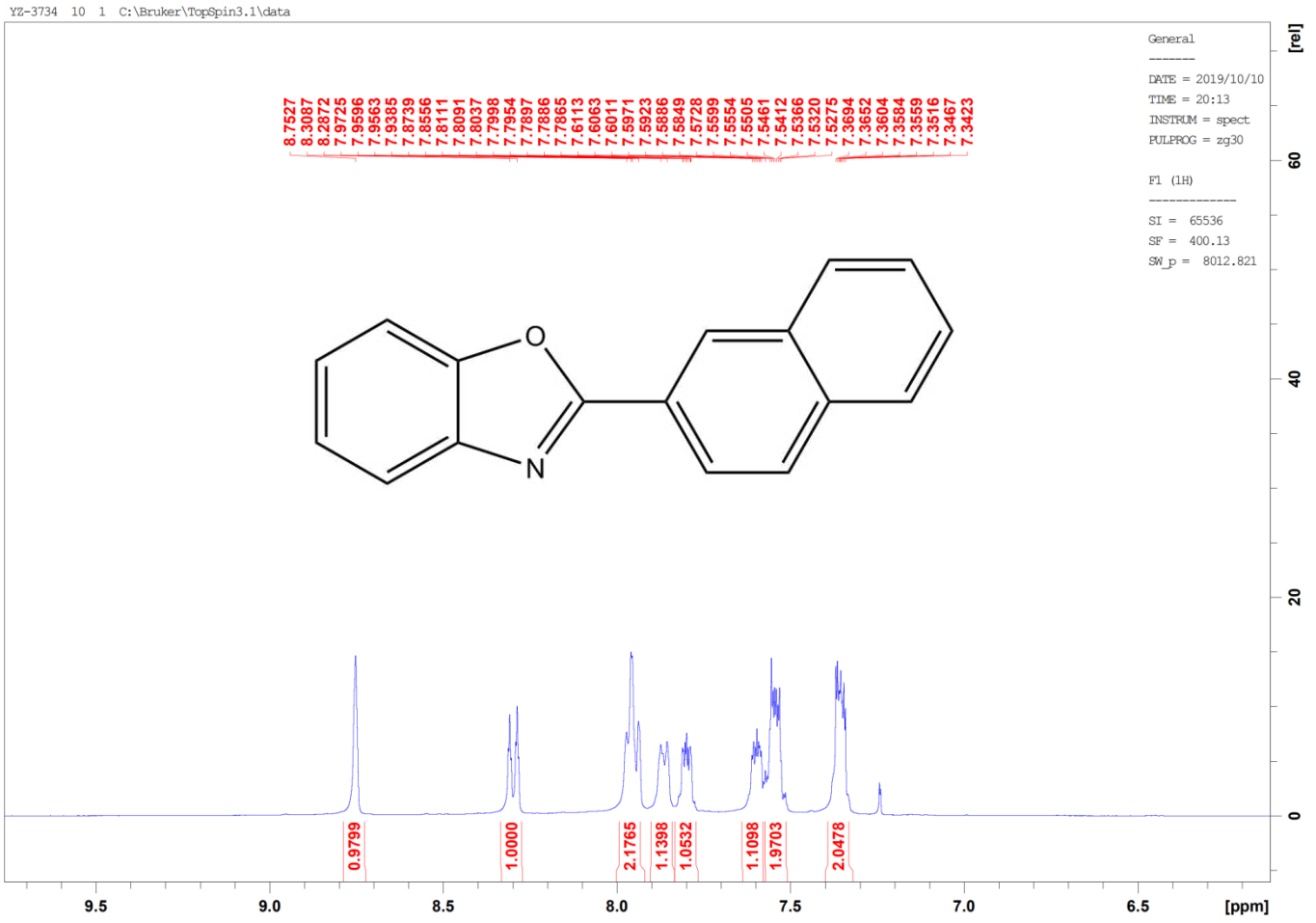
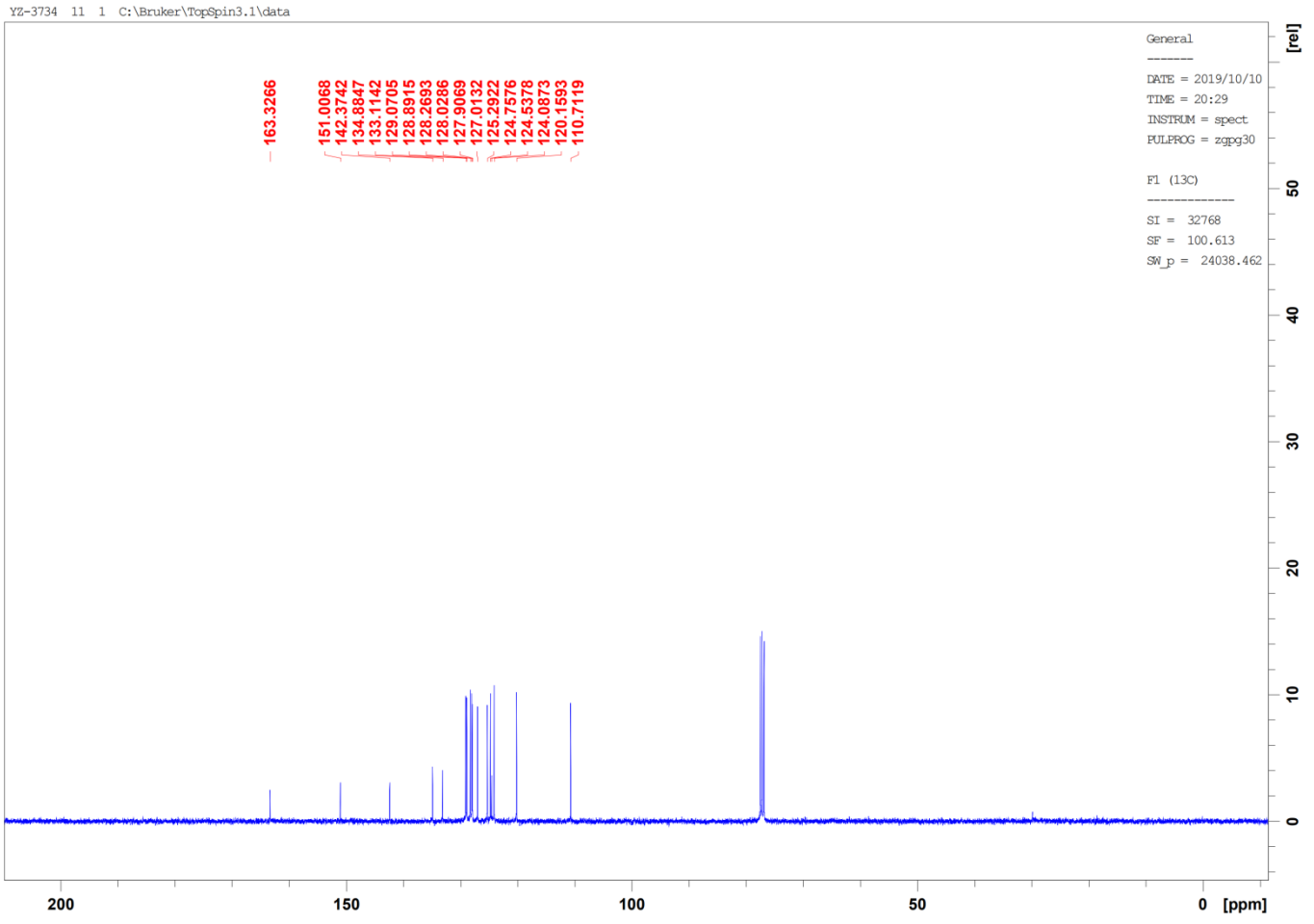
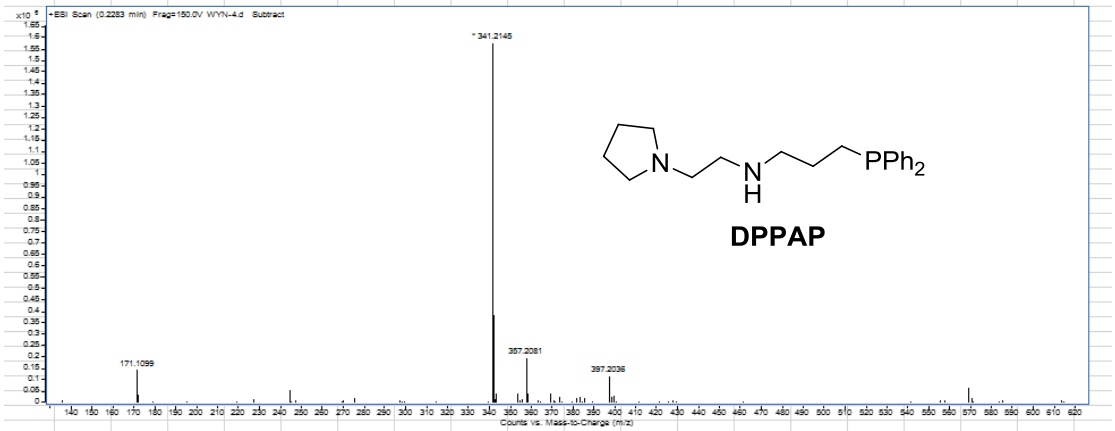

YZ-3734 10 1 C:\Bruker\TopSpin3.1\data
8.7527
8.3087
8.2872
7.9725
7.9596
7.9563
7.9385
7.8739
7.8556
7.8111
7.8091
7.8037
7.7998
7.7954
7.7897
7.7897
7.7886
7.7865
7.6113
7.6063
7.6011
7.5971
7.5923
7.5886
7.5849
7.5728
7.5599
7.5554
7.5505
7.5461
7.5412
7.5366
7.5320
7.5275
7.3694
7.3652
7.3604
7.3584
7.3559
7.3516
7.3467
7.3423
O
N
0.9799
1.0000
2.1765
1.1398
1.0532
1.1098
1.9703
2.0478
9.5
9.0
8.5
8.0
7.5
7.0
6.5
[ppm]
[rel]
General
DATE = 2019/10/10
TIME = 20:13
INSTRUM = spect
PULPROG = zg30
F1 (1H)
SI = 65536
SF = 400.13
SW_p = 8012.821


YZ-3734 11 1 C:\Bruker\TopSpin3.1\data
163.3266
151.0068
142.3742
134.8847
133.1142
129.0705
128.8915
128.2693
128.0286
127.9069
127.0132
125.2922
124.7576
124.5378
124.0873
120.1593
110.7119
200
150
100
50
0
[ppm]
[rel]
General
DATE = 2019/10/10
TIME = 20:29
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 100.613
SW_p = 24038.462

3. HRMS spectra



MS Formula Results: + Scan (0.2283 min) Sub (WYN-4.d)

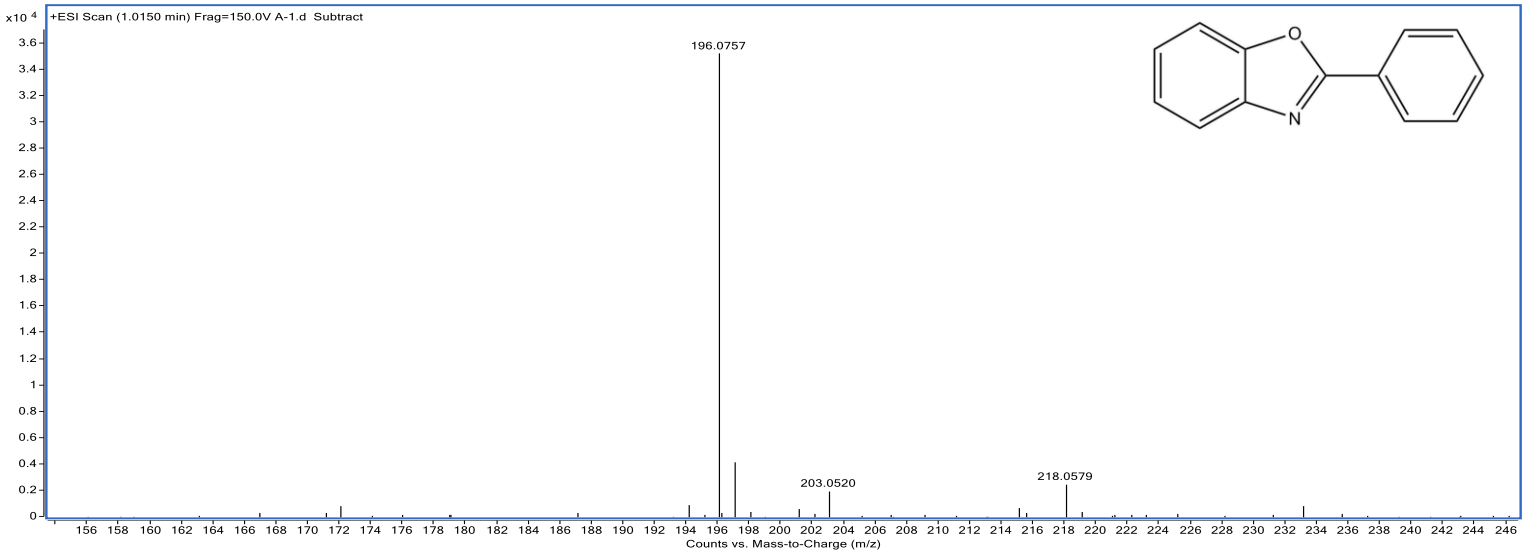
m/z	Ion	Formula	Abundance
341.2145	(M+H)+	C21 H30 N2 P	1576775

Best	Formula (M)	Ion Formula	Score	Cross Score	Calc m/z	Diff (ppm)	Mass Match	Abund Match	Spacing Match
✓	C21 H29 N2 P	C21 H30 N2 P	97.22		341.2141	-0.98	99.28	99.44	90.46

MS Formula Results: + Scan (1.0476 min) Sub (A-1.d)

m/z	Ion	Formula	Abundance
196.0759	(M+H)+	C13 H10 N O	36052.2

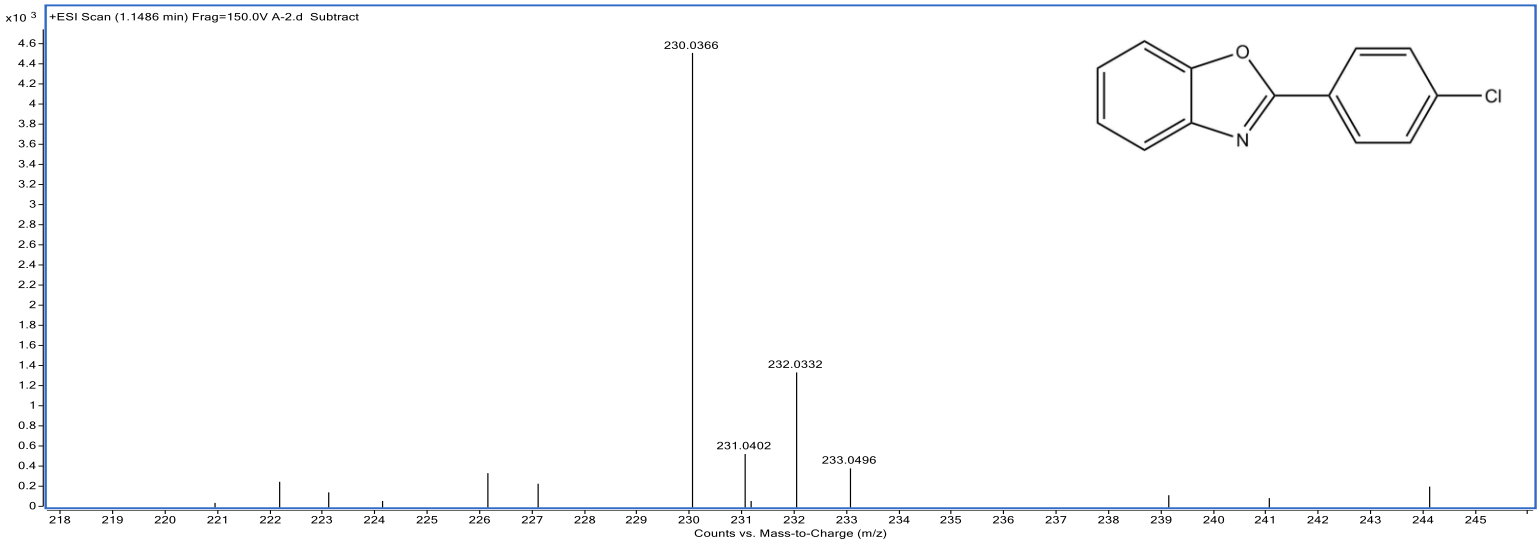
Best	Formula (M)	Ion Formula	Score	Cross Score	Calc m/z	Diff (ppm)	Mass Match	Abund Match	Spacing Match
☑	C13 H9 N O	C13 H10 N O	98.71		196.0757	-0.82	99.74	99.51	95.7



MS Formula Results: + Scan (1.1486 min) Sub (A-2.d)

m/z	Ion	Formula	Abundance
230.0366	(M+H)+	C13 H9 Cl N O	4513.2

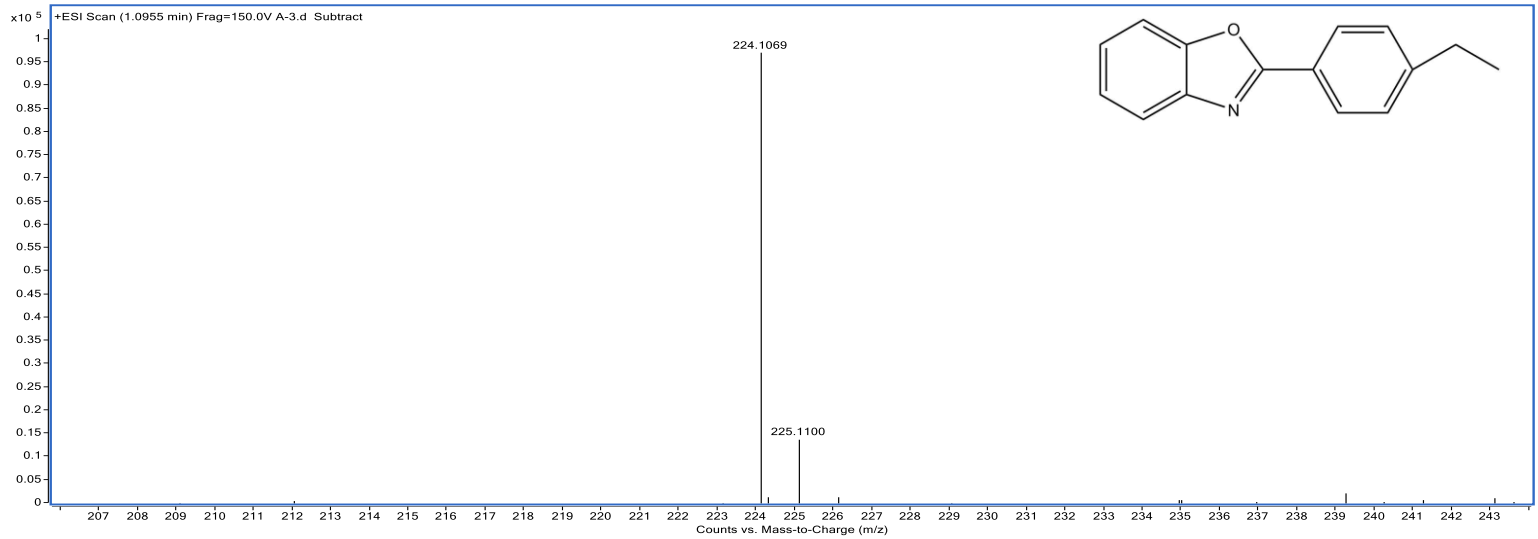
Best	Formula (M)	Ion Formula	Score	Cross Score	Calc m/z	Diff (ppm)	Mass Match	Abund Match	Spacing Match
☑	C13 H8 Cl N O	C13 H9 Cl N O	93.71		230.0367	0.8	99.69	81.13	96.85



MS Formula Results: + Scan (1.0955 min) Sub (A-3.d)

m/z	Ion	Formula	Abundance
224.1069	(M+H)+	C15 H14 N O	97181.7

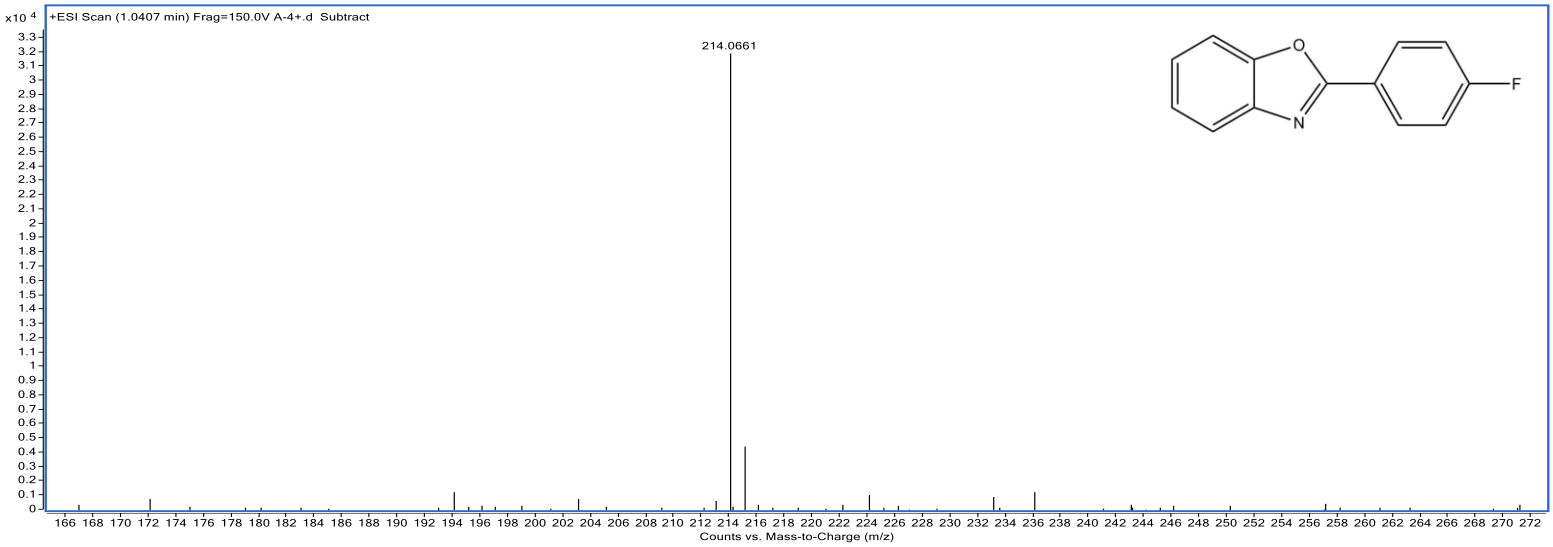
Best	Formula (M)	Ion Formula	Score	Cross Score	Calc m/z	Diff (ppm)	Mass Match	Abund Match	Spacing Match
☑	C15 H13 N O	C15 H14 N O	98.22		224.107	0.21	99.98	94.13	99.58



MS Formula Results: + Scan (1.0407 min) Sub (A-4+.d)

m/z	Ion	Formula	Abundance
214.0661	(M+H)+	C13 H9 F N O	31931.8

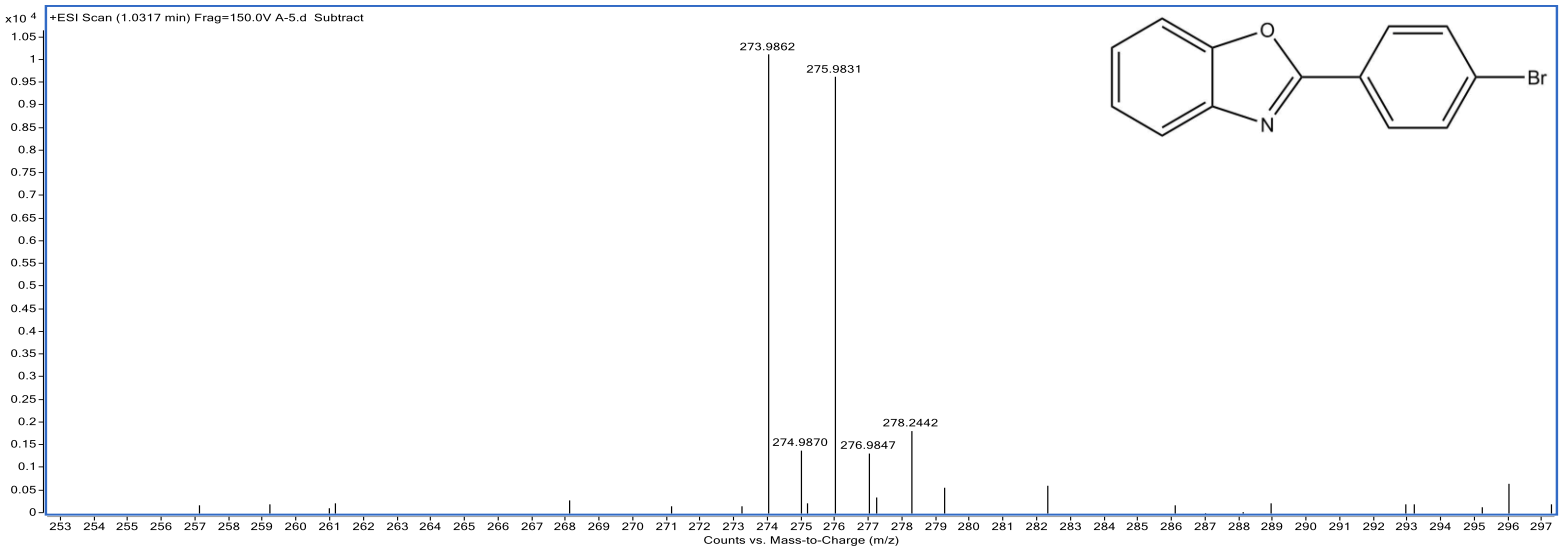
Best	Formula (M)	Ion Formula	Score	Cross Score	Calc m/z	Diff (ppm)	Mass Match	Abund Match	Spacing Match
☑	C13 H8 F N O	C13 H9 F N O	99.56		214.0663	0.75	99.75	99.75	98.96



MS Formula Results: + Scan (1.0317 min) Sub (A-5.d)

m/z	Ion	Formula	Abundance
273.9862	(M+H)+	C13 H9 Br N O	10135.1

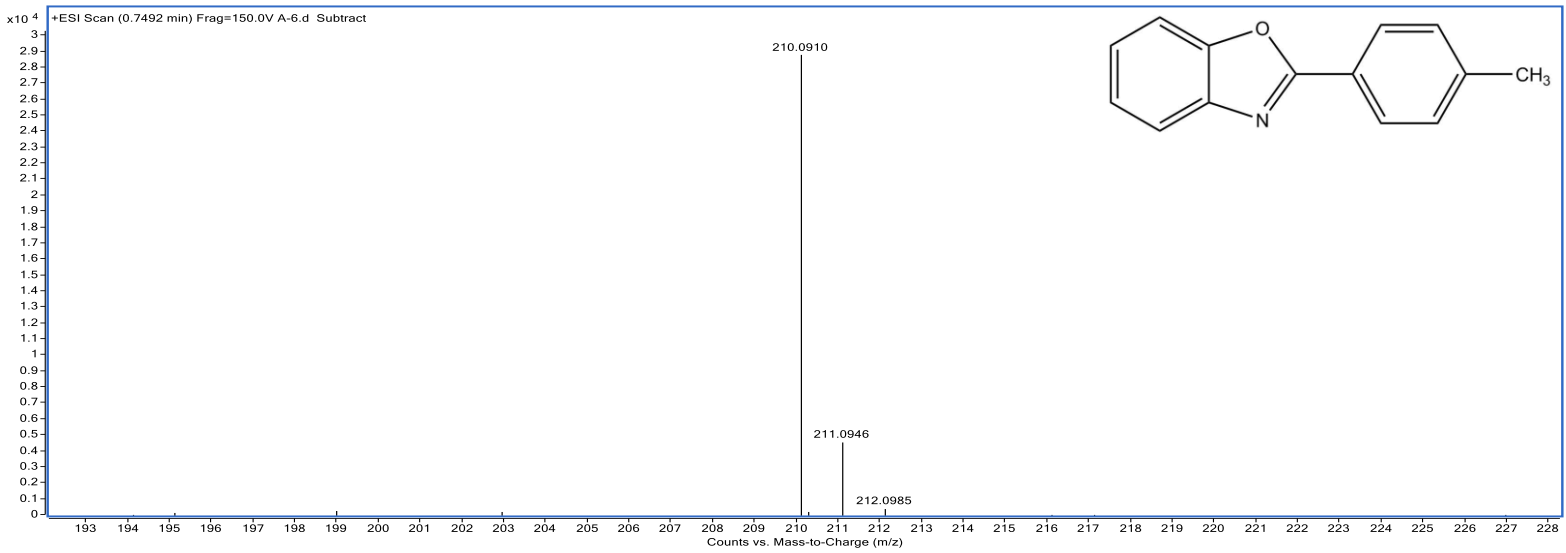
Best	Formula (M)	Ion Formula	Score	Cross Score	Calc m/z	Diff (ppm)	Mass Match	Abund Match	Spacing Match
☑	C13 H8 Br N O	C13 H9 Br N O	91.94		273.9862	2.04	97.55	99.18	72.05



MS Formula Results: + Scan (0.7492 min) Sub (A-6.d)

m/z	Ion	Formula	Abundance
210.091	(M+H)+	C14 H12 N O	28819.7

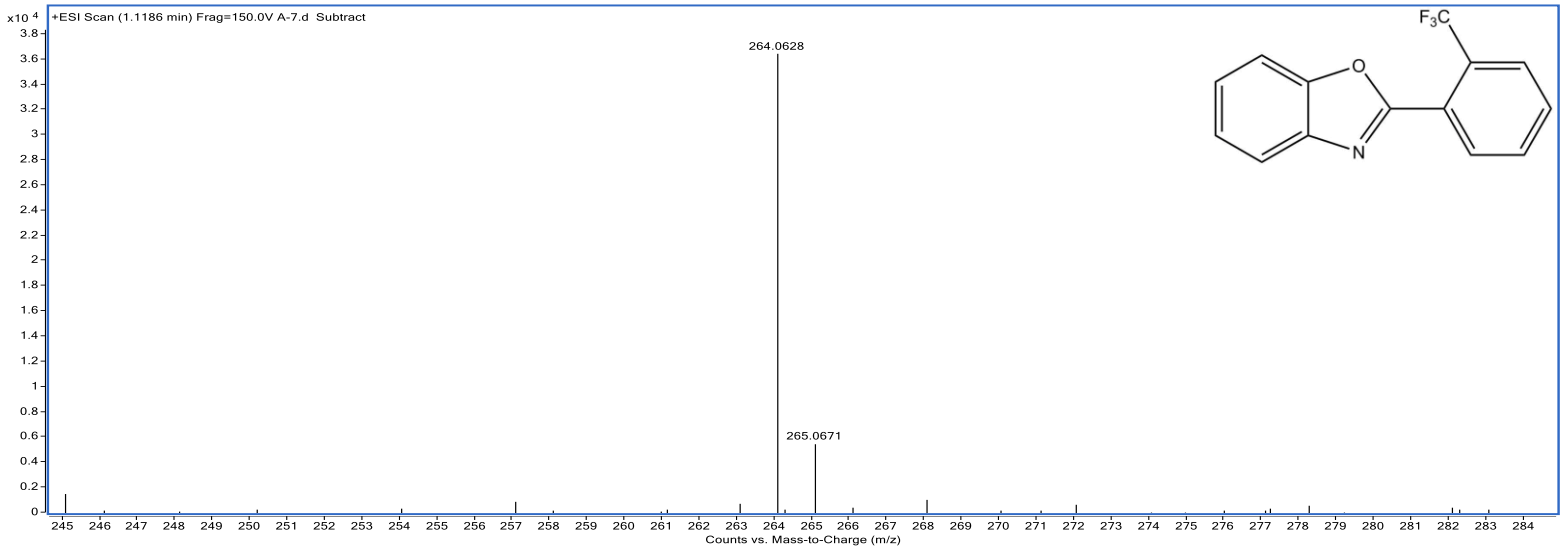
Best	Formula (M)	Ion Formula	Score	Cross Score	Calc m/z	Diff (ppm)	Mass Match	Abund Match	Spacing Match
☑	C14 H11 N O	C14 H12 N O	99.05		210.0913	1.74	98.7	99.87	98.76



MS Formula Results: + Scan (1.1186 min) Sub (A-7.d)

m/z	Ion	Formula	Abundance
264.0628	(M+H)+	C14 H9 F3 N O	36473.3

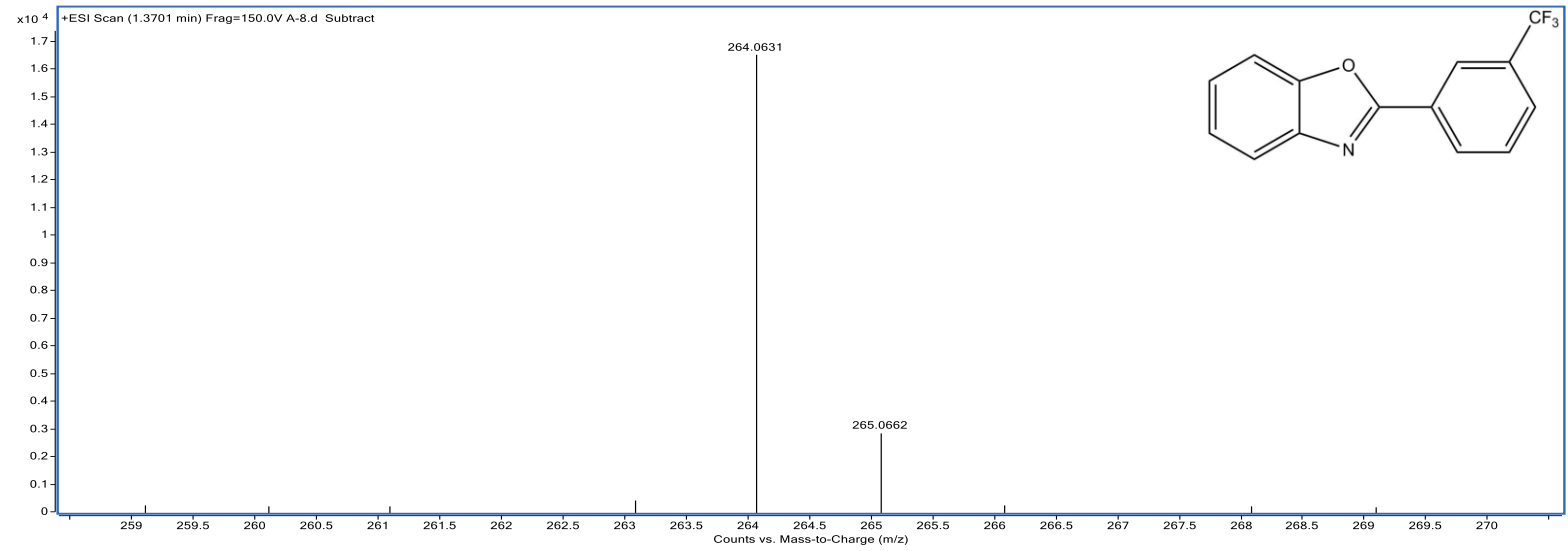
Best	Formula (M)	Ion Formula	Score	Cross Score	Calc m/z	Diff (ppm)	Mass Match	Abund Match	Spacing Match
☑	C14 H8 F3 N O	C14 H9 F3 N O	97.94		264.0631	1.02	99.41	99.73	92.84



MS Formula Results: + Scan (1.3701 min) Sub (A-8.d)

m/z	Ion	Formula	Abundance
264.0631	(M+H)+	C14 H9 F3 N O	16555.1

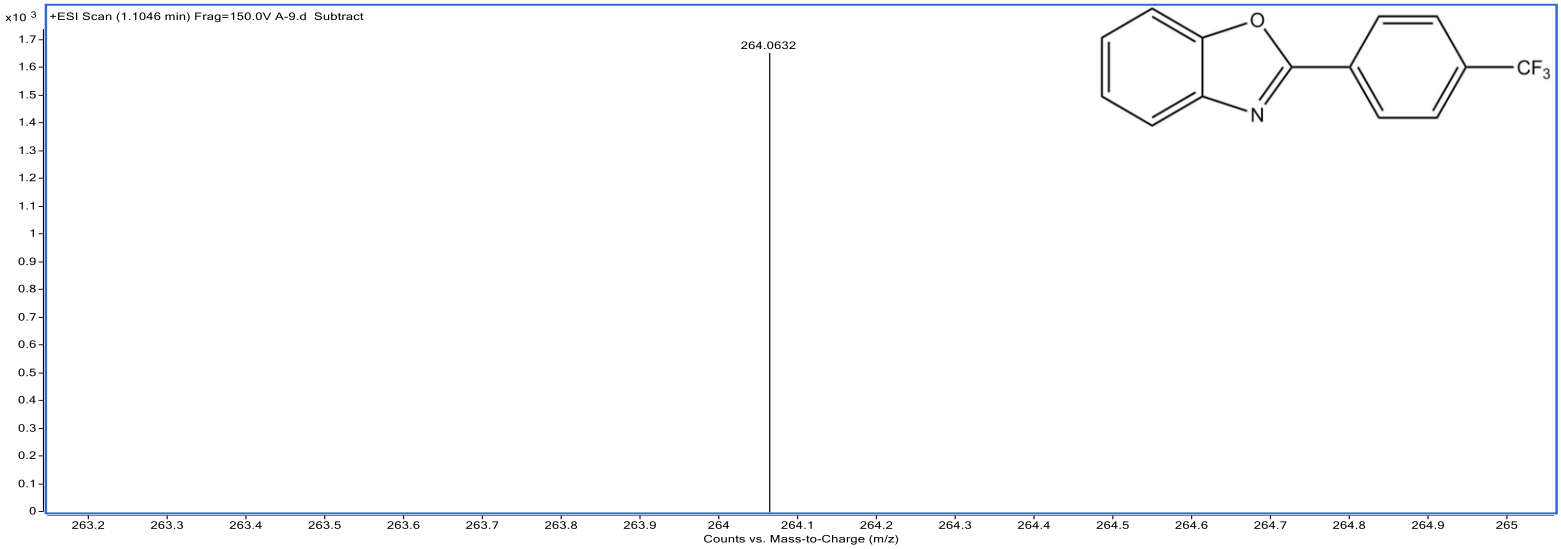
Best	Formula (M)	Ion Formula	Score	Cross Score	Calc m/z	Diff (ppm)	Mass Match	Abund Match	Spacing Match
☑	C14 H8 F3 N O	C14 H9 F3 N O	99.05		264.0631	-0.13	99.99	97.36	99.19



MS Formula Results: + Scan (1.1046 min) Sub (A-9.d)

m/z	Ion	Formula	Abundance
264.0632	(M+H)+	C14 H9 F3 N O	1655.3

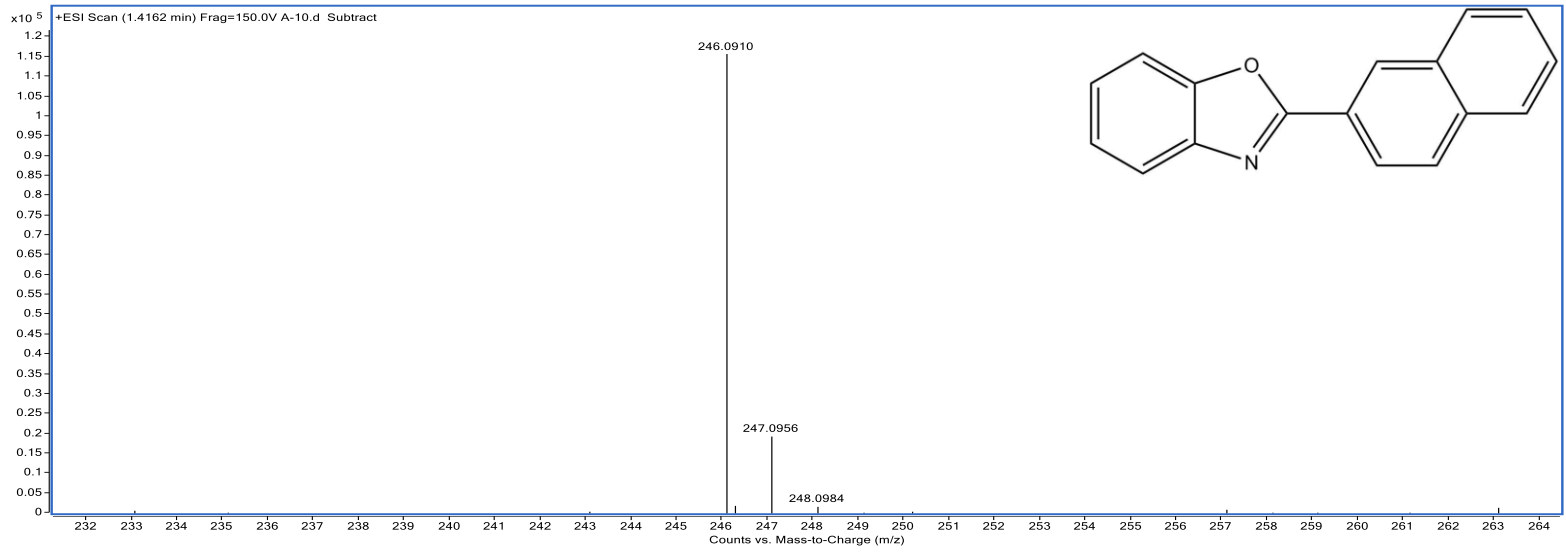
Best	Formula (M)	Ion Formula	Score	Cross Score	Calc m/z	Diff (ppm)	Mass Match	Abund Match	Spacing Match
☑	C14 H8 F3 N O	C14 H9 F3 N O	75.51		264.0631	-0.31	99.94	67.04	36.81



MS Formula Results: + Scan (1.4162 min) Sub (A-10.d)

m/z	Ion	Formula	Abundance
246.091	(M+H)+	C17 H12 N O	115798.4

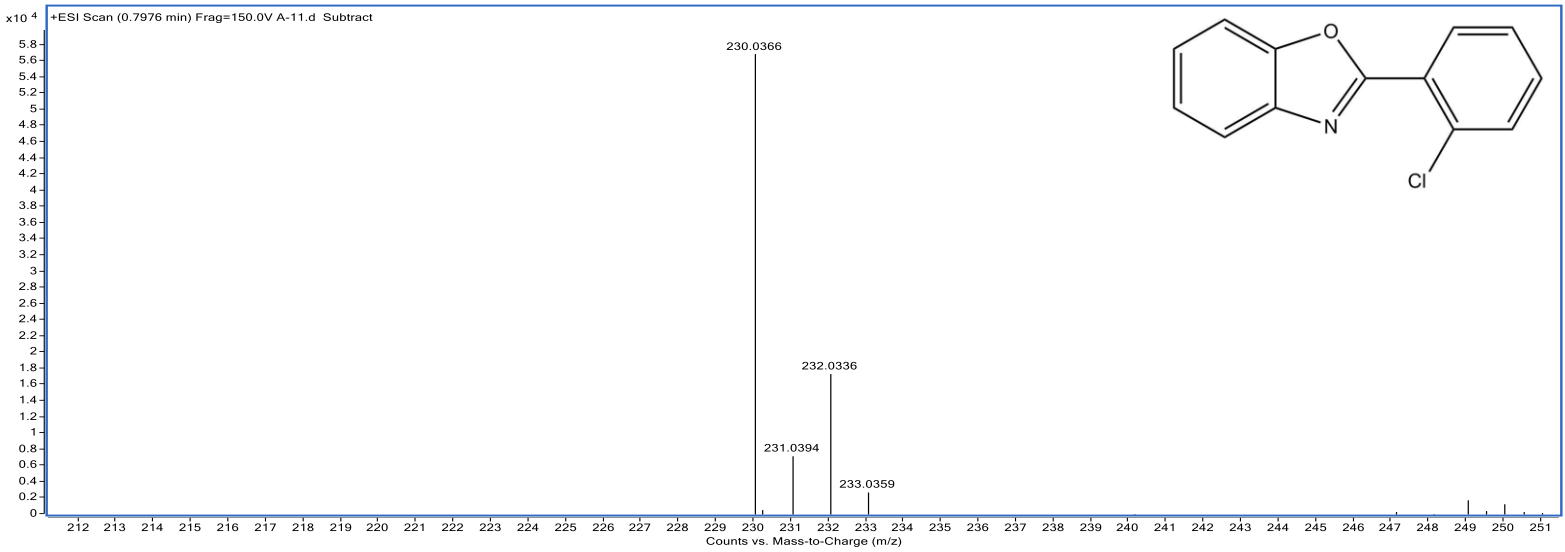
Best	Formula (M)	Ion Formula	Score	Cross Score	Calc m/z	Diff (ppm)	Mass Match	Abund Match	Spacing Match
☑	C17 H11 N O	C17 H12 N O	95.64		246.0913	1.32	99.08	95.84	88.51



MS Formula Results: + Scan (0.7976 min) Sub (A-11.d)

m/z	Ion	Formula	Abundance
230.0366	(M+H)+	C13 H9 Cl N O	56916.5

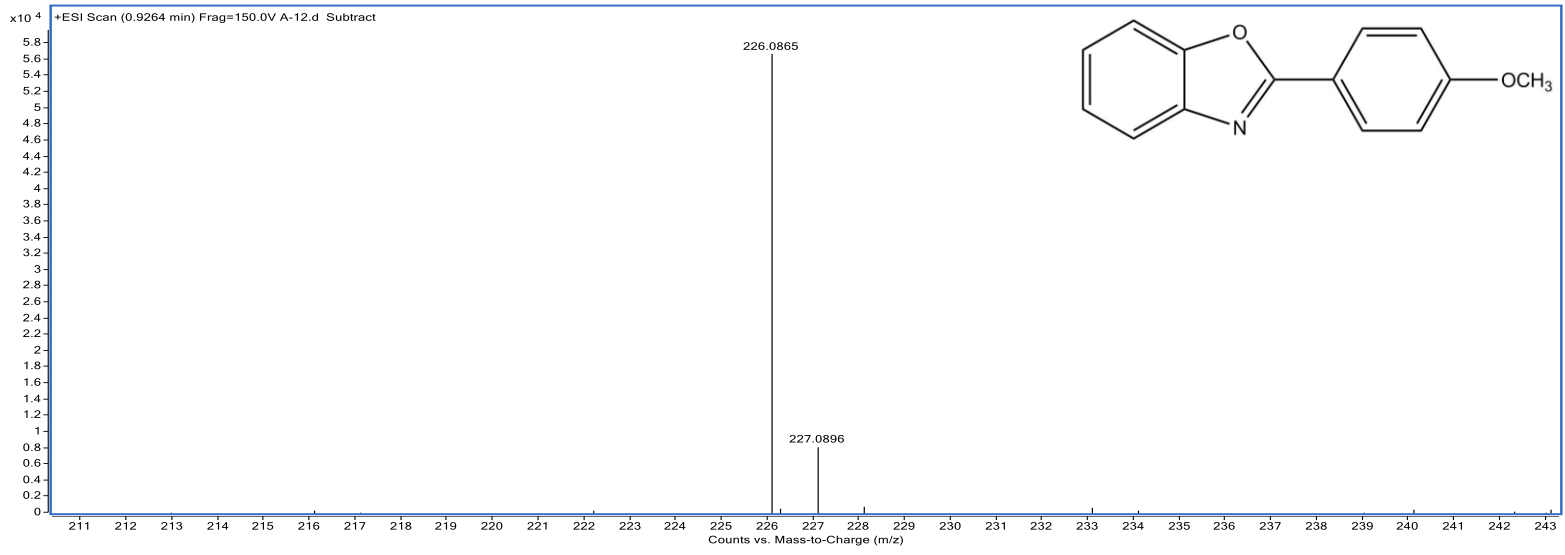
Best	Formula (M)	Ion Formula	Score	Cross Score	Calc m/z	Diff (ppm)	Mass Match	Abund Match	Spacing Match
☑	C13 H8 Cl N O	C13 H9 Cl N O	98.31		230.0367	0.42	99.92	96.08	97.75



MS Formula Results: + Scan (0.9264 min) Sub (A-12.d)

m/z	Ion	Formula	Abundance
226.0865	(M+H)+	C14 H12 N O2	56757

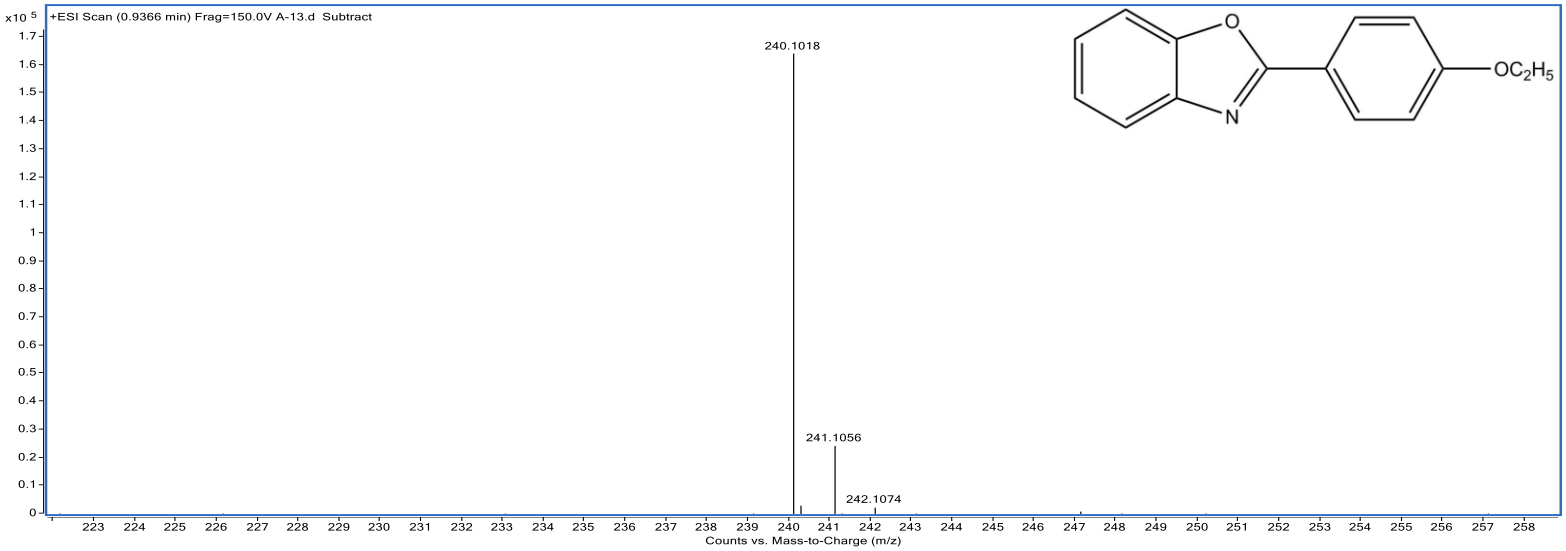
Best	Formula (M)	Ion Formula	Score	Cross Score	Calc m/z	Diff (ppm)	Mass Match	Abund Match	Spacing Match
☑	C14 H11 N O2	C14 H12 N O2	99.27		226.0863	-0.95	99.57	98.29	99.86



MS Formula Results: + Scan (0.9366 min) Sub (A-13.d)

m/z	Ion	Formula	Abundance
240.1018	(M+H)+	C15 H14 N O2	164253.1

Best	Formula (M)	Ion Formula	Score	Cross Score	Calc m/z	Diff (ppm)	Mass Match	Abund Match	Spacing Match
☑	C15 H13 N O2	C15 H14 N O2	98.37		240.1019	0.42	99.91	96.06	98.06



MS Formula Results: + Scan (1.1206 min) Sub (A-14.d)

m/z	Ion	Formula	Abundance
263.9975	(M+H)+	C13 H8 Cl2 N O	1181.2

Best	Formula (M)	Ion Formula	Score	Cross Score	Calc m/z	Diff (ppm)	Mass Match	Abund Match	Spacing Match
☑	C13 H7 Cl2 N O	C13 H8 Cl2 N O	47.29		263.9977	1.1	99.31	0	0