Supporting Information

Copper(II)-Catalyzed Dehydrogenative Cross-Coupling between Two Azoles

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I. General Information

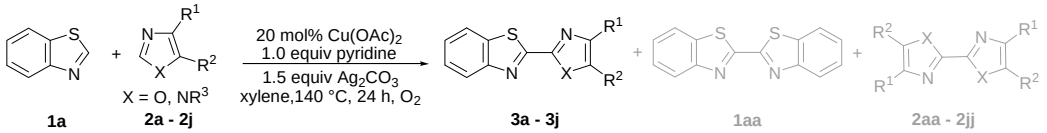
All reagents were purchased from commercial suppliers and used without further purification. 5-Substituted oxazoles,[1] ethyl 4-methyloxazole-5-carboxylate,[2] ethyl 4-methylthiazole-5-carboxylate,[2] ethyl thiazole-5-carboxylate,[2] and 1-methyl-1H-benzoimidazole[3] were prepared according to the literature procedures. All solvents were purified and dried according to standard methods prior to use. The ^{1}H NMR (400 MHz or 600 MHz) chemical shifts were measured relative to $CDCl_3$ as the internal reference ($CDCl_3$: δ = 7.26 ppm). The ^{13}C NMR (100 MHz or 150 MHz) chemical shifts were given using $CDCl_3$ as the internal standard ($CDCl_3$: δ = 77.16 ppm). The following abbreviations were used to designate the multiplicities: s = singlet, d = doublet, t = triplet, bs = broad signal, m = multiplet. GC-MS analyses were performed using naphthalene as internal standard.

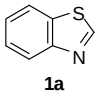
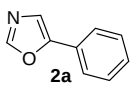
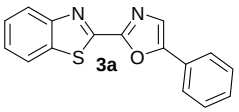
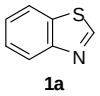
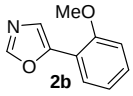
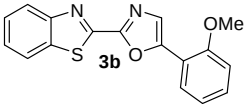
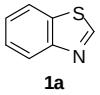
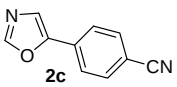
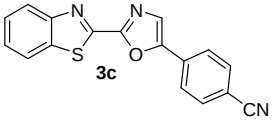
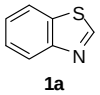
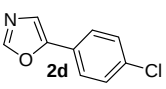
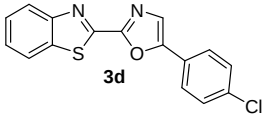
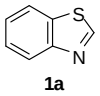
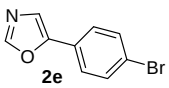
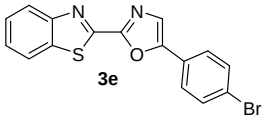
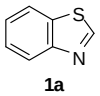
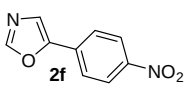
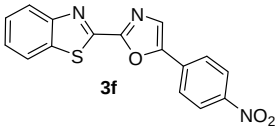
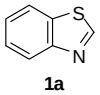
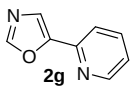
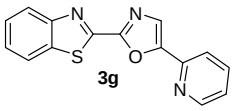
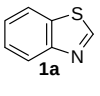
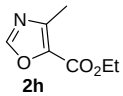
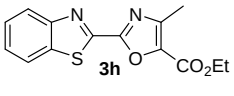
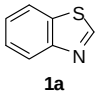
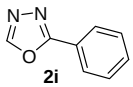
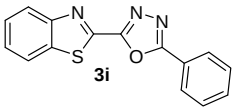
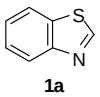
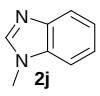
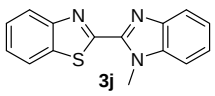
II. Optimization of the Dehydrogenative Cross-Coupling of Benzothiazole with 5-Phenyloxazole

A flame-dried Schlenk test tube with a magnetic stirring bar was charged with Cu salt (20 mol%), base (1.5 equiv), oxidant (1.5 equiv), additive (1.0 equiv), benzothiazole (0.25 mmol), 5-phenyloxazole (0.25 mmol) and solvent (1.0 mL) under O_2 (1 atm) atmosphere. The resulting mixture was stirred for 10 min at room temperature, and then heated at 140 ºC for the indicated time. The reaction mixture was then cooled to ambient temperature, diluted with 20 mL of CH_2Cl_2, filtered through a Celite pad, and washed with 10-20 mL of CH_2Cl_2. The combined organic extracts were concentrated, and the resulting residue was purified by column chromatography on silica gel (petroleum/ethyl acetate = 10/1-5/1 v/v) to provide the desired product **3a**.

III. Detailed Hetero-Couplings and Homo-Couplings for all Described Reactions

Table S1. Selective Cross-Couplings of Benzothiazole with Azoles[a,b]

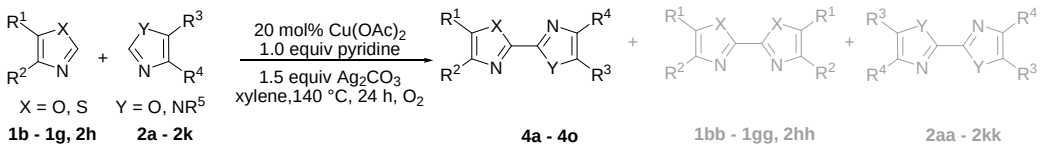


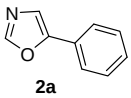
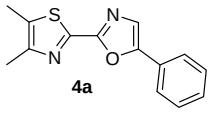
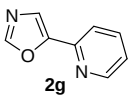
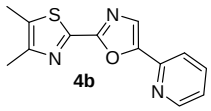
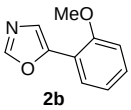
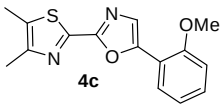
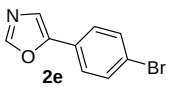
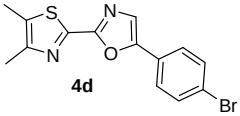
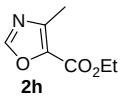
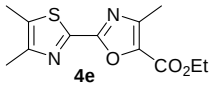
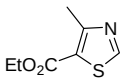
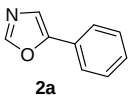
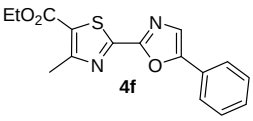
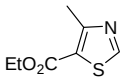
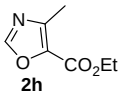
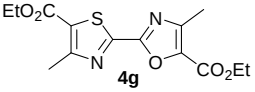
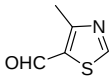
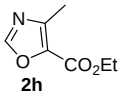
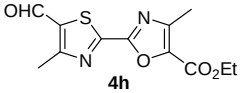
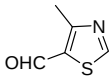
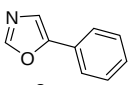
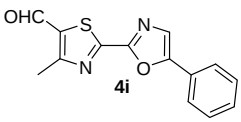
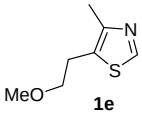
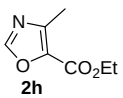
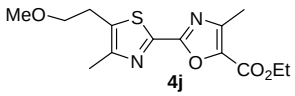
entry	benzothiazole	azole **2**	heterocoupling product	yield (%)
1	 **1a**	 **2a**	 **3a**	76 (10, 17)
2	 **1a**	 **2b**	 **3b**	75 (13, 15)
3	 **1a**	 **2c**	 **3c**	75 (10, <5)
4	 **1a**	 **2d**	 **3d**	69 (10, 8)
5	 **1a**	 **2e**	 **3e**	69 (13, <5)
6	 **1a**	 **2f**	 **3f**	71 (13, <5)
7	 **1a**	 **2g**	 **3g**	70 (12, 18)
8	 **1a**	 **2h**	 **3h**	64 (10, <5)
9	 **1a**	 **2i**	 **3i**	78 (12, <5)
10	 **1a**	 **2j**	 **3j**	67 (13, 18)

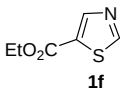
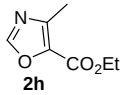
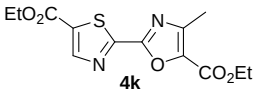
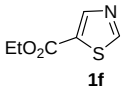
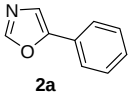
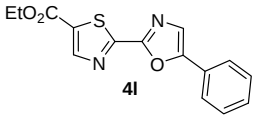
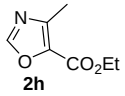
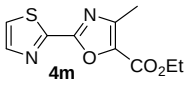
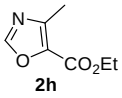
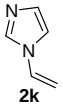
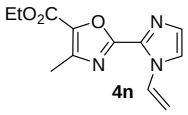
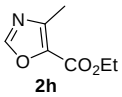
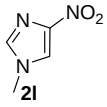
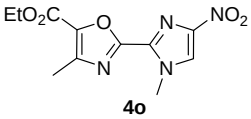
[a] Reactions were carried out using $Cu(OAc)_2$ (20 mol%), Ag_2CO_3 (1.5 equiv), pyridine (1.0 equiv), benzothiazole (0.5 mmol), and azole **2** (0.5 mmol) at 140 ^oC for 24 h under oxygen atmosphere. [b]

Yields of isolated product. The yields in parentheses refer to the homocoupling products of benzothiazole (**1a**) and azole **2**, respectively.

Table S2. Selective Cross-Couplings between Two Non-benzofused Azoles[a,b]



entry	azole **1**	azole **2**	heterocoupling Product	yield (%)
1	 **1b**	 **2a**	 **4a**	65 (13, 19)
2	 **1b**	 **2g**	 **4b**	62 (16, 18)
3	 **1b**	 **2b**	 **4c**	70 (21, trace)
4	 **1b**	 **2e**	 **4d**	73 (23, trace)
5	 **1b**	 **2h**	 **4e**	73 (18, 8)
6	 **1c**	 **2a**	 **4f**	61 (23, 12)
7	 **1c**	 **2h**	 **4g**	63 (21, <5)
8	 **1d**	 **2h**	 **4h**	70 (trace, <5)
9	 **1d**	 **2a**	 **4i**	65 (trace, 19)
10	 **1e**	 **2h**	 **4j**	66 (<5, trace)

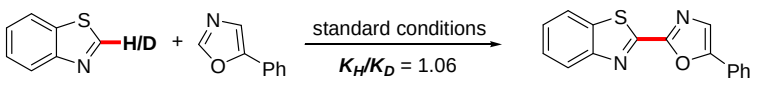
11	 1f	 2h	 4k	63 (15, 19)
12	 1f	 2a	 4l	65 (13, 11)
13	 1g	 2h	 4m	60 (<5, trace)
14	 2h	 2k	 4n	58 (<5, n.d)
15	 2h	 2l	 4o	52[c] (<5, n.d)

[a] Reactions were carried out using $Cu(OAc)_2$ (20 mol%), Ag_2CO_3 (1.5 equiv), pyridine (1.0 equiv), azole **1** (0.5 mmol), and azole **2** (0.5 mmol) at 140 ^oC for 24 h under oxygen atmosphere. [b] Yields of isolated product. The yields in parentheses refer to the homocoupling products of azole **1** and azole **2**, respectively. [c] Oxazole **1** (0.5 mmol), and imidazole **2** (0.75 mmol).

IV. Experimental Procedures for the KIE Study for Cross-Coupling of Benzothiazole with 5-Phenyloxazole

Two sets of reactions were carried out in a parallel manner. In each case 5-phenyloxazole was allowed to react with benzothiazole and 2-deuterio-benzothiazole, respectively.[4] The conversion was measured carefully after designated time (0 h, 0.5 h, 1 h, 2 h) by GC-MS analyses (naphthalene as internal standard) to compare the initial reaction rates.

Table S3. Conversion (%) of the Reaction of Benzothiazole (2-H and 2-D)



reaction time (h)	2-deuterio-benzothiazole	benzothiazole
0	0.0%	0.0%

0.5	2.8%	5.6%
1	11.1%	14.1%
2	34.9%	37.5%

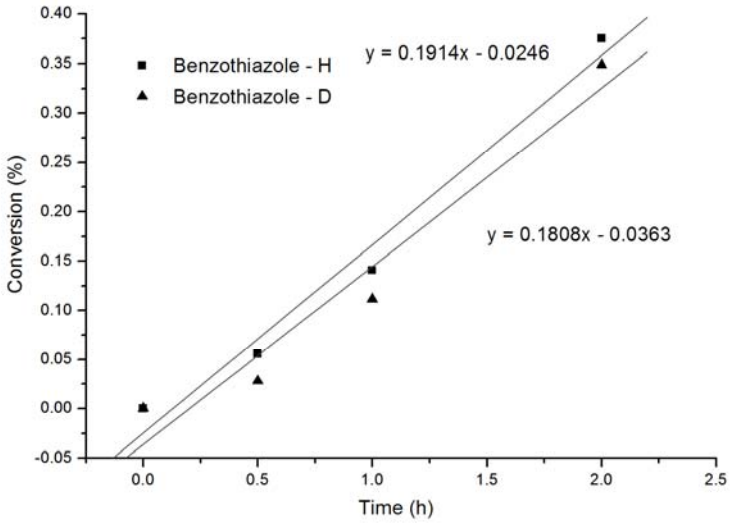
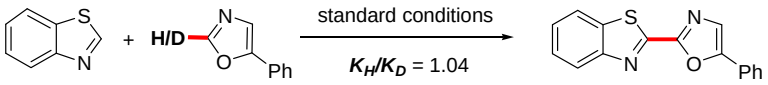


Figure S1 Conversion (%) versus Time (h)

Two sets of reactions were carried out in a parallel manner. In each case benzothiazole was allowed to react with 5-phenyloxazole and 2-deuterio-5-phenyloxazole, respectively.[4] The conversion was measured carefully after designated time (0 h, 0.5 h, 1 h, 2 h) by GC-MS analyses (naphthalene as internal standard) to compare the initial reaction rates.

Table S4. Conversion (%) of the Reaction of 5-Phenyloxazole (2-H and 2-D)



reaction time (h)	2-deuterio-5-phenyloxazole	5-phenyloxazole
0	0.0%	0.0%
0.5	3.5%	6.3%

1	12.6%	15.2%
2	29.3%	31.1%

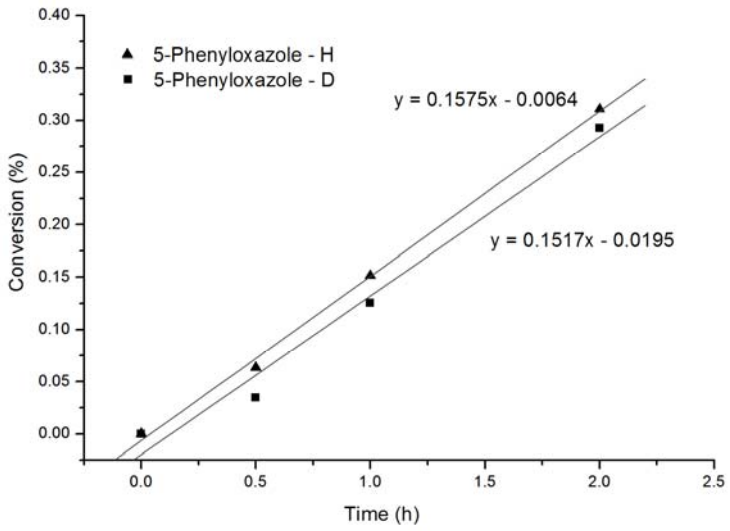


Figure S2 Conversion (%) versus Time (h).

V. References

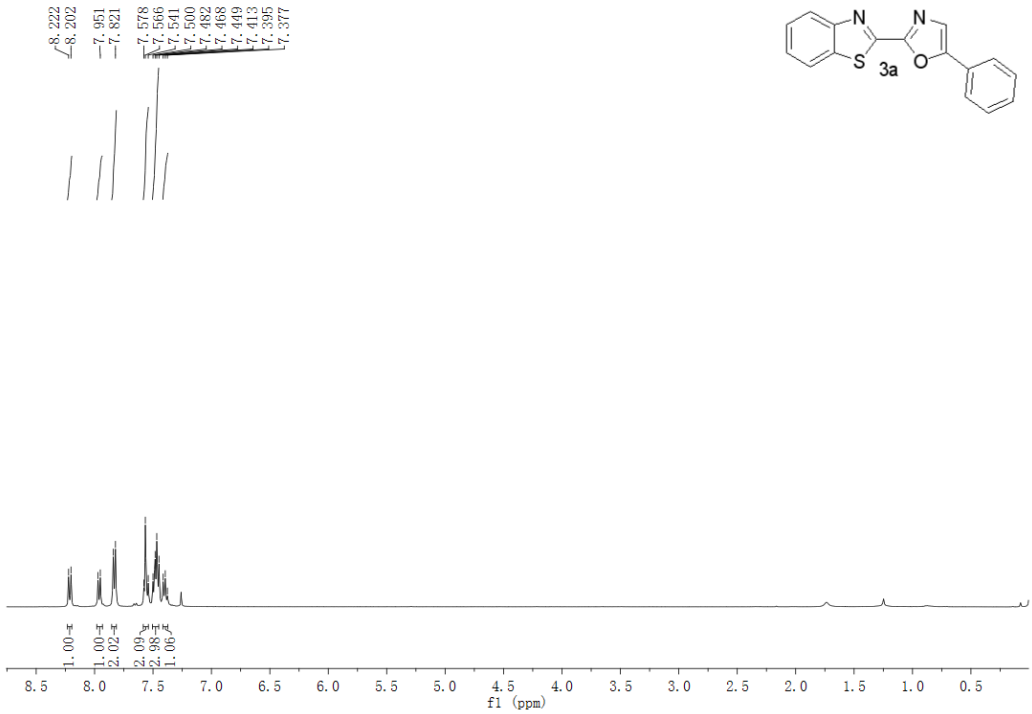
(1) Besselièvre, F.; Mahuteau-Betzer, F.; Grierson, D. S.; Piguel, S. *J. Org. Chem*. **2008**, *73*, 3278.

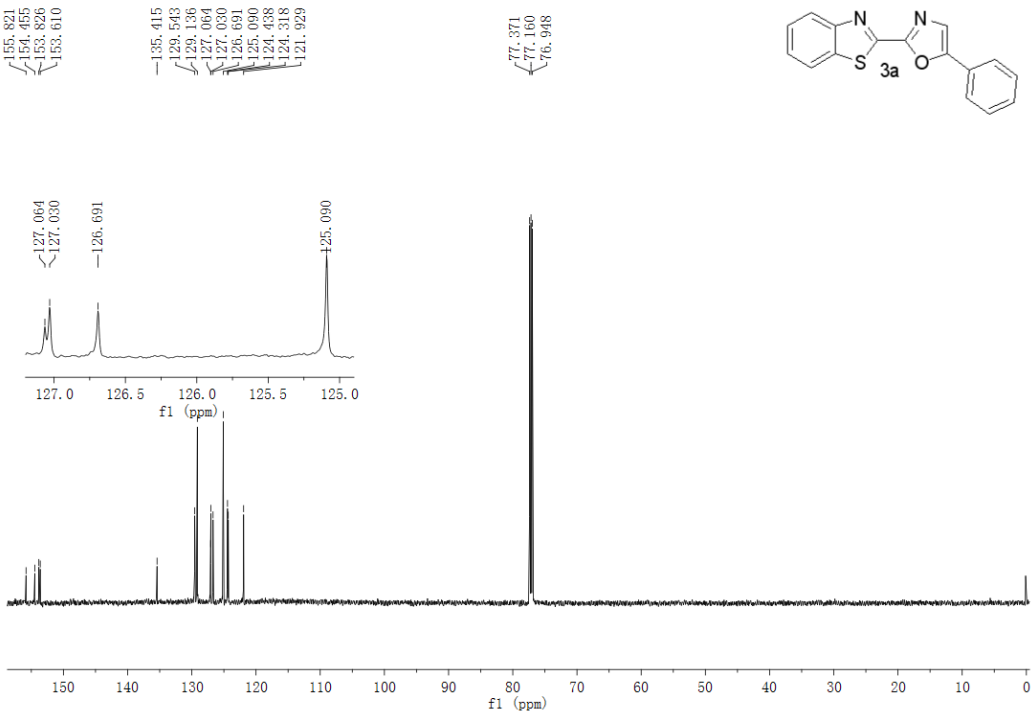
(2) Boulos, J. *J. Heterocyclic Chem*. **1998**, *35*, 859.

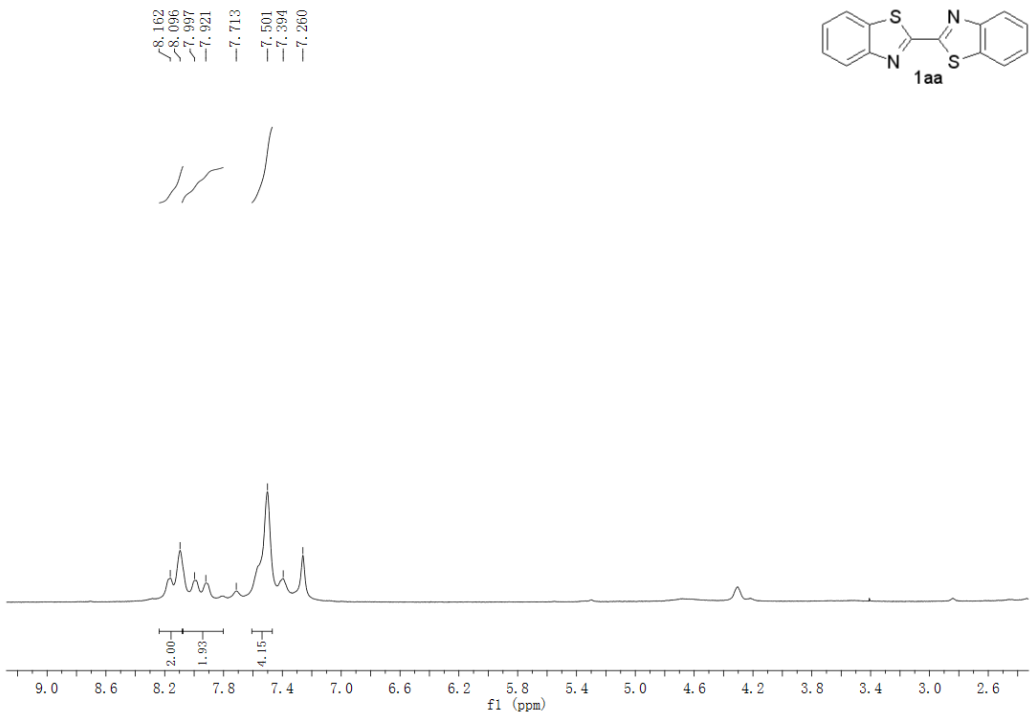
(3) Petzer, J. P.; Steyn, S.; Castagnoli, K. P.; Chen, J. –F.; Schwarzschild, M. A.; Schyf, C. J. W.; Castagnoli, N. *Bio. Med. Chem.* **2003**, *11*, 1299.

(4) (a) Crowe, E.; Hossner, F.; Hughes, M. J. *Tetrahedron* **1995**, *51*, 8889. (b) Bayh, O.; Awad, H.; Mongin, F.; Hoarau, C.; Bischoff, L.; Trécourt, F.; Quéguiner, G.; Marsais, F.; Blanco, F.; Abarca, B.; Ballesteros, R. *J. Org. Chem*. **2005**, *70*, 5190.

VI. Copies of ^{1}H and ^{13}C NMR Spectra



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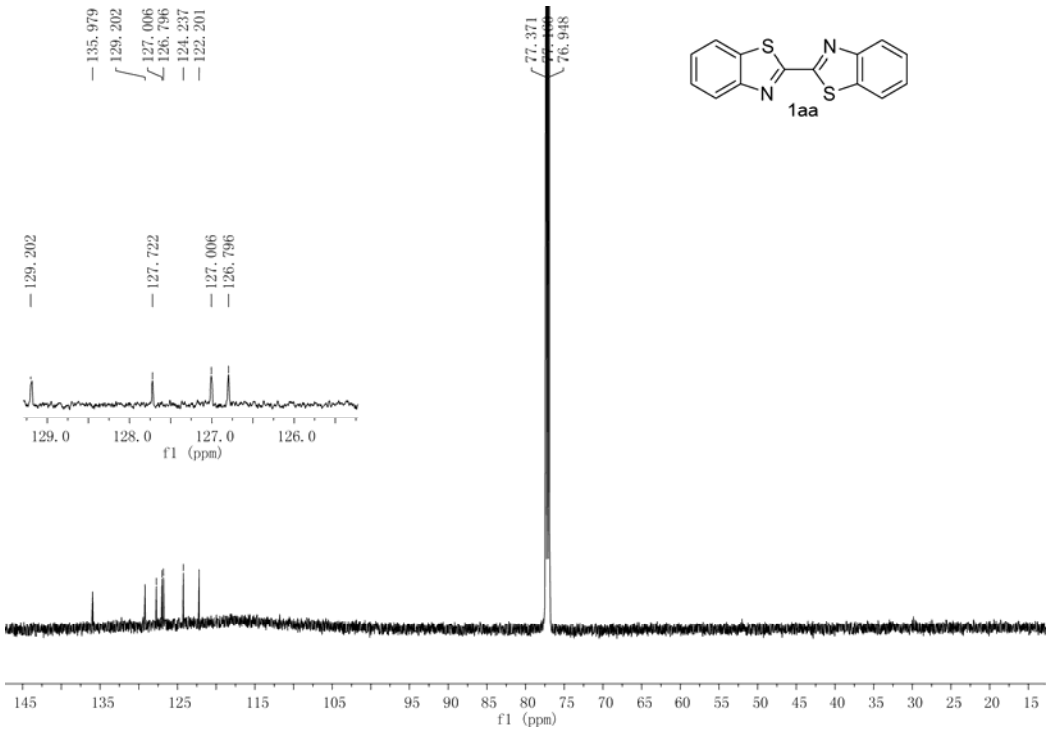
7.997
7.921
7.713
7.501
7.394
7.260
1aa
2.00
1.93
4.15
f1 (ppm)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127.006
126.796
124.237
122.201
77.371
76.948
1aa
129.202
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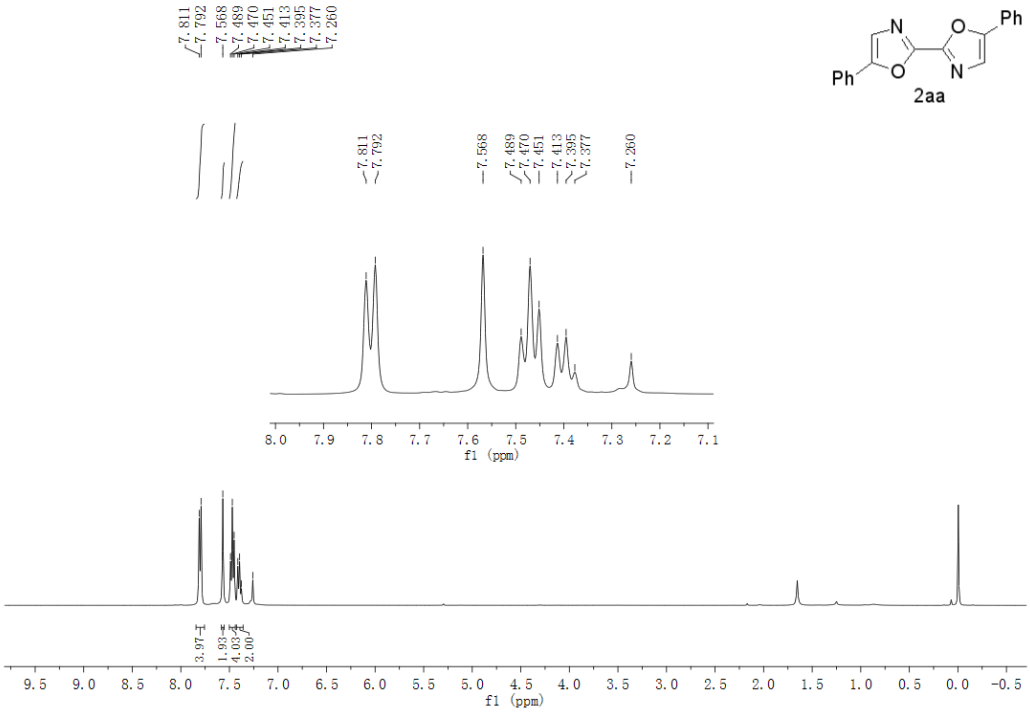
127.006
126.796
f1 (ppm)
f1 (ppm)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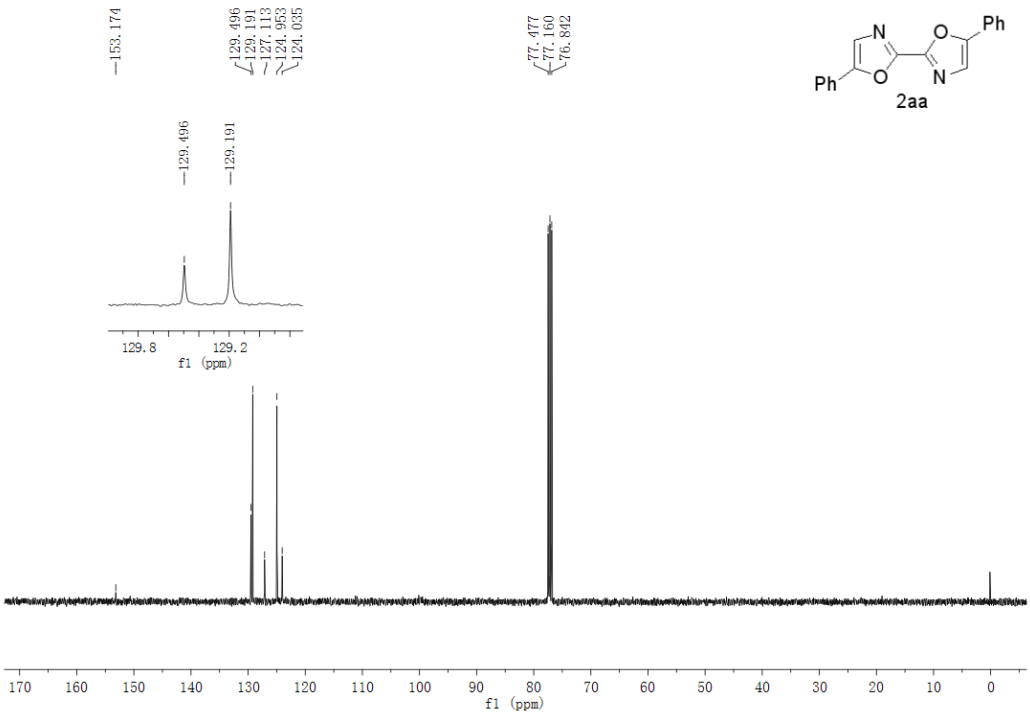
7.792
7.568
7.489
7.470
7.451
7.413
7.395
7.377
7.260
Ph
Ph
2aa
f1 (ppm)
3.97
1.93
4.03
2.00
f1 (ppm)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129.191
127.113
124.953
124.035
77.477
77.160
76.842
Ph
Ph
2aa
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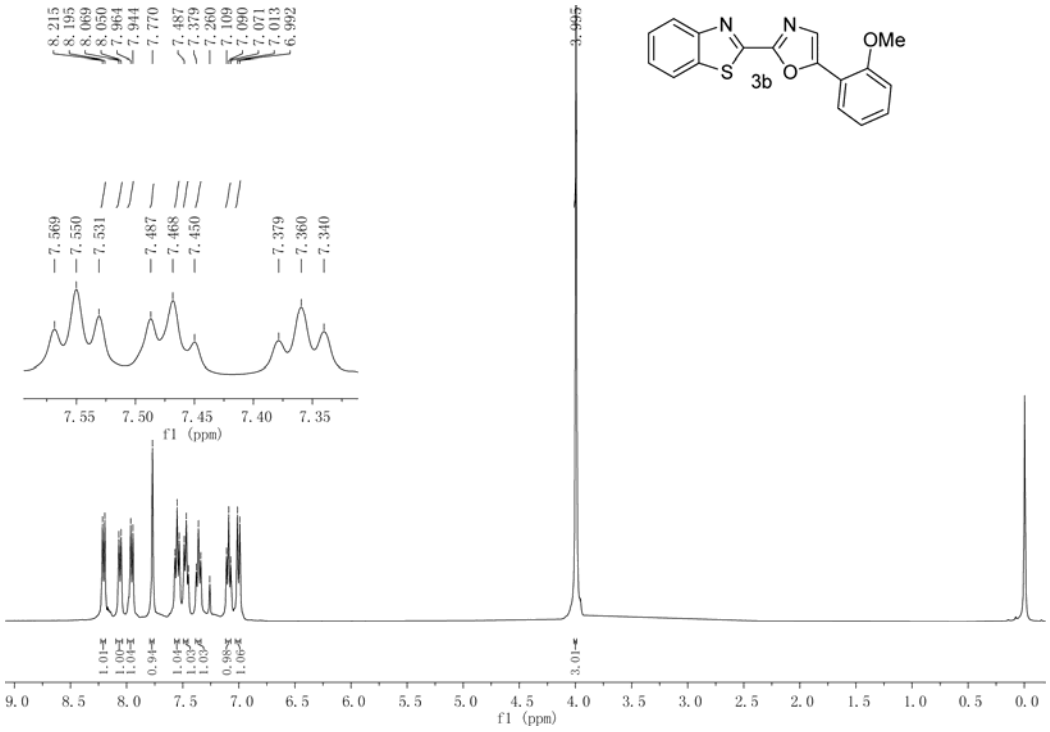
129.191
129.8
129.2
f1 (ppm)
f1 (ppm)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7.944
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7.487
7.379
7.260
7.109
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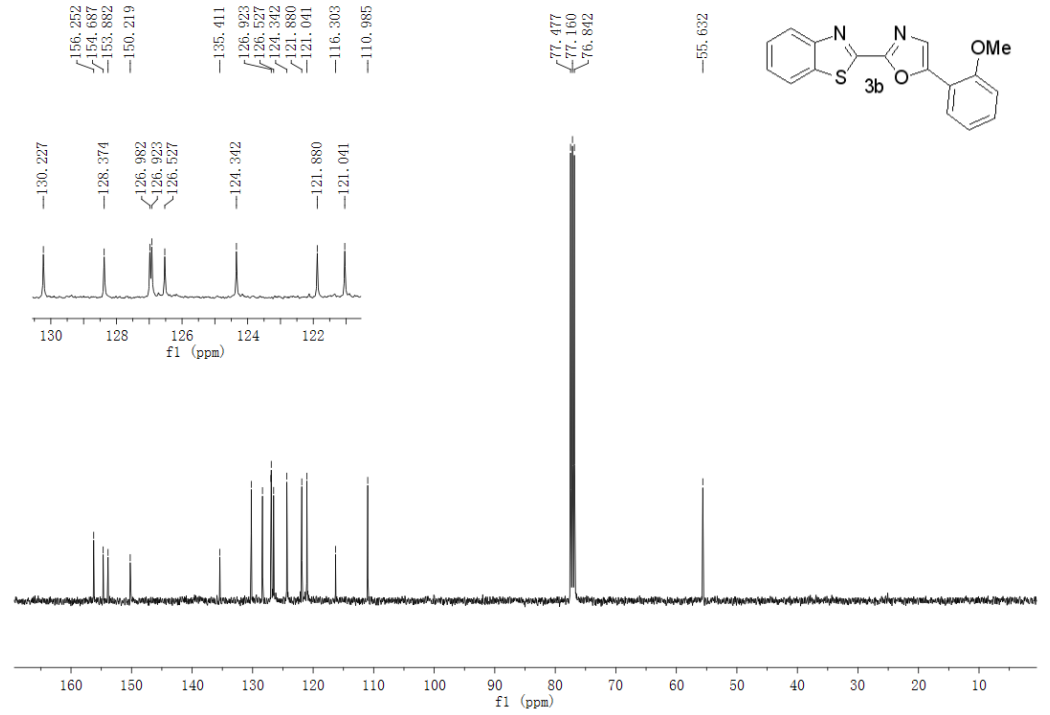
7.071
7.013
6.992
3.995
7.569
7.550
7.531
7.487
7.468
7.450
7.379
7.360
7.340
7.55 7.50 7.45 7.40 7.35
f1 (ppm)
1.01
1.00
1.04
0.94
1.04
1.03
1.02
0.98
1.06
3.01
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
N
S
N
O
OMe
3b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121.041
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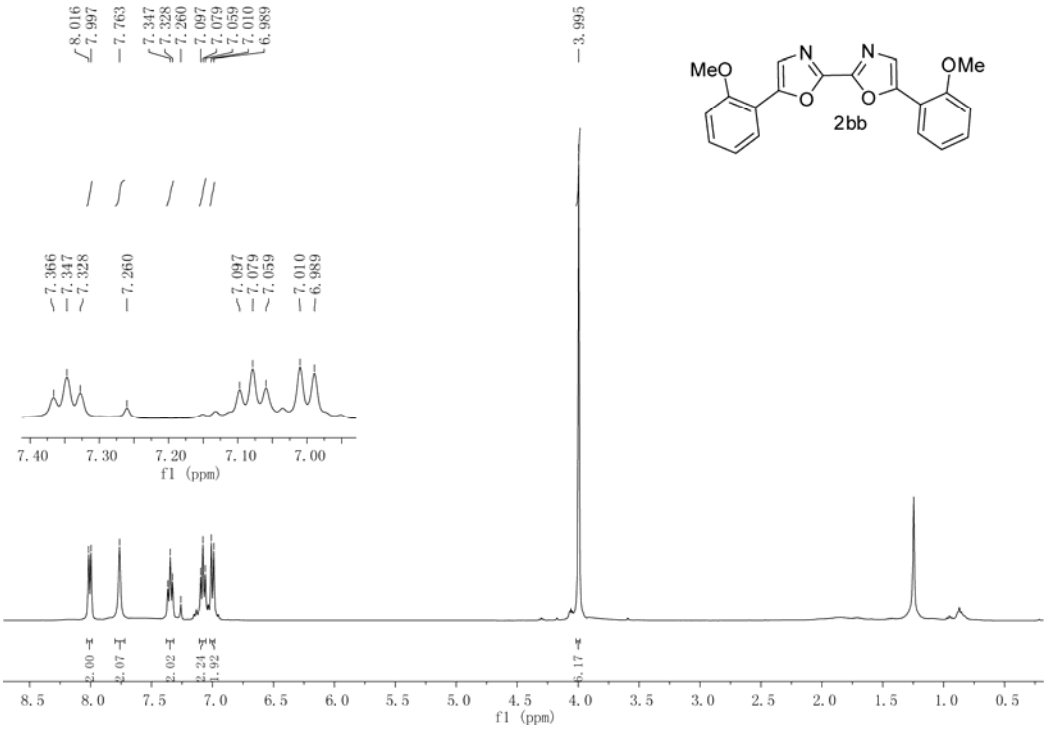
110.985
77.477
77.160
76.842
55.632
130.227
128.374
126.982
126.923
126.527
124.342
121.880
121.041
130 128 126 124 122
f1 (ppm)
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)
N
S
N
O
OMe
3b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7.328
7.260
7.097
7.079
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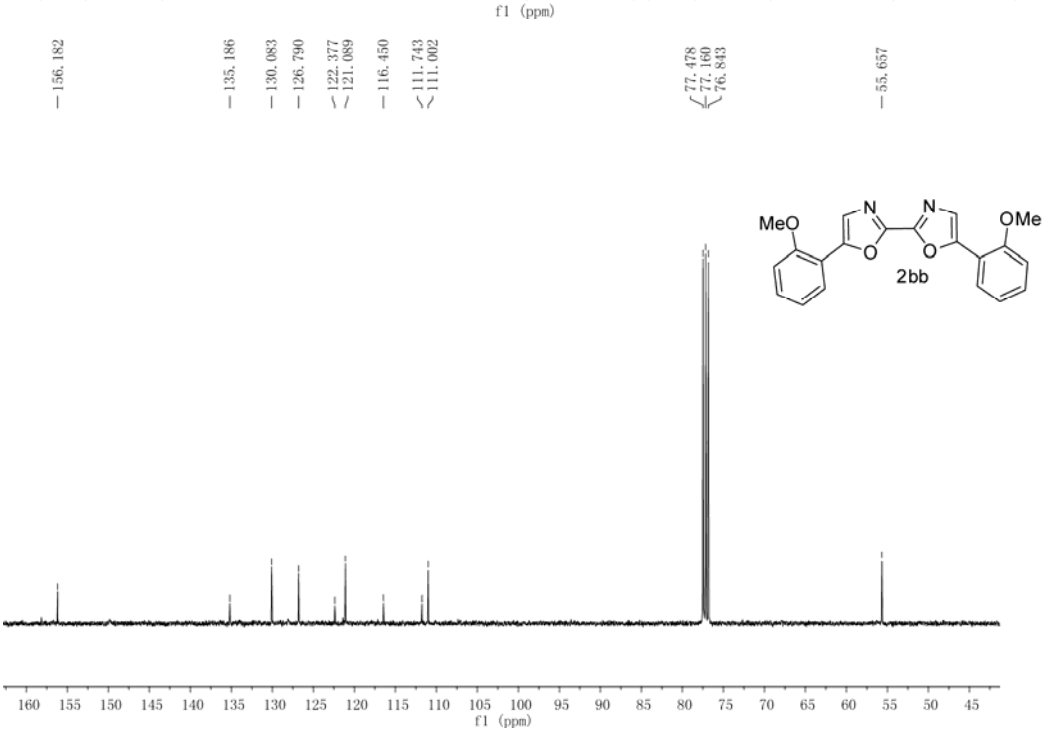
7.010
6.989
3.995
MeO
OMe
2bb
7.366
7.347
7.328
7.260
7.097
7.079
7.059
7.010
6.989
7.40
7.30
7.20
7.10
7.00
f1 (ppm)
2.00
2.07
2.02
2.24
1.92
6.17
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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135.186
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77.478
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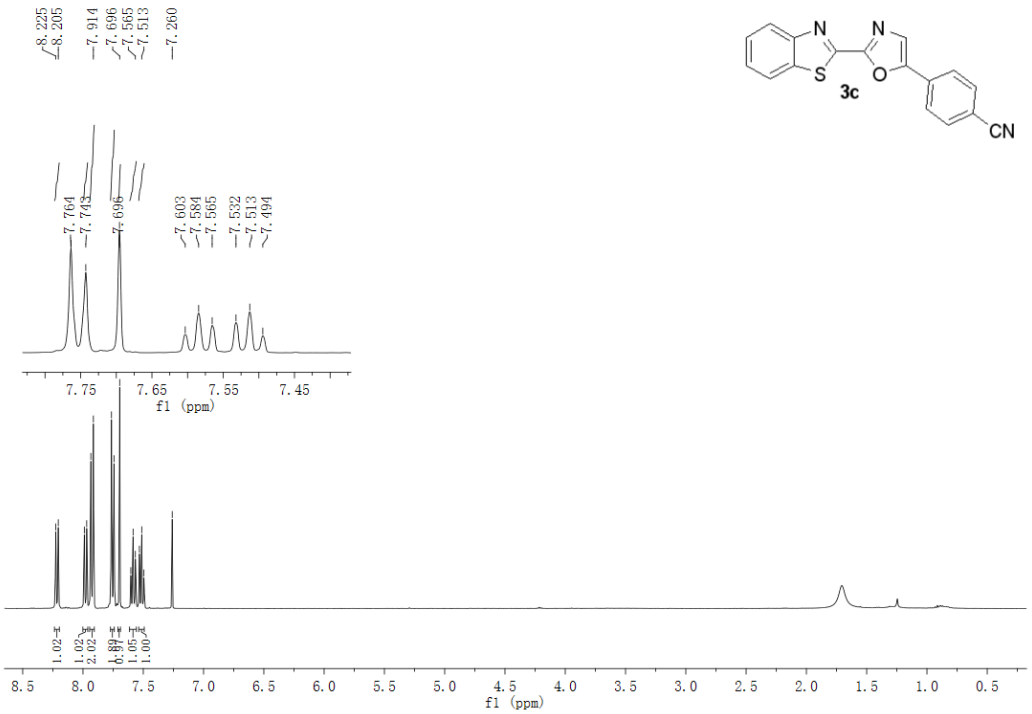
55.657
MeO
OMe
2bb
160
155
150
145
140
135
130
125
120
115
110
105
100
95
90
85
80
75
70
65
60
55
50
45
f1 (ppm)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7.565
7.532
7.513
7.494
7.75
7.65
7.55
7.45
f1 (ppm)
1.02
1.02
2.02
0.89
1.05
1.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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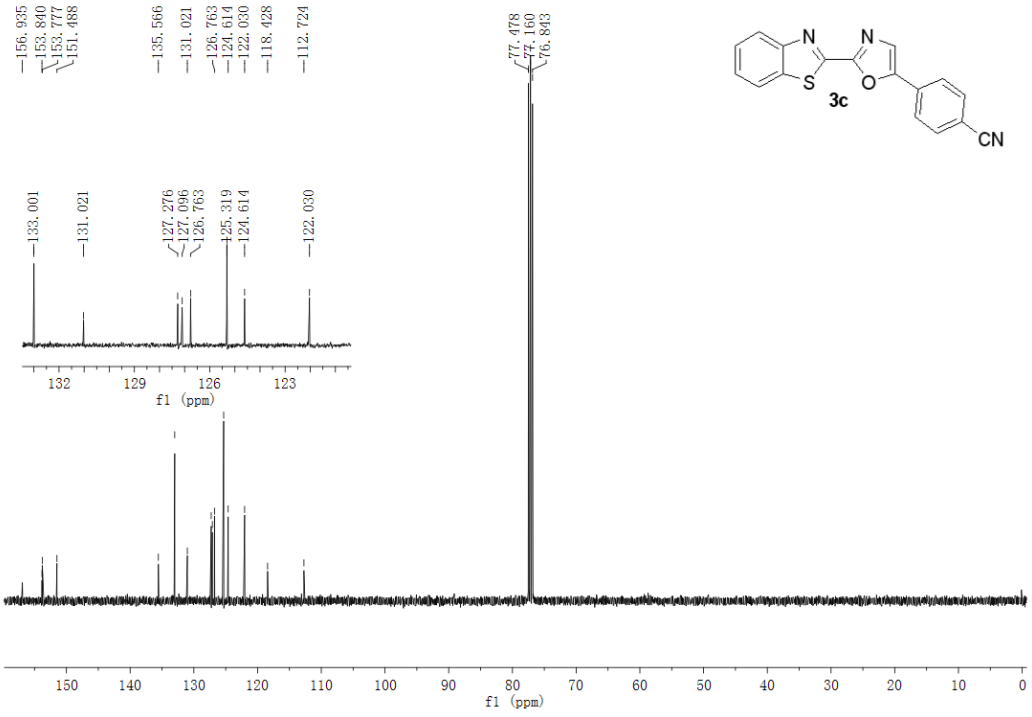
f1 (ppm)
N
S
N
O
3c
CN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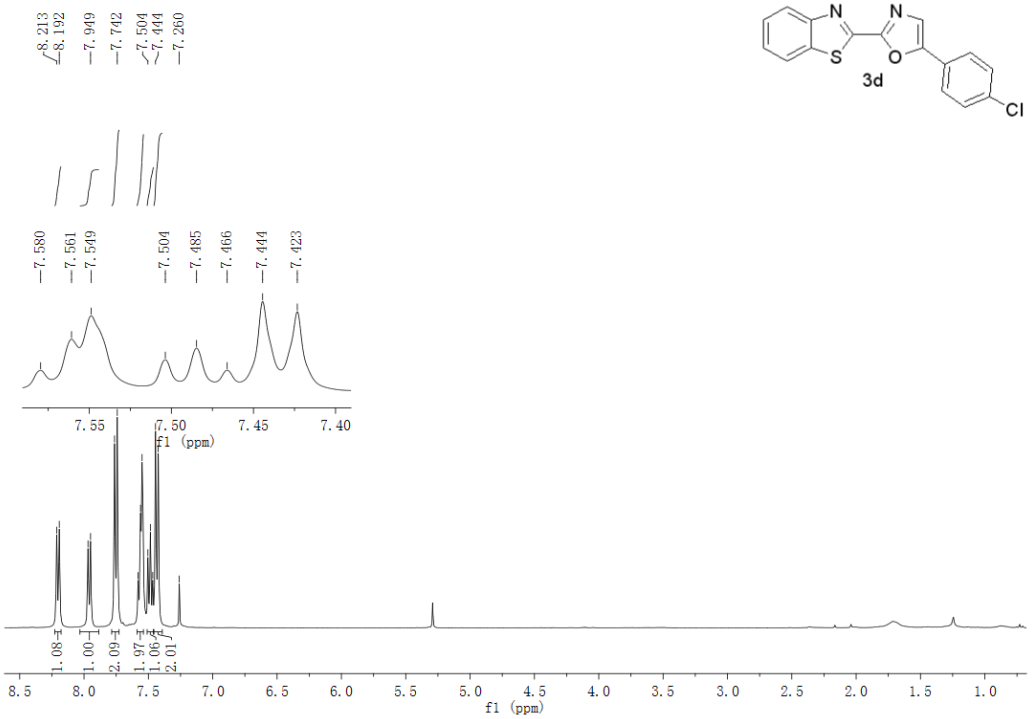
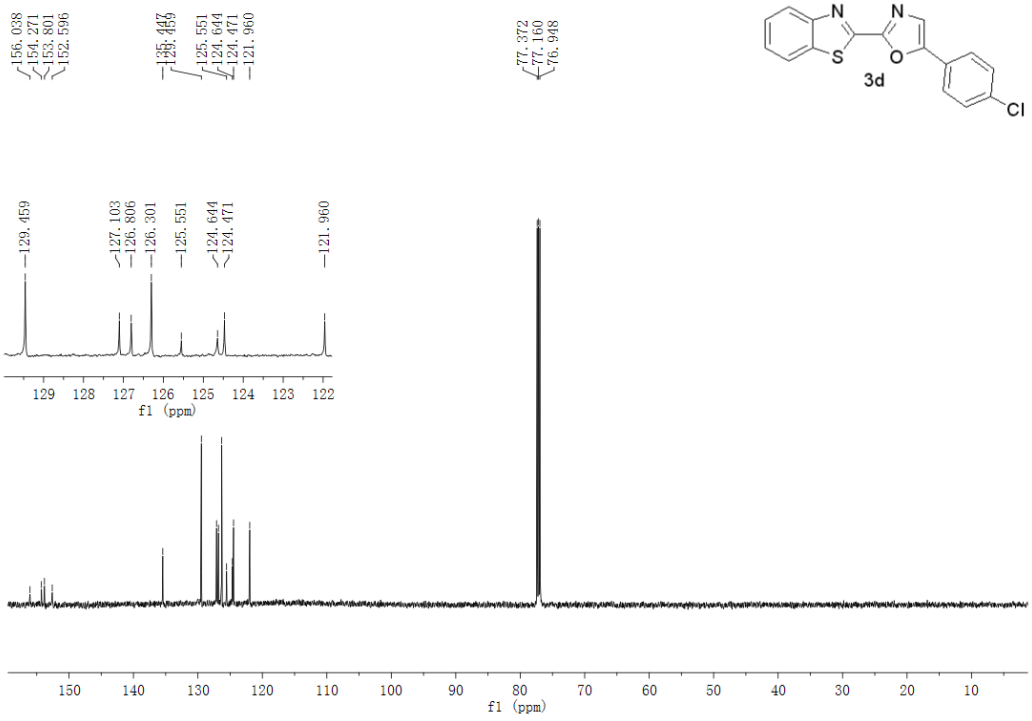
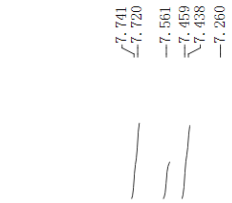
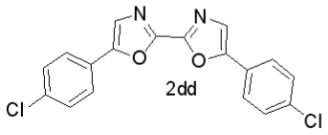
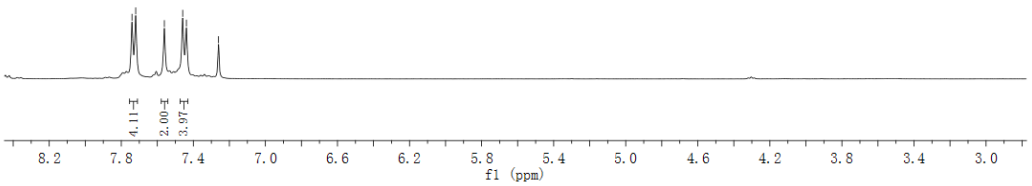
77.160
76.843
133.001
131.021
127.276
127.096
126.763
125.319
124.614
122.030
132
129
126
123
f1 (ppm)
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
N
S
N
O
3c
CN

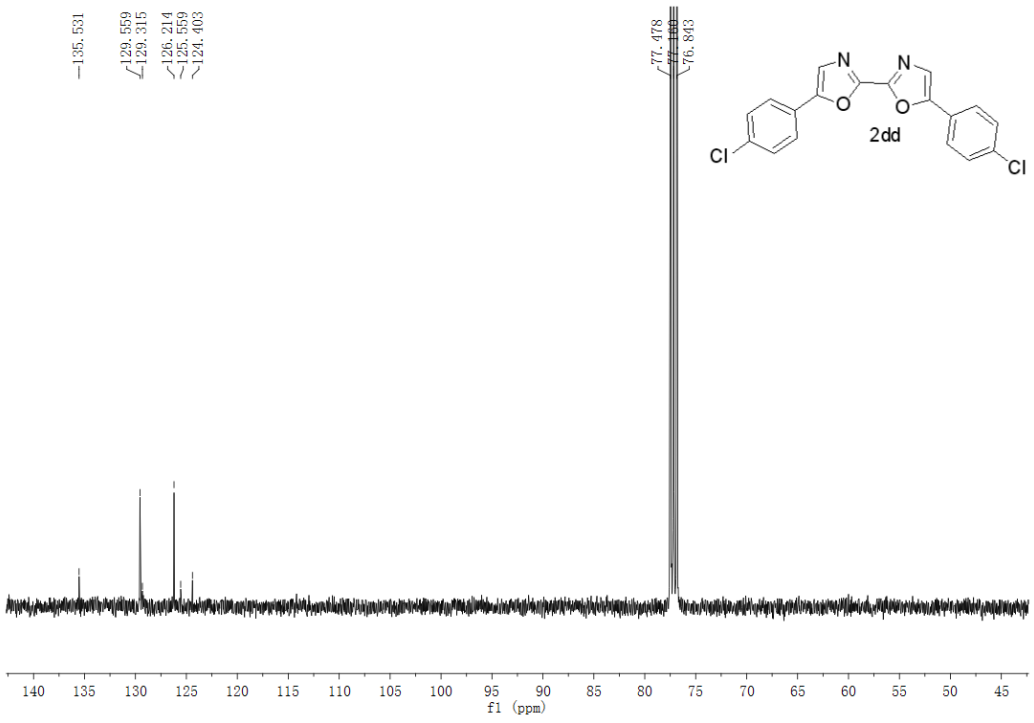

8.213
8.192
7.949
7.742
7.504
7.444
7.260
7.580
7.561
7.549
7.504
7.485
7.466
7.444
7.423
7.55
7.50
7.45
7.40
f1 (ppm)
1.08
1.00
2.09
1.97
1.06
2.01
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
f1 (ppm)
N
N
S
O
3d
Cl

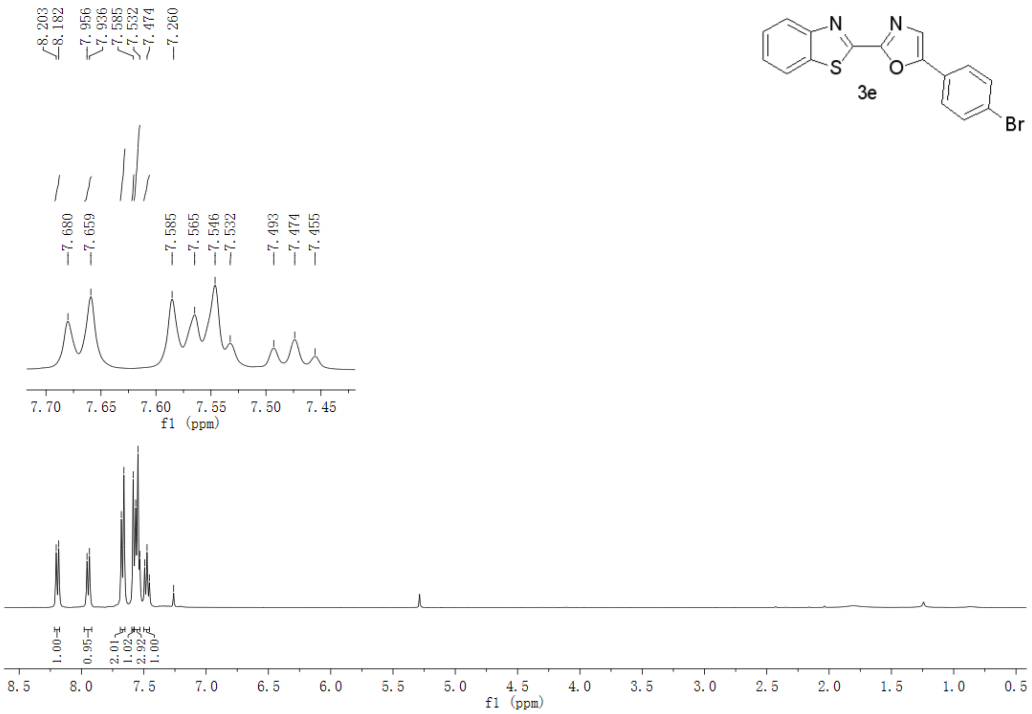

156.038
154.271
153.801
152.596
135.447
129.459
125.551
124.644
124.471
121.960
77.372
77.160
76.948
129.459
127.103
126.806
126.301
125.551
124.644
124.471
121.960
129
128
127
126
125
124
123
122
f1 (ppm)
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)
N
N
S
O
3d
Cl

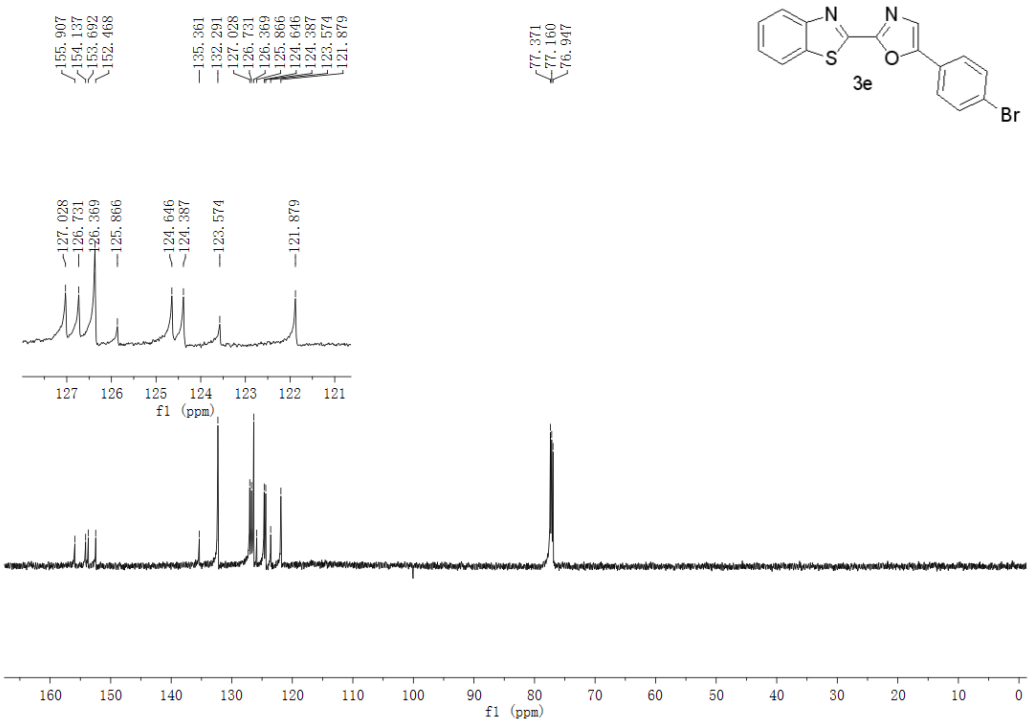

7.741
7.720
7.561
7.459
7.438
7.260

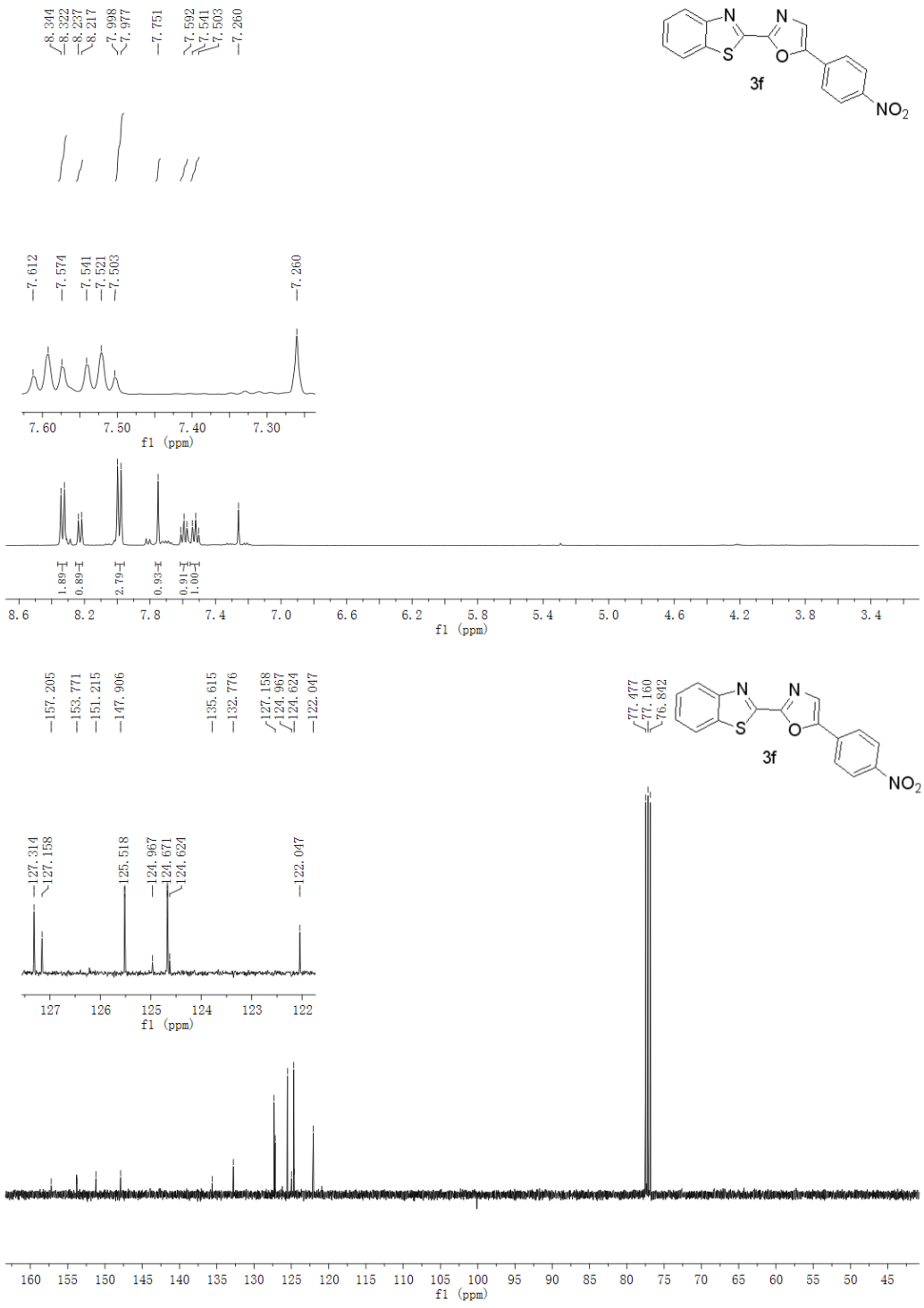

N
N
O
O
Cl
Cl
2dd

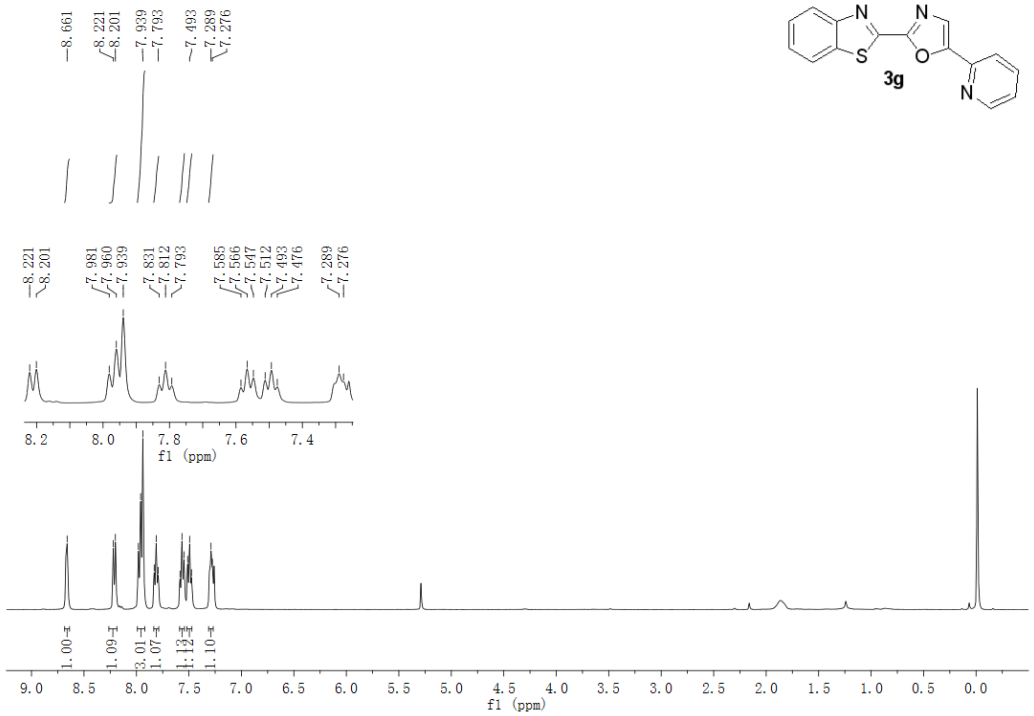

4.11
2.00
3.97
8.2
7.8
7.4
7.0
6.6
6.2
5.8
5.4
5.0
4.6
4.2
3.8
3.4
3.0
f1 (ppm)

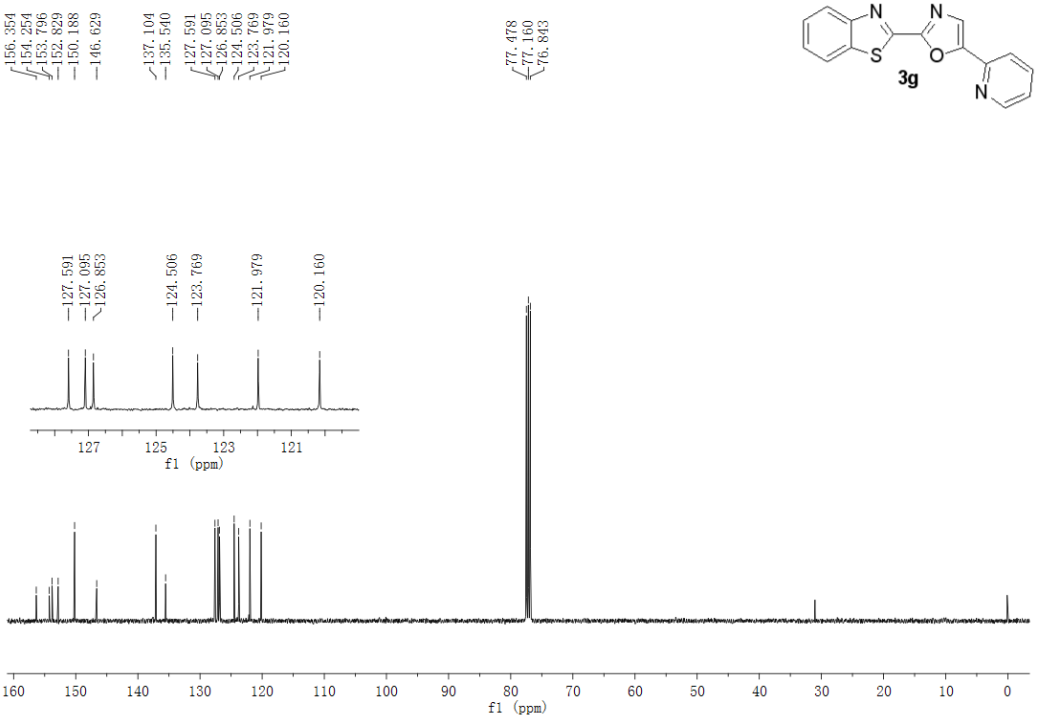

135.531
129.559
129.315
126.214
125.559
124.403
77.478
77.160
76.843
N
N
O
O
Cl
Cl
2dd
140
135
130
125
120
115
110
105
100
95
90
85
80
75
70
65
60
55
50
45
f1 (ppm)

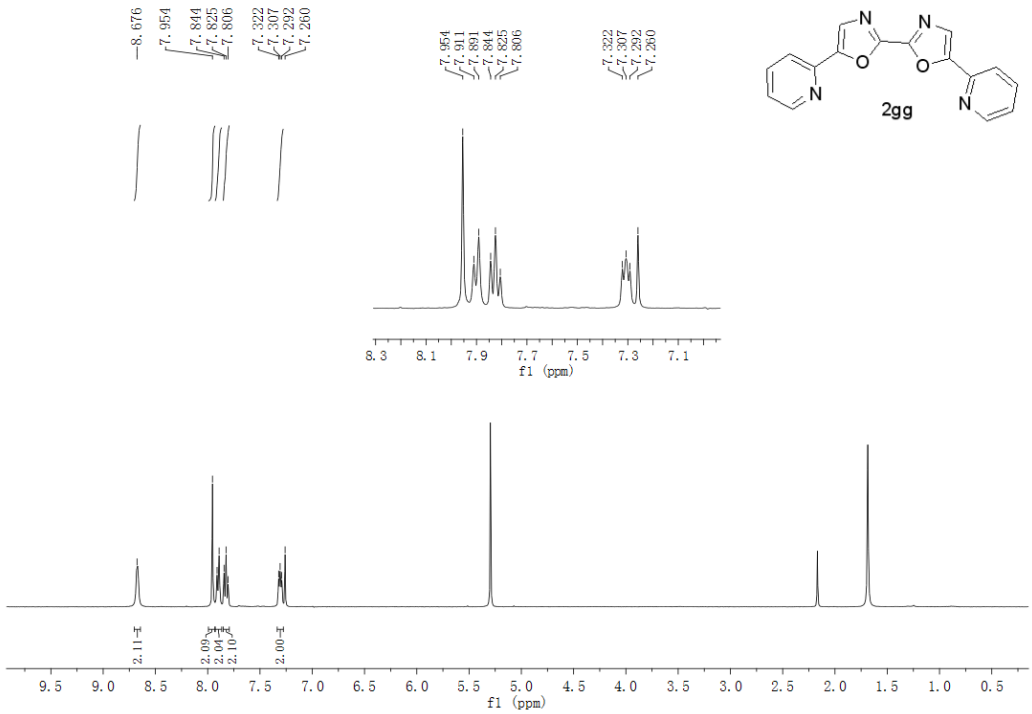

8.203
8.182
7.956
7.936
7.585
7.532
7.474
7.260
3e
Br
7.680
7.659
7.585
7.565
7.546
7.532
7.493
7.474
7.455
f1 (ppm)
1.00
0.95
2.01
1.02
2.92
1.00
f1 (ppm)

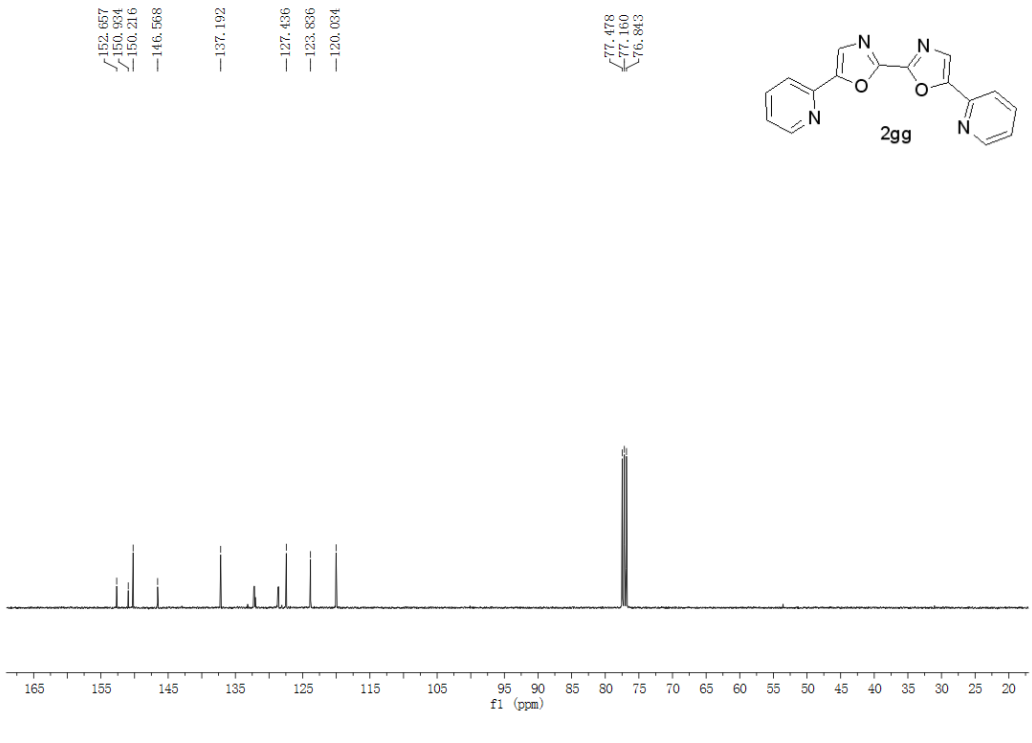

155.907
154.137
153.692
152.468
135.361
132.291
127.028
126.731
126.369
125.866
124.646
124.387
123.574
121.879
77.371
77.160
76.947
3e
Br
127.028
126.731
126.369
125.866
124.646
124.387
123.574
121.879
f1 (ppm)
f1 (ppm)

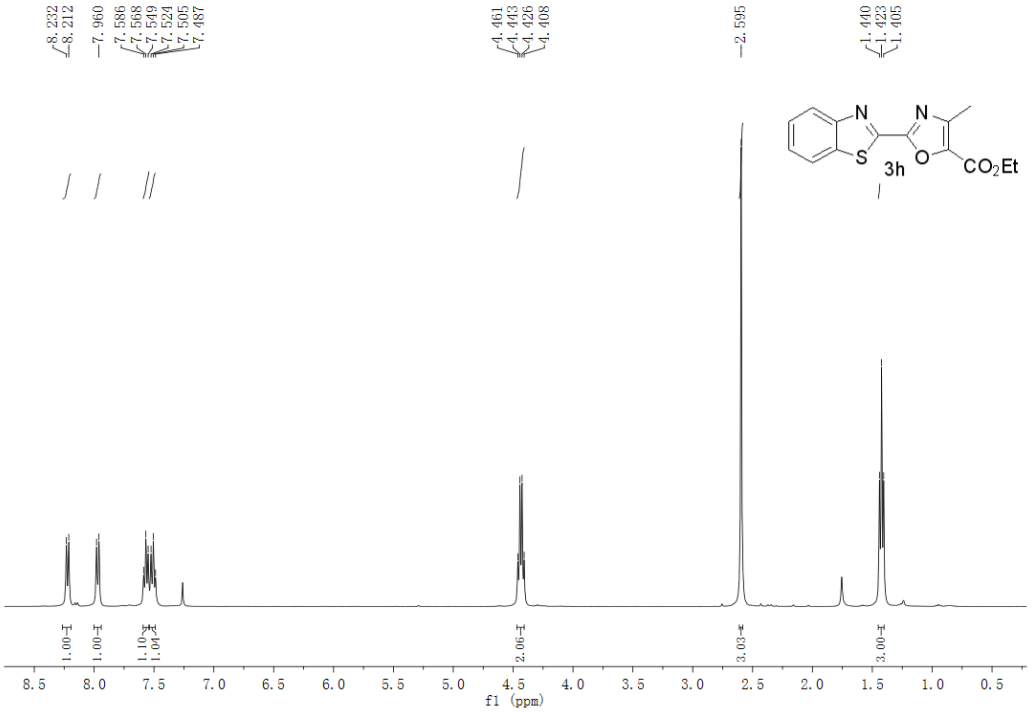

8.344
8.322
8.237
8.217
7.998
7.977
7.751
7.592
7.541
7.503
7.260
3f
NO2
7.612
7.574
7.541
7.521
7.503
7.260
7.60
7.50
7.40
7.30
f1 (ppm)
1.89
0.89
2.79
0.93
0.91
1.00
8.6
8.2
7.8
7.4
7.0
6.6
6.2
5.8
5.4
5.0
4.6
4.2
3.8
3.4
f1 (ppm)
157.205
153.771
151.215
147.906
135.615
132.776
127.158
124.967
124.624
122.047
77.477
77.160
76.842
3f
NO2
127.314
127.158
125.518
124.967
124.671
124.624
122.047
127
126
125
124
123
122
f1 (ppm)
160
155
150
145
140
135
130
125
120
115
110
105
100
95
90
85
80
75
70
65
60
55
50
45
f1 (ppm)

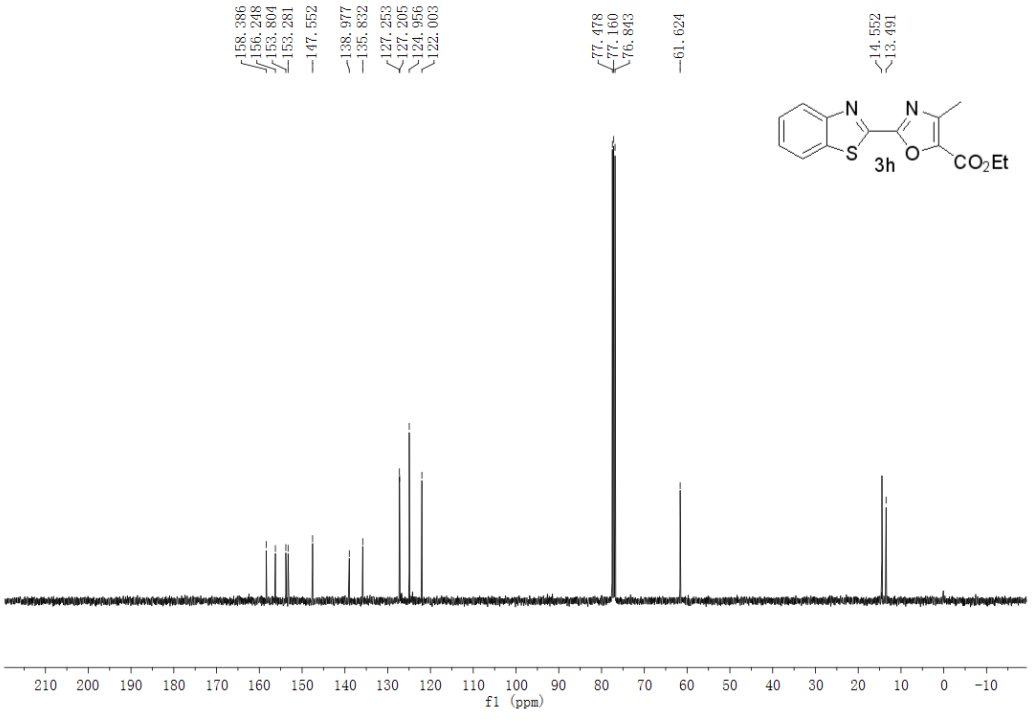

8.661
8.221
8.201
7.939
7.793
7.493
7.289
7.276
3g
f1 (ppm)
1.00
1.09
3.01
1.07
1.13
1.10

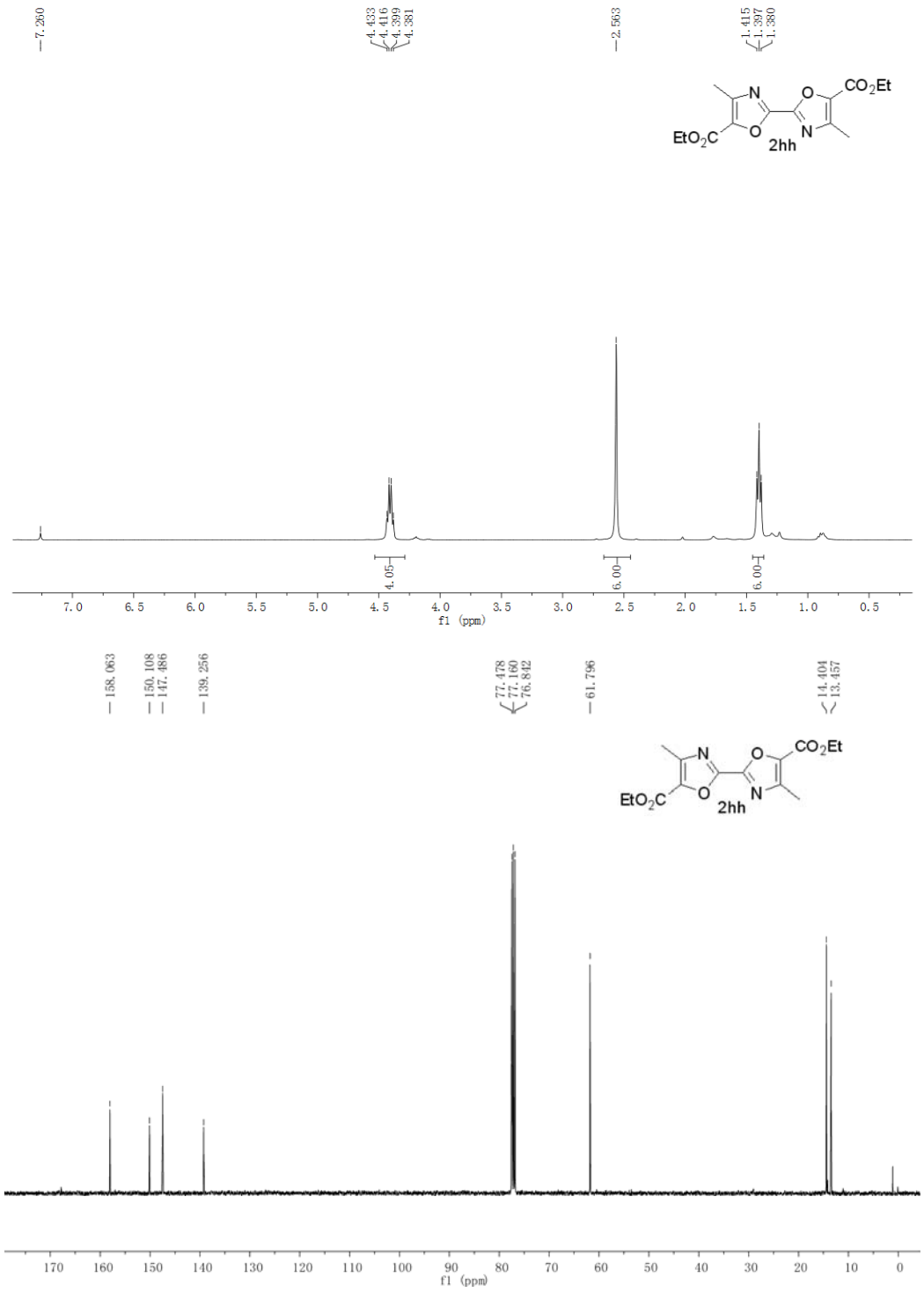

156.354
154.254
153.796
152.829
150.188
146.629
137.104
135.540
127.591
127.095
126.853
124.506
123.769
121.979
120.160
77.478
77.160
76.843
3g
f1 (ppm)

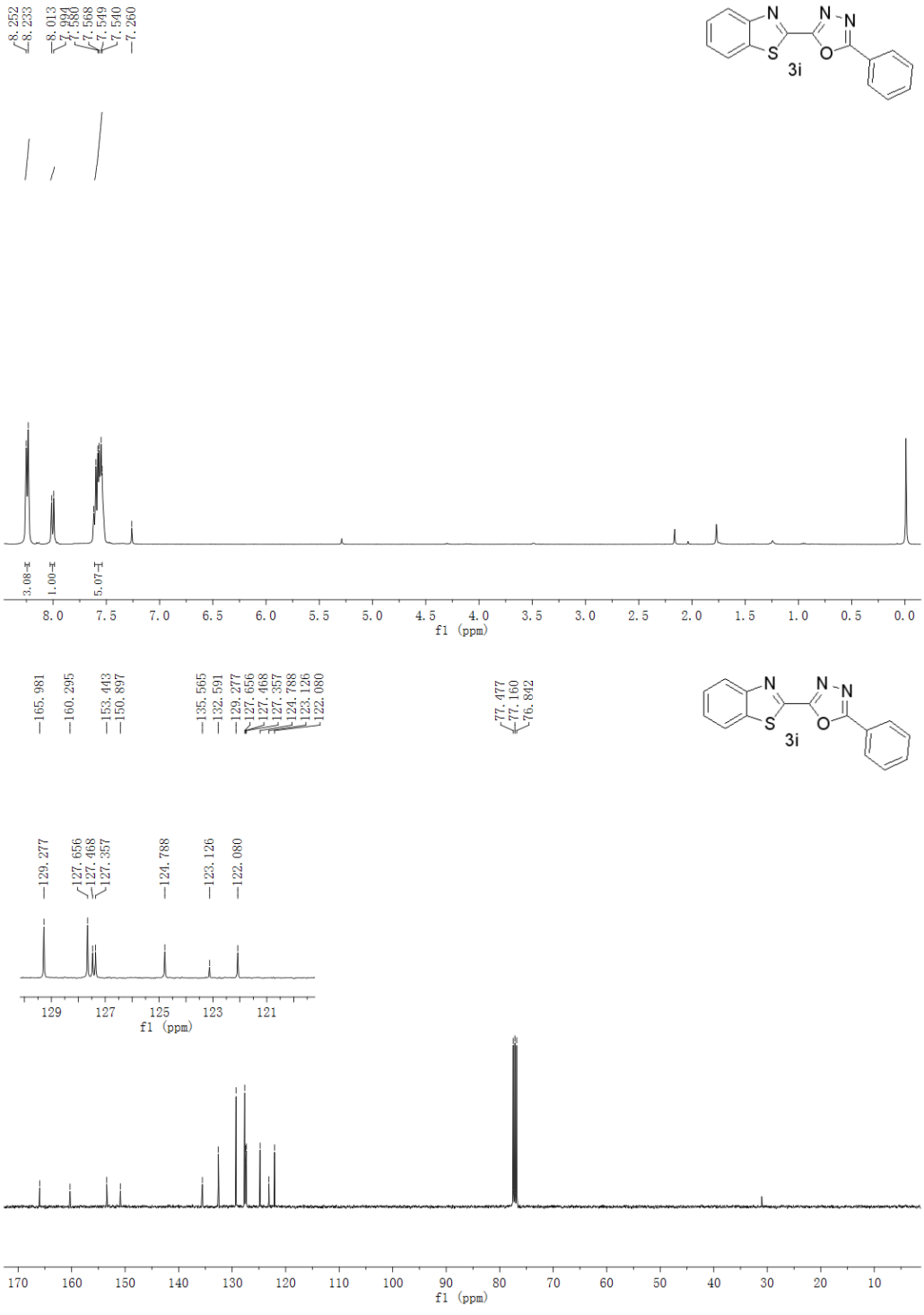

8.676
7.954
7.844
7.825
7.806
7.322
7.307
7.292
7.260
2gg
f1 (ppm)
2.11
2.09
2.04
2.10
2.00

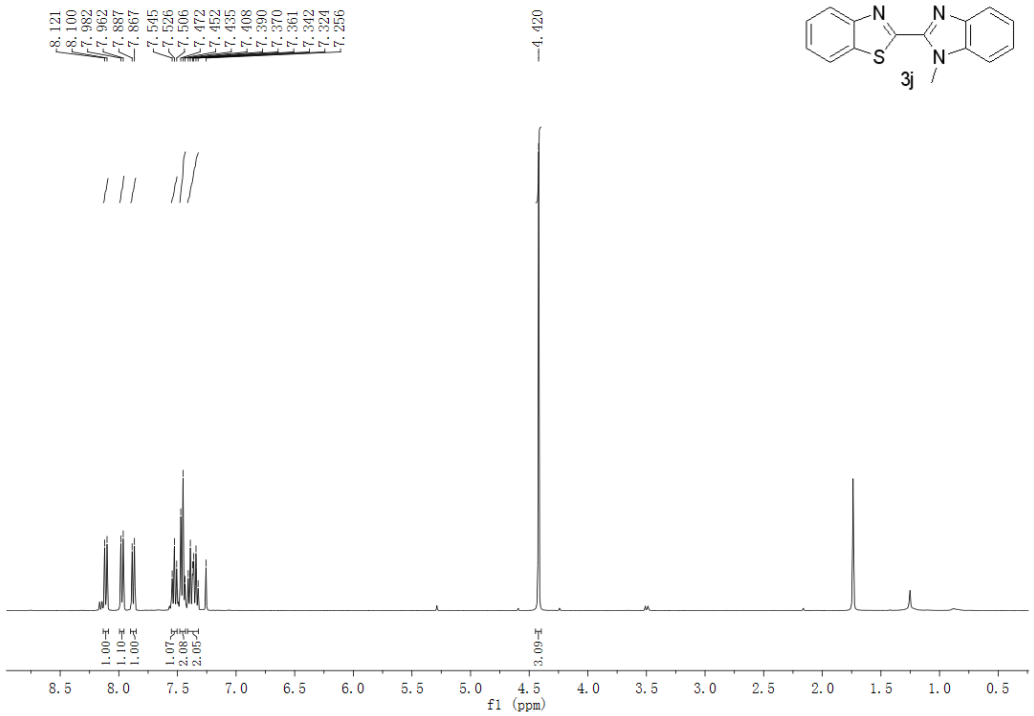

152.657
150.934
150.216
146.568
137.192
127.436
123.836
120.034
77.478
77.160
76.843
2gg
f1 (ppm)

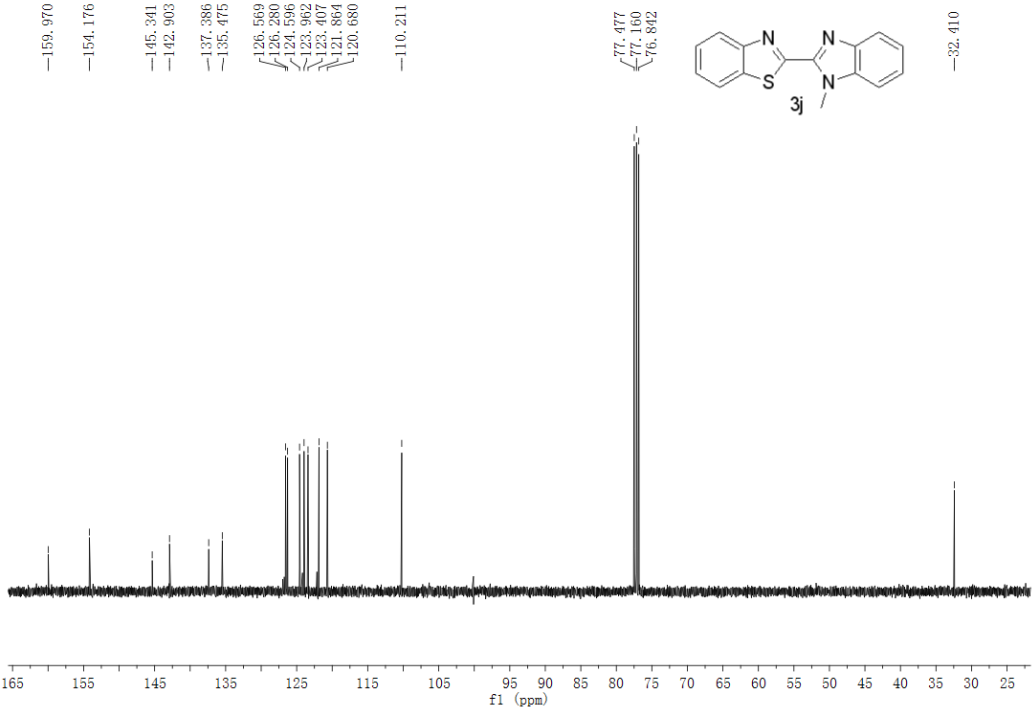

8.232
8.212
7.960
7.586
7.568
7.549
7.524
7.505
7.487
4.461
4.443
4.426
4.408
2.595
1.440
1.423
1.405
3h
CO2Et
1.00
1.00
1.10
1.04
2.06
3.03
3.00
f1 (ppm)

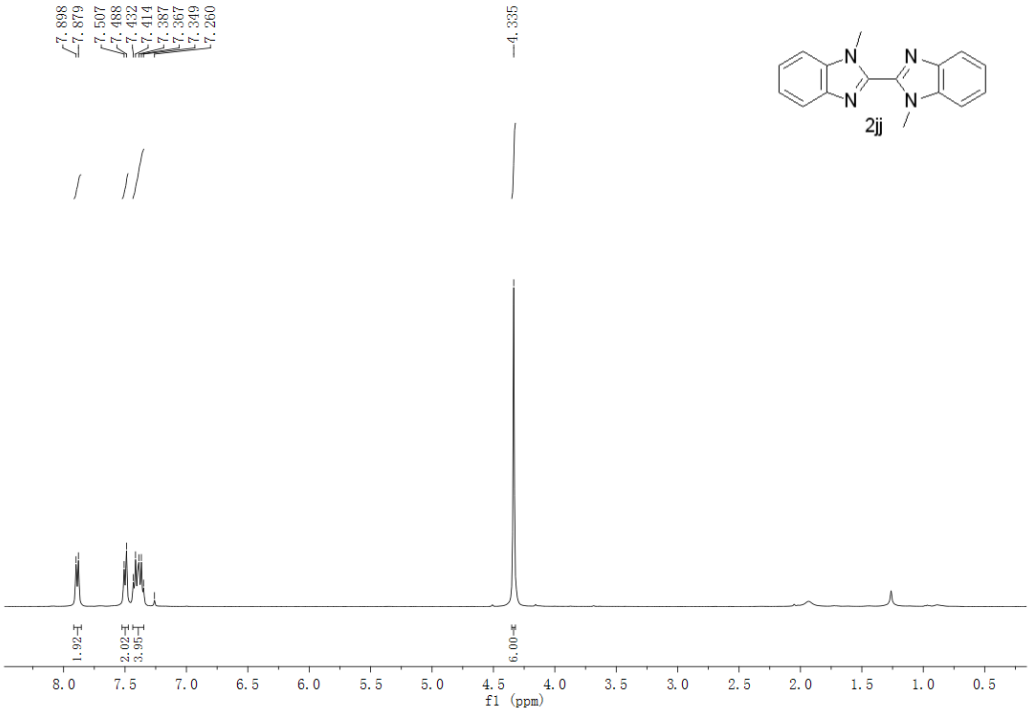

158.386
156.248
153.804
153.281
147.552
138.977
135.832
127.253
127.205
124.956
122.003
77.478
77.160
76.843
61.624
14.552
13.491
3h
CO2Et
f1 (ppm)

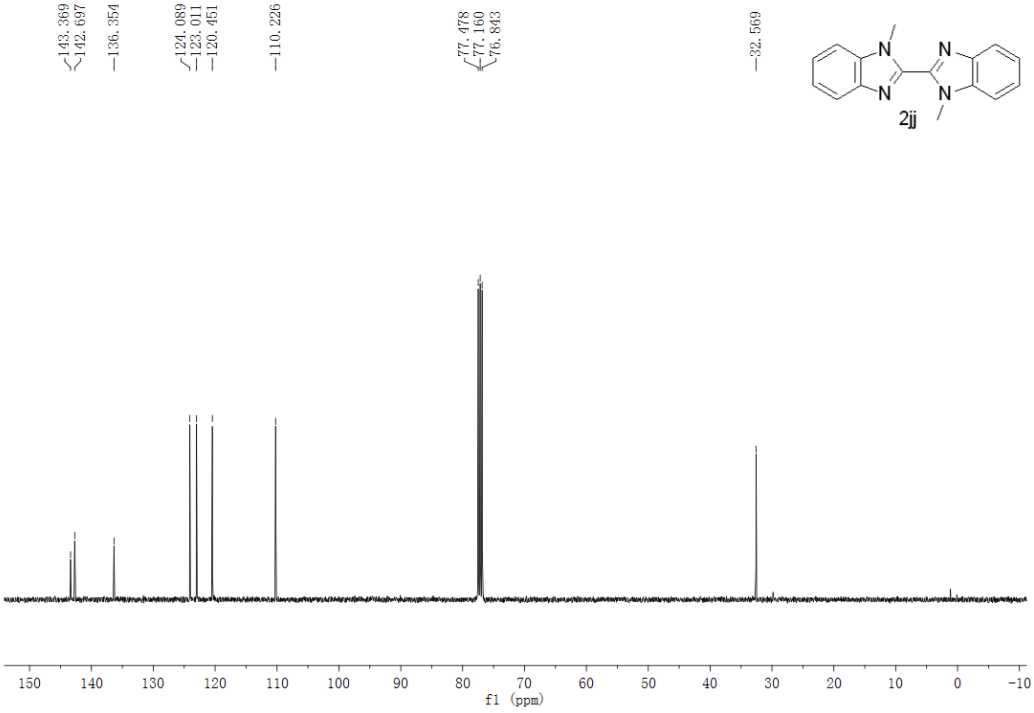

7.260
4.433
4.416
4.399
4.381
2.563
1.415
1.397
1.380
CO2Et
EtO2C
2hh
4.05
6.00
6.00
f1 (ppm)
158.063
150.108
147.486
139.256
77.478
77.160
76.842
61.796
14.404
13.457
CO2Et
EtO2C
2hh
f1 (ppm)

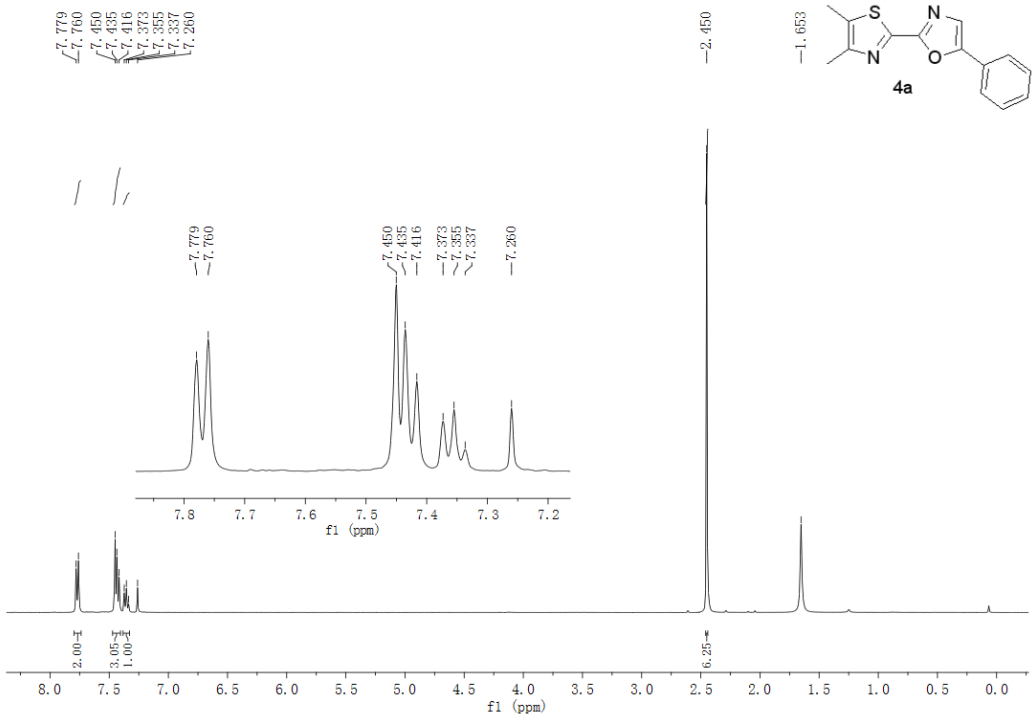

8.252
8.233
8.013
7.994
7.580
7.568
7.549
7.540
7.260
3i
3.08
1.00
5.07
f1 (ppm)
165.981
160.295
153.443
150.897
135.565
132.591
129.277
127.656
127.468
127.357
124.788
123.126
122.080
77.477
77.160
76.842
3i
f1 (ppm)
f1 (ppm)

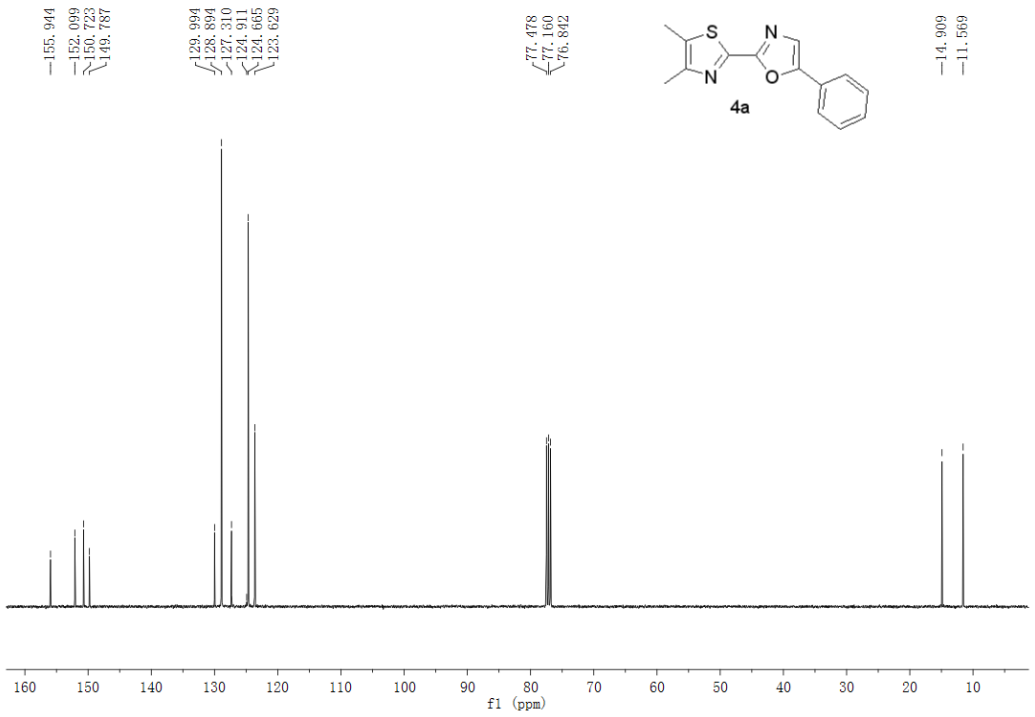

8.121
8.100
7.982
7.962
7.887
7.867
7.545
7.526
7.506
7.472
7.452
7.435
7.408
7.390
7.370
7.361
7.342
7.324
7.256
4.420
3j
1.00
1.10
1.00
1.07
2.08
2.05
3.09
f1 (ppm)

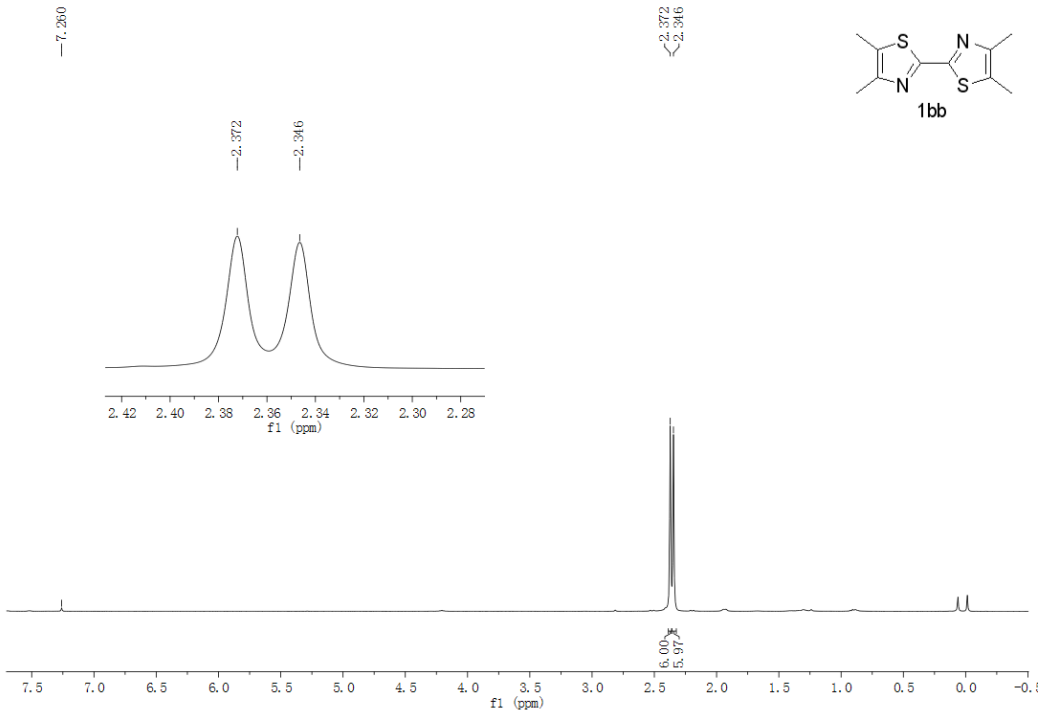

159.970
154.176
145.341
142.903
137.386
135.475
126.569
126.280
124.596
123.962
123.407
121.864
120.680
110.211
77.477
77.160
76.842
32.410
3j
f1 (ppm)

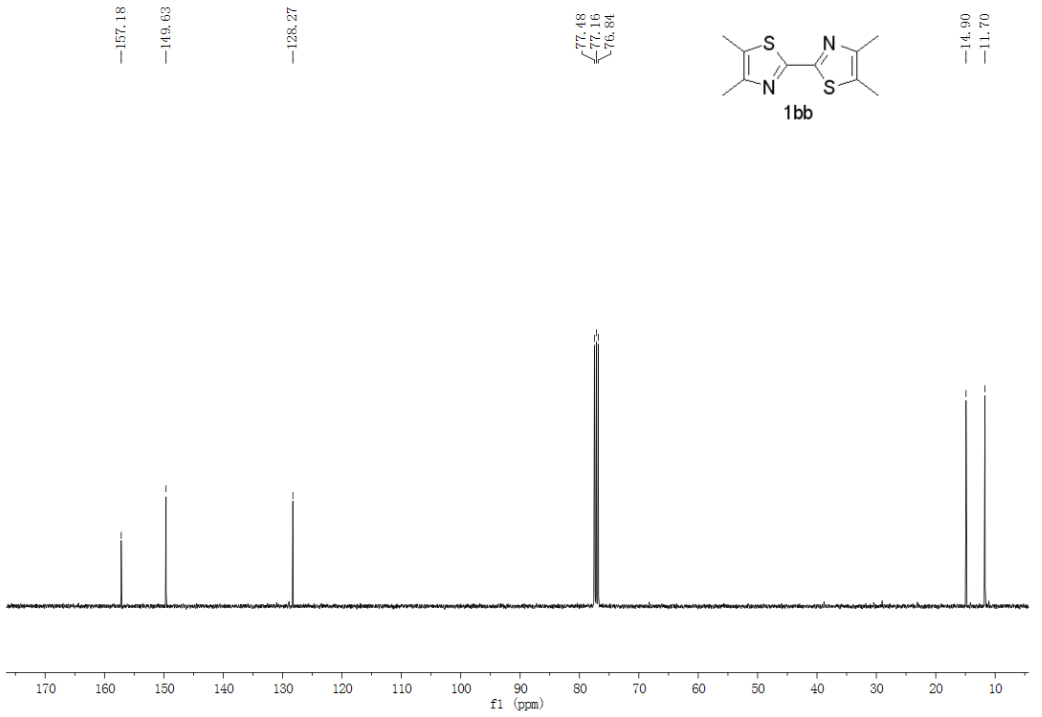

7.898
7.879
7.507
7.488
7.432
7.414
7.387
7.367
7.349
7.260
4.335
2jj
1.92
2.02
3.96
6.00
f1 (ppm)

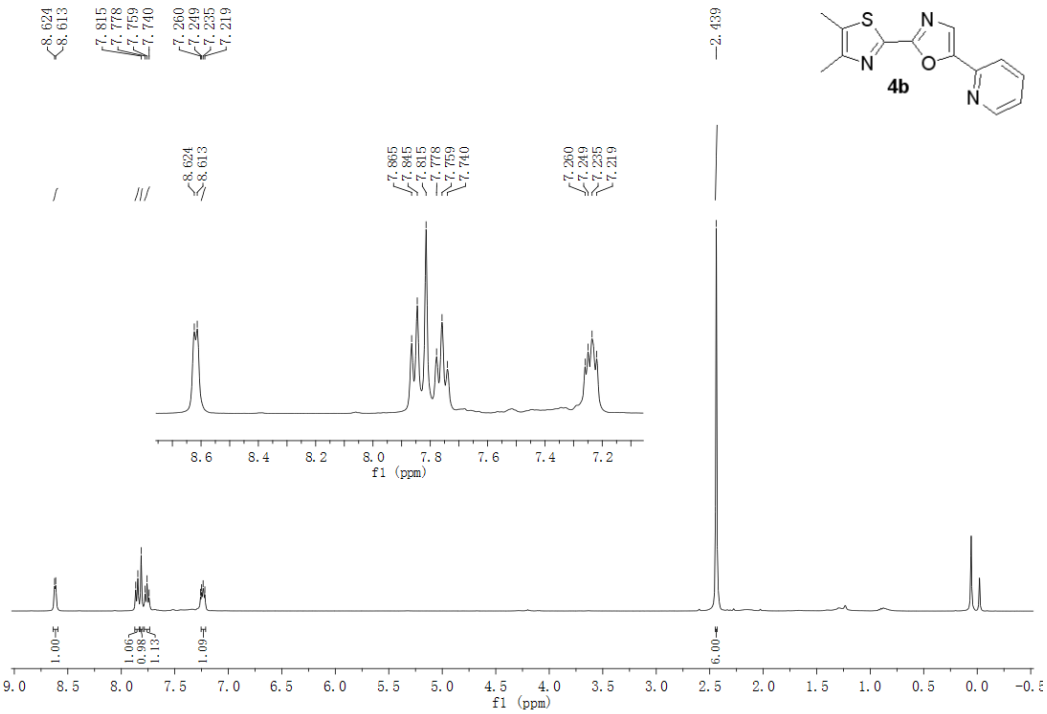

143.369
142.697
136.354
124.089
123.011
120.451
110.226
77.478
77.160
76.843
32.569
2jj
f1 (ppm)

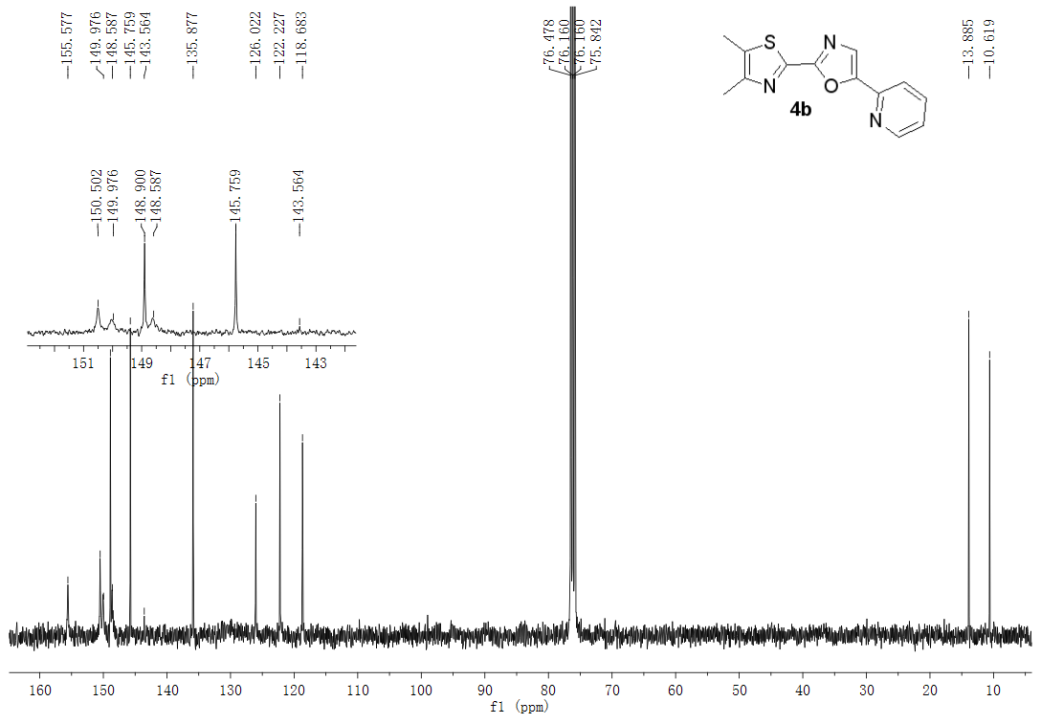

7.779
7.760
7.450
7.435
7.416
7.373
7.355
7.337
7.260
2.450
1.653
4a
f1 (ppm)
2.00
3.05
1.00
6.25

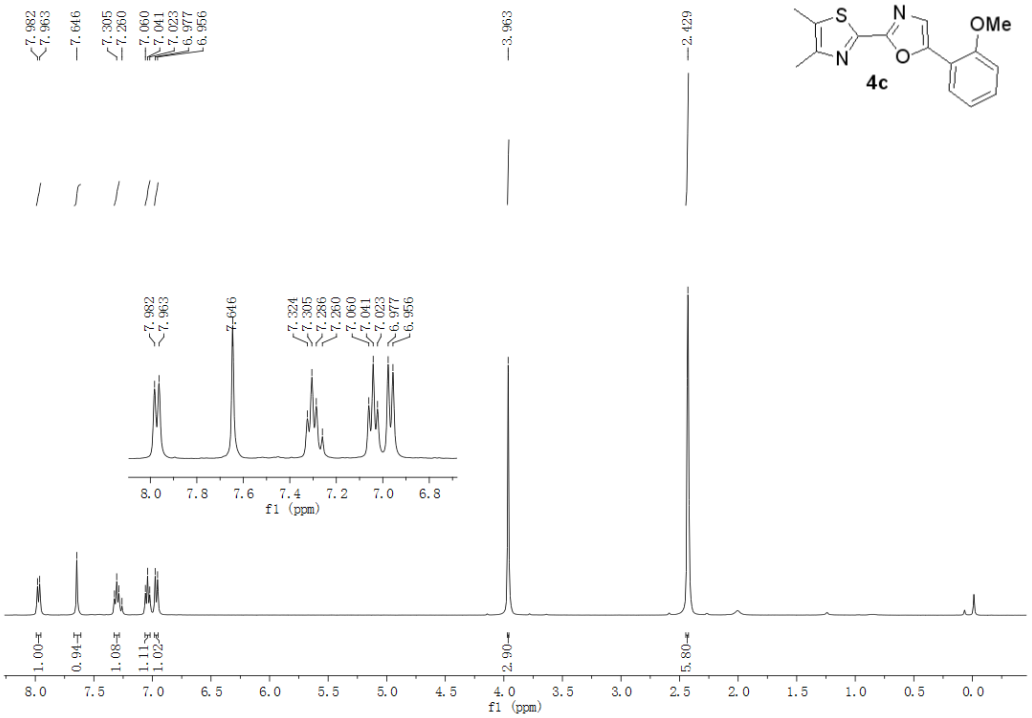

155.944
152.099
150.723
149.787
129.994
128.894
127.310
124.911
124.665
123.629
77.478
77.160
76.842
14.909
11.569
4a
f1 (ppm)

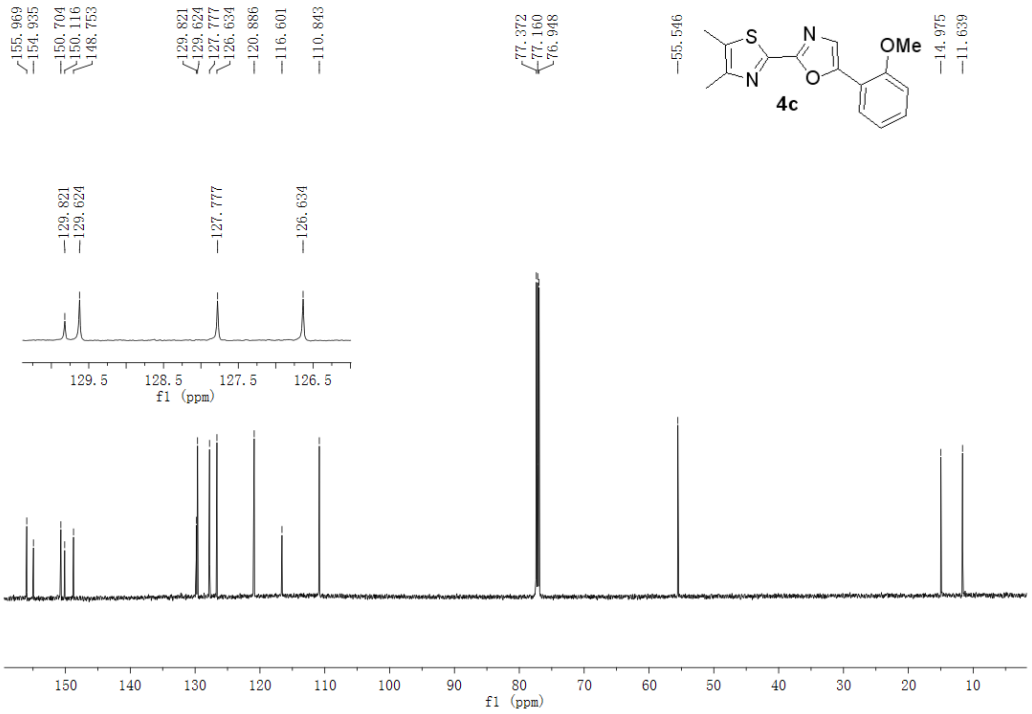

7.260
2.372
2.346
1bb
2.372
2.346
2.42 2.40 2.38 2.36 2.34 2.32 2.30 2.28
f1 (ppm)
6.00
5.97
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

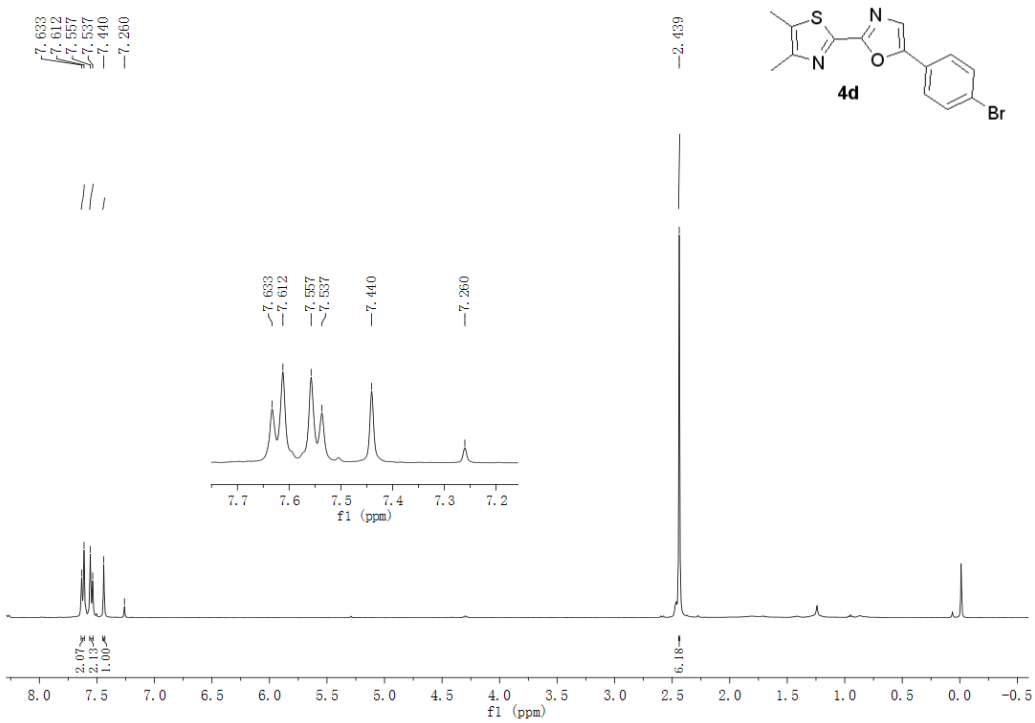

157.18
149.63
128.27
77.48
77.16
76.84
1bb
14.90
11.70
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

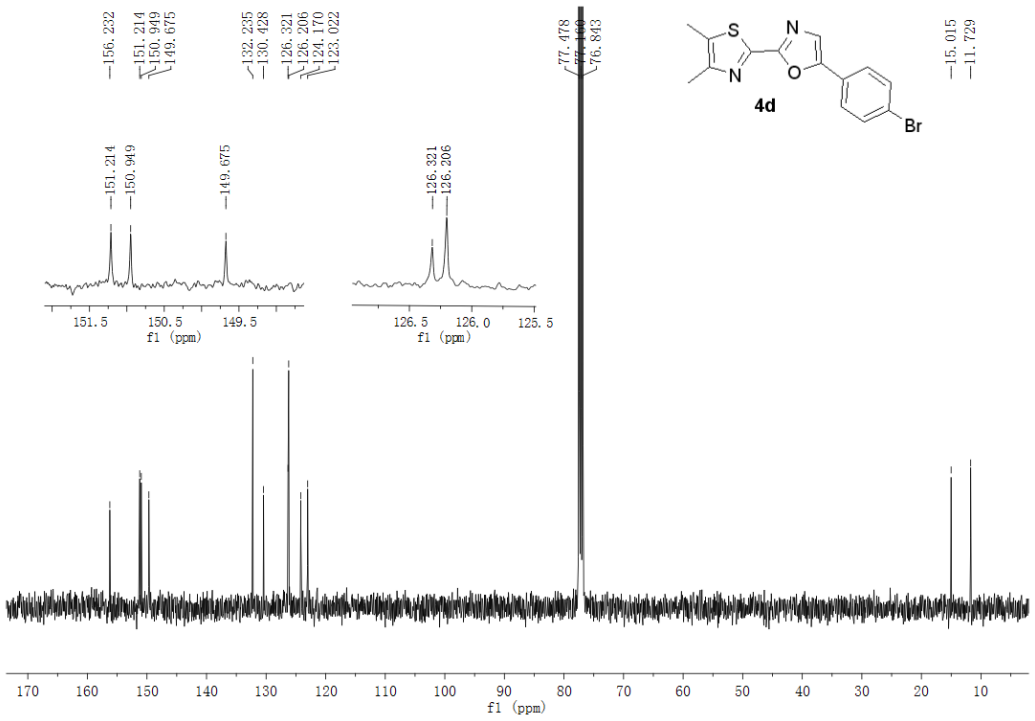

8.624
8.613
7.815
7.778
7.759
7.740
7.260
7.249
7.235
7.219
2.439
4b
f1 (ppm)
1.00
1.06
0.98
1.13
1.09
6.00

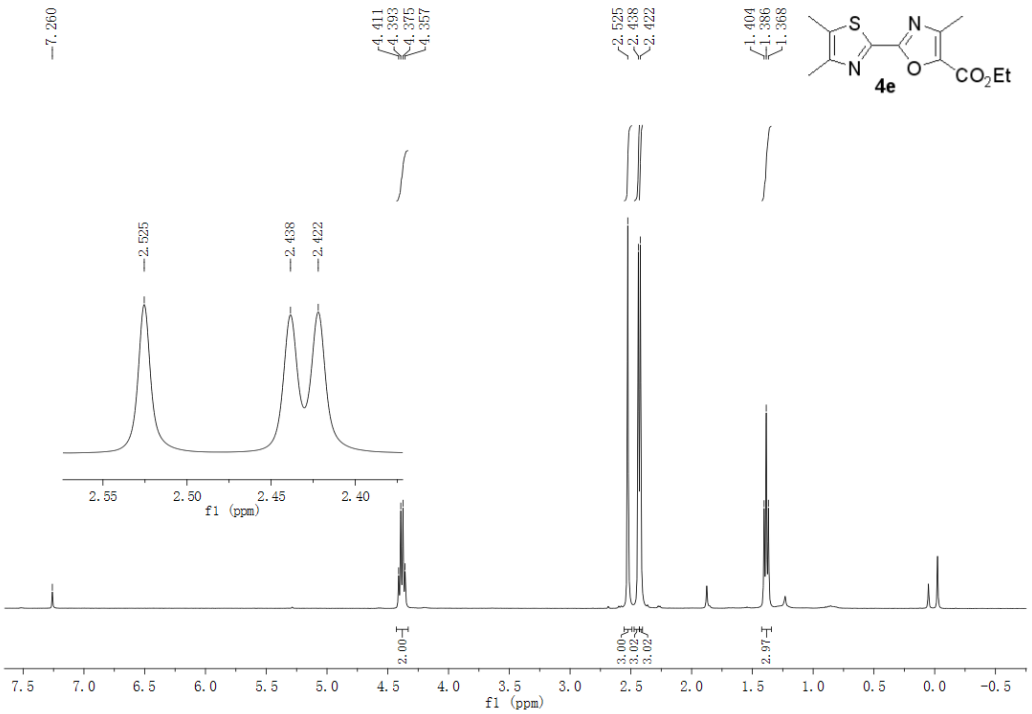

155.577
149.976
148.587
145.759
143.564
135.877
126.022
122.227
118.683
76.478
76.160
75.842
13.885
10.619
4b
150.502
149.976
148.900
148.587
145.759
143.564
f1 (ppm)

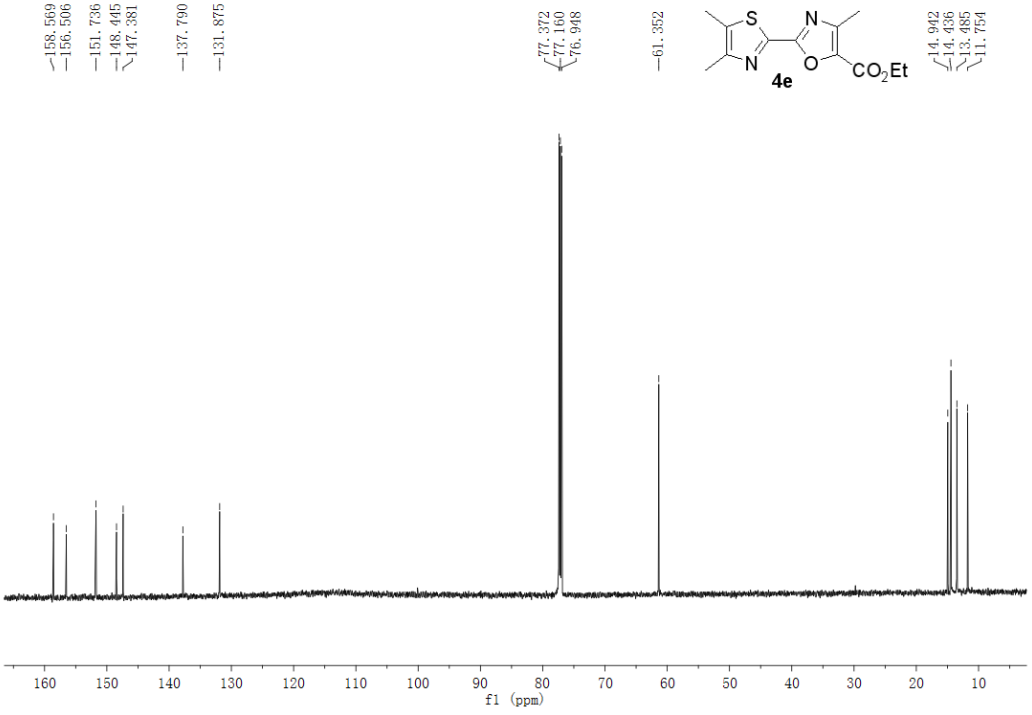

7.982
7.963
7.646
7.305
7.260
7.060
7.041
7.023
6.977
6.956
3.963
2.429
S
N
N
O
OMe
4c
f1 (ppm)
1.00
0.94
1.08
1.11
1.02
2.90
5.80


155.969
154.935
150.704
150.116
148.753
129.821
129.624
127.777
126.634
120.886
116.601
110.843
77.372
77.160
76.948
55.546
14.975
11.639
S
N
N
O
OMe
4c
f1 (ppm)


7.633
7.612
7.557
7.537
7.440
7.260
2.439
4d
Br
2.07
2.13
1.00
6.18
f1 (ppm)


156.232
151.214
150.949
149.675
132.235
130.428
126.321
126.206
124.170
123.022
77.478
77.160
76.843
15.015
11.729
4d
Br
f1 (ppm)


7.260
4.411
4.393
4.375
4.357
2.525
2.438
2.422
1.404
1.386
1.368
4e
2.525
2.438
2.422
2.55
2.50
2.45
2.40
f1 (ppm)
2.00
3.00
3.02
3.02
2.97
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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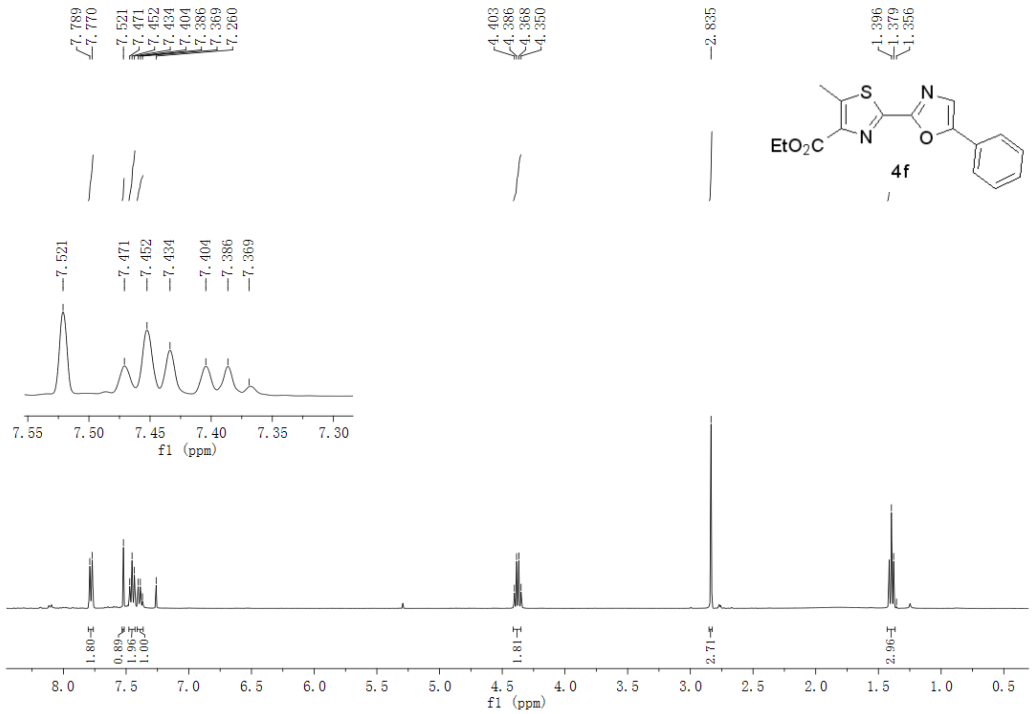
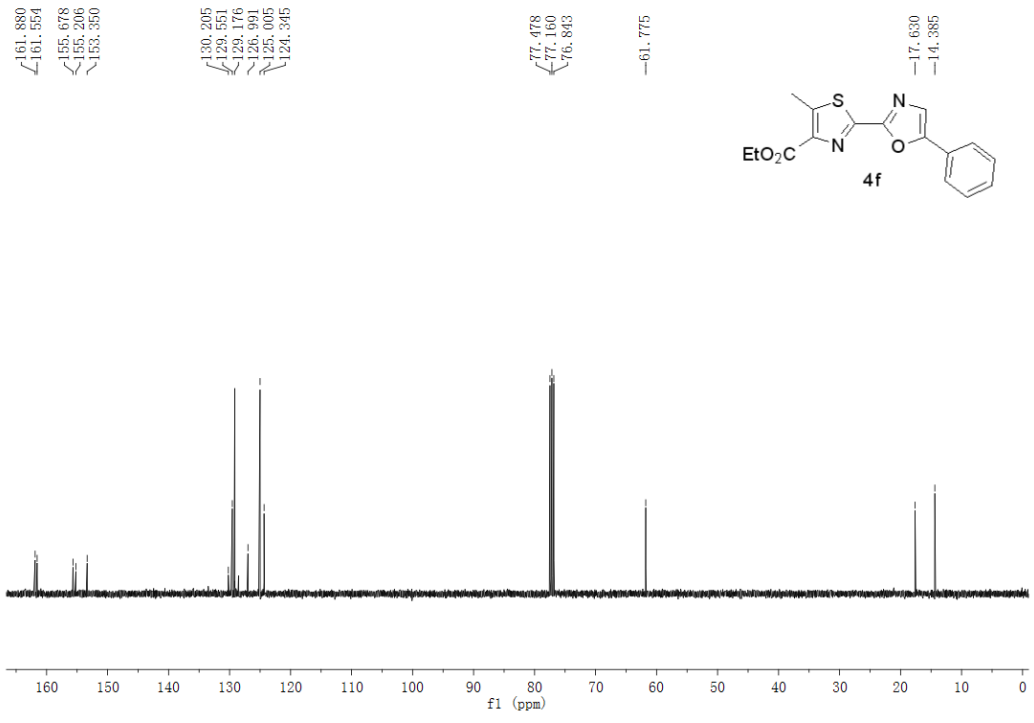
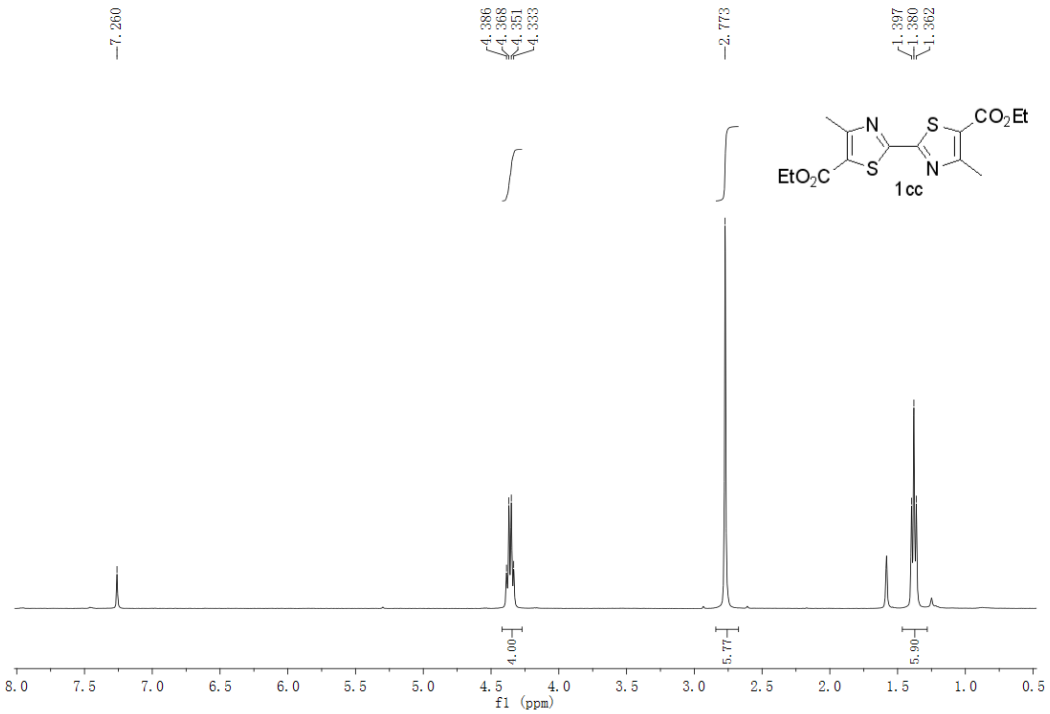
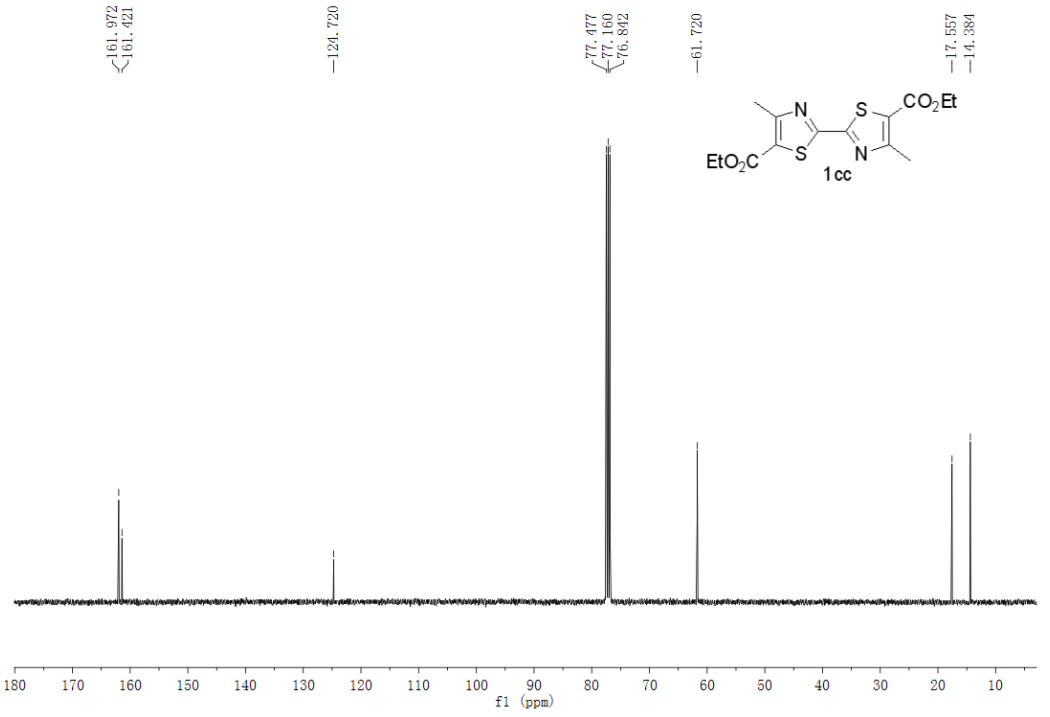
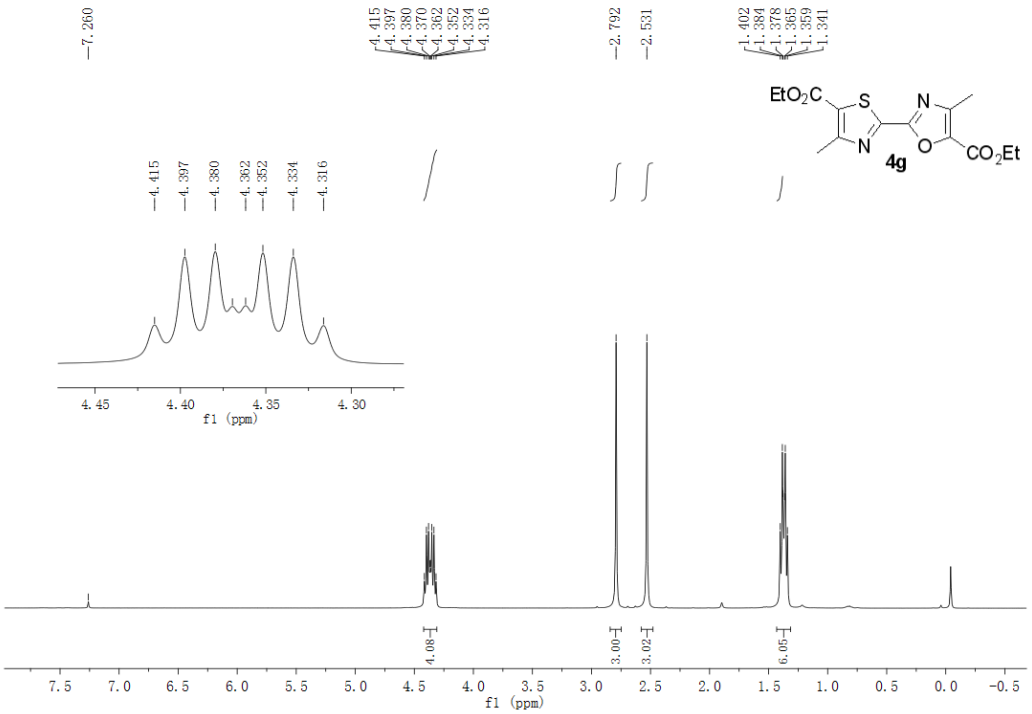
156.506
151.736
148.445
147.381
137.790
131.875
77.372
77.160
76.948
61.352
14.942
14.436
13.485
11.754
4e
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

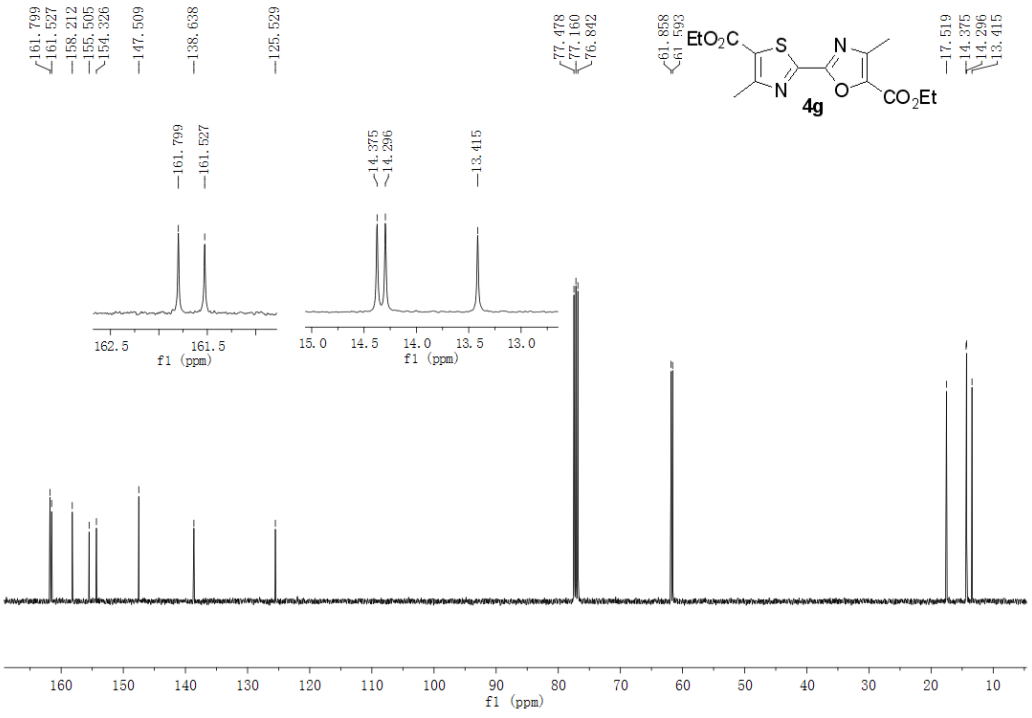

7.789
7.770
7.521
7.471
7.452
7.434
7.404
7.386
7.369
7.260
4.403
4.386
4.368
4.350
2.835
1.396
1.379
1.356
EtO2C
4f
f1 (ppm)
1.80
0.89
1.96
1.00
1.81
2.71
2.96

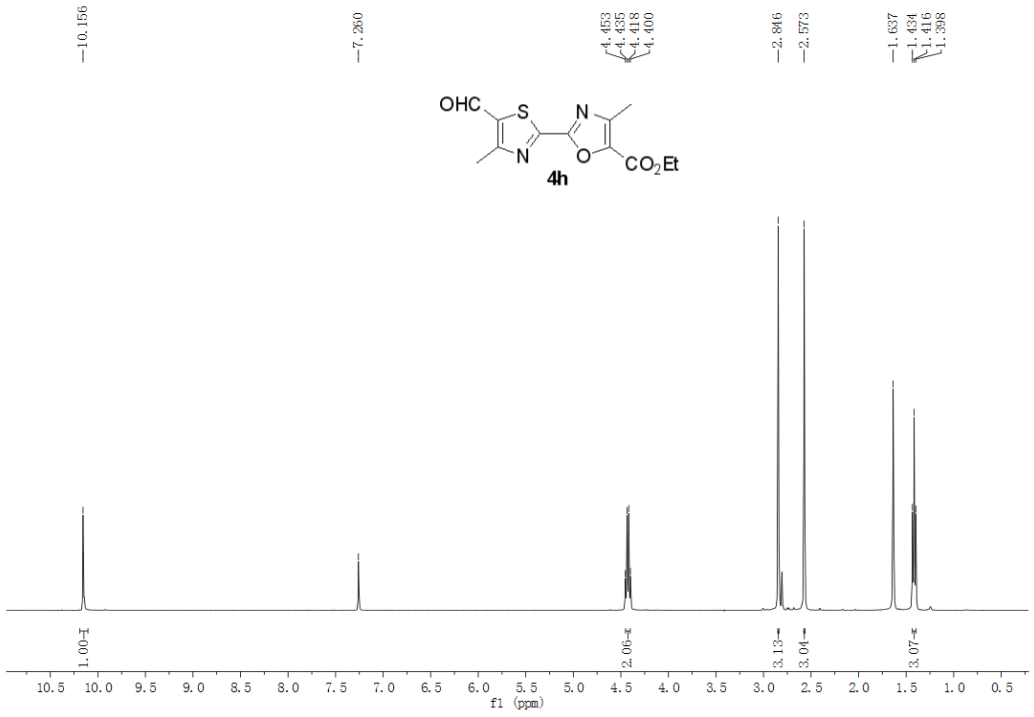

161.880
161.554
155.678
155.206
153.350
130.205
129.551
129.176
126.991
125.005
124.345
77.478
77.160
76.843
61.775
17.630
14.385
EtO2C
4f
f1 (ppm)

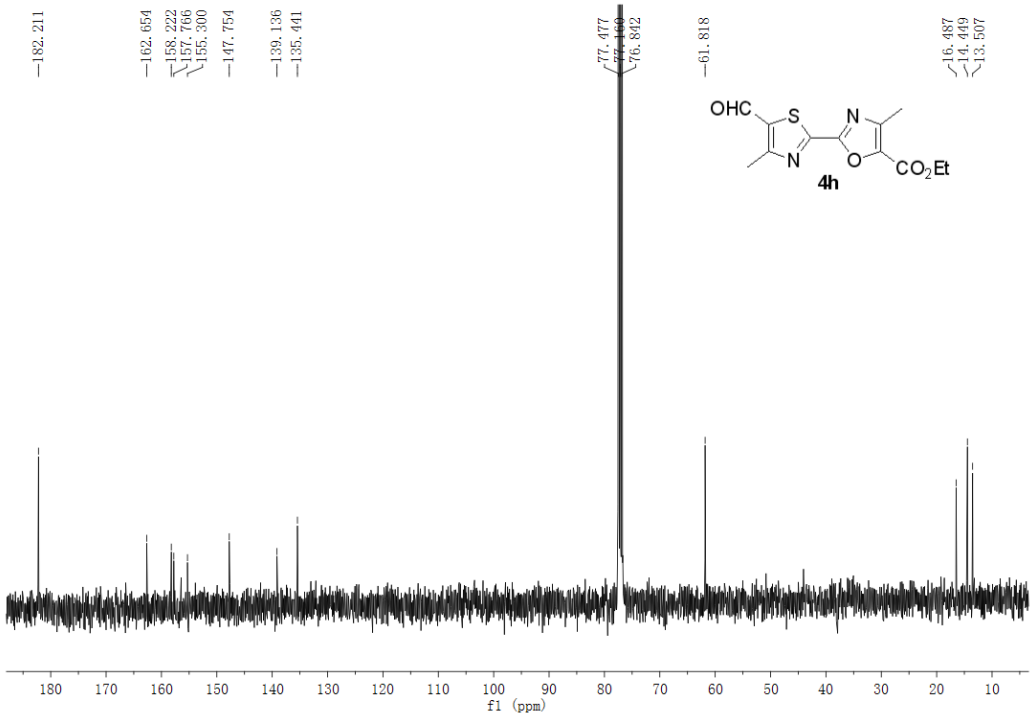

7.260
4.386
4.368
4.351
4.333
2.773
1.397
1.380
1.362
4.00
5.77
5.90
f1 (ppm)
1cc

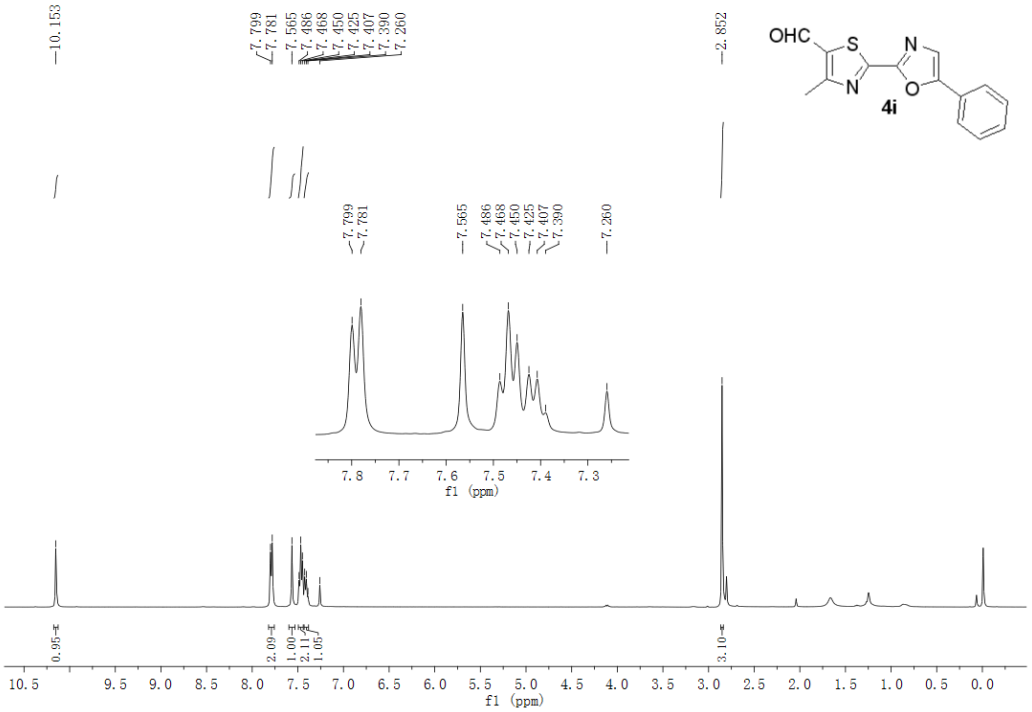

161.972
161.421
124.720
77.477
77.160
76.842
61.720
17.557
14.384
f1 (ppm)
1cc

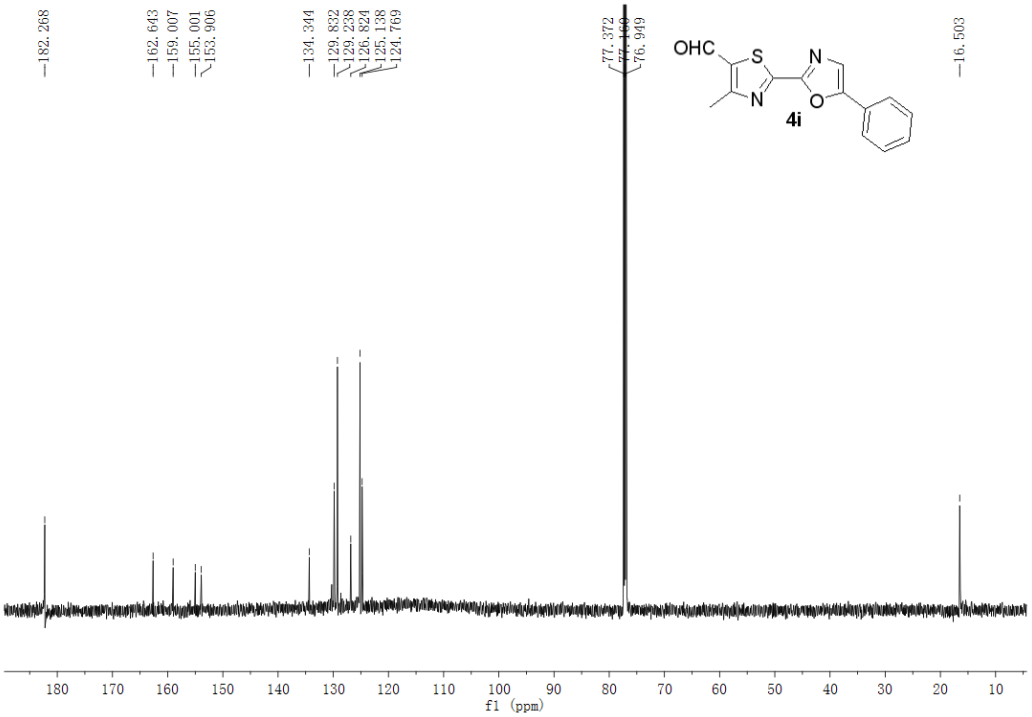

7.260
4.415
4.397
4.380
4.370
4.362
4.352
4.334
4.316
2.792
2.531
1.402
1.384
1.378
1.365
1.359
1.341
EtO2C
S
N
N
O
CO2Et
4g
4.08
3.00
3.02
6.05
f1 (ppm)

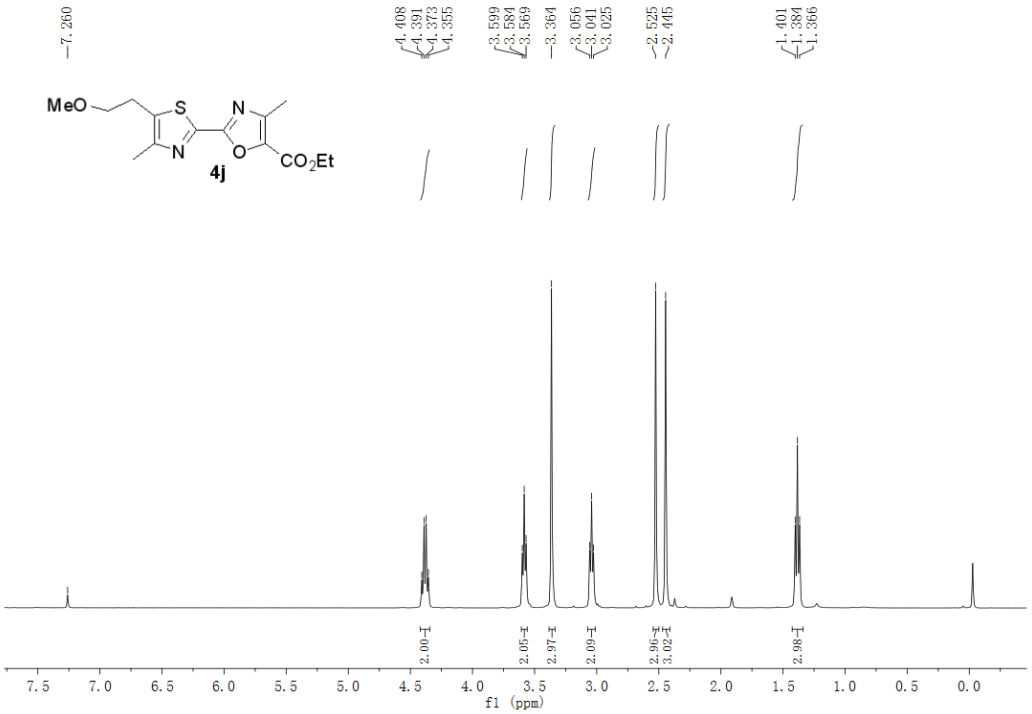

161.799
161.527
158.212
155.505
154.326
147.509
138.638
125.529
77.478
77.160
76.842
61.858
61.593
17.519
14.375
14.296
13.415
EtO2C
S
N
N
O
CO2Et
4g
f1 (ppm)

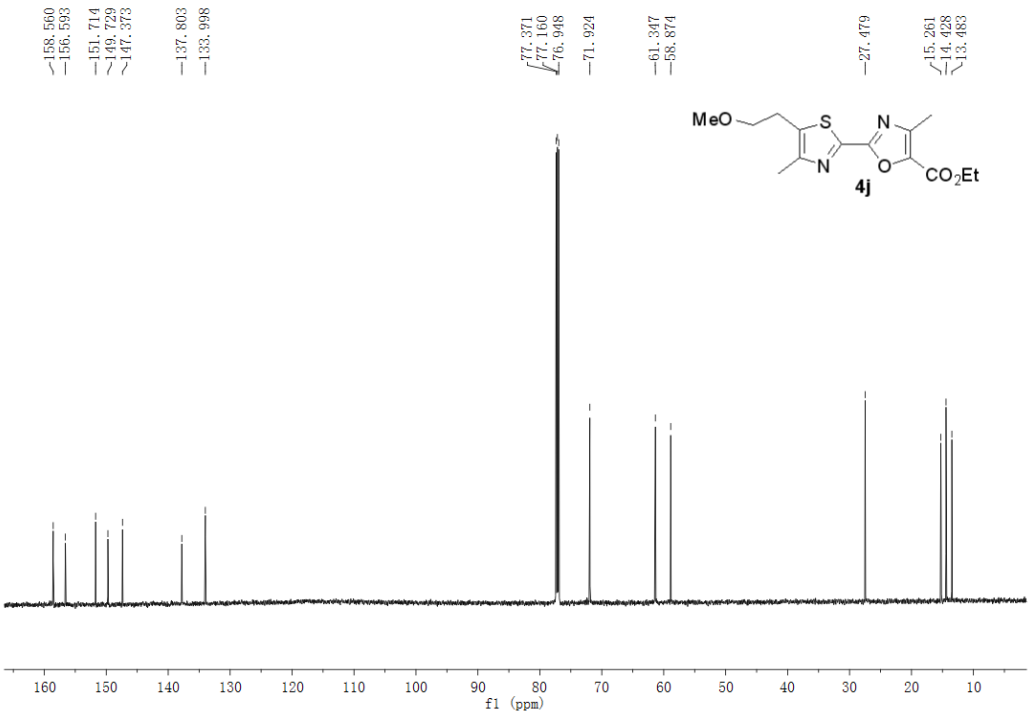

10.156
7.260
4.453
4.435
4.418
4.400
2.846
2.573
1.637
1.434
1.416
1.398
OHC
S
N
N
O
CO2Et
4h
1.00
2.06
3.13
3.04
3.07
f1 (ppm)

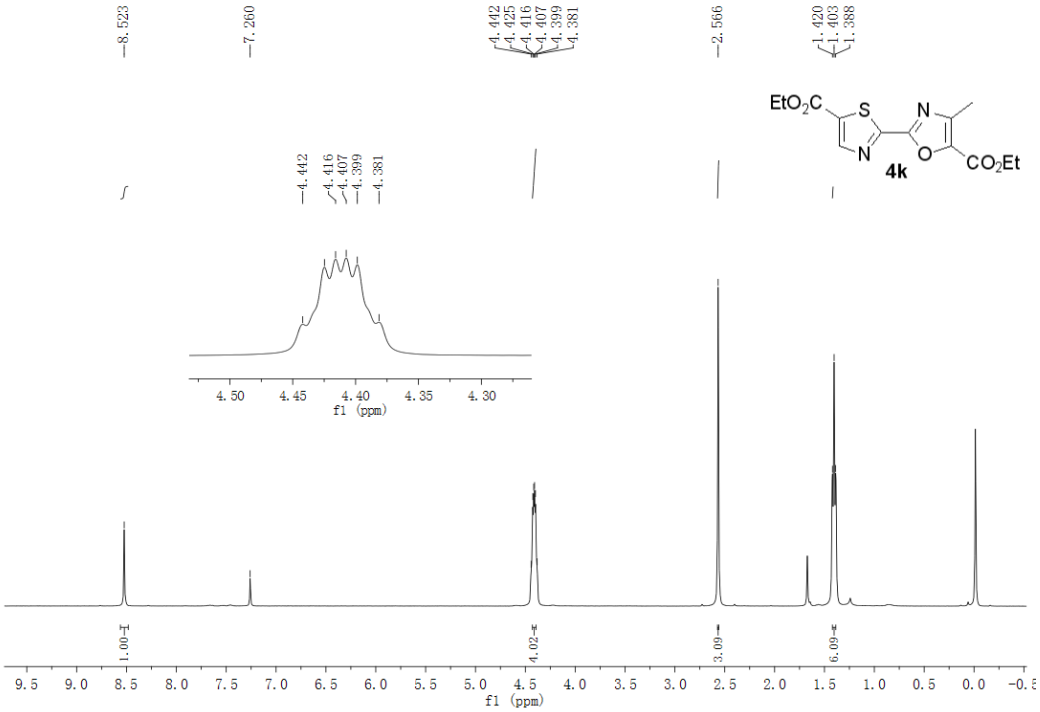

182.211
162.654
158.222
157.766
155.300
147.754
139.136
135.441
77.477
77.160
76.842
61.818
16.487
14.449
13.507
OHC
S
N
N
O
CO2Et
4h
f1 (ppm)

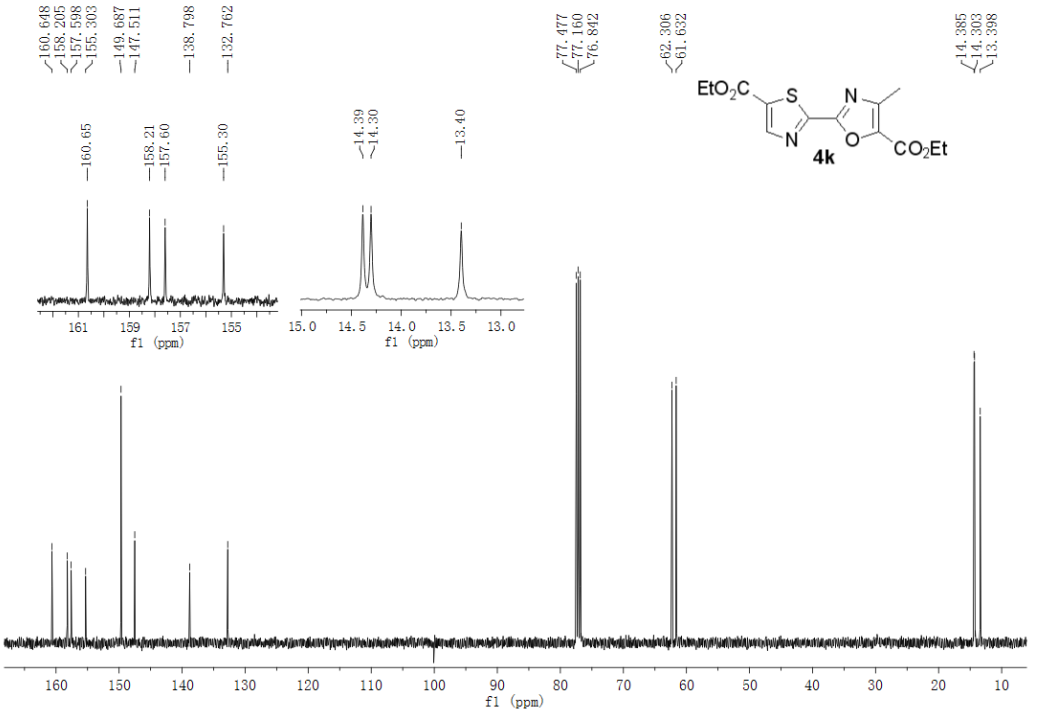

10.153
7.799
7.781
7.565
7.486
7.468
7.450
7.425
7.407
7.390
7.260
2.852
OHC
S
N
N
O
4i
0.95
2.09
1.00
2.11
1.05
3.10
f1 (ppm)

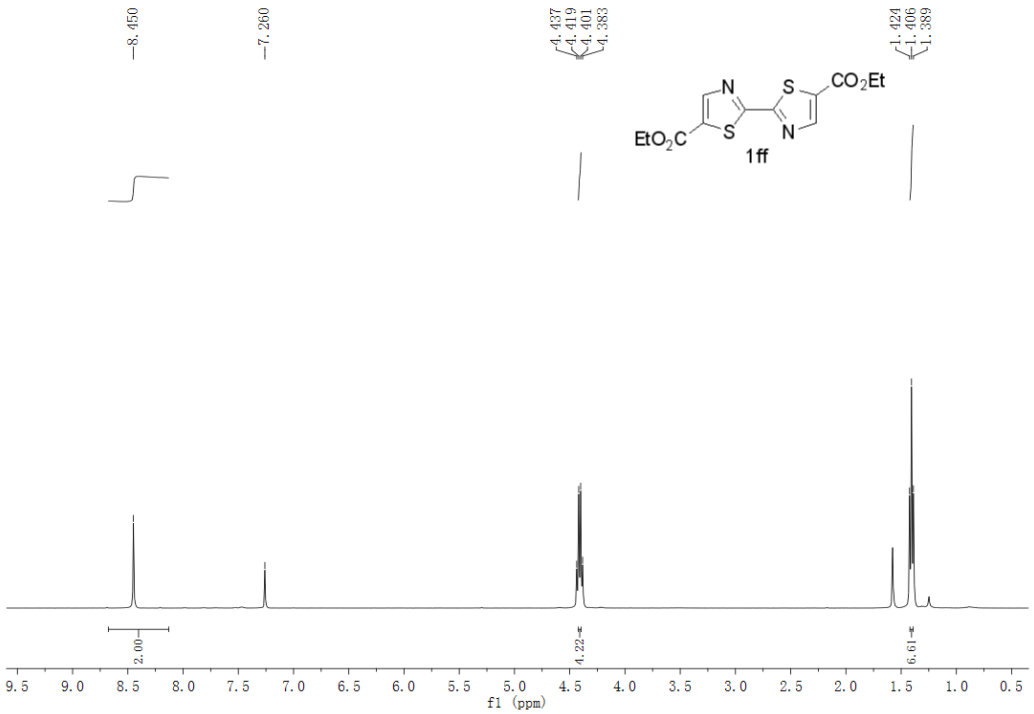

182.268
162.643
159.007
155.001
153.906
134.344
129.832
129.238
126.824
125.138
124.769
77.372
77.160
76.949
16.503
OHC
S
N
N
O
4i
f1 (ppm)

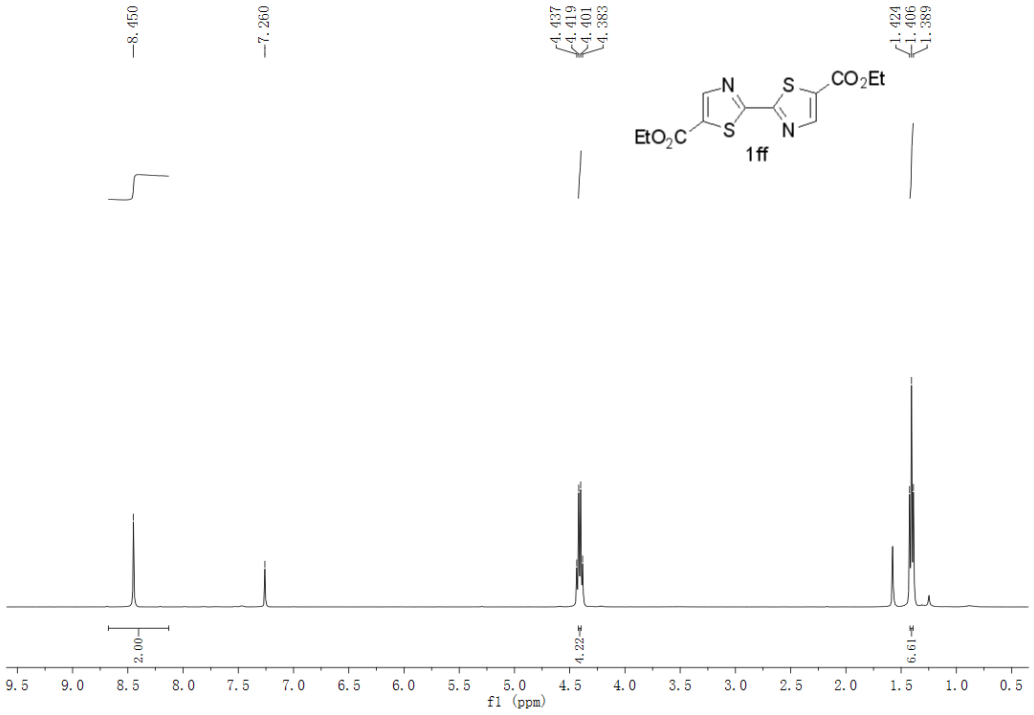

7.260
4.408
4.391
4.373
4.355
3.599
3.584
3.569
3.364
3.056
3.041
3.025
2.525
2.445
1.401
1.384
1.366
MeO
S
N
N
O
CO2Et
4j
2.00
2.05
2.97
2.09
2.96
3.02
2.98
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

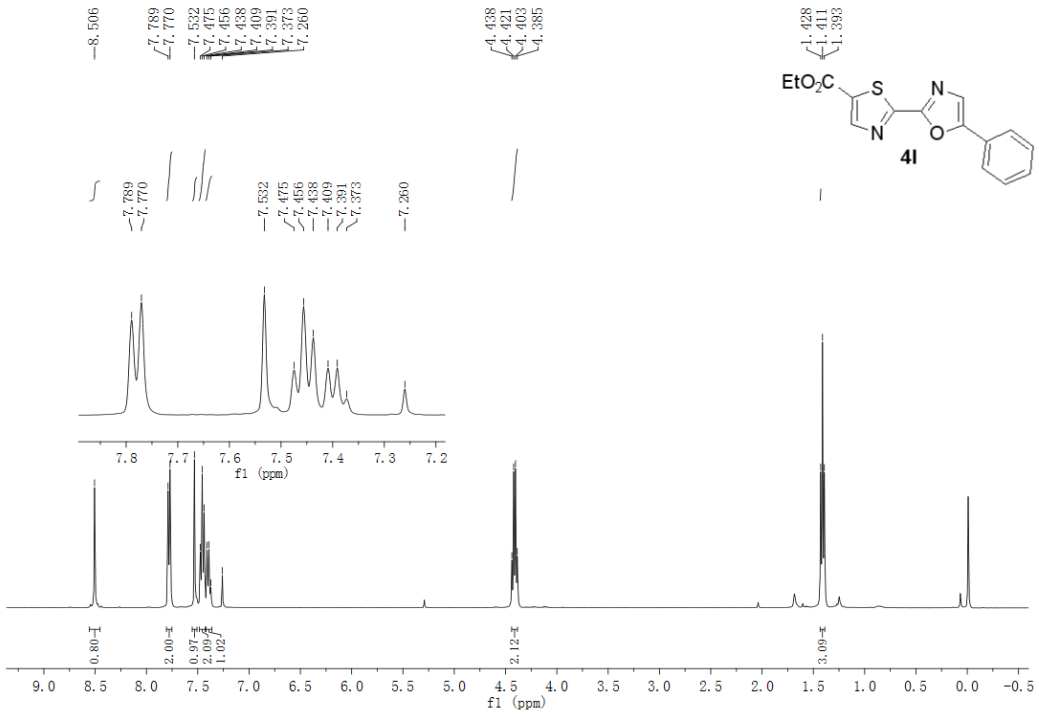

158.560
156.593
151.714
149.729
147.373
137.803
133.998
77.371
77.160
76.948
71.924
61.347
58.874
27.479
15.261
14.428
13.483
MeO
S
N
N
O
CO2Et
4j
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

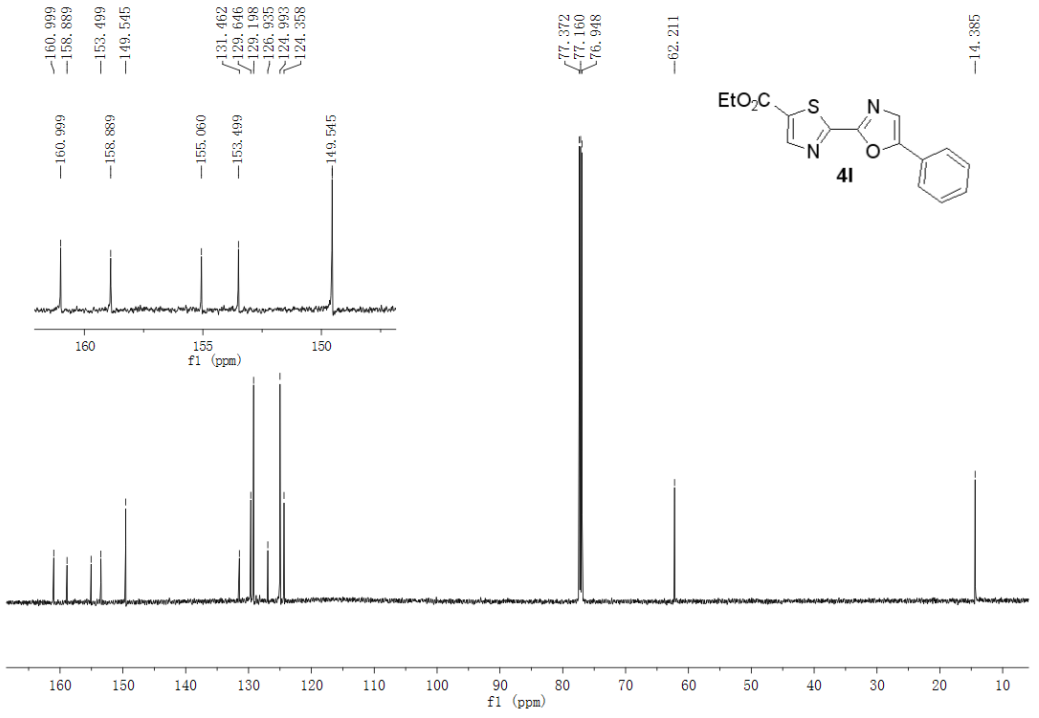

8.523
7.260
4.442
4.425
4.416
4.407
4.399
4.381
2.566
1.420
1.403
1.388
EtO2C
S
N
N
O
CO2Et
4k
4.50
4.45
4.40
4.35
4.30
f1 (ppm)
1.00
4.02
3.09
6.09
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

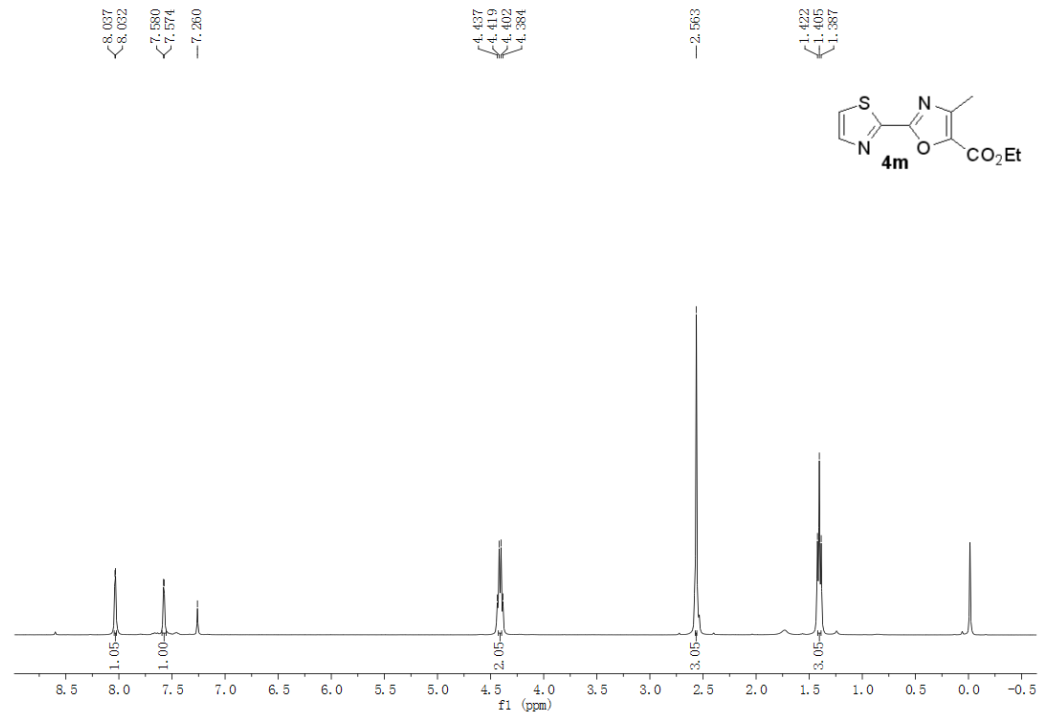

160.648
158.205
157.598
155.303
149.687
147.511
138.798
132.762
77.477
77.160
76.842
62.306
61.632
14.385
14.303
13.398
160.65
158.21
157.60
155.30
14.39
14.30
13.40
EtO2C
S
N
N
O
CO2Et
4k
161
159
157
155
f1 (ppm)
15.0
14.5
14.0
13.5
13.0
f1 (ppm)
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

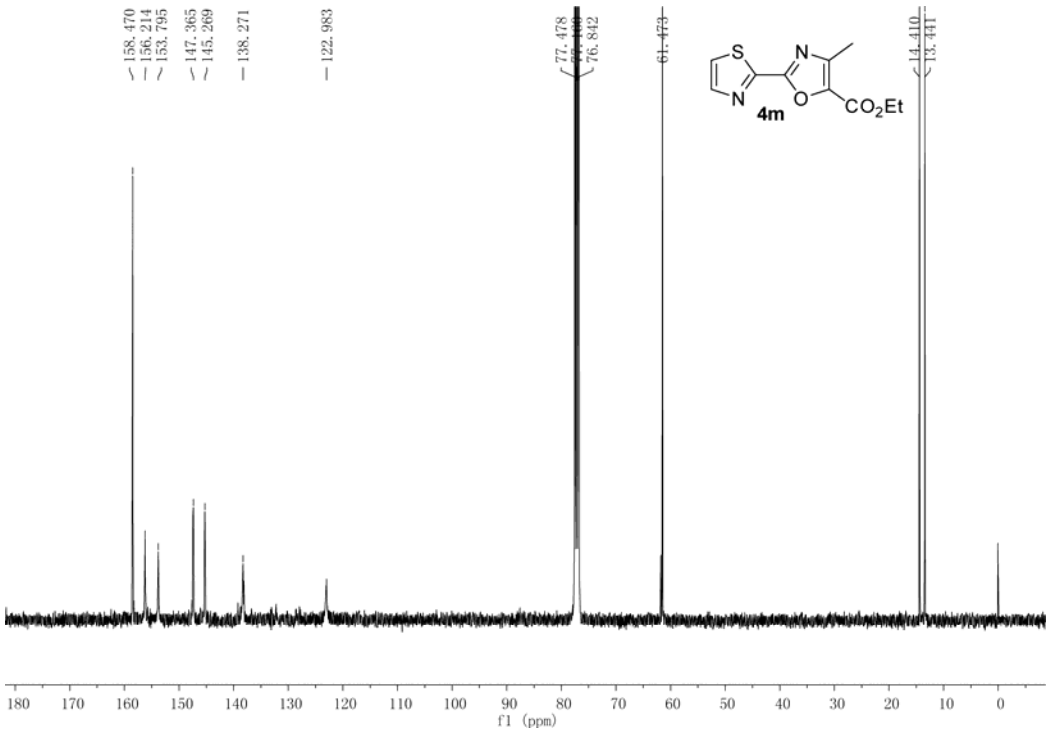

8.450
7.260
4.437
4.419
4.401
4.383
1.424
1.406
1.389
CO2Et
EtO2C
1ff
2.00
4.22
6.61
f1 (ppm)

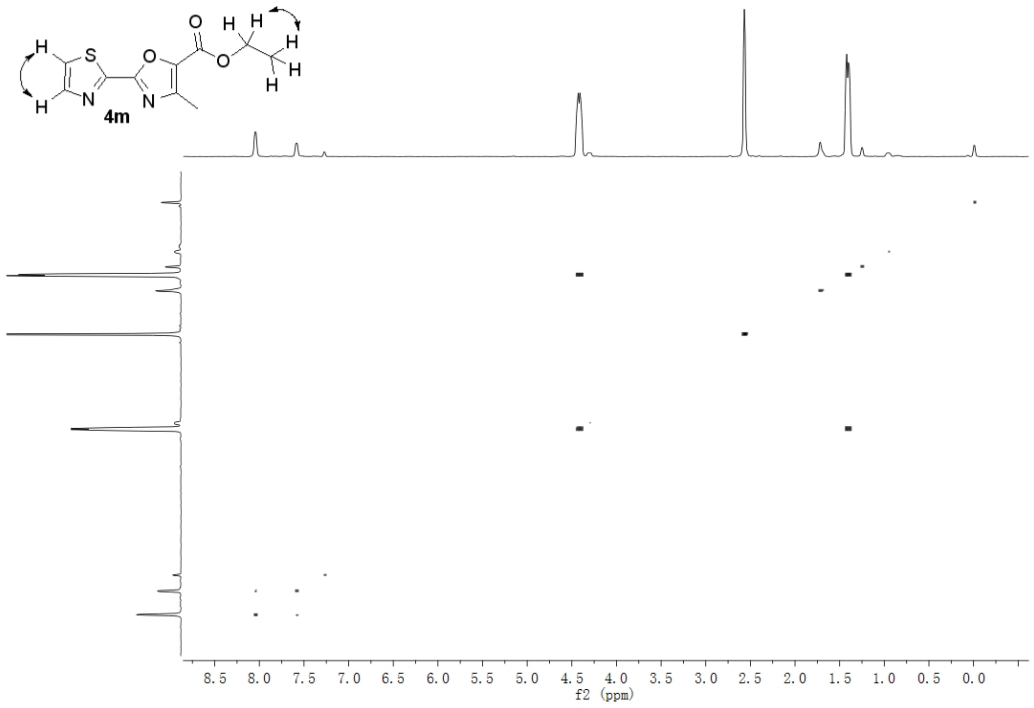

8.450
7.260
4.437
4.419
4.401
4.383
1.424
1.406
1.389
CO2Et
EtO2C
1ff
2.00
4.22
6.61
f1 (ppm)

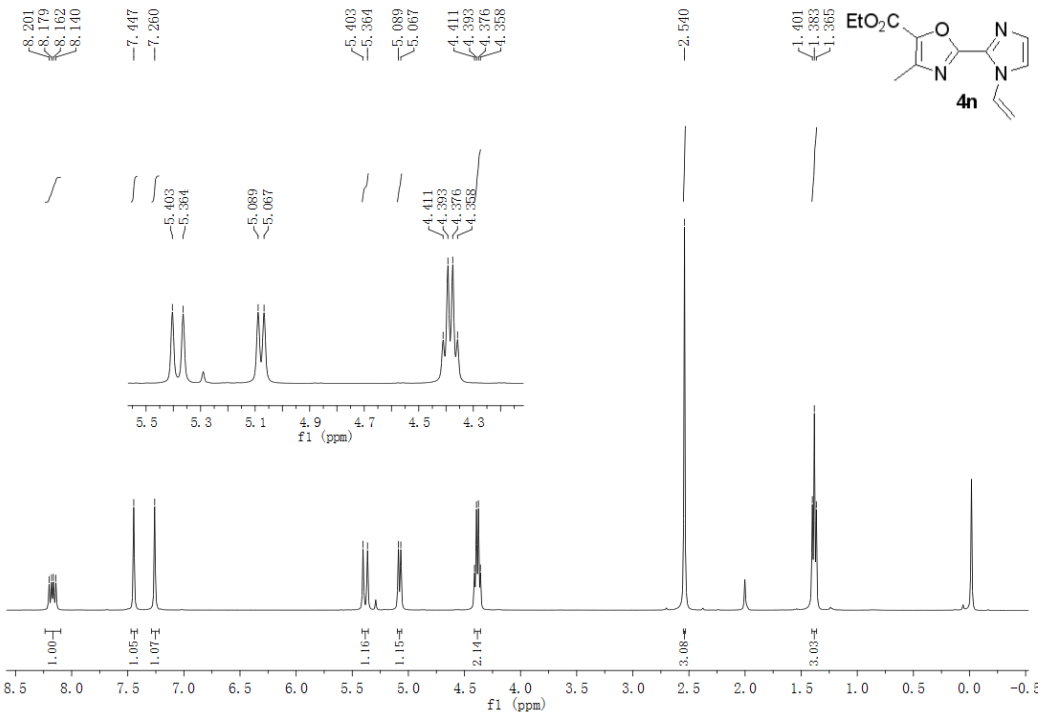

8.506
7.789
7.770
7.532
7.475
7.456
7.438
7.409
7.391
7.373
7.260
4.438
4.421
4.403
4.385
1.428
1.411
1.393
EtO2C
S
N
N
O
4l
f1 (ppm)
0.80
2.00
0.97
2.09
1.02
2.12
3.09

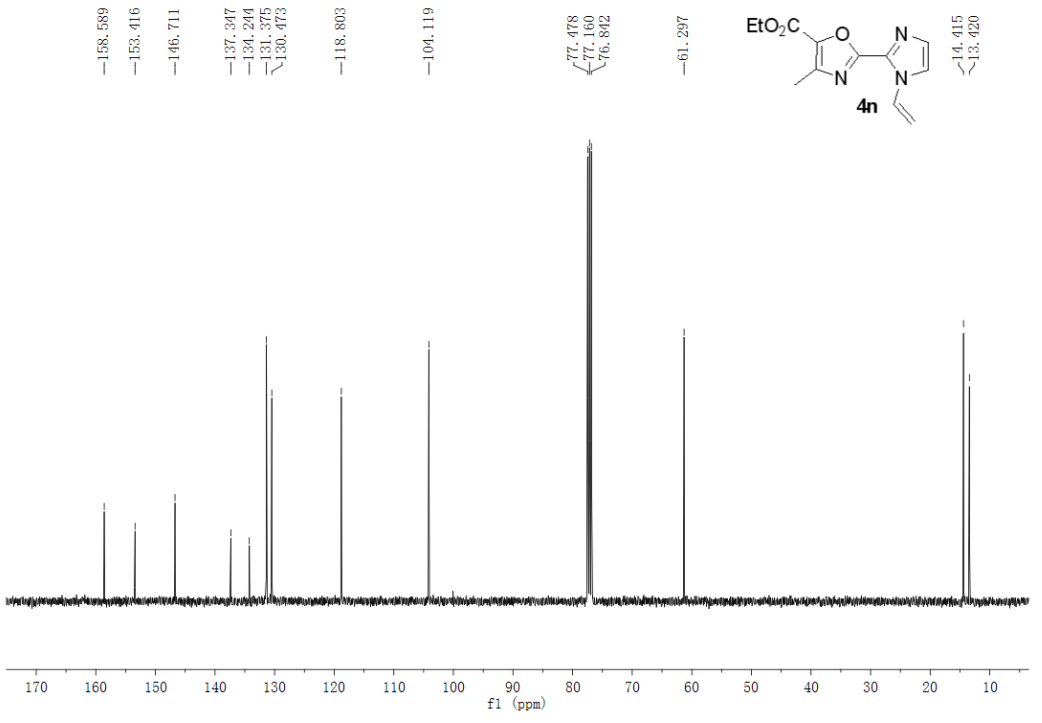

160.999
158.889
153.499
149.545
131.462
129.646
129.198
126.935
124.993
124.358
77.372
77.160
76.948
62.211
14.385
155.060
EtO2C
S
N
N
O
4l
f1 (ppm)

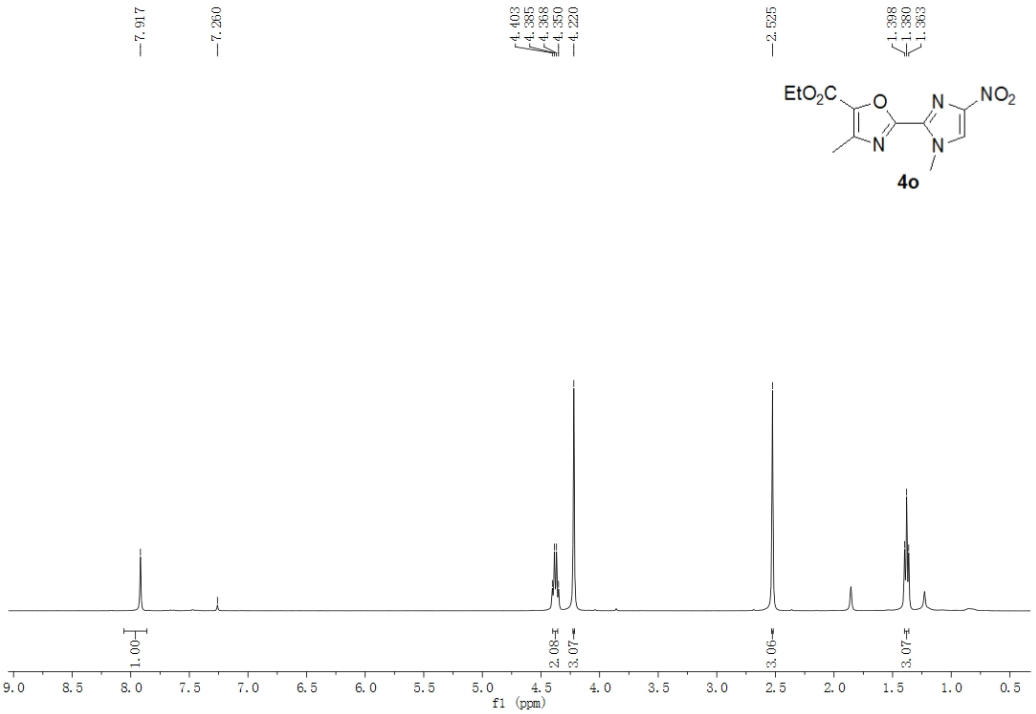

8.037
8.032
7.580
7.574
7.260
4.437
4.419
4.402
4.384
2.563
1.422
1.405
1.387
4m
1.05
1.00
2.05
3.05
3.05
f1 (ppm)


158.470
156.214
153.795
147.365
145.269
138.271
122.983
77.478
76.842
61.473
14.410
13.441
4m
f1 (ppm)


4m
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f2 (ppm)


8.201
8.179
8.162
8.140
7.447
7.260
5.403
5.364
5.089
5.067
4.411
4.393
4.376
4.358
2.540
1.401
1.383
1.365
EtO2C
O
N
N
N
4n
f1 (ppm)
1.00
1.05
1.07
1.16
1.15
2.14
3.08
3.03


158.589
153.416
146.711
137.347
134.244
131.375
130.473
118.803
104.119
77.478
77.160
76.842
61.297
14.415
13.420
EtO2C
O
N
N
N
4n
f1 (ppm)


7.917
7.260
4.403
4.385
4.368
4.350
4.220
2.525
1.398
1.380
1.363
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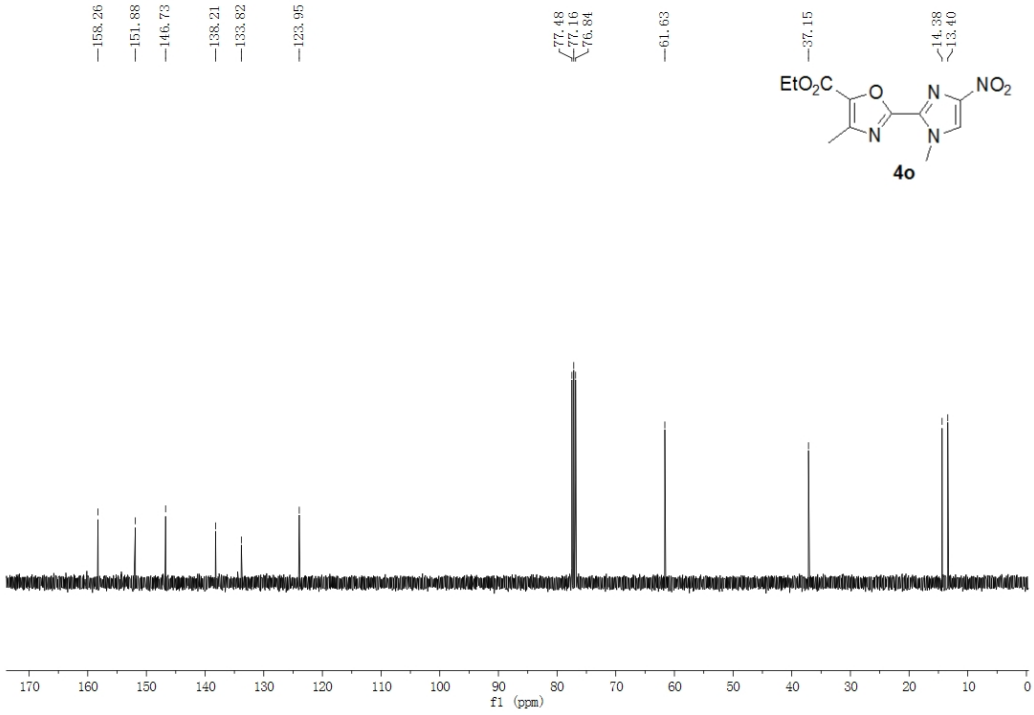
O
N
N
NO2
4o
1.00
2.08
3.07
3.06
3.07
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)


158.26
151.88
146.73
138.21
133.82
123.95
77.48
77.16
76.84
61.63
37.15
14.38
13.40
EtO2C
O
N
N
NO2
4o
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)