Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Reaction of Alkenecarboxylic Acids with Isocyanates via Rhodium(III)-Catalyzed C-H Activation: A Versatile Route to Cyclic Imides

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General Procedure 2

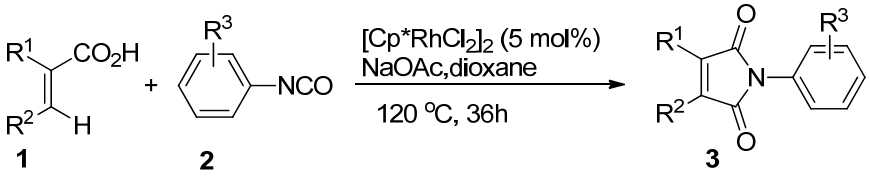
^{1}H, ^{13}C NMR and GCMS Spectra 9

Experimental Section

Solvents and reagents were purchased from Sigma-Aldrich and were used without further purification unless otherwise specified. ^{1}H and ^{13}C NMR spectra were recorded on Bruker 400 MHz, or 500 MHz spectrometers; internal reference of δ = 7.28 or 77.0 $CHCl_3$ as standard. HRMS was conducted using electro-spraying ionization (ESI), and was performed by McGill University on a Thermo-Scientific Exactive Orbitrap. Protonated molecular ions $[M + H]^+$ or sodium adducts $[M + Na]^+$, were used for empirical formula confirmation.

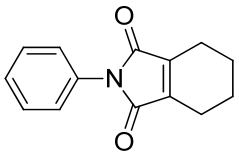
General Synthetic Procedure for Compounds 3a – 3o

An oven-dried reaction vessel was charged with $[Cp^*RhCl_2]_2$ (6.18 mg, 5 mol%, 0.01 mmol), NaOAc (16.4 mg, 0.2 mmol), substituted alkenecarboxylic acids (0.2 mmol) and isocyanate (0.6 mmol). The tube was evacuated and purged with argon three times, and then dioxane (0.5 mL) was added to the vial by syringe. The mixture was stirred at 120 °C (oil bath temperature) for 36 h. After this time, the resulting mixture was cooled down to room temperature, filtered through a short pad of silica gel, and then concentrated under vacuum. The residue was purified by preparative TLC (eluent: hexane/ethyl acetate = 10 : 1) to afford the corresponding product.



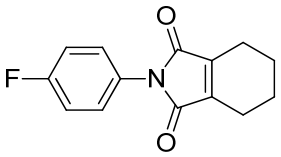
1a $R^1R^2 = CH_2CH_2CH_2CH_2$;
1b $R^1R^2 = OCH_2CH_2CH_2$;
1C $R^1 = CH_3$; R^2= H.

2-Phenyl-4,5,6,7-tetrahydro-1H-isoindole-1,3(2H)-dione (3a) [1]



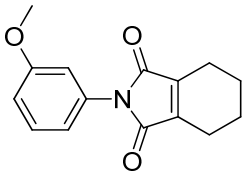
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41- 7.48(m, 2H), 7.30 - 7.37(m, 3H), 2.43(s, 4H), 1.84(s, 4H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 169.9, 141.8, 131.9, 129.0, 127.4, 126.0, 21.4, 20.2.

2-(4-Fluorophenyl)-4,5,6,7-tetrahydro-1H-isoindole-1,3(2H)-dione (3b) [1]



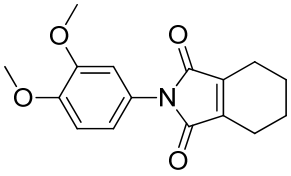
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 - 7.36(m, 2H), 7.12 - 7.19(m, 2H), 2.40 – 2.50(m, 4H), 1.80 - 1.90(m, 4H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 169.8, 162.5, 160.5, 141.8, 127.9, 127.8, 127.8, 127.7, 116.1, 115.9, 21.4, 20.2.

2-(3-Methoxyphenyl)-4,5,6,7-tetrahydro-1H-isoindole-1,3(2H)-dione (3c) [1]



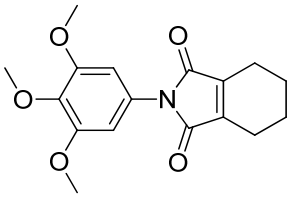
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.34 - 7.39(t, J = 7.5Hz, 1H), 6.88 - 6.97(m, 3H), 3.84(s, 1H), 2.46(s, 4H), 1.84(s, 4H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 169.9, 160.0, 141.8, 133.0, 129.7, 118.3, 113.4, 111.7, 55.4, 21.4, 20.2.

2-(3,4-Dimethoxyphenyl)-4,5,6,7-tetrahydro-1H-isoindole-1,3(2H)-dione (3d) [2]



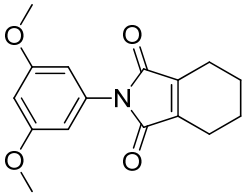
^{1}H NMR (400 MHz, $CDCl_3$) δ 6.84- 6.96(m, 3H), 3.92(s, 3H), 3.89(s, 3H), 2.45(s, 4H), 1.85(s, 4H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 170.2, 149.1, 148.4, 141.7, 124.7, 118.8, 111.2, 110.0, 56.1, 56.0, 21.4, 20.2.

2-(3,4,5-Trimethoxyphenyl)-4,5,6,7-tetrahydro-1H-isoindole-1, 3(2H)-dione (3e)



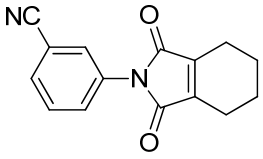
^{1}H NMR (500 MHz, $CDCl_3$) δ 6.58(s, 2H), 3.87(s, 9H), 2.45(s, 4H), 1.85(s, 4H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 170.0, 153.3, 141.8, 137.4, 127.5, 103.9, 60.9, 56.2, 21.4, 20.2. HRMS Calcd for $[C_{17}H_{20}NO_5]^+$ (M + H^+) 318.1336, found 318.1333.

2-(3, 5-Dimethoxyphenyl)-4,5,6,7-tetrahydro-1H-isoindole-1,3(2H)-dione (3f) [3]



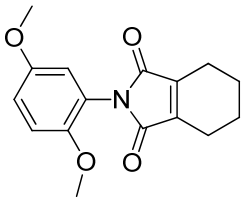
^{1}H NMR (400 MHz, $CDCl_3$) δ 6.53 (d, *J* = 2.3 Hz, 2H), 6.46 (t, *J* = 2.2 Hz, 1H), 3.81(s, 6H), 2.44(s, 4H), 1.84(s, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.8, 160.8, 141.7, 133.4, 104.4, 100.0, 55.5, 21.4, 20.2.

2-(3-Cyanophenyl)-4,5,6,7-tetrahydro-1H-isoindole-1,3(2H)-dione (3g)



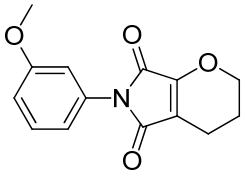
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.75 – 7.79(m, 1H), 7.68 - 7.73(m, 1H), 7.54 – 7.64(m, 2H), 2.47(s, 4H), 1.86(s, 4H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 169.1, 142.2, 133.0, 130.4, 129.9, 129.6, 128.7, 118.0, 113.2, 21.3, 20.2. HRMS Calcd for $[C_{15}H_{13}N_2O_2]^+$ (M + H^+) 253.0972, found 253.0969.

2-(2, 5-Dimethoxyphenyl)-4,5,6,7-tetrahydro-1H-isoindole-1,3(2H)-dione (3h)



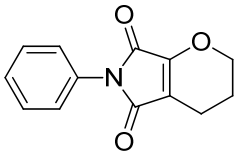
^{1}H NMR (500 MHz, $CDCl_3$) δ 6.92 - 6.98(m, 2H), 6.75 (d, *J* = 2.0 Hz, 1H), 3.79(s, 3H), 3.78(s, 3H), 2.45(s, 4H), 1.84(s, 4H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 170.0, 153.6, 149.9, 142.0, 121.0, 115.8, 115.4, 113.1, 56.5, 55.8, 21.4, 20.3. HRMS Calcd for $[C_{16}H_{18}NO_4]^+$ (M + H^+) 288.1230, found 288.1229.

6-(3-methoxyphenyl)-3,4-dihydropyrano[2,3-c]pyrrole-5,7(2H, 6H)-dione (3i)



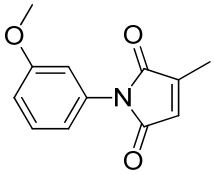
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 – 7.39 (m, 1H), 6.88 – 6.98 (m, 3H), 4.43 (t, *J* = 5.2 Hz, 2H), 3.83 (s, 3H), 2.47 (t, *J* = 6.1 Hz, 2H), 2.14 – 2.03 (m, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 168.7, 163.8, 160.0, 155.6, 132.4, 129.7, 118.4, 113.4, 111.9, 111.1, 69.7, 55.4, 21.1, 16.15. HRMS Calcd for $[C_{14}H_{13}NNaO_4]^+$ (M + Na^+) 282.0737, found 282.0734.

6-phenyl-3,4-dihydropyrano[2,3-c]pyrrole-5,7(2H,6H)-dione (3j)



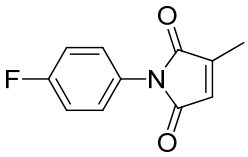
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 - 7.51(m, 2H), 7.33 - 7.38 (m, 3H), 4.44 (t, *J* = 5.2Hz, 2H), 2.48 (t, *J* = 6.0 Hz, 2H), 2.06 – 2.13 (m, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 168.8, 163.9, 155.6, 131.4, 129.0, 127.5, 126.1, 111.1, 69.7, 21.1, 16.2. HRMS Calcd for $[C_{13}H_{11}NNaO_3]^+$ (M + Na^+) 252.0631, found 252.0628.

1-(3-Methoxyphenyl)-3-methyl-1H-pyrrole-2,5-dione (3k) [4]



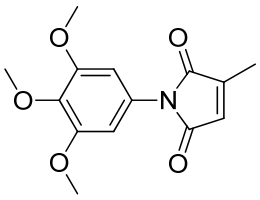
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.35-7.40(m, 1H), 6.90-6.98(m, 3H), 6.49 – 6.51(m, 1H), 3.84(s, 3H), 2.20 (d, *J* = 2.0 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 170.5, 169.5, 160.0, 145. 8, 132.7, 129.7, 127.5, 118.2, 113.6, 111.8, 55.4, 11.2.

1-(4-Fluorophenyl)-3-methyl-1H-pyrrole-2,5-dione (3l) [5]



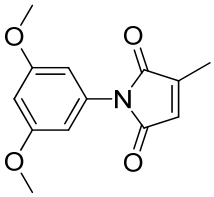
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.32-7.37(m, 2H), 7.14-7.19(m, 2H), 6.49 – 6.52(m, 1H), 2.20(d, *J* = 2.0 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 170.5, 169.5, 162.7, 160.7, 145.9, 127.8, 127.7, 127.6, 127.5, 116.1, 116.0, 11.2.

1-(3,4,5-Trimethoxyphenyl)-3-methyl-1H-pyrrole-2,5-dione (3m)



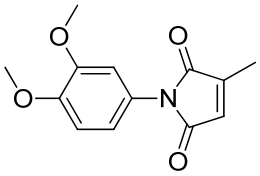
^{1}H NMR (400 MHz, $CDCl_3$) δ 6.57(s, 2H), 6.49 - 6.51(m, 1H), 3.88(s, 3H), 3.88(s, 6H), 2.20 (d, *J* = 1.6 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.9, 169.7, 153.4, 145.8, 137.8, 128.6, 127.6, 127.2, 104.0, 100.0, 61.0, 56.0, 11.4. HRMS Calcd for $[C_{14}H_{15}NO_5]^+$ (M + H^+) 278.1023, found 278.1023.

1-(3,5-Dimethoxyphenyl)-3-methyl-1H-pyrrole-2,5-dione (3n) [6]



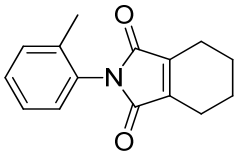
^{1}H NMR (500 MHz, $CDCl_3$) δ 6.53 (d, *J* = 2.5 Hz, 2H), 6.47 - 6.50(m, 2H), 3.80(s, 6H), 2.19 (d, *J* = 2.0 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 170.5, 169.4, 160.9, 145.8, 133.1, 127.5, 104.5, 100.2, 55.5, 11.2.

1-(3,4-Dimethoxyphenyl)-3-methyl-1H-pyrrole-2,5-dione (3o)



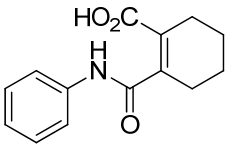
^{1}H NMR (400 MHz, $CDCl_3$) δ 6.87 - 6.98(m, 2H), 6.83 -6.87(s, 1H), 6.49 (d, *J* = 1.6 Hz, 1H), 3.92(s, 3H), 3.90(s, 3H), 2.19(d, *J* = 1.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.9, 169.9, 149.2, 148.7, 145.7, 127.4, 124.4, 118.7, 111.1, 109.9, 56.1, 56.0, 11.2. HRMS Calcd for $[C_{13}H_{14}NO_4]^+$ (M + H^+) 248.0917, found 248.0919.

2-(o-Tolyl)-4,5,6,7-tetrahydro-1H-isoindole-1,3(2H)-dione (3p) [7]



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 - 7.35(m, 3H), 7.11 (d, *J* = 7.2 Hz, 1H), 2.48(s, 4H), 2.19(s, 3H), 1.85(s, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.1, 141.9, 136.7, 131.0, 130.7, 129.0, 128.8, 126.7, 21.4, 20.2, 18.1.

2-(Phenylcarbamoyl)cyclohex-1-enecarboxylic acid (F) [8]



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 - 7. 45 (m, 4H), 7.20 - 7.26(m, 1H), 2.57 – 2.63 (m, 2H), 2.39 – 2.46 (m, 2H), 1.80 – 1.90 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.5, 150.9, 150.2, 144.0, 136.2, 128.8, 126.4, 124.5, 21.4, 21.4, 21.2, 20.4.

Notes and references

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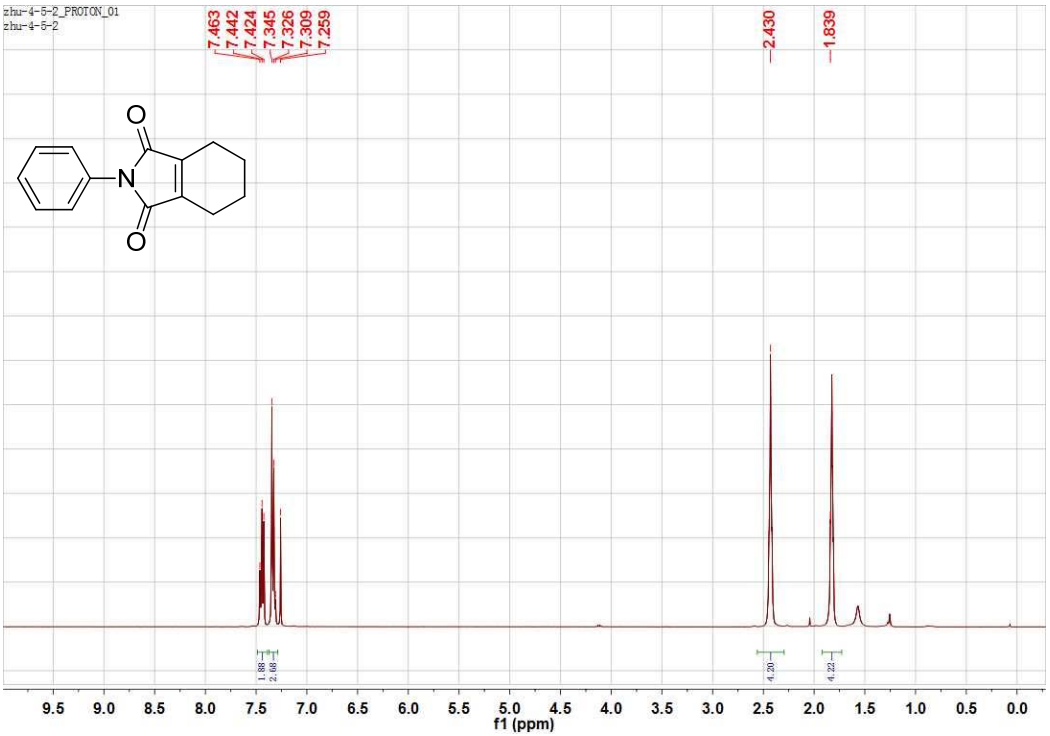
8. T. Katagi, *Nippon Noyaku Gakkaishi*, 1989, **14**, 497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7.424
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7.309
7.259
2.430
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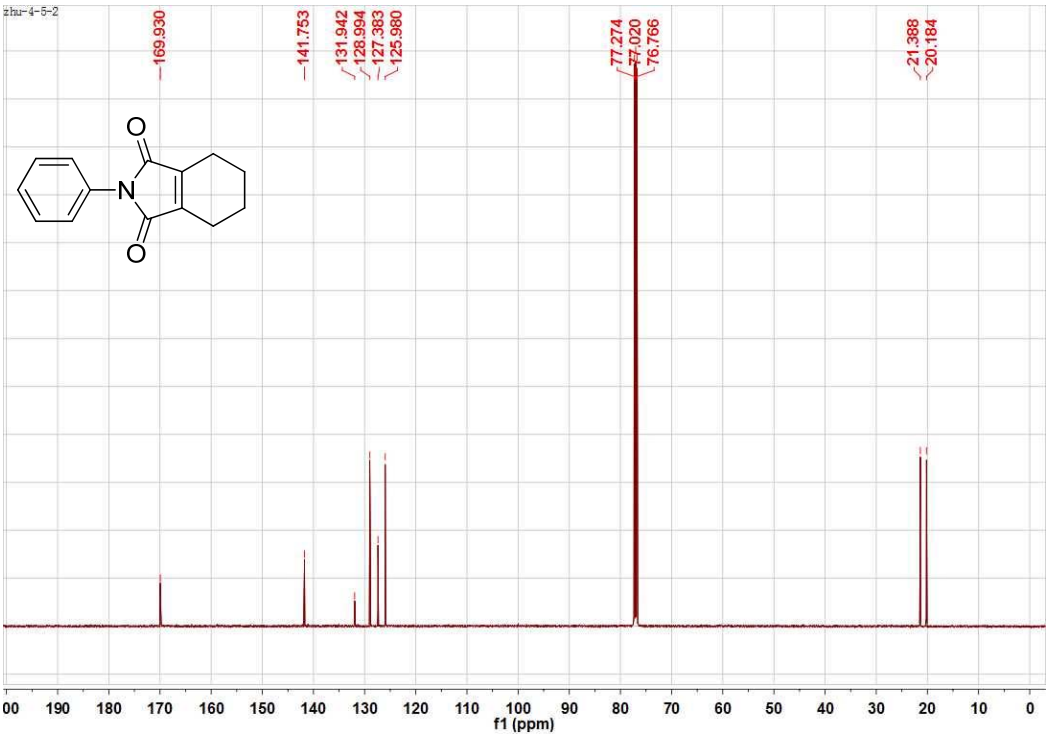
1.88
2.68
4.20
4.22
f1 (ppm)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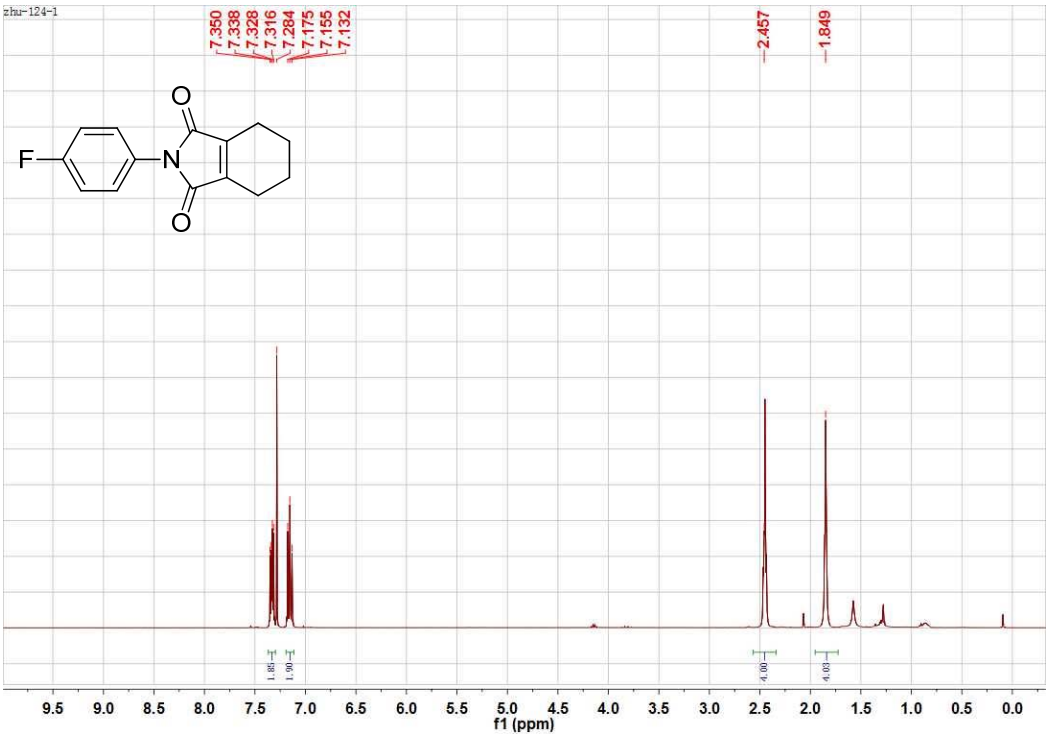
f1 (ppm)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7.316
7.284
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7.155
7.132
2.457
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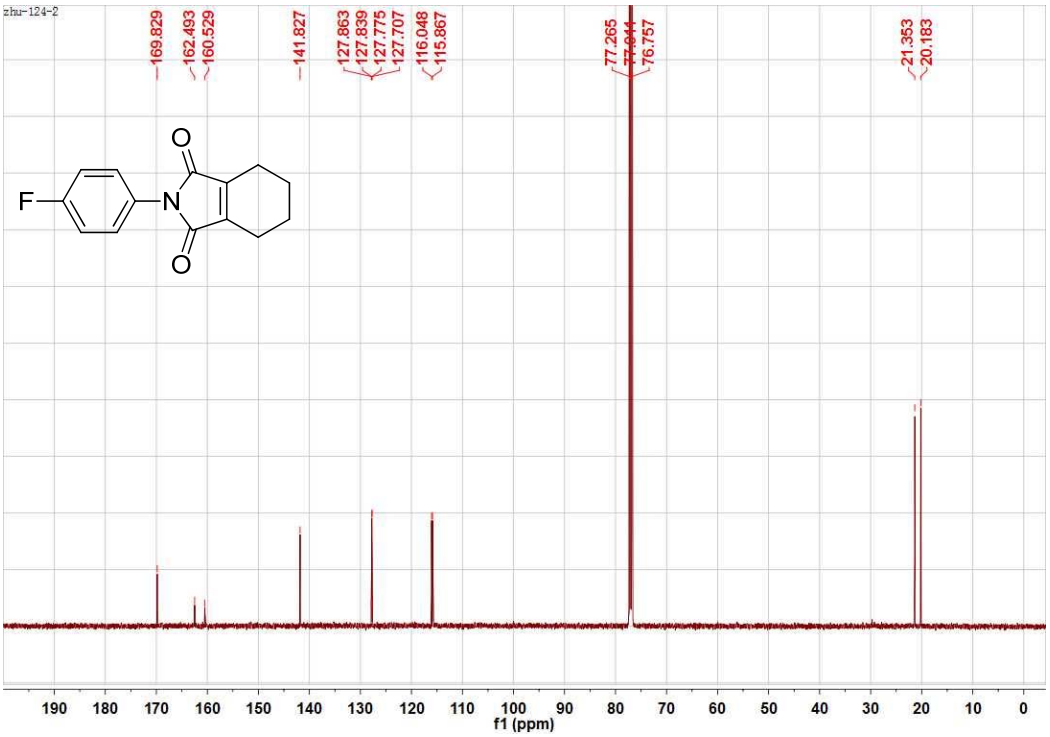
F
N
O
O
1.85
1.90
4.00
4.03
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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21.353
20.183
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N
O
O
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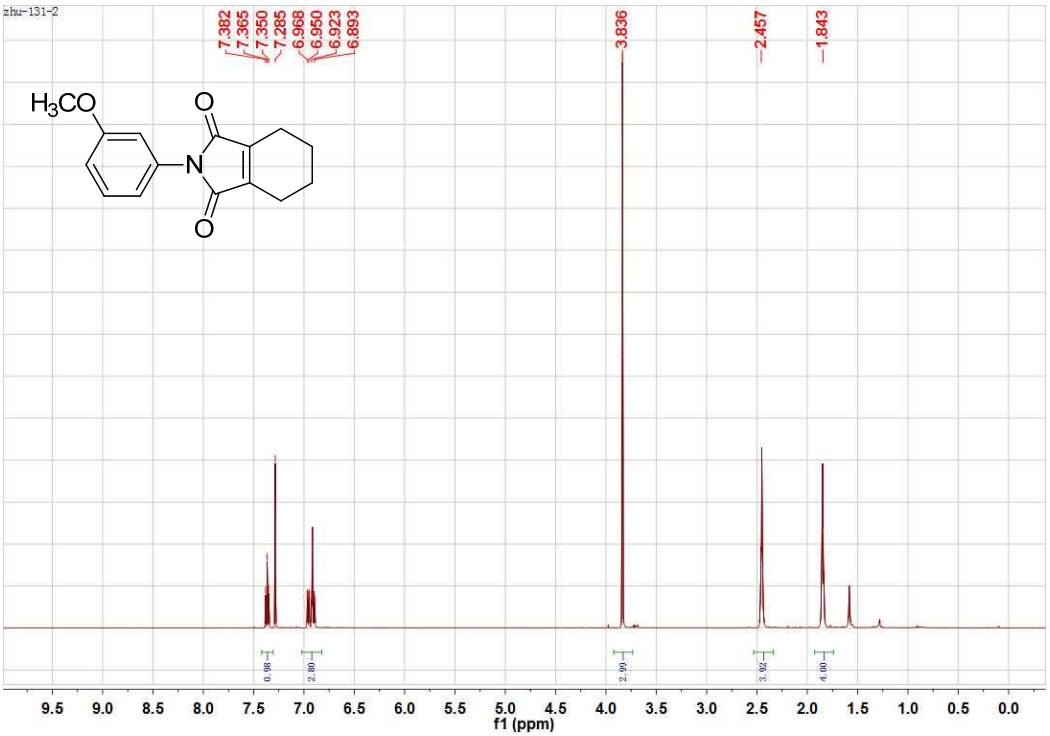
f1 (ppm)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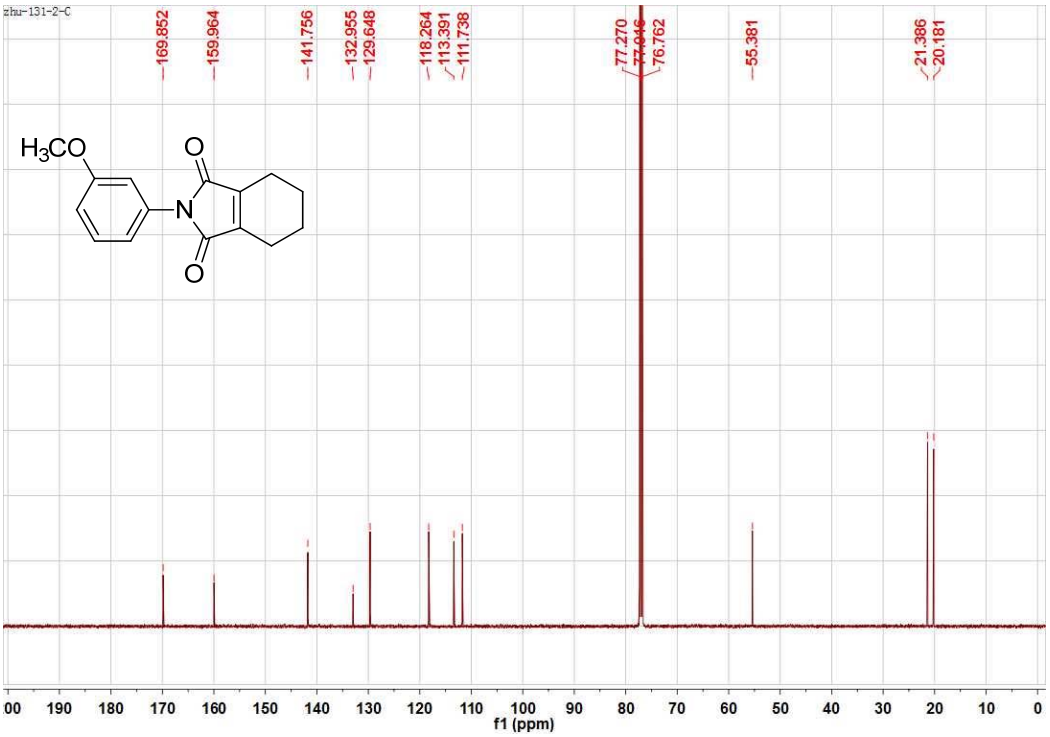
1.843
H3CO
O
N
O
0.88
2.80
2.99
3.92
4.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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111.738
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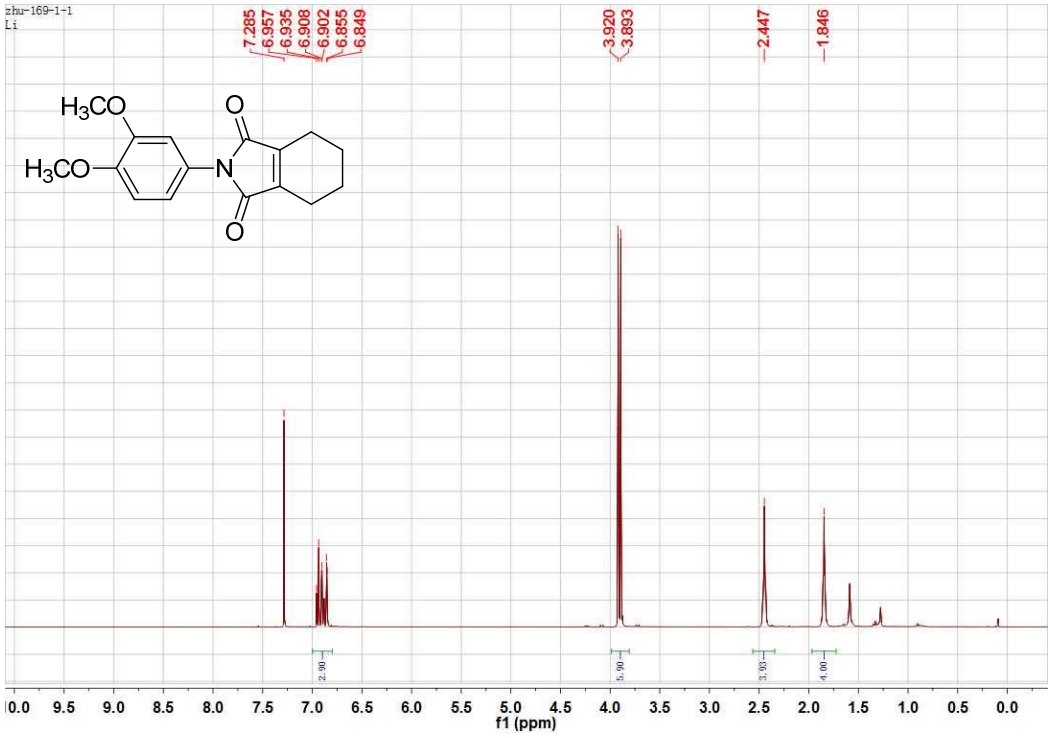
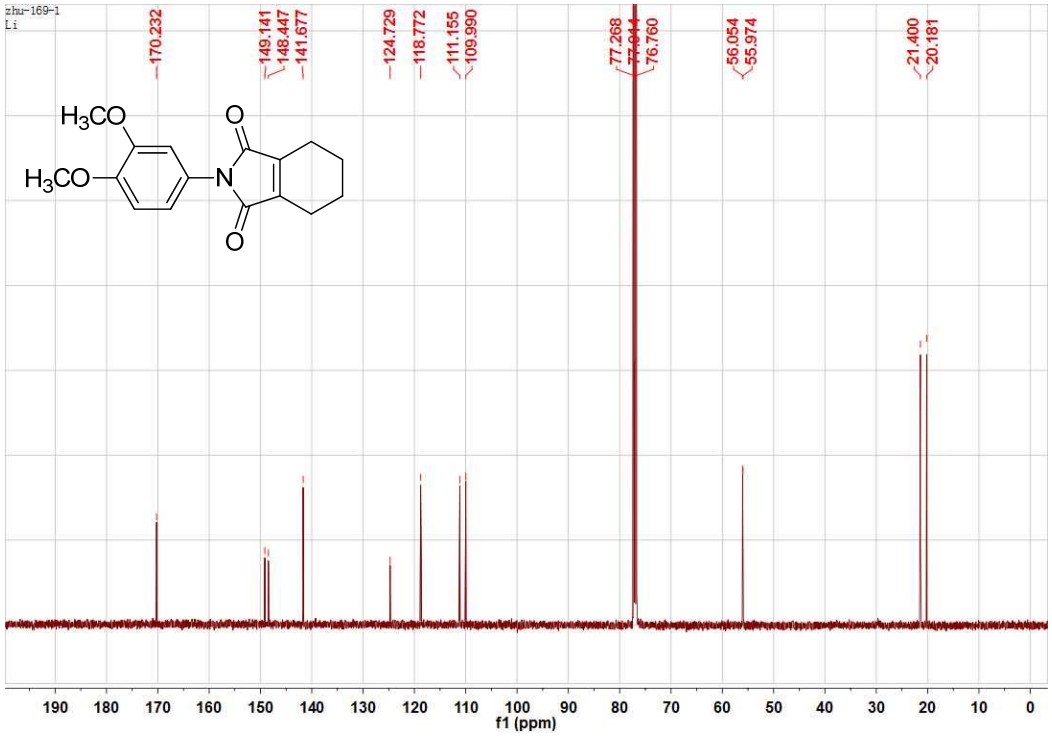
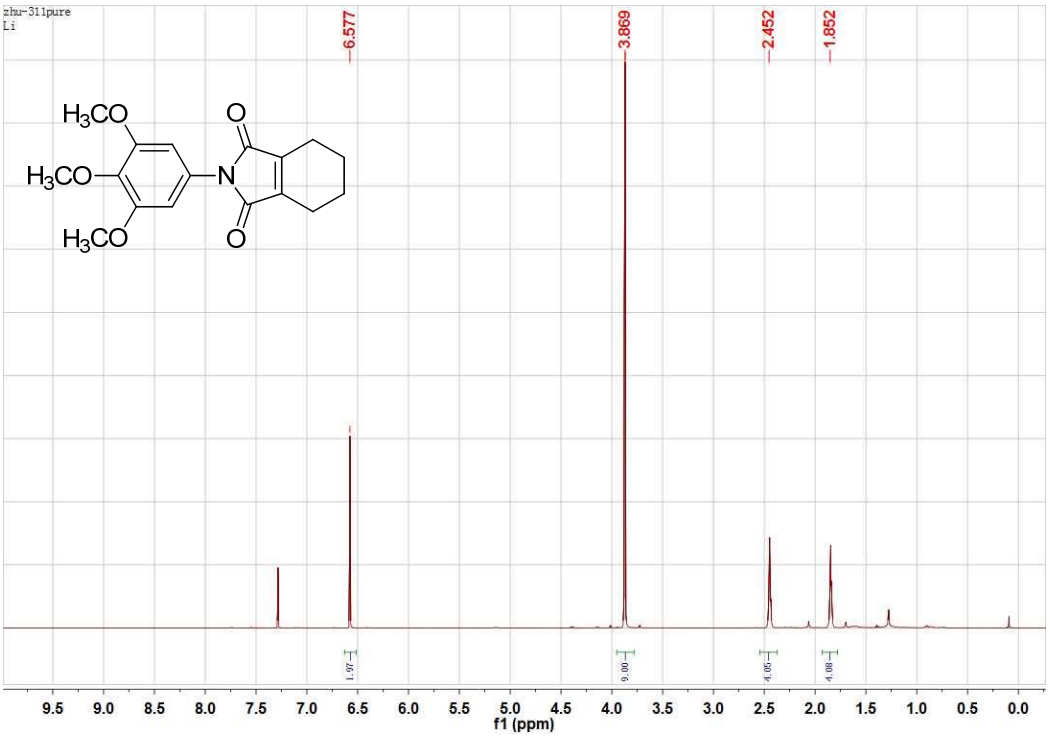
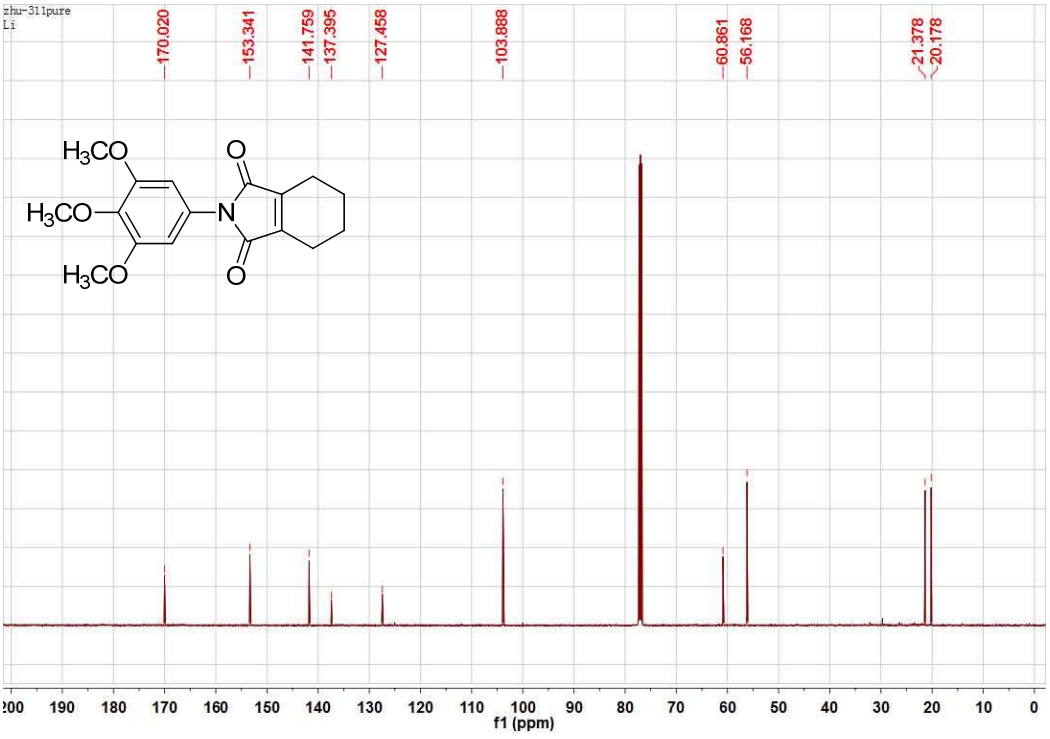
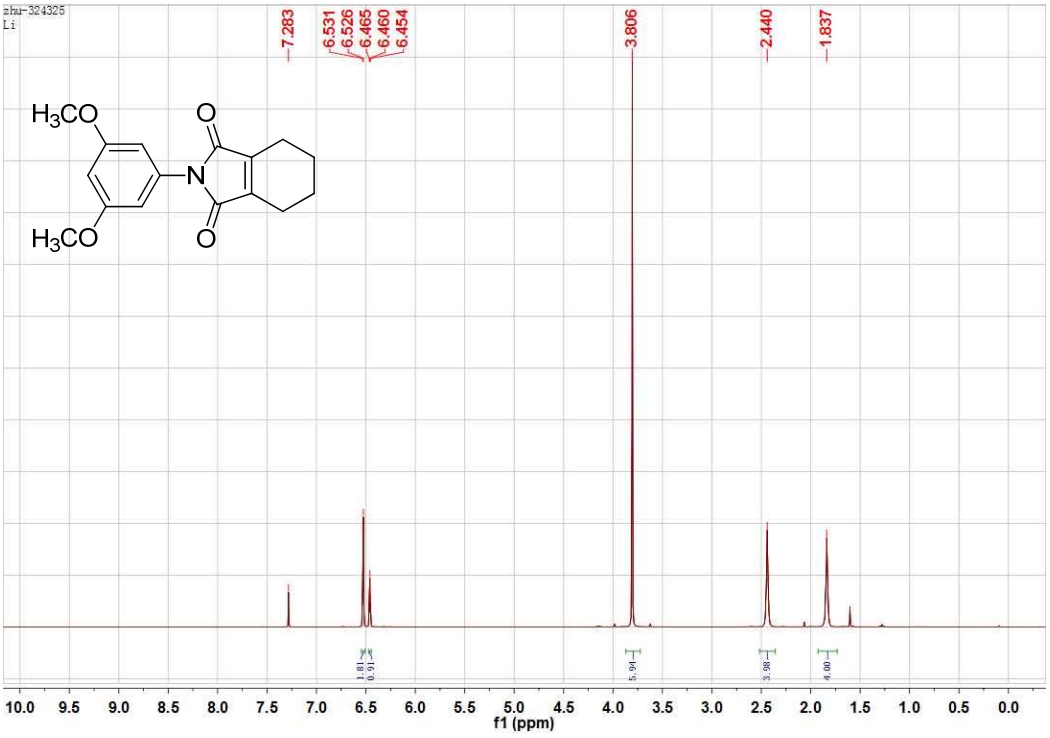
55.381
21.386
20.181
H3CO
O
N
O
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

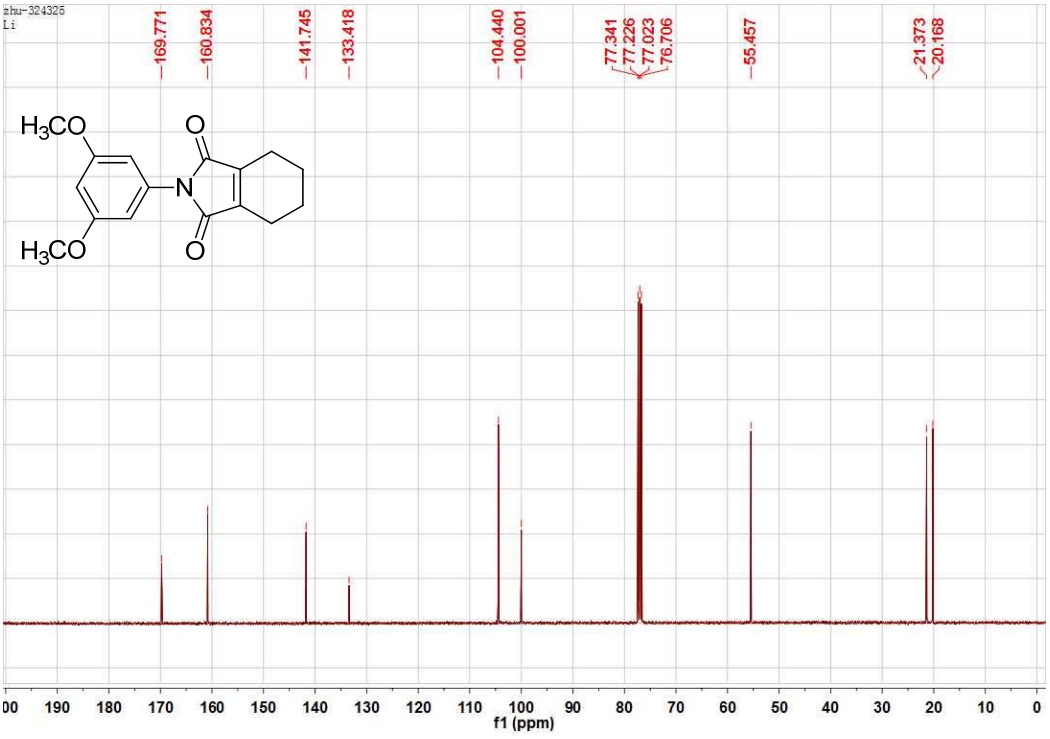

zhu-169-1-1
Li
7.285
6.957
6.935
6.908
6.902
6.855
6.849
3.920
3.893
2.447
1.846
H3CO
H3CO
O
N
O
2.90
5.90
3.93
4.00
f1 (ppm)

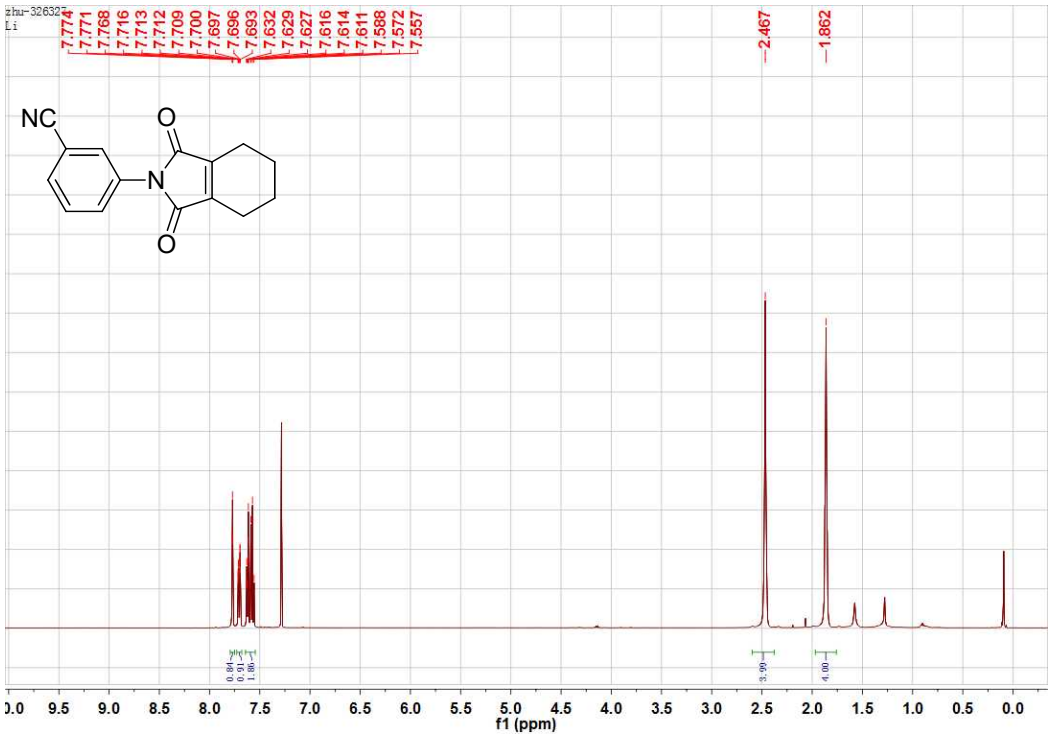

zhu-169-1
Li
170.232
149.141
148.447
141.677
124.729
118.772
111.155
109.990
77.268
77.044
76.760
56.054
55.974
21.400
20.181
H3CO
H3CO
O
N
O
f1 (ppm)

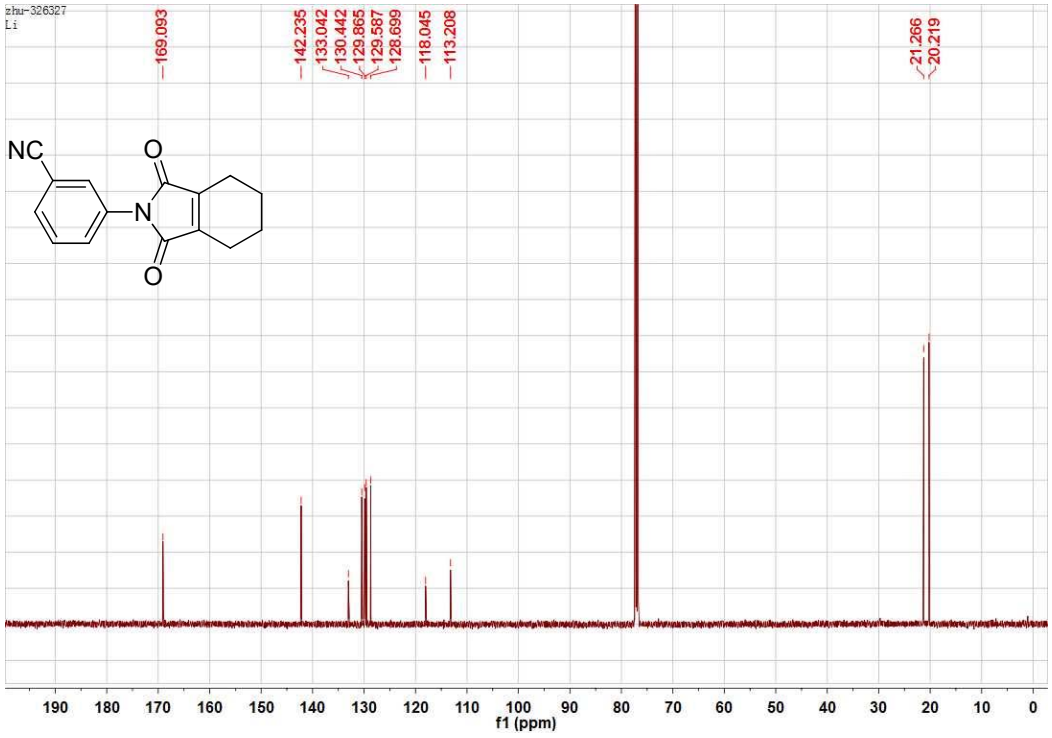

zhu-311pure
Li
6.577
3.869
2.452
1.852
1.97
9.00
4.05
4.08
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

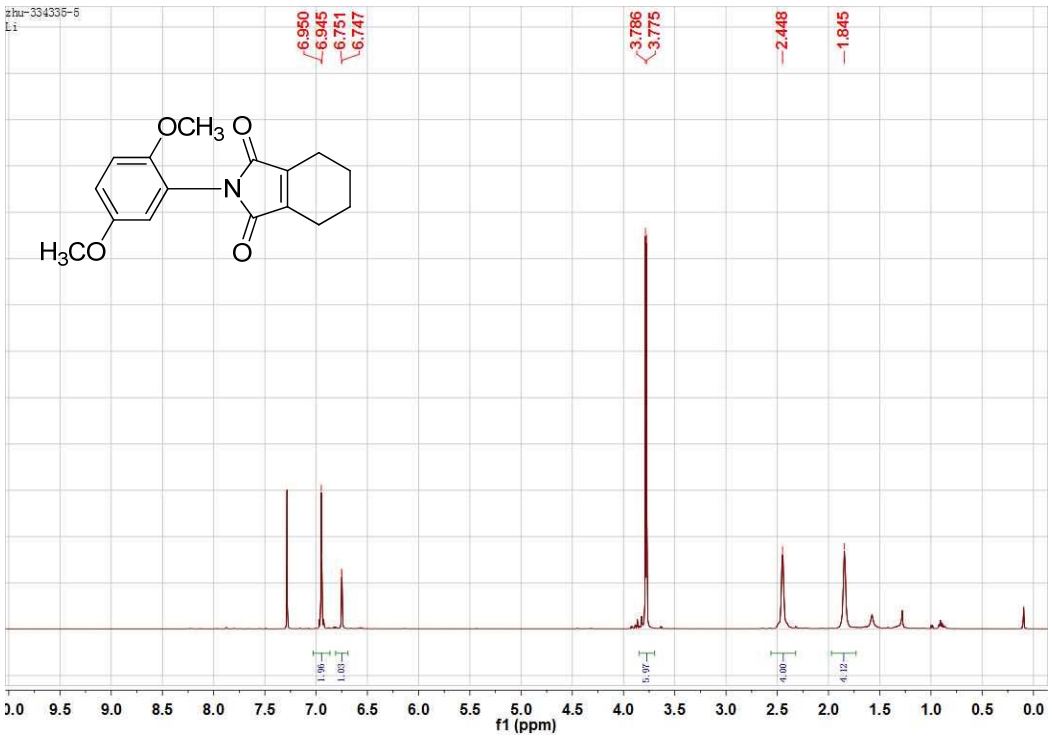

zhu-311pure
Li
170.020
153.341
141.759
137.395
127.458
103.888
60.861
56.168
21.378
20.178
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

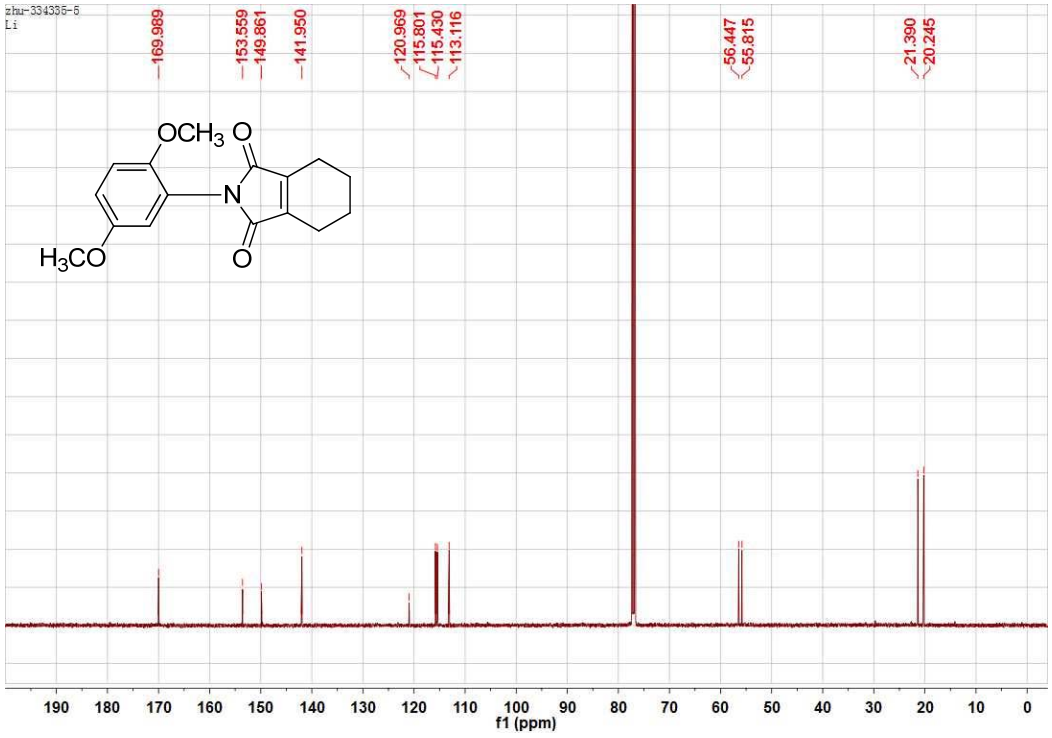

zhu-324325
Li
7.283
6.531
6.526
6.465
6.460
6.454
3.806
2.440
1.837
1.81
0.91
5.94
3.98
4.00
H3CO
O
N
H3CO
O
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

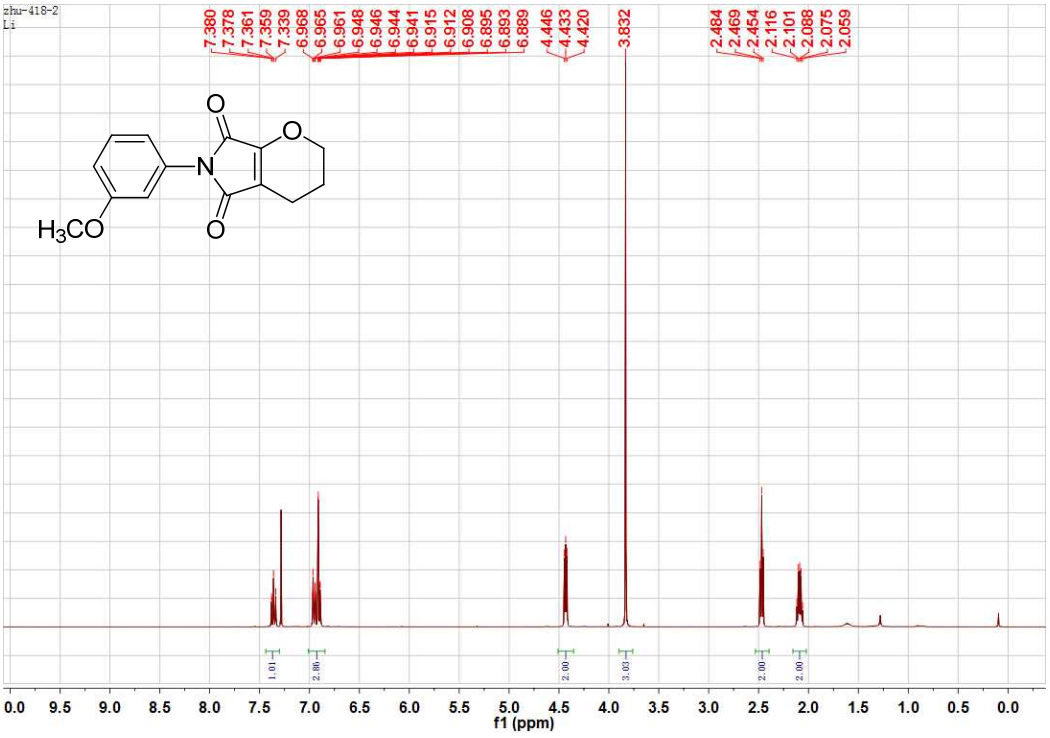

zhu-324325
Li
169.771
160.834
141.745
133.418
104.440
100.001
77.341
77.226
77.023
76.706
55.457
21.373
20.168
H3CO
O
N
H3CO
O
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

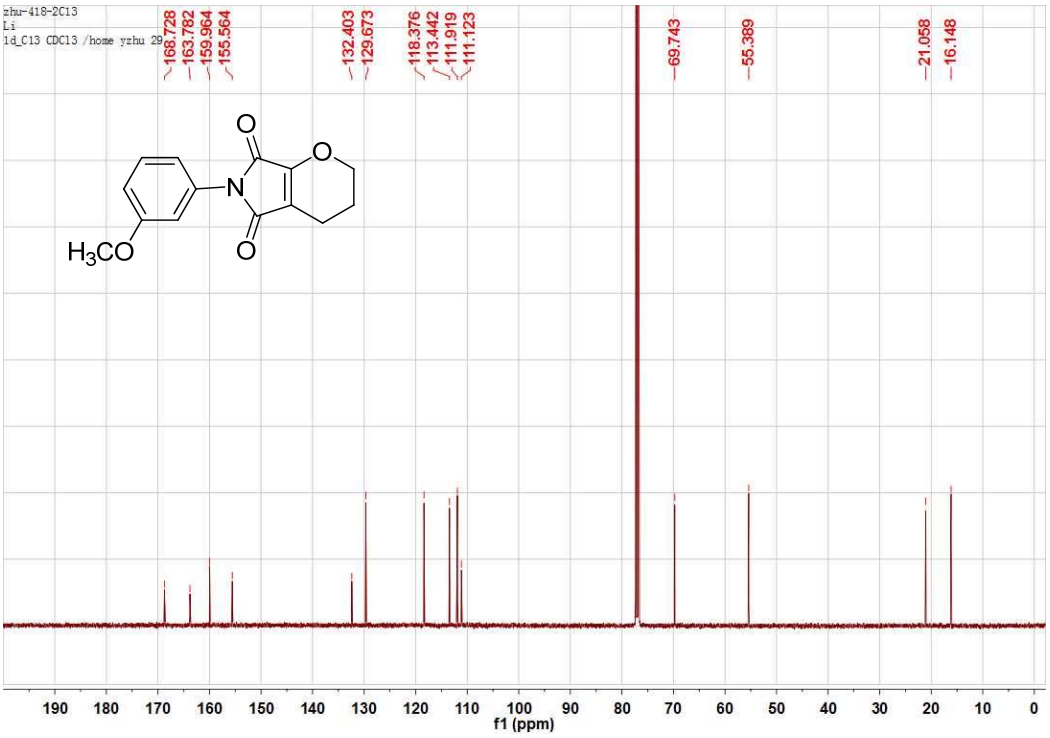

zhu-326327
Li
7.774
7.771
7.768
7.716
7.713
7.712
7.709
7.700
7.697
7.696
7.693
7.632
7.629
7.627
7.616
7.614
7.611
7.588
7.572
7.557
2.467
1.862
NC
O
N
O
0.99
0.97
1.00
3.99
4.00
f1 (ppm)

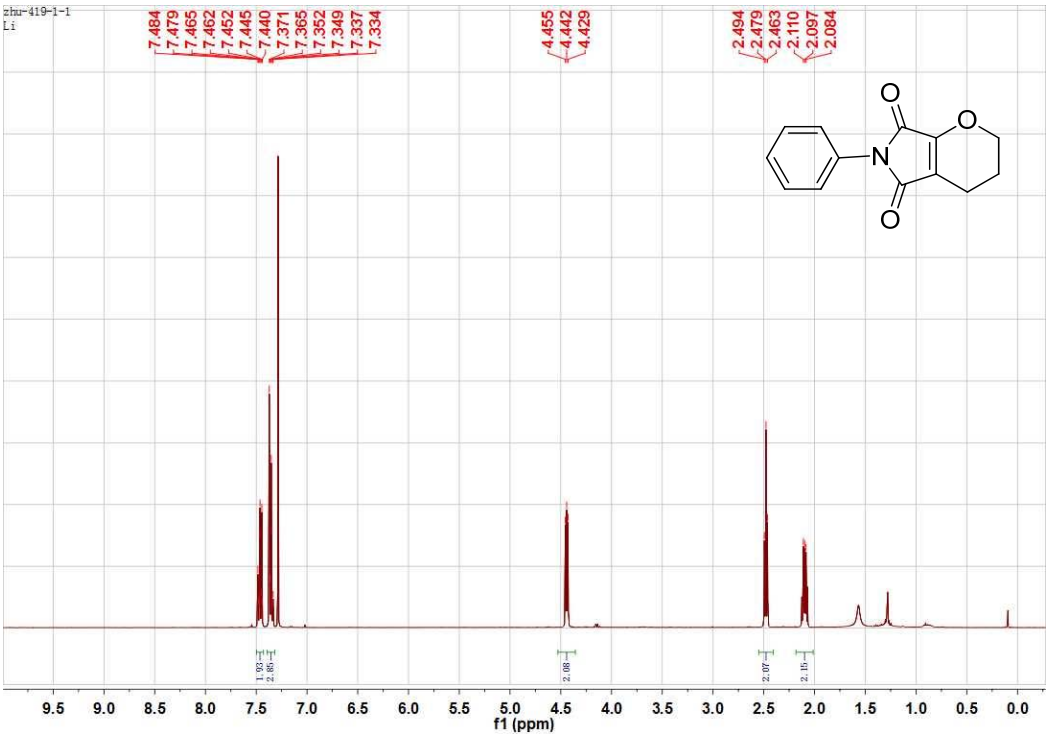

zhu-326327
Li
169.093
142.235
133.042
130.442
129.865
129.587
128.699
118.045
113.208
21.266
20.219
NC
O
N
O
f1 (ppm)

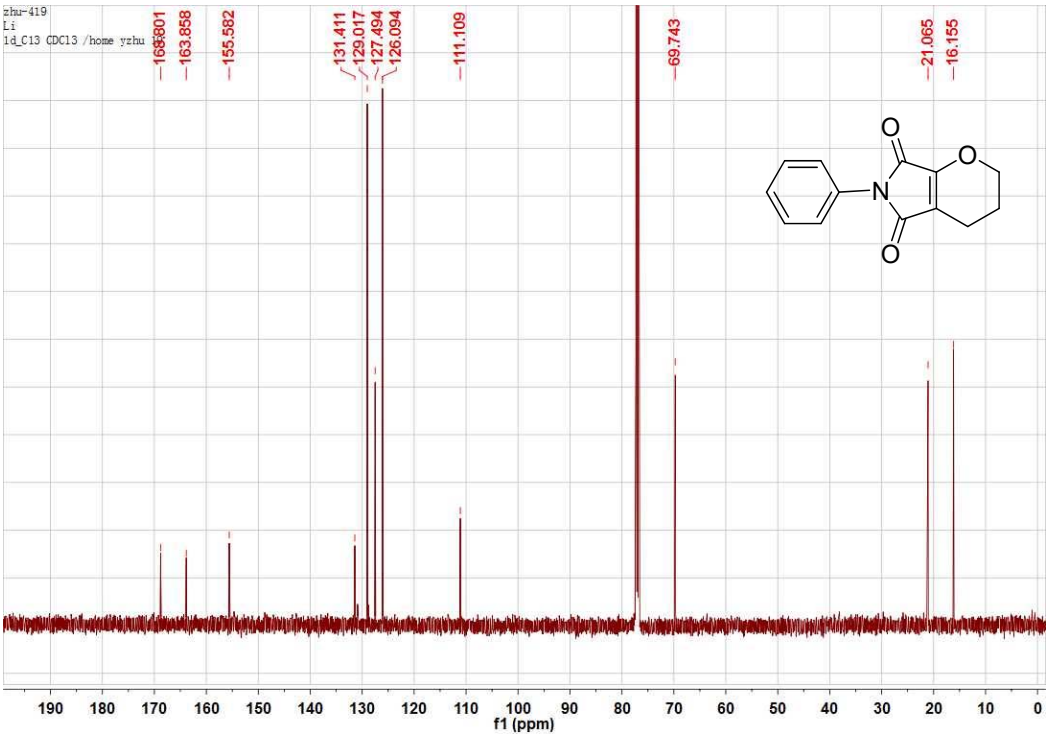

zhu-334336-5
Li
6.950
6.945
6.751
6.747
3.786
3.775
2.448
1.845
OCH3
O
N
O
H3CO
1.90
1.00
5.97
4.00
4.12
f1 (ppm)

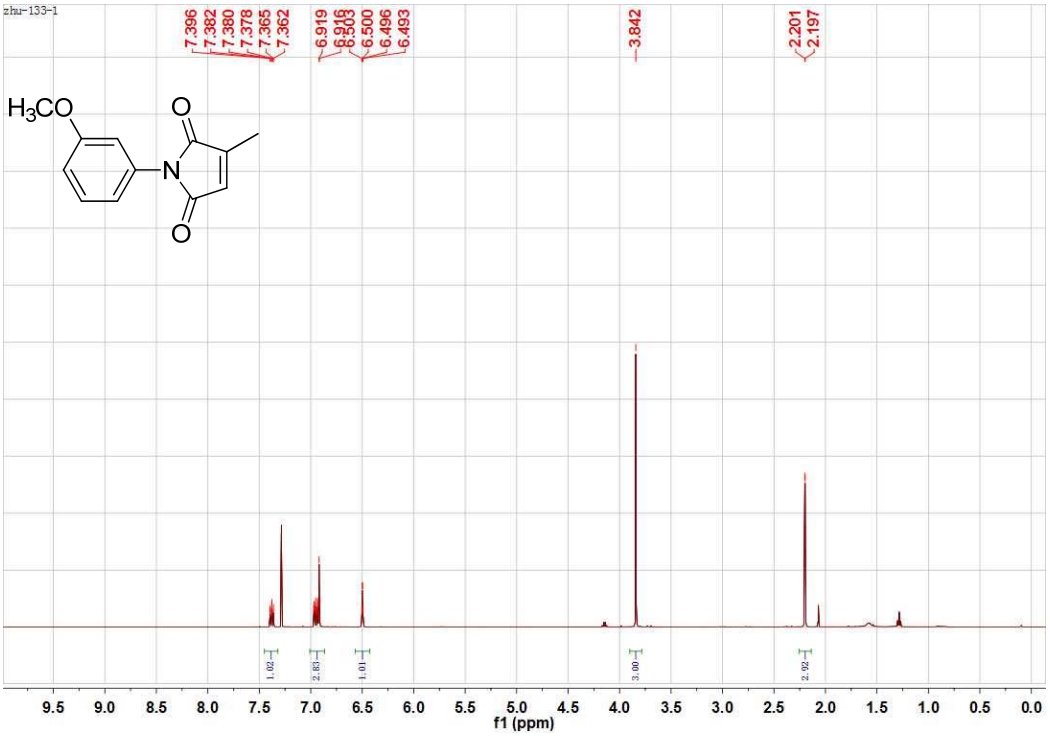

zhu-334336-5
Li
169.989
153.559
149.861
141.950
120.969
115.801
115.430
113.116
56.447
55.815
21.390
20.245
OCH3
O
N
O
H3CO
f1 (ppm)

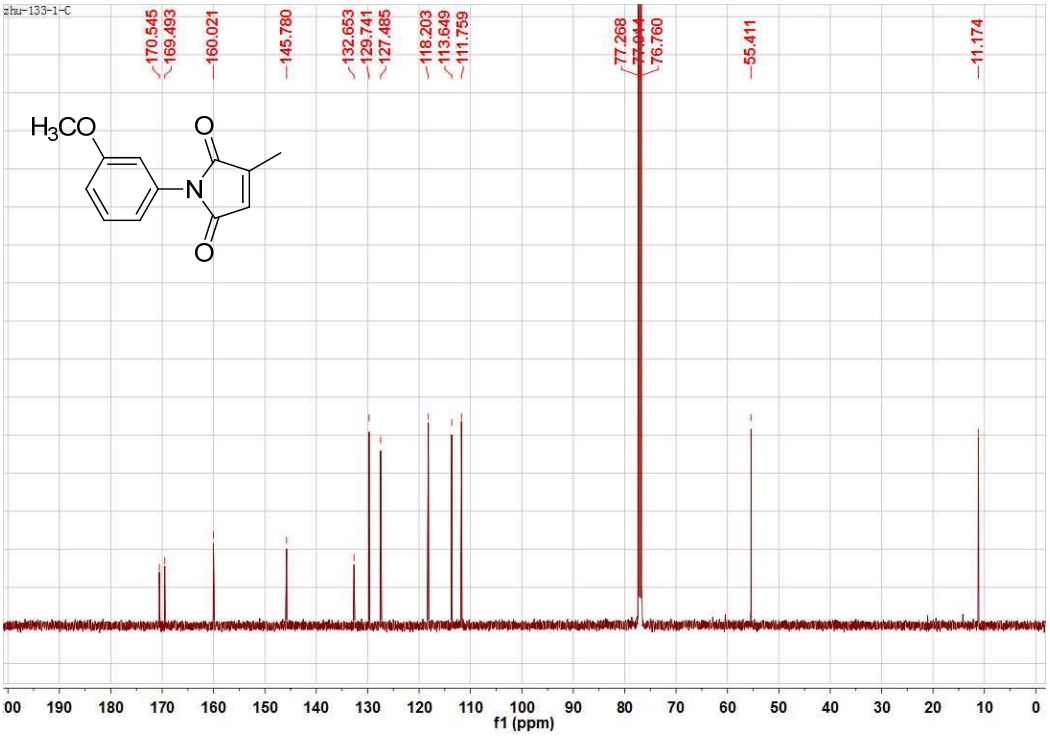

zhu-418-2
Li
7.380
7.378
7.361
7.359
7.339
6.968
6.965
6.961
6.948
6.946
6.944
6.941
6.915
6.912
6.908
6.895
6.893
6.889
4.446
4.433
4.420
3.832
2.484
2.469
2.454
2.116
2.101
2.088
2.075
2.059
O
O
N
O
H3CO
1.01
2.86
2.00
3.03
2.00
2.00
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

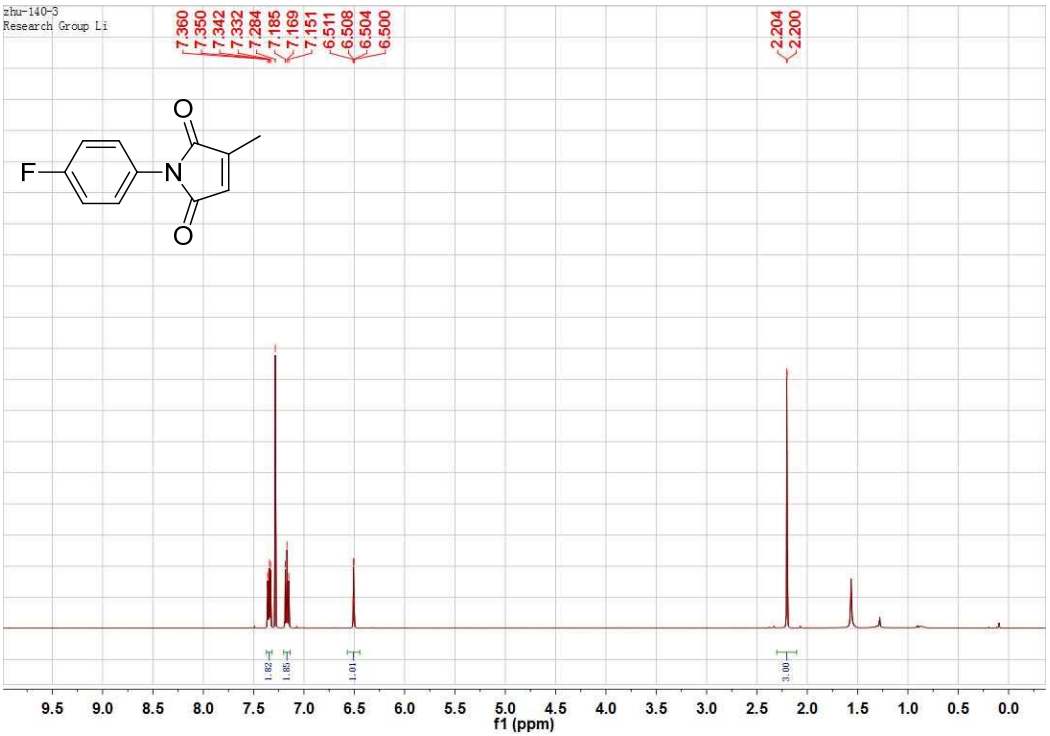

zhu-418-2C13
Li
1d_C13 CDC13 /home yzhu 29
168.728
163.782
159.964
155.564
132.403
129.673
118.376
113.442
111.919
111.123
69.743
55.389
21.058
16.148
O
O
N
O
H3CO
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

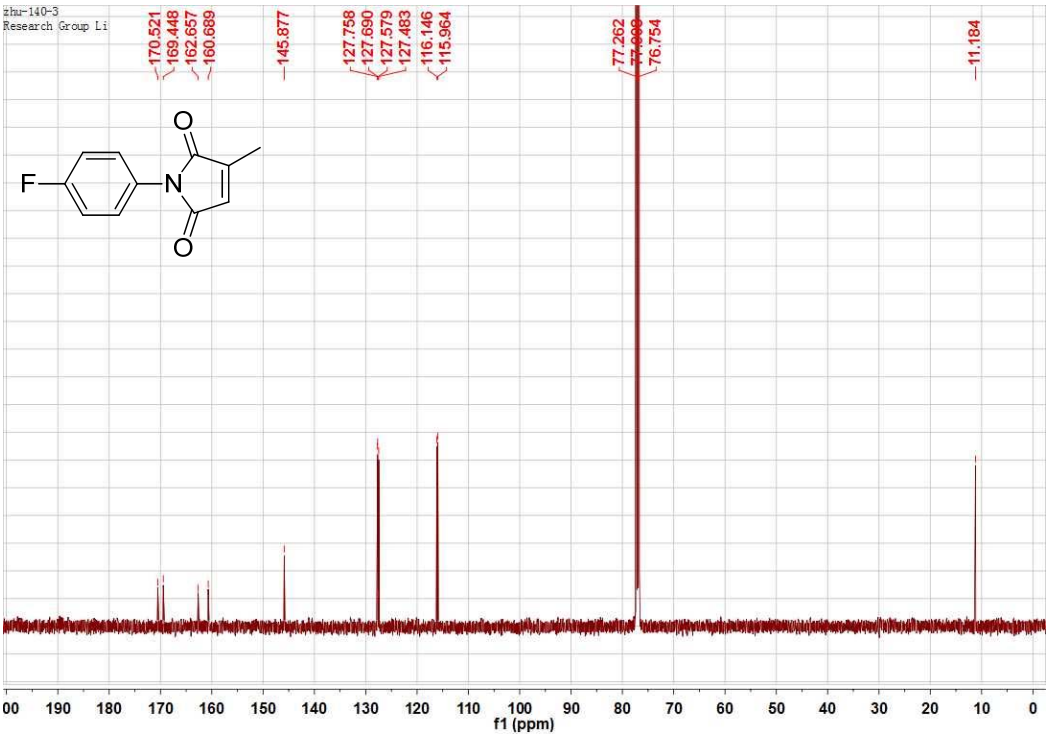

zhu-419-1-1
Li
7.484
7.479
7.465
7.462
7.452
7.445
7.440
7.371
7.365
7.352
7.349
7.337
7.334
4.455
4.442
4.429
2.494
2.479
2.463
2.110
2.097
2.084
O
O
N
O
1.93
2.85
2.08
2.07
2.15
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

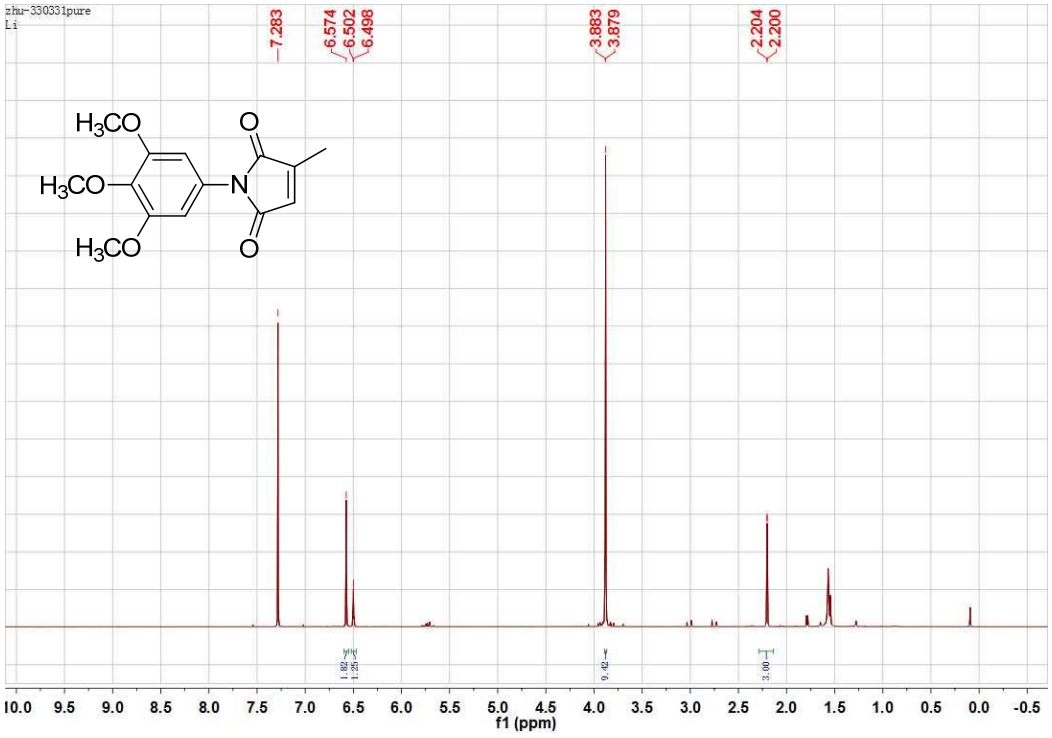

zhu-419
Li
1d_C13 CDCl3 /home yzhu
168.801
163.858
155.582
131.411
129.017
127.494
126.094
111.109
69.743
21.065
16.155
O
O
N
O
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

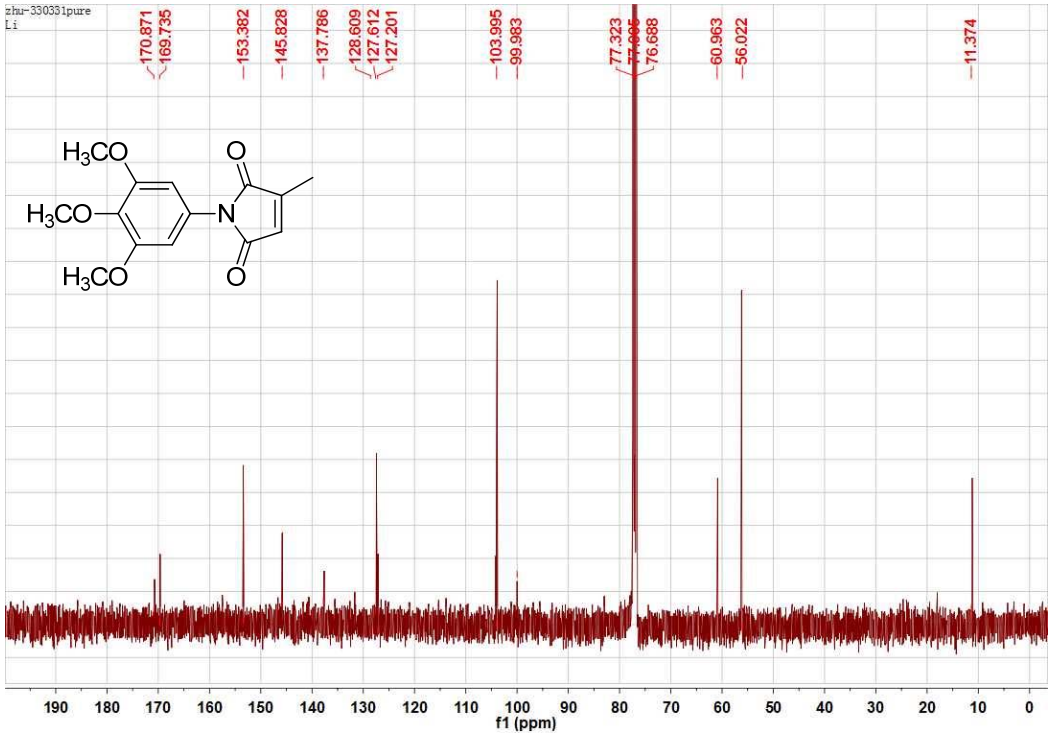

zhu-133-1
7.396
7.382
7.380
7.378
7.365
7.362
6.919
6.918
6.500
6.496
6.493
3.842
2.201
2.197
H3CO
O
N
O
1.02
2.83
1.01
3.00
2.92
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

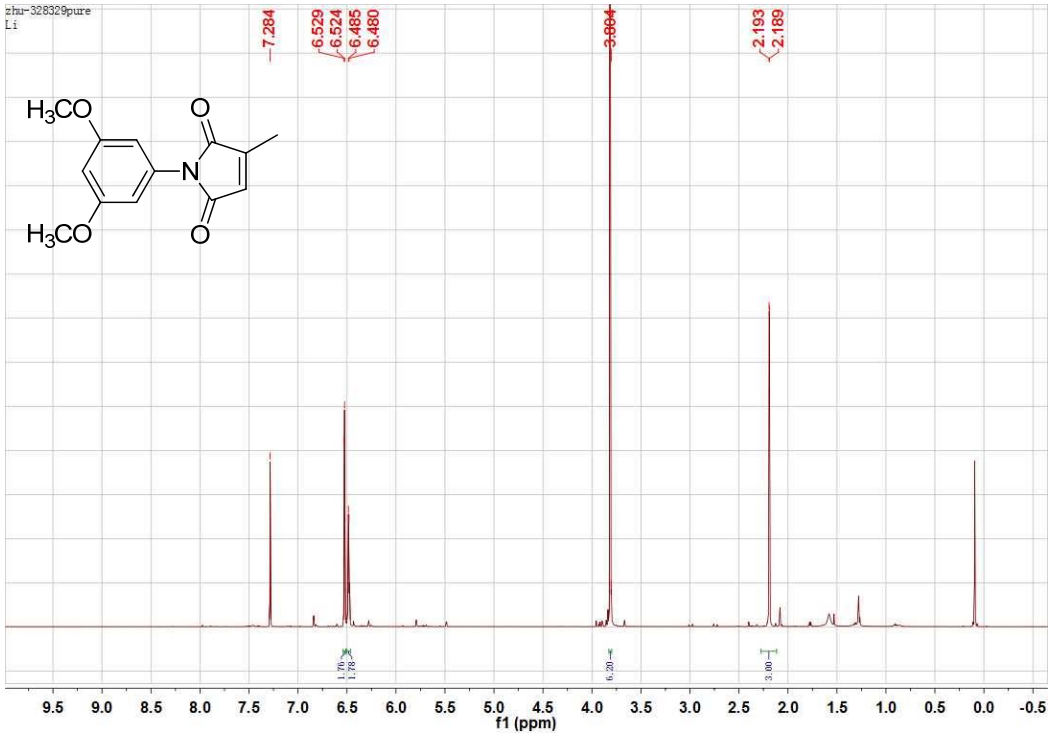

zhu-133-1-C
170.545
169.493
160.021
145.780
132.653
129.741
127.485
118.203
113.649
111.759
77.268
77.044
76.760
55.411
11.174
H3CO
O
N
O
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

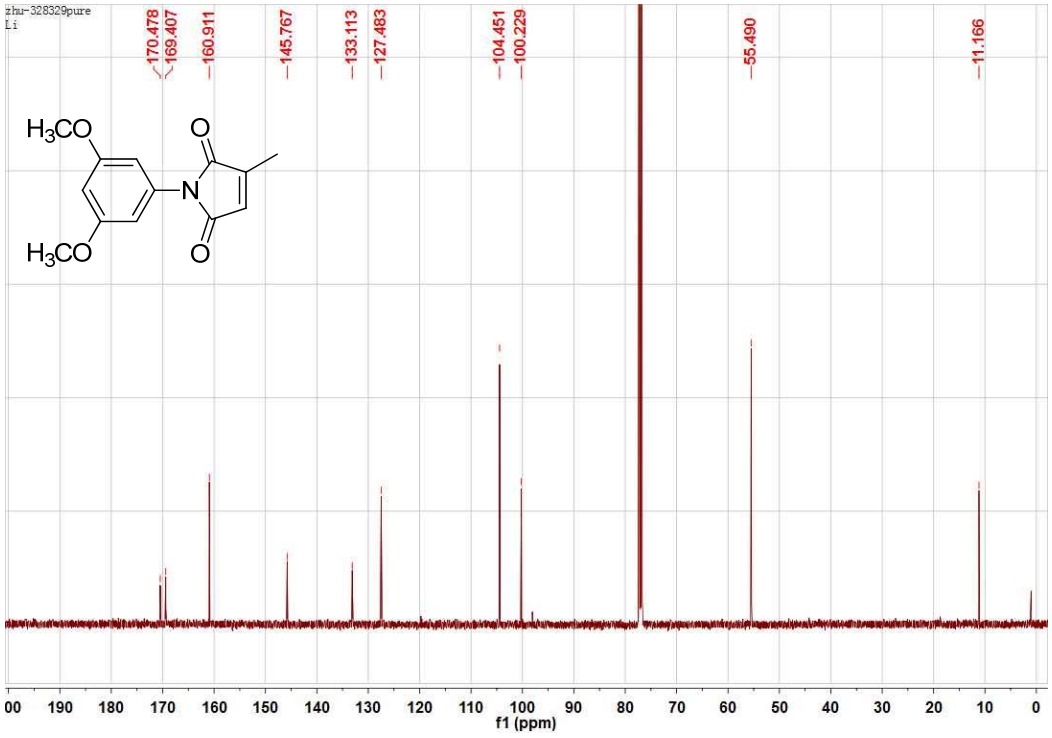

zhu-140-3
Research Group Li
7.360
7.350
7.342
7.332
7.284
7.185
7.169
7.151
6.511
6.508
6.504
6.500
2.204
2.200
F
N
O
O
1.82
1.85
1.01
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

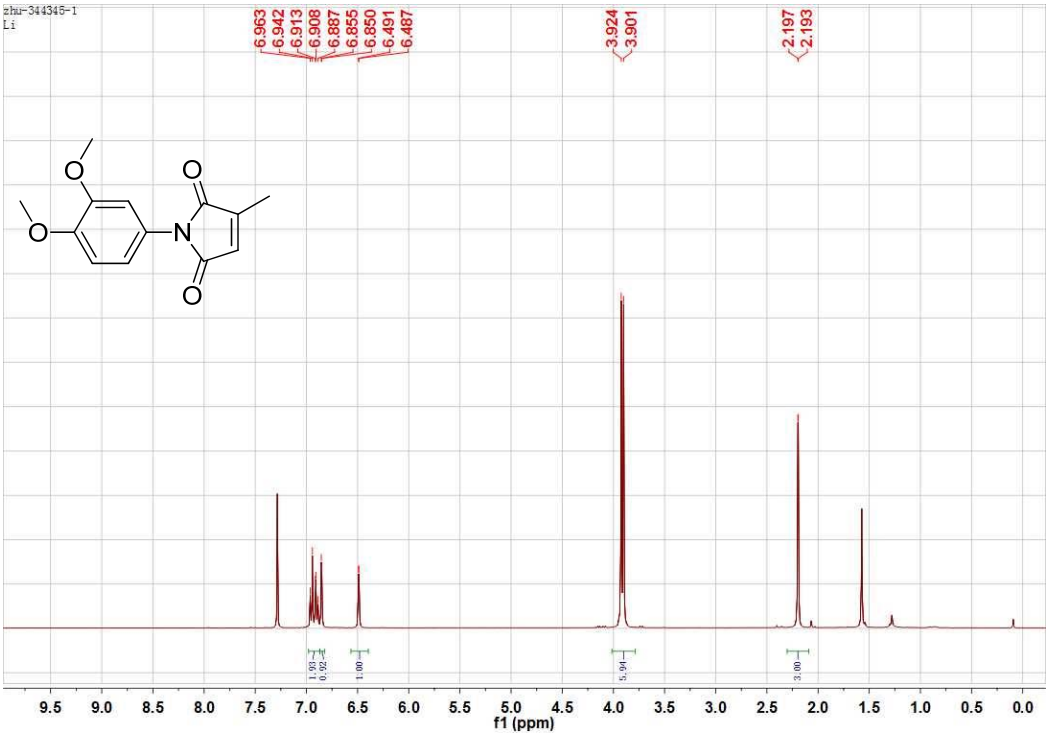

zhu-140-3
Research Group Li
170.521
169.448
162.657
160.689
145.877
127.758
127.690
127.579
127.483
116.146
115.964
77.262
77.000
76.754
11.184
F
N
O
O
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

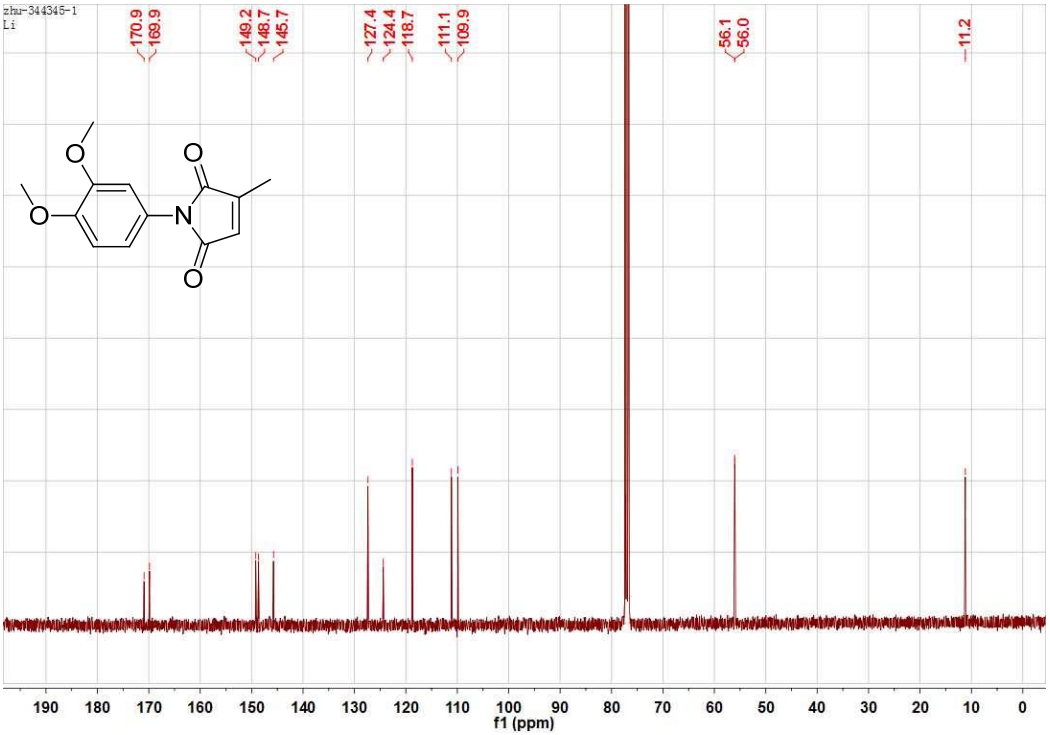

zhu-330331pure
Li
7.283
6.574
6.502
6.498
3.883
3.879
2.204
2.200
H3CO
H3CO
H3CO
O
N
O
1.82
1.25
9.42
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

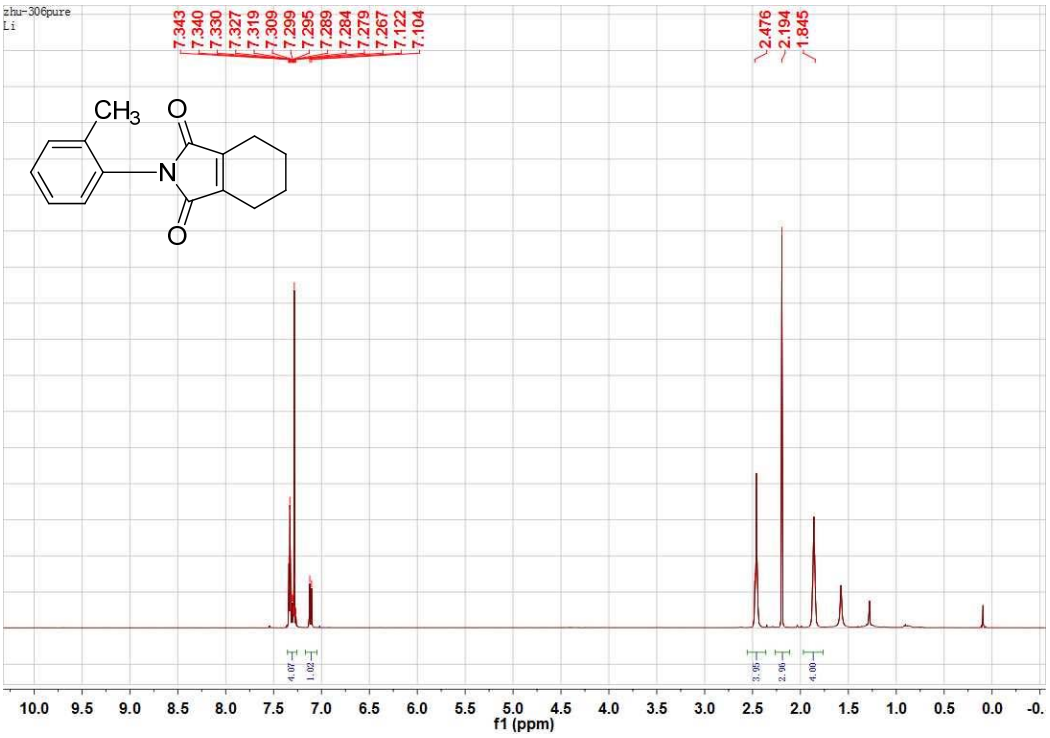

zhu-330331pure
Li
170.871
169.735
153.382
145.828
137.786
128.609
127.612
127.201
103.995
99.983
77.323
77.086
76.688
60.963
56.022
11.374
H3CO
H3CO
H3CO
O
N
O
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

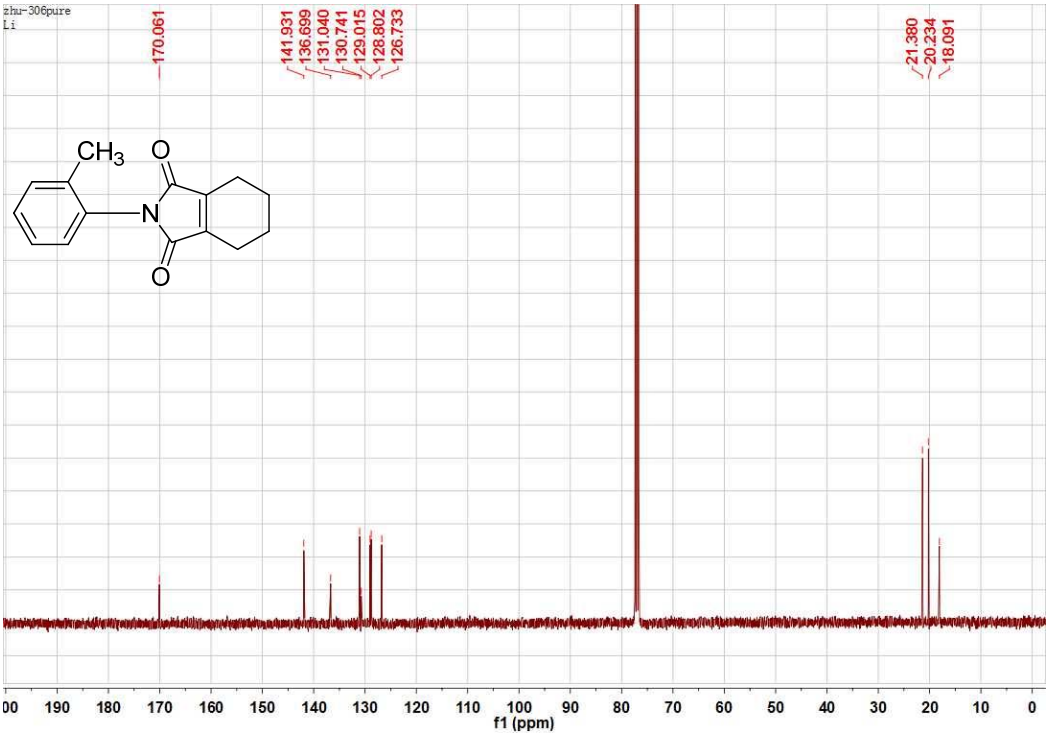

zhu-328329pure
Li
7.284
6.529
6.524
6.485
6.480
3.804
2.193
2.189
H3CO
O
N
H3CO
O
1.78
1.78
6.20
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

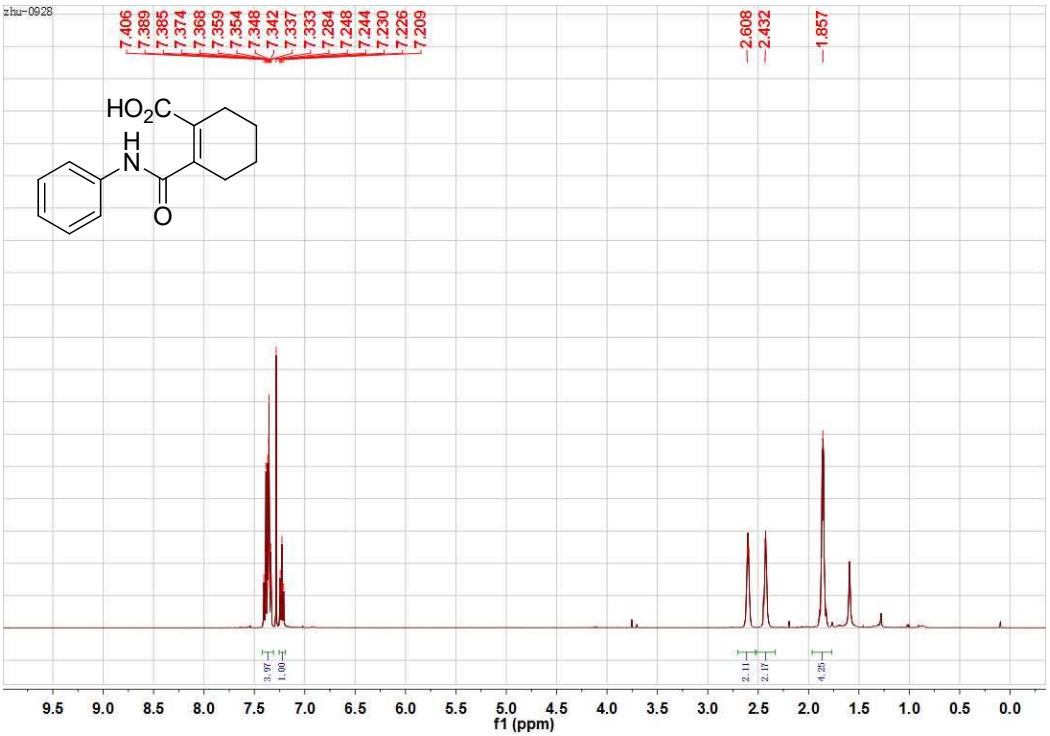

zhu-328329pure
Li
170.478
169.407
160.911
145.767
133.113
127.483
104.451
100.229
55.490
11.166
H3CO
O
N
H3CO
O
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

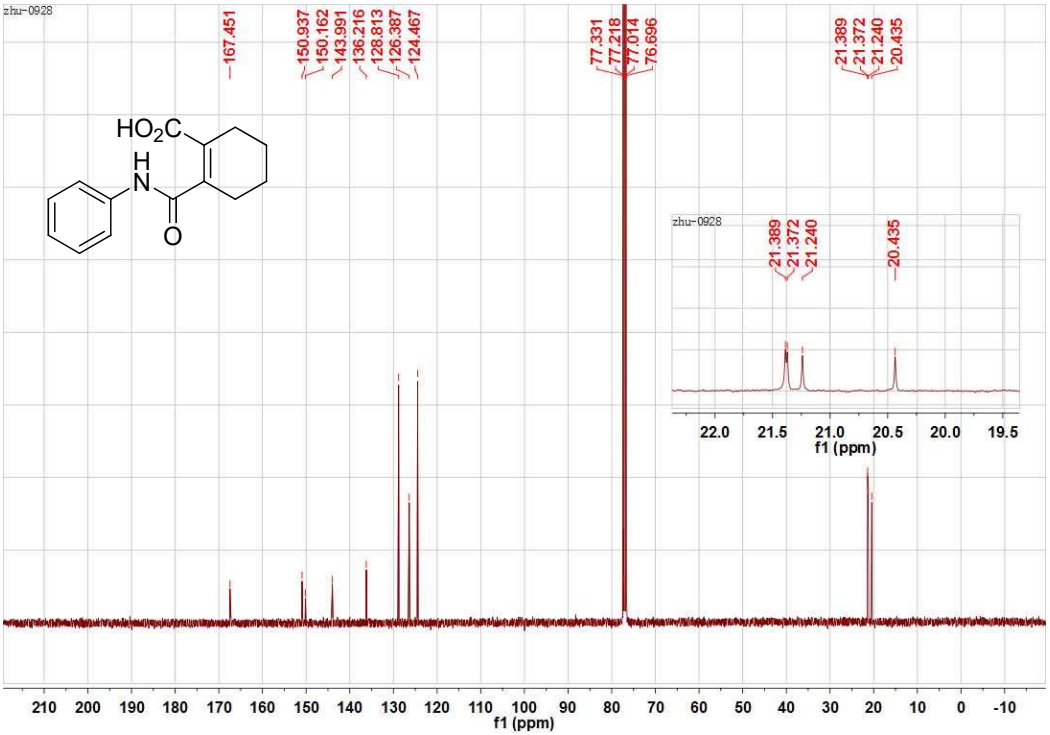

zhu-344345-1
Li
6.963
6.942
6.913
6.908
6.887
6.855
6.850
6.491
6.487
3.924
3.901
2.197
2.193
O
O
O
N
O
1.93
0.92
1.00
5.94
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

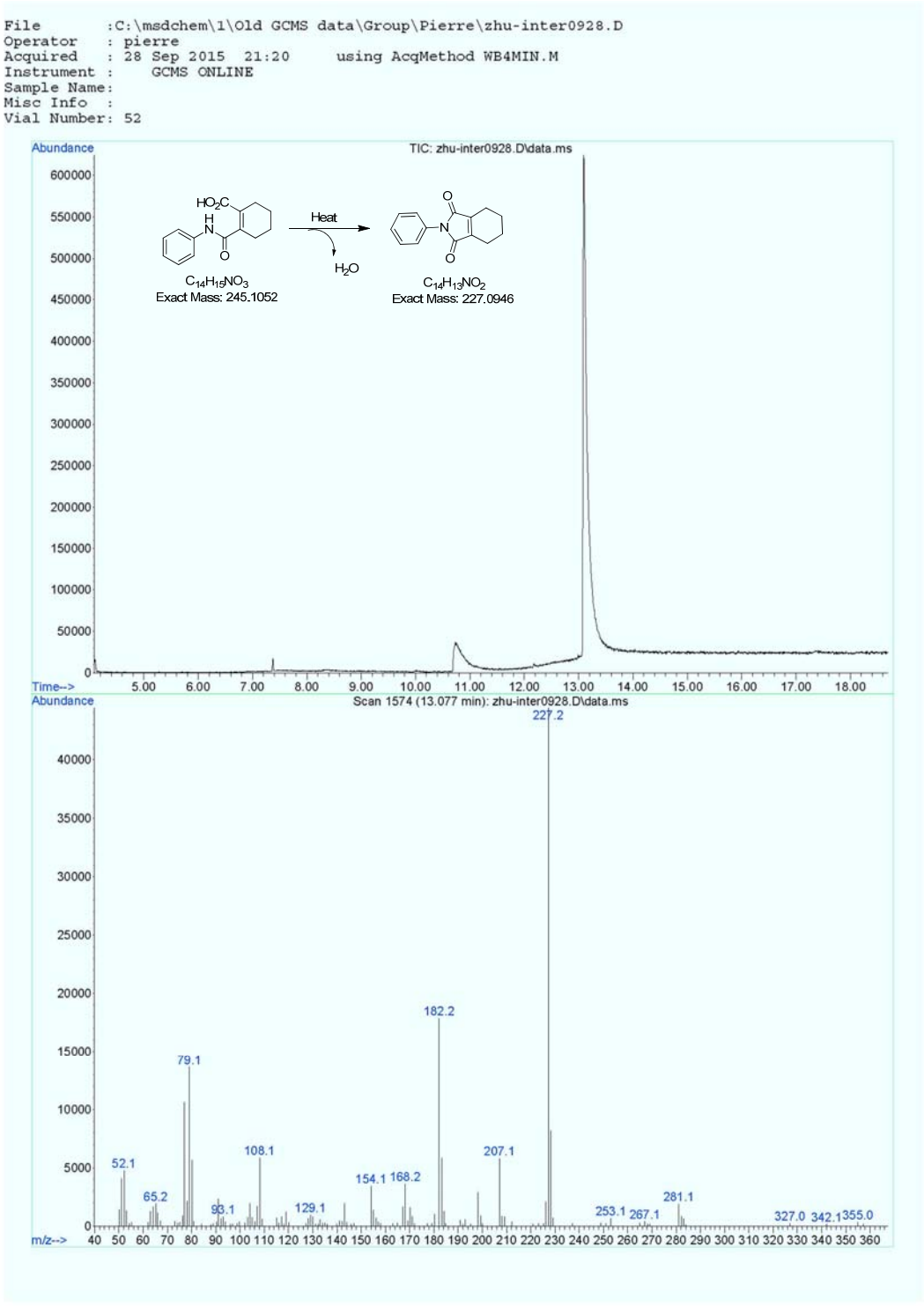

zhu-344345-1
Li
170.9
169.9
149.2
148.7
145.7
127.4
124.4
118.7
111.1
109.9
56.1
56.0
11.2
O
O
O
N
O
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


zhu-306pure
Li
7.343
7.340
7.330
7.327
7.319
7.309
7.299
7.295
7.289
7.284
7.279
7.267
7.122
7.104
2.476
2.194
1.845
CH3
O
N
O
4.07
1.02
3.05
2.00
4.00
10.0 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 -0.
f1 (ppm)

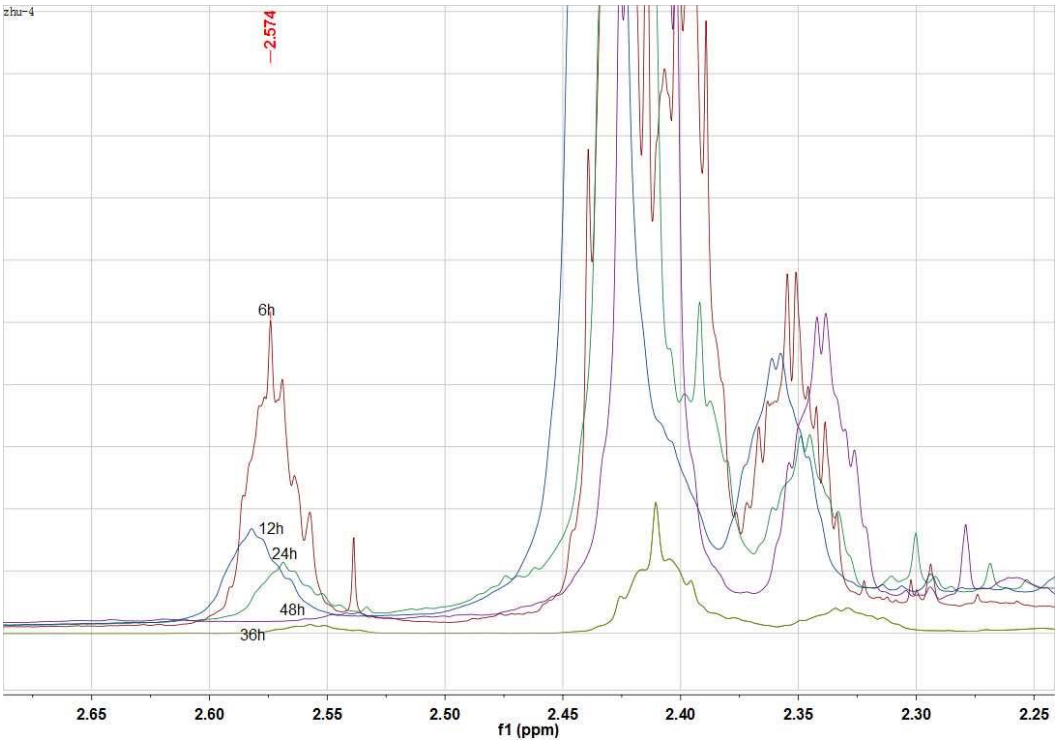

zhu-306pure
Li
170.061
141.931
136.699
131.040
130.741
129.015
128.802
126.733
21.380
20.234
18.091
CH3
O
N
O
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


zhu-0928
7.406
7.389
7.385
7.374
7.368
7.359
7.354
7.348
7.342
7.337
7.333
7.284
7.248
7.244
7.230
7.226
7.209
2.608
2.432
1.857
HO2C
H
N
O
3.97
1.00
2.11
2.17
4.25
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)


zhu-0928
167.451
150.937
150.162
143.991
136.216
128.813
126.387
124.467
77.331
77.218
77.014
76.696
21.389
21.372
21.240
20.435
HO2C
H
N
O
zhu-0928
21.389
21.372
21.240
20.435
22.0 21.5 21.0 20.5 20.0 19.5
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



The GCMS of Compound **F**.



The ^{1}HNMRs of crude products at different time.