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Electronic Supporting Information

One-pot Synthesis of Indolizine via 1,3-Dipolar Cycloaddition Using Sub-equivalent Amount of $K_2Cr_2O_7$ as an Efficient Oxidant under Base Free Conditions

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General methods and materials:

Unless otherwise noted, all commercial reagents and solvents were obtained from the commercial provider and used without further purification. ^{1}H NMR and ^{13}C NMR spectra were recorded on Bruker 400 MHz spectrometers. Chemical shifts were reported relative to internal tetramethylsilane (δ 0.00 ppm) or $CDCl_3$ (δ 7.26 ppm) for ^{1}H NMR and $CDCl_3$ (δ 77.0 ppm) for ^{13}C NMR. Flash column chromatography was performed on 300-400 mesh silica gels. Analytical thin layer chromatography was performed with pre-coated glass baked plates (250μ) and visualized by fluorescence. HRMS were recorded on Bruker micrOTOF-Q spectrometer. IR spectra were recorded by Nicolet iS50 spectrometer.

General procedure for synthesis of indolizines:

Pyridine derivative (**1**, 0.21 mmol) and α-halide carbonyl compound (**2**, 0.20 mmol) in 0.20 mL of DMF were heated at 60 ^{o}C in a test tube with a stopper for 2 h to form **3** in situ. Then alkene (**4**, 0.30 mmol), potassium dichromate (0.15 mmol) and another 1.80 mL of DMF were added to the tube. Then the mixture was heated at 80 ^{o}C for another 8h (the reaction course was monitored by TLC). Then the mixture was cooled to r.t., passed through a layer of silica gel and washed with ethyl acetate to remove the inorganic by-products. Then solvent was removed by reduce pressure. The residue was purified by flash chromatogram on silica gel using petroleum ether/ ethyl acetate as eluate to give the corresponding indolizine.

Characteristic data of new compounds

Compound ***5k*** {3-benzoyl-2-(*p*-tolyl)indolizine-1-carbonitrile}: 46.5 mg (69%, PE/ EA = 8/1); yellow solid; m. p. 65-67 ^{o}C; H NMR (400 MHz, $CDCl_3$) δ 9.65 (d, *J* = 7.1 Hz, 1H), 7.82 (d, *J* = 8.8 Hz, 1H), 7.46 (d, *J* = 7.5 Hz, 1H), 7.42 (d, *J* = 7.9 Hz, 2H), 7.22 (t, *J* = 7.4 Hz, 1H), 7.09 – 7.03 (m, 5H), 6.89 (d, *J* = 7.9 Hz, 2H), 2.21 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 187.4, 140.3, 138.6, 138.2, 131.6, 130.2, 129.5, 128.7, 128.6, 127.6, 127.4, 117.3, 115.4, 31.9, 31.0, 30.9, 29.7, 29.4, 22.7; IR (KBr): 2917, 2849, 2214, 1614, 1563, 1507, 1463, 1433; HRMS (ESI): m/z calcd for $C_{23}H_{16}N_2O$: 336.1263 $[M+Na]^+$; found: 359.1155.

Compound ***5l*** {1-(3-benzoylindolizin-1-yl)propan-1-one}: 46.8 mg (85%, PE/ EA = 6/ 1); white solid; m. p. 133-135 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.95 (d, *J* = 7.0 Hz, 1H), 8.65 (d, *J* = 8.9 Hz, 1H), 7.80 (d, *J* = 7.1 Hz, 2H), 7.70 (s, 1H), 7.61 – 7.56 (m, 1H), 7.55 – 7.45 (m, 3H), 7.12 (t, *J* = 6.8 Hz, 1H), 2.87 (q, *J* = 7.3 Hz, 2H), 1.21 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.2, 185.5, 140.0, 139.6, 131.5, 129.0, 128.9, 128.8, 128.5, 128.2, 122.3, 120.5, 116.1, 114.3, 32.9, 29.7; IR (KBr): 2974, 2935, 1652, 1623, 1574, 1512, 1478, 1458, 1439, 1411; HRMS (ESI): m/z calcd for $C_{18}H_{15}NO_2$: 277.1103 $[M+Na]^+$; found: 300.0995.

Compound ***5o*** {phenyl(1-(phenylsulfonyl)indolizin-3-yl)methanone}: 30.9 mg (43%, PE/ EA = 8/ 1); white solid; m. p. 193-194 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.96 (d, *J* = 7.0 Hz, 1H), 8.25 (d, *J* = 9.0 Hz, 1H), 7.98 (d, *J* = 7.7 Hz, 2H), 7.89 – 7.78 (m, 3H), 7.65 (t, *J* = 7.3 Hz, 1H), 7.59 – 7.53 (m, 3H), 7.53 – 7.48 (m, 3H), 7.17 (t, *J* = 7.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 185.6,

143.2, 139.2, 137.1, 132.8, 132.0, 129.4, 129.2, 129.0, 128.6, 128.3, 127.5, 126.5, 122.7, 117.7, 115.9, 113.9; IR (KBr): 2918, 2849, 1621, 1563, 1500, 1479, 1447; HRMS (ESI): m/z calcd for $C_{21}H_{15}NO_3S$: 361.0773 $[M+Na]^+$; found: 384.0665

Compound ***6a*** {butyl 3-benzoyl-5-methylindolizine-1-carboxylate}: 31.3 mg (47%, PE/ EA = 8/1); yellow sticky oil; ^1H NMR (400 MHz, $CDCl_3$): 8.39 (d, J = 8.8 Hz, 1H), 8.07 (d, J = 7.3 Hz, 2H), 7.75 (s, 1H), 7.65 (t, J = 7.4 Hz, 1H), 7.56 (t, J = 7.6 Hz, 2H), 7.48 – 7.42 (m, 1H), 6.94 (d, J = 6.9 Hz, 1H), 4.33 (t, J = 6.7 Hz, 2H), 2.62 (s, 3H), 1.80 – 1.73 (m, 2H), 1.52 – 1.44 (m, 2H), 0.98 (t, J = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 182.9, 164.2, 141.8, 139.8, 138.6, 132.6, 130.3, 129.6, 128.4, 127.4, 125.4, 117.1, 116.7, 105.5, 63.9, 31.0, 29.7, 23.2, 19.3; IR (KBr): 2959, 1670, 1632, 1561, 1522, 1480, 1421; HRMS (ESI): m/z calcd for $C_{21}H_{21}NO_3$: 335.1521 $[M+Na]^+$; found: 358.1414.

Compound ***6b*** {butyl 3-benzoyl-5,7-dimethylindolizine-1-carboxylate}: 25.9 mg (37%, PE/ EA = 8/1); yellow solid; m. p. 56-59 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 8.19 (s, 1H), 8.05 (d, J = 7.2 Hz, 2H), 7.70 (s, 1H), 7.64 (t, J = 7.4 Hz, 1H), 7.55 (t, J = 7.5 Hz, 2H), 6.79 (s, 1H), 4.32 (t, J = 6.8 Hz, 2H), 2.60 (s, 3H), 2.50 (s, 3H), 1.79 – 1.72 (m, 2H), 1.51 – 1.42 (m, 2H), 0.98 (t, J = 7.4 Hz, 3H); ^{13}C NMR (100MHz, $CDCl_3$) δ 182.6, 164.4, 142.5, 139.3, 139.0, 138.8, 132.4, 130.2, 128.4, 125.0, 119.2, 116.1, 104.3, 63.8, 31.0, 30.9, 29.7, 23.0, 21.3, 19.3; IR (KBr): 2957, 2917, 2849, 1687, 1626, 1538, 1514, 1482, 1465; HRMS (ESI): m/z calcd for $C_{22}H_{23}NO_3$: 349.1678 $[M+Na]^+$; found: 372.1570.

Compound ***6d*** {butyl 3-benzoylpyrrolo[2,1-*a*]isoquinoline-1-carboxylate}: 52.5 mg (71%, PE/ EA = 10/1); yellow solid; m. p. 109-111 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 9.84 (d, J = 7.6 Hz, 1H), 9.66 (d, J = 7.4 Hz, 1H), 7.90 (d, J = 7.4 Hz, 2H), 7.84 (s, 1H), 7.79 – 7.74 (m, 1H), 7.68 – 7.66 (m, 2H), 7.63 (d, J = 7.1 Hz, 1H), 7.56 (t, J = 7.4 Hz, 2H), 7.27 (d, J = 7.6 Hz, 1H), 4.37 (t, J = 6.8 Hz, 2H), 1.80 – 1.76 (m, 2H), 1.53 – 1.43 (m, 2H), 1.00 (t, J = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 185.9, 164.7, 139.8, 136.9, 131.8, 130.5, 130.1, 129.3, 129.3, 128.4, 128.1, 127.8, 126.7, 125.1, 124.6, 123.3, 115.5, 110.3, 64.6, 30.9, 19.4, 13.9; IR (KBr): 2961, 1710, 1622, 1524, 1459, 1424, 1362; HRMS (ESI): m/z calcd for $C_{24}H_{21}NO_3$: 371.1521 $[M+Na]^+$; found: 394.1414.

Compound ***6f*** {1-butyl 7-methyl 3-benzoylindolizine-1,7-dicarboxylate}: 43.2 mg (57%, PE/ EA = 8/ 1); yellow solid; m. p. 112-113 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 9.92 (d, J = 7.4 Hz, 1H), 9.12 – 8.97 (m, 1H), 7.87 (s, 1H), 7.86 – 7.81 (m, 2H), 7.61 (dd, J = 7.3, 1.6 Hz, 2H), 7.54 (t, J = 7.4 Hz, 2H), 4.37 (t, J = 6.7 Hz, 2H), 4.00 (s, 3H), 1.87 – 1.73 (m, 2H), 1.58 – 1.45 (m, 2H), 1.01 (t, J = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 185.9, 165.2, 163.7, 139.4, 138.2, 131.9, 129.1, 129.1, 128.5, 128.5, 128.0, 123.7, 121.9, 114.1, 109.2, 64.4, 52.7, 30.9, 19.4, 13.8; IR (KBr): 2957, 1725, 1702, 1618, 1529, 1473, 1433; HRMS (ESI): m/z calcd for $C_{22}H_{21}NO_5$: 379.1420 $[M+Na]^+$; found: 402.1312.

Compound ***6g*** {butyl 3-(4-nitrobenzoyl)indolizine-1-carboxylate}: 65.2mg (89%, PE/ EA = 6/ 1); yellow solid; m. p. 87-89 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 9.99 (d, J = 6.9 Hz, 1H), 8.44 (d, J = 8.9 Hz 1H), 8.38 (d, J = 8.5 Hz, 2H), 7.96 (d, J = 8.5 Hz, 2H), 7.75 (s, 1H), 7.55 (t, J = 7.8 Hz, 1H), 7.18 (t, J = 6.9 Hz, 1H), 4.34 (t, J = 6.7 Hz, 2H), 1.81 – 1.74 (m, 2H), 1.52 – 1.42 (m, 2H),

0.99 (t, J = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 182.9, 163.8, 149.4, 145.4, 140.4, 129.7, 129.3, 129.2, 128.6, 123.7, 121.9, 119.7, 116.0, 107.3, 64.3, 30.9, 19.3, 13.8; IR (KBr): 2959, 2873, 1702, 1634, 1619, 1598, 1562, 1522, 1484; HRMS (ESI): m/z calcd for $C_{20}H_{18}N_2O_5$: 366.1216 $[M+Na]^+$; found: 389.1108

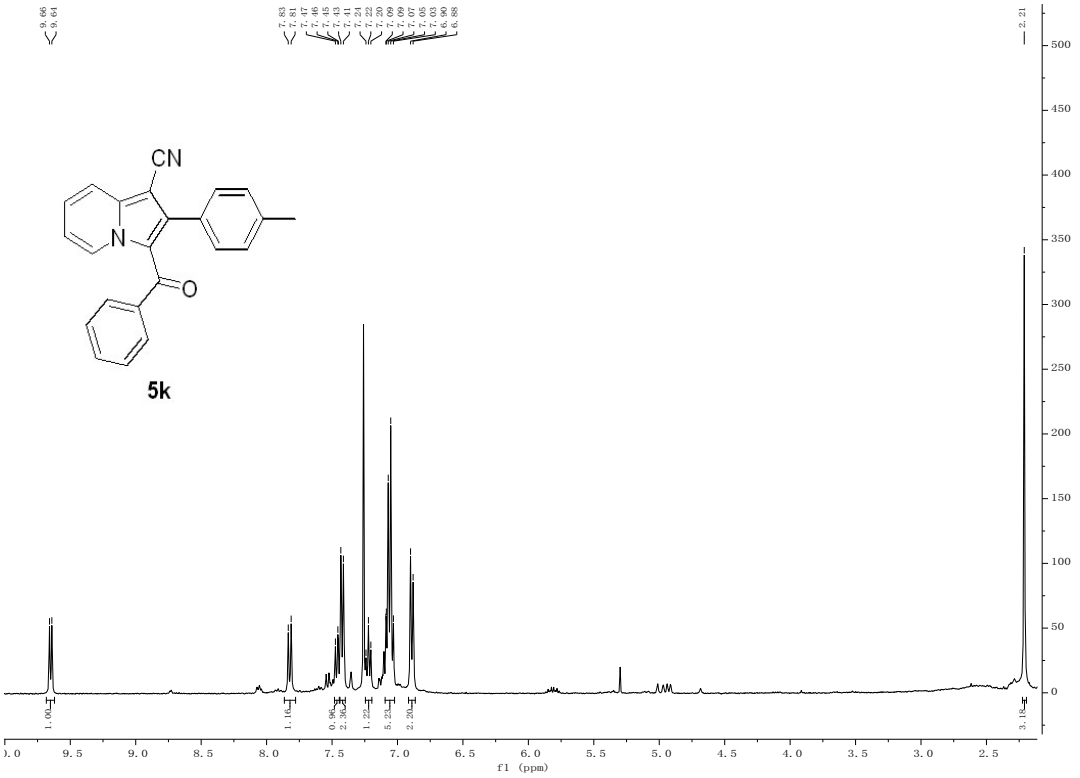
Compound ***6h*** {butyl 3-(4-methoxybenzoyl)indolizine-1-carboxylate}: 43.8 mg (62%, PE/ EA = 6/ 1); white solid; m. p. 72-73 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.88 (d, J = 7.0 Hz, 1H), 8.35 (d, J = 8.9 Hz, 1H), 7.87 – 7.78 (m, 3H), 7.40 (t, J = 7.8 Hz, 1H), 7.03 (t, J = 7.0 Hz, 1H), 7.00 (d, J = 8.7 Hz, 2H), 4.32 (t, J = 6.7 Hz, 2H), 3.89 (s, 3H), 1.79 –1.72 (m, 2H), 1.51 – 1.41 (m, 2H), 0.97 (t, J = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 184.5, 164.3, 162.5, 139.6, 132.3, 131.2, 129.1, 128.3, 127.3, 122.7, 119.5, 115.0, 113.7, 106.0, 64.0, 55.5, 31.0, 29.7, 19.4; IR (KBr): 2952, 2918, 1711, 1616, 1600, 1523, 1485; HRMS (ESI): m/z calcd for $C_{21}H_{21}NO_4$: 351.1471 $[M+Na]^+$; found: 374.1363.

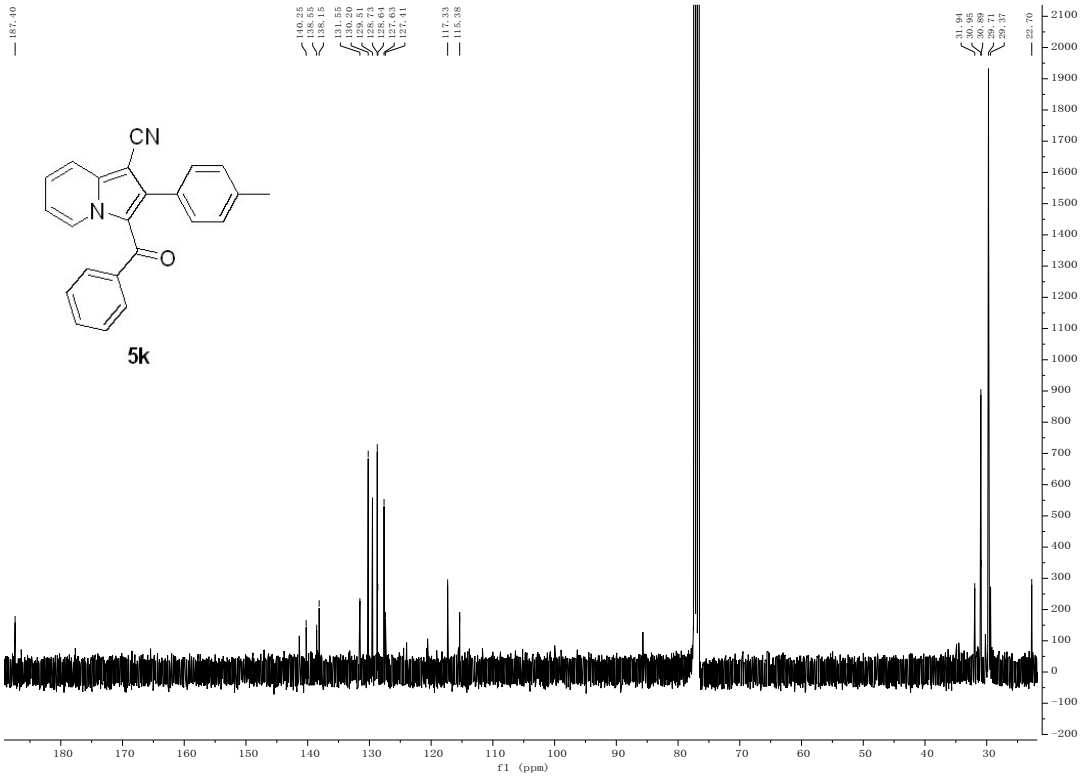
Compound ***6i*** {1-butyl 3-ethyl indolizine-1,3-dicarboxylate}: 33.0 mg (57%, PE/ EA = 8/ 1); yellow solid; m. p. 53-55 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.53 (d, J = 7.0 Hz, 1H), 8.34 (d, J = 9.0 Hz, 1H), 7.99 (s, 1H), 7.34 – 7.30 (m, 1H), 6.98 (t, J = 6.8 Hz, 1H), 4.40 (q, J = 7.1 Hz, 2H), 4.35 (t, J = 6.7 Hz, 2H), 1.83 – 1.76 (m, 2H), 1.57 – 1.49 (m, 2H), 1.43 (t, J = 7.1 Hz, 3H), 1.01 (t, J = 7.4 Hz, 3H); ^{13}C NMR (100MHz, $CDCl_3$) δ 164.3, 161.2, 139.0, 127.9, 125.6, 124.2, 119.6, 114.7, 114.3, 105.2, 63.8, 60.3, 31.0, 19.4, 14.5, 13.8; IR ((KBr): 2961, 1692, 1525, 1492, 1433; HRMS (ESI): m/z calcd for $C_{16}H_{19}NO_4$: 289.1314 $[M+Na]^+$; found: 312.1206.

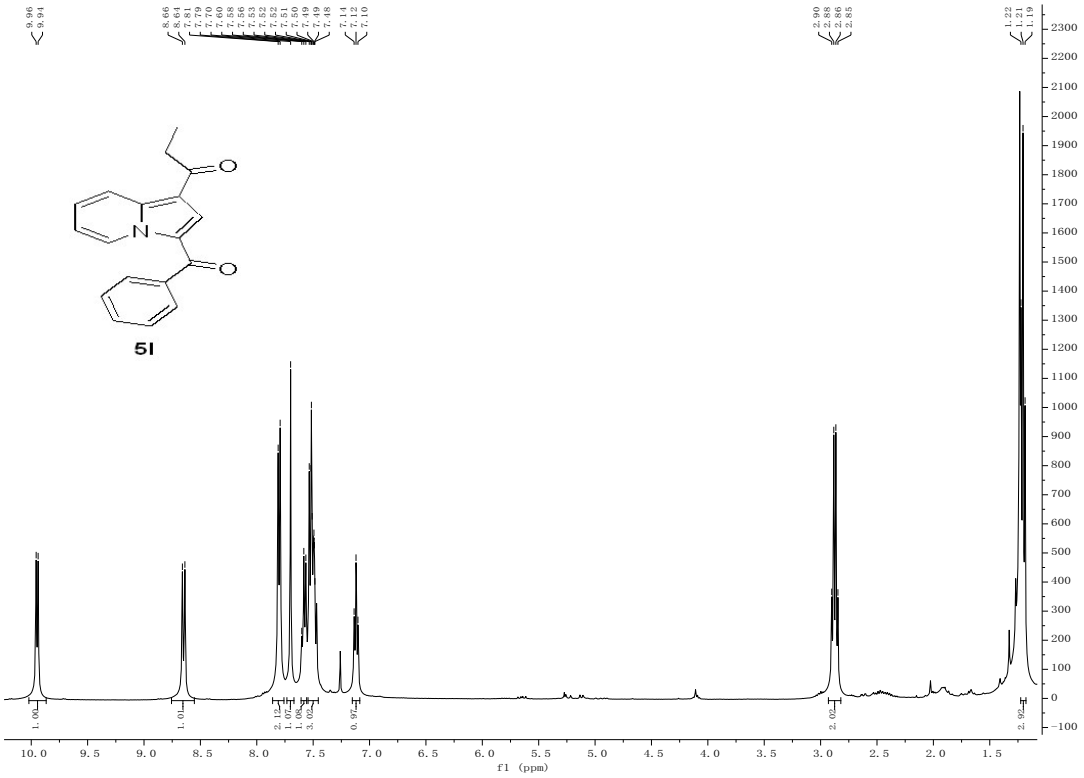
Compound ***6j*** {1-butyl 3-phenyl indolizine-1,3-dicarboxylate}: 25.6 mg (38%, PE/ EA = 8/ 1); white solid; m. p. 91-93 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.53 (d, J = 7.0 Hz, 1H), 8.42 (d, J = 9.0 Hz, 1H), 8.25 (s, 1H), 7.47 (t, J = 7.8 Hz, 2H), 7.43 – 7.38 (m, 1H), 7.32 (d, J = 7.4 Hz, 1H), 7.29 – 7.25 (m, 2H), 7.05 (t, J = 6.9 Hz, 1H), 4.38 (t, J = 6.6 Hz, 2H), 1.85 – 1.78 (m, 2H), 1.59 – 1.50 (m, 2H), 1.03 (t, J = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.1, 159.5, 150.5, 139.7, 129.5, 128.1, 126.3, 125.9, 125.4, 121.9, 119.7, 114.8, 113.6, 105.9, 77.3, 64.0, 31.0, 19.4, 13.8; IR (KBr): 2958, 1711, 1687, 1633, 1526, 1488, 1445, 1434; HRMS (ESI): m/z calcd for $C_{20}H_{19}NO_4$: 337.1314 $[M+Na]^+$; found: 360.1206.

Compound ***6k*** {butyl 3-cyanoindolizine-1-carboxylate}: 44.6 mg (92%, PE/ EA = 8/ 1); yellow solid; m. p. 71-73 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.32 (t, J = 8.1 Hz, 2H), 7.78 (s, 1H), 7.38 – 7.29 (m, 1H), 7.03 (t, J = 6.9 Hz, 1H), 4.32 (t, J = 6.6 Hz, 2H), 1.81 – 1.71 (m, 2H), 1.53 – 1.43 (m, 2H), 0.98 (t, J = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.4, 137.8, 126.0, 125.7, 125.2, 120.4, 115.0, 112.7, 106.1, 96.6, 64.2, 30.9, 29.7, 19.4; IR (KBr): 2963, 2930, 2212, 1702, 1521, 1488, 1448, 1435; HRMS (ESI): m/z calcd for $C_{14}H_{14}N_2O_2$: 242.1055 $[M+Na]^+$; found: 265.0947.

Copies of compounds' NMR spectra



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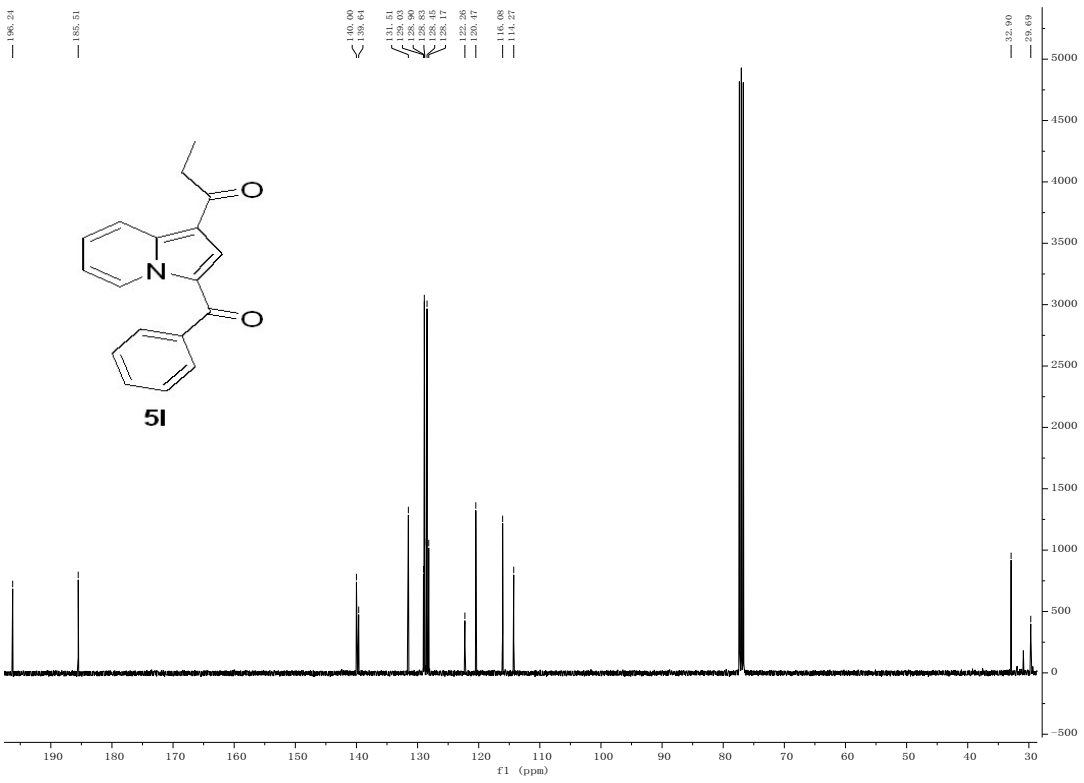
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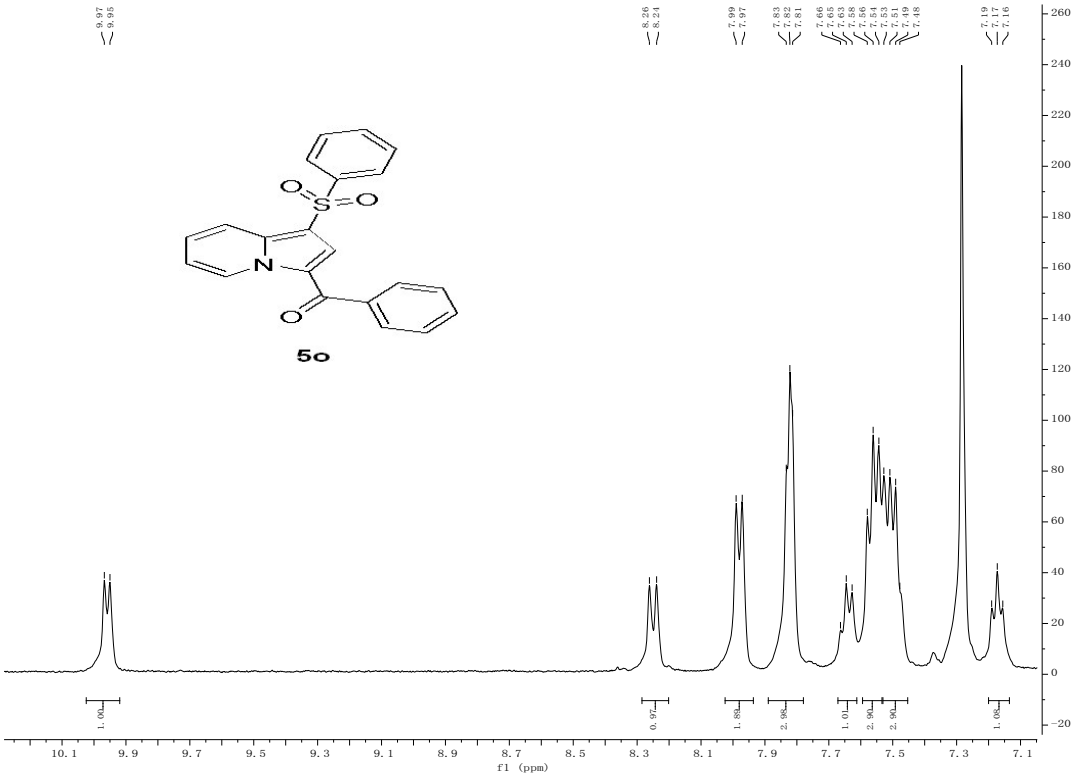
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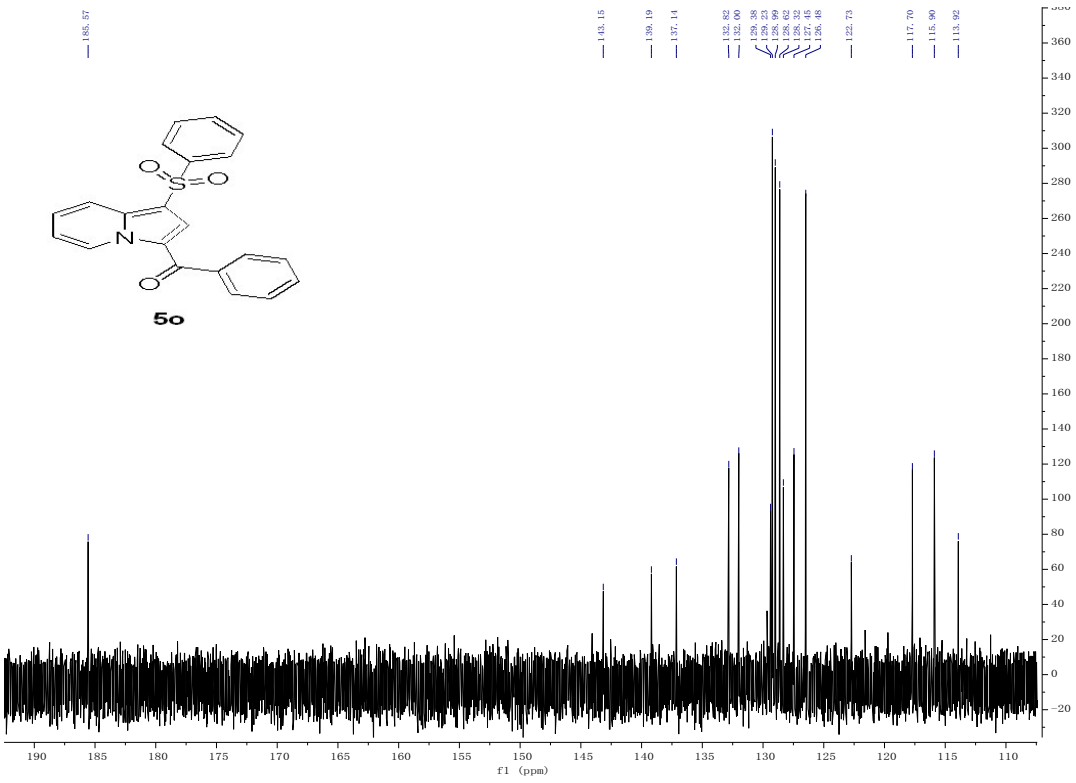
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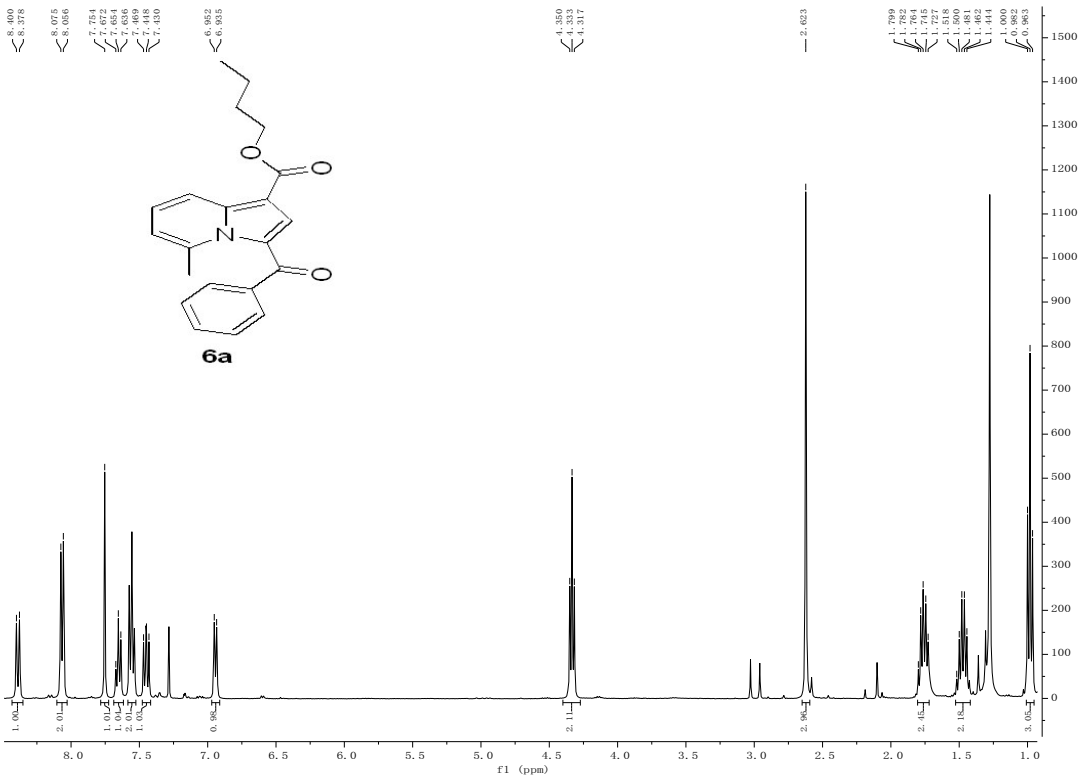
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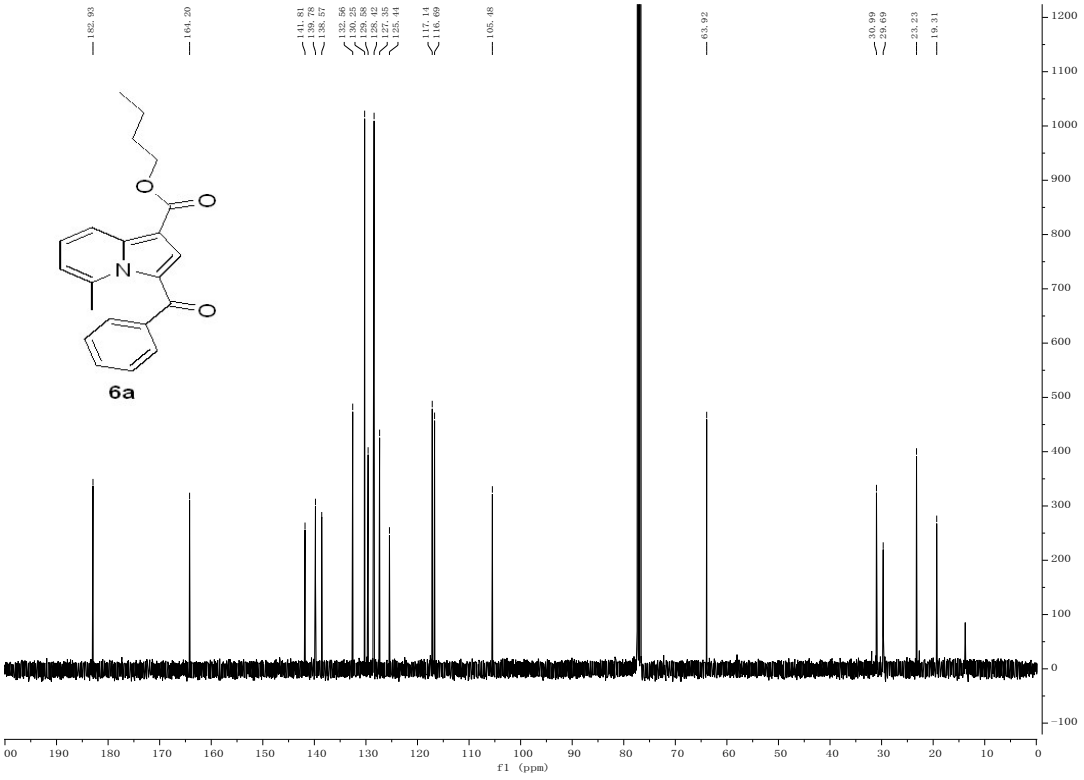
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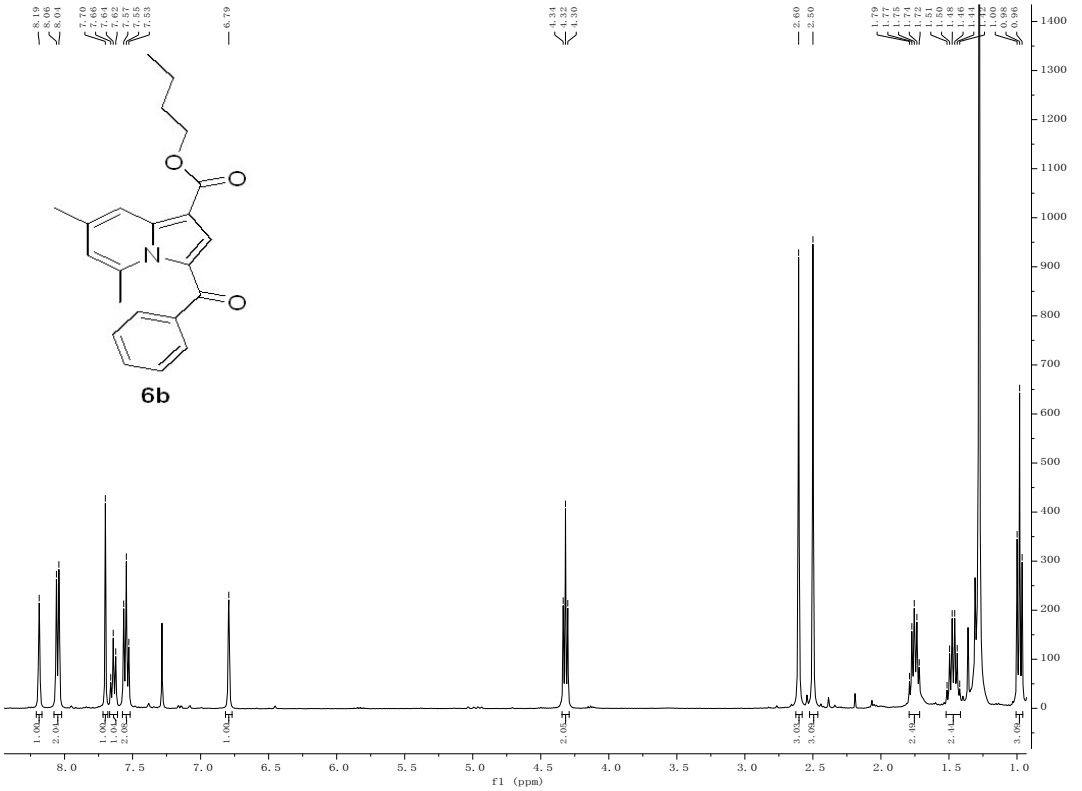
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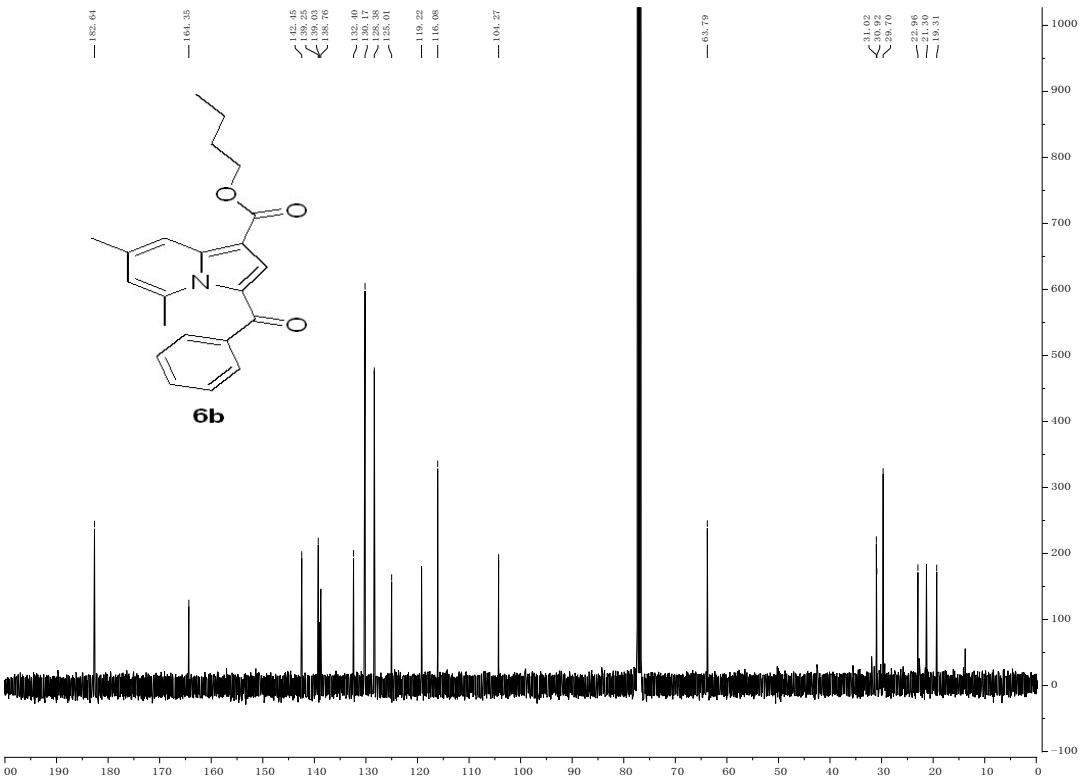
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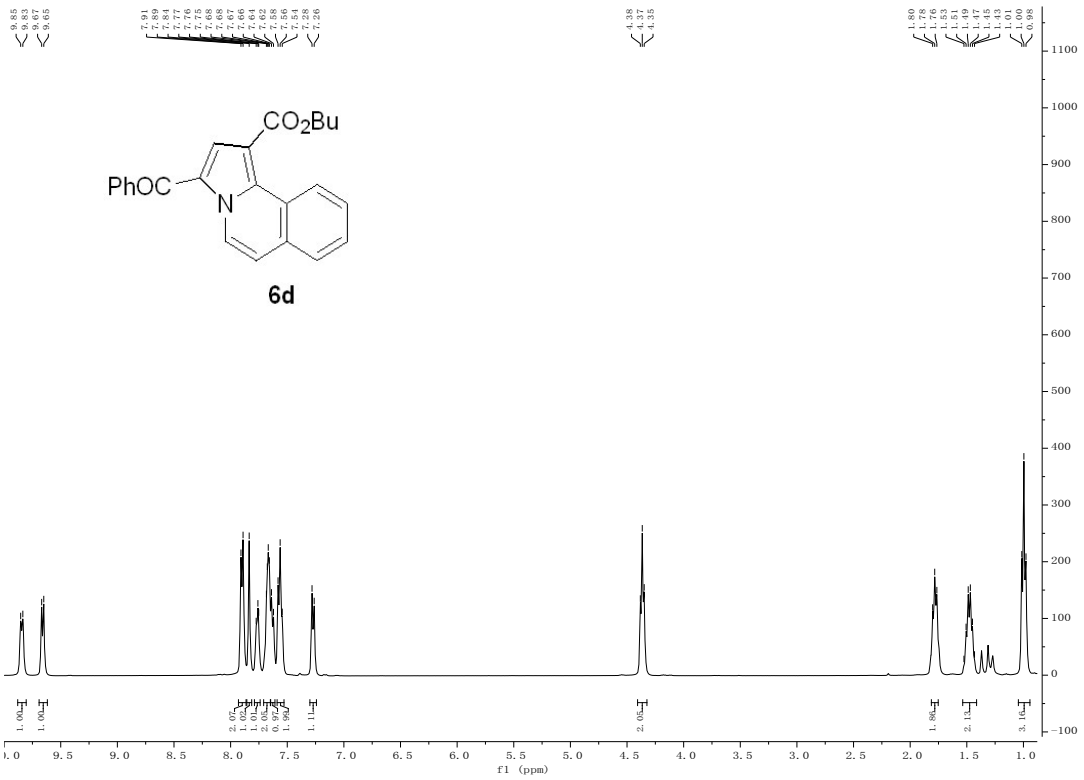
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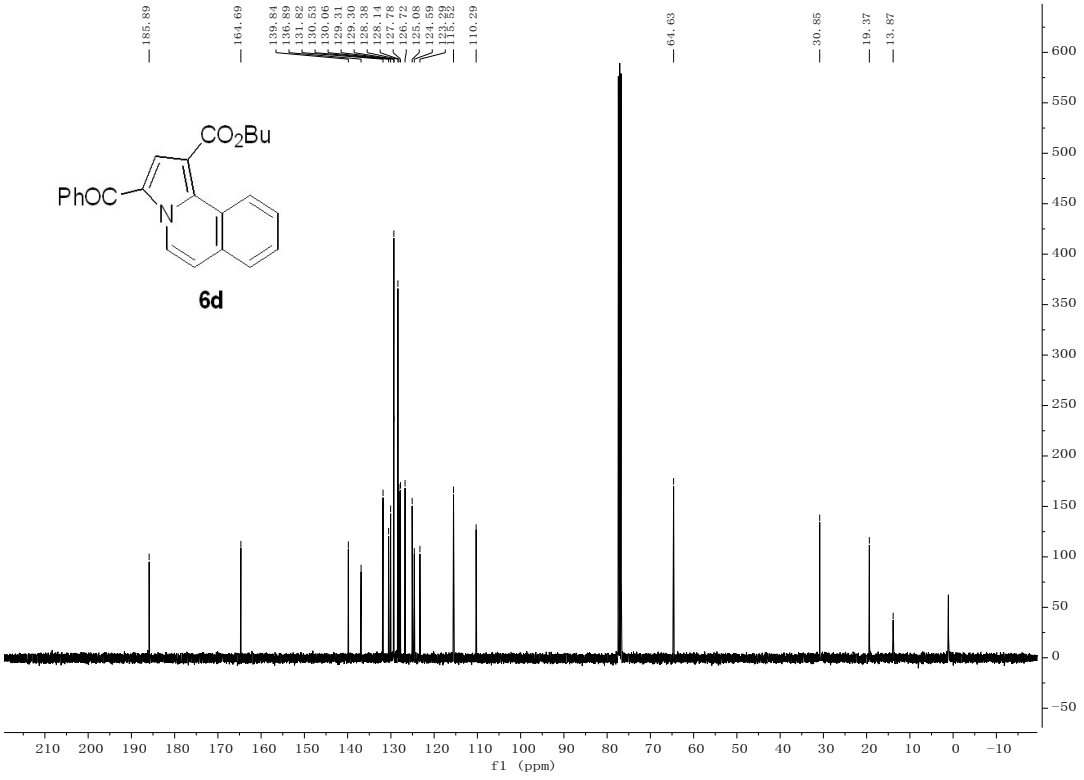
6d
f1 (ppm)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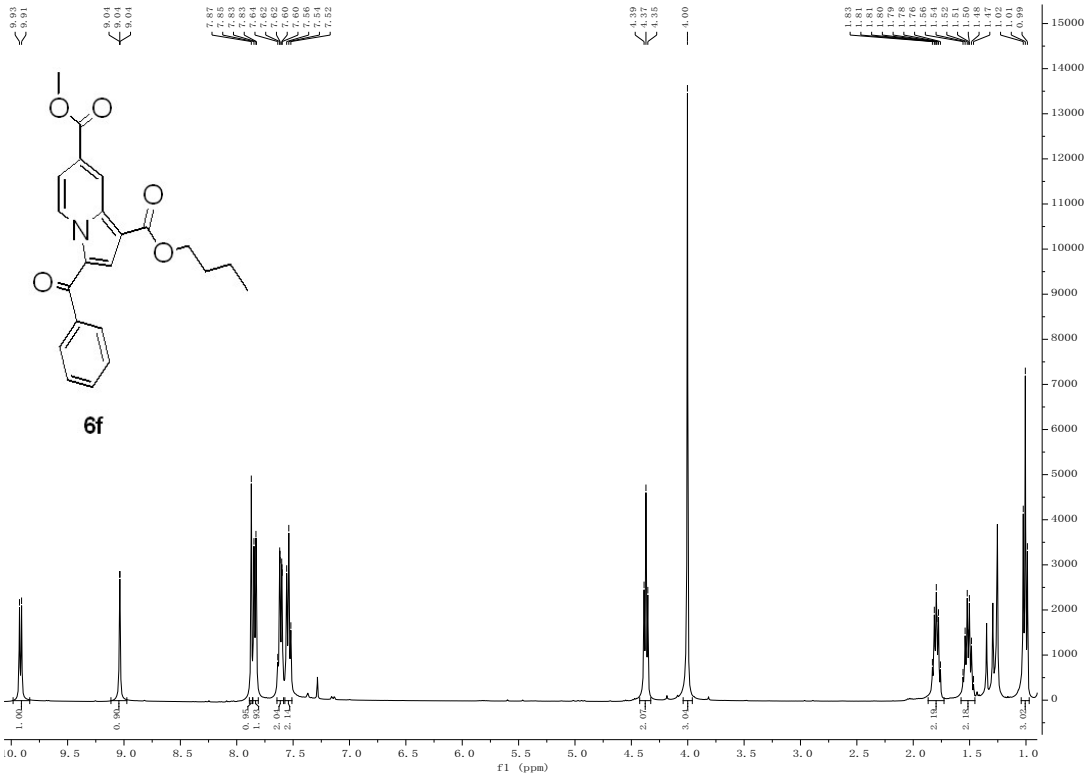
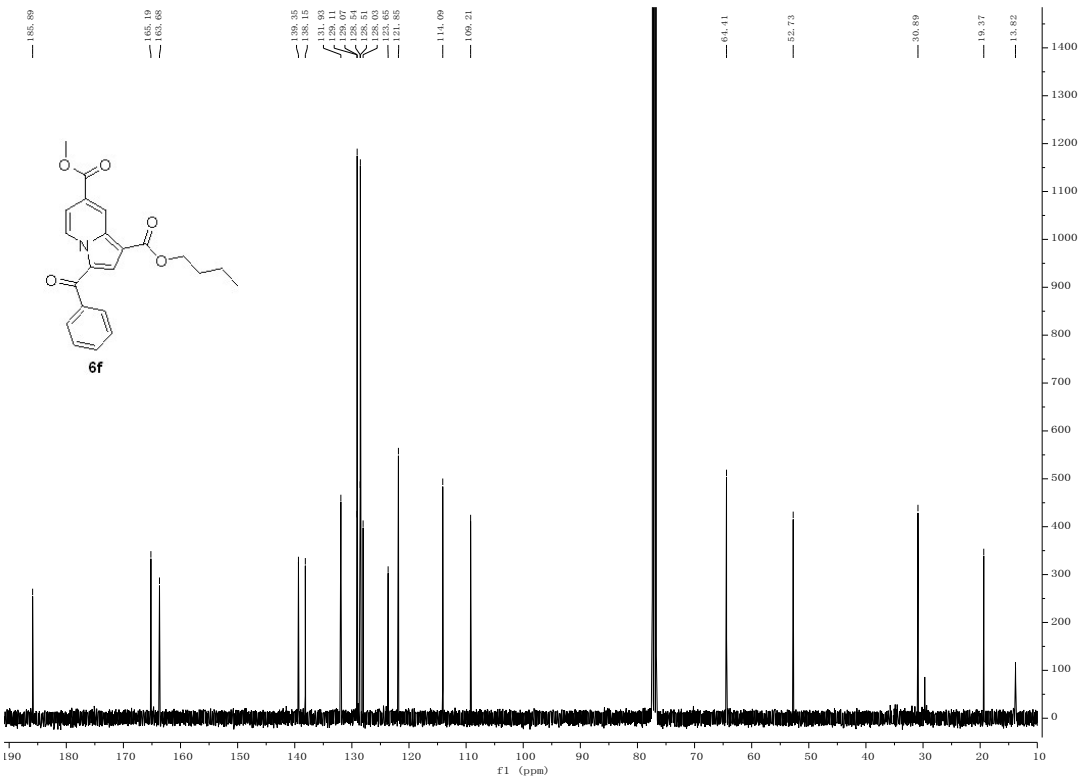
164.69
139.84
136.89
131.82
130.53
130.06
129.31
129.30
128.38
128.14
127.78
126.72
125.08
124.59
123.29
123.22
115.32
110.29
64.63
30.85
19.37
13.87
CO2Bu
PhOC
N
6d
f1 (ppm)


9.93
9.91
9.04
9.04
9.04
7.87
7.85
7.83
7.83
7.64
7.62
7.60
7.60
7.56
7.54
7.52
4.39
4.37
4.35
4.00
1.83
1.81
1.81
1.80
1.79
1.78
1.76
1.56
1.54
1.52
1.51
1.50
1.48
1.47
1.02
1.01
0.99
1.00
0.90
1.95
2.04
2.14
2.07
3.04
2.19
2.18
3.02
f1 (ppm)

6f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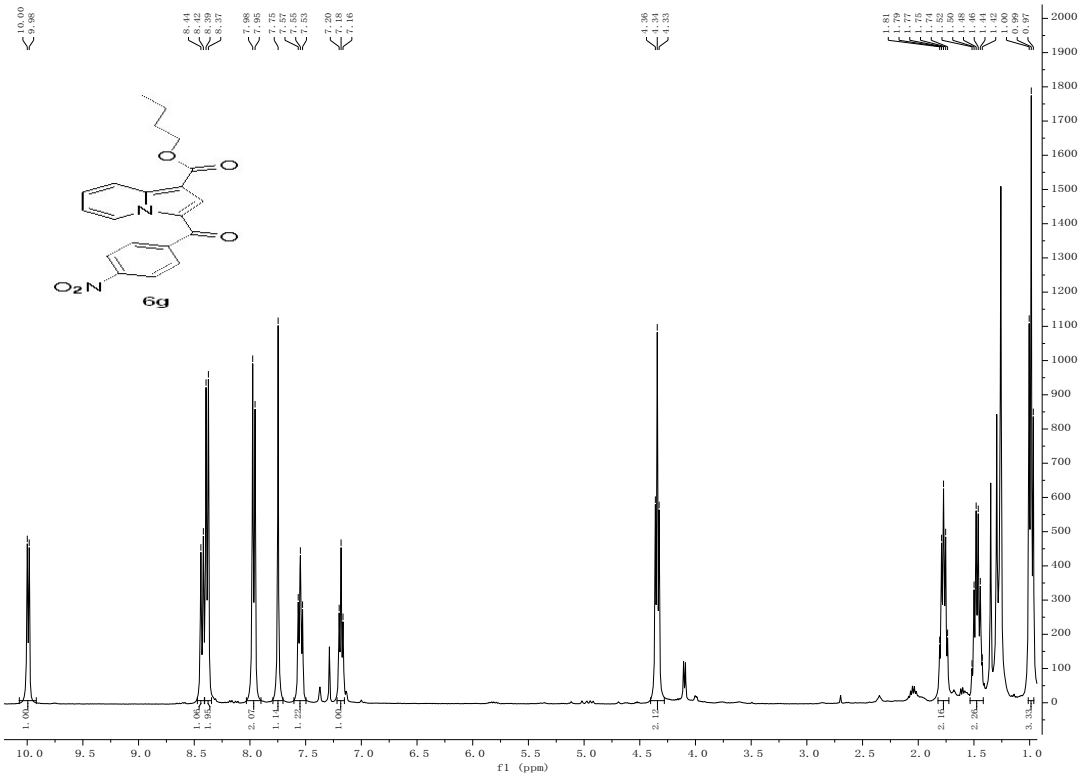
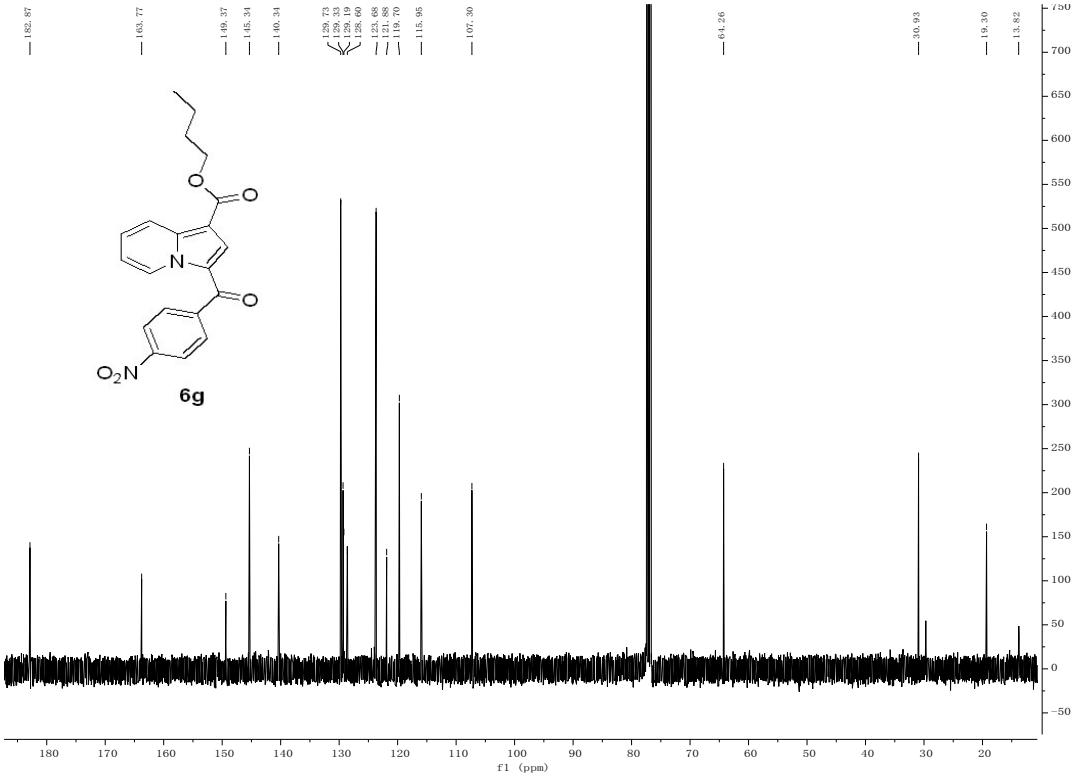
165.19
163.68
139.35
138.15
131.93
129.11
129.07
128.84
128.51
128.03
123.65
121.85
114.09
109.21
64.41
52.73
30.89
19.37
13.82
f1 (ppm)

6f


10.00
9.98
8.44
8.42
8.39
8.37
7.98
7.95
7.75
7.57
7.55
7.53
7.20
7.18
7.16
4.36
4.34
4.33
1.81
1.79
1.77
1.75
1.74
1.52
1.50
1.48
1.46
1.44
1.42
1.00
0.99
0.97
1.00
1.90
2.07
1.14
1.22
1.04
2.13
2.16
2.20
3.33
f1 (ppm)

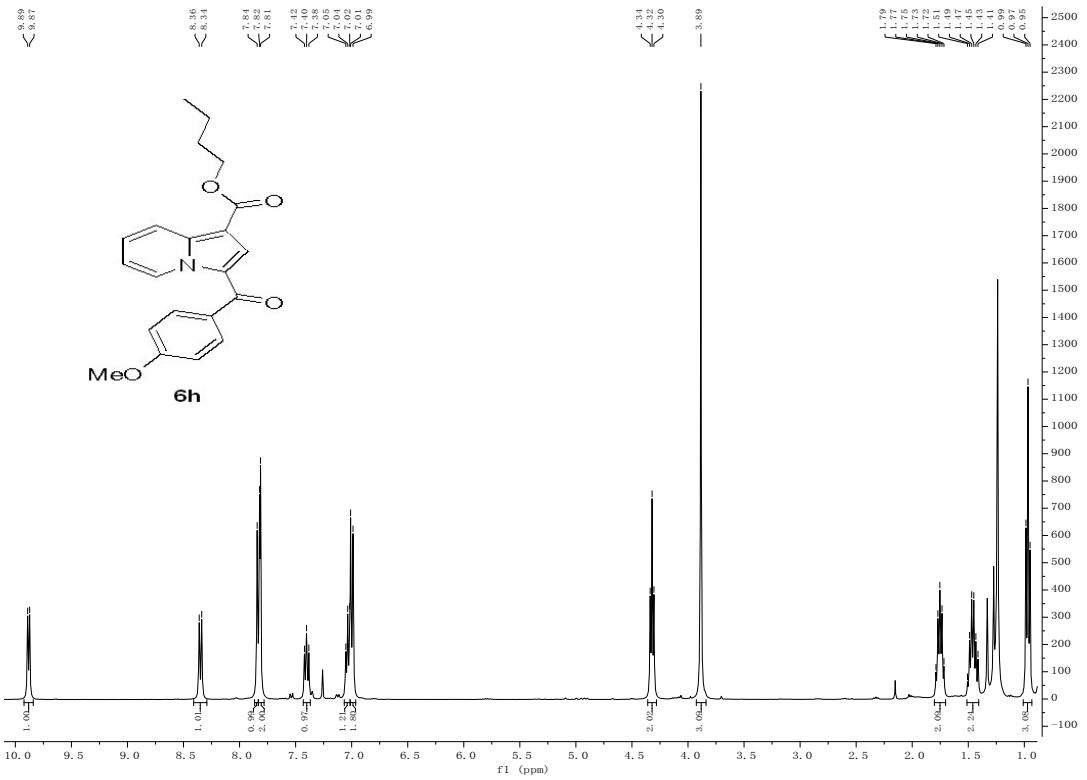
O2N

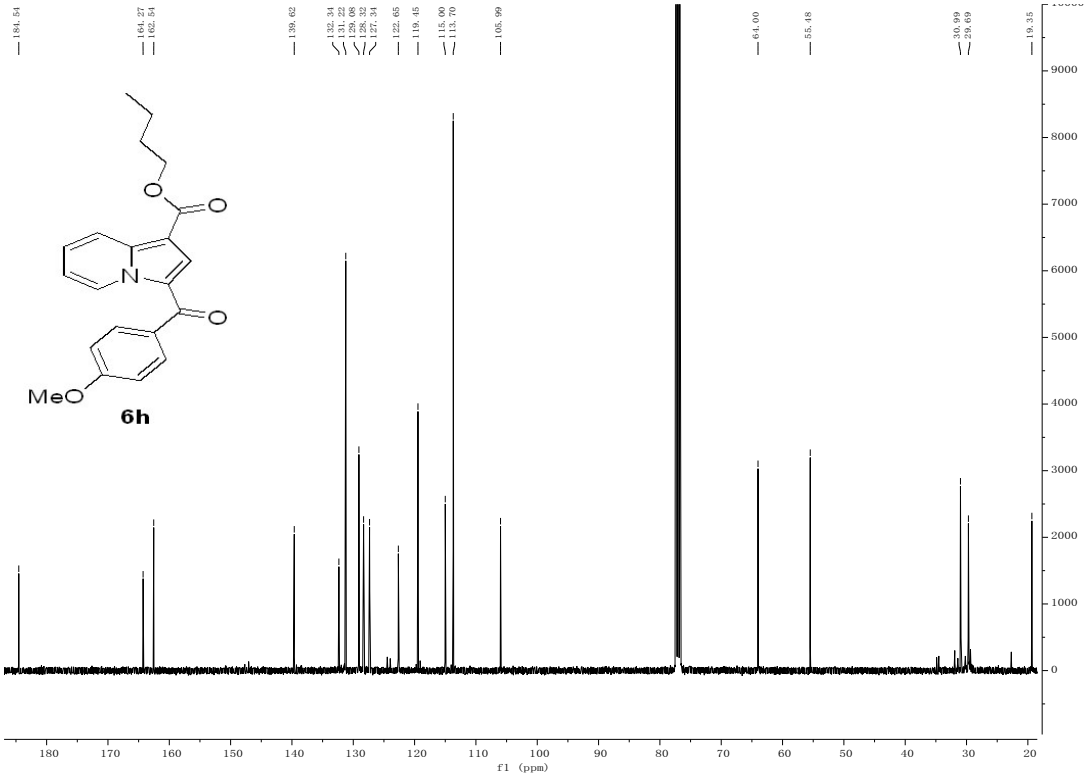
6g


182.87
163.77
149.37
145.34
140.34
129.73
129.33
129.19
128.60
123.68
121.88
119.70
115.95
107.30
64.26
30.93
19.30
13.82
f1 (ppm)

O2N

6g


9.89
9.87
8.36
8.34
7.84
7.82
7.81
7.42
7.40
7.38
7.05
7.04
7.02
7.01
6.99
4.34
4.32
4.30
3.89
1.79
1.77
1.75
1.73
1.72
1.51
1.49
1.47
1.45
1.43
1.41
0.99
0.97
0.95
MeO
6h
f1 (ppm)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162.54
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132.34
131.22
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128.32
127.34
122.65
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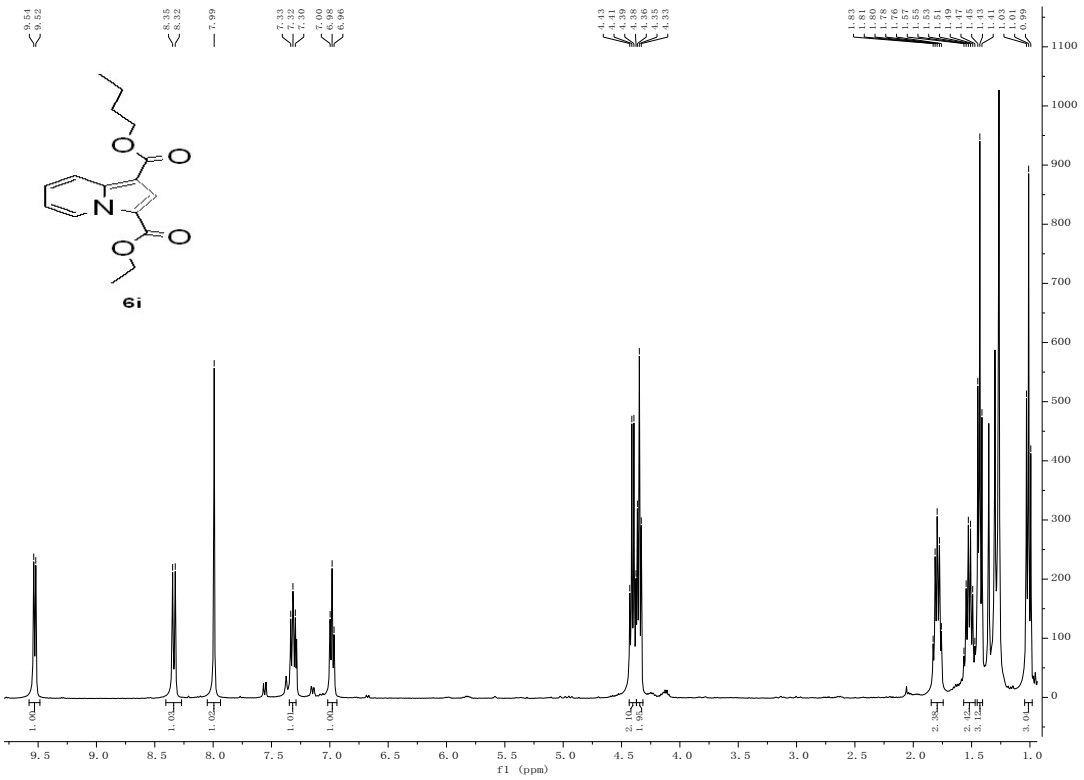
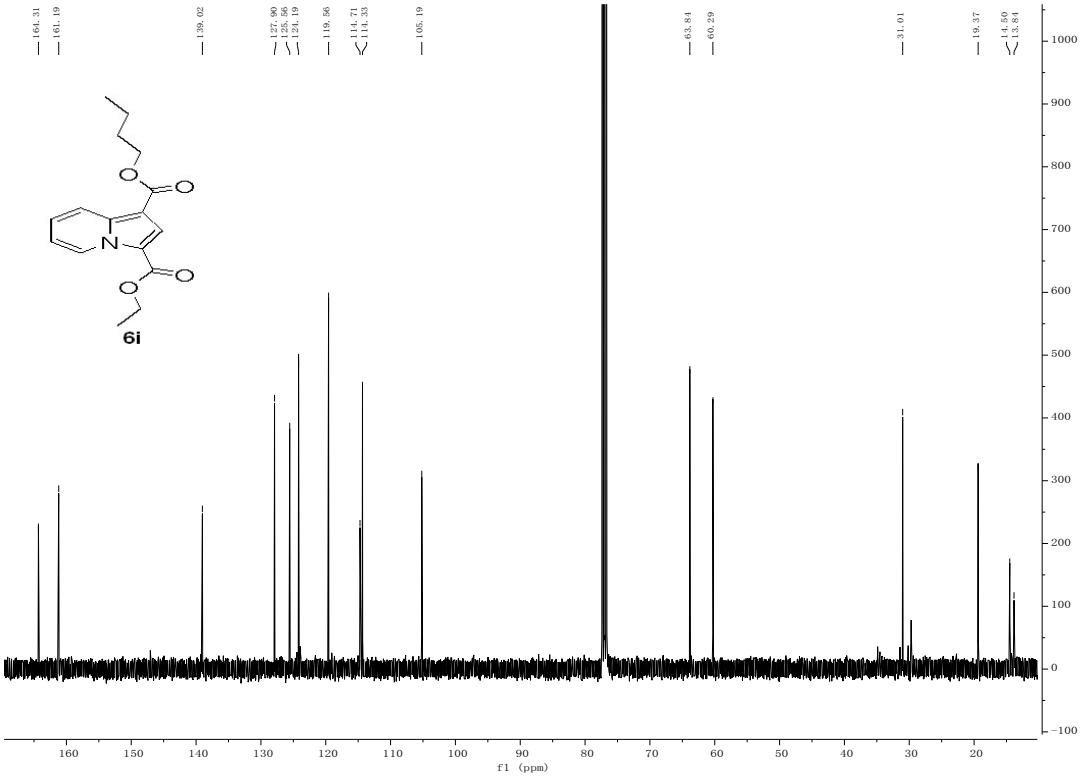
115.00
113.70
105.99
64.00
55.48
30.99
29.69
19.35
MeO
6h
f1 (ppm)


9.54
9.52
8.35
8.32
7.99
7.33
7.32
7.30
7.00
6.98
6.96
4.43
4.41
4.39
4.38
4.36
4.35
4.33
1.83
1.81
1.80
1.78
1.76
1.57
1.55
1.53
1.51
1.49
1.47
1.45
1.43
1.41
1.03
1.01
0.99
1.00
1.02
1.02
1.01
1.00
2.10
1.90
2.38
2.42
3.12
3.00
f1 (ppm)
6i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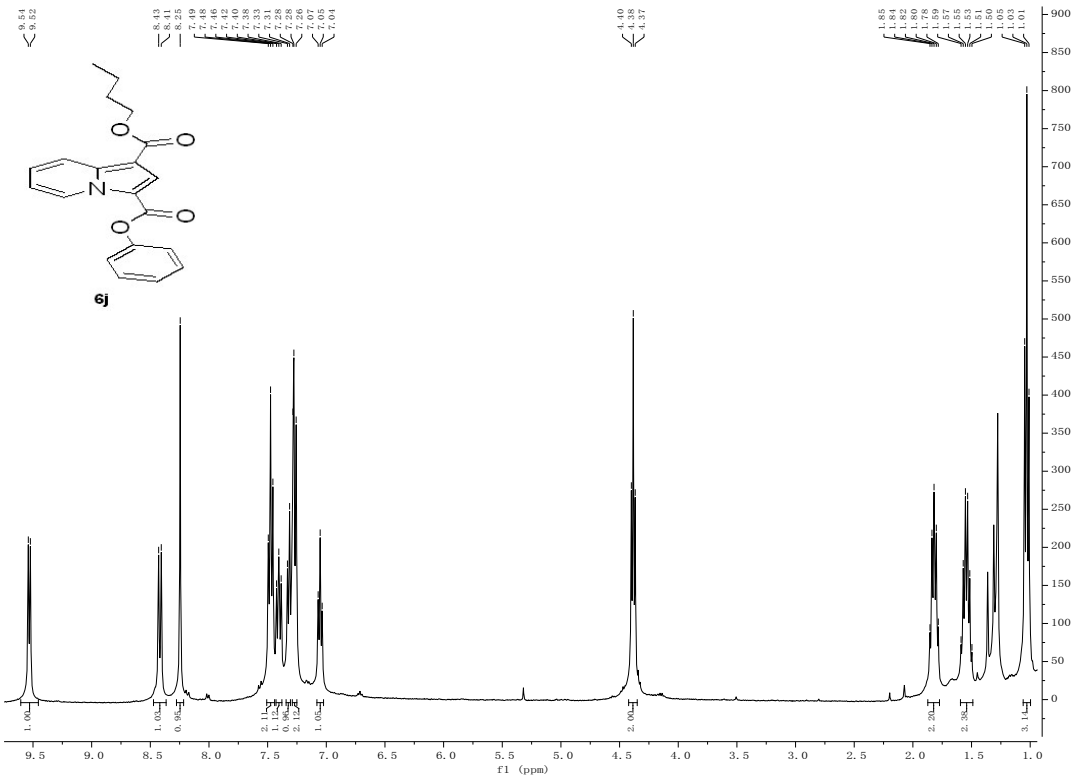
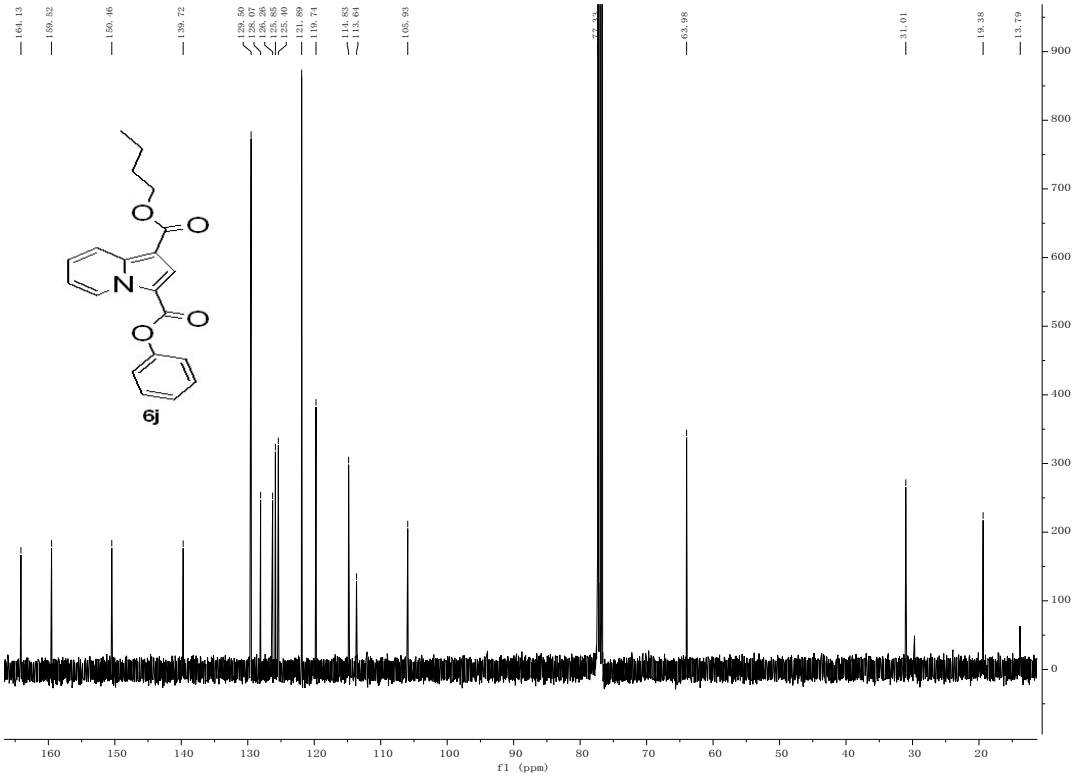
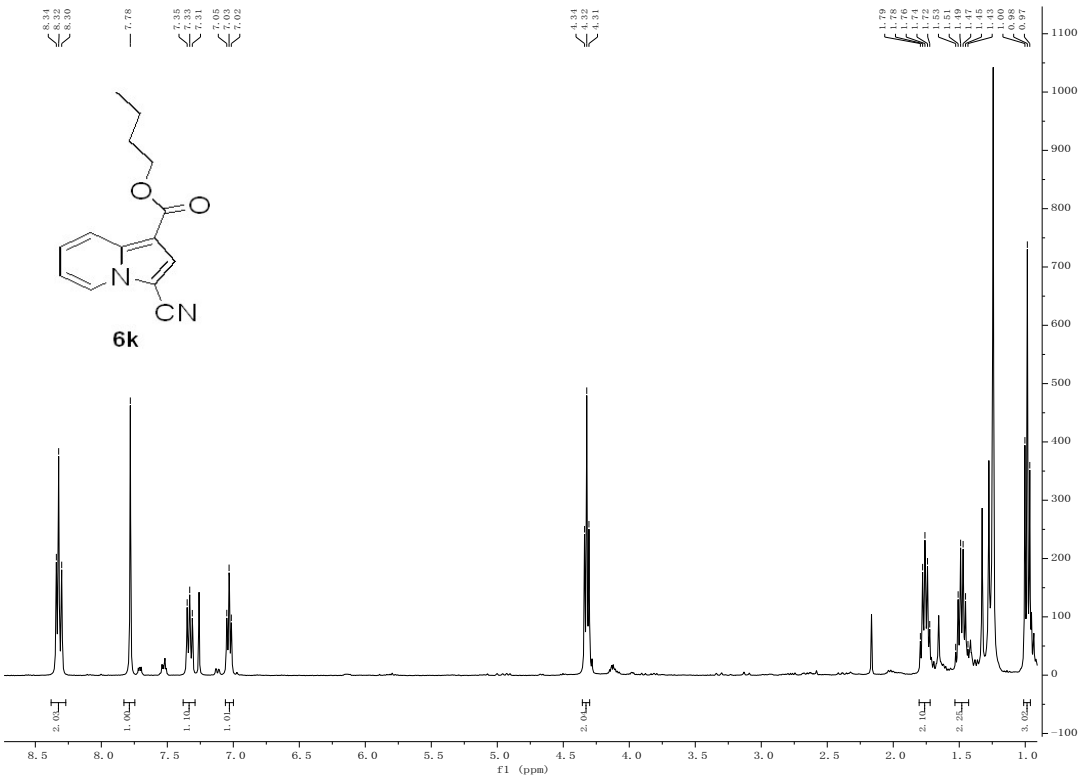
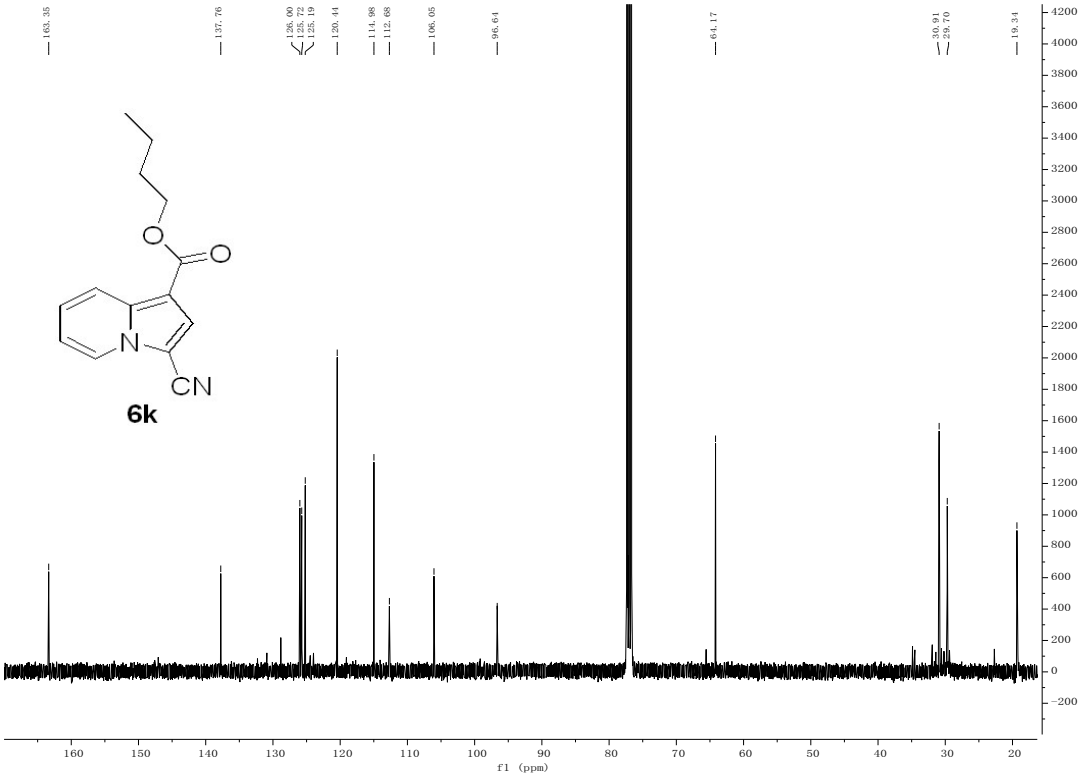
161.19
139.02
127.90
125.96
124.19
119.56
114.71
114.33
105.19
63.84
60.29
31.01
19.37
14.50
13.84
f1 (ppm)
6i


9.54
9.52
8.43
8.41
8.25
7.49
7.48
7.46
7.42
7.40
7.38
7.33
7.31
7.28
7.26
7.07
7.05
7.04
4.40
4.38
4.37
1.85
1.84
1.82
1.80
1.78
1.59
1.57
1.55
1.53
1.51
1.50
1.05
1.03
1.01
6j
f1 (ppm)


164.13
159.52
150.46
139.72
129.50
128.07
126.26
125.85
125.40
121.89
119.74
114.83
113.64
105.93
77.33
63.98
31.01
19.38
13.79
6j
f1 (ppm)


8.34
8.32
8.30
7.78
7.35
7.33
7.31
7.05
7.03
7.02
4.34
4.32
4.31
1.79
1.78
1.76
1.74
1.72
1.53
1.51
1.49
1.47
1.45
1.43
1.00
0.98
0.97
O
O
N
CN
6k
2.03
1.00
1.10
1.01
2.04
2.10
2.25
3.02
f1 (ppm)


163.35
137.76
126.00
125.72
125.19
120.44
114.98
112.68
106.05
96.64
64.17
30.91
29.70
19.34
O
O
N
CN
6k
f1 (ppm)