

Supporting Information

TfOH-catalyzed synthesis of 3-aryl isoindolinones via tandem reaction

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Supporting Information

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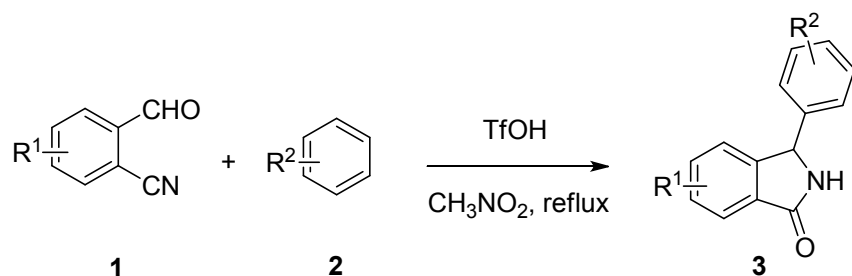
4 Copies of ^1H NMR and ^{13}C NMR of products

1. General experimental details

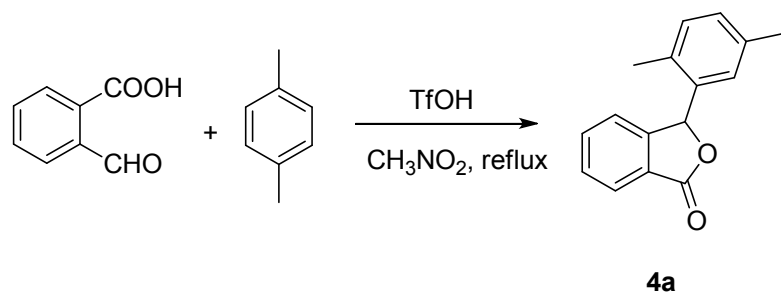
Some 2-formylbenzonitrile compounds were prepared according to the reported method, other chemicals were purchased from Aladdin. All the reactions and manipulations were performed in atmosphere using standard schlenk techniques. All solvents before use needed drying treatment. All reactions were monitored by TLC with silica gel-coated plates.

NMR spectra were recorded on BRUKER DRX 400 spectrometers. Chemical shifts are reported in parts per million (ppm) down field from TMS with the solvent resonance as the internal standard. Coupling constants (J) were reported in Hz and refer to apparent peak multiplications. High resolution mass spectra (HRMS) were recorded on Bruker micrOTOF mass instrument (ESI). IR spectra were recorded on BRUKER TENSOR 27 spectrometers.

2. Synthesis of substituted isoindolinones and isobenzofuran

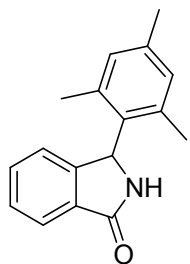


20% equiv TfOH was added to a stirred 5 mL CH_3NO_2 of 2-formylbenzonitrile derivatives **1** (1 mmol) and benzene derivatives **2** (5 mmol), The solution was stirred and heated to reflux, after reaction was completed (as indicated by TLC), the mixture was purified by flash chromatography on silica gel eluting with petroleum ether/ethyl acetate.



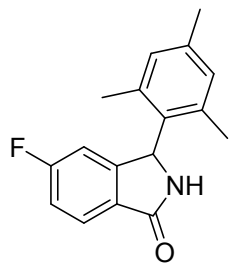
2-formylbenzoic acid (150 mg, 1 mmol) and p-xylene (530 mg, 5 mmol) was dissolved in dry CH_3NO_2 (5 mL), 20% equiv TfOH (30 mg, 0.2 mmol) was slowly added and the mixture was stirred at room temperature until the reaction was completed (monitored by TLC). The mixture was purified by chromatography on silica gel eluting with petroleum ether/ethyl acetate to afford the desired products **4a**.

3. Experimental characterization data for products

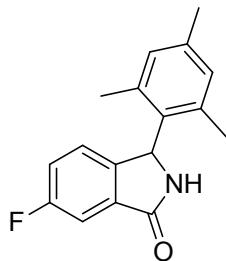


3-mesitylisoindolin-1-one (3a). The product was obtained as a light yellow solid (218 mg, 87%): ^1H -NMR (400 MHz, DMSO) δ 8.86 (s, 1H), 7.74 (d, J = 6.9 Hz, 1H), 7.52 (t, J = 7.5 Hz, 2H), 7.17 (d, J = 7.0 Hz, 1H), 6.95 (s, 1H), 6.69 (s, 1H), 6.08 (s, 1H), 2.54 (s, 3H), 2.20 (s, 3H), 1.51 (s, 3H); ^{13}C -NMR (100 MHz, DMSO) δ 170.1, 147.8, 137.8, 137.4, 137.2, 133.4,

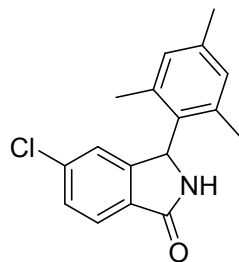
132.3, 131.3, 131.2, 129.7, 128.7, 128.3, 123.2, 56.3, 21.2, 20.8, 18.9. IR $\nu_{\text{max}}(\text{KBr})/\text{cm}^{-1}$: 3076, 2952, 2920, 1686, 1475, 1382, 730. HRMS (ESI) calcd for $[\text{C}_{17}\text{H}_{17}\text{NO}+\text{Na}]^+$: 274.1202, found: 274.1206.



5-fluoro-3-mesitylisoindolin-1-one (3b). The product was obtained as a white solid (221mg, 82%): ^1H -NMR (400 MHz, CDCl_3) δ 7.86 (m, 1H), 7.17 (d, J = 8.8 Hz, 1H), 7.07 (s, 1H), 6.95 (s, 1H), 6.86 (d, J = 7.2 Hz, 1H), 6.75 (s, 1H), 6.10 (s, 1H), 2.57 (s, 3H), 2.27 (s, 3H), 1.68 (s, 3H); ^{13}C -NMR (100 MHz, CDCl_3) δ 170.1, 149.9, 138.3, 138.1, 137.3, 131.6, 129.6, 129.1, 128.3, 125.9, 125.8, 116.0, 109.8, 56.4, 21.1, 20.8, 19.0. IR $\nu_{\text{max}}(\text{KBr})/\text{cm}^{-1}$: 3076, 2972, 2920, 2850, 1687, 1624, 1384, 1263, 1147, 837, 767, 702. HRMS (ESI) calcd for $[\text{C}_{17}\text{H}_{16}\text{NOF}+\text{Na}]^+$: 292.1108, found: 292.1107.

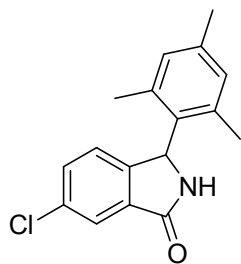


6-fluoro-3-mesitylisoindolin-1-one (3c). The product was obtained as a white solid (213 mg, 79%): ^1H -NMR (400 MHz, CDCl_3) δ 7.54 (dd, J = 7.6, 2.2 Hz, 1H), 7.29 (s, 1H), 7.23 (m, 1H), 7.15 (m, 1H), 6.94 (s, 1H), 6.72 (s, 1H), 6.11 (s, 1H), 2.58 (s, 3H), 2.27 (s, 3H), 1.66 (s, 3H); ^{13}C -NMR (100 MHz, CDCl_3) δ 170.1, 142.7, 138.2, 138.0, 137.3, 134.4, 131.6, 129.6, 129.2, 124.2, 124.1, 119.9, 110.6, 56.5, 21.2, 20.8, 19.0. IR $\nu_{\text{max}}(\text{KBr})/\text{cm}^{-1}$: 3068, 2954, 2923, 2852, 1695, 1604, 1384, 1321, 1236, 1191, 1026, 754, 702. HRMS (ESI) calcd for $[\text{C}_{17}\text{H}_{16}\text{NOF}+\text{Na}]^+$: 292.1108, found: 292.1106.

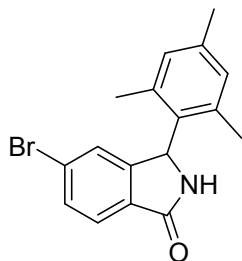


5-chloro-3-mesitylisoindolin-1-one (3d). The product was obtained as a pale yellow oil (211 mg, 74%): ^1H -NMR (400 MHz, CDCl_3) δ 7.81 (d, J = 8.1 Hz, 1H), 7.46 (d, J = 8.0 Hz, 1H), 7.28 (s, 1H), 7.16 (s, 1H), 6.94 (s, 1H), 6.75 (s, 1H), 6.11 (s, 1H), 2.58 (s, 3H), 2.28 (s, 3H), 1.69 (s, 3H); ^{13}C -NMR (100 MHz, CDCl_3) δ 169.8, 148.9, 138.7, 138.4, 138.1, 137.3,

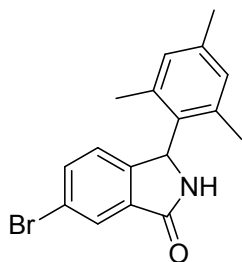
131.6, 130.7, 129.7, 128.9, 128.8, 125.1, 123.0, 56.3, 21.2, 20.8, 19.1. IR $\nu_{\text{max}}(\text{KBr})/\text{cm}^{-1}$: 3072, 2954, 2923, 2858, 1687, 1608, 1384, 1188, 852, 763, 609. HRMS (ESI) calcd for $[\text{C}_{17}\text{H}_{16}\text{NOCl}+\text{Na}]^+$: 308.0813, found: 308.0816.



6-chloro-3-mesitylisoindolin-1-one (3e). The product was obtained as a yellow solid (206 mg, 72%): ^1H -NMR (400 MHz, CDCl_3) δ 7.85 (s, 1H), 7.48 (d, $J = 4.6$ Hz, 1H), 7.17 (s, 1H), 7.13 (d, $J = 8.1$ Hz, 1H), 6.95 (s, 1H), 6.73 (s, 1H), 6.11 (s, 1H), 2.59 (s, 3H), 2.27 (s, 3H), 1.66 (s, 3H); ^{13}C -NMR (100 MHz, CDCl_3) δ 169.8, 145.5, 138.3, 138.0, 137.3, 134.4, 134.0, 132.4, 131.6, 129.6, 128.9, 124.0, 123.9, 56.6, 21.2, 20.8, 19.1. IR $\nu_{\text{max}}(\text{KBr})/\text{cm}^{-1}$: 3082, 2967, 2923, 2860, 1693, 1382, 1191, 1048, 680, 615. HRMS (ESI) calcd for $[\text{C}_{17}\text{H}_{16}\text{NOCl}+\text{Na}]^+$: 308.0813, found: 308.0812.

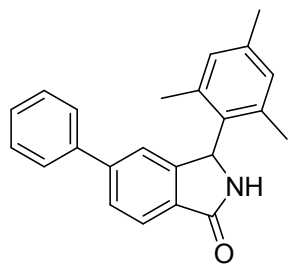


5-bromo-3-mesitylisoindolin-1-one (3f). The product was obtained as a light yellow oil (251 mg, 76%): ^1H -NMR (400 MHz, CDCl_3) δ 7.70 (d, $J = 8.1$ Hz, 1H), 7.60 (dd, $J = 8.1, 0.7$ Hz, 1H), 7.42 (s, 1H), 7.33 (s, 1H), 6.92 (s, 1H), 6.74 (s, 1H), 6.08 (s, 1H), 2.57 (s, 3H), 2.26 (s, 3H), 1.68 (s, 3H); ^{13}C -NMR (100 MHz, CDCl_3) δ 170.3, 149.2, 138.3, 138.0, 137.3, 131.6, 131.6, 131.3, 129.6, 129.0, 127.0, 125.9, 125.2, 56.4, 21.2, 20.8, 19.1. IR $\nu_{\text{max}}(\text{KBr})/\text{cm}^{-1}$: 3062, 2966, 2925, 2862, 1689, 1608, 1384, 1193, 1051, 852, 763. HRMS (ESI) calcd for $[\text{C}_{17}\text{H}_{16}\text{NOBr}+\text{Na}]^+$: 352.0307, found: 352.0309.



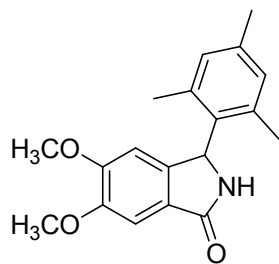
6-bromo-3-mesitylisoindolin-1-one (3g). The product was obtained as a light yellow solid (248 mg, 75%): ^1H -NMR (400 MHz, CDCl_3) δ 8.02 (s, 1H), 7.64 (d, $J = 8.0$ Hz, 1H), 7.08 (d, $J = 8.1$ Hz, 1H), 6.96 (d, $J = 9.2$ Hz, 2H), 6.74 (s, 1H), 6.09 (s, 1H), 2.59 (s, 3H), 2.27 (s, 3H), 1.67 (s, 3H); ^{13}C -NMR (100 MHz, CDCl_3) δ 169.5, 146.0, 138.3, 138.0, 137.3, 135.2, 134.3, 131.6, 129.6, 128.9, 127.0, 124.3, 122.1, 56.5, 21.2, 20.8, 19.1. IR $\nu_{\text{max}}(\text{KBr})/\text{cm}^{-1}$: 3074, 2956, 2920, 2850, 1691,

1610, 1456, 1382, 1311, 1195, 1029, 852, 757, 640. HRMS (ESI) calcd for $[C_{17}H_{16}NOBr+Na]^+$: 352.0307, found: 352.0306.

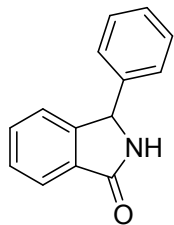


3-mesityl-5-phenylisoindolin-1-one (3h). The product was obtained as a white solid (318 mg, 97%): 1H -NMR (400 MHz, DMSO) δ 8.87 (s, 1H), 7.83 – 7.76 (m, 2H), 7.64 (d, J = 7.2 Hz, 2H), 7.47 – 7.33 (m, 4H), 6.96 (s, 1H), 6.69 (s, 1H), 6.14 (s, 1H), 2.59 (s, 3H), 2.19 (s, 3H), 1.57 (s, 3H); ^{13}C -NMR (100 MHz, DMSO) δ 169.9, 148.8, 144.3, 139.8, 138.0, 137.5, 137.3, 132.6, 131.3, 131.1, 129.7, 129.5, 128.7, 128.5, 127.6, 127.2, 123.8, 121.3, 56.4, 21.3, 20.9, 19.0. IR $\nu_{max}(KBr)/cm^{-1}$: 3058, 2927, 2918, 1720, 1630, 1463, 1390, 1328, 1246, 1191, 732. HRMS (ESI) calcd for

$[C_{23}H_{21}NO+Na]^+$: 350.1515, found: 350.1518.

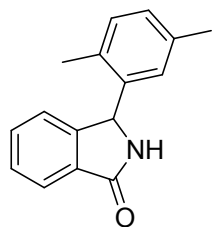


3-mesityl-5,6-dimethoxyisoindolin-1-one (3i). The product was obtained as a white solid (227 mg, 73%): 1H NMR (400 MHz, DMSO) δ 8.58 (s, 1H), 7.22 (s, 1H), 6.93 (s, 1H), 6.68 (d, J = 3.0 Hz, 2H), 5.95 (s, 1H), 3.84 (s, 3H), 3.71 (s, 3H), 2.55 (s, 3H), 2.20 (s, 3H), 1.56 (s, 3H). ^{13}C NMR (100 MHz, DMSO) δ 170.4, 153.1, 149.7, 141.4, 137.9, 137.7, 137.1, 131.3, 131.2, 129.7, 125.4, 105.4, 105.2, 56.3, 56.1, 55.9, 21.2, 20.8, 18.8. IR $\nu_{max}(KBr)/cm^{-1}$: 3063, 2958, 2918, 2852, 1690, 1611, 1388, 1186, 1038, 734. HRMS (ESI) calcd for $[C_{19}H_{21}NO_3+Na]^+$: 334.1414, found: 334.1418.

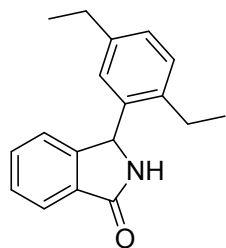


3-phenylisoindolin-1-one (3j). The product was obtained as a yellow oil (69 mg, 33%): 1H -NMR (400 MHz, DMSO) δ 9.10 (s, 1H), 7.72 (d, J = 7.3 Hz, 1H), 7.54 (t, J = 6.9 Hz, 1H), 7.48 (t, J = 7.2 Hz, 1H), 7.37 (t, 2H), 7.30 (t, J = 7.8 Hz, 4H), 5.74 (s, 1H); ^{13}C -NMR (100 MHz, DMSO) δ 170.2, 148.6, 140.0, 132.3, 131.8, 129.2, 128.6, 128.4, 127.0, 123.9, 123.3, 60.0. IR

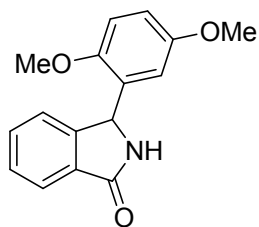
$\nu_{\text{max}}(\text{KBr})/\text{cm}^{-1}$: 3053, 2918, 1718, 1463, 1384, 1328, 1242, 1191, 702. HRMS (ESI) calcd for $[\text{C}_{14}\text{H}_{11}\text{NO}+\text{Na}]^+$: 232.0733, found: 232.0730.



3-(2,5-dimethylphenyl)isoindolin-1-one (3k). The product was obtained as a yellow solid (195 mg, 82%): ^1H -NMR (400 MHz, DMSO) δ 8.97 (s, 1H), 7.75 (d, J = 6.8 Hz, 1H), 7.51 (t, J = 7.9 Hz, 2H), 7.24 (d, J = 6.7 Hz, 1H), 7.12 (d, J = 7.4 Hz, 1H), 7.00 (d, J = 7.1 Hz, 1H), 6.75 (s, 1H), 5.91 (s, 1H), 2.36 (s, 3H), 2.14 (s, 3H); ^{13}C -NMR (100 MHz, DMSO) δ 170.2, 148.6, 137.4, 135.6, 133.2, 132.5, 132.3, 131.4, 128.9, 128.5, 127.5, 123.8, 123.4, 57.5, 21.0, 19.0. IR $\nu_{\text{max}}(\text{KBr})/\text{cm}^{-1}$: 3045, 2968, 2918, 1757, 1612, 1463, 1384, 1286, 1068, 804, 748. HRMS (ESI) calcd for $[\text{C}_{16}\text{H}_{15}\text{NO}+\text{Na}]^+$: 260.1046, found: 260.1048.

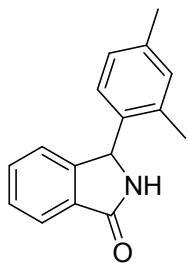


3-(2,5-diethylphenyl)isoindolin-1-one (3l). The product was obtained as a yellow solid (204 mg, 77%): ^1H -NMR (400 MHz, CDCl_3) δ 7.92 (d, J = 7.0 Hz, 1H), 7.54 – 7.47 (m, 2H), 7.24 (d, J = 7.3 Hz, 1H), 7.21 (d, J = 7.9 Hz, 1H), 7.11 (d, J = 9.3 Hz, 1H), 6.95 (s, 1H), 6.78 (s, 1H), 5.95 (s, 1H), 2.88 – 2.80 (m, 2H), 2.53 – 2.45 (m, 2H), 1.33 (t, J = 7.5 Hz, 3H), 1.12 (t, J = 7.6 Hz, 3H); ^{13}C -NMR (100 MHz, CDCl_3) δ 171.2, 148.4, 142.7, 139.4, 135.1, 132.2, 131.3, 129.4, 128.2, 128.0, 126.5, 123.9, 123.3, 57.1, 28.3, 25.4, 16.2, 15.4. IR $\nu_{\text{max}}(\text{KBr})/\text{cm}^{-1}$: 3087, 2960, 2929, 2857, 1699, 1471, 1386, 1192, 1031, 831, 768. HRMS (ESI) calcd for $[\text{C}_{18}\text{H}_{19}\text{NO}+\text{Na}]^+$: 288.1359, found: 288.1361.

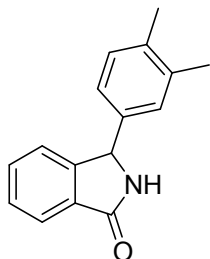


3-(2,5-dimethoxyphenyl)isoindolin-1-one (3m). The product was obtained as a white solid (221 mg, 82%): ^1H -NMR (400 MHz, DMSO) δ 8.91 (s, 1H), 7.70 (d, J = 7.2 Hz, 1H), 7.52 (d, J = 7.5 Hz, 1H), 7.46 (t, J = 7.2 Hz, 1H), 7.39 (d, J = 7.3 Hz, 1H), 7.05 (d, J = 8.9 Hz, 1H), 6.85 (d, J = 8.9 Hz, 1H), 6.55 (s, 1H), 6.00 (s, 1H), 3.85 (s, 3H), 3.62 (s, 3H); ^{13}C -NMR (100 MHz, DMSO) δ 170.4, 153.6, 151.3, 148.5, 132.3, 132.0, 128.9, 128.5, 123.8, 123.4, 113.5, 113.1, 112.4,

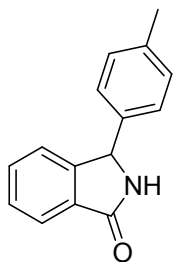
56.6, 55.8, 54.6. IR $\nu_{\text{max}}(\text{KBr})/\text{cm}^{-1}$: 3084, 2958, 2920, 2848, 1693, 1382, 1218, 1165, 1029, 825, 727. HRMS (ESI) calcd for $[\text{C}_{16}\text{H}_{15}\text{NO}_3+\text{Na}]^+$: 292.0944, found: 292.0944.



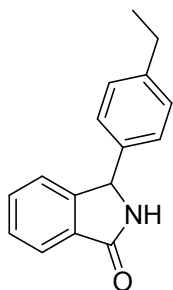
3-(2,4-dimethylphenyl)isoindolin-1-one (3n). The product was obtained as a yellow solid (220 mg, 93%): ^1H -NMR (400 MHz, DMSO) δ 8.80 (s, 1H), 7.57 (d, $J = 7.0$ Hz, 1H), 7.30 (t, $J = 7.8$ Hz, 2H), 7.02 (d, $J = 7.1$ Hz, 1H), 6.82 (s, 1H), 6.71 (d, $J = 7.7$ Hz, 1H), 6.61 (d, $J = 7.8$ Hz, 1H), 5.70 (s, 1H), 2.15 (s, 3H), 2.02 (s, 3H); ^{13}C -NMR (100 MHz, DMSO) δ 170.2, 148.8, 137.3, 137.0, 136.3, 132.2, 131.8, 130.2, 128.5, 127.9, 124.5, 123.9, 123.3, 59.9, 19.8, 19.5. IR $\nu_{\text{max}}(\text{KBr})/\text{cm}^{-1}$: 3076, 2922, 1685, 1463, 1382, 1037, 823, 763. HRMS (ESI) calcd for $[\text{C}_{16}\text{H}_{15}\text{NO}+\text{Na}]^+$: 260.1046, found: 260.1048.



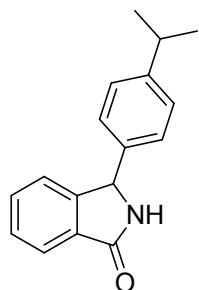
3-(3,4-dimethylphenyl)isoindolin-1-one (3o). The product was obtained as a white solid (145 mg, 61%): ^1H -NMR (400 MHz, DMSO) δ 8.87 (s, 1H), 7.56 (d, $J = 7.3$ Hz, 1H), 7.36 (t, $J = 7.2$ Hz, 1H), 7.30 (t, $J = 7.4$ Hz, 1H), 7.10 (d, $J = 7.6$ Hz, 1H), 6.95 (d, $J = 7.4$ Hz, 1H), 6.85 (d, $J = 7.9$ Hz, 2H), 5.48 (s, 1H), 2.01 (s, 6H); ^{13}C -NMR (100 MHz, DMSO) δ 170.3, 148.6, 137.4, 136.3, 134.6, 132.6, 132.3, 132.0, 128.5, 127.3, 127.3, 123.8, 123.4, 57.5, 21.0, 19.3. IR $\nu_{\text{max}}(\text{KBr})/\text{cm}^{-1}$: 3080, 2927, 2854, 1693, 1463, 1380, 1352, 1134, 1026, 827, 765. HRMS (ESI) calcd for $[\text{C}_{16}\text{H}_{15}\text{NO}+\text{Na}]^+$: 260.1046, found: 260.1046.



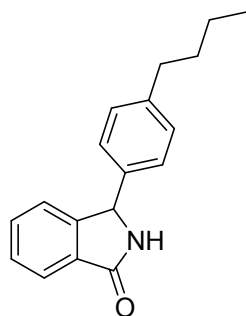
3-(p-tolyl)isoindolin-1-one (3p). The product was obtained as a yellow oil (158 mg, 71%): ^1H -NMR (400 MHz, DMSO) δ 8.88 (s, 1H), 7.54 (d, $J = 7.1$ Hz, 1H), 7.37 – 7.21 (m, 2H), 7.11 – 6.83 (m, 5H), 5.49 (s, 1H), 2.06 (s, 3H); ^{13}C -NMR (100 MHz, DMSO) δ 170.3, 148.6, 137.7, 137.0, 132.3, 131.8, 129.8, 128.5, 126.8, 123.9, 123.3, 59.9, 21.1. IR $\nu_{\text{max}}(\text{KBr})/\text{cm}^{-1}$: 3062, 2922, 1697, 1656, 1382, 1205, 1029, 827, 732. HRMS (ESI) calcd for $[\text{C}_{15}\text{H}_{13}\text{NO}+\text{Na}]^+$: 246.0889, found: 246.0890.



3-(4-ethylphenyl)isoindolin-1-one (3q). The product was obtained as a white solid (171 mg, 72%): $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 7.87 (d, $J = 7.4$ Hz, 1H), 7.50 (t, $J = 7.4$ Hz, 1H), 7.46 (t, $J = 7.3$ Hz, 1H), 7.29 (d, $J = 5.9$ Hz, 1H), 7.27 – 7.21 (m, 2H), 7.20 – 7.16 (m, 3H), 5.61 (s, 1H), 2.64 (m, 2H), 1.22 (t, $J = 7.6$ Hz, 3H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 171.2, 148.2, 144.6, 135.6, 132.2, 130.9, 128.5, 128.2, 126.8, 123.7, 123.3, 60.7, 28.5, 15.5. IR $\nu_{\text{max}}(\text{KBr})/\text{cm}^{-1}$: 3060, 2962, 2922, 2861, 1697, 1460, 1376, 1195, 1033, 841, 761. HRMS (ESI) calcd for $[\text{C}_{16}\text{H}_{15}\text{NO}+\text{Na}]^+$: 260.1046, found: 260.1048.

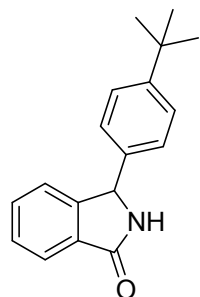


3-(4-isopropylphenyl)isoindolin-1-one (3r). The product was obtained as a yellow solid (206 mg, 82%): $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 7.86 (d, $J = 7.4$ Hz, 1H), 7.81 (s, 1H), 7.50 (t, $J = 7.4$ Hz, 1H), 7.45 (t, $J = 7.4$ Hz, 1H), 7.26 (d, $J = 7.5$ Hz, 1H), 7.21 (s, 4H), 5.62 (s, 1H), 2.89 (m, 1H), 1.24 (d, $J = 2.7$ Hz, 3H), 1.23 (d, $J = 2.7$ Hz, 3H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 171.5, 149.2, 148.2, 135.7, 132.2, 131.0, 128.2, 127.1, 126.8, 123.7, 123.3, 60.8, 33.8, 23.9. IR $\nu_{\text{max}}(\text{KBr})/\text{cm}^{-1}$: 3066, 2960, 2861, 2820, 1692, 1462, 1380, 1192, 1026, 810, 754. HRMS (ESI) calcd for $[\text{C}_{17}\text{H}_{17}\text{NO}+\text{Na}]^+$: 274.1202, found: 274.1206.

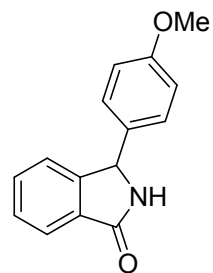


3-(4-butylphenyl)isoindolin-1-one (3s). The product was obtained as a yellow oil (164 mg, 62%): $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 7.86 (d, $J = 7.4$ Hz, 1H), 7.79 – 7.66 (m, 1H), 7.50 (t, $J = 7.4$ Hz, 1H), 7.45 (t, $J = 7.4$ Hz, 1H), 7.25 (d, $J = 7.5$ Hz, 1H), 7.19 (d, $J = 8.1$ Hz, 2H), 7.16 (d, $J = 8.1$ Hz, 2H), 5.61 (s, 1H), 2.63 – 2.55 (t, $J = 6.2$ Hz, 2H), 1.63 – 1.53 (m, 2H), 1.40 – 1.31 (m, 2H), 0.93 (t, $J = 7.4$ Hz, 3H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 171.5, 148.2, 143.3, 135.5, 132.2, 131.0, 129.0, 128.2, 126.7, 123.7, 123.3, 60.8, 35.3, 33.5, 22.4, 14.0. IR $\nu_{\text{max}}(\text{KBr})/\text{cm}^{-1}$: 3061, 2954, 2930, 2854, 2821, 1693,

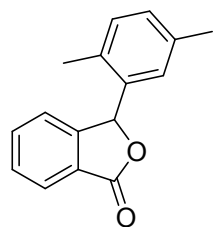
1466, 1372, 1195, 1021, 810, 772. HRMS (ESI) calcd for $[C_{18}H_{19}NO+Na]^+$: 288.1359, found: 288.1363.



3-(4-(tert-butyl)phenyl)isoindolin-1-one (3t). The product was obtained as a yellow solid (212 mg, 80%): 1H -NMR (400 MHz, $CDCl_3$) δ 7.87 (d, $J = 4.7$ Hz, 1H), 7.50 (t, $J = 4.9$ Hz, 1H), 7.46 (t, $J = 4.9$ Hz, 1H), 7.36 (d, $J = 5.4$ Hz, 2H), 7.26 (d, $J = 4.9$ Hz, 1H), 7.20 (d, $J = 5.5$ Hz, 2H), 5.60 (s, 1H), 1.30 (s, 9H); ^{13}C -NMR (100 MHz, $CDCl_3$) δ 171.2, 151.5, 148.1, 135.3, 132.2, 130.9, 128.2, 126.5, 126.0, 123.7, 123.4, 60.6, 34.6, 31.3. IR $\nu_{max}(KBr)/cm^{-1}$: 3058, 2962, 2920, 2860, 1681, 1456, 1380, 1189, 1019, 806, 744. HRMS (ESI) calcd for $[C_{18}H_{19}NO+Na]^+$: 288.1359, found: 288.1360.



3-(4-methoxyphenyl)isoindolin-1-one (3u). The product was obtained as a white solid (201 mg, 84%): 1H -NMR (400 MHz, $CDCl_3$) δ 7.96 (d, $J = 10.1$ Hz, 1H), 7.84 (d, $J = 7.3$ Hz, 1H), 7.52 – 7.41 (m, 2H), 7.22 (d, $J = 7.5$ Hz, 1H), 7.17 (d, $J = 8.6$ Hz, 2H), 6.85 (d, $J = 8.7$ Hz, 2H), 5.58 (s, 1H), 3.75 (d, $J = 7.3$ Hz, 3H); ^{13}C -NMR (100 MHz, $CDCl_3$) δ 171.4, 159.7, 148.4, 132.2, 131.1, 130.3, 128.2, 128.1, 123.7, 123.3, 114.4, 60.5, 55.3. IR $\nu_{max}(KBr)/cm^{-1}$: 3062, 2956, 2922, 2848, 1685, 1606, 1512, 1463, 1382, 1176, 1033, 825, 732, 590. HRMS (ESI) calcd for $[C_{15}H_{13}NO_2+Na]^+$: 262.0838, found: 288. 262.0835.

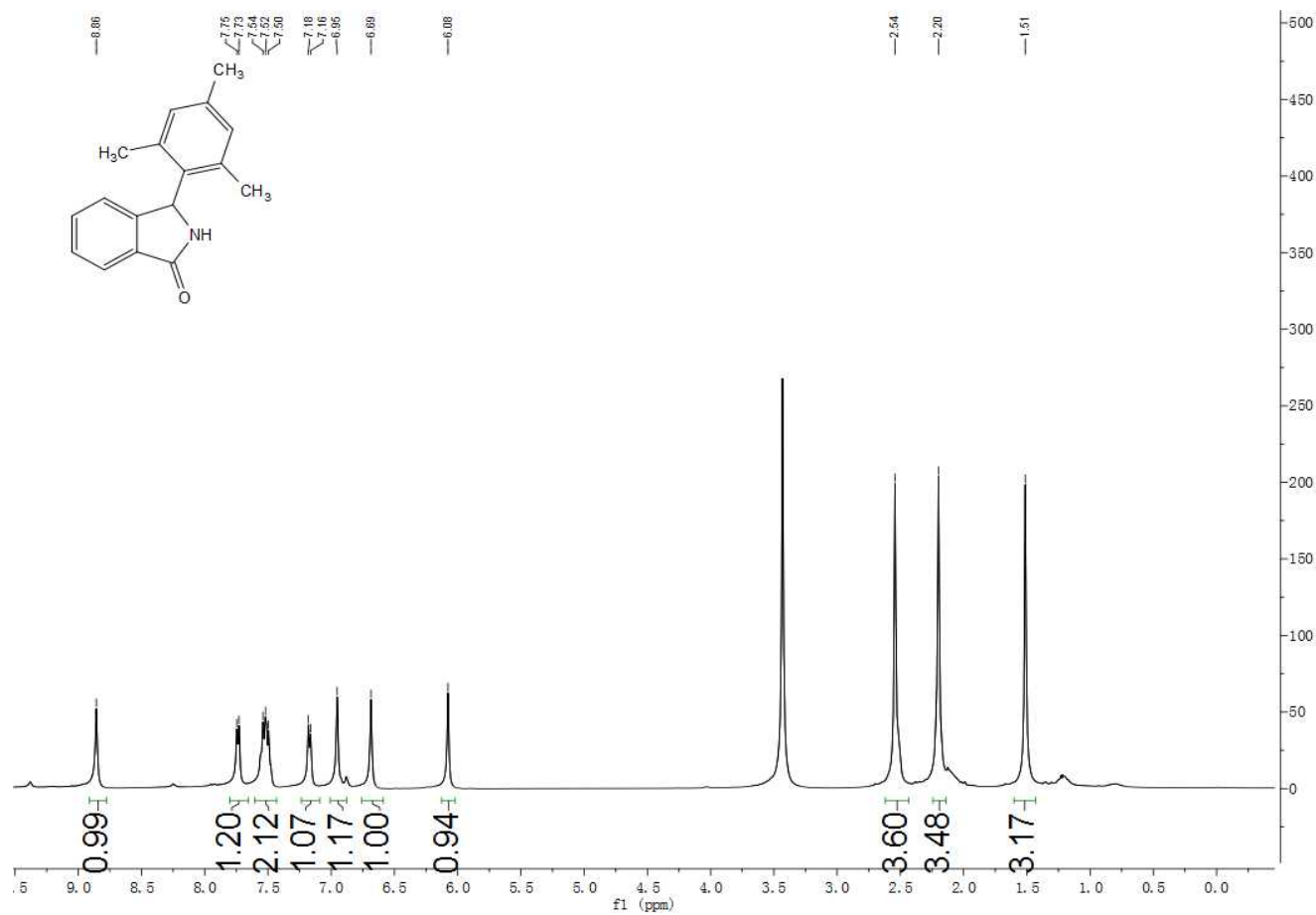


3-(2,5-dimethylphenyl)isobenzofuran-1(3H)-one (4a). The product was obtained as a pale yellow solid (226 mg, 95%): 1H -NMR (400 MHz, $CDCl_3$) δ 7.97 (d, $J = 7.6$ Hz, 1H), 7.66 (t, $J = 7.5$ Hz, 1H), 7.57 (t, $J = 7.5$ Hz, 1H), 7.35 (d, $J = 7.6$ Hz, 1H), 7.14 (d, $J = 7.7$ Hz, 1H), 7.07 (d, $J = 7.3$ Hz, 1H), 6.75 (s, 1H), 6.65 (s, 1H), 2.45 (s, 3H), 2.21 (s, 3H); ^{13}C -NMR (100 MHz, $CDCl_3$) δ 170.8, 149.6, 136.0, 134.3, 133.9, 133.8, 131.1, 130.0, 129.3, 127.7, 126.2, 125.6, 123.1, 80.6, 20.9, 18.9. IR $\nu_{max}(KBr)/cm^{-1}$: 3038, 2968, 2918, 1755, 1610, 1463, 1382, 1064, 740. HRMS (ESI) calcd for $[C_{16}H_{14}O_2+Na]^+$: 261.0886, found: 261.0888.

4 Copies of ^1H NMR and ^{13}C NMR of products

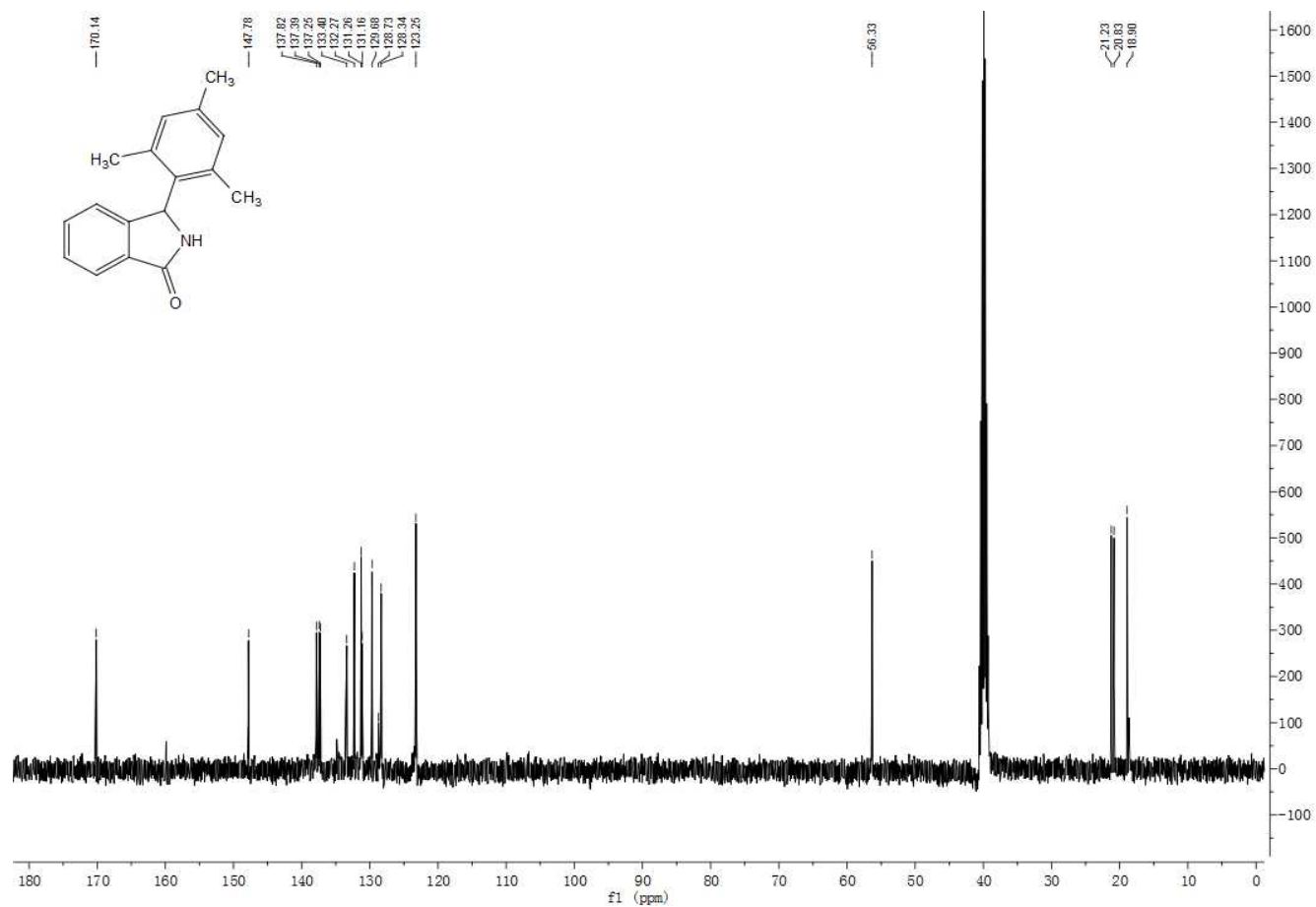
3-mesitylisoindolin-1-one (3a)

^1H NMR



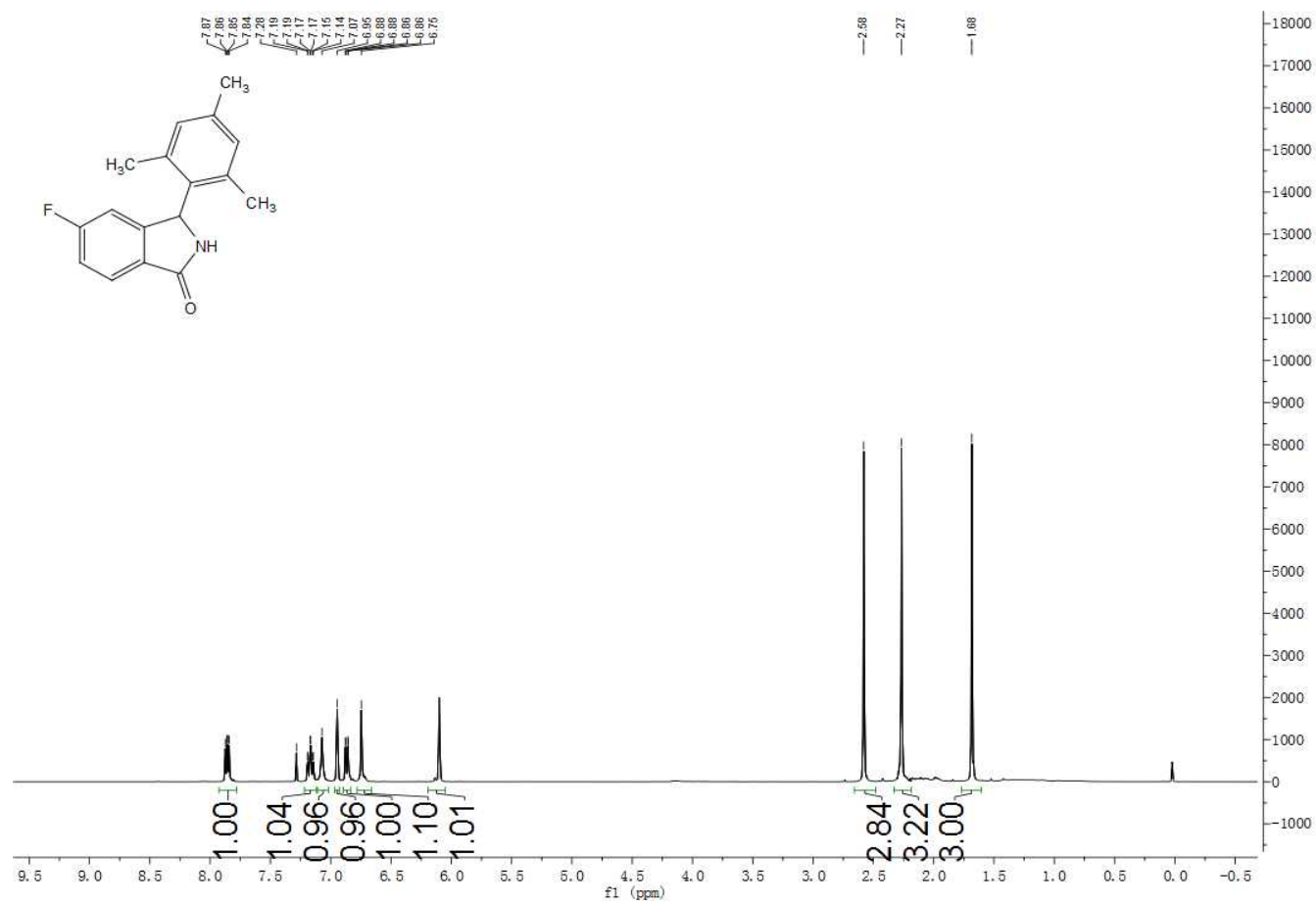
3-mesitylisoindolin-1-one (3a)

^{13}C NMR



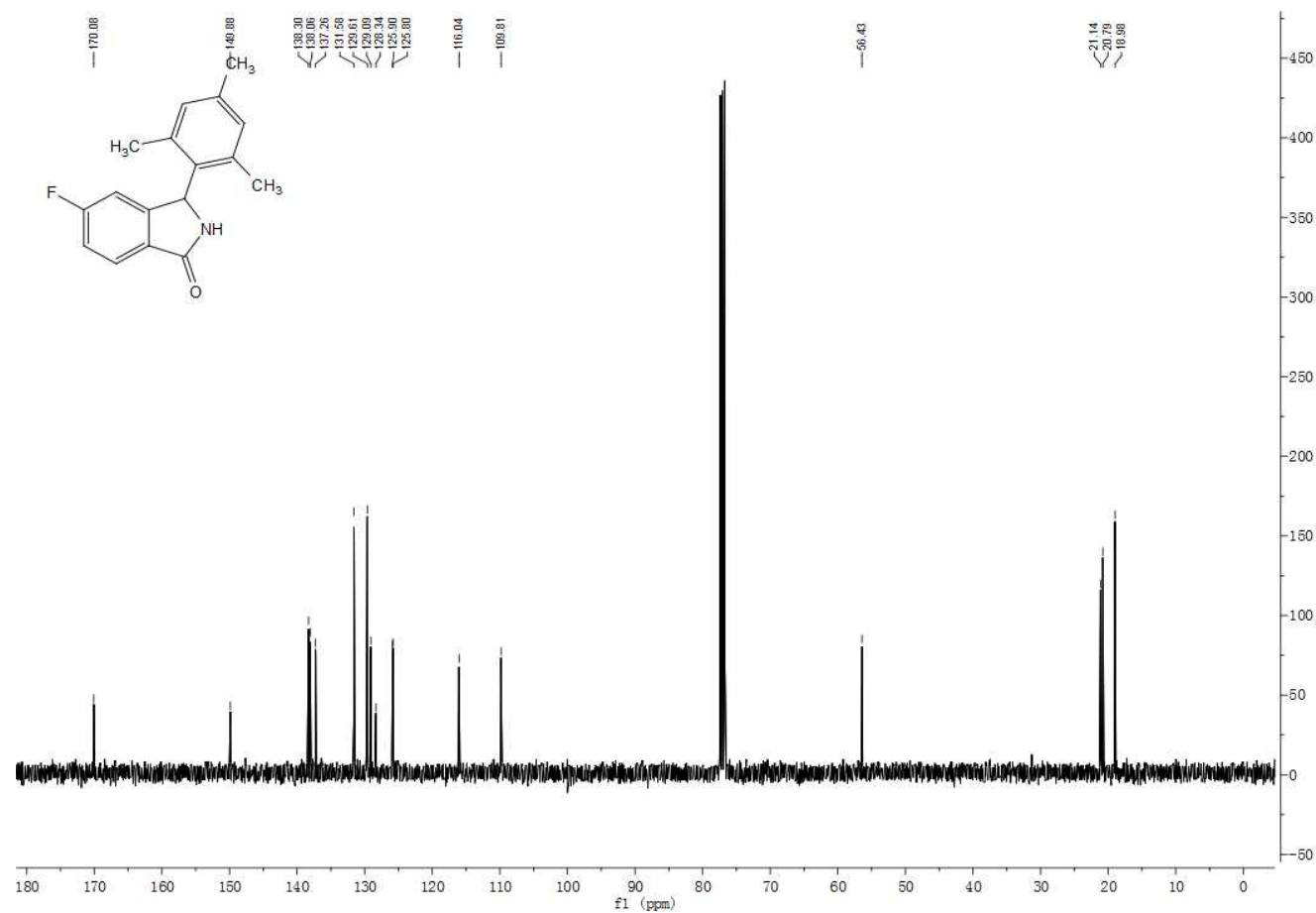
5-fluoro-3-mesitylisoindolin-1-one (3b)

^1H NMR



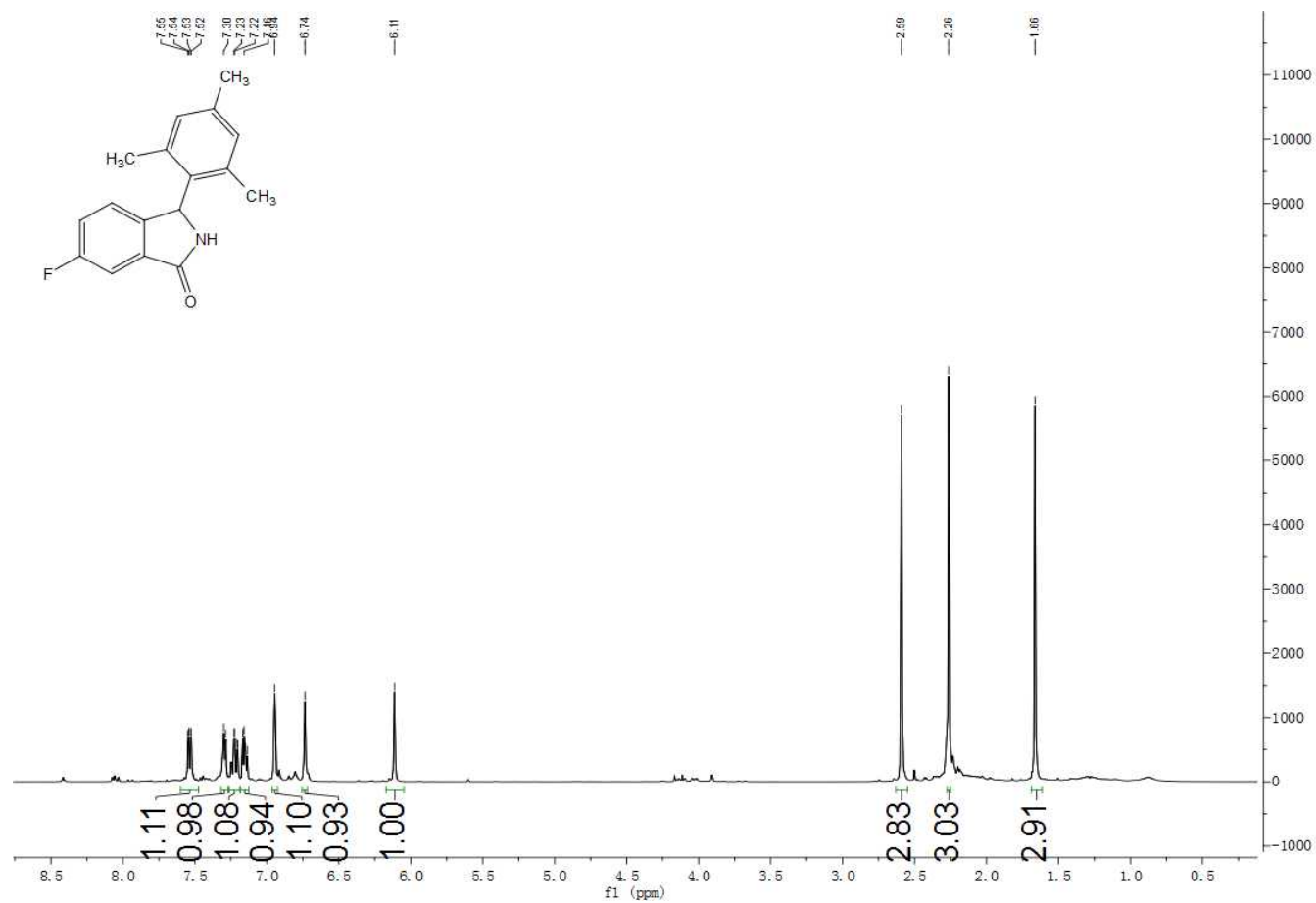
5-fluoro-3-mesitylisoindolin-1-one (3b)

^{13}C NMR



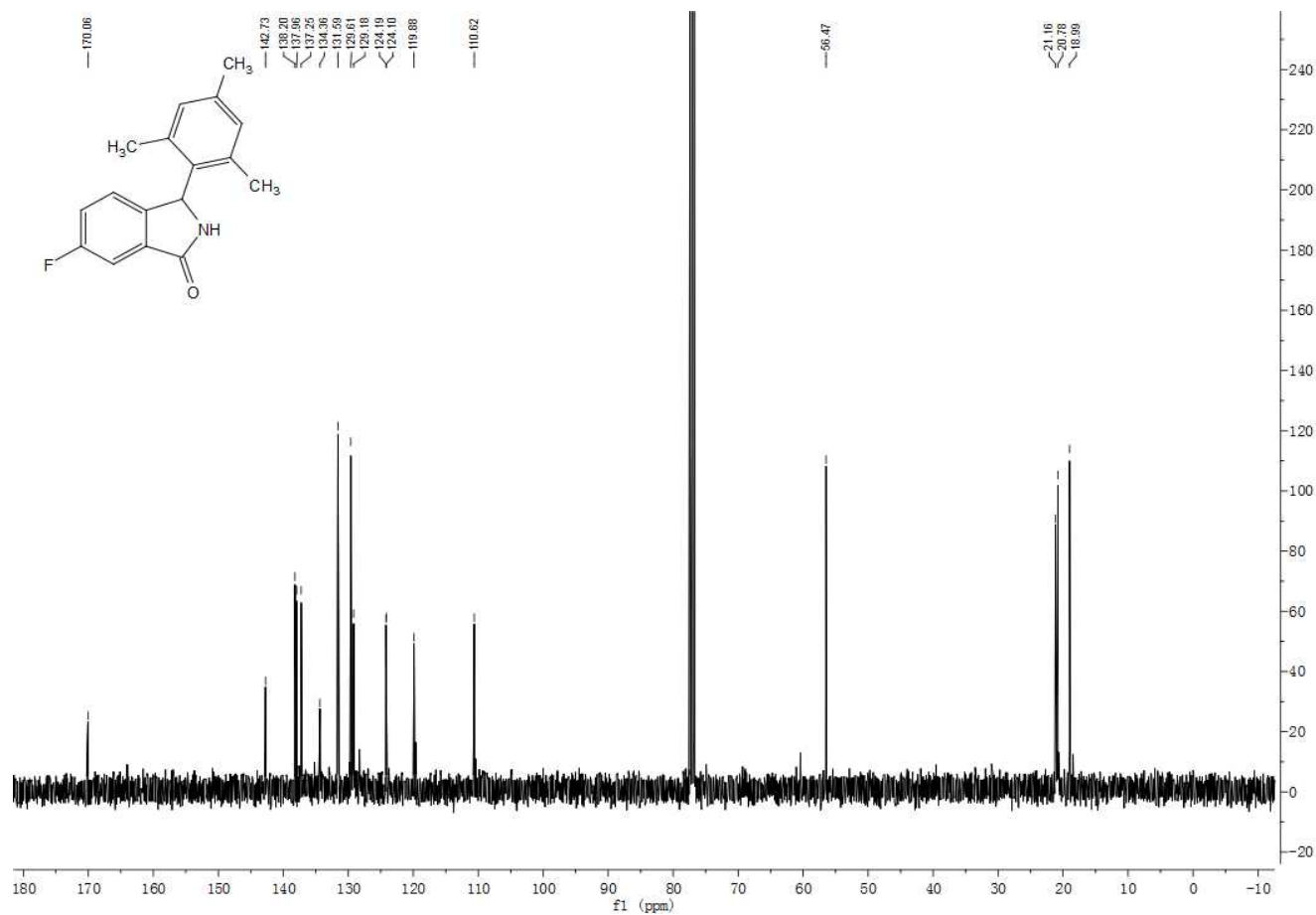
6-fluoro-3-mesitylisoindolin-1-one (3c)

^1H NMR



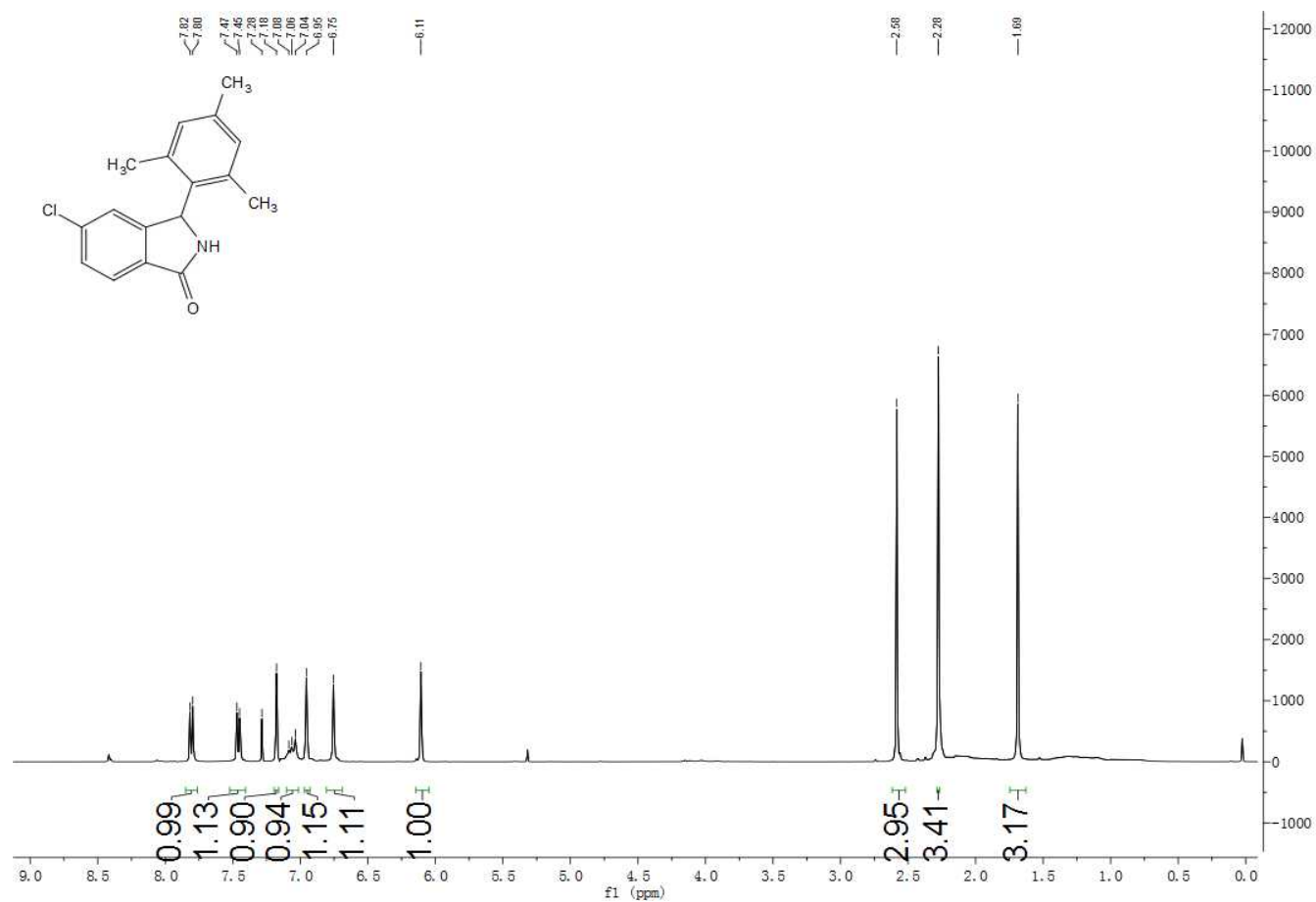
6-fluoro-3-mesitylisoindolin-1-one (3c)

^{13}C NMR



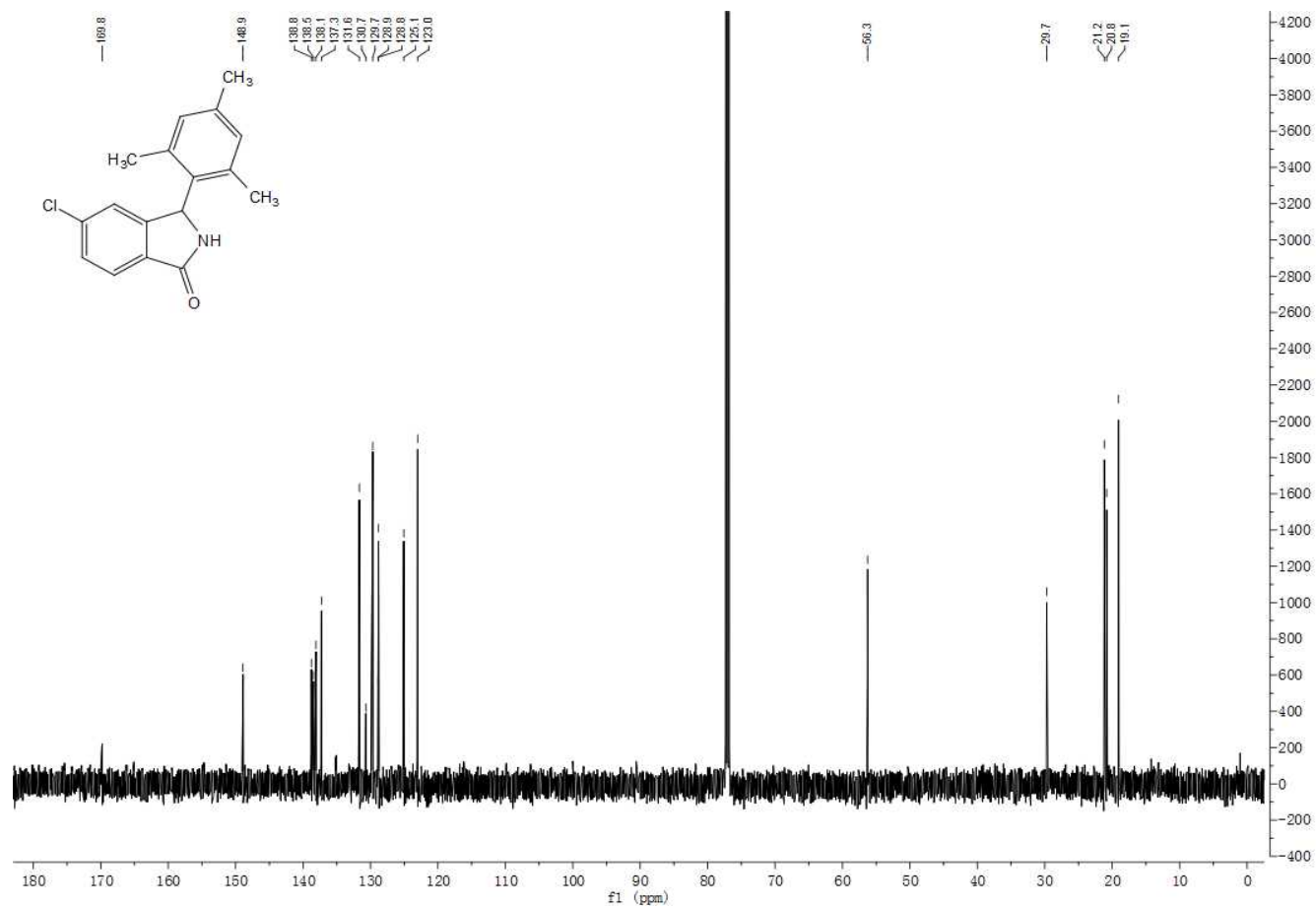
5-chloro-3-mesitylisoindolin-1-one (3d)

^1H NMR



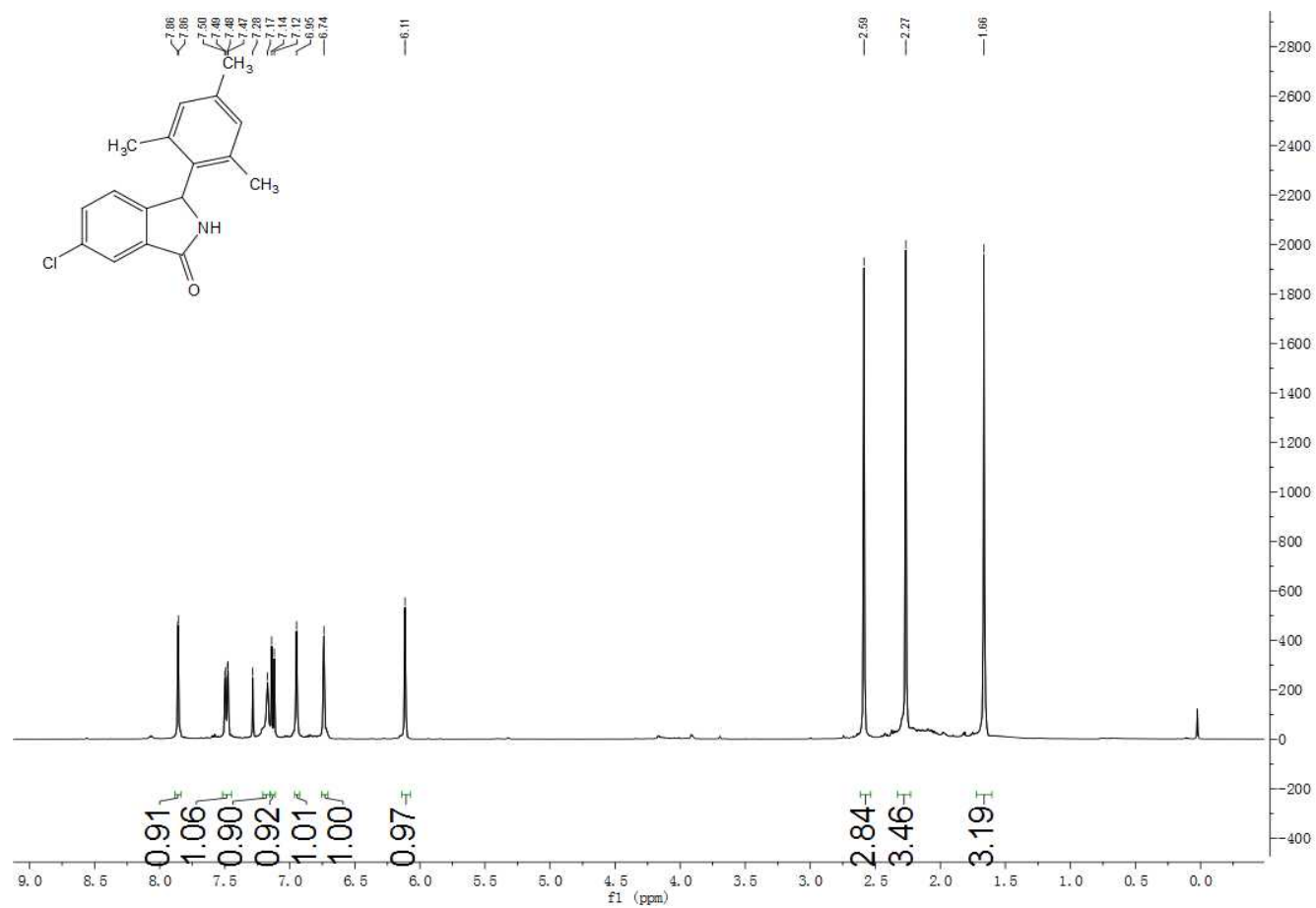
5-chloro-3-mesitylisoindolin-1-one (3d)

^{13}C NMR



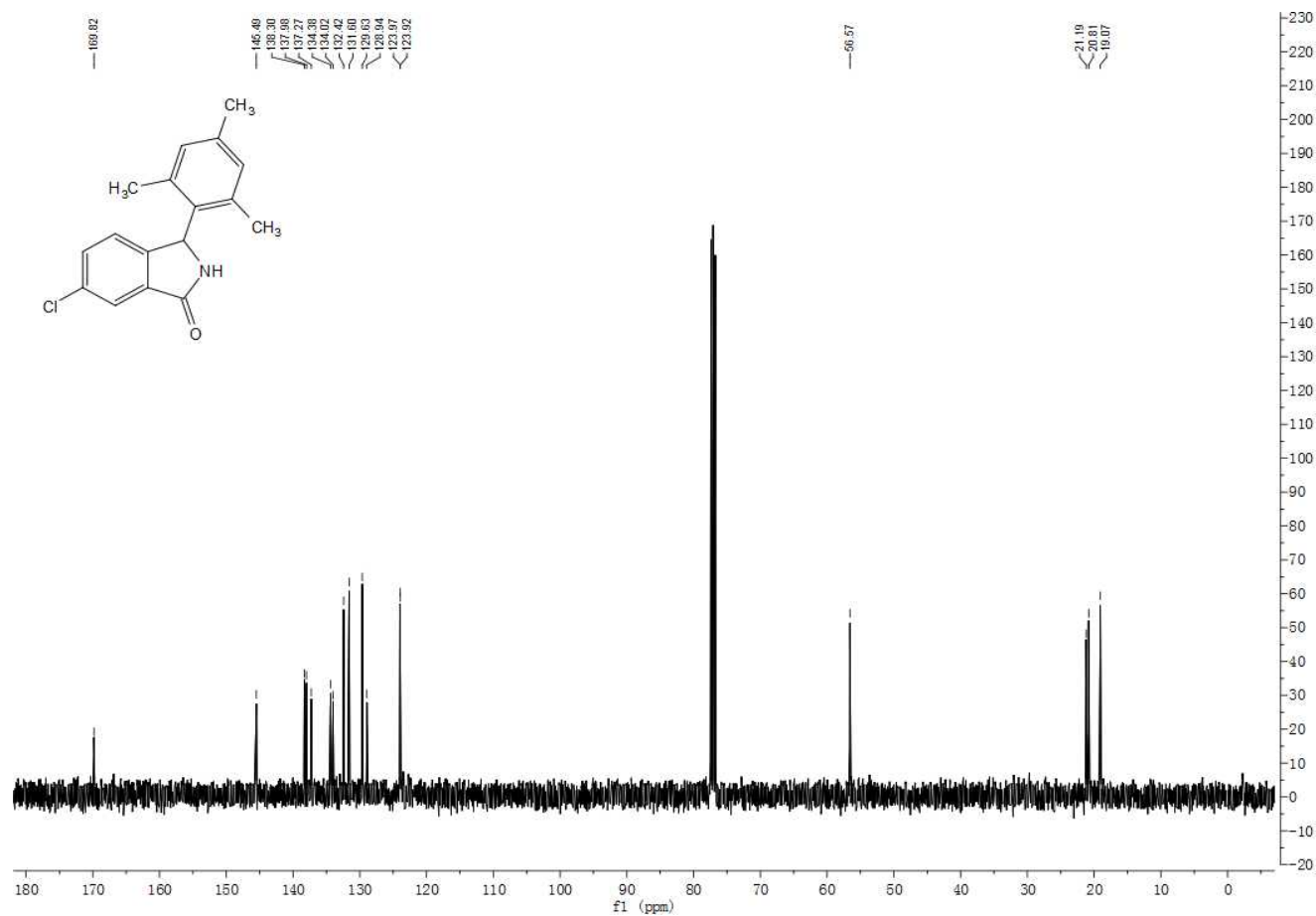
6-chloro-3-mesitylisoindolin-1-one (3e)

^1H NMR



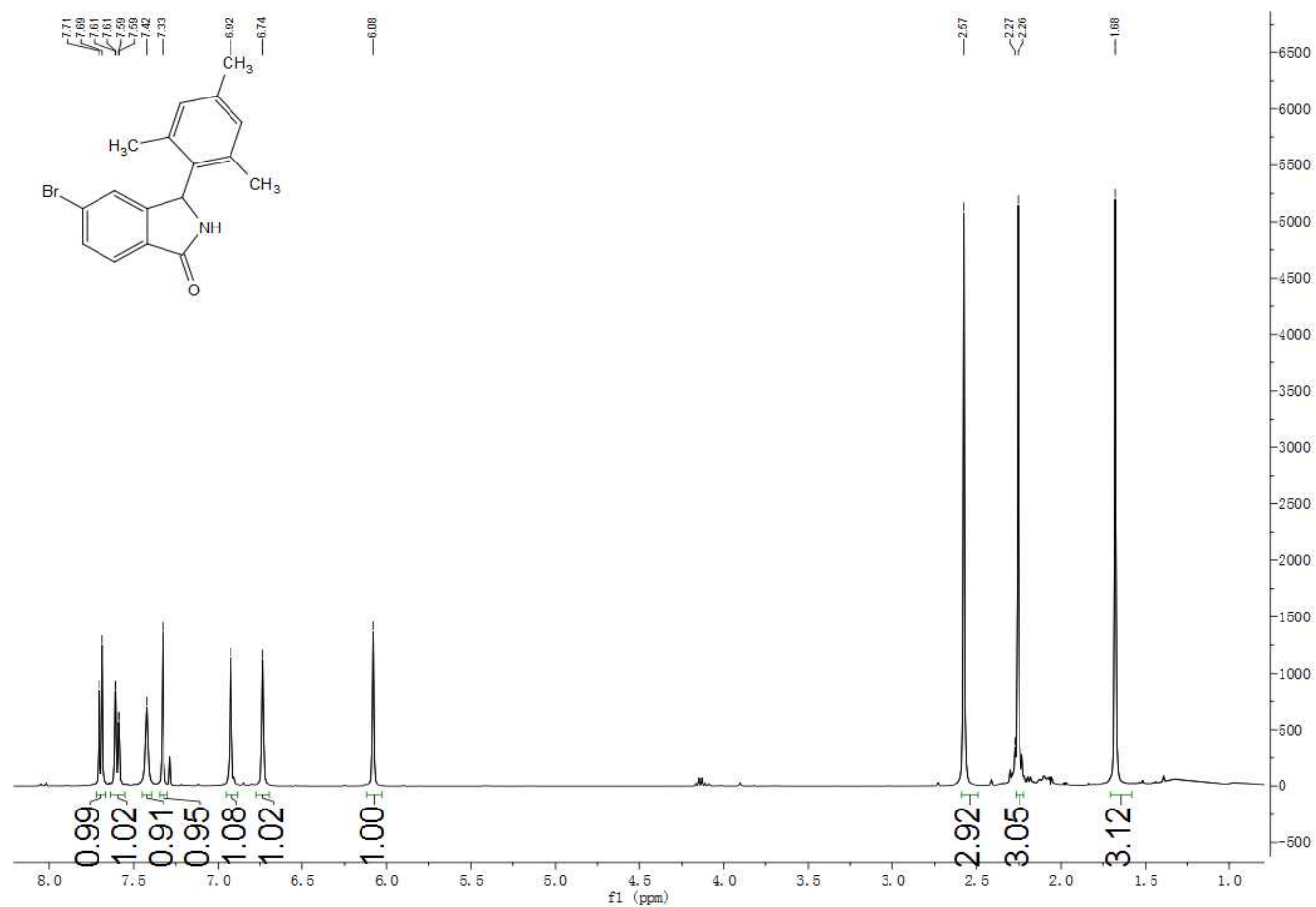
6-chloro-3-mesitylisoindolin-1-one (3e)

^{13}C NMR



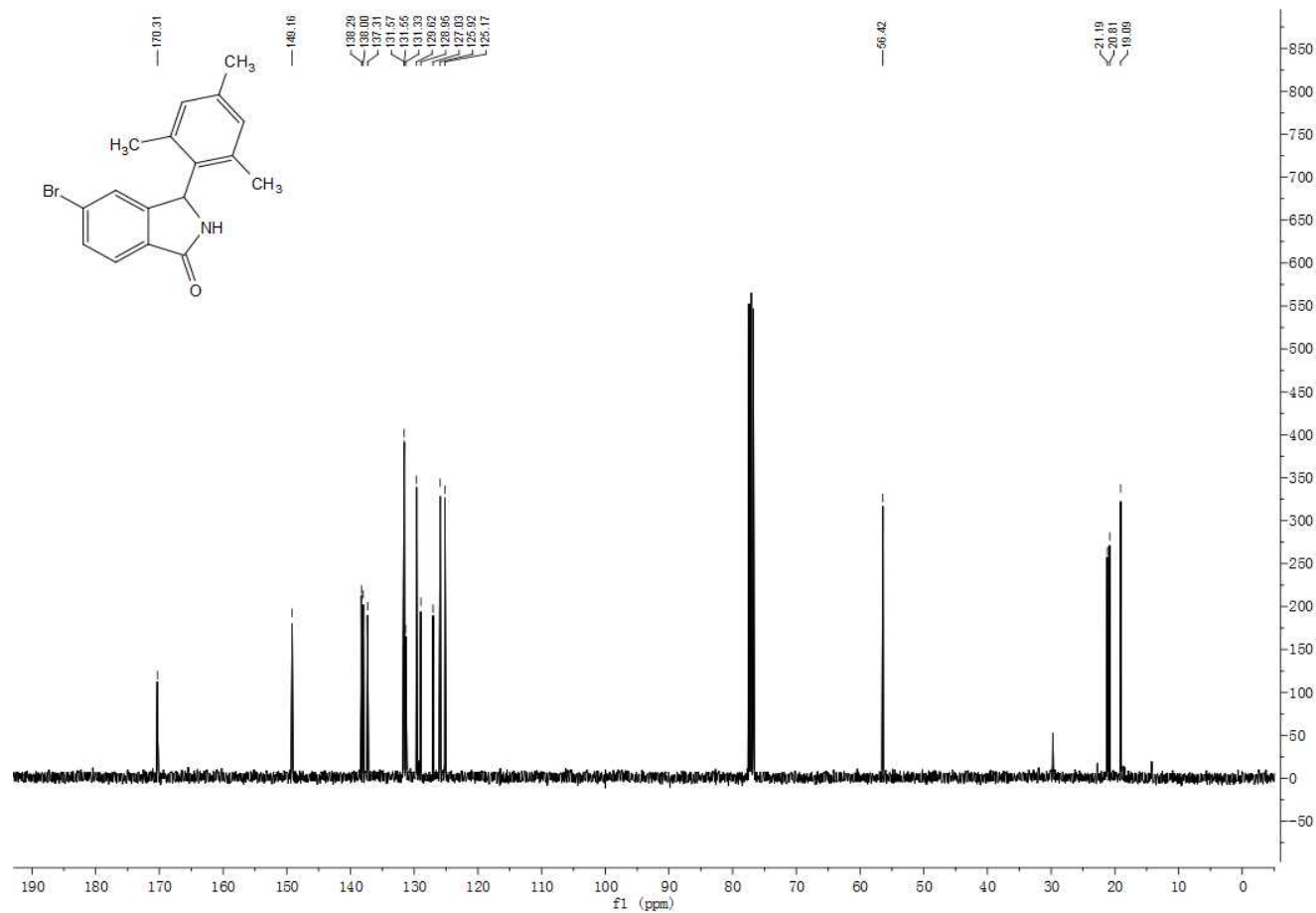
5-bromo-3-mesitylisoindolin-1-one (3f)

^1H NMR



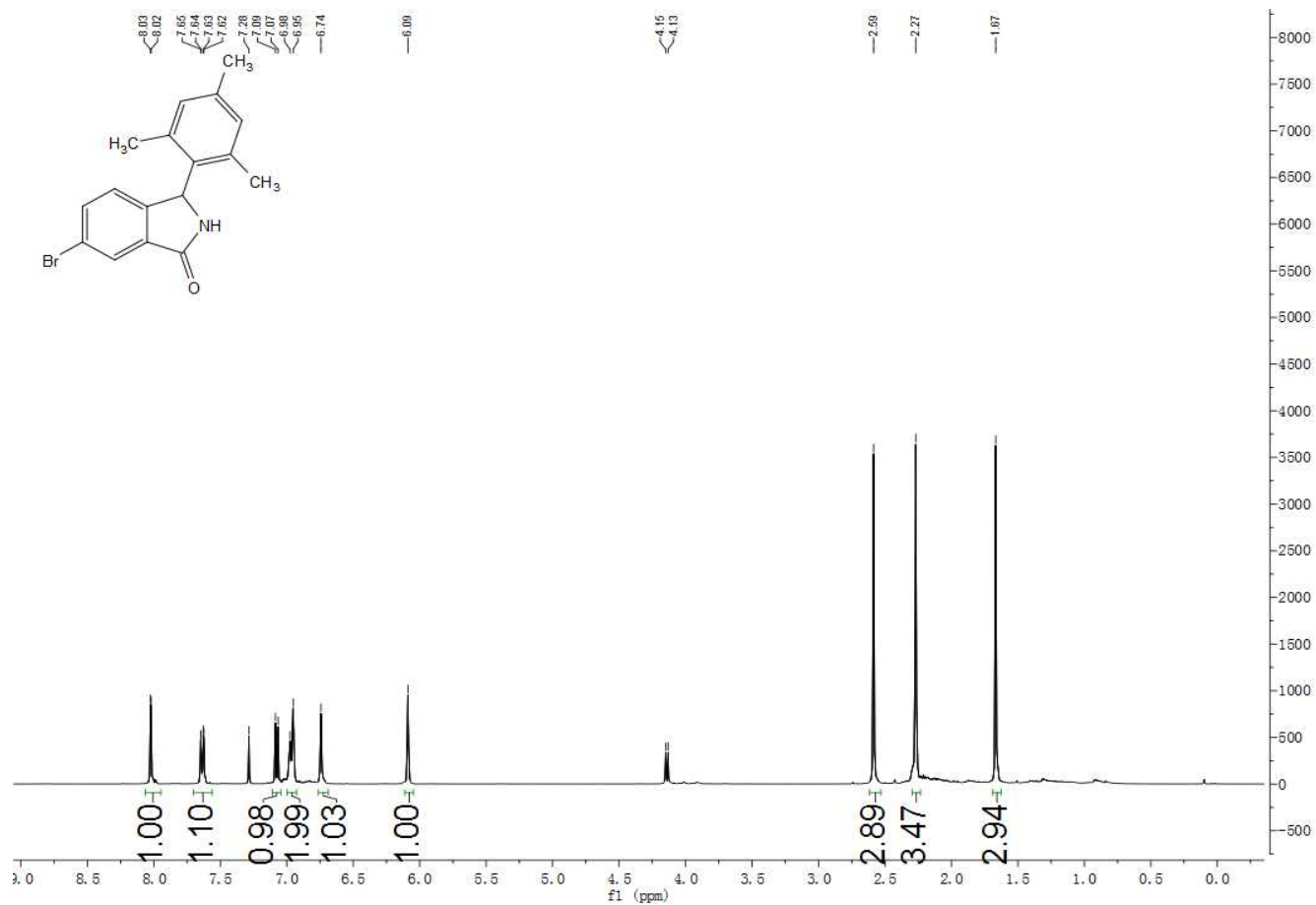
5-bromo-3-mesitylisoindolin-1-one (3f)

^{13}C NMR



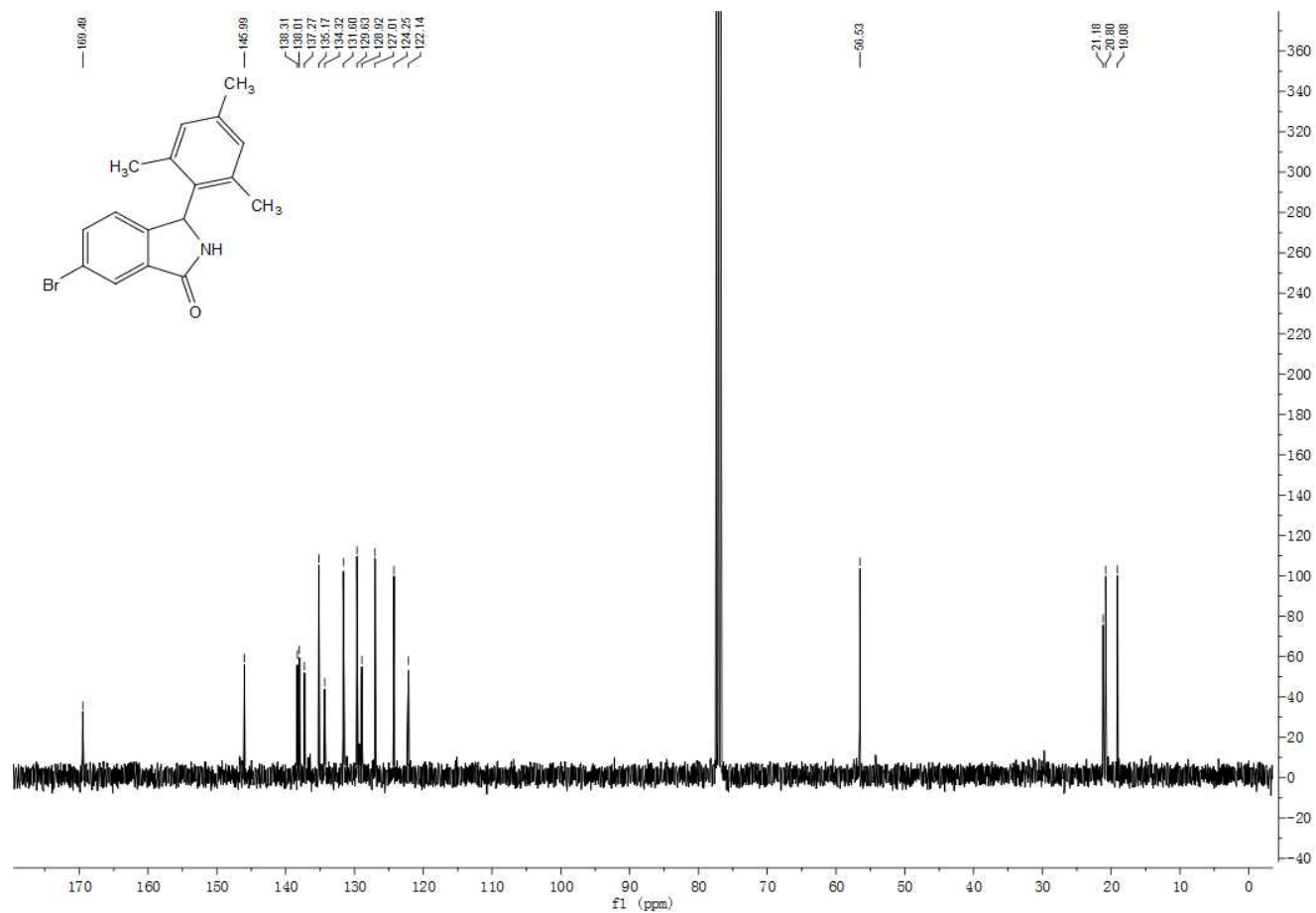
6-bromo-3-mesitylisoindolin-1-one (3g)

^1H NMR



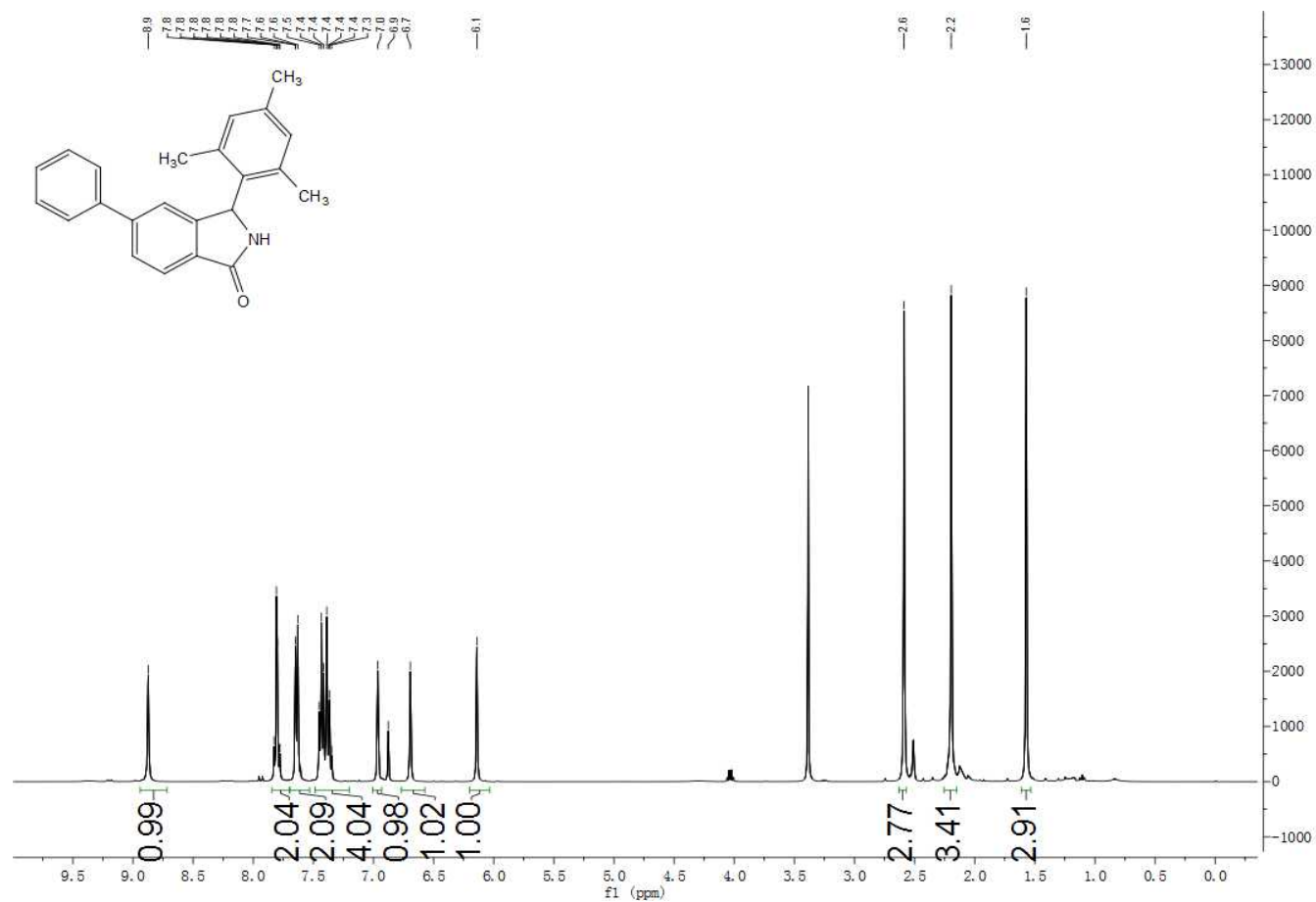
6-bromo-3-mesitylisoindolin-1-one (3g)

^{13}C NMR



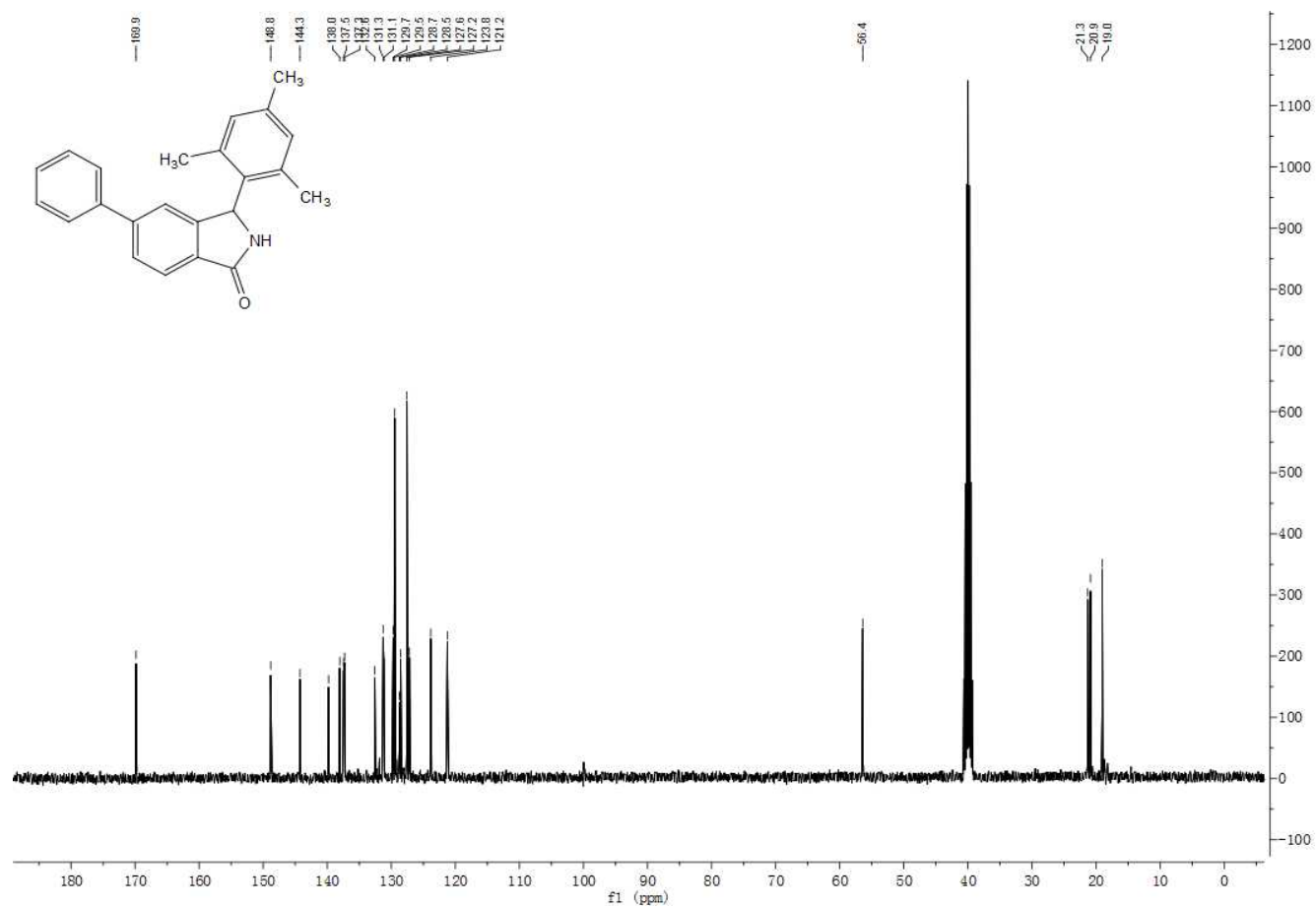
3-mesityl-5-phenylisoindolin-1-one (3h)

^1H NMR



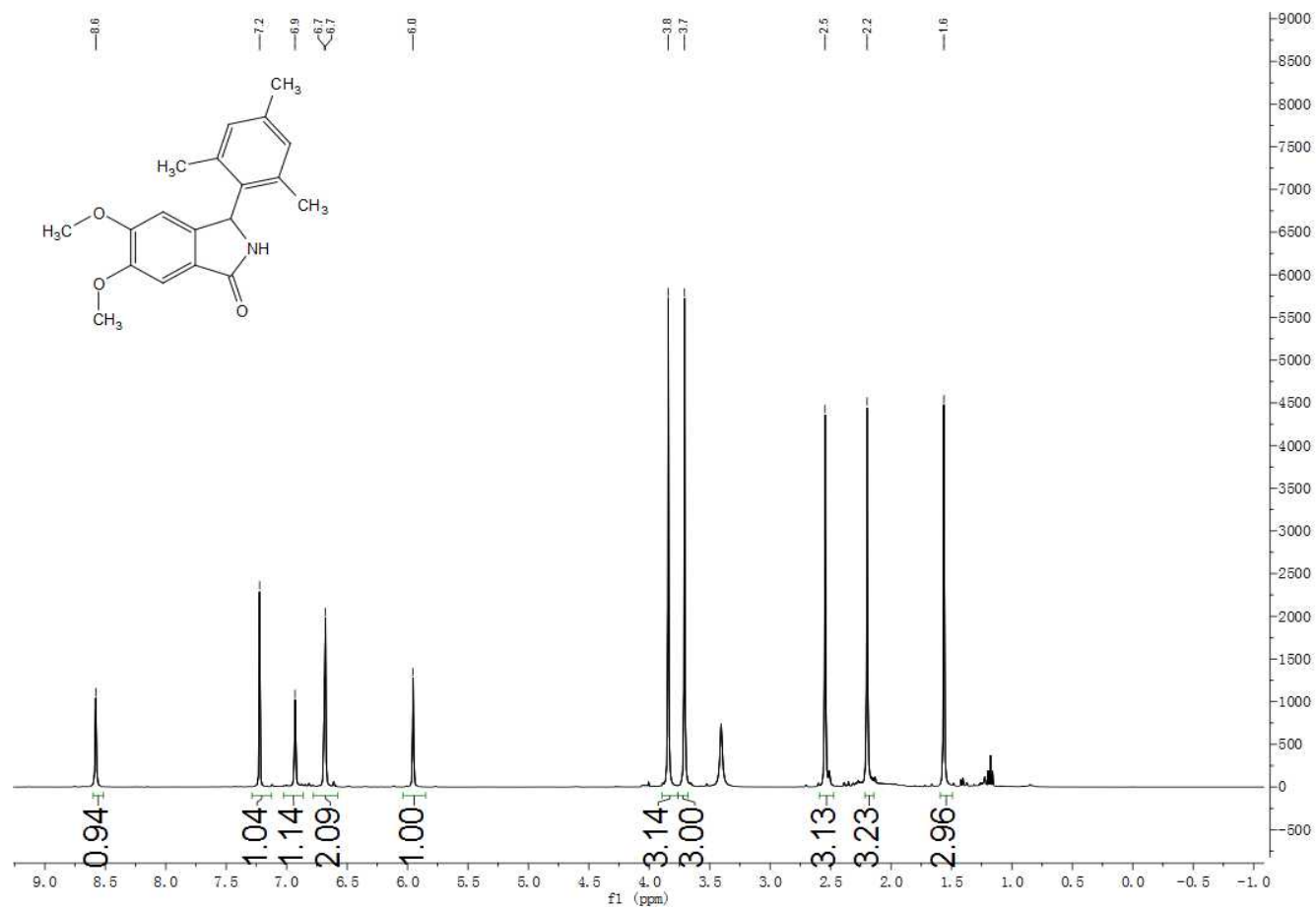
3-mesityl-5-phenylisoindolin-1-one (3h)

^{13}C NMR



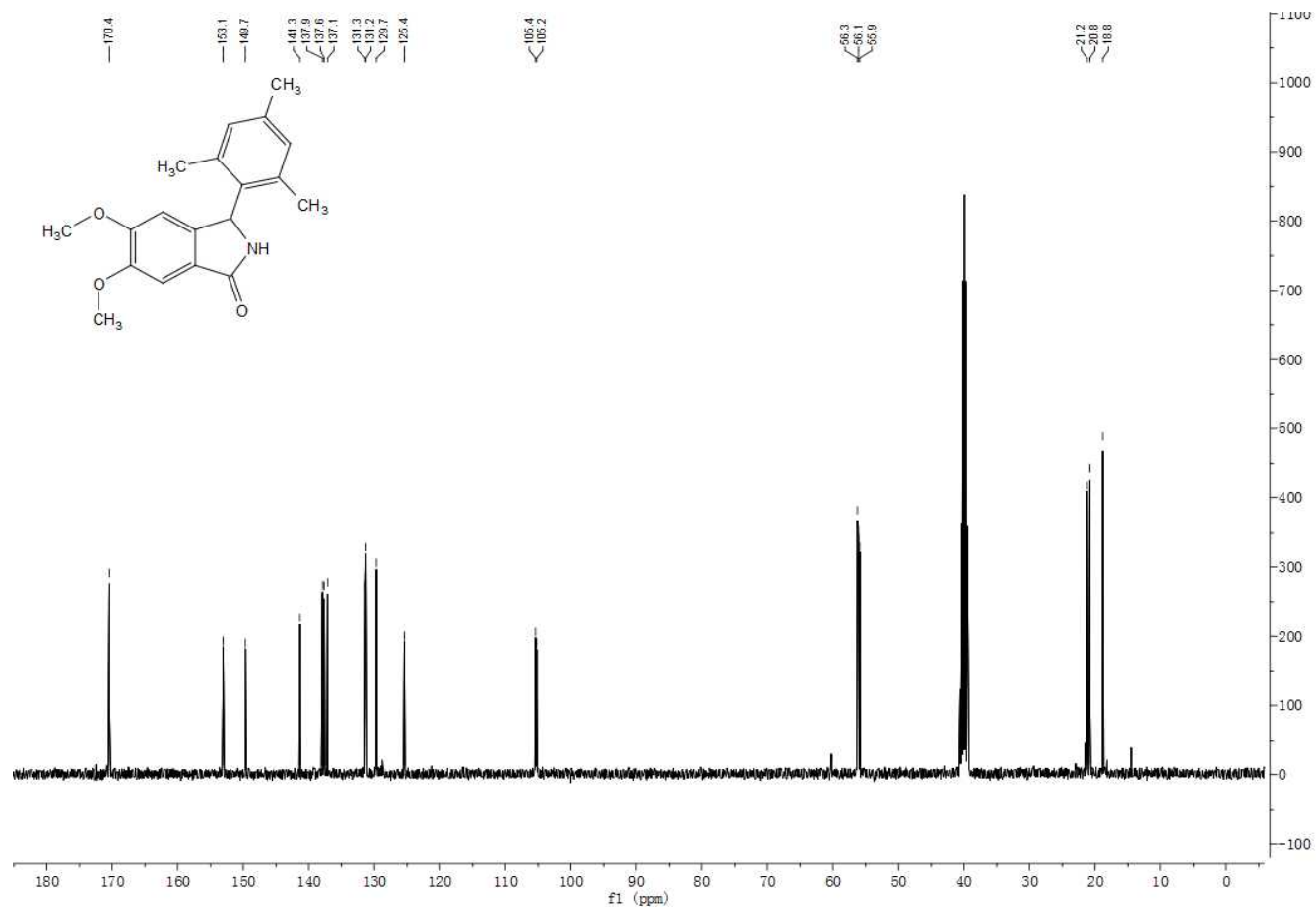
3-mesityl-5,6-dimethoxyisoindolin-1-one (3i)

^1H NMR



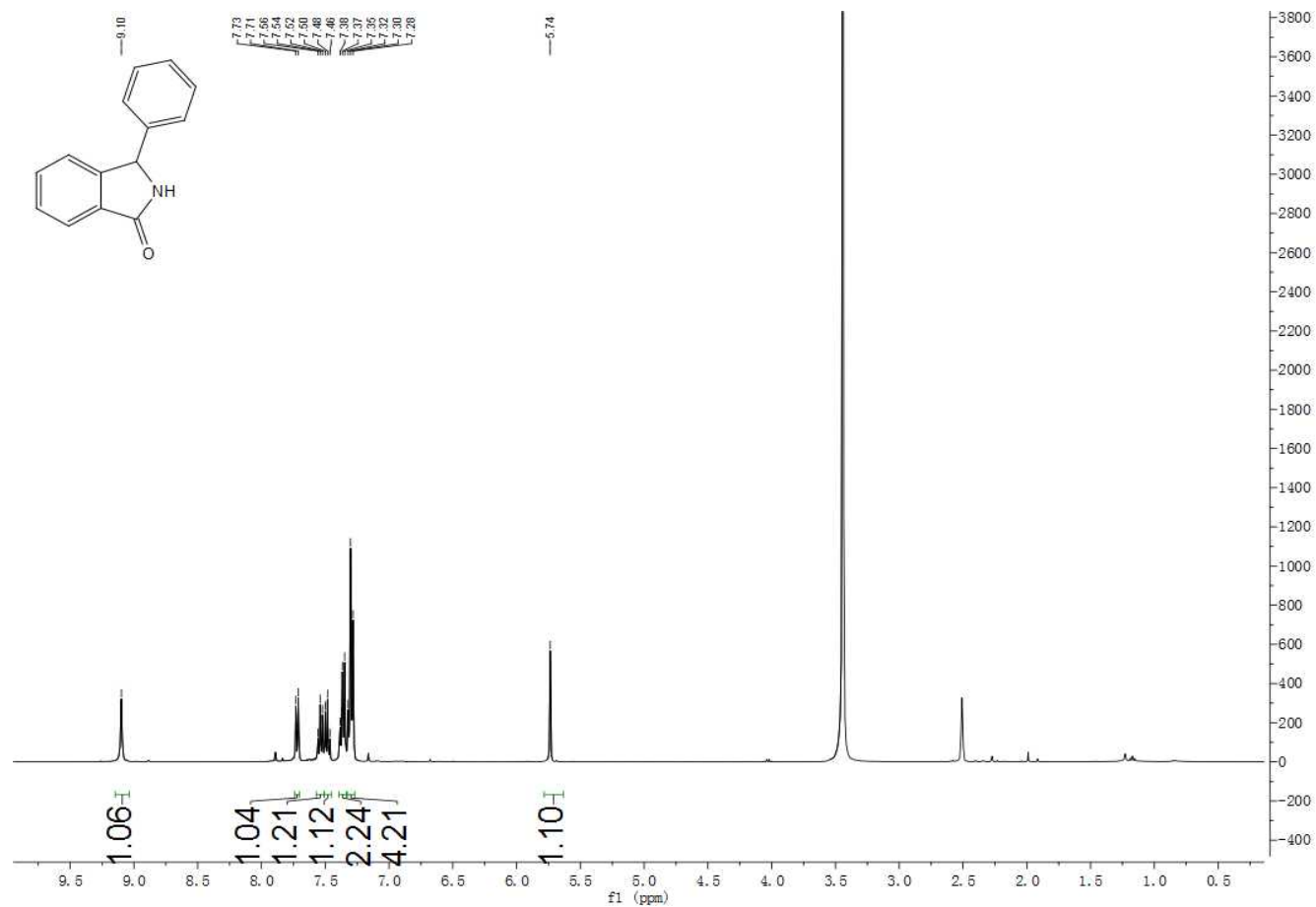
3-mesityl-5,6-dimethoxyisoindolin-1-one (3i)

^{13}C NMR



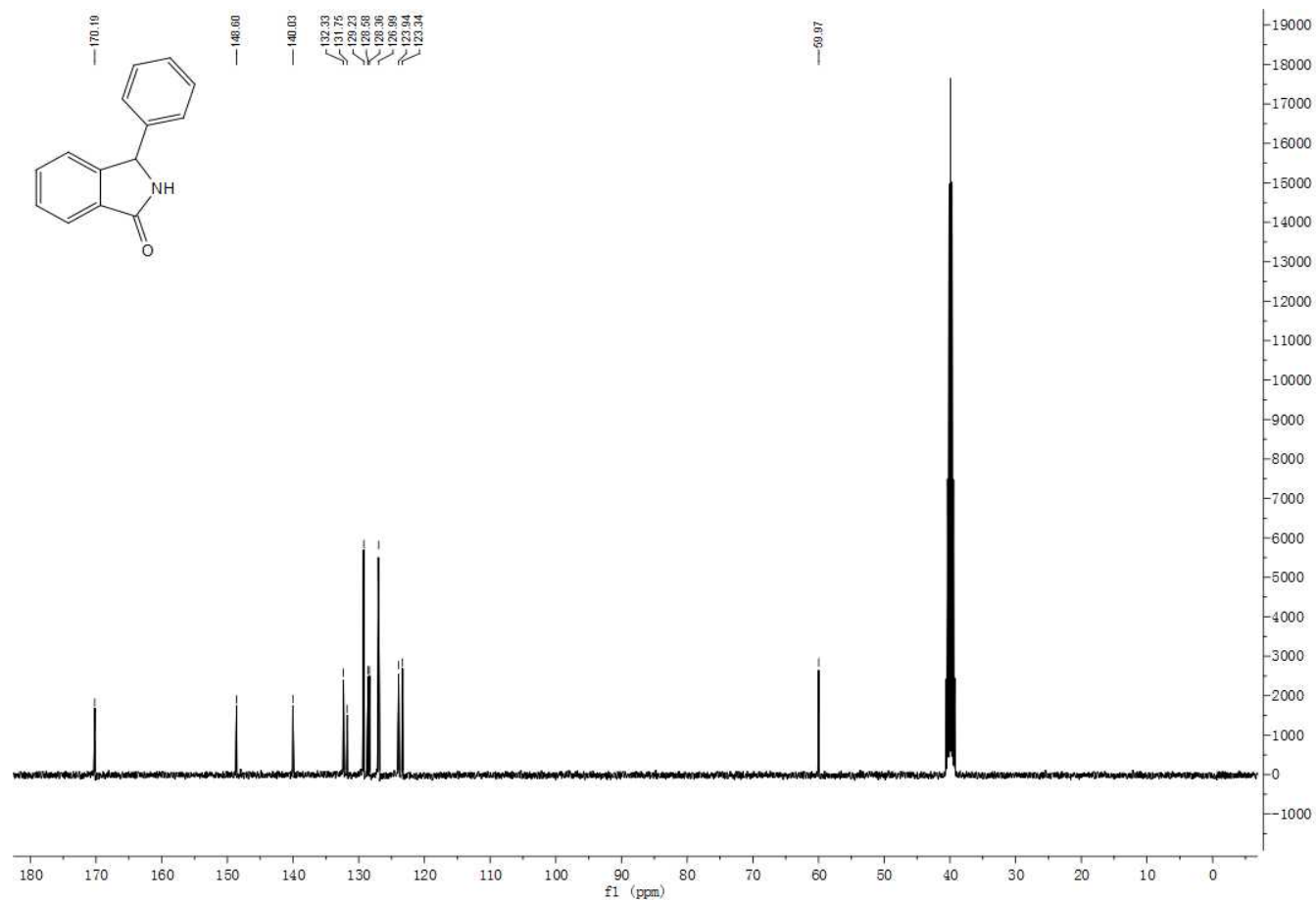
3-phenylisoindolin-1-one (3j)

^1H NMR



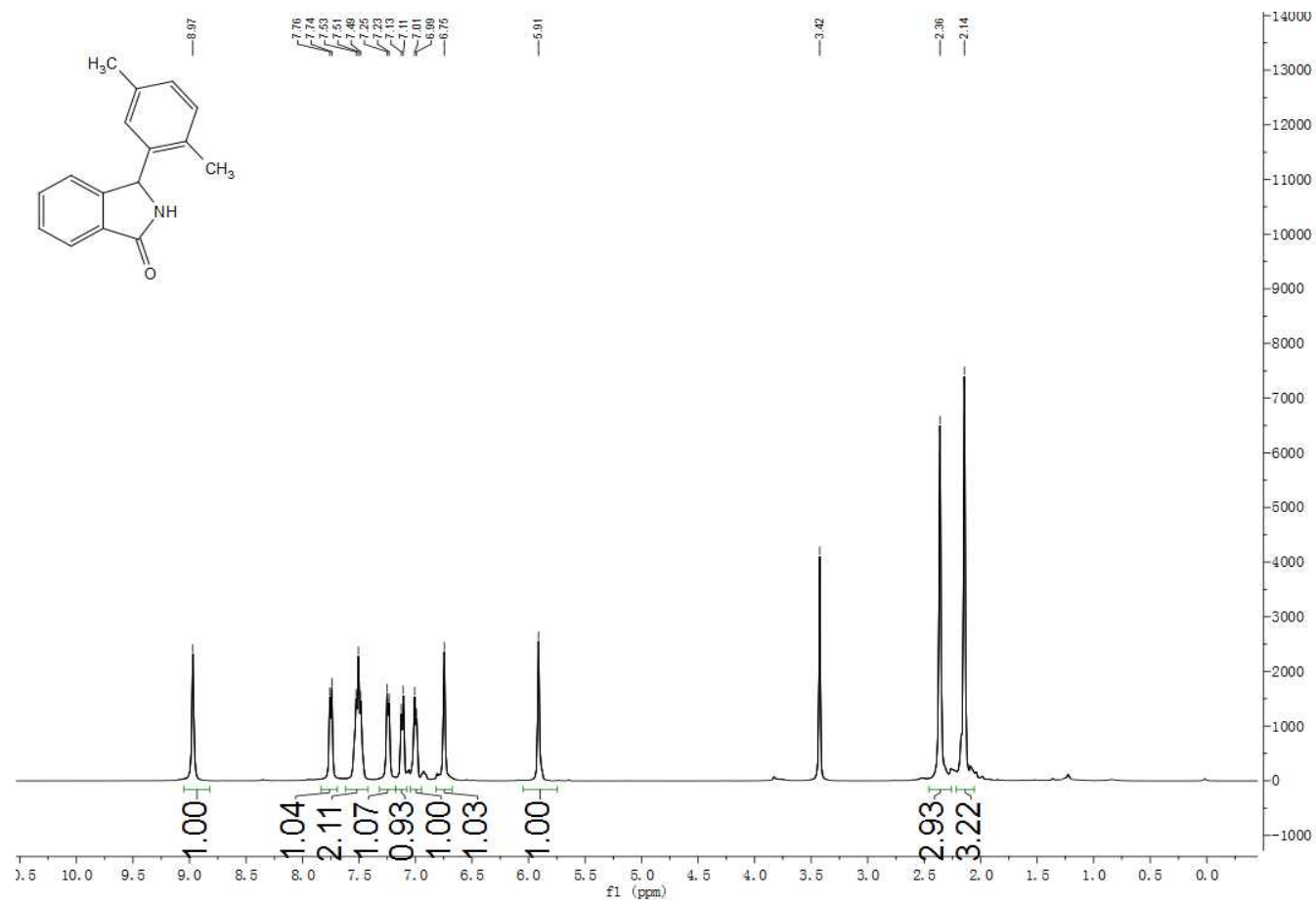
3-phenylisoindolin-1-one (3j)

^{13}C NMR



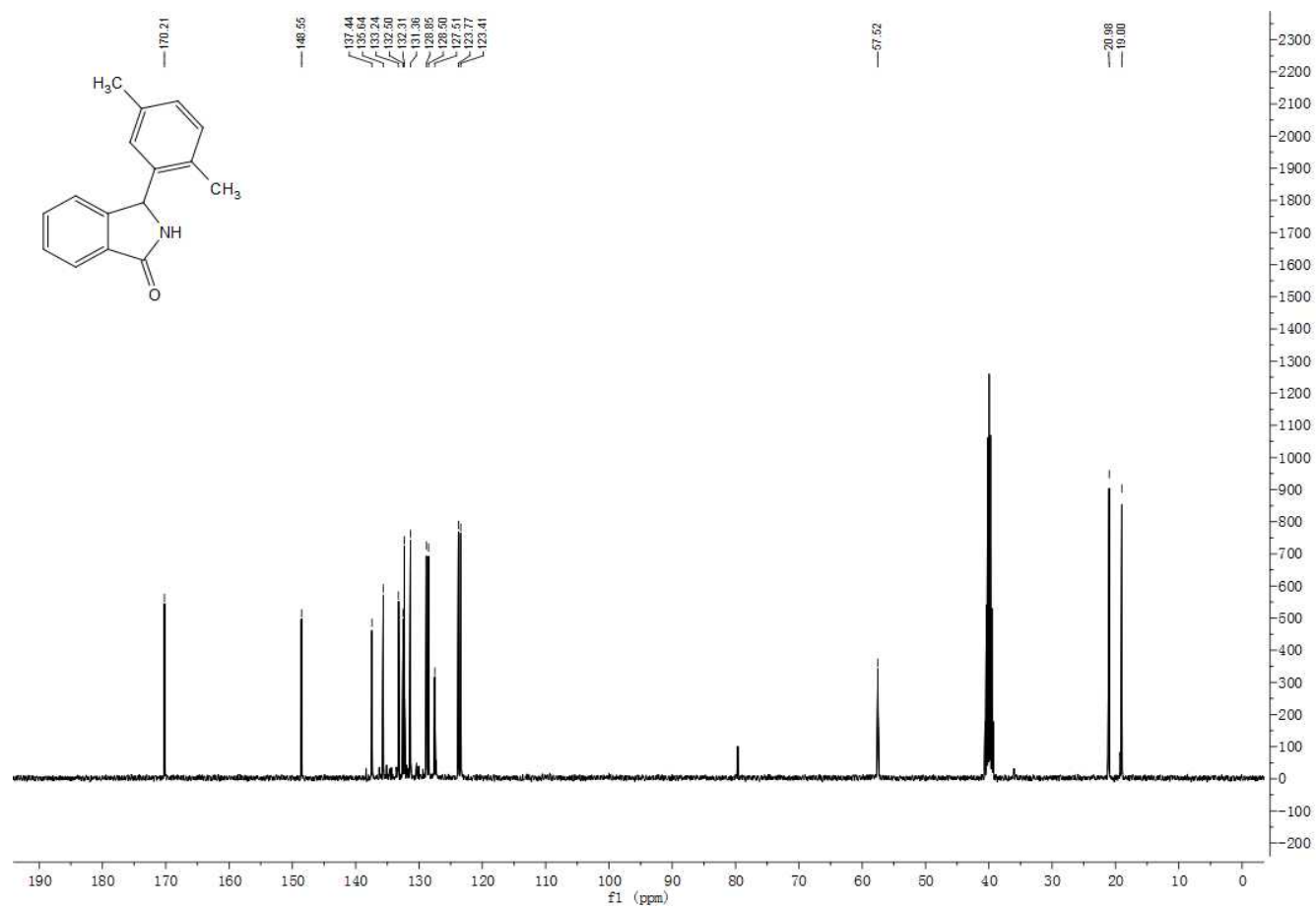
3-(2,5-dimethylphenyl)isoindolin-1-one (3k)

^1H NMR



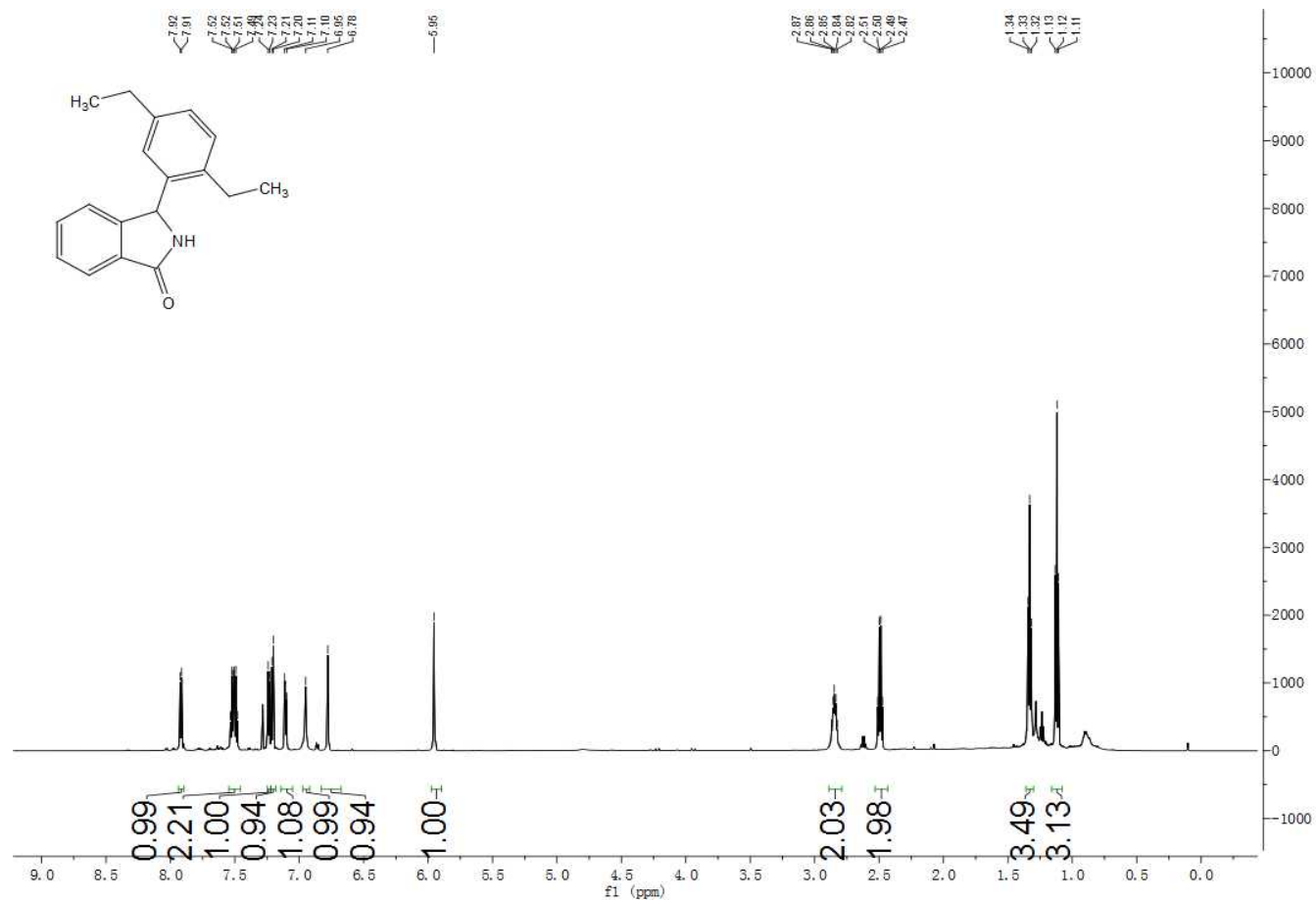
3-(2,5-dimethylphenyl)isoindolin-1-one (3k)

^{13}C NMR



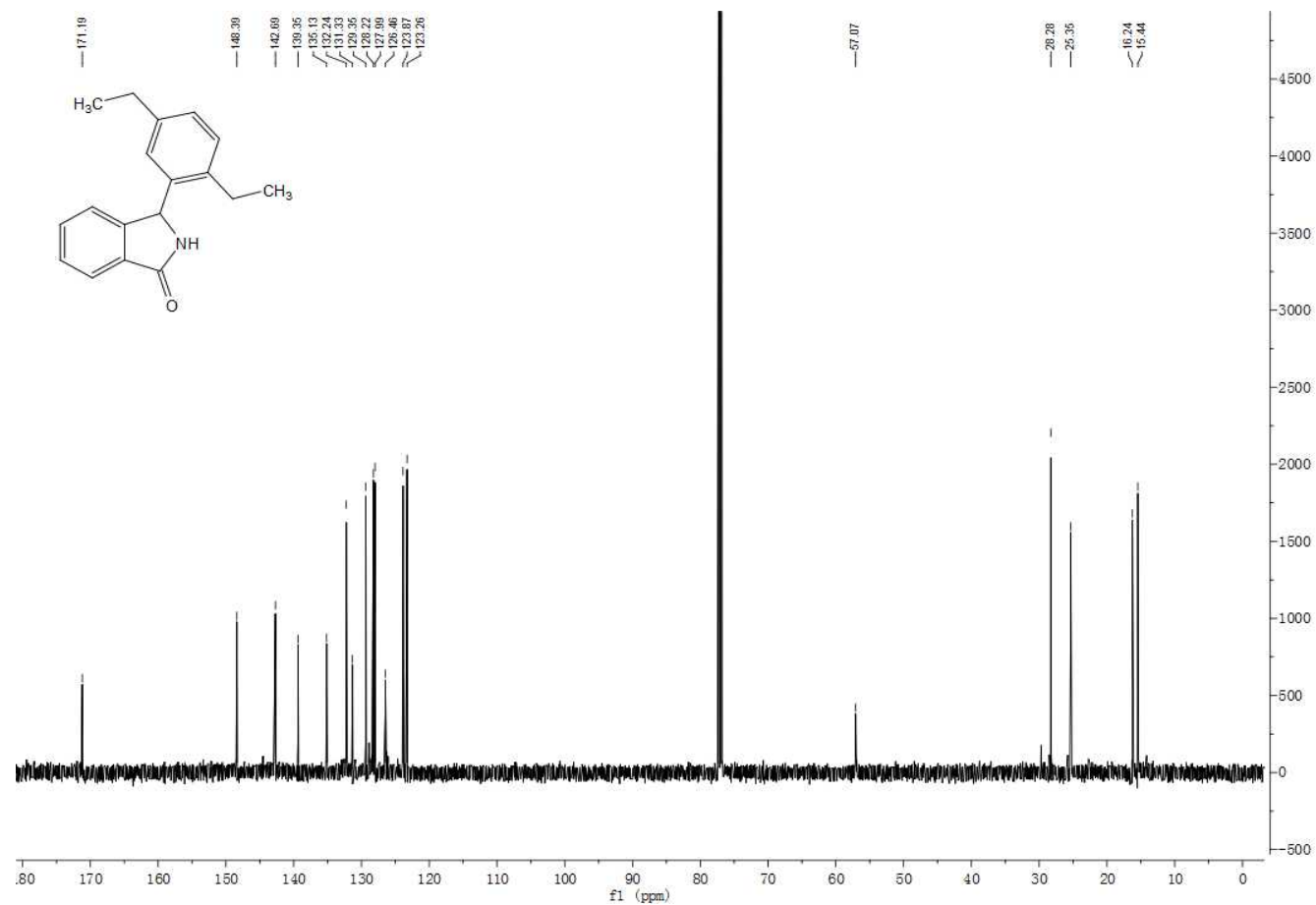
3-(2,5-diethylphenyl)isoindolin-1-one (3l)

^1H NMR



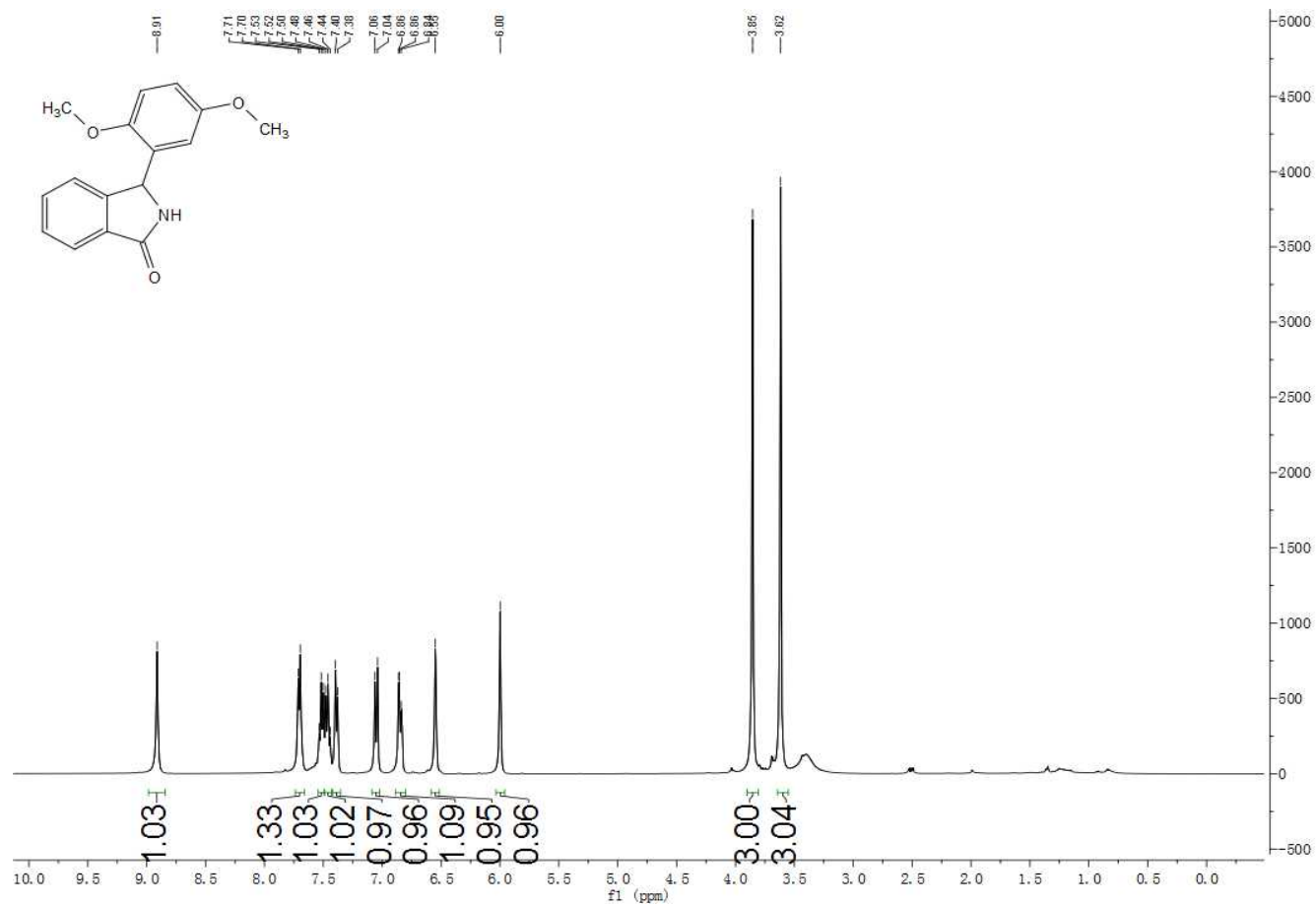
3-(2,5-diethylphenyl)isoindolin-1-one (3l)

^{13}C NMR



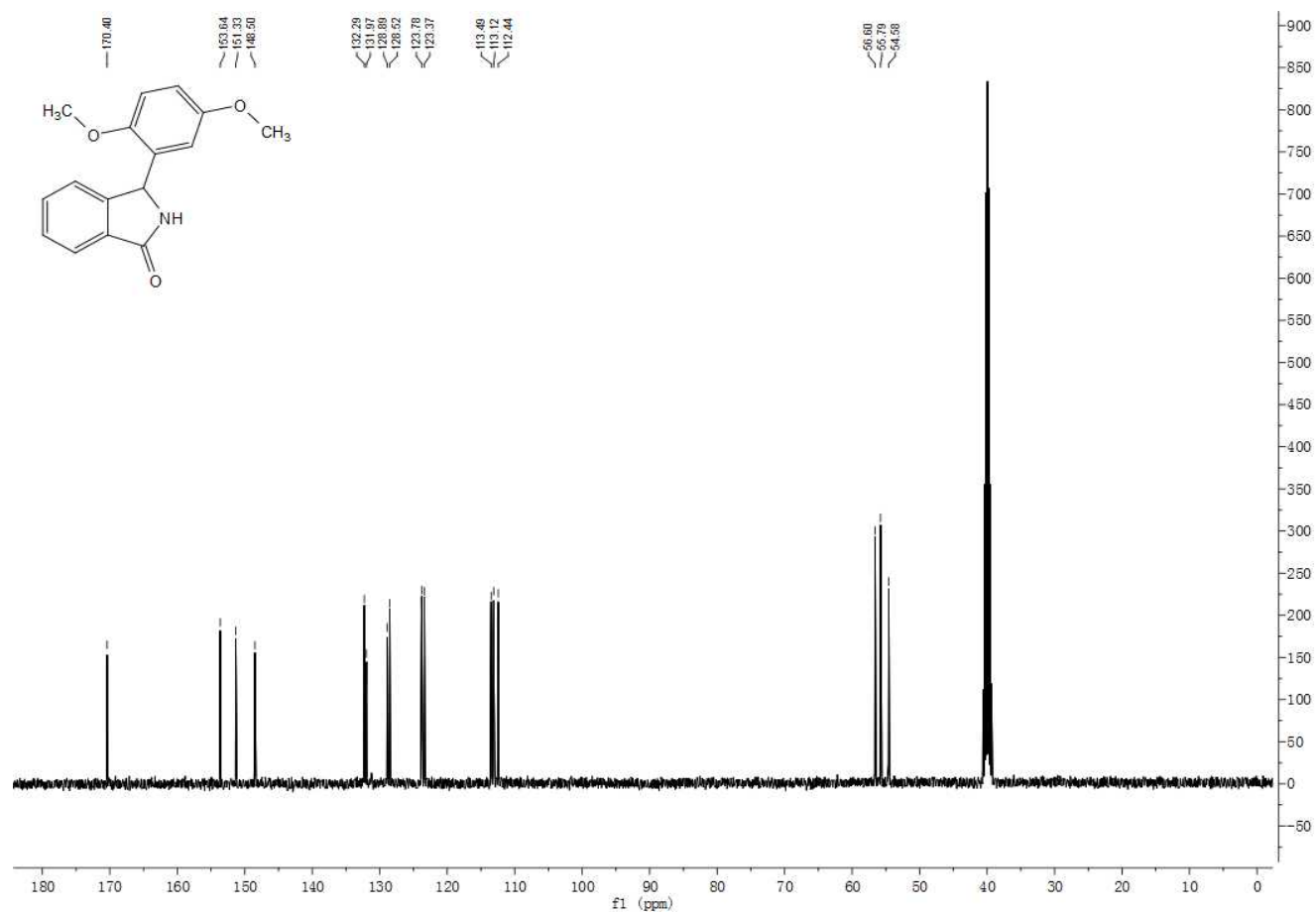
3-(2,5-dimethoxyphenyl)isoindolin-1-one (3m)

^1H NMR



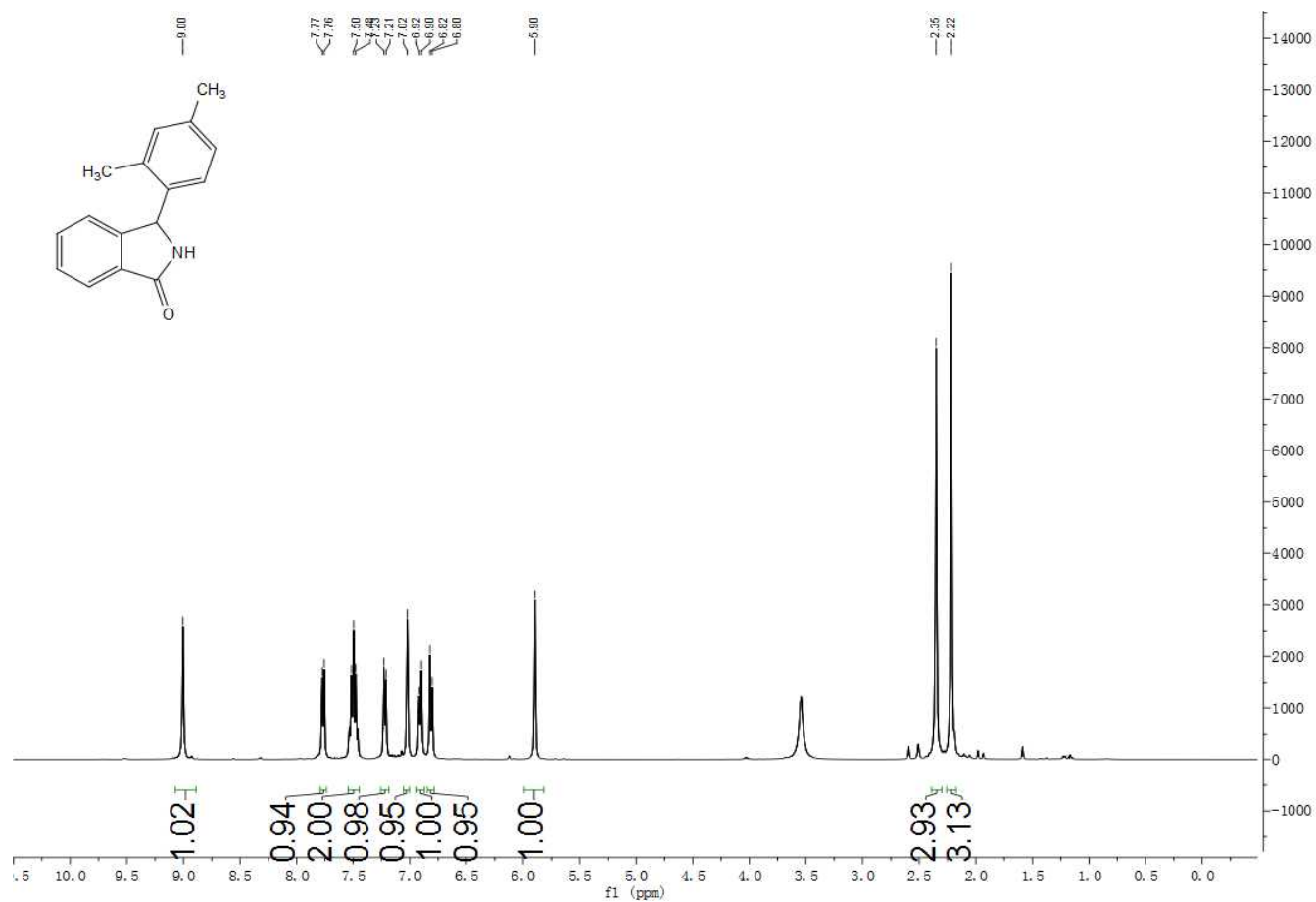
3-(2,5-dimethoxyphenyl)isoindolin-1-one (3m)

^{13}C NMR



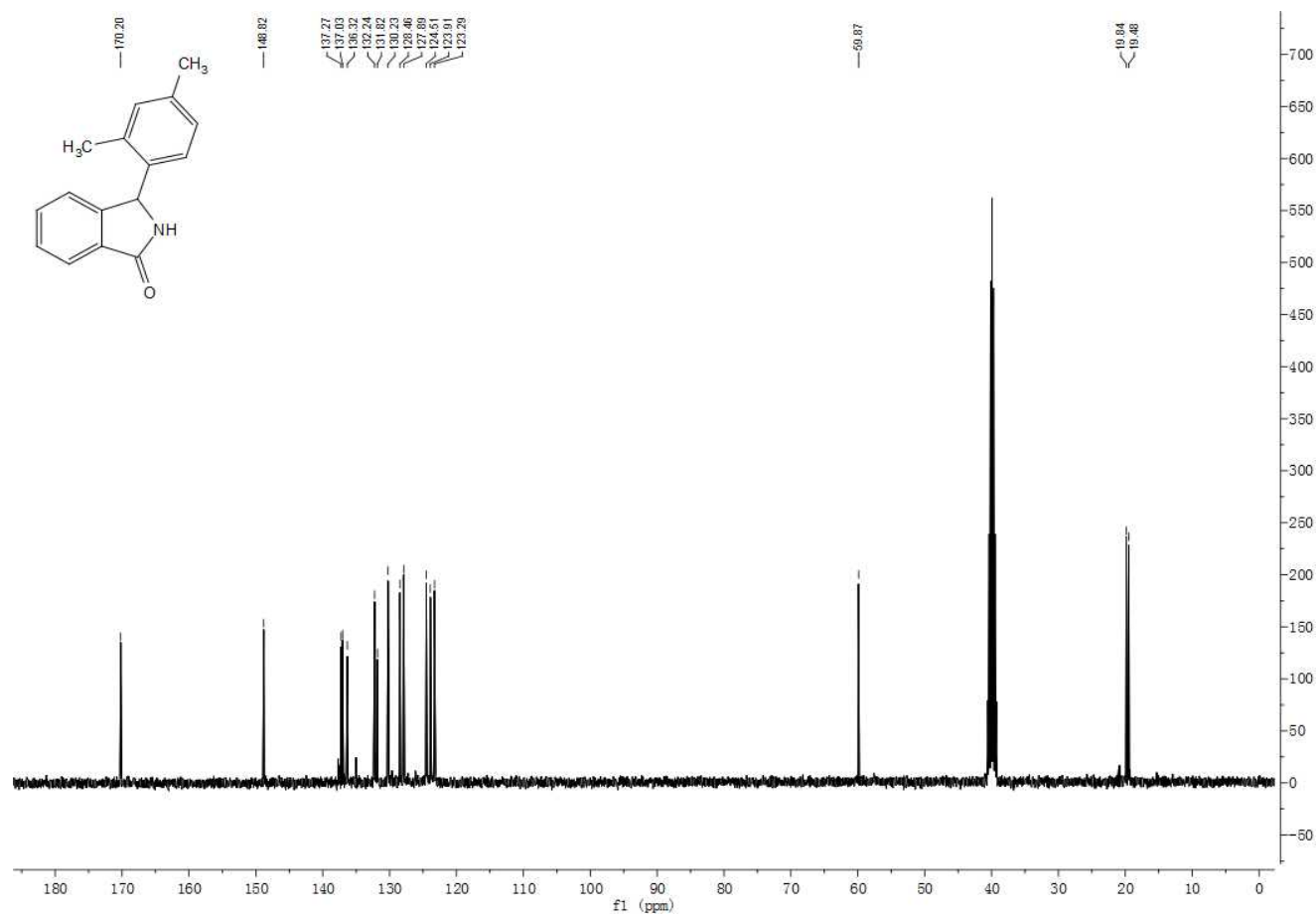
3-(2,4-dimethylphenyl)isoindolin-1-one (3n)

^1H NMR



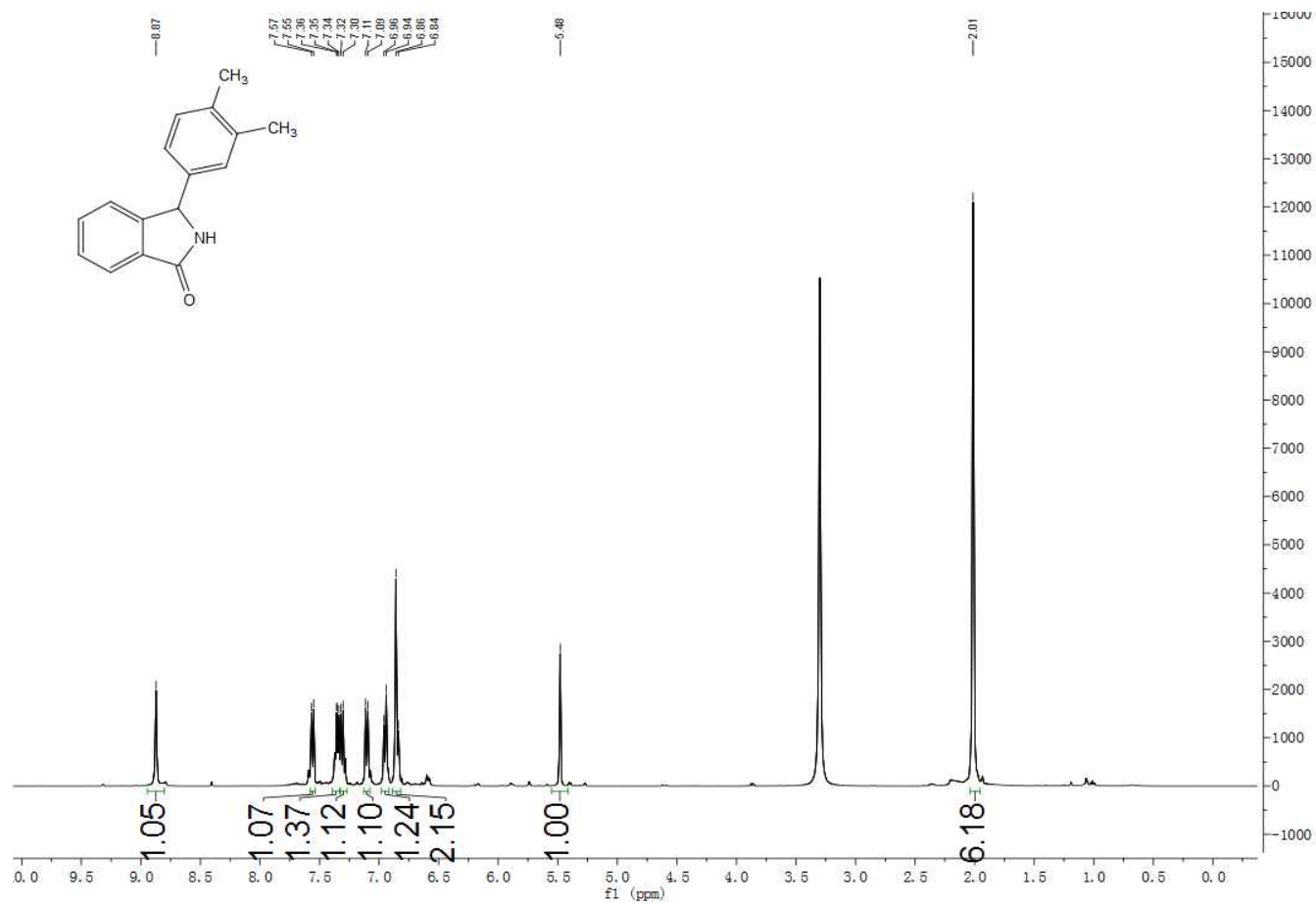
3-(2,4-dimethylphenyl)isoindolin-1-one (3n)

^{13}C NMR



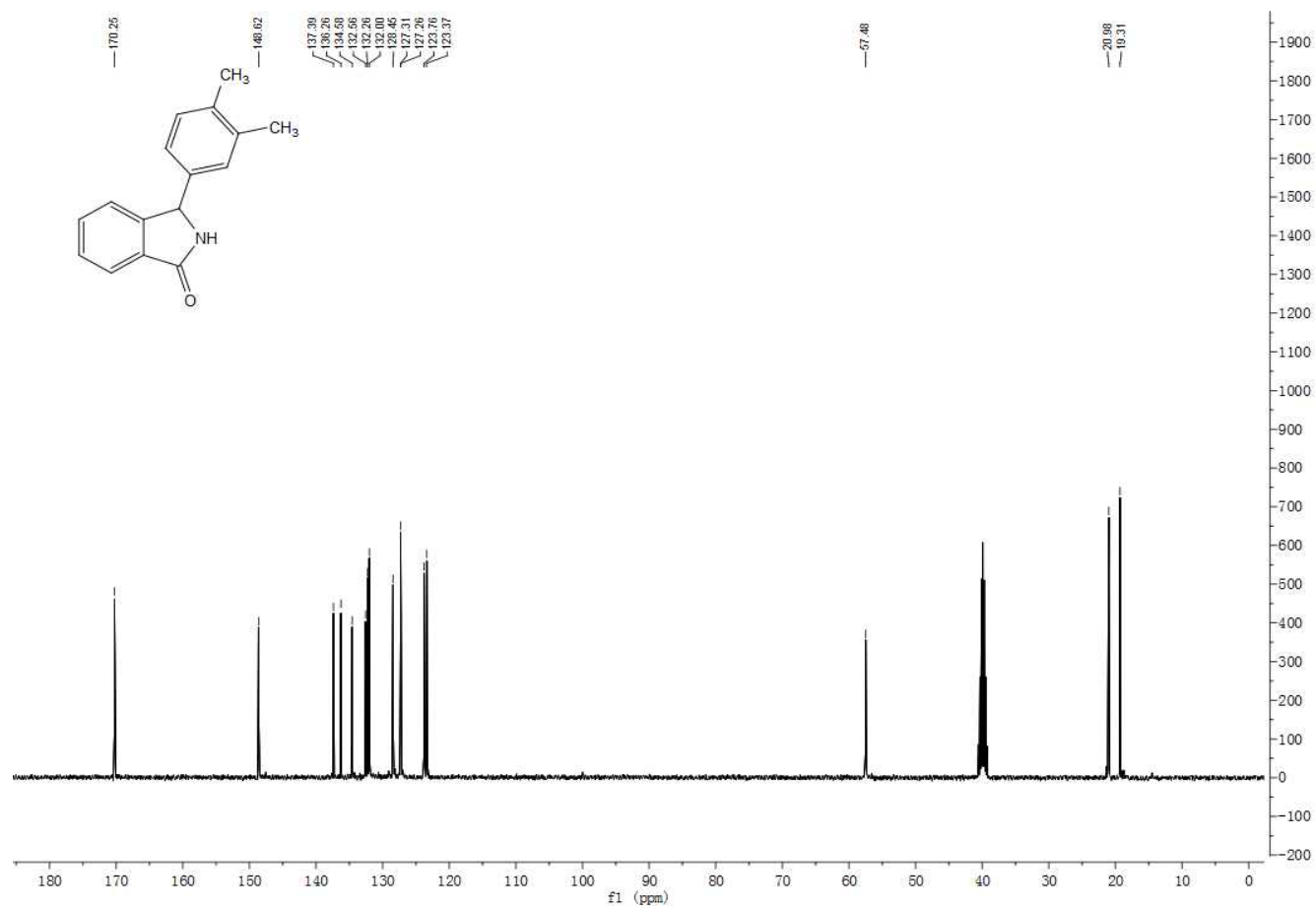
3-(3,4-dimethylphenyl)isoindolin-1-one (3o)

^1H NMR



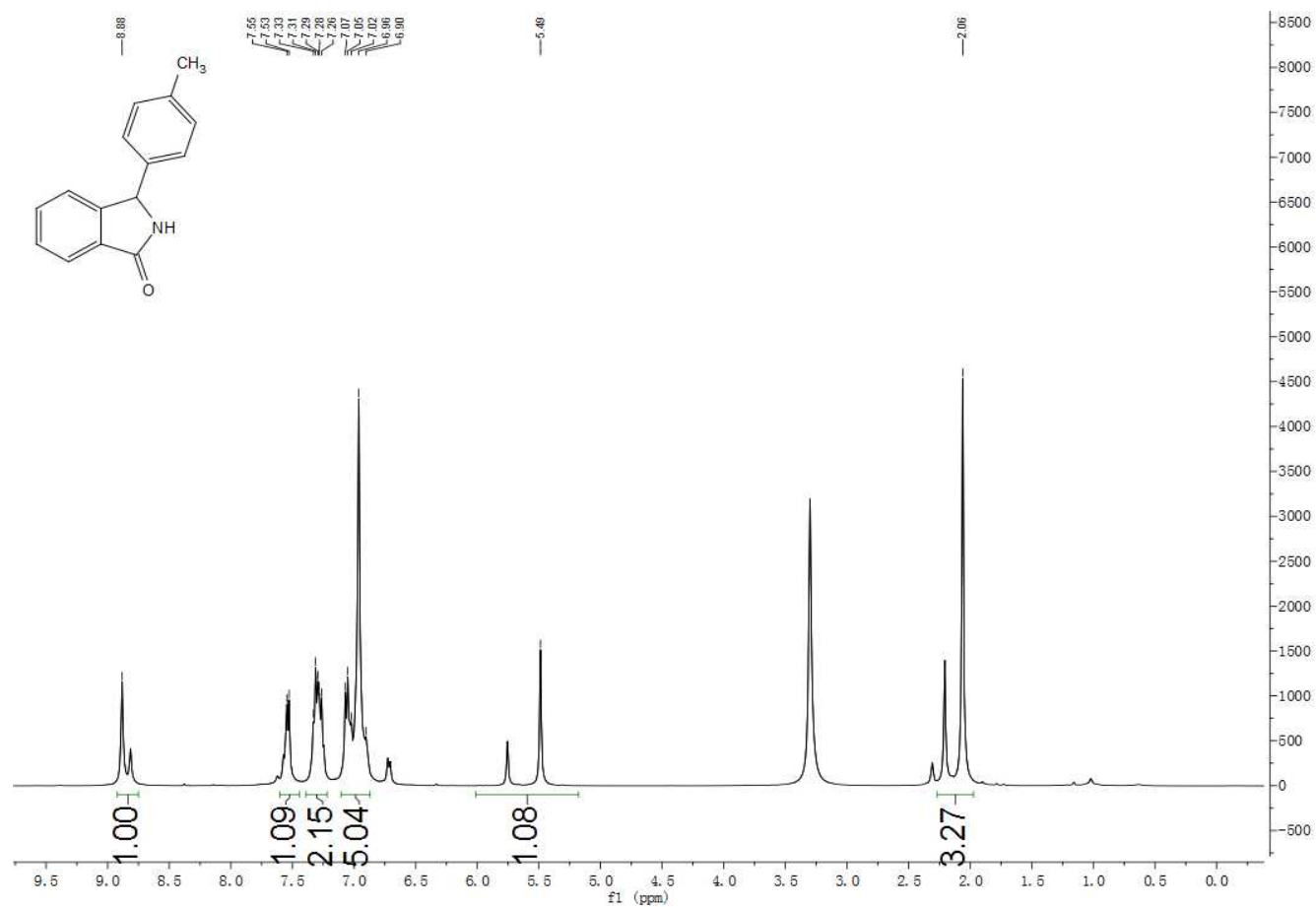
3-(3,4-dimethylphenyl)isoindolin-1-one (3o)

^{13}C NMR



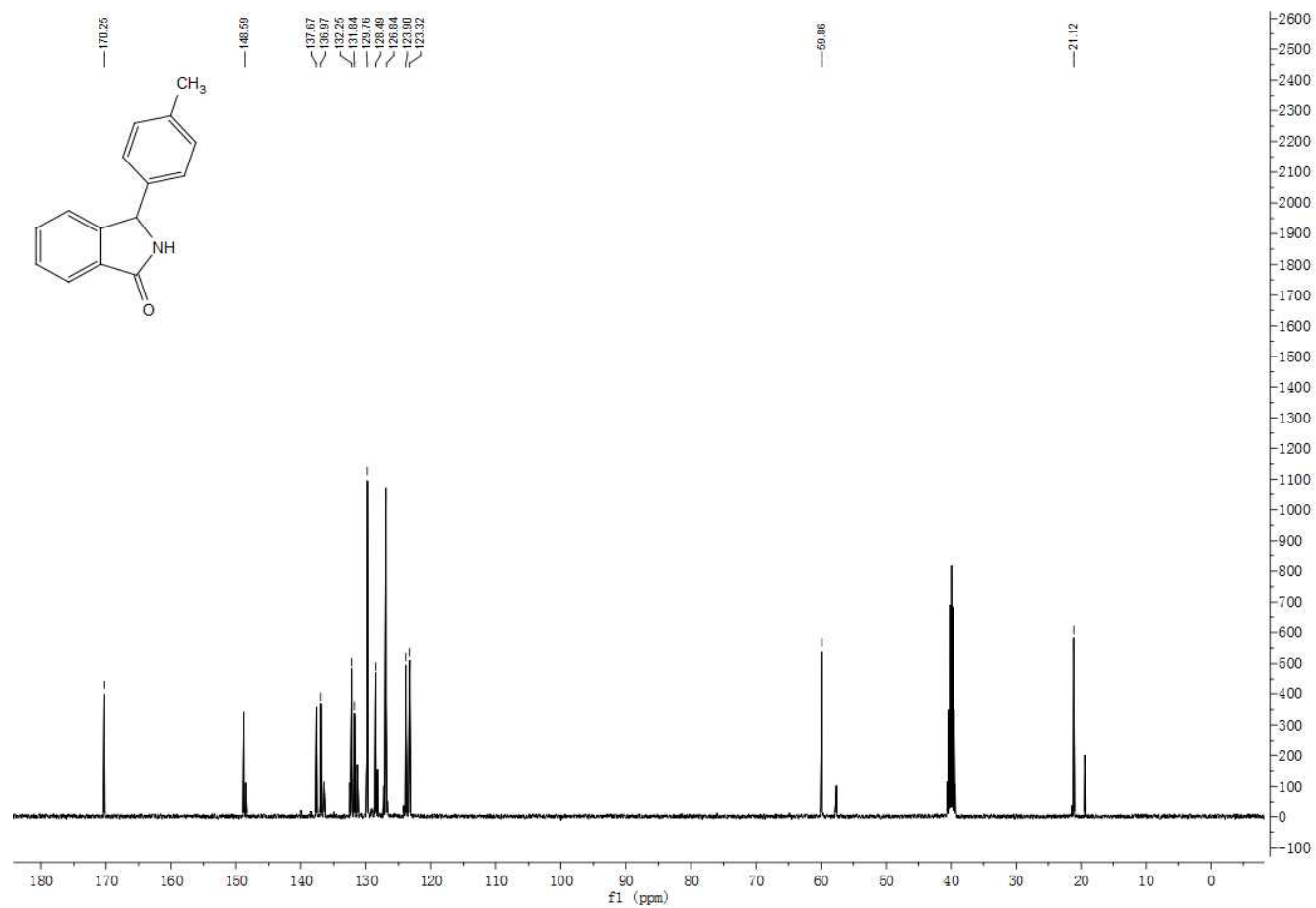
3-(p-tolyl)isoindolin-1-one (3p)

^1H NMR



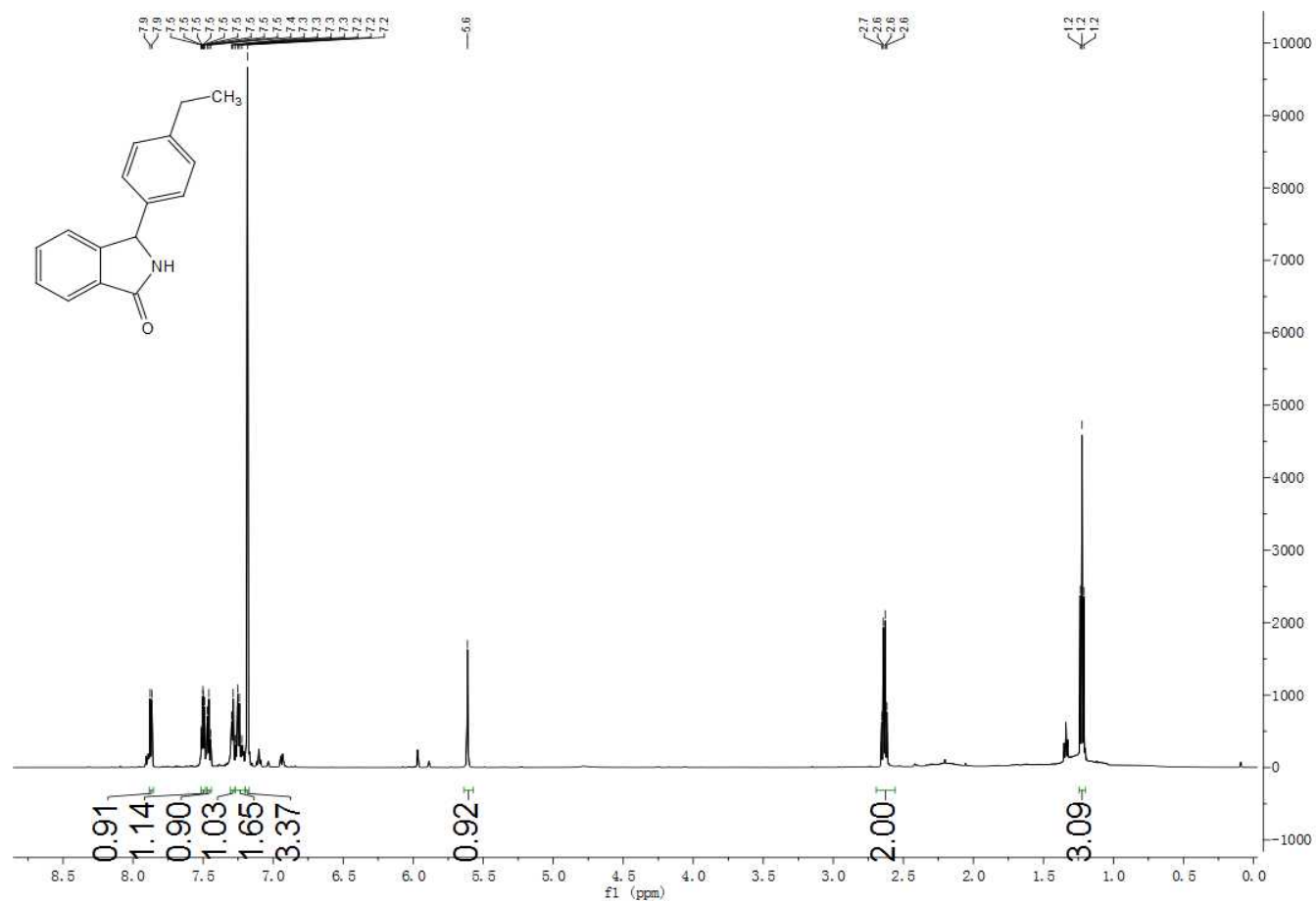
3-(p-tolyl)isoindolin-1-one (3p)

^{13}C NMR



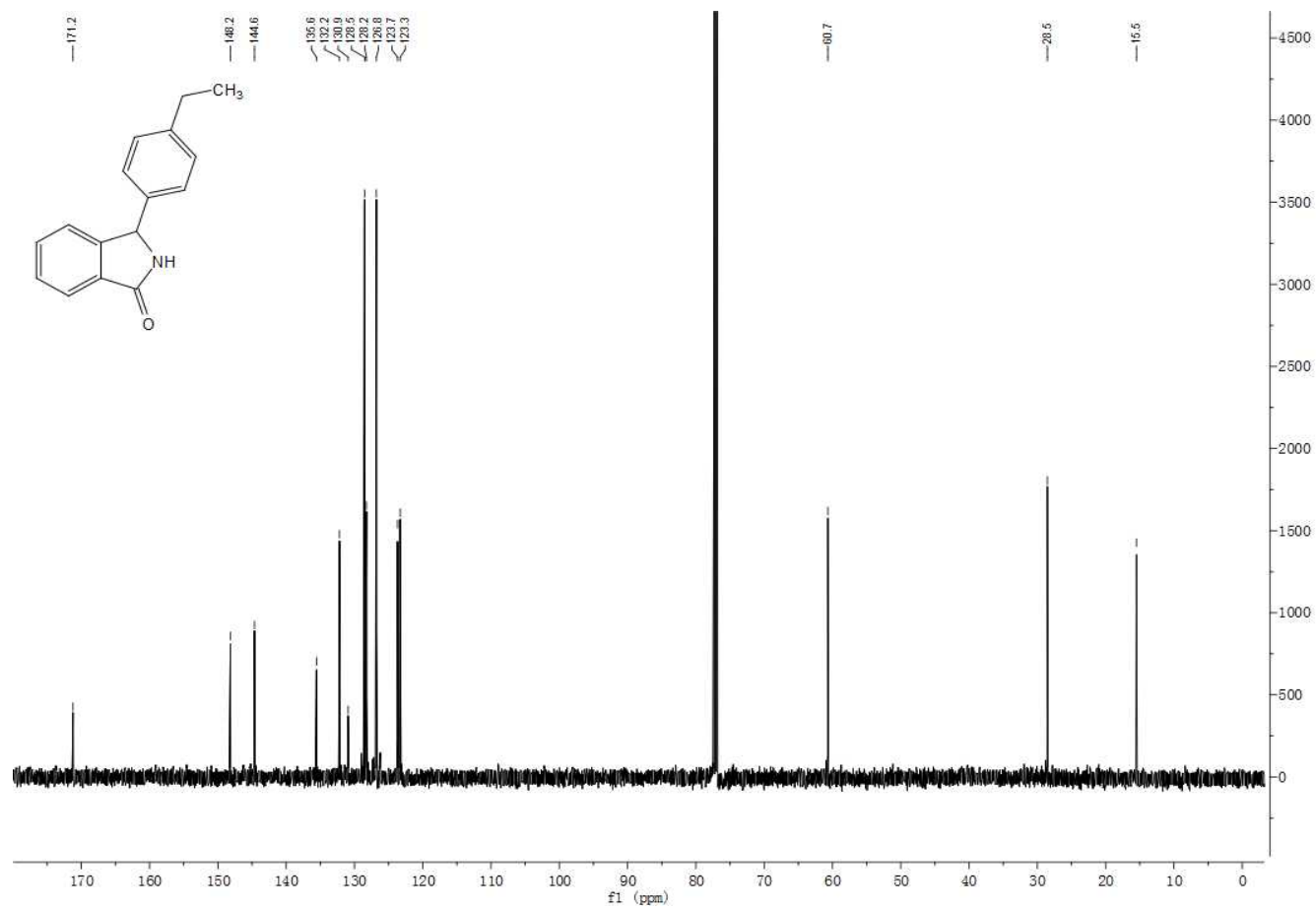
3-(4-ethylphenyl)isoindolin-1-one (3q)

^1H NMR



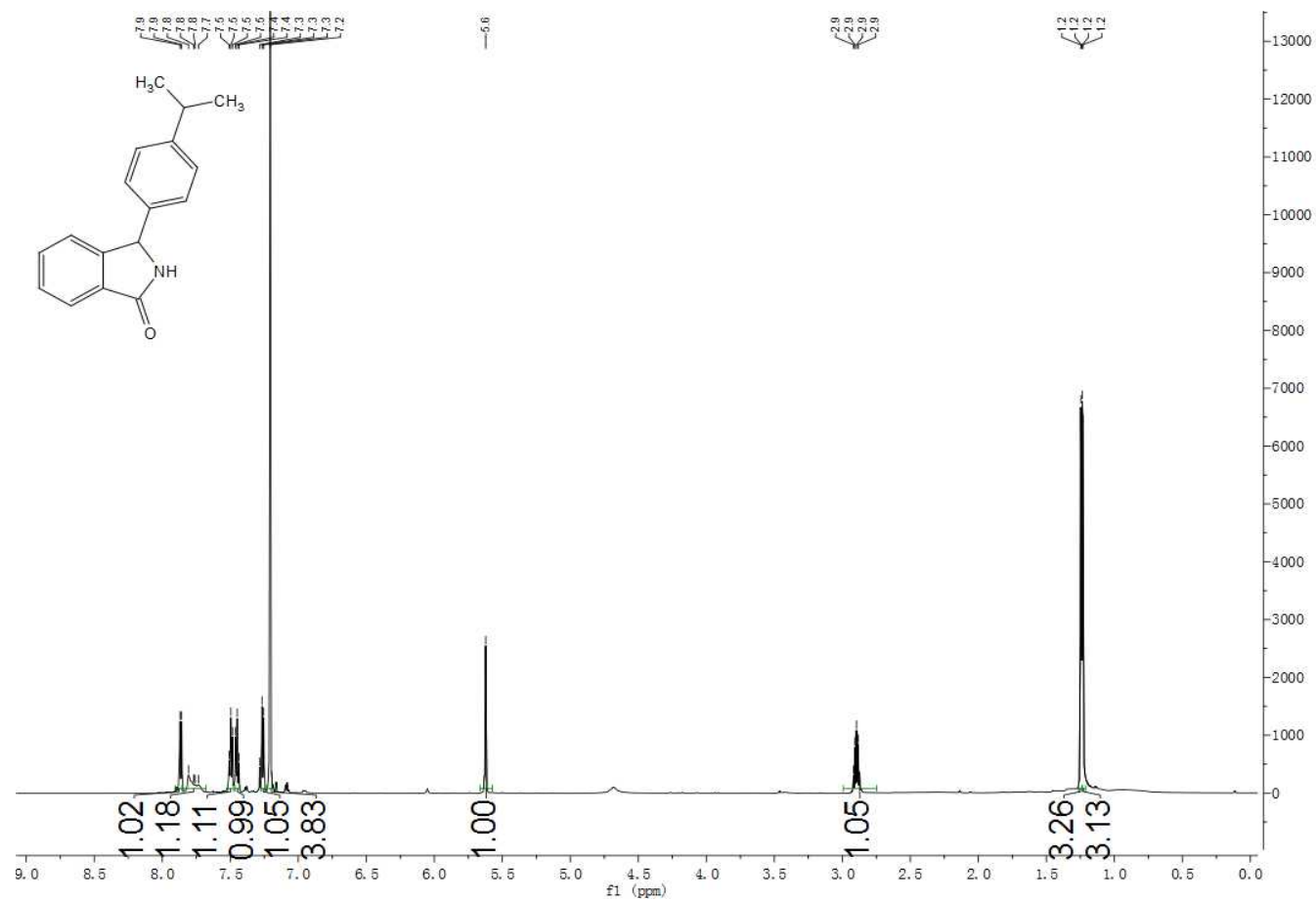
3-(4-ethylphenyl)isoindolin-1-one (3q)

^{13}C NMR



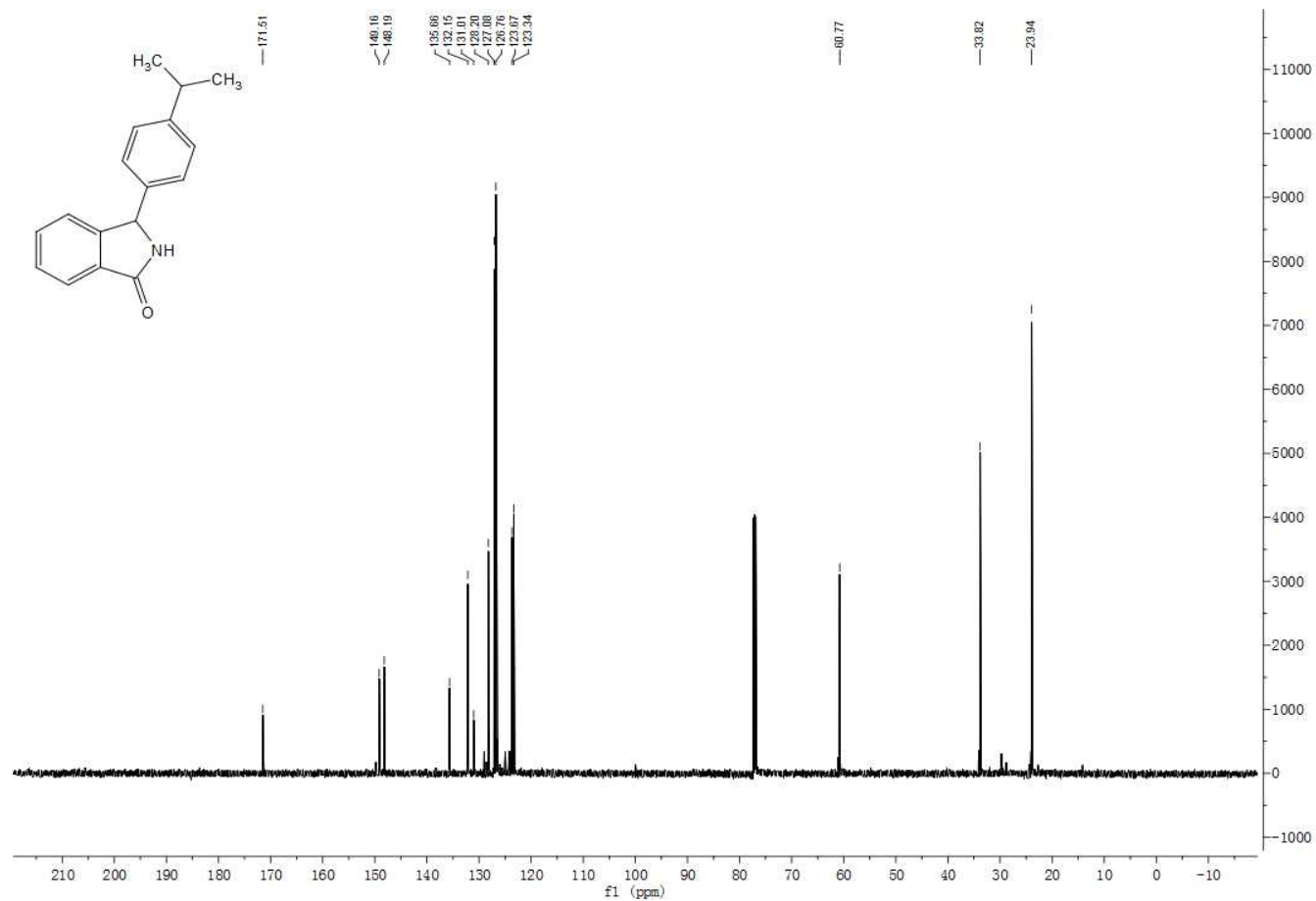
3-(4-isopropylphenyl)isoindolin-1-one (3r)

¹H NMR



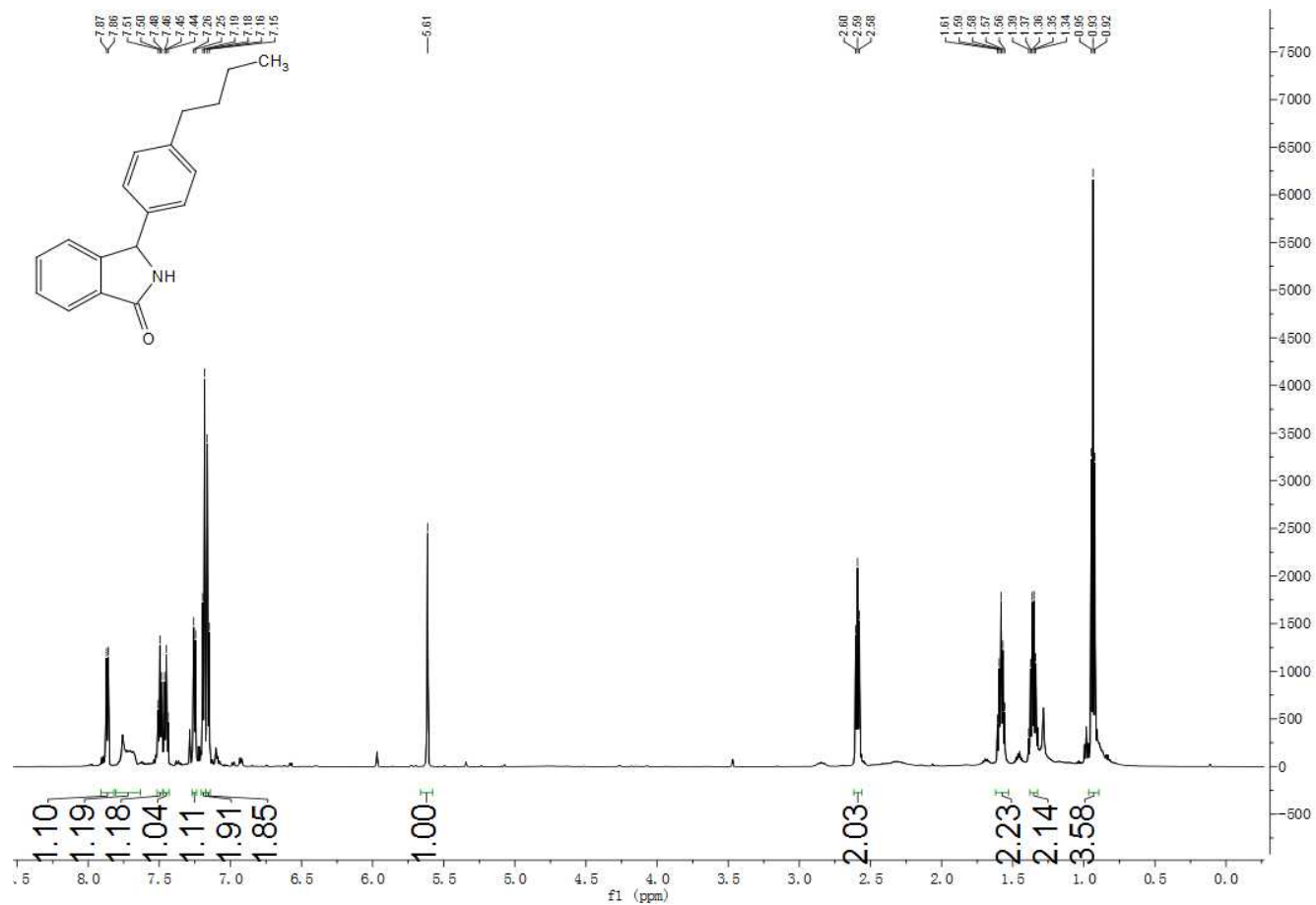
3-(4-isopropylphenyl)isoindolin-1-one (3r)

^{13}C NMR



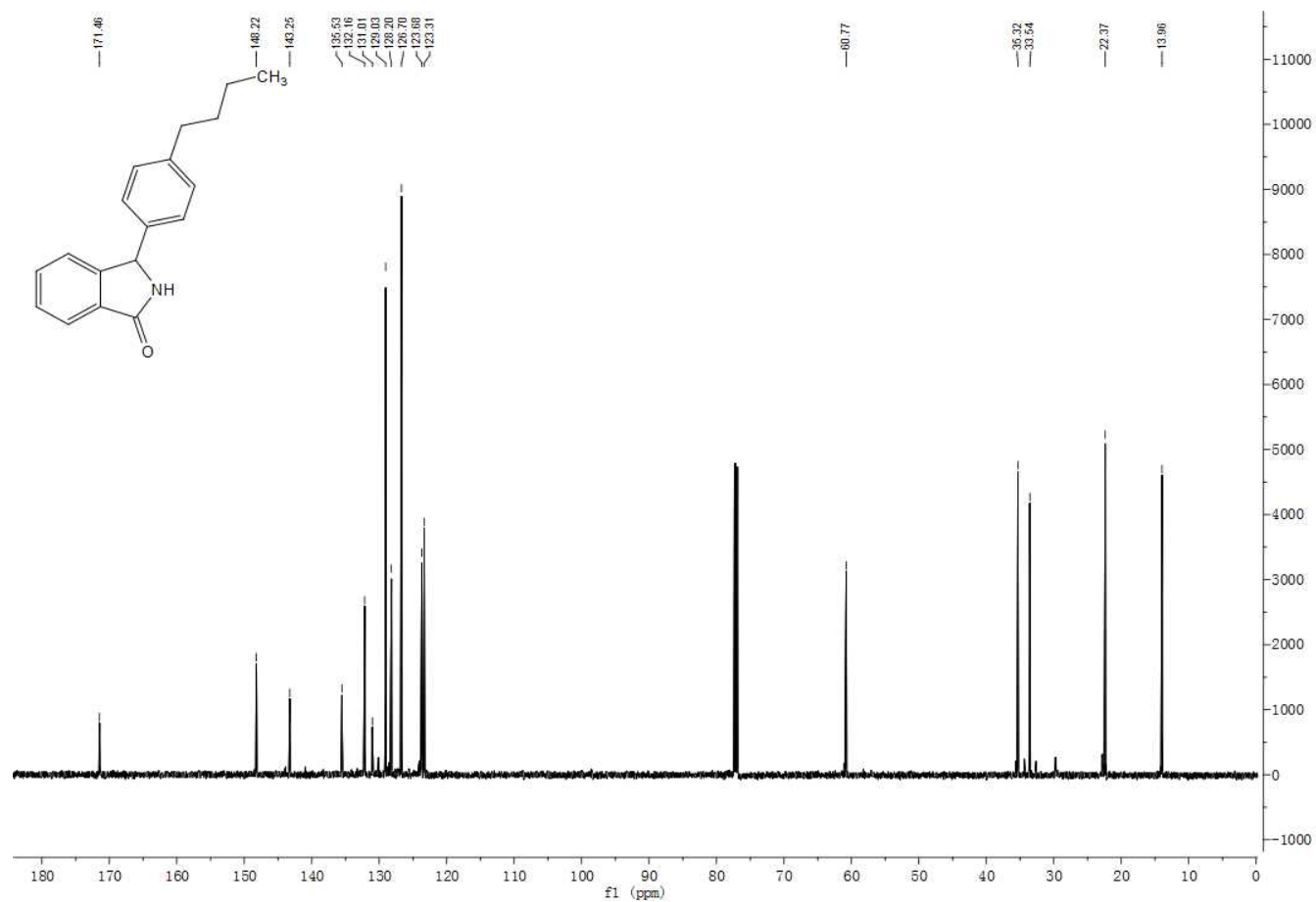
3-(4-butylphenyl)isoindolin-1-one (3s)

^1H NMR



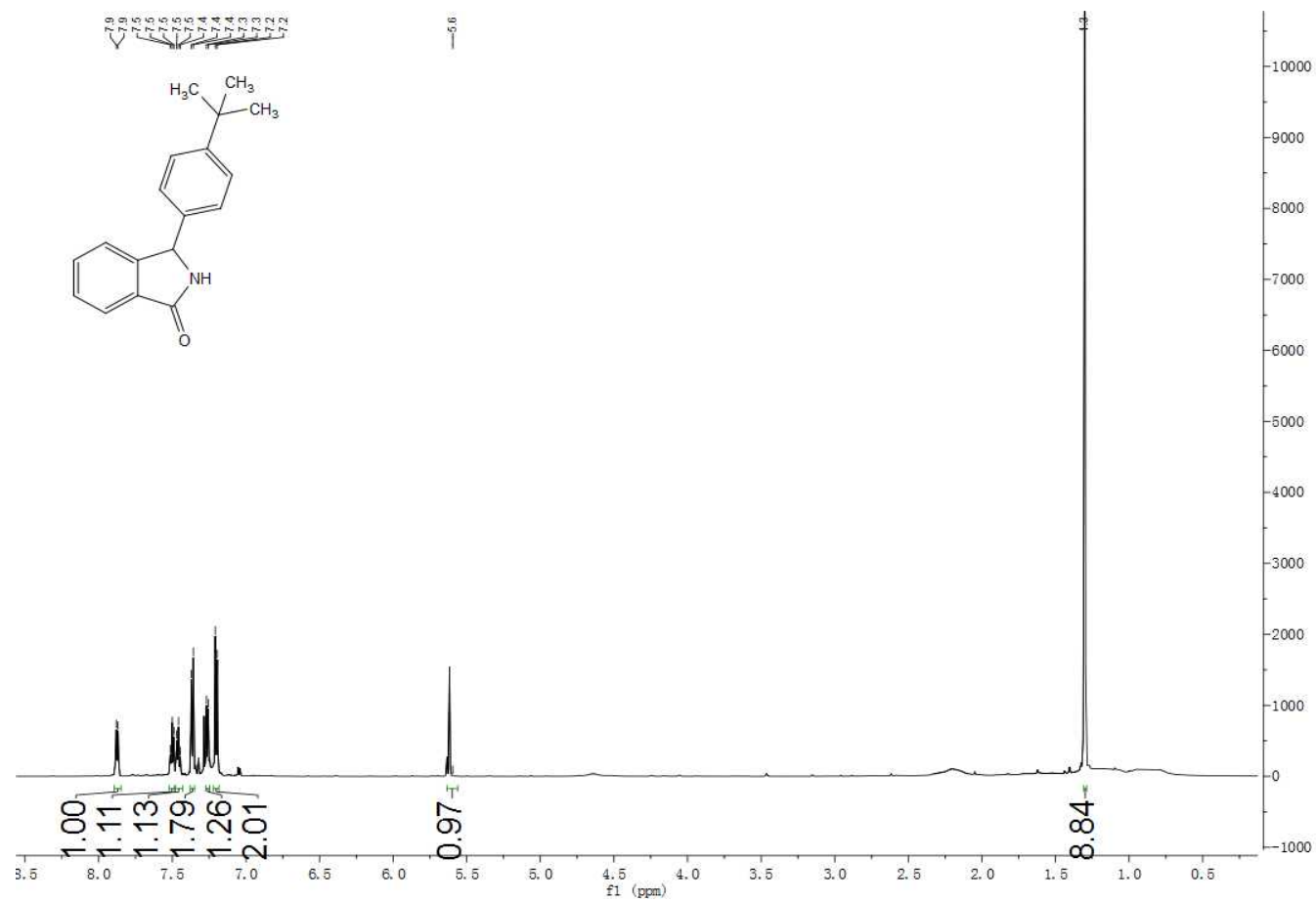
3-(4-butylphenyl)isoindolin-1-one (3s)

^{13}C NMR



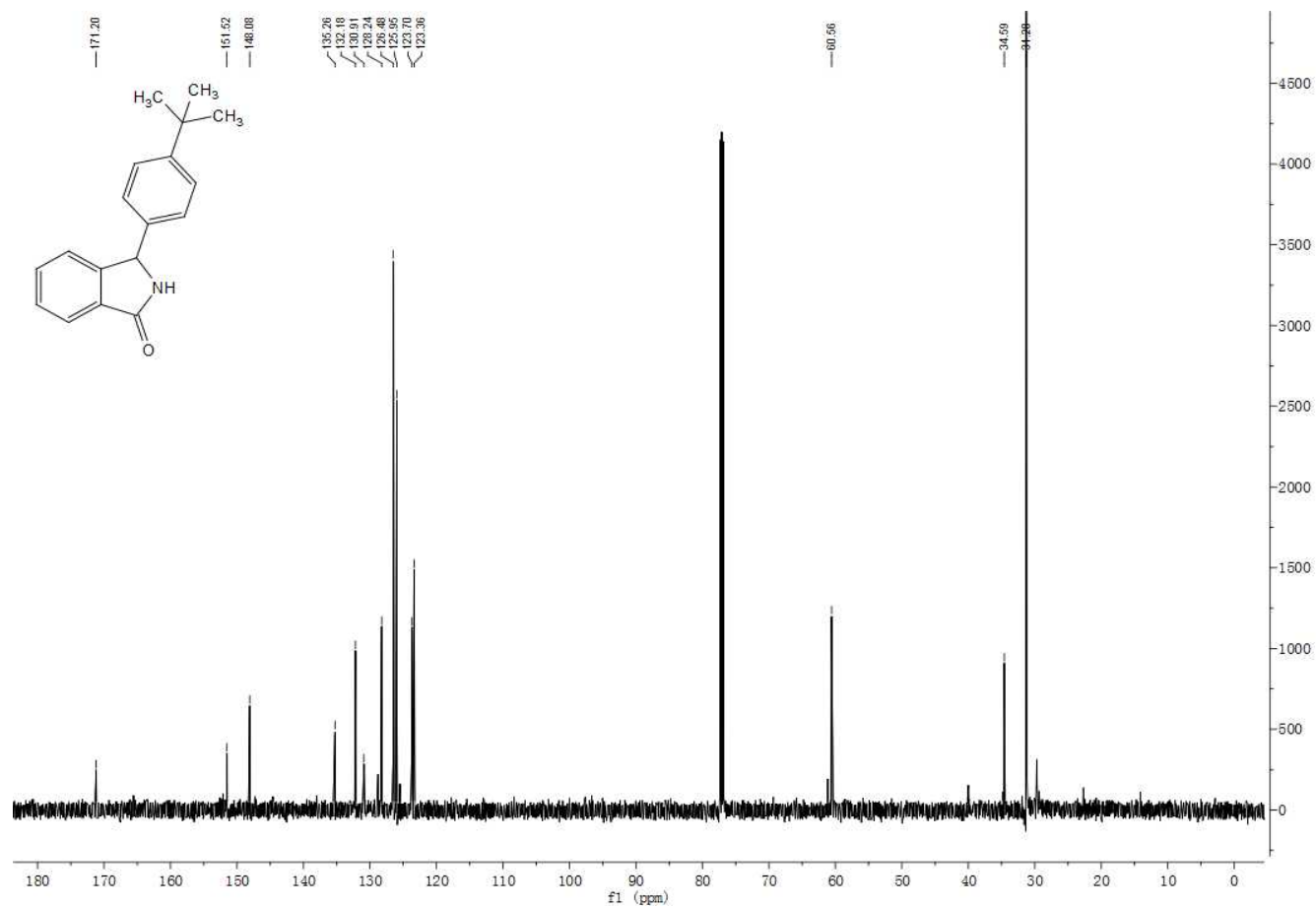
3-(4-(tert-butyl)phenyl)isoindolin-1-one (3t)

^1H NMR



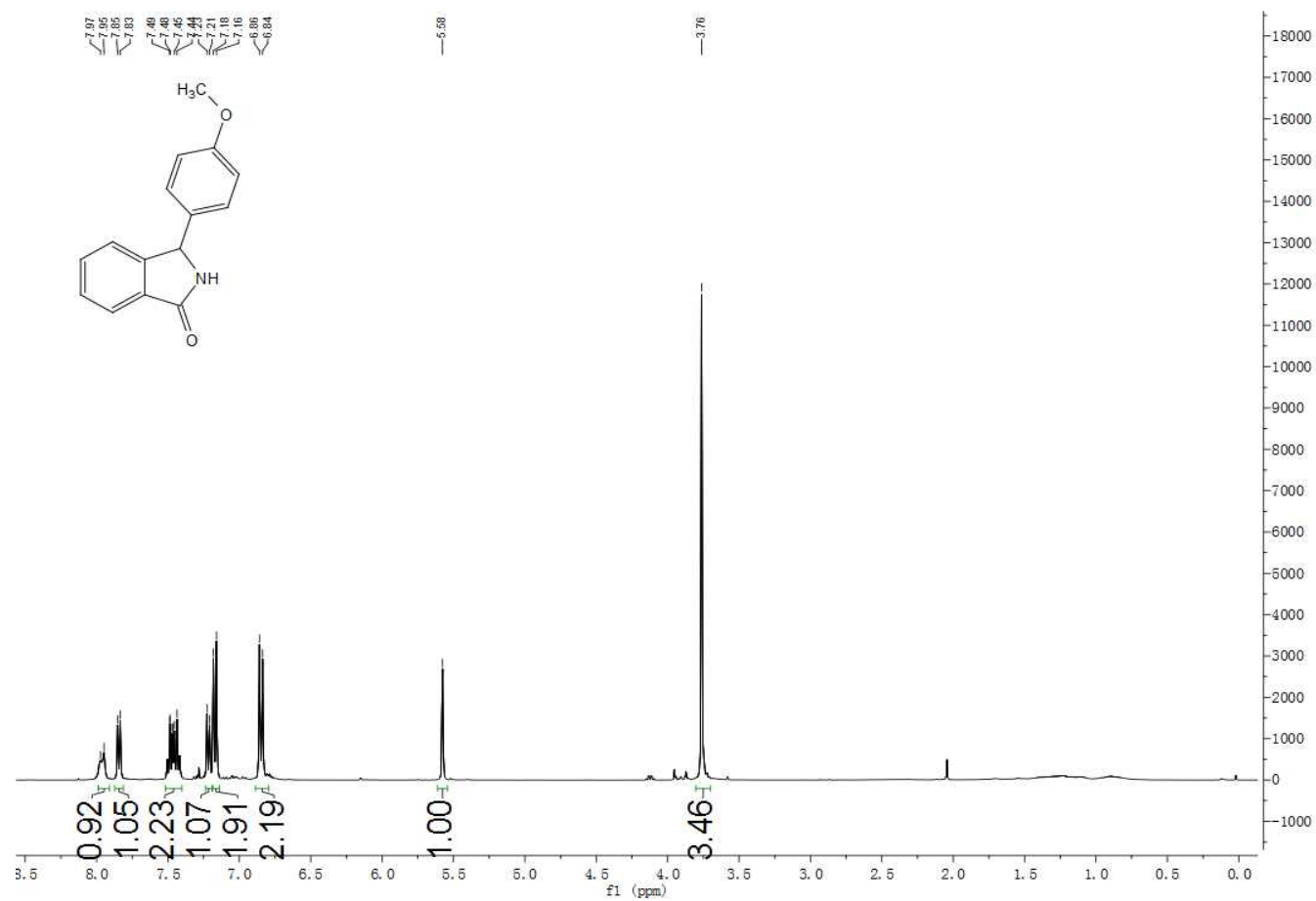
3-(4-(tert-butyl)phenyl)isoindolin-1-one (3t)

^{13}C NMR



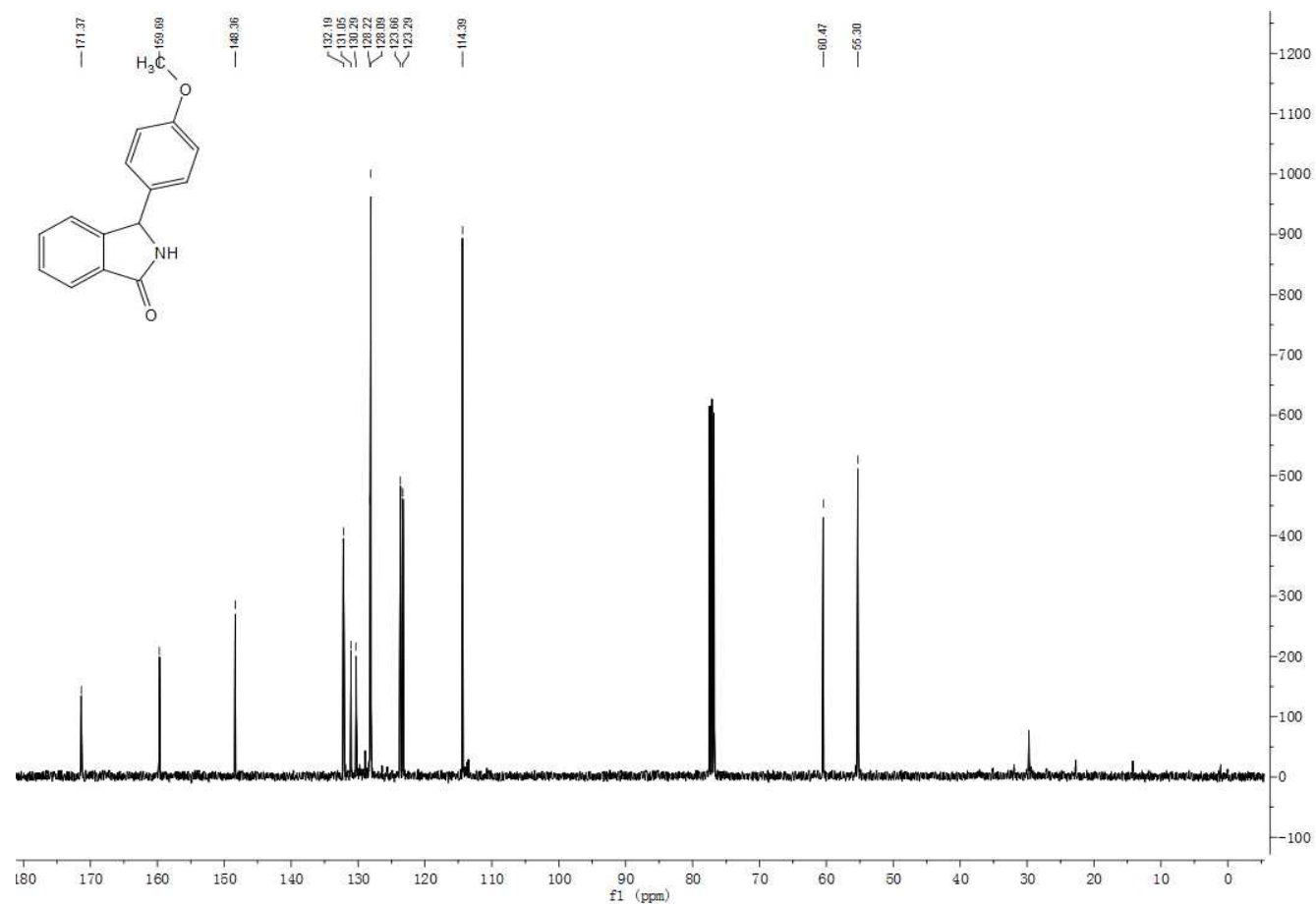
3-(4-methoxyphenyl)isoindolin-1-one (3u)

^1H NMR



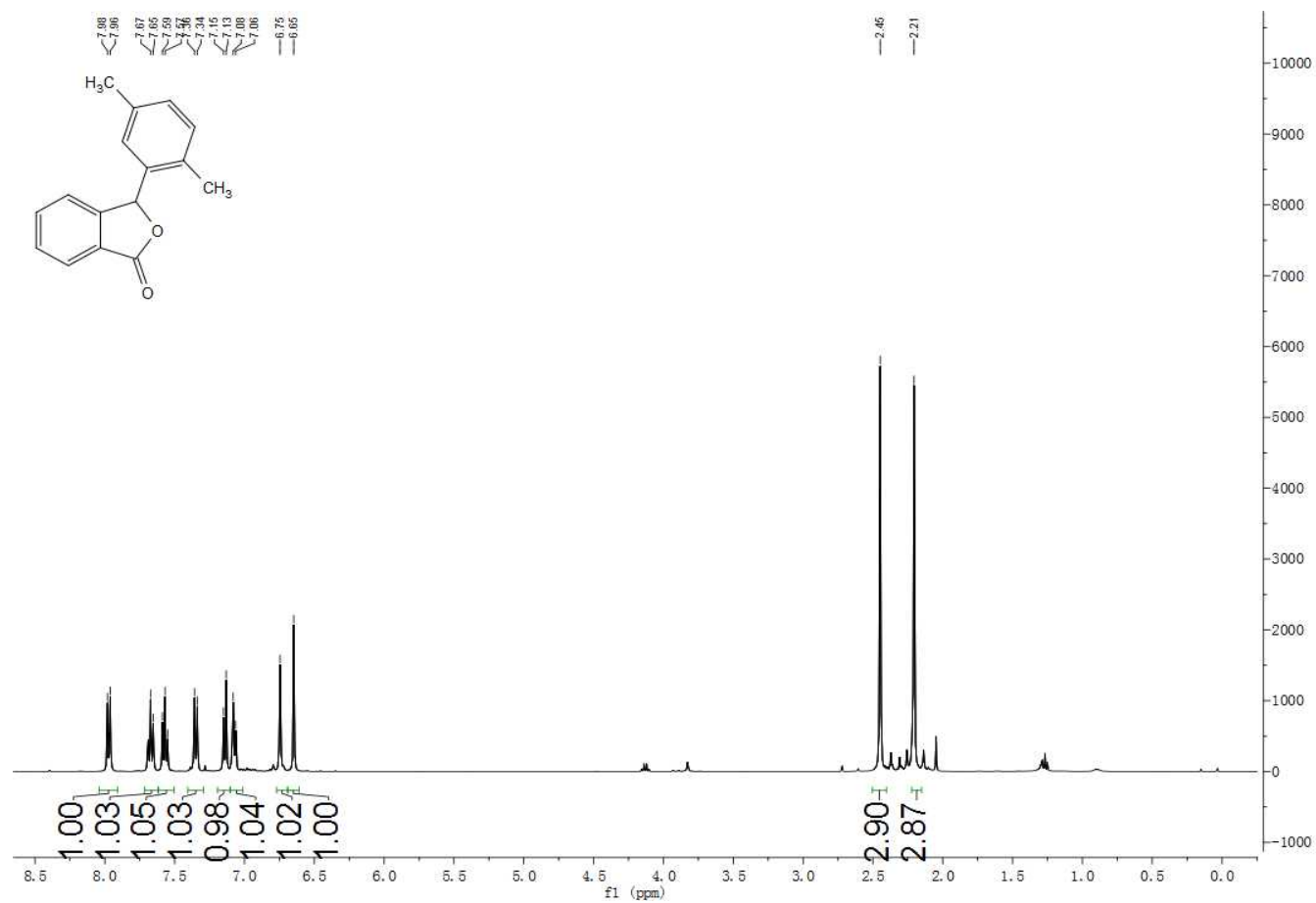
3-(4-methoxyphenyl)isoindolin-1-one (3u)

^{13}C NMR



3-(2,5-dimethylphenyl)isobenzofuran-1(3H)-one (4a)

^1H NMR



3-(2,5-dimethylphenyl)isobenzofuran-1(3H)-one (4a)

^{13}C NMR

