Supporting Information

Cobalt(III)-Catalyzed C-C Coupling of Arenes with *7*-Oxabenzonorbornadiene and *2*-Vinyloxirane via C-H Activation

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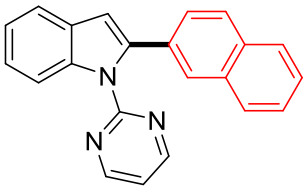
Content

I. General

All chemicals were obtained from commercial sources and were used as received unless otherwise noted. *N*-pyrimidinylindoles,[1] *7*-Oxabenzonorbornadienes,[2] $[Cp^*CoCl_2]_2$,[3] $[Cp^*Co(MeCN)_3](SbF_6)_2$[4] were prepared by following literature reports. All reactions were carried out using Schlenk techniques or in an N_2-filled glovebox. NMR Spectra were recorded on a 400 MHz NMR spectrometer in the solvent indicated. The chemical shift is given in dimensionless δ values and is frequency referenced relative to TMS in ^1H and ^{13}C NMR spectroscopy. HRMS data were obtained on a Thermo Scientific LTQ Orbitrap Discovery spectrometer (Bremen, Germany). Column chromatography was performed on silica gel (300-400 mesh) using Ethyl acetate (EA)/petroleum ether (PE).

II. General procedures for the synthesis of compound 3

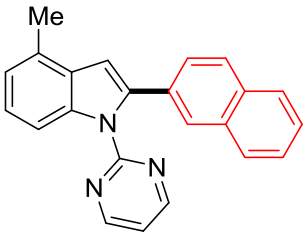
Reaction conditions: indole (0.2 mmol), *7*-oxabenzonorbornadiene (0.4 mmol), $[Cp^*CoCl_2]_2$ (5 mol %), $AgSbF_6$ (30 mol %), HOAc (2 equiv), and DCE (2 mL) were charged into the pressure tube. The reaction mixture was stirred under N_2 at 50 ℃ for 12 h. After the solvent was removed under reduced pressure, the residue was purified by silica gel chromatography using PE/EA to afford the product **3**.



2-(Naphthalen-2-yl)-1-(pyrimidin-2-yl)-1H-indole (**3aa**)

3aa was obtained according to the general procedure in 86% yield (52.1 mg). white solid;

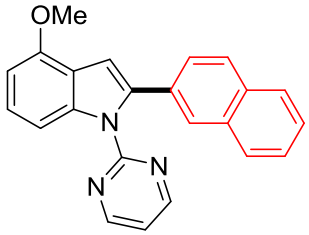
^1H NMR (400 MHz, $CDCl_3$) δ 8.59 (d, J = 4.5 Hz, 2H), 8.20 (d, J = 7.9 Hz, 1H), 7.88 (s, 1H), 7.79 – 7.76 (m, 2H), 7.68 (t, J = 9.0 Hz, 2H), 7.49 – 7.40 (m, 2H), 7.32 – 7.22 (m, 3H), 7.03 (t, J = 4.9 Hz, 1H), 6.90 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.3, 158.2, 140.6, 138.3, 133.4, 132.5, 131.6, 129.5, 128.2, 127.7, 127.5, 126.7, 126.6, 126.3, 126.1, 123.7, 122.3, 120.8, 117.6, 113.0, 108.9. HRMS: $[M + H]^+$ calculated for $C_{22}H_{16}N_3^+$: 322.1339, found: 322.1341.



4-Methyl-2-(naphthalen-2-yl)-1-(pyrimidin-2-yl)-1H-indole (**3ba**)

3ba was obtained according to the general procedure in 77% yield (51.7 mg). white solid;

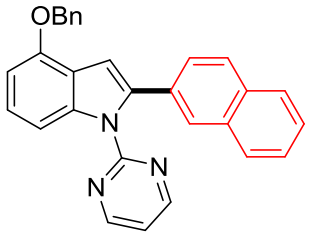
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.58 (d, J = 4.6 Hz, 2H), 8.02 (d, J = 8.3 Hz, 1H), 7.89 (s, 1H), 7.79 – 7.76 (m, 2H), 7.68 (d, J = 8.4 Hz, 1H), 7.48 – 7.39 (m, 2H), 7.27 (d, J = 8.3 Hz, 1H), 7.21 (t, J = 7.7 Hz, 1H), 7.05 (d, J = 7.1 Hz, 1H), 7.01 (t, J = 4.6 Hz, 1H), 6.94 (s, 1H), 2.61 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.3, 158.28, 140.0, 138.1, 133.4, 132.5, 131.8, 130.2, 129.2, 128.2, 127.7, 127.5, 126.6, 126.3, 126.0, 123.9, 122.6, 117.6, 110.6, 107.4, 18.8. HRMS: $[M + H]^+$ calculated for $C_{23}H_{18}N_3^+$: 336.1495, found: 336.1497.



4-Methoxy-2-(naphthalen-2-yl)-1-(pyrimidin-2-yl)-1H-indole (**3ca**)

3ca was obtained according to the general procedure in 70% yield (49.2 mg). white solid;

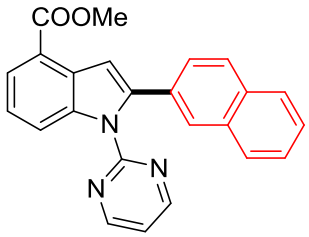
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.59 (d, J = 4.7 Hz, 2H), 7.86 (s, 1H), 7.79 – 7.74 (m, 3H), 7.67 (d, J = 8.5 Hz, 1H), 7.52 – 7.37 (m, 2H), 7.31 – 7.17 (m, 2H), 7.09 – 6.97 (m, 2H), 6.67 (d, J = 7.8 Hz, 1H), 3.97 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.31, 158.3, 153.2, 139.6, 139.1, 133.4, 132.4, 131.6, 128.2, 127.7, 127.4, 126.6, 126.6, 126.2, 126.0, 124.6, 120.0, 117.7, 106.2, 105.8, 102.4, 55.5. HRMS: $[M + H]^+$ calculated for $C_{23}H_{18}N_3O^+$: 352.1444, found: 352.1448.



4-(Benzyloxy)-2-(naphthalen-2-yl)-1-(pyrimidin-2-yl)-1H-indole (**3da**)

3da was obtained according to the general procedure in 83% yield (70.9 mg). white solid;

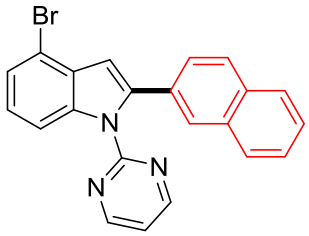
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.61 (d, J = 4.8 Hz, 2H), 7.87 (s, 1H), 7.80 – 7.74 (m, 3H), 7.68 (d, J = 8.5 Hz, 1H), 7.52 (d, J = 7.3 Hz, 2H), 7.47 – 7.36 (m, 4H), 7.34 – 7.30 (m, 1H), 7.26 (d, J = 8.5 Hz, 1H), 7.23 – 7.17 (m, 1H), 7.11 (s, 1H), 7.05 (t, J = 4.8 Hz, 1H), 6.74 (d, J = 7.9 Hz, 1H), 5.26 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.3, 152.3, 139.7, 139.1, 137.5, 133.4, 132.4, 131.6, 128.6, 128.2, 127.9, 127.7, 127.5, 127.4, 126.6, 126.57, 126.2, 126.0, 124.5, 120.4, 117.7, 106.4, 106.1, 103.9, 70.1. One signal is missing due to overlap. HRMS: $[M + H]^+$ calculated for $C_{29}H_{22}N_3O^+$: 428.1757, found: 428.1754.



Methyl 2-(naphthalen-2-yl)-1-(pyrimidin-2-yl)-1H-indole-4-carboxylate (**3ea**)

3ea was obtained according to the general procedure in 80% yield (60.1 mg). white solid;

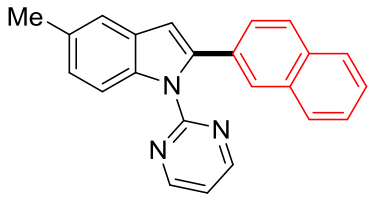
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.62 (d, J = 4.6 Hz, 2H), 8.37 (d, J = 8.2 Hz, 1H), 8.02 (d, J = 7.5 Hz, 1H), 7.94 (s, 1H), 7.85 – 7.74 (m, 2H), 7.70 (d, J = 8.5 Hz, 1H), 7.62 (s, 1H), 7.47 (d, J = 4.1 Hz, 2H), 7.33 (t, J = 7.9 Hz, 1H), 7.27 (d, J = 8.3 Hz, 1H), 7.09 (t, J = 4.6 Hz, 1H), 4.01 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.8, 158.5, 158.0, 142.7, 139.0, 133.4, 132.7, 131.1, 129.3, 128.3, 127.7, 127.6, 127.3, 126.5, 126.4, 126.3, 125.4, 122.9, 121.6, 118.2, 117.7, 109.4, 52.0. HRMS: $[M + H]^+$ calculated for $C_{24}H_{18}N_3O_2^+$: 380.1394, found: 380.1393.



4-Bromo-2-(naphthalen-2-yl)-1-(pyrimidin-2-yl)-1H-indole (**3fa**)

3fa was obtained according to the general procedure in 84% yield (67.0 mg). white solid;

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.62 (d, J = 4.7 Hz, 2H), 8.11 (d, J = 8.3 Hz, 1H), 7.90 (s, 1H), 7.80 – 7.77 (m, 2H), 7.70 (d, J = 8.5 Hz, 1H), 7.54 – 7.44 (m, 2H), 7.41 (d, J = 7.7 Hz, 1H), 7.25 (d, J = 9.3 Hz, 1H), 7.15 (t, J = 8.0 Hz, 1H), 7.09 (t, J = 4.7 Hz, 1H), 6.97 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.4, 158.0, 141.3, 138.4, 133.3, 132.6, 131.0, 130.0, 128.2, 127.7, 127.6, 127.0, 126.4, 126.37, 126.3, 125.1, 124.5, 118.1, 114.5, 112.2, 108.3. HRMS: $[M + H]^+$ calculated for $C_{22}H_{15}BrN_3^+$: 400.0444, found: 400.0447.

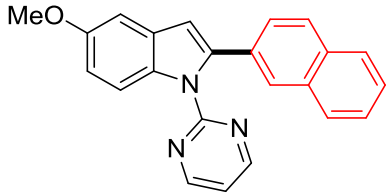


5-Methyl-2-(naphthalen-2-yl)-1-(pyrimidin-2-yl)-1H-indole (**3ga**)

3ga was obtained according to the general procedure in 82% yield (55.0 mg). white solid;

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.59 (d, J = 4.8 Hz, 2H), 8.10 (d, J = 8.5 Hz, 1H), 7.88 (s, 1H), 7.78 (dd, J = 9.5, 6.5 Hz, 2H), 7.69 (d, J = 8.5 Hz, 1H), 7.46 – 7.44 (m, 3H), 7.27 (dd, J = 8.5, 1.7 Hz, 1H), 7.12 (dd, J = 8.5, 1.2 Hz, 1H), 7.04 (t, J = 4.8 Hz, 1H), 6.83 (s, 1H), 2.47 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.3, 158.2, 140.5, 136.6, 133.4, 132.5, 131.8, 131.6, 129.7, 128.2,

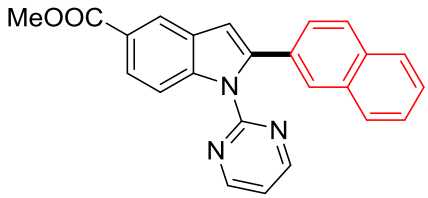
127.7, 127.4, 126.6, 126.5, 126.2, 126.0, 125.2, 120.6, 117.4, 112.8, 108.8, 21.4. HRMS: $[M + H]^+$ calculated for $C_{23}H_{18}N_3^+$: 336.1495, found: 336.1496.



5-Methoxy-2-(naphthalen-2-yl)-1-(pyrimidin-2-yl)-1H-indole (**3ha**)

3ha was obtained according to the general procedure in 58% yield (40.7 mg). white solid;

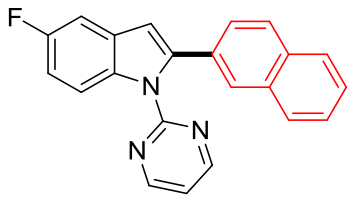
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.57 (d, J = 4.8 Hz, 2H), 8.14 (d, J = 9.0 Hz, 1H), 7.88 (s, 1H), 7.79 (dd, J = 8.9, 4.9 Hz, 2H), 7.69 (d, J = 8.5 Hz, 1H), 7.48 – 7.43 (m, 2H), 7.27 (d, J = 8.5 Hz, 1H), 7.12 (d, J = 2.2 Hz, 1H), 7.02 (t, J = 4.7 Hz, 1H), 6.94 (dd, J = 9.0, 2.3 Hz, 1H), 6.83 (s, 1H), 3.88 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.2, 155.7, 141.1, 133.3, 133.2, 132.5, 131.8, 130.1, 128.2, 127.7, 127.4, 126.6, 126.6, 126.2, 126.0, 117.4, 114.1, 113.0, 108.9, 102.7, 55.8. One signal is missing due to overlap. HRMS: $[M + H]^+$ calculated for $C_{23}H_{18}N_3O^+$: 352.1444, found: 352.1448.



Methyl 2-(naphthalen-2-yl)-1-(pyrimidin-2-yl)-1H-indole-5-carboxylate (**3ia**)

3ia was obtained according to the general procedure in 75% yield (56.5 mg). white solid;

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.61 (d, J = 4.8 Hz, 2H), 8.41 (s, 1H), 8.17 (d, J = 8.8 Hz, 1H), 8.00 (d, J = 8.8 Hz, 1H), 7.86 (s, 1H), 7.80 – 7.76 (m, 2H), 7.69 (d, J = 8.5 Hz, 1H), 7.47 – 7.44 (m, 2H), 7.27 – 7.19 (m, 1H), 7.09 (t, J = 4.8 Hz, 1H), 6.95 (s, 1H), 3.94 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.9, 158.5, 157.9, 142.0, 140.7, 133.3, 132.7, 131.0, 129.1, 128.2, 127.7, 127.6, 127.0, 126.44, 126.4, 126.3, 125.0, 124.2, 123.3, 118.2, 112.7, 109.0, 52.1. HRMS: $[M + H]^+$ calculated for $C_{24}H_{18}N_3O_2^+$: 380.1394, found: 380.1397.

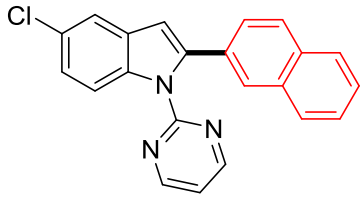


5-Fluoro-2-(naphthalen-2-yl)-1-(pyrimidin-2-yl)-1H-indole (**3ja**)

3ja was obtained according to the general procedure in 73% yield (49.5 mg). white solid;

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.60 (d, J = 4.8 Hz, 2H), 8.17 – 8.14 (m, 1H), 7.88 (s, 1H), 7.79 (dd, J = 9.5, 6.3 Hz, 2H), 7.70 (d, J = 8.5 Hz, 1H), 7.52 – 7.42 (m, 2H), 7.30 (dd, J = 8.9, 2.4 Hz, 1H),

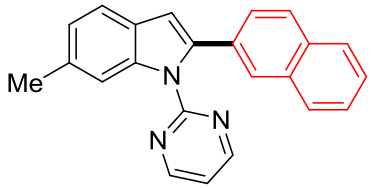
7.28 – 7.23 (m, 1H), 7.08 – 7.00 (m, 2H), 6.85 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.31, 158.3, 158.0, 142.1, 133.6 (d, $J_{C\text{-}F}$ = 203.9 Hz), 133.3, 131.3, 130.0 (d, $J_{C\text{-}F}$ = 10.2 Hz), 128.2, 127.7, 127.5, 126.8, 126.5, 126.3, 126.2, 117.7, 114.1 (d, $J_{C\text{-}F}$ = 9.3 Hz), 111.5 (d, $J_{C\text{-}F}$ = 25.4 Hz), 108.5 (d, $J_{C\text{-}F}$ = 4.2 Hz), 105.9, 105.7. HRMS: $[M + H]^+$ calculated for $C_{22}H_{15}FN_3^+$: 340.1245, found: 340.1249.



5-Chloro-2-(naphthalen-2-yl)-1-(pyrimidin-2-yl)-1H-indole (**3ka**)

3ka was obtained according to the general procedure in 70% yield (49.8 mg). white solid;

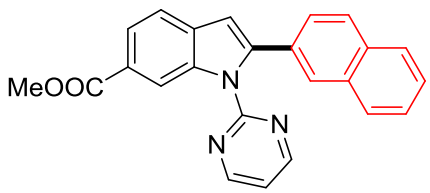
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.59 (d, J = 4.5 Hz, 2H), 8.12 (d, J = 8.8 Hz, 1H), 7.86 (s, 1H), 7.78 – 7.76 (m, 2H), 7.69 (d, J = 8.5 Hz, 1H), 7.61 (s, 1H), 7.47 – 7.45 (m, 2H), 7.24 (d, J = 8.4 Hz, 2H), 7.06 – 7.05 (m, 1H), 6.81 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.3, 157.9, 141.9, 136.5, 133.3, 132.6, 131.2, 130.5, 128.2, 127.7, 127.5, 126.9, 126.44, 126.4, 126.3, 123.8, 120.1, 117.9, 114.3, 108.0. One signal is missing due to overlap. HRMS: $[M + H]^+$ calculated for $C_{22}H_{15}ClN_3^+$: 356.0949, found: 356.0950.



6-Methyl-2-(naphthalen-2-yl)-1-(pyrimidin-2-yl)-1H-indole (**3la**)

3la was obtained according to the general procedure in 62% yield (41.1 mg). white solid;

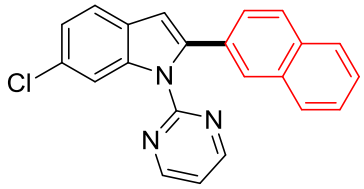
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.59 (d, J = 4.8 Hz, 2H), 8.00 (s, 1H), 7.85 (s, 1H), 7.78 – 7.75 (m, 2H), 7.67 (d, J = 8.5 Hz, 1H), 7.54 (d, J = 7.9 Hz, 1H), 7.46 – 7.41 (m, 2H), 7.27 – 7.24 (m, 1H), 7.08 (d, J = 7.9 Hz, 1H), 7.02 (t, J = 4.8 Hz, 1H), 6.86 (s, 1H), 2.50 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.3, 158.26, 140.0, 138.7, 133.7, 133.4, 132.4, 131.8, 128.2, 127.7, 127.4, 127.3, 126.6, 126.5, 126.2, 125.9, 123.9, 120.4, 117.5, 112.9, 108.8, 22.2. HRMS: $[M + H]^+$ calculated for $C_{23}H_{18}N_3^+$: 336.1495, found: 336.1498.



Methyl 2-(naphthalen-2-yl)-1-(pyrimidin-2-yl)-1H-indole-6-carboxylate (**3ma**)

3ma was obtained according to the general procedure in 67% yield (50.1 mg). white solid;

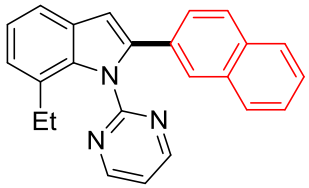
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.84 (s, 1H), 8.64 (d, J = 4.8 Hz, 2H), 7.95 (dd, J = 8.2, 1.3 Hz, 1H), 7.88 (s, 1H), 7.80 – 7.76 (m, 2H), 7.69 (t, J = 8.6 Hz, 2H), 7.51 – 7.42 (m, 2H), 7.28 – 7.21 (m, 1H), 7.09 (t, J = 4.8 Hz, 1H), 6.92 (s, 1H), 3.93 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.1, 158.6, 157.8, 143.7, 137.6, 133.3, 133.1, 132.8, 130.9, 128.3, 127.8, 127.7, 127.2, 126.5, 126.4, 126.4, 125.2, 123.4, 120.4, 118.2, 115.1, 108.4, 52.1. HRMS: $[M + H]^+$ calculated for $C_{24}H_{18}N_3O_2^+$: 380.1394, found: 380.1397.



6-Chloro-2-(naphthalen-2-yl)-1-(pyrimidin-2-yl)-1H-indole (**3na**)

3na was obtained according to the general procedure in 74% yield (52.6 mg). white solid;

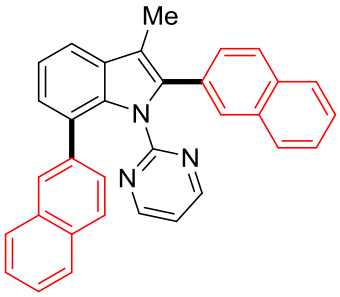
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.59 (d, J = 4.8 Hz, 2H), 8.24 (s, 1H), 7.85 (s, 1H), 7.79 – 7.75 (m, 2H), 7.68 (d, J = 8.5 Hz, 1H), 7.54 (d, J = 8.3 Hz, 1H), 7.48 – 7.42 (m, 2H), 7.25 – 7.21 (m, 2H), 7.05 (t, J = 4.8 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.4, 157.8, 141.3, 138.5, 133.3, 132.6, 131.2, 129.5, 128.2, 128.0, 127.7, 127.5, 126.7, 126.4, 126.4, 126.2, 122.9, 121.5, 117.9, 113.4, 108.5. HRMS: $[M + H]^+$ calculated for $C_{22}H_{15}ClN_3^+$: 356.0949, found: 356.0951.



7-Ethyl-2-(naphthalen-2-yl)-1-(pyrimidin-2-yl)-1H-indole (**3oa**)

3oa was obtained in the condition of indole (0.2 mmol), *7*-oxabenzonorbornadiene (0.4 mmol), $[Cp^*CoCl_2]_2$ (5 mol %), $AgSbF_6$ (30 mol %), AgOAc (30 mol %), HOAc (2 equiv), DCE (2 mL), 110 ^{o}C for 12 h in 53 yield (37.1 mg). white solid;

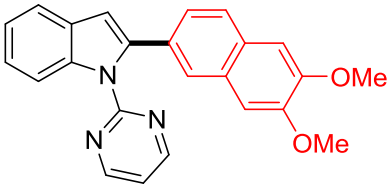
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.70 (d, J = 4.8 Hz, 2H), 7.82 (s, 1H), 7.78 – 7.69 (m, 2H), 7.66 (d, J = 8.5 Hz, 1H), 7.56 (d, J = 7.7 Hz, 1H), 7.46 – 7.35 (m, 3H), 7.21 – 7.15 (m, 2H), 7.07 (d, J = 7.2 Hz, 1H), 6.87 (s, 1H), 2.36 (q, J = 7.5 Hz, 2H), 0.94 (t, J = 7.5 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.5, 158.3, 142.2, 137.4, 133.1, 132.5, 130.5, 129.8, 128.3, 128.2, 128.0, 127.6, 127.6, 126.8, 126.2, 126.1, 123.8, 121.6, 119.8, 118.9, 25.4, 14.4. HRMS: $[M + H]^+$ calculated for $C_{24}H_{20}N_3^+$: 350.1652, found: 350.1654.



3-Methyl-2,7-di(naphthalen-2-yl)-1-(pyrimidin-2-yl)-1H-indole (**3pa**)

3pa was obtained according to the procedure of **3oa** in 67% yield (61.9 mg). white solid;

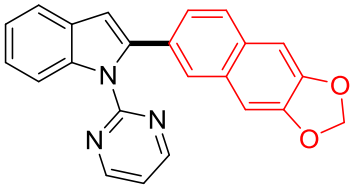
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50 (d, J = 4.8 Hz, 2H), 8.23 (d, J = 8.1 Hz, 1H), 8.13 (d, J = 7.5 Hz, 1H), 7.82 – 7.77 (m, 4H), 7.71 (d, J = 8.5 Hz, 1H), 7.64 (d, J = 7.3 Hz, 1H), 7.50 – 7.23 (m, 7H), 7.23 – 7.16 (m, 1H), 6.93 (t, J = 4.8 Hz, 1H), 6.63 (d, J = 7.4 Hz, 1H), 2.39 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.1, 158.09, 151.6, 137.1, 135.8, 134.8, 133.2, 132.3, 131.3, 130.7, 128.4, 128.2, 127.9, 127.7, 127.66, 127.3, 126.4, 126.1, 126.0, 125.9, 125.2, 124.5, 124.0, 121.9, 121.7, 120.5, 119.1, 117.0, 115.8, 113.0, 108.6, 9.7. HRMS: $[M + H]^+$ calculated for $C_{33}H_{24}N_3^+$: 462.1965, found: 462.1968.



2-(6,7-Dimethoxynaphthalen-2-yl)-1-(pyrimidin-2-yl)-1H-indole (**3ab**)

3ab was obtained according to the general procedure in 48% yield (36.6 mg). white solid;

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.63 (d, J = 4.7 Hz, 2H), 8.17 (d, J = 8.1 Hz, 1H), 7.75 (s, 1H), 7.66 (d, J = 7.4 Hz, 1H), 7.54 (d, J = 8.4 Hz, 1H), 7.31 – 7.23 (m, 2H), 7.12 (d, J = 8.3 Hz, 1H), 7.08 – 7.06 (m, 3H), 6.86 (s, 1H), 3.98 (s, 3H), 3.97 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.3, 149.8, 149.7, 140.9, 138.2, 130.0, 129.5, 129.1, 128.3, 125.9, 125.4, 124.9, 123.5, 122.2, 120.6, 117.6, 112.9, 108.2, 106.6, 106.2, 77.4, 77.1, 76.8, 55.93, 55.9. One signal is missing due to overlap. HRMS: $[M + H]^+$ calculated for $C_{24}H_{20}N_3O_2^+$: 382.1550, found: 382.1552.



2-(Naphtho[2,3-d][1,3]dioxol-6-yl)-1-(pyrimidin-2-yl)-1H-indole (**3ac**)

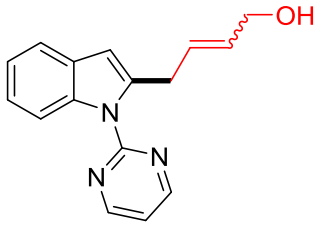
3ac was obtained according to the general procedure in 52% yield (38.0 mg). white solid;

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.62 (d, J = 4.6 Hz, 2H), 8.16 (d, J = 8.0 Hz, 1H), 7.76 – 7.61 (m, 2H), 7.51 (d, J = 8.3 Hz, 1H), 7.31 – 7.22 (m, 2H), 7.12 (d, J = 8.2 Hz, 1H), 7.09 – 7.00 (m, 3H),

6.86 (s, 1H), 6.00 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.3, 147.9, 147.8, 140.7, 138.2, 130.4, 130.1, 129.6, 129.5, 126.6, 126.0, 125.0, 123.5, 122.2, 120.7, 117.6, 112.9, 108.3, 104.2, 103.8, 101.1. One signal is missing due to overlap. HRMS: $[M + H]^+$ calculated for $C_{23}H_{16}N_3O_2^+$: 366.1237, found: 366.1240.

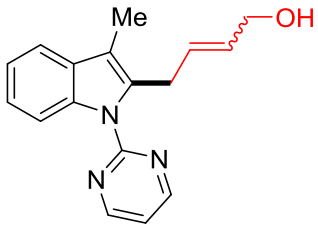
III. General procedures for the synthesis of compound 5

Reaction conditions: indole (0.2 mmol), *2*-vinyloxirane (0.4 mmol), $[Cp^*Co(MeCN)_3](SbF_6)_2$ (5 mol %), NaOAc (20 mol %), and DCE (2 mL) were charged into the pressure tube. The reaction mixture was stirred under N_2 at 40 ℃ for 12 h. After the solvent was removed under reduced pressure, the residue was purified by silica gel chromatography using PE/EA to afford the product **5**.



4-(1-(Pyrimidin-2-yl)-1H-indol-2-yl)but-2-en-1-ol (**5a**), 2.8:1.

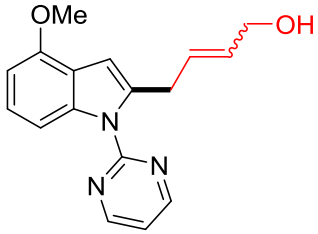
5a was obtained according to the general procedure in 99% yield (52.5 mg). colorless liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.73 (d, *J* = 4.8 Hz, 2H), 8.25 – 8.20 (m, 1H), 7.52 (d, *J* = 7.7 Hz, 1H), 7.24 – 7.15 (m, 2H), 7.08 (t, *J* = 4.8 Hz, 1H), 6.46 (s, 1H), 5.81 (dt, *J* = 15.4, 6.6 Hz, 1H), 5.61 (dt, *J* = 15.3, 5.8 Hz, 1H), 4.22 – 3.98 (m, 2H), 3.95 – 3.90 (m, 2H), 1.71 (1H, OH). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.2, 158.1, 139.6, 137.0, 131.1, 129.5, 129.2, 122.7, 121.9, 119.9, 117.2, 113.7, 106.5, 63.3, 32.5. Minor: δ 139.7, 137.1, 130.3, 129.1, 129.0, 122.8, 122.0, 117.1, 113.9, 106.3, 58.6, 28.1. The NMR data agree with those in a literature report.[5]



4-(3-Methyl-1-(pyrimidin-2-yl)-1H-indol-2-yl)but-2-en-1-ol (**5b**), 2.7:1.

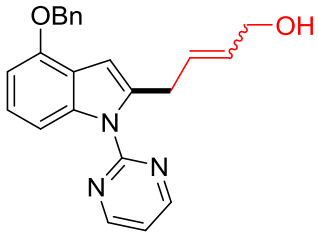
5b was obtained according to the general procedure in 98% yield (55.1 mg). colorless liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.74 – 8.72 (m, 2H), 8.21 – 8.18 (m, 1H), 7.55 – 7.46 (m, 1H), 7.27 – 7.16 (m, 2H), 7.08 – 7.06 (m, 1H), 5.73 (dt, *J* = 15.4, 6.6 Hz, 1H), 5.52 – 5.42 (m, 1H), 4.19 – 3.88 (m, 4H), 2.29 (s, 3H), 1.41 (1H, OH). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.2, 158.1, 136.2, 134.1, 130.1, 129.8, 128.7, 123.0, 121.5, 118.2, 116.9, 113.8, 113.5, 63.4, 29.0, 8.86. Minor: δ 136.3, 134.6, 130.3, 129.9, 123.1, 121.6, 118.1, 116.8, 113.6, 113.4, 58.7, 25.1, 8.9. The NMR data

agree with those in a literature report.[5]



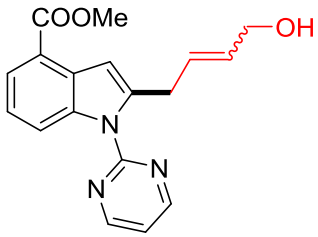
4-(4-Methoxy-1-(pyrimidin-2-yl)-1H-indol-2-yl)but-2-en-1-ol (**5c**), 3.0:1.

5c was obtained according to the general procedure in 98% yield (57.9 mg). colorless liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.74 – 8.73 (m, 2H), 7.90 – 7.76 (m, 1H), 7.14 (t, J = 8.1 Hz, 1H), 7.11 – 7.07 (m, 1H), 6.62 (d, J = 7.9 Hz, 1H), 6.58 (s, 1H), 5.82 (dt, J = 15.4, 6.6 Hz, 1H), 5.61 (dt, J = 15.4, 5.8 Hz, 1H), 4.21 – 3.98 (m, 2H), 3.93 (s, 3H), 3.91 – 3.88 (m, 2H), 1.69 (1H, OH). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.2, 152.4, 138.3, 138.2, 131.1, 129.5, 123.47, 119.4, 117.32, 107.1, 103.2, 102.16, 63.4, 55.4, 32.5. One signal is missing due to overlap. Minor: δ 152.3, 138.4, 130.3, 129.0, 123.52, 117.27, 107.2, 103.1, 102.22, 58.6, 28.1. The NMR data agree with those in a literature report.[5]



4-(4-(Benzyloxy)-1-(pyrimidin-2-yl)-1H-indol-2-yl)but-2-en-1-ol (**5d**), 3.2:1.

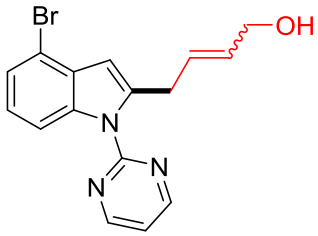
5d was obtained according to the general procedure in 87% yield (64.6 mg). colorless liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.74 (d, J = 4.8 Hz, 2H), 7.86 – 7.81 (m, 1H), 7.50 – 7.48 (m, 2H), 7.40 – 7.36 (m, 2H), 7.33 – 7.30 (m, 1H), 7.14 – 7.08 (m, 2H), 6.68 (d, J = 7.9 Hz, 1H), 6.64 (s, 1H), 5.81 (dt, J = 15.4, 5.3 Hz, 1H), 5.62 (dt, J = 15.4, 5.8 Hz, 1H), 5.20 (s, 2H), 4.22 – 3.89 (m, 4H), 1.53 (1H, OH). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.2, 158.19, 151.6, 138.47, 138.2, 137.52, 131.1, 129.6, 128.5, 127.8, 127.5, 123.4, 119.8, 117.3, 107.3, 103.7, 103.5, 70.1, 63.4, 32.5. Minor: δ 151.5, 138.5, 138.3, 137.5, 130.2, 129.1, 127.47, 123.5, 117.27, 107.5, 103.8, 103.4, 58.6, 28.1. The NMR data agree with those in a literature report.[5]



Methyl 2-(4-hydroxybut-2-en-1-yl)-1-(pyrimidin-2-yl)-1H-indole-4-carboxylate (**5e**), 2.6:1.

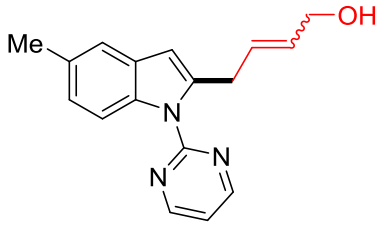
5e was obtained according to the general procedure in 93% yield (60.1 mg). colorless liquid;

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.83 – 8.72 (m, 2H), 8.43 – 8.38 (m, 1H), 7.93 (d, J = 7.6 Hz, 1H), 7.28 – 7.21 (m, 1H), 7.20 – 7.12 (m, 2H), 5.85 (dt, J = 15.4, 6.5 Hz, 1H), 5.64 (dt, J = 15.4, 5.8 Hz, 1H), 4.25 – 3.94 (m, 7H), 1.95 (1H, OH). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.9, 158.3, 157.8, 142.1, 137.76, 131.5, 129.2, 128.9, 124.8, 121.9, 120.59, 118.3, 117.7, 107.0, 63.3, 51.8, 32.5. Minor: δ 137.8, 130.6, 129.1, 128.5, 124.9, 122.0, 120.6, 118.4, 117.68, 106.8, 58.6, 28.1. HRMS: $[M + H]^+$ calculated for $C_{18}H_{18}N_3O_3^+$: 324.1343, found: 324.1345.



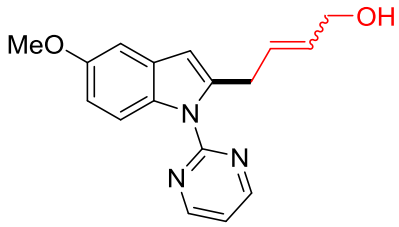
4-(4-Bromo-1-(pyrimidin-2-yl)-1H-indol-2-yl)but-2-en-1-ol (**5f**), 2.7:1.

5f was obtained according to the general procedure in 97% yield (66.4 mg). colorless liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.76 (d, J = 4.8 Hz, 2H), 8.18 – 8.13 (m, 1H), 7.33 (d, J = 7.7 Hz, 1H), 7.16 – 7.13 (m, 1H), 7.08 – 7.04 (m, 1H), 6.52 (s, 1H), 5.82 (dt, J = 15.4, 6.6 Hz, 1H), 5.64 (dt, J = 15.4, 5.7 Hz, 1H), 4.24 – 3.90 (m, 4H), 1.69 (1H, OH). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.3, 157.8, 140.66, 137.28, 131.5, 129.7, 128.8, 124.7, 123.6, 117.73, 113.7, 112.9, 106.1, 63.3, 32.5. Minor: δ 140.7, 137.3, 130.6, 129.6, 128.5, 124.8, 123.7, 117.7, 113.0, 106.0, 58.6, 28.1. The NMR data agree with those in a literature report.[5]



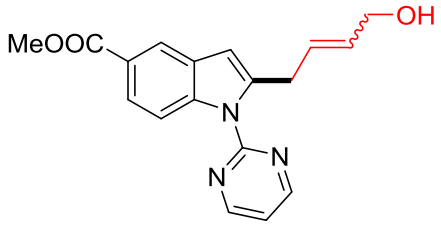
4-(5-Methyl-1-(pyrimidin-2-yl)-1H-indol-2-yl)but-2-en-1-ol (**5g**), 3.0:1.

5g was obtained according to the general procedure in 99% yield (55.3 mg). colorless liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.73 (d, J = 4.8 Hz, 2H), 8.17 – 8.12 (m, 1H), 7.30 (s, 1H), 7.07 (t, J = 4.8 Hz, 1H), 7.04 (d, J = 8.5 Hz, 1H), 6.38 (s, 1H), 5.83 (dt, J = 15.4, 6.5 Hz, 1H), 5.63 (dt, J = 15.4, 5.8 Hz, 1H), 4.24 – 3.91 (m, 4H), 2.43 (s, 3H), 1.50 (1H, OH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.1, 158.08, 139.7, 135.3, 131.2, 130.9, 129.7, 129.5, 124.1, 119.7, 116.9, 113.7, 106.4, 63.4, 32.7, 21.4. Minor: δ 158.2, 139.8, 135.4, 131.3, 130.1, 129.4, 129.3, 124.2, 116.8, 113.8, 106.2, 58.6, 28.3. The NMR data agree with those in a literature report.[5]



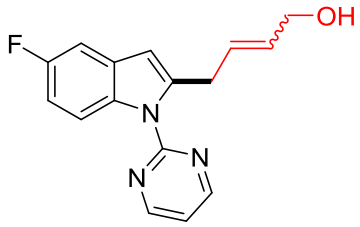
4-(5-Methoxy-1-(pyrimidin-2-yl)-1H-indol-2-yl)but-2-en-1-ol (**5h**), 3.1:1.

5h was obtained according to the general procedure in 99% yield (58.5 mg). colorless liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.71 (d, J = 4.8 Hz, 2H), 8.22 – 8.18 (m, 1H), 7.06 (t, J = 4.8 Hz, 1H), 6.98 (d, J = 2.4 Hz, 1H), 6.86 – 6.83 (m, 1H), 6.39 (s, 1H), 5.83 (dt, J = 15.4, 6.6 Hz, 1H), 5.64 (dt, J = 15.4, 5.8 Hz, 1H), 4.24 – 3.92 (m, 4H), 3.83 (s, 3H), 1.72 (1H, OH). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.08, 158.07, 155.4, 140.5, 131.96, 131.0, 130.0, 129.6, 116.9, 115.0, 111.6, 106.5, 102.4, 63.4, 55.7, 32.8. Minor: δ 158.1, 155.44, 132.0, 130.2, 129.96, 129.1, 116.8, 115.2, 111.7, 106.4, 102.3, 58.6, 28.4. The NMR data agree with those in a literature report.[5]



Methyl 2-(4-hydroxybut-2-en-1-yl)-1-(pyrimidin-2-yl)-1H-indole-5-carboxylate (**5i**), 2.6:1.

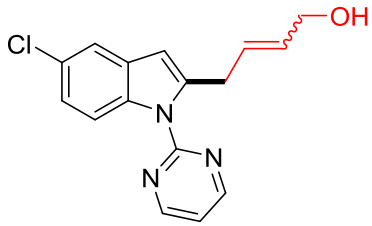
5i was obtained according to the general procedure in 98% yield (63.4 mg). colorless liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.77 (d, J = 4.8 Hz, 2H), 8.29 – 8.16 (m, 2H), 7.92 – 7.89 (m, 1H), 7.18 – 7.15 (m, 1H), 6.52 (s, 1H), 5.80 (dt, J = 15.4, 6.6 Hz, 1H), 5.63 (dt, J = 15.4, 5.7 Hz, 1H), 4.24 – 3.89 (m, 7H), 1.94 – 1.87 (1H, OH). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.0, 158.3, 157.7, 141.27, 139.66, 131.5, 128.8, 128.7, 124.09, 123.6, 122.33, 117.8, 113.3, 106.8, 63.2, 51.9, 32.4. Minor: δ 141.3, 139.7, 130.7, 128.4, 124.1, 123.7, 122.3, 117.78, 113.5, 106.6, 58.5, 28.0. The NMR data agree with those in a literature report.[5]



4-(5-Fluoro-1-(pyrimidin-2-yl)-1H-indol-2-yl)but-2-en-1-ol (**5j**), 2.7:1.

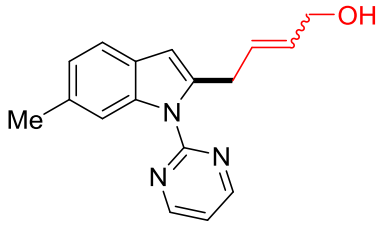
5j was obtained according to the general procedure in 99% yield (56.1 mg). colorless liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.74 (d, J = 4.8 Hz, 2H), 8.27 – 8.15 (m, 1H), 7.20 – 7.07 (m, 2H), 6.96 – 6.91 (m, 1H), 6.41 (s, 1H), 5.82 (dt, J = 15.4, 6.6 Hz, 1H), 5.64 (dt, J = 15.4, 5.8 Hz, 1H), 4.23 – 3.91 (m, 4H), 1.67 (1H, OH). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.9 (d, $J_{C\text{-}F}$ = 237.9 Hz),

158.2, 158.0, 141.5, 133.4 (d, J_{C-F} = 0.6 Hz), 131.3, 129.9 (d, J_{C-F} = 10.1 Hz), 129.1, 117.3, 114.9 (d, J_{C-F} = 9.1 Hz), 110.4 (d, J_{C-F} = 25.1 Hz), 106.3 (d, J_{C-F} = 4.0 Hz), 105.0 (d, J_{C-F} = 23.7 Hz), 63.3, 32.7. Minor: δ 160.1, 158.19, 157.97, 157.8, 133.5, 133.45, 130.4, 129.94, 129.84, 128.8, 117.2, 115.1, 115.0, 110.6, 110.3, 106.2, 106.1, 105.2, 104.9, 58.6, 28.3. HRMS: $[M + H]^+$ calculated for $C_{16}H_{15}FN_3O^+$: 284.1194, found: 284.1194.



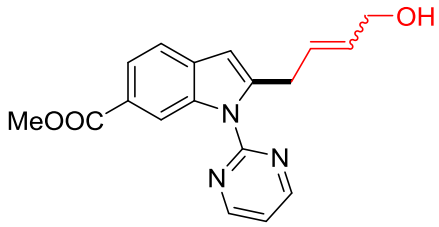
4-(5-Chloro-1-(pyrimidin-2-yl)-1H-indol-2-yl)but-2-en-1-ol (**5k**), 2.7:1.

5k was obtained according to the general procedure in 98% yield (58.8 mg). colorless liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.74 (d, J = 4.7 Hz, 2H), 8.20 – 8.15 (m, 1H), 7.46 (d, J = 1.1 Hz, 1H), 7.16 – 7.12 (m, 2H), 6.38 (s, 1H), 5.80 (dt, J = 15.4, 6.5 Hz, 1H), 5.63 (dt, J = 15.4, 5.8 Hz, 1H), 4.23 – 3.90 (m, 4H), 1.69 (1H, OH). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.2, 157.9, 141.3, 135.4, 131.4, 130.4, 129.0, 127.3, 122.7, 119.3, 117.5, 115.07, 105.8, 63.3, 32.6. Minor: δ 135.42, 130.49, 130.3, 128.7, 127.4, 122.8, 117.4, 115.2, 105.7, 58.6, 28.3. The NMR data agree with those in a literature report.[5]



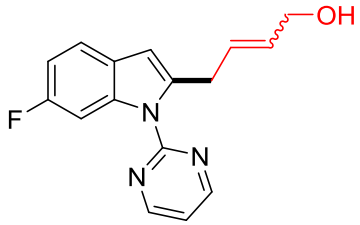
4-(6-Methyl-1-(pyrimidin-2-yl)-1H-indol-2-yl)but-2-en-1-ol (**5l**), 3.0:1.

5l was obtained according to the general procedure in 99% yield (55.6 mg). colorless liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.75 (d, J = 4.8 Hz, 2H), 8.04 – 8.01 (m, 1H), 7.39 (d, J = 7.9 Hz, 1H), 7.09 (t, J = 4.8 Hz, 1H), 7.01 (d, J = 7.9 Hz, 1H), 6.41 (s, 1H), 5.80 (dt, J = 15.4, 6.5 Hz, 1H), 5.60 (dt, J = 15.4, 5.8 Hz, 1H), 4.21 – 3.88 (m, 4H), 2.46 (s, 3H), 1.66 (1H, OH). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.2, 158.1, 138.9, 137.4, 132.57, 130.9, 129.6, 126.93, 123.4, 119.5, 117.1, 113.7, 106.3, 63.4, 32.4, 22.1. Minor: δ 139.0, 137.5, 132.6, 130.1, 129.2, 126.9, 123.5, 119.49, 117.0, 113.9, 106.2, 58.6, 28.1. HRMS: $[M + H]^+$ calculated for $C_{17}H_{18}N_3O^+$: 280.1444, found: 280.1448.



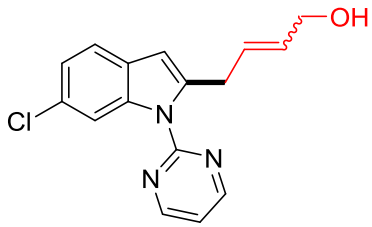
Methyl 2-(4-hydroxybut-2-en-1-yl)-1-(pyrimidin-2-yl)-1H-indole-6-carboxylate (**5m**), 2.8:1.

5m was obtained according to the general procedure in 95% yield (61.4 mg). colorless liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.90 – 8.88 (m, 1H), 8.80 (d, J = 4.8 Hz, 2H), 7.89 – 7.86 (m, 1H), 7.52 (d, J = 8.2 Hz, 1H), 7.18 – 7.15 (m, 1H), 6.50 (s, 1H), 5.82 (dt, J = 15.4, 6.6 Hz, 1H), 5.65 (dt, J = 15.4, 5.7 Hz, 1H) 4.24 – 4.02 (m, 2H), 3.97 – 3.91 (m, 5H), 1.94 – 1.87 (1H, OH). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.2, 158.4, 157.7, 143.3, 136.5, 133.0, 131.6, 128.5, 124.27, 123.08, 119.4, 117.8, 115.8, 106.3, 63.2, 52.0, 32.5. Minor: δ 143.27, 136.4, 132.9, 130.8, 128.2, 124.3, 123.1, 117.7, 116.0, 106.1, 58.5, 28.2. The NMR data agree with those in a literature report.[5]



4-(6-Fluoro-1-(pyrimidin-2-yl)-1H-indol-2-yl)but-2-en-1-ol (**5n**), 2.8:1.

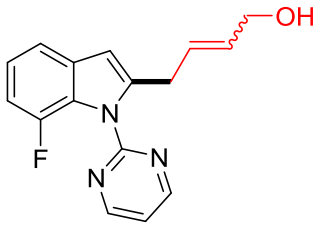
5n was obtained according to the general procedure in 97% yield (54.8 mg). white solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.75 (d, J = 4.8 Hz, 2H), 8.08 – 8.02 (m, 1H), 7.41 (dd, J = 8.5, 5.6 Hz, 1H), 7.13 (t, J = 4.8 Hz, 1H), 6.94 (td, J = 9.1, 2.3 Hz, 1H), 6.43 (s, 1H), 5.83 (dt, J = 15.4, 6.6 Hz, 1H), 5.64 (dt, J = 15.4, 5.8 Hz, 1H), 4.25 – 3.92 (m, 4H), 1.58 (1H, OH). ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.2 (d, $J_{C\text{-}F}$ = 237.8 Hz), 158.2, 158.0, 140.2 (d, $J_{C\text{-}F}$ = 3.9 Hz), 137.1 (d, $J_{C\text{-}F}$ = 12.8 Hz), 131.1, 129.4, 125.5(d, $J_{C\text{-}F}$ = 1.2 Hz), 120.2 (d, $J_{C\text{-}F}$ = 9.9 Hz), 117.4, 110.1 (d, $J_{C\text{-}F}$ = 24.3 Hz), 106.3, 101.3 (d, $J_{C\text{-}F}$ = 28.8 Hz), 63.36, 32.67. Minor: δ 140.3, 140.21, 137.2, 137.06, 130.3, 129.0, 117.3, 110.3, 110.0, 106.1, 101.6, 101.4, 58.6, 28.3. HRMS: $[M + H]^+$ calculated for $C_{16}H_{15}FN_3O^+$: 284.1194, found: 284.1198.



4-(6-Chloro-1-(pyrimidin-2-yl)-1H-indol-2-yl)but-2-en-1-ol (**5o**), 2.7:1.

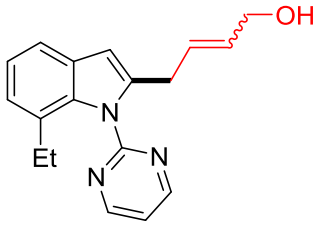
5o was obtained according to the general procedure in 94% yield (56.1 mg). colorless liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.76 (d, J = 4.8 Hz, 2H), 8.32 – 8.29 (m, 1H), 7.40 (d, J = 8.3 Hz,

1H), 7.19 – 7.10 (m, 2H), 6.42 (s, 1H), 5.82 (dt, J = 15.4, 6.6 Hz, 1H), 5.64 (dt, J = 15.4, 5.8 Hz, 1H), 4.24 – 4.01 (m, 2H), 3.95 – 3.90 (m, 2H), 1.76 – 1.59 (1H, OH). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.2, 157.8, 140.6, 137.3, 131.3, 129.1, 128.5, 122.4, 120.5, 117.5, 114.2, 106.2, 63.3, 32.6. One signal is missing due to overlap. Minor: δ 157.9, 137.4, 130.4, 128.7, 128.6, 122.4, 117.4, 114.3, 106.1, 58.6, 28.2. The NMR data agree with those in a literature report.[5]



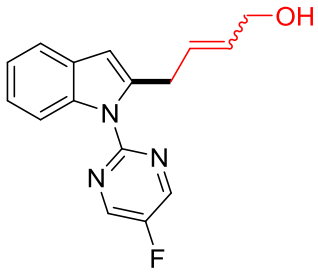
4-(7-Fluoro-1-(pyrimidin-2-yl)-1H-indol-2-yl)but-2-en-1-ol (**5p**), 2.8:1.

5p was obtained according to the general procedure in 92% yield (52.1 mg). colorless liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.80 – 8.78 (m, 2H), 7.31 (d, J = 7.8 Hz, 1H), 7.27 – 7.21 (m, 1H), 7.08 – 7.03 (m, 1H), 6.90 – 6.86 (m, 1H), 6.47 – 6.42 (m, 1H), 5.71 – 5.58 (m, 1H), 5.44 (dt, J = 15.4, 5.8 Hz, 1H), 4.10 – 3.62 (m, 4H), 1.87 (1H, OH). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.4, 158.3, 149.6 (d, $J_{C\text{-}F}$ = 248.0 Hz), 140.5, 132.5 (d, $J_{C\text{-}F}$ = 4.3 Hz), 131.5, 128.1, 124.7 (d, $J_{C\text{-}F}$ = 9.1 Hz), 121.6 (d, $J_{C\text{-}F}$ = 6.9 Hz), 119.1, 115.9 (d, $J_{C\text{-}F}$ = 3.5 Hz), 108.8 (d, $J_{C\text{-}F}$ = 19.0 Hz), 104.8 (d, $J_{C\text{-}F}$ = 2.0 Hz), 63.0, 30.6. Minor: δ 157.6, 140.7, 130.8, 127.7, 124.8, 124.66, 121.7, 121.67, 119.0, 109.0, 108.8, 104.6, 104.5, 58.3, 26.2. HRMS: $[M + H]^+$ calculated for $C_{16}H_{15}FN_3O^+$: 284.1194, found: 284.1196.



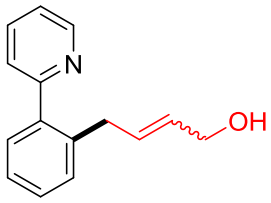
4-(7-Ethyl-1-(pyrimidin-2-yl)-1H-indol-2-yl)but-2-en-1-ol (**5q**), 3.1:1.

5q was obtained according to the general procedure in 95% yield (55.9 mg). colorless liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.80 – 8.79 (m, 2H), 7.41 (d, J = 7.7 Hz, 1H), 7.26 – 7.23 (m, 1H), 7.10 (t, J = 7.5 Hz, 1H), 7.01 (d, J = 7.3 Hz, 1H), 6.42 – 6.41 (m, 1H), 5.64 – 5.51 (m, 1H), 5.35 (dt, J = 15.4, 5.7 Hz, 1H), 4.03 – 3.45 (m, 4H), 2.30 – 2.23 (m, 2H), 1.93 (1H, OH), 0.94 (t, J = 7.5 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.5, 158.4, 139.7, 136.0, 131.1, 129.7, 128.4, 128.0, 122.97, 121.5, 119.5, 118.1, 104.2, 63.0, 30.7, 25.7, 14.0. Minor: δ 159.1, 140.0, 136.1, 130.5, 129.71, 128.03, 127.9, 123.0, 121.6, 119.4, 104.0, 58.2, 26.2. The NMR data agree with those in a literature report.[5]



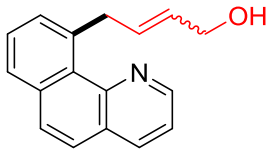
4-(1-(5-Fluoropyrimidin-2-yl)-1H-indol-2-yl)but-2-en-1-ol (**5r**), 2.8:1.

5r was obtained according to the general procedure in 99% yield (56.1mg). colorless liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.61 (s, 2H), 8.15 – 8.11 (m, 1H), 7.56 – 7.48 (m, 1H), 7.24 – 7.16 (m, 2H), 6.46 (s, 1H), 5.82 (dt, J = 15.4, 6.5 Hz, 1H), 5.63 (dt, J = 15.4, 5.8 Hz, 1H), 4.23 – 3.87 (m, 4H), 1.53 (1H, OH). ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.2 (d, $J_{C\text{-}F}$ = 206.0 Hz), 153.9 (d, $J_{C\text{-}F}$ = 52.8 Hz), 145.8 (d, $J_{C\text{-}F}$ = 21.6 Hz), 139.5, 136.99, 131.2, 129.2, 129.1, 122.8, 122.0, 120.0, 113.3, 106.4, 63.3, 32.3, 28.0. Minor: δ 153.6, 146.0, 145.8, 139.6, 137.0, 130.4, 129.0, 128.9, 122.9, 122.1, 113.5, 106.2, 58.6, HRMS: $[M + H]^+$ calculated for $C_{16}H_{15}FN_3O^+$: 284.1194, found: 284.1198.



4-(2-(Pyridin-2-yl)phenyl)but-2-en-1-ol (**7a**), 1.8:1

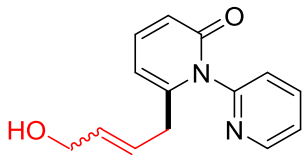
7a was obtained according to the general procedure in 80% yield (36.4 mg). colorless liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.67 – 8.66 (m, 1H), 7.81 – 7.67 (m, 1H), 7.38 – 7.23 (m, 6H), 5.68 (dt, J = 15.3, 6.5 Hz, 1H), 5.42 (dt, J = 15.3, 5.8 Hz, 1H), 4.01 – 3.45 (m, 4H), 2.02 (1H, OH). ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.8, 149.1, 140.3, 137.8, 136.3, 131.4, 130.2, 130.1, 129.9, 128.5, 126.4, 124.2, 121.8, 63.3, 36.0. Minor: δ 160.0, 149.0, 140.1, 138.3, 136.6, 131.2, 130.0, 129.8, 129.1, 128.7, 126.3, 124.4, 121.9, 58.0, 31.1. The NMR data agree with those in a literature report.[5]



4-(Benzo[h]quinolin-10-yl)but-2-en-1-ol (**7b**), 1.7;1

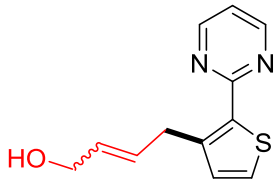
7b was obtained according to the general procedure in 52% yield (26.0 mg). colorless liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.08 – 8.93 (m, 1H), 8.14 – 8.12 (m, 1H), 7.80 – 7.77 (m, 2H), 7.67 – 7.52 (m, 3H), 7.48 – 7.44 (m, 1H), 6.23 (dt, J = 15.4, 6.5 Hz, 1H), 5.99 – 5.66 (m, 1H), 4.78-4.03 (m, 4H), 1.31 (1H, OH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.2, 147.3, 140.4, 135.7, 135.5, 134.2, 130.8, 129.2, 128.93, 128.9, 128.0, 127.6, 127.4, 125.6, 120.8, 64.0, 41.0. Minor: δ 148.3,

147.2, 140.6, 135.5, 135.4, 133.7, 130.5, 129.3, 129.0, 127.6, 127.5, 127.4, 125.6, 120.9, 59.2, 26.2. HRMS: $[M + H]^+$ calculated for $C_{17}H_{16}NO^+$: 250.1226, found: 250.1229.



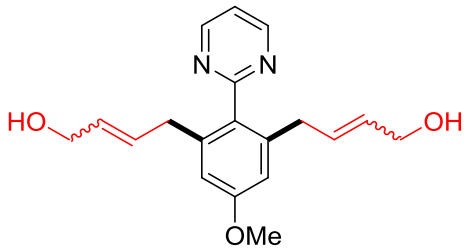
6-(4-Hydroxybut-2-en-1-yl)-2H-[1,2'-bipyridin]-2-one (**7c**), 3.2:1

7c was obtained according to the general procedure in 78% yield (37.7 mg). colorless liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.64 – 8.63 (m, 1H), 7.91 – 7.85 (m, 1H), 7.46 – 7.30 (m, 3H), 6.53 (d, J = 9.2 Hz, 1H), 6.12 (d, J = 6.9 Hz, 1H), 5.74 – 5.32 (m, 2H), 3.97 – 3.00 (m, 4H), 2.42 (1H, OH). ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.9, 151.4, 149.7, 147.8, 140.3, 138.5, 133.4, 125.1, 124.4, 124.2, 119.0, 105.9, 62.6, 36.0. Minor: δ 163.7, 151.5, 149.9, 147.6, 138.7, 132.6, 125.2, 124.3, 105.6, 105.6, 57.9, 31.3. HRMS: $[M + H]^+$ calculated for $C_{14}H_{15}N_2O_2^+$: 243.1128, found: 243.1129.



4-(2-(Pyrimidin-2-yl)thiophen-3-yl)but-2-en-1-ol (**7d**), 2.0:1

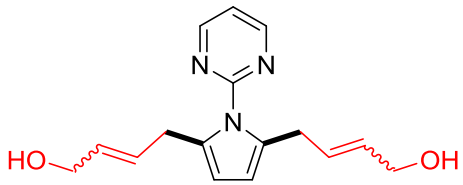
7d was obtained according to the general procedure in 27% yield (12.5 mg). colorless liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.70 – 8.69 (m, 2H), 7.39 – 7.35 (m, 1H), 7.14 – 6.94 (m, 2H), 5.95 (dt, J = 15.4, 6.6 Hz, 1H), 5.81 – 5.71 (m, 1H), 4.35 – 3.99 (m, 4H), 1.34 (1H, OH). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.6, 156.8, 142.9, 136.3, 131.6, 131.3, 129.9, 128.2, 117.8, 63.7, 32.9. Minor: δ 162.5, 156.9, 142.8, 131.4, 131.1, 128.8, 128.6, 117.9, 58.6, 28.4. The NMR data agree with those in a literature report.[5]



4,4'-(5-Methoxy-2-(pyrimidin-2-yl)-1,3-phenylene)bis(but-2-en-1-ol) (**7e**)

7e was obtained according to the general procedure in 77% yield (50.2 mg). yellow liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.81 – 8.80 (m, 2H), 7.31 – 7.21 (m, 1H), 6.75 – 6.64 (m, 2H), 5.62 – 5.11 (m, 4H), 3.89 – 3.86 (m, 4H), 3.81 (s, 3H), 3.23 – 3.08 (m, 4H), 2.66 – 2.49 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.5, 159.8, 157.0, 140.02, 139.9, 131.3, 130.3, 129.5, 119.0, 113.1, 112.8, 63.1, 55.3, 36.7. Minor: δ 167.6, 159.7, 157.1, 156.9, 140.1, 140.0, 131.4, 130.4, 130.1,

119.1, 113.2, 63.0, 57.9, 57.8, 36.74, 31.8. HRMS: $[M + H]^+$ calculated for $C_{19}H_{23}N_2O_3^+$: 327.1703, found: 327.1706.



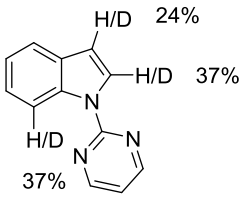
4,4'-(1-(Pyrimidin-2-yl)-1H-pyrrole-2,5-diyl)bis(but-2-en-1-ol) (**7f**)

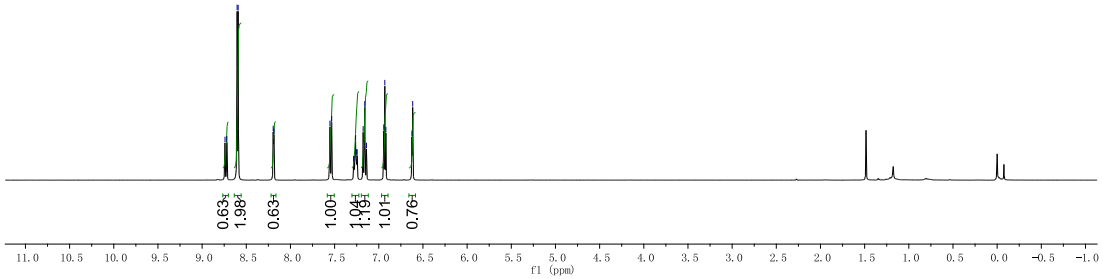
7f was obtained according to the general procedure in 93% yield (53.5 mg). yellow liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.76 – 8.74 (m, 2H), 7.21 (t, J = 4.8 Hz, 1H), 6.02 – 5.88 (m, 2H), 5.69 – 5.24 (m, 4H), 4.07 – 4.04 (m, 1H), 3.89 – 3.87 (m, 3H), 3.55 – 3.50 (m, J = 13.5, 5.7 Hz, 4H), 2.06 – 2.00 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.5, 158.4, 132.3, 130.2, 130.0, 129.6, 129.3, 118.7, 108.6, 63.2, 30.8. Minor: δ 157.8, 132.5, 132.4, 118.6, 108.8, 108.5, 108.4, 58.3, 58.2, 30.9, 26.5, 26.5. HRMS: $[M + H]^+$ calculated for $C_{16}H_{20}N_3O_2^+$: 286.1550, found: 286.1552.

IV. Mechanistic Studies

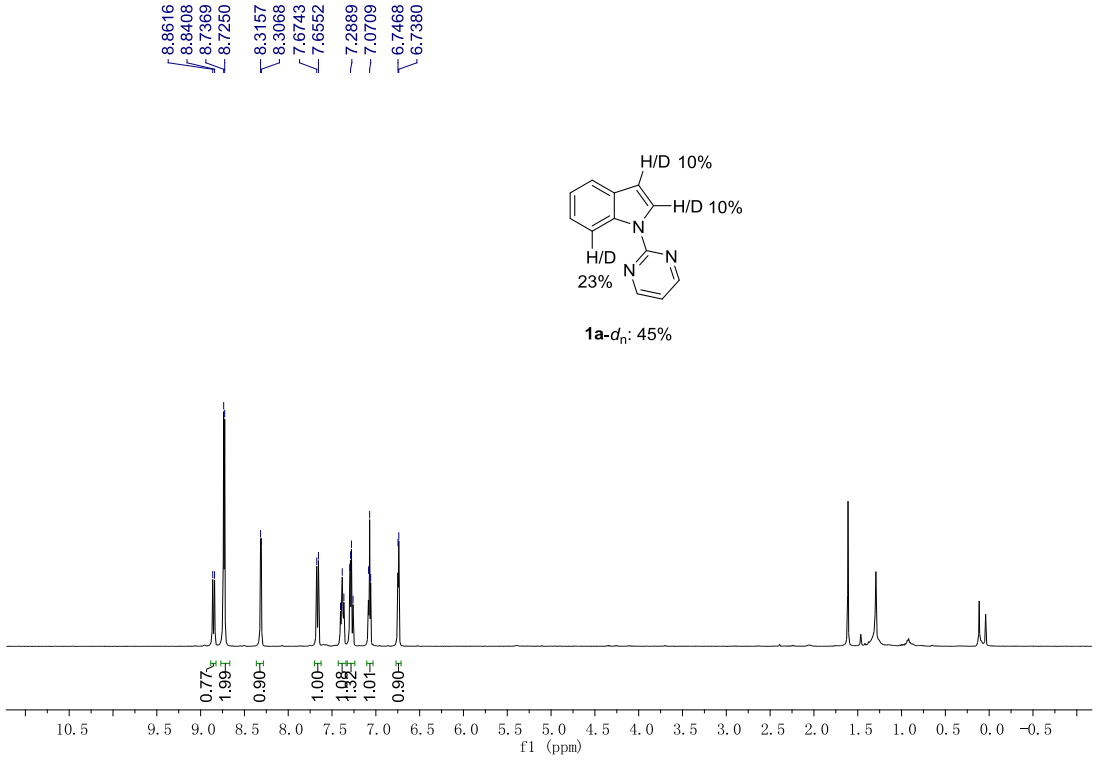
1. The experiment of H/D exchange

(a) *N*-pyrimidyl indole (0.2 mmol), $[Cp^*CoCl_2]_2$ (5 mol %), $AgSbF_6$ (30 mol %), CD_3COOD (0.4 mmol), and DCE (2 mL) were charged into the pressure tube. The reaction mixture was stirred under N_2 at 50 ℃ for 12 h. After the solvent was removed under reduced pressure, the residue was purified by silica gel chromatography using PE/EA. The ratio of H/D was determined on the basis of ^{1}H NMR analysis.

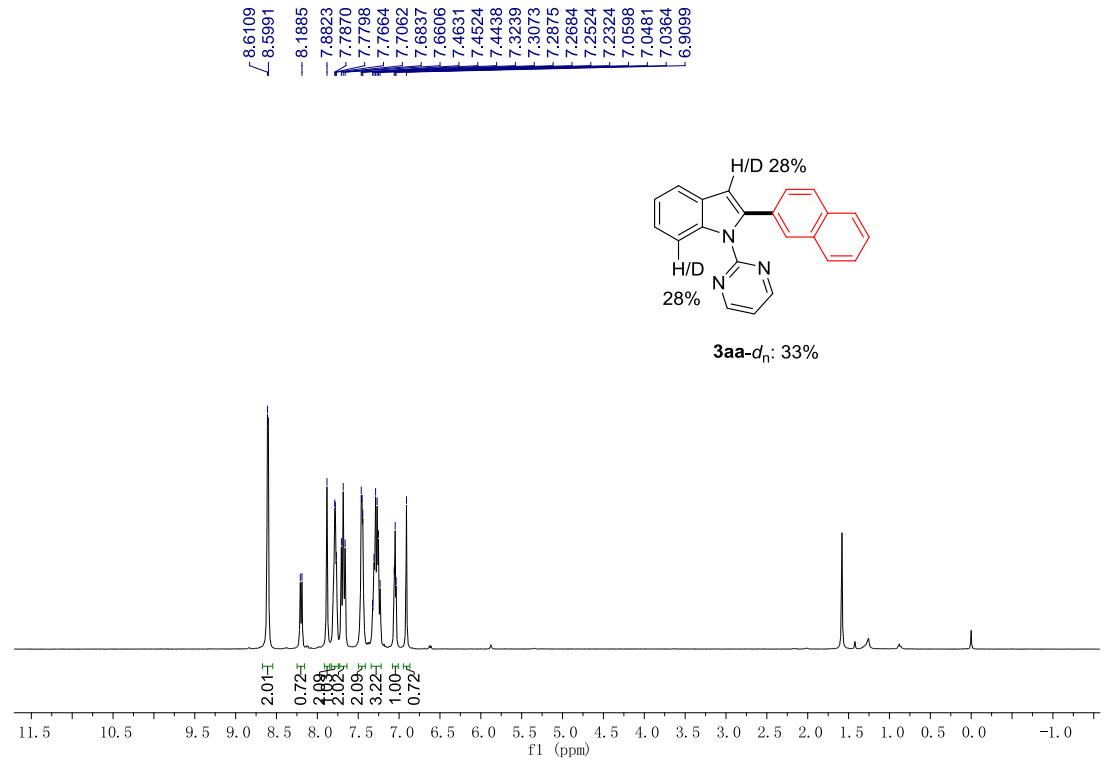




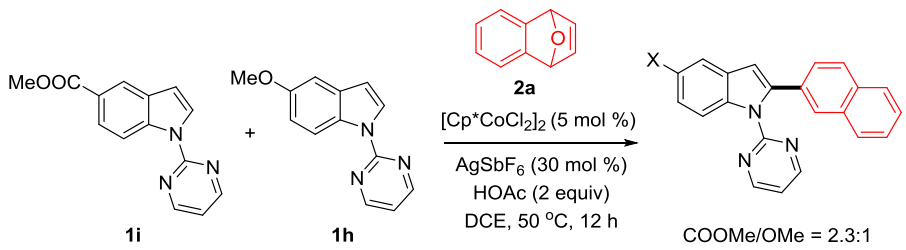
(b) *N*-pyrimidyl indole (0.2 mmol), *7*-oxabenzonorbornadiene (0.4 mmol), $[Cp^*CoCl_2]_2$ (5 mol %), $AgSbF_6$ (30 mol %), CD_3COOD (0.4 mmol), and DCE (2 mL) were charged into the pressure tube. The reaction mixture was stirred under N_2 at 50 ℃ for 1 h. After the solvent was removed under reduced pressure, the residue was purified by silica gel chromatography using PE/EA. The ratio of H/D was determined on the basis of ^{1}H NMR analysis.



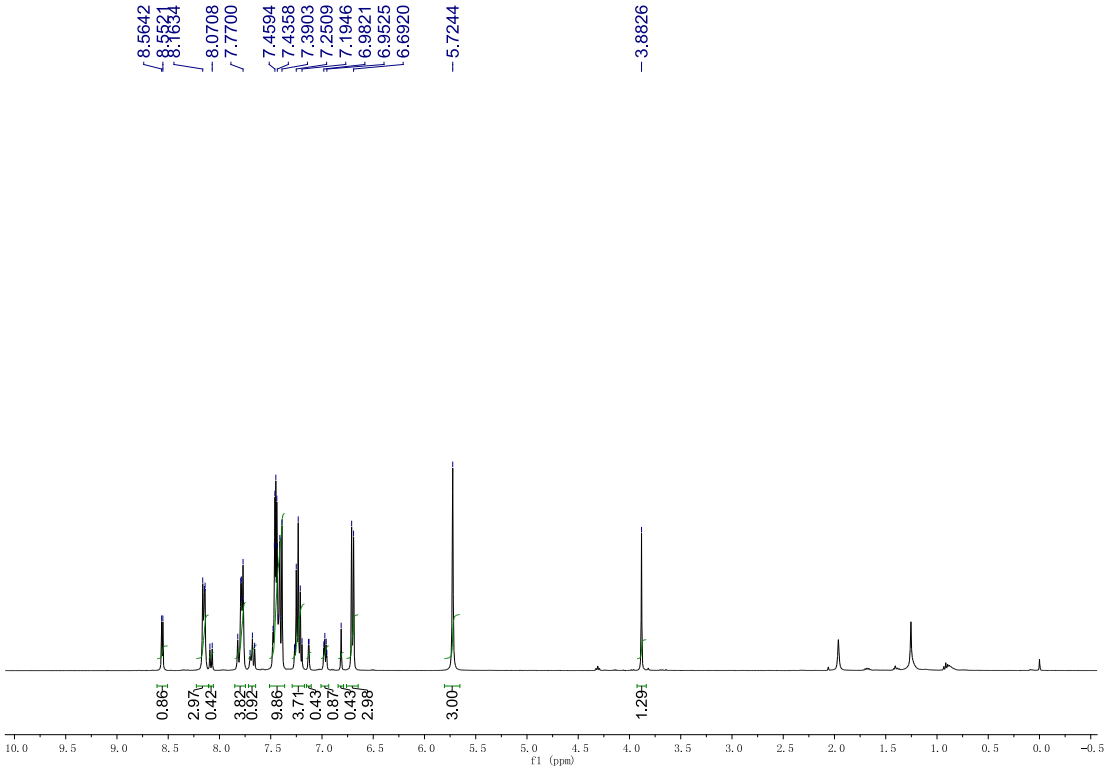
1a-d_n: 45%



2. Competitive Experiment



An equimolar mixture of acetanilide **1i** (0.1 mmol) and **1h** (0.1 mmol), 7-oxabenzonorbornadiene (0.2 mmol), $[Cp^*CoCl_2]_2$ (5 mol %), $AgSbF_6$ (30 mol %), HOAc (0.4 mmol), and DCE (2.0 mL) were charged into a pressure tube under N_2. The reaction mixture was stirred at 50 ℃ for 12 h. The solvent was rapidly removed under reduced pressure and the residue was purified by silica gel chromatography using PE/EA to afford the mixed product. The yield ratio (**3ia**/**3ha** = 2.3:1) was determined on the basis of ^{1}H NMR analysis.



V. References

[1] Ackermann, L.; Lygin, A. V. Org. Lett., **2011**, *13*, 3332.

[2]) Lautens, M.; Fagnou, K.; Yang, D. *J. Am. Chem. Soc.* **2003**, *125*, 14884.

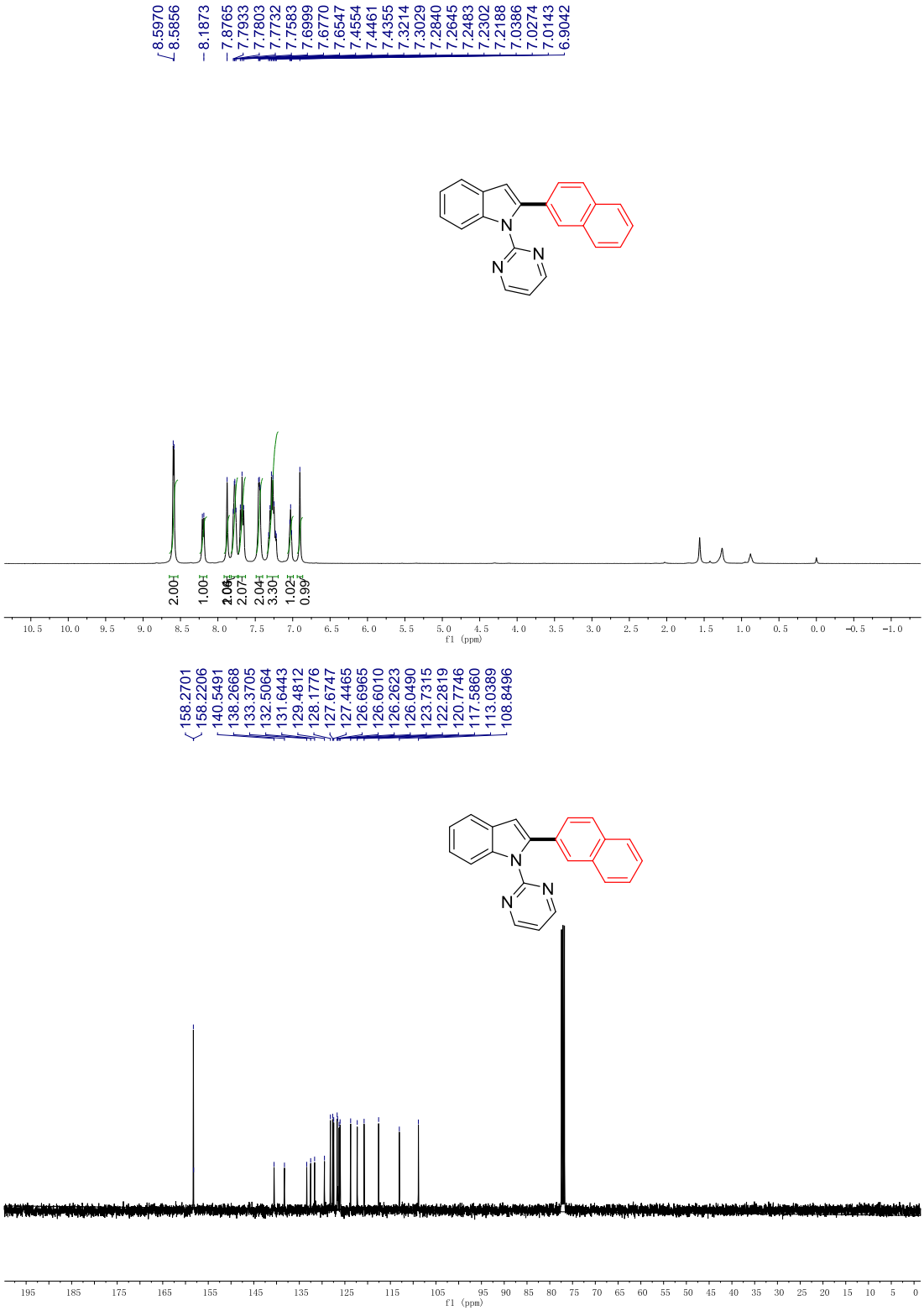
[3] Yoshino, T.; Ikemoto, H., Matsunaga, S.; Kanai, M. *Angew. Chem., Int. Ed*. **2013**, *52*, 2207.

[4] Yu, D.-G.; Gensch, T.; Azambuja, F.; Vá squez-Cé spedes, S.; Glorius, F. *J Am Chem Soc* **2014**, 136, 17722.

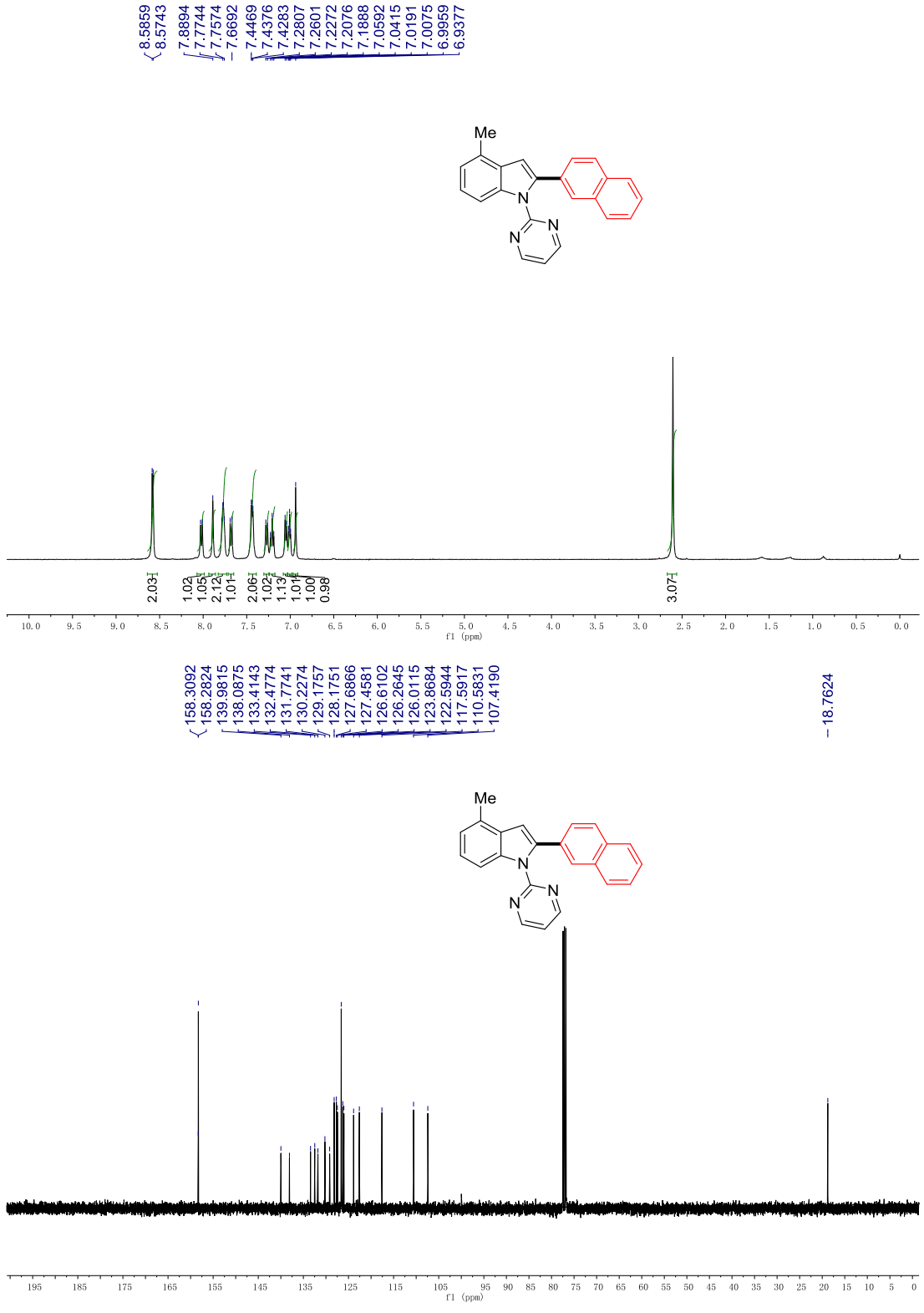
[5] Yu, S.; Li, X. *Org. Lett.* **2014**, *16*, 1200.

VI. NMR Spectra

3aa



3ba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7.7744
7.7574
7.6692
7.4469
7.4376
7.4283
7.2807
7.2601
7.2272
7.2076
7.1888
7.0592
7.0415
7.0191
7.0075
6.9959
6.9377
Me
N
N
N
2.03
1.02
1.05
2.12
1.01
2.06
1.02
1.19
1.01
1.00
0.98
3.07
f1 (ppm)
158.3092
158.2824
139.9815
138.0875
133.4143
132.4774
131.7741
130.2274
129.1757
128.1751
127.6866
127.4581
126.6102
126.2645
126.0115
123.8684
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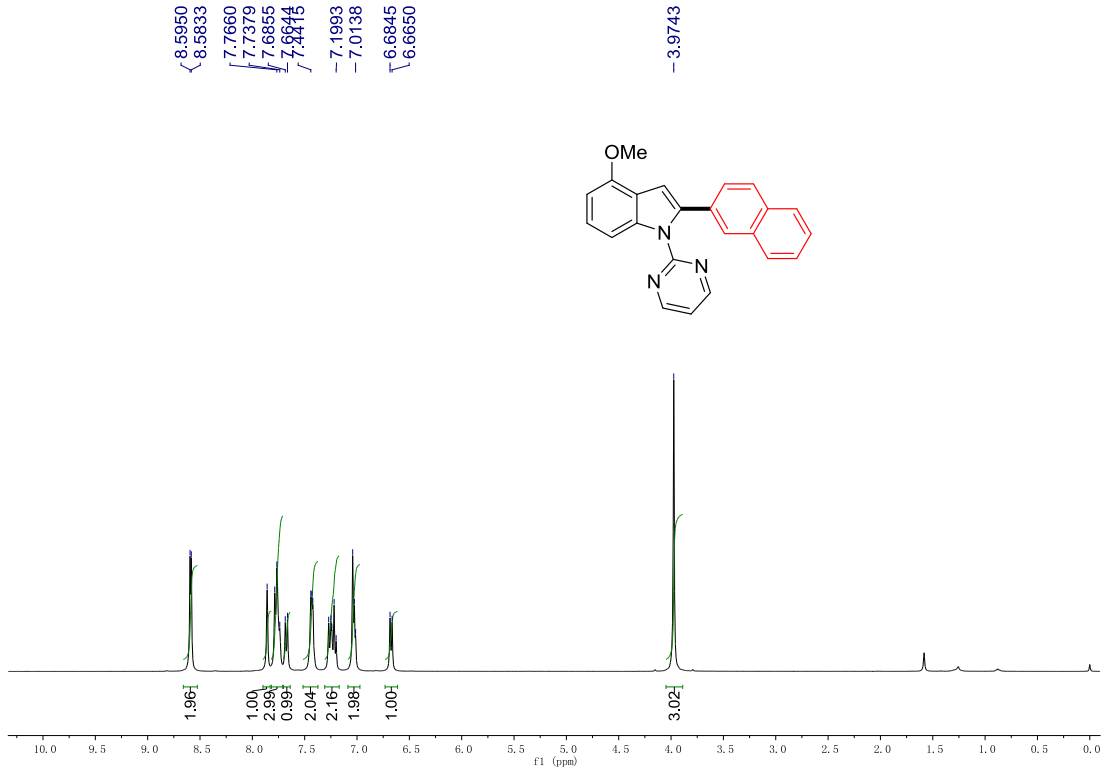
117.5917
110.5831
107.4190
18.7624
Me
N
N
N
f1 (ppm)

3ca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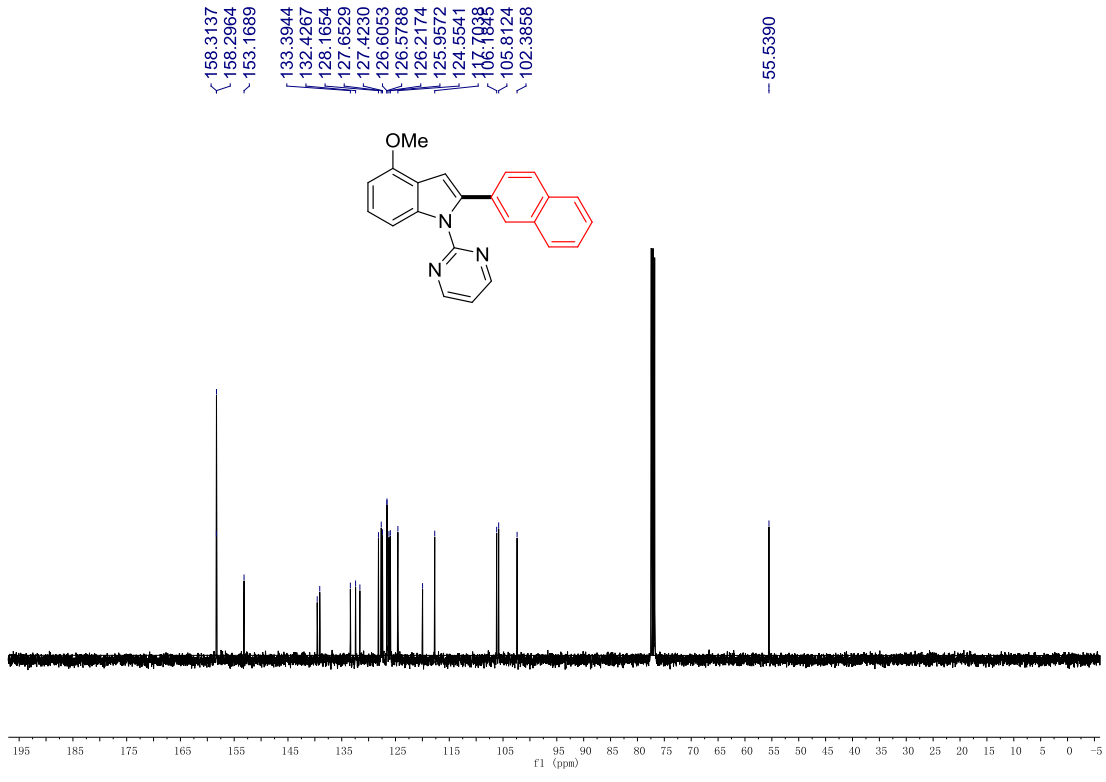
8.5833
7.7660
7.7379
7.6855
7.6644
7.4415
7.1993
7.0138
6.6845
6.6650
3.9743
OMe
N
N
N
1.96
1.00
2.90
0.99
2.04
2.16
1.98
1.00
3.02
f1 (ppm)


158.3137
158.2964
153.1689
133.3944
132.4267
128.1654
127.6529
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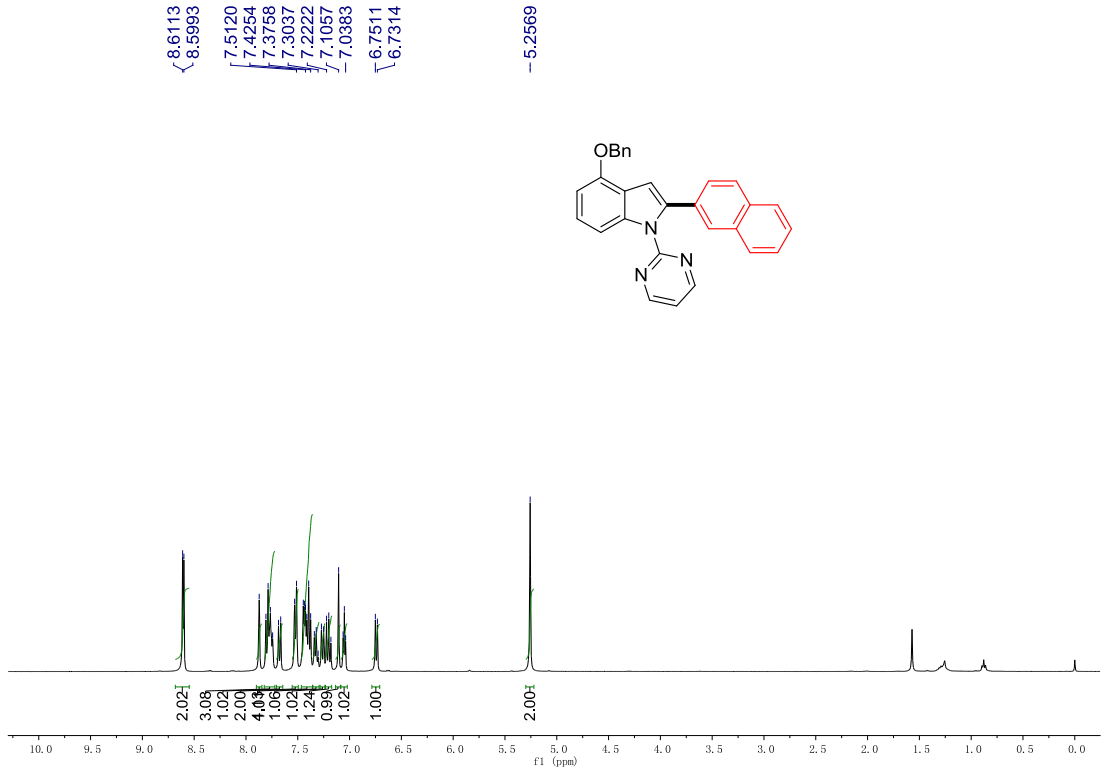
126.2174
125.9572
124.5541
106.1845
105.8124
102.3858
55.5390
OMe
N
N
N
f1 (ppm)

3da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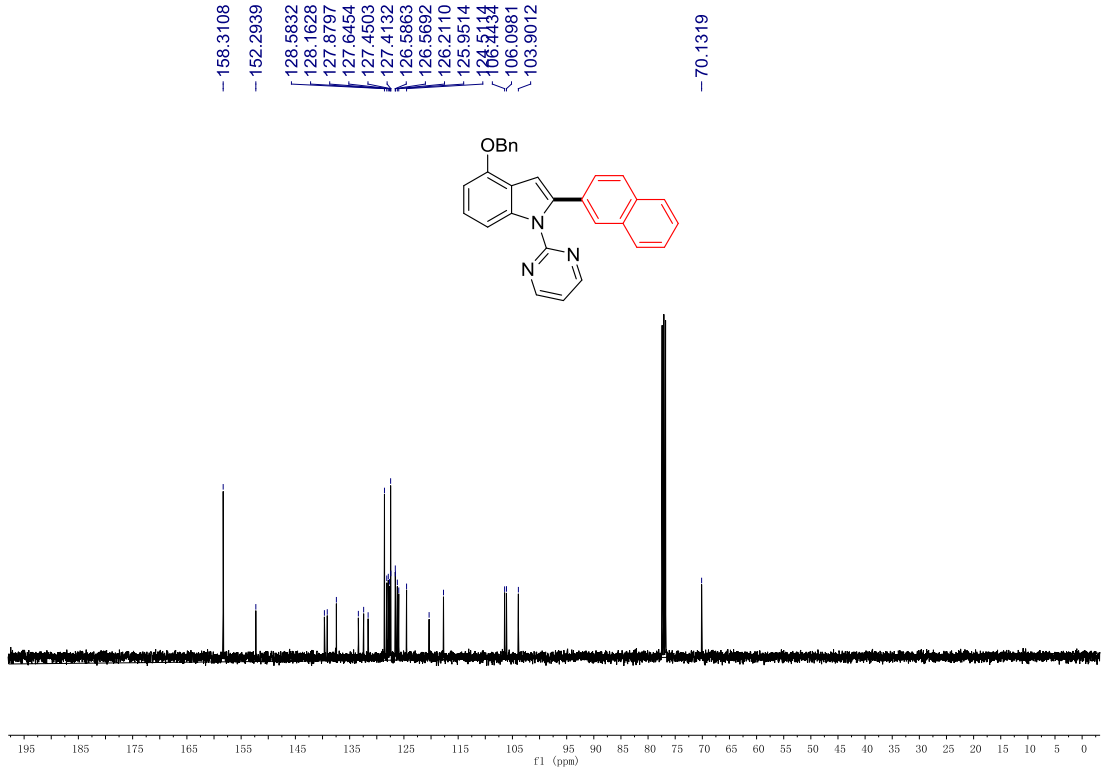
8.5993
7.5120
7.4254
7.3758
7.3037
7.2222
7.1057
7.0383
6.7511
6.7314
5.2569
OBn
N
N
N
2.02
3.08
1.02
2.00
4.03
1.08
1.02
1.24
0.99
1.02
1.00
2.00
f1 (ppm)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152.2939
128.5832
128.1628
127.8797
127.6454
127.4503
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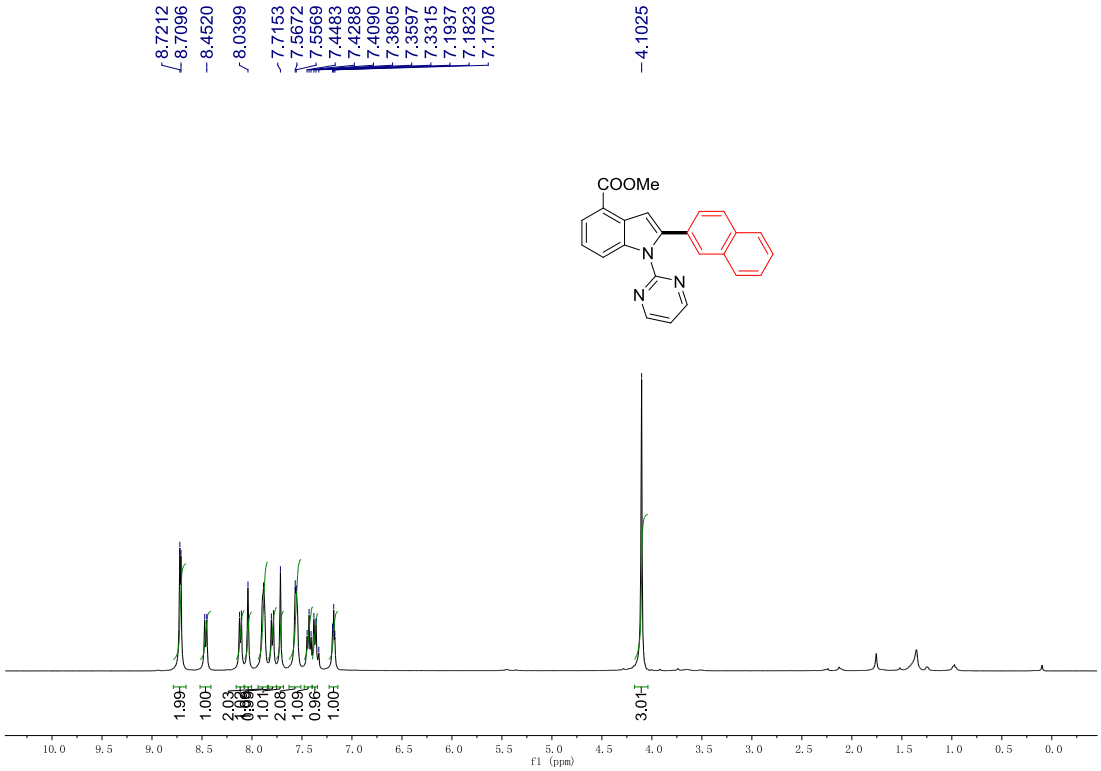
126.5863
126.5692
126.2110
125.9514
124.5134
106.4434
106.0981
103.9012
70.1319
OBn
N
N
N
f1 (ppm)

3ea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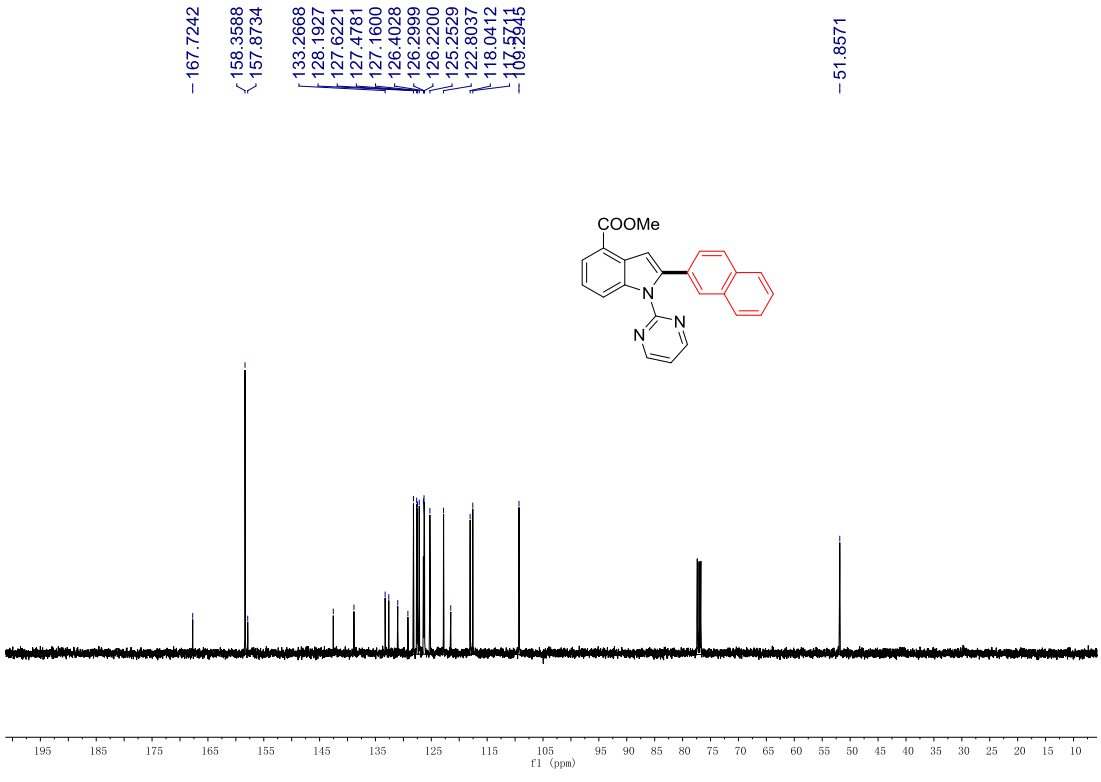
8.7096
8.4520
8.0399
7.7153
7.5672
7.5569
7.4483
7.4288
7.4090
7.3805
7.3597
7.3315
7.1937
7.1823
7.1708
4.1025
COOMe
N
N
1.99
1.00
2.03
1.01
2.08
1.09
0.96
1.00
3.01
f1 (ppm)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128.1927
127.6221
127.4781
127.1600
126.4028
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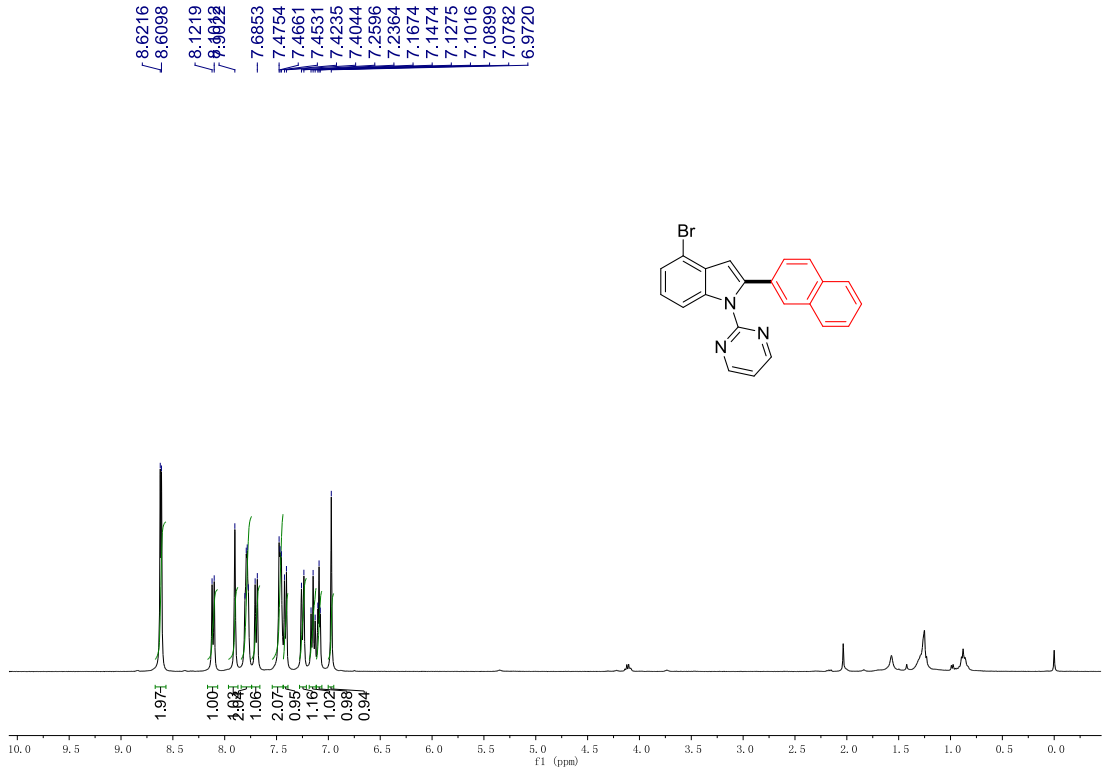
125.2529
122.8037
118.0412
51.8571
COOMe
N
N
f1 (ppm)

3fa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8.6098
8.1219
7.6853
7.4754
7.4661
7.4531
7.4235
7.4044
7.2596
7.2364
7.1674
7.1474
7.1275
7.1016
7.0899
7.0782
6.9720
Br
N
N
N
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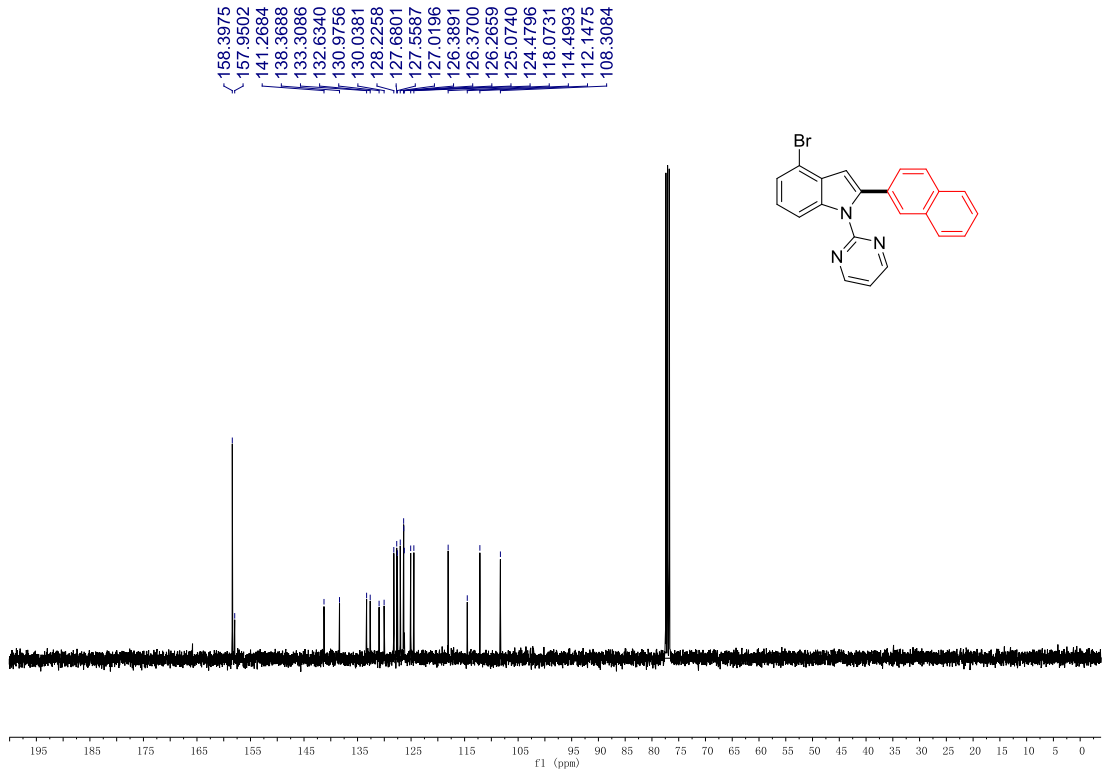
2.03
1.06
2.07
0.95
1.16
1.02
0.98
0.94
f1 (ppm)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127.5587
127.0196
126.3891
126.3700
126.2659
125.0740
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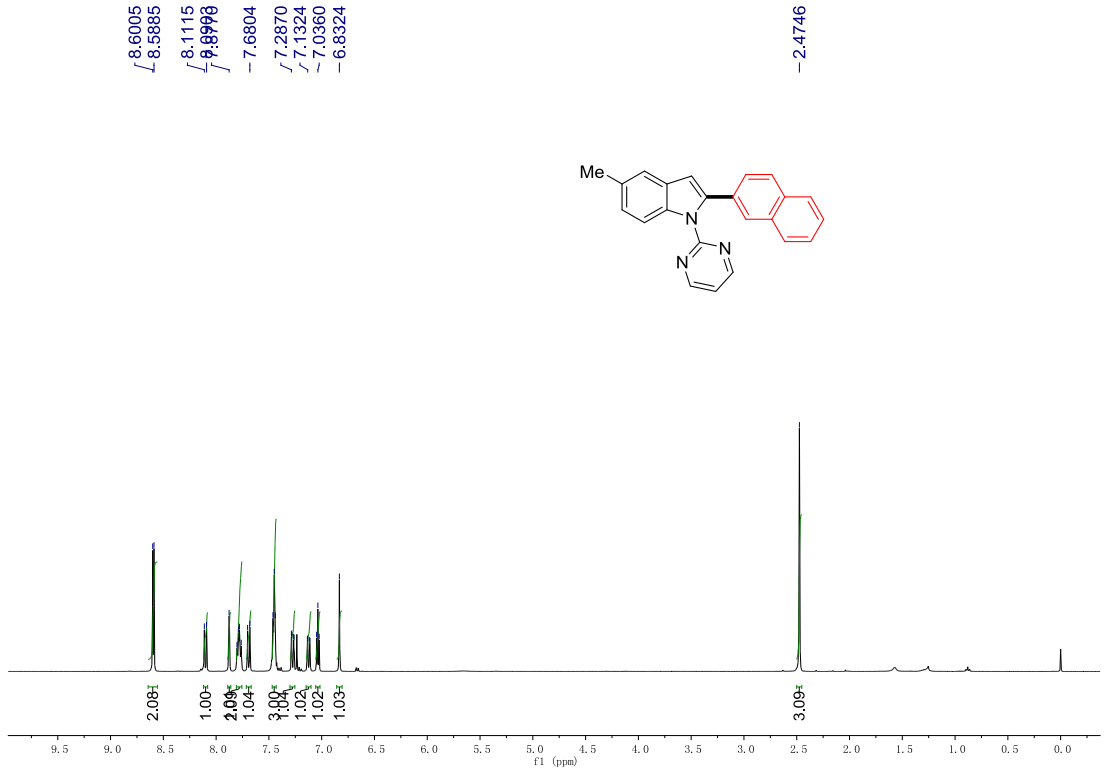
118.0731
114.4993
112.1475
108.3084
Br
N
N
N
f1 (ppm)

3ga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7.2870
7.1324
7.0360
6.8324
2.4746
Me
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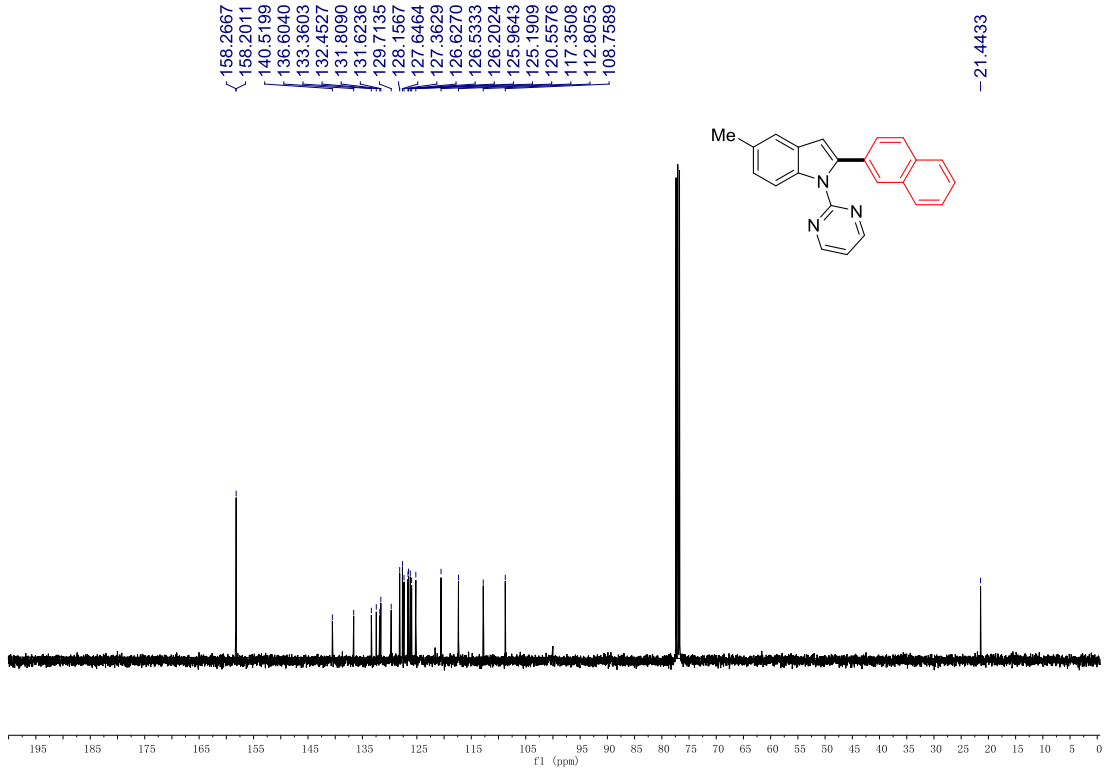
N
2.08
1.00
1.04
3.00
1.02
1.03
3.09
f1 (ppm)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127.6464
127.3629
126.6270
126.5333
126.2024
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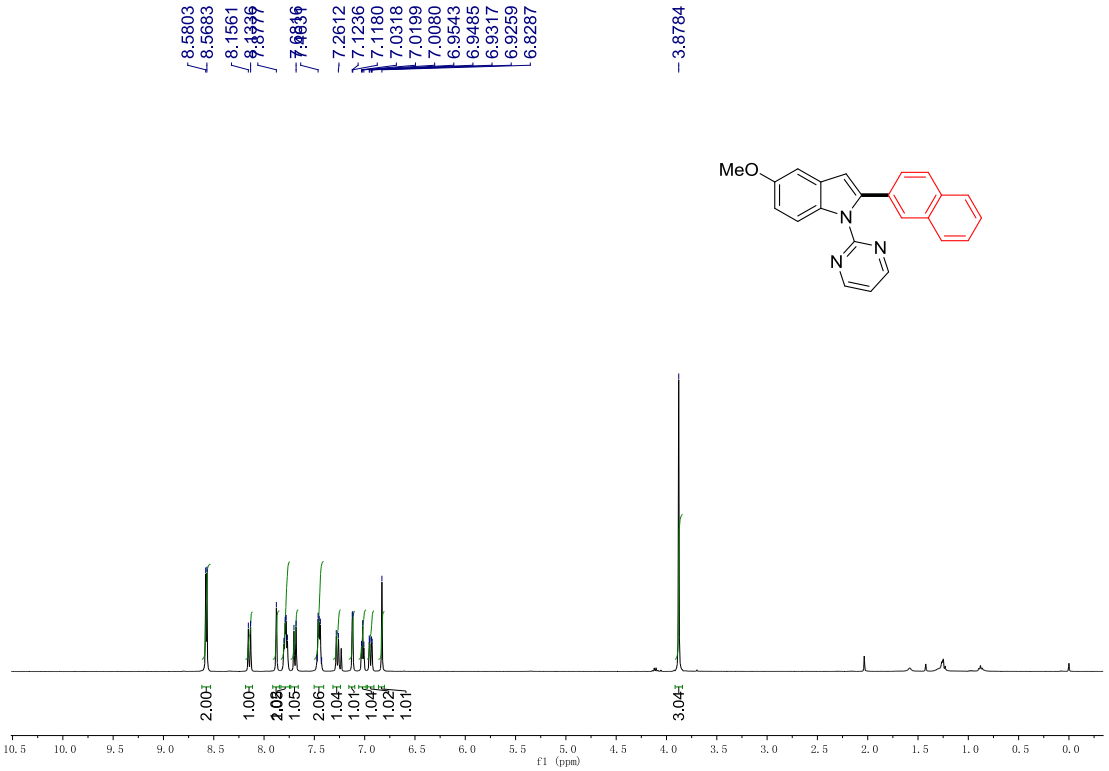
125.1909
120.5576
117.3508
112.8053
108.7589
21.4433
Me
N
N
f1 (ppm)

3ha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6.9485
6.9317
6.9259
6.8287
3.8784
MeO
N
N
N
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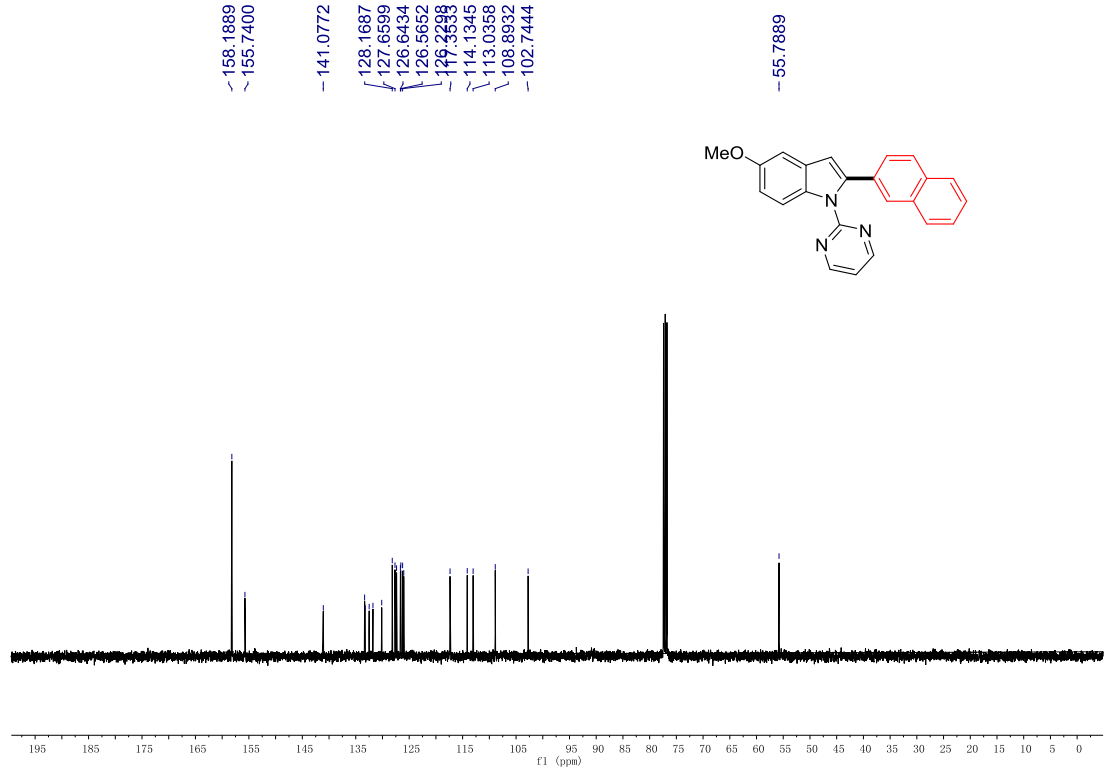
1.05
2.06
1.04
1.01
1.04
1.02
1.01
3.04
f1 (ppm)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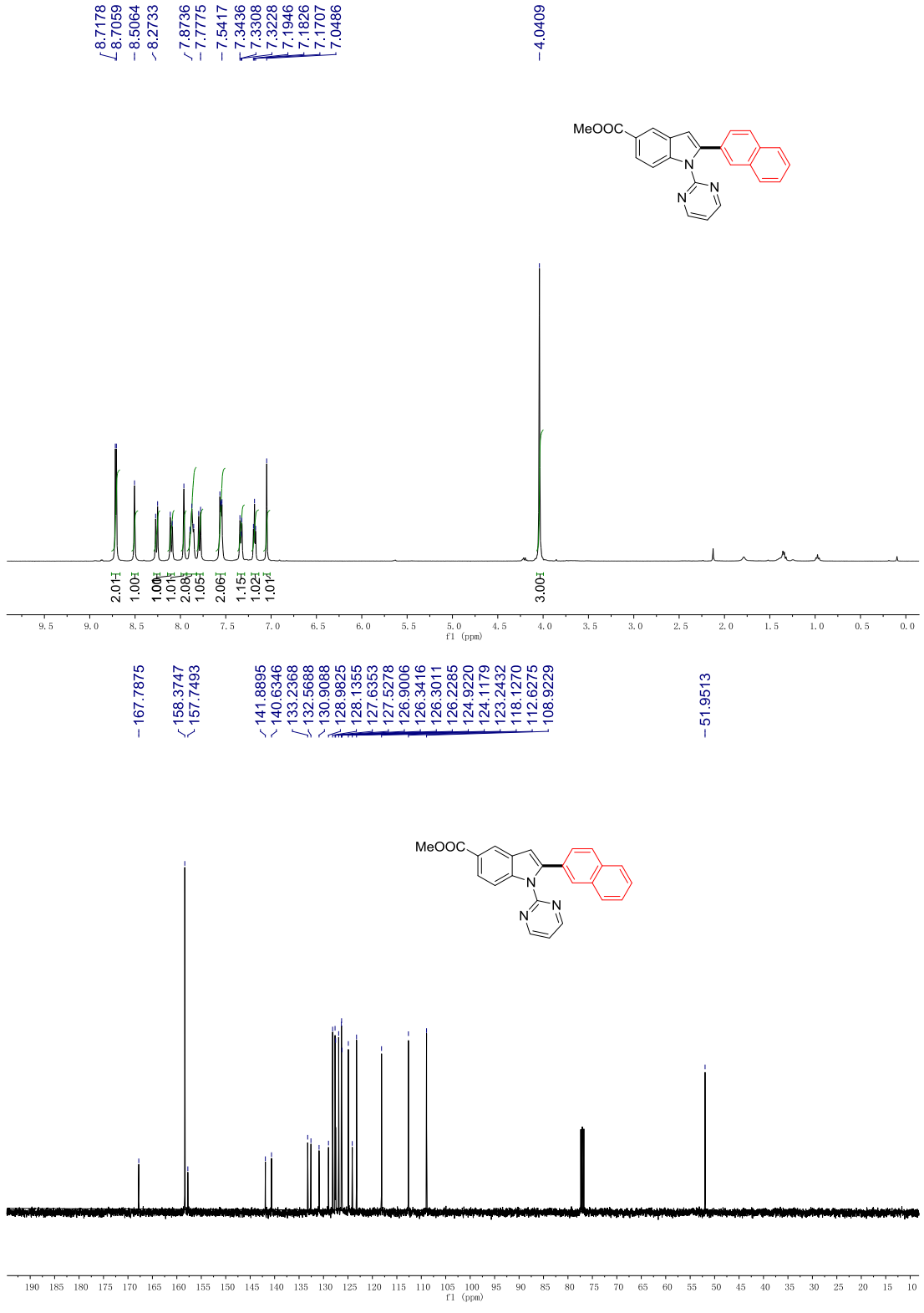
N
N
f1 (ppm)

3ia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7.1946
7.1826
7.1707
7.0486
4.0409
MeOOC
N
N
N
2.01
1.00
1.00
1.01
2.08
1.05
2.06
1.15
1.02
1.01
3.00
f1 (ppm)
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158.3747
157.7493
141.8895
140.6346
133.2368
132.5688
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128.9825
128.1355
127.6353
127.5278
126.9006
126.3416
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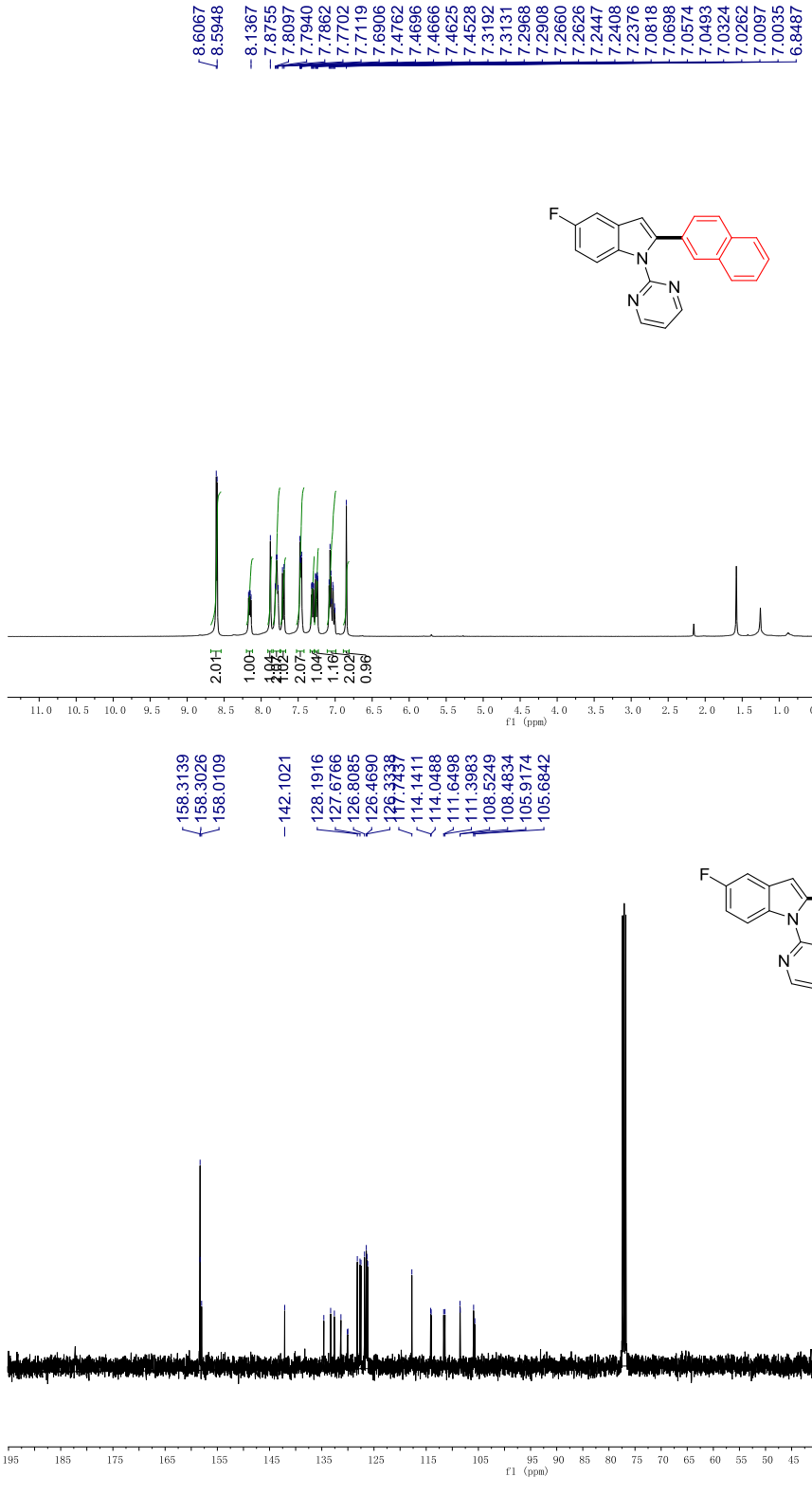
3ja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7.4762
7.4696
7.4666
7.4625
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7.2968
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7.2626
7.2447
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7.2376
7.0818
7.0698
7.0574
7.0493
7.0324
7.0262
7.0097
7.0035
6.8487
F
N
N
N
2.01
1.00
2.07
1.04
1.16
2.02
0.96
f1 (ppm)
158.3139
158.3026
158.0109
142.1021
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126.4690
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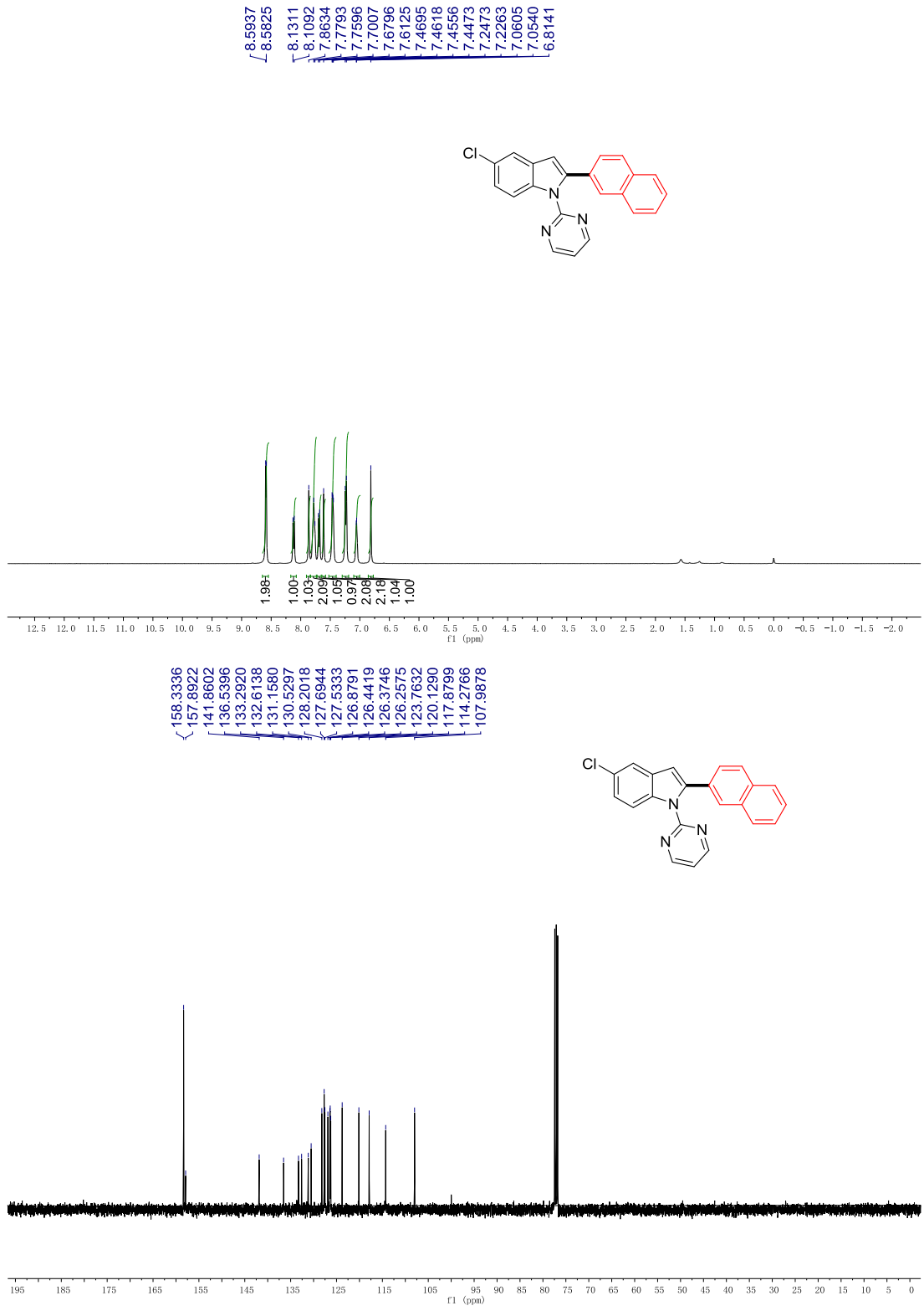
3ka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7.7596
7.7007
7.6796
7.6125
7.4695
7.4618
7.4556
7.4473
7.2473
7.2263
7.0605
7.0540
6.8141
Cl
N
N
N
1.98
1.00
1.03
2.09
1.05
0.97
2.08
2.18
1.04
1.00
f1 (ppm)
158.3336
157.8922
141.8602
136.5396
133.2920
132.6138
131.1580
130.5297
128.2018
127.6944
127.5333
126.8791
126.4419
126.3746
126.2575
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120.1290
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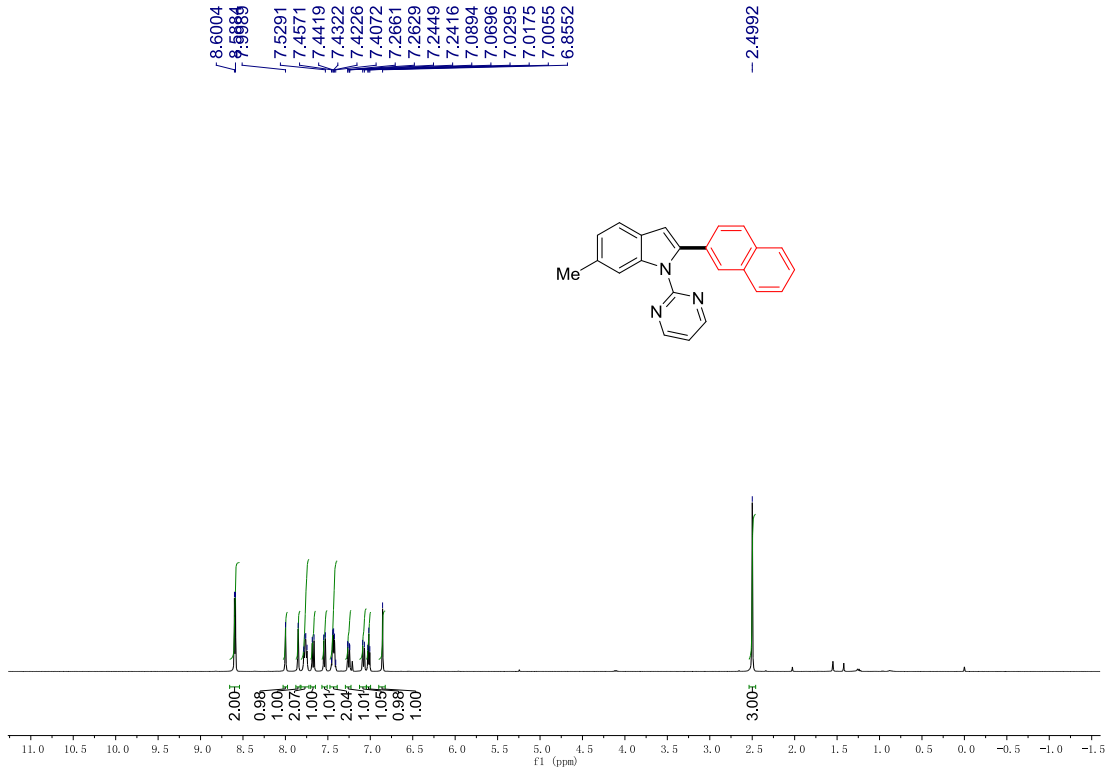
N
f1 (ppm)

3la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7.4226
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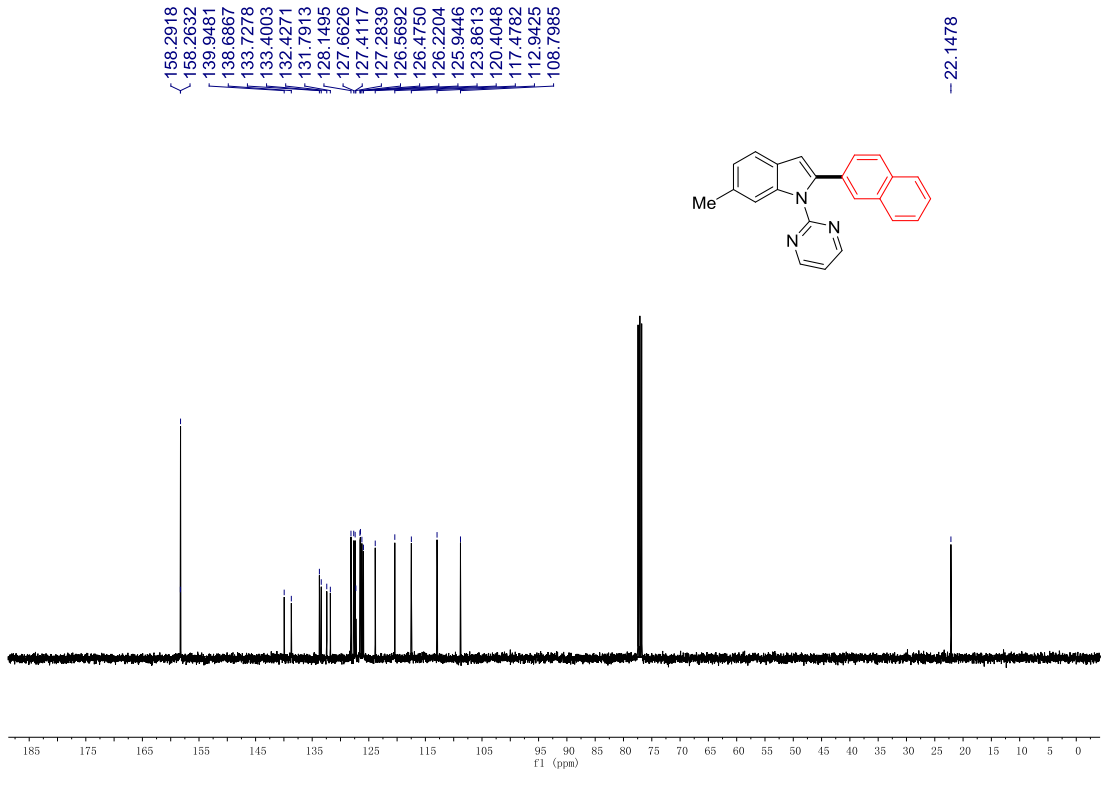
7.2661
7.2629
7.2449
7.2416
7.0894
7.0696
7.0295
7.0175
7.0055
6.8552
2.4992
Me
N
N
N
2.00
0.98
1.00
2.07
1.00
1.01
2.04
1.01
1.05
0.98
1.00
3.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1.0 −1.5
f1 (ppm)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127.4117
127.2839
126.5692
126.4750
126.2204
125.9446
123.8613
120.4048
117.4782
112.9425
108.7985
22.1478
Me
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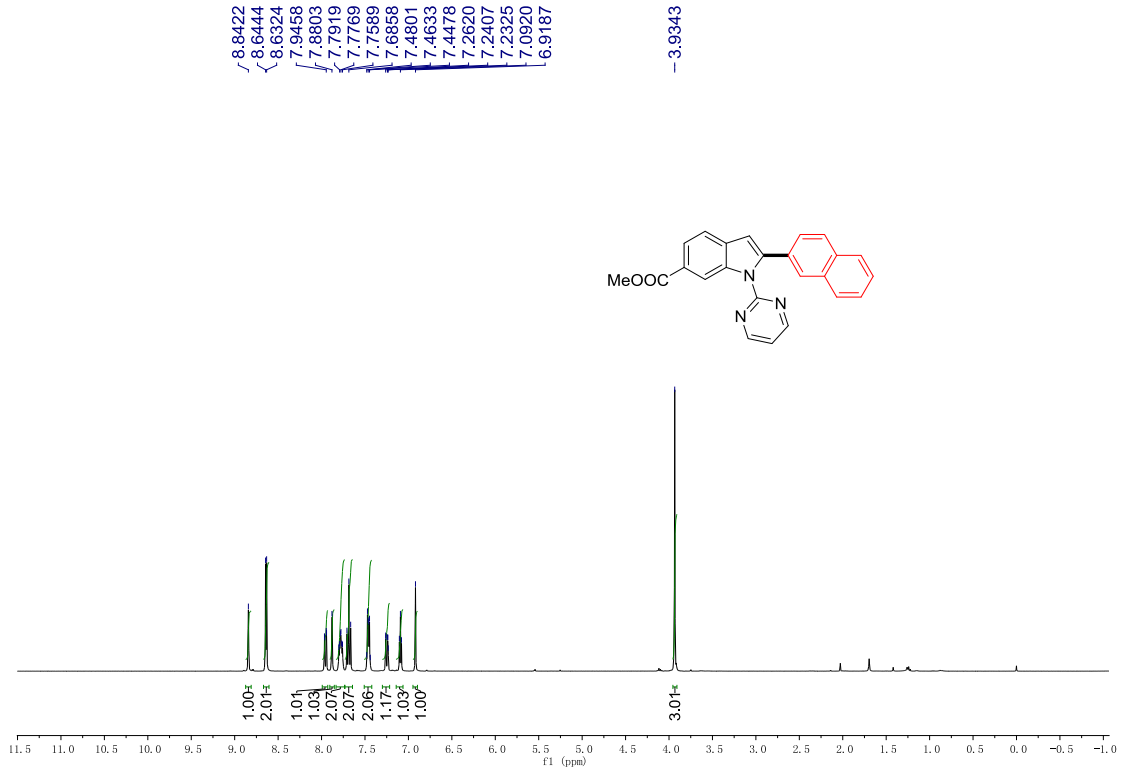
N
N
185 175 165 155 145 135 125 115 105 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)

3ma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7.8803
7.7919
7.7769
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7.6858
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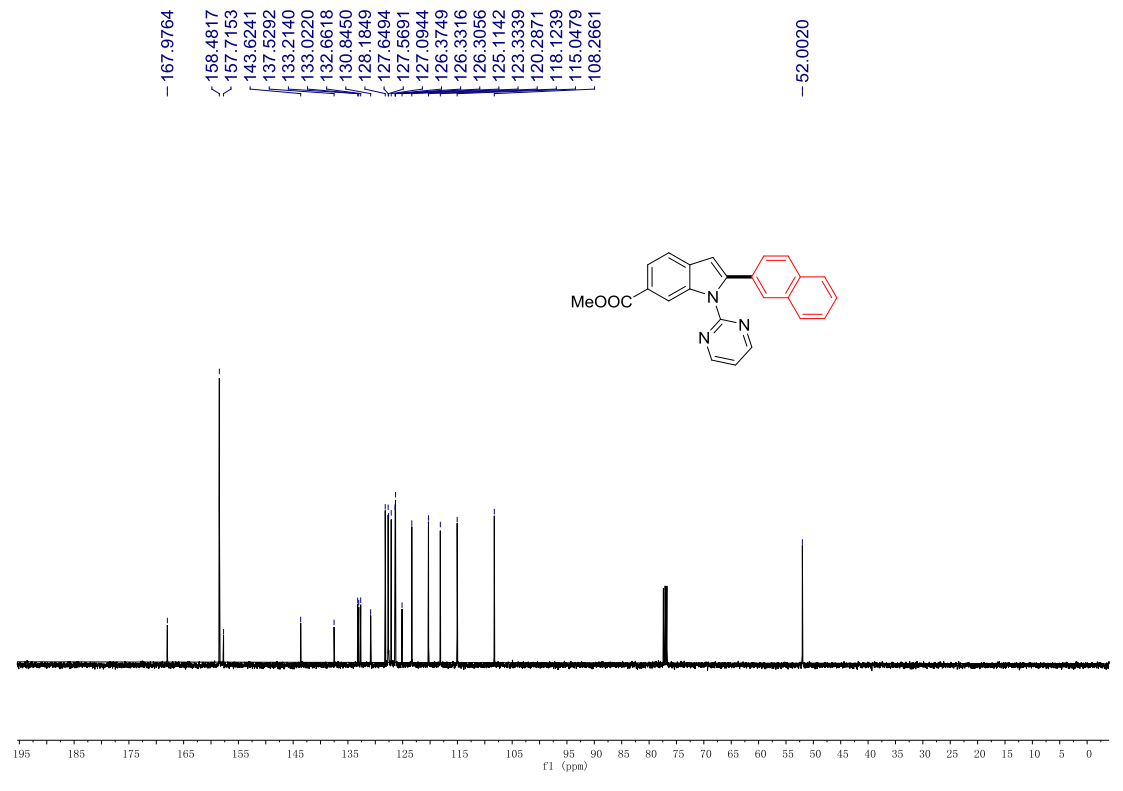
7.4633
7.4478
7.2620
7.2407
7.2325
7.0920
6.9187
3.9343
MeOOC
N
N
N
1.00
2.01
1.01
1.03
2.07
2.07
2.06
1.17
1.03
1.00
3.01
f1 (ppm)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127.5691
127.0944
126.3749
126.3316
126.3056
125.1142
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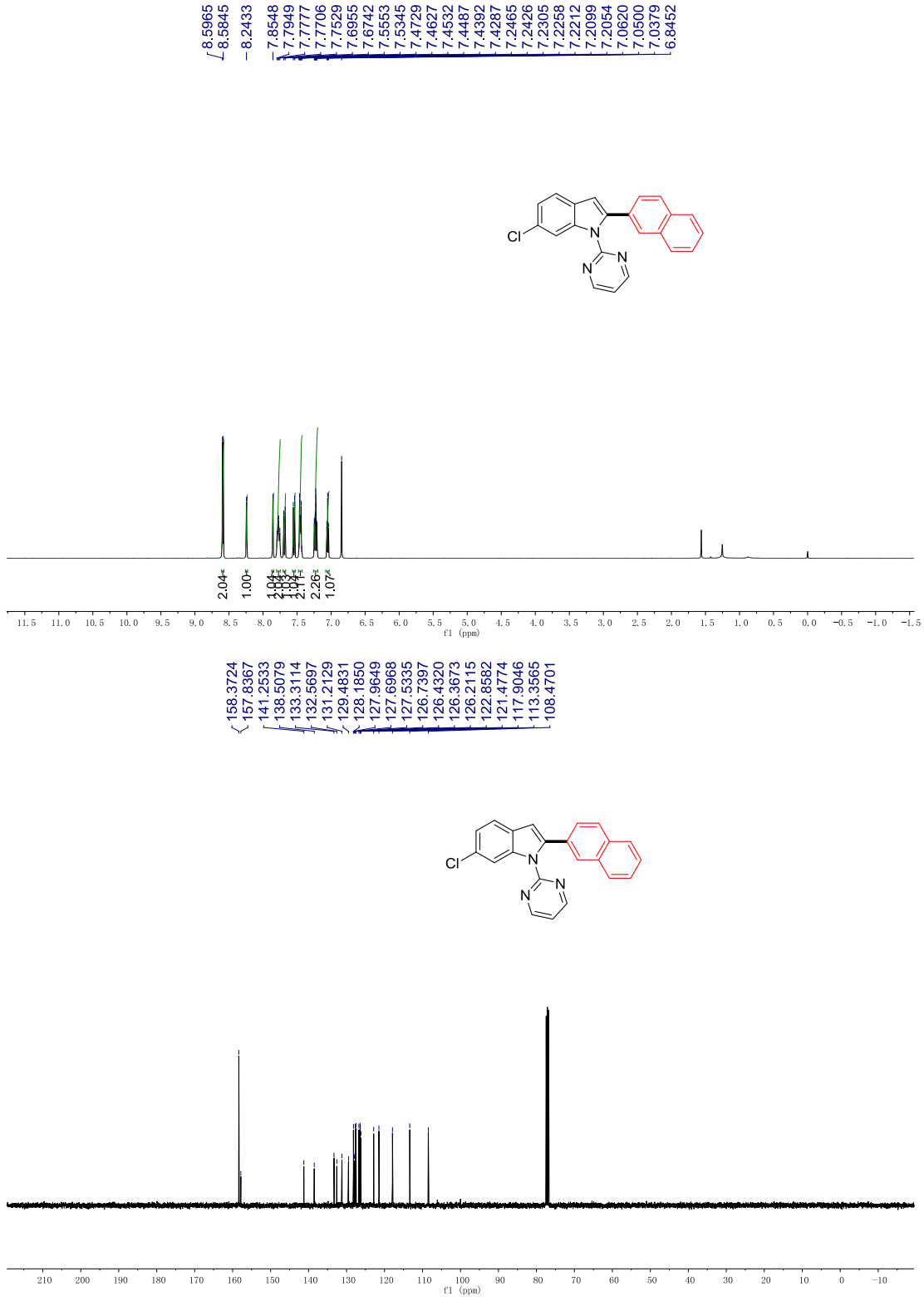
N
f1 (ppm)

3na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7.5345
7.4729
7.4627
7.4532
7.4487
7.4392
7.4287
7.2465
7.2426
7.2305
7.2258
7.2212
7.2099
7.2054
7.0620
7.0500
7.0379
6.8452
Cl
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N
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1.00
1.07
f1 (ppm)
158.3724
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138.5079
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132.5697
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126.4320
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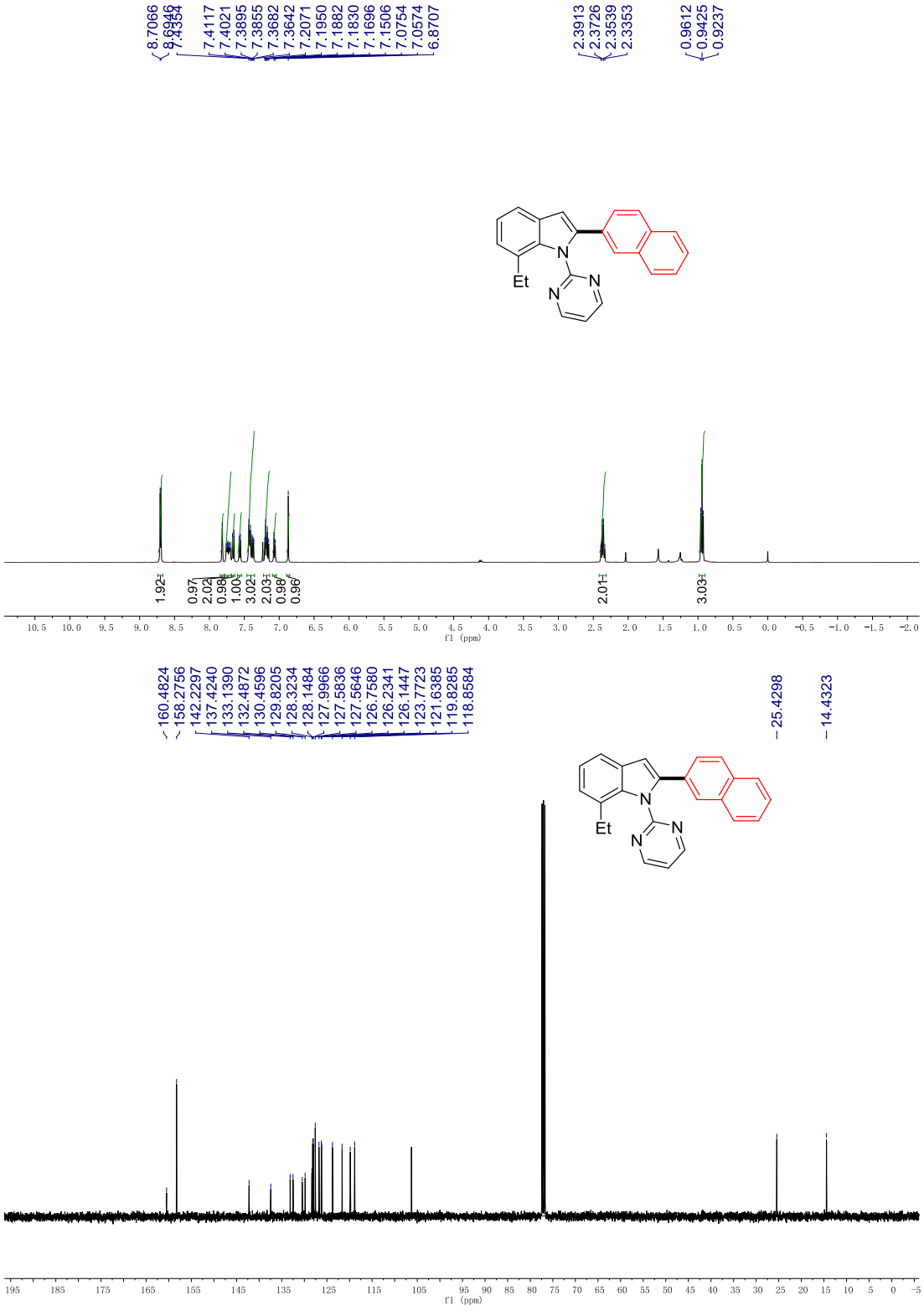
N
f1 (ppm)

3oa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7.3682
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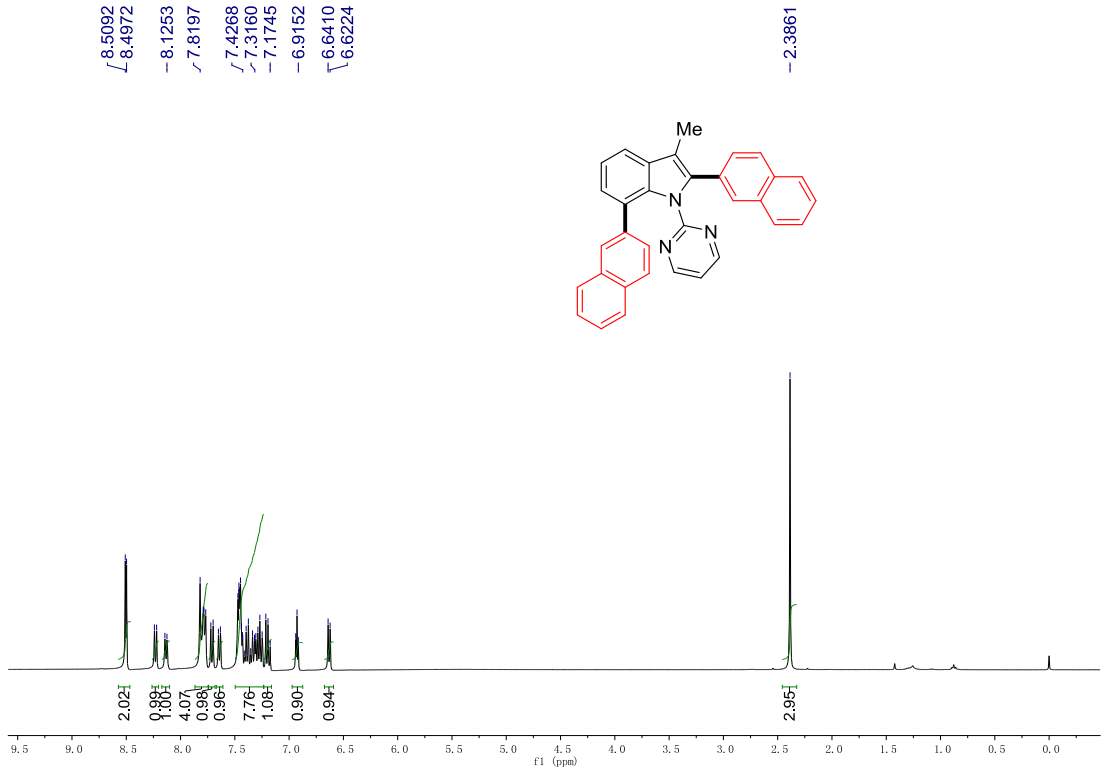
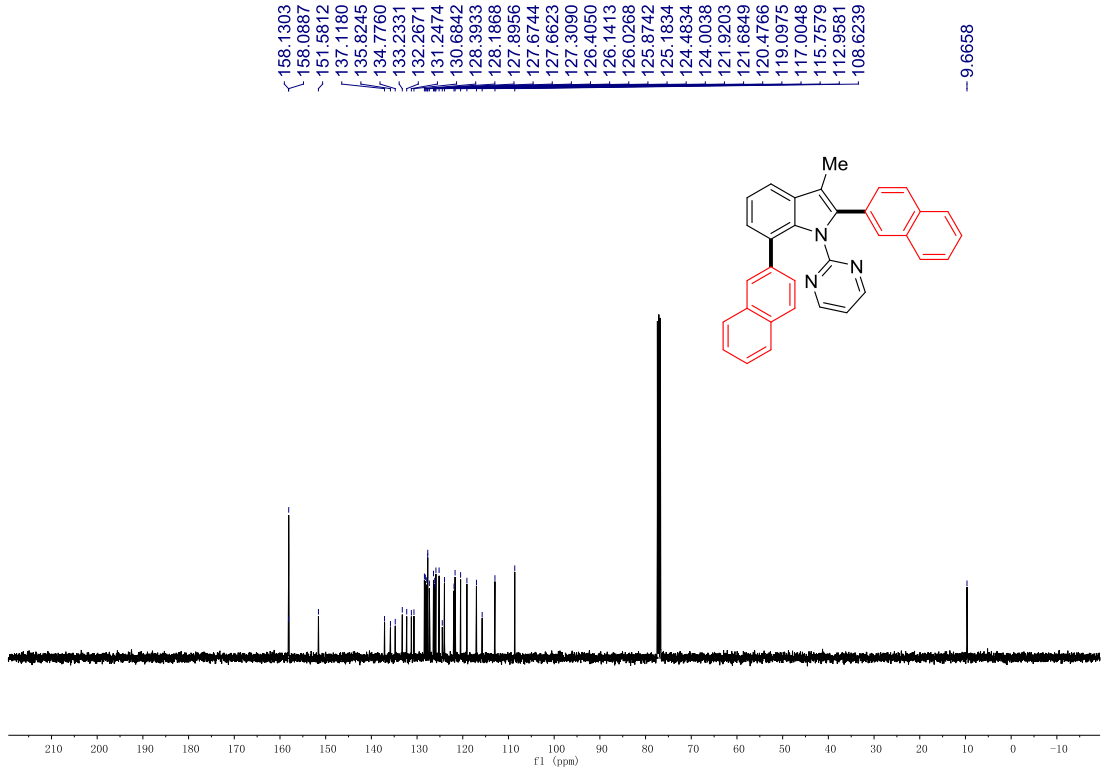
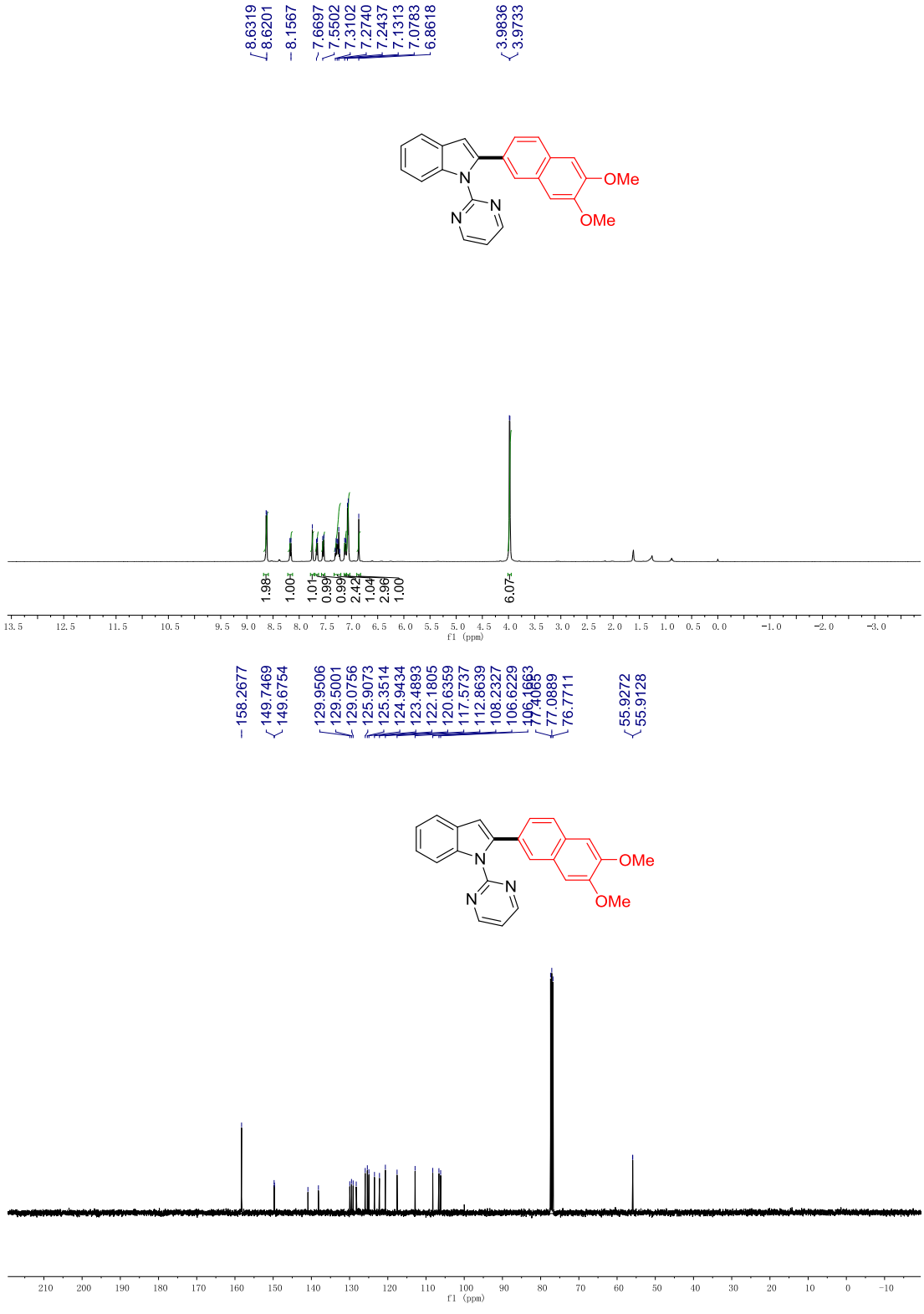
7.2071
7.1950
7.1882
7.1830
7.1696
7.1506
7.0754
7.0574
6.8707
2.3913
2.3726
2.3539
2.3353
0.9612
0.9425
0.9237
Et
N
N
N
1.92
0.97
2.02
0.98
1.00
3.02
2.03
0.98
0.96
2.01
3.03
f1 (ppm)
160.4824
158.2756
142.2297
137.4240
133.1390
132.4872
130.4596
129.8205
128.3234
128.1484
127.9966
127.5836
127.5646
126.7580
126.2341
126.1447
123.7723
121.6385
119.8285
118.8584
25.4298
14.4323
Et
N
N
N
f1 (ppm)

3pa

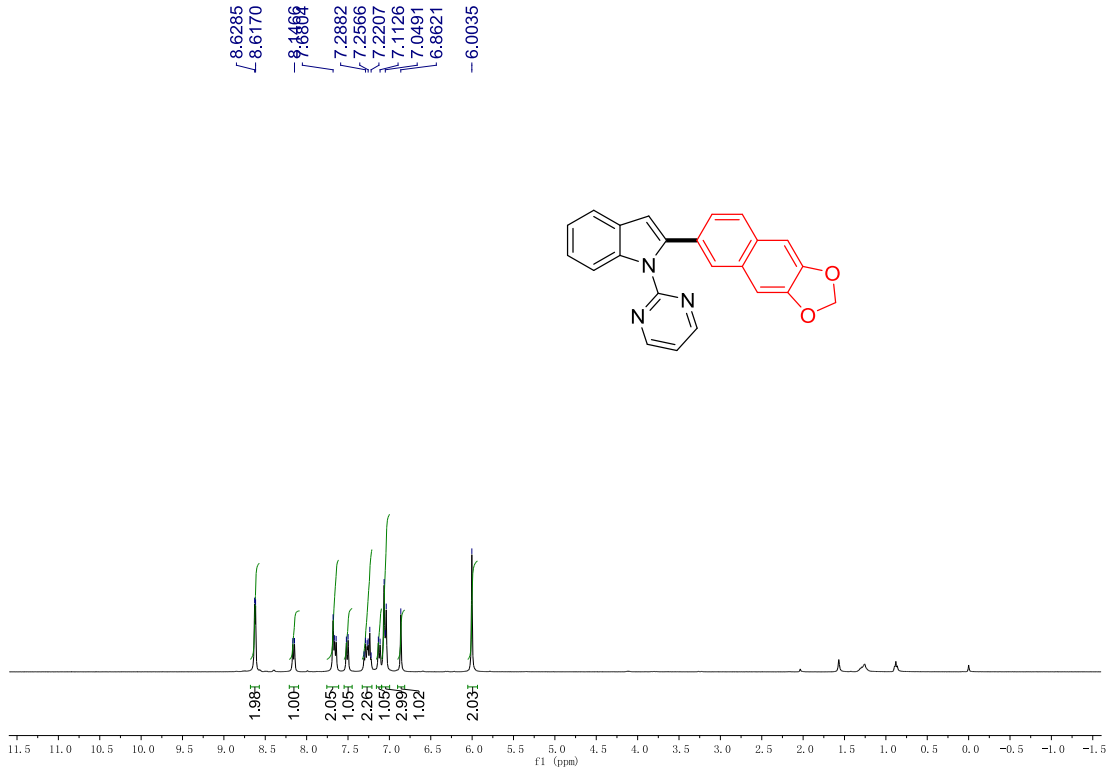

8.5092
8.4972
8.1253
7.8197
7.4268
7.3160
7.1745
6.9152
6.6410
6.6224
2.3861
Me
N
N
N
2.02
0.98
1.01
4.07
0.98
0.96
7.76
1.08
0.90
0.94
2.95
f1 (ppm)

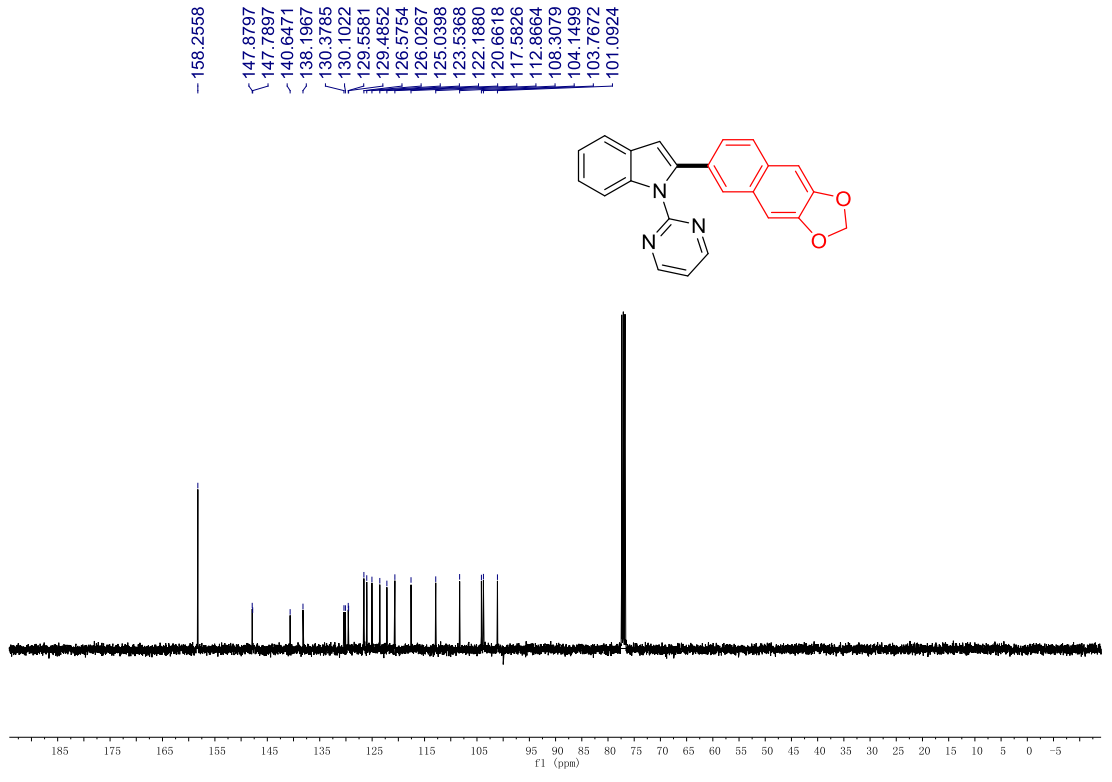

158.1303
158.0887
151.5812
137.1180
135.8245
134.7760
133.2331
132.2671
131.2474
130.6842
128.3933
128.1868
127.8956
127.6744
127.6623
127.3090
126.4050
126.1413
126.0268
125.8742
125.1834
124.4834
124.0038
121.9203
121.6849
120.4766
119.0975
117.0048
115.7579
112.9581
108.6239
9.6658
Me
N
N
N
f1 (ppm)

3ab

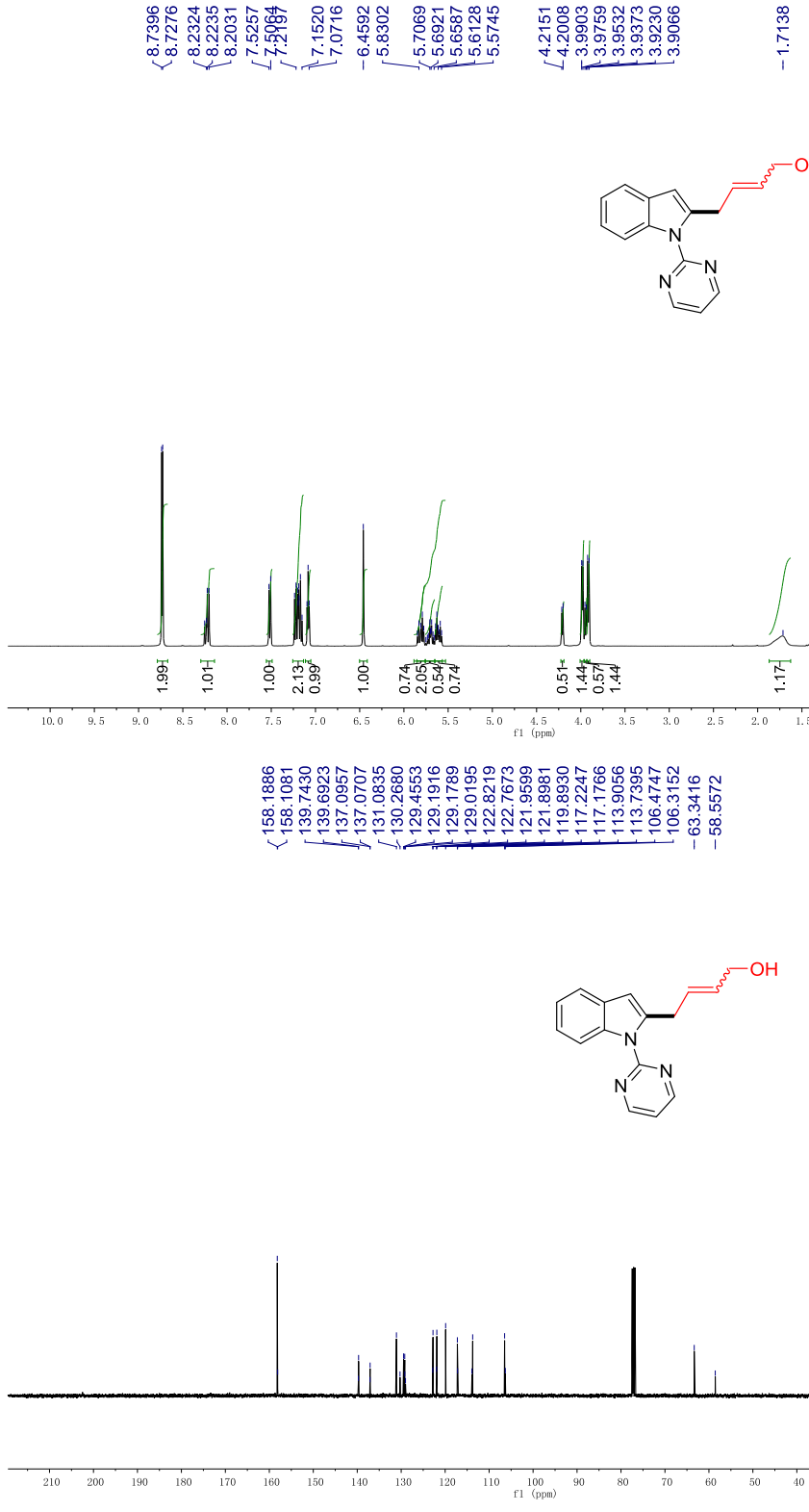

8.6319
8.6201
8.1567
7.6697
7.5502
7.3102
7.2740
7.2437
7.1313
7.0783
6.8618
3.9836
3.9733
OMe
OMe
1.98
1.00
1.01
0.99
0.99
2.42
1.04
2.96
1.00
6.07
f1 (ppm)
158.2677
149.7469
149.6754
129.9506
129.5001
129.0756
125.9073
125.3514
124.9434
123.4893
122.1805
120.6359
117.5737
112.8639
108.2327
106.6229
106.1683
77.4065
77.0889
76.7711
55.9272
55.9128
OMe
OMe
f1 (ppm)

3ac

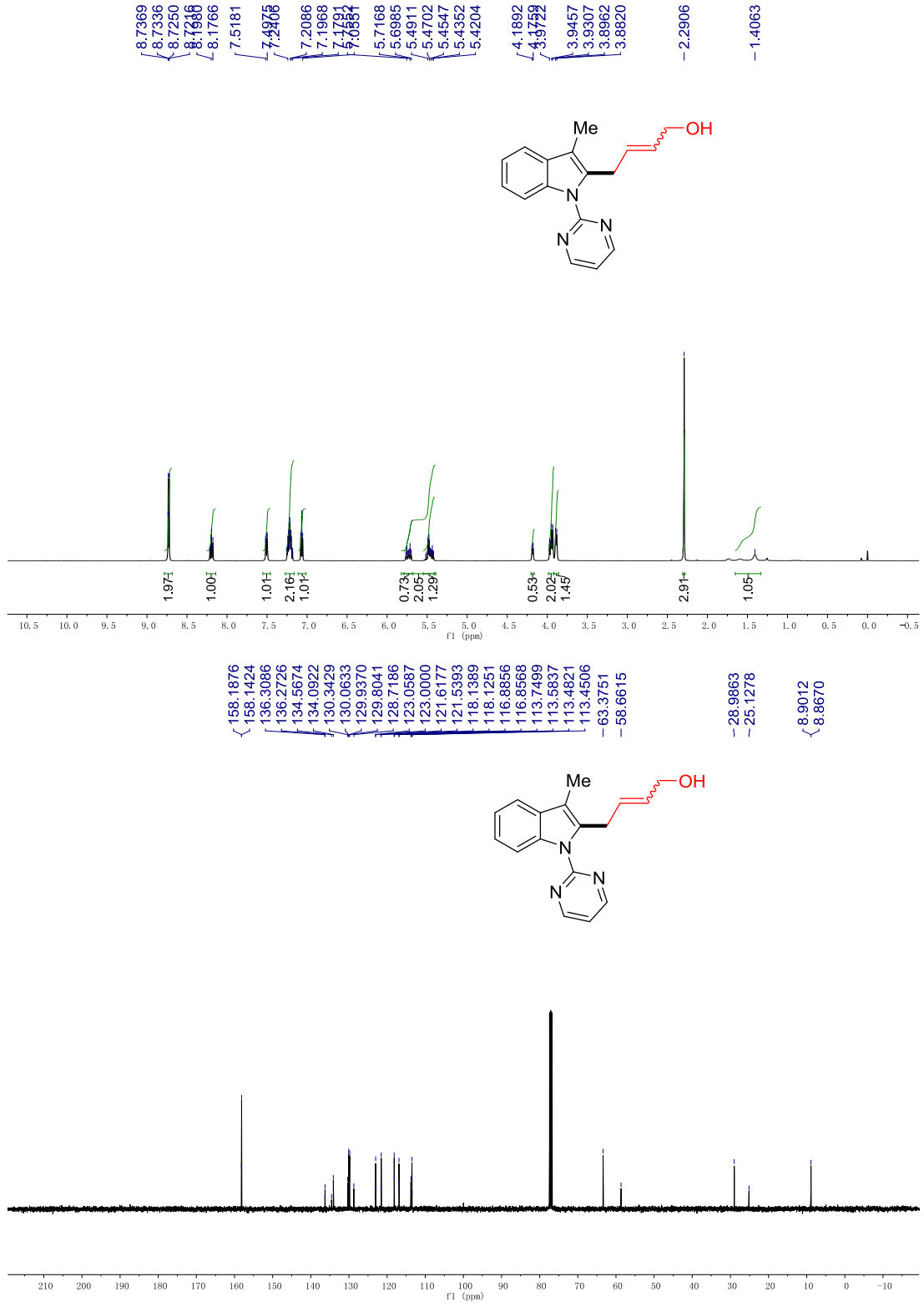

8.6285
8.6170
8.1466
8.1354
7.8864
7.2882
7.2566
7.2207
7.1126
7.0491
6.8621
6.0035
1.98
1.00
2.05
1.05
2.26
1.05
2.99
1.02
2.03
f1 (ppm)


158.2558
147.8797
147.7897
140.6471
138.1967
130.3785
130.1022
129.5581
129.4852
126.5754
126.0267
125.0398
123.5368
122.1880
120.6618
117.5826
112.8664
108.3079
104.1499
103.7672
101.0924
f1 (ppm)

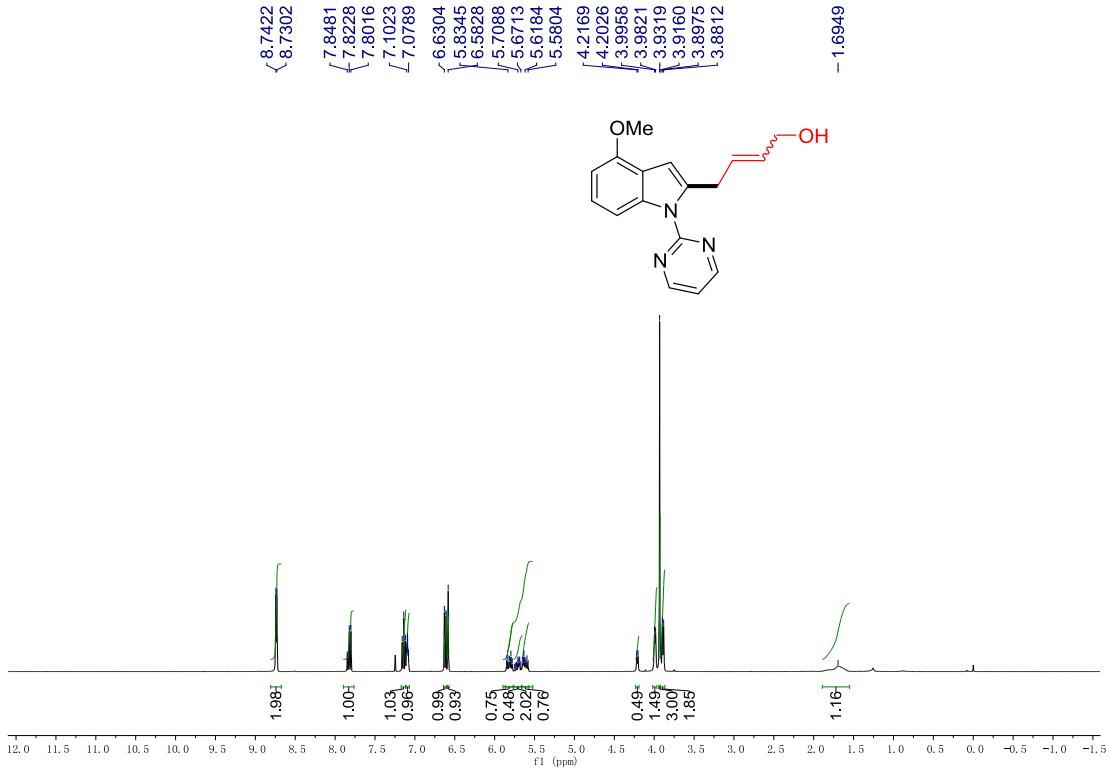
5a

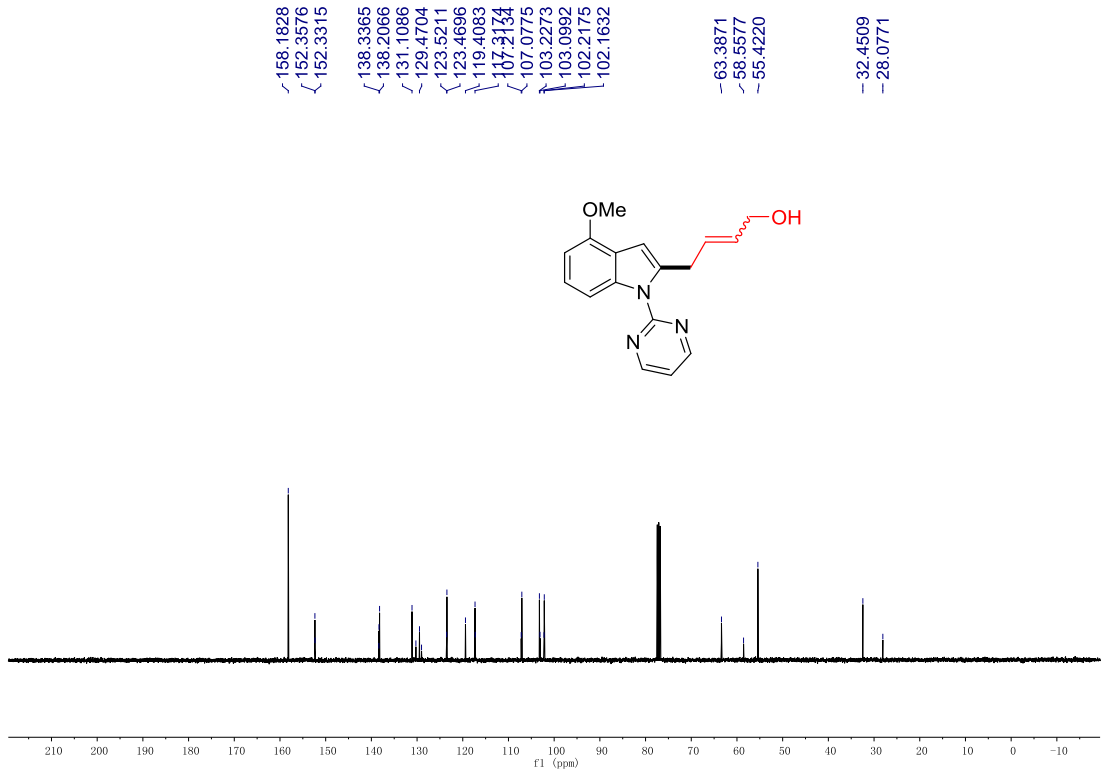

8.7396
8.7276
8.2324
8.2235
8.2031
7.5257
7.5064
7.2197
7.1520
7.0716
6.4592
5.8302
5.7069
5.6921
5.6587
5.6128
5.5745
4.2151
4.2008
3.9903
3.9759
3.9532
3.9373
3.9230
3.9066
1.7138
OH
N
N
N
1.99
1.01
1.00
2.13
0.99
1.00
0.74
2.05
0.54
0.74
0.51
1.44
0.57
1.44
1.17
f1 (ppm)
158.1886
158.1081
139.7430
139.6923
137.0957
137.0707
131.0835
130.2680
129.4553
129.1916
129.1789
129.0195
122.8219
122.7673
121.9599
121.8981
119.8930
117.2247
117.1766
113.9056
113.7395
106.4747
106.3152
63.3416
58.5572
32.4814
28.1432
OH
N
N
N
f1 (ppm)

5b

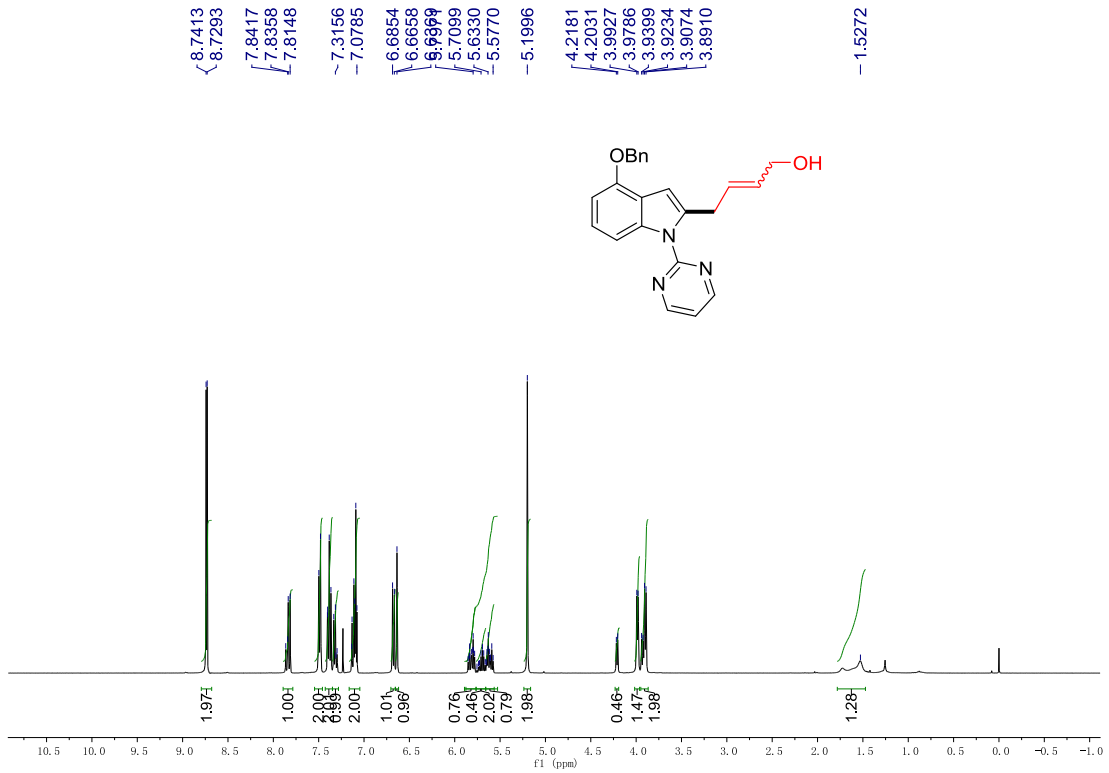

8.7369
8.7336
8.7250
8.1766
7.5181
7.2086
7.1968
5.7168
5.6985
5.4911
5.4702
5.4547
5.4352
5.4204
4.1892
3.9722
3.9457
3.9307
3.8962
3.8820
2.2906
1.4063
Me
OH
N
N
N
1.97
1.00
1.01
2.16
1.01
0.73
2.05
1.29
0.53
2.02
1.45
2.91
1.05
f1 (ppm)
158.1876
158.1424
136.3086
136.2726
134.5674
134.0922
130.3429
130.0633
129.9370
129.8041
128.7186
123.0587
123.0000
121.6177
121.5393
118.1389
118.1251
116.8856
116.8568
113.7499
113.5837
113.4821
113.4506
63.3751
58.6615
28.9863
25.1278
8.9012
8.8670
Me
OH
N
N
N
f1 (ppm)

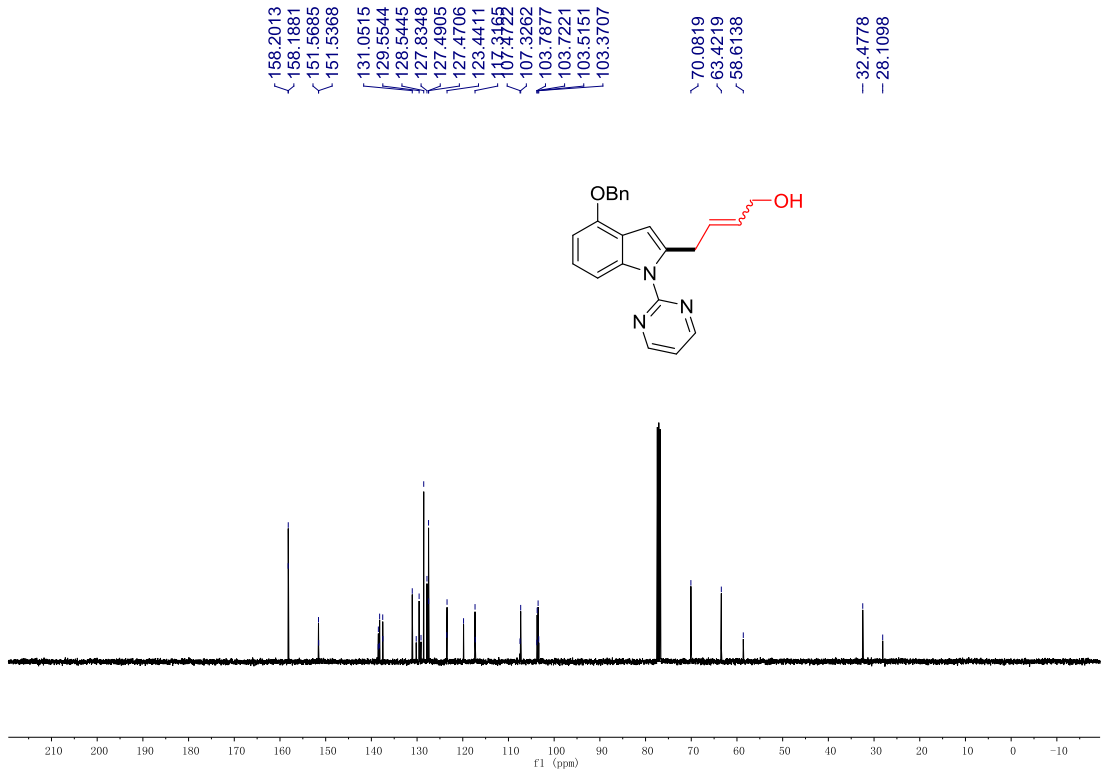
5c


8.7422
8.7302
7.8481
7.8228
7.8016
7.1023
7.0789
6.6304
5.8345
6.5828
5.7088
5.6713
5.6184
5.5804
4.2169
4.2026
3.9958
3.9821
3.9319
3.9160
3.8975
3.8812
1.6949
OMe
OH
N
N
N
1.98
1.00
1.03
0.96
0.99
0.93
0.75
0.48
2.02
0.76
0.49
1.49
3.00
1.85
1.16
f1 (ppm)

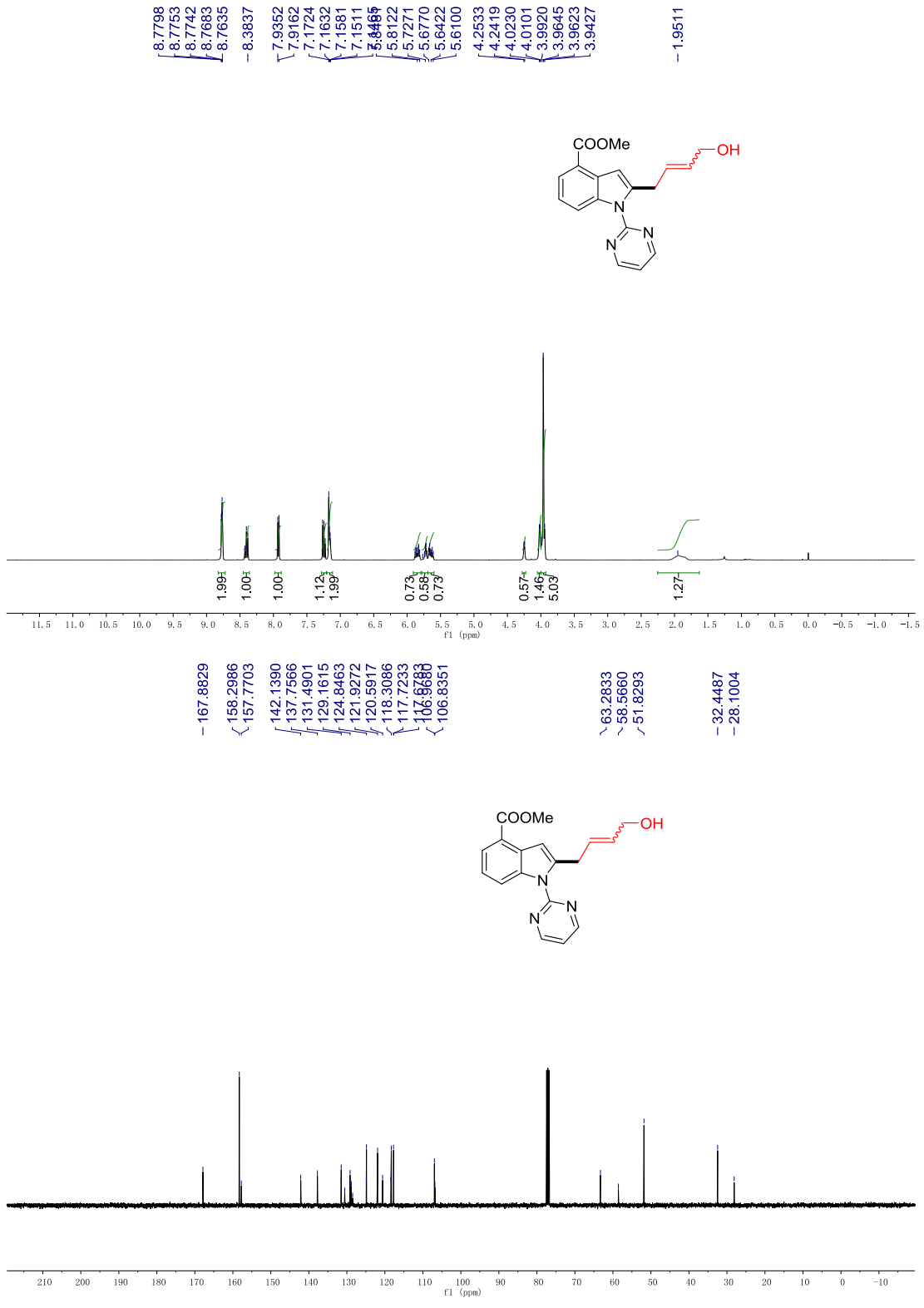

158.1828
152.3576
152.3315
138.3365
138.2066
131.1086
129.4704
123.5211
123.4696
119.4083
117.3174
117.2134
107.0775
103.2273
103.0992
102.2175
102.1632
63.3871
58.5577
55.4220
32.4509
28.0771
OMe
OH
N
N
N
f1 (ppm)

5d

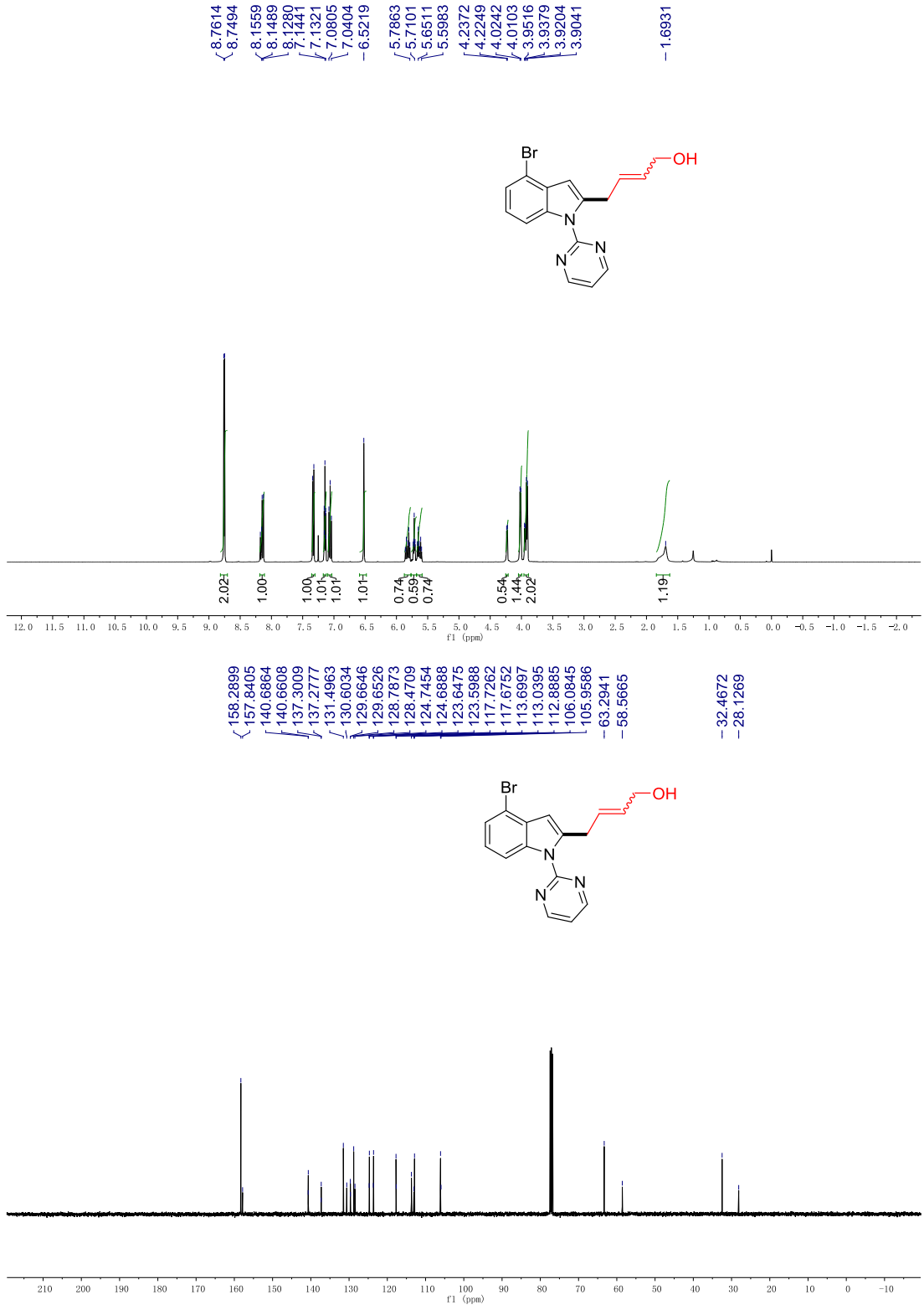

8.7413
8.7293
7.8417
7.8358
7.8148
7.3156
7.0785
6.6854
6.6658
5.7099
5.6330
5.5770
5.1996
4.2181
4.2031
3.9927
3.9786
3.9399
3.9234
3.9074
3.8910
1.5272
OBn
OH
N
N
N
1.97
1.00
2.00
2.00
1.01
0.98
0.76
0.46
2.02
0.79
1.98
0.46
1.47
1.98
1.28
f1 (ppm)


158.2013
158.1881
151.5685
151.5368
131.0515
129.5544
128.5445
127.8348
127.4905
127.4706
123.4411
107.3262
103.7877
103.7221
103.5151
103.3707
70.0819
63.4219
58.6138
32.4778
28.1098
OBn
OH
N
N
N
f1 (ppm)

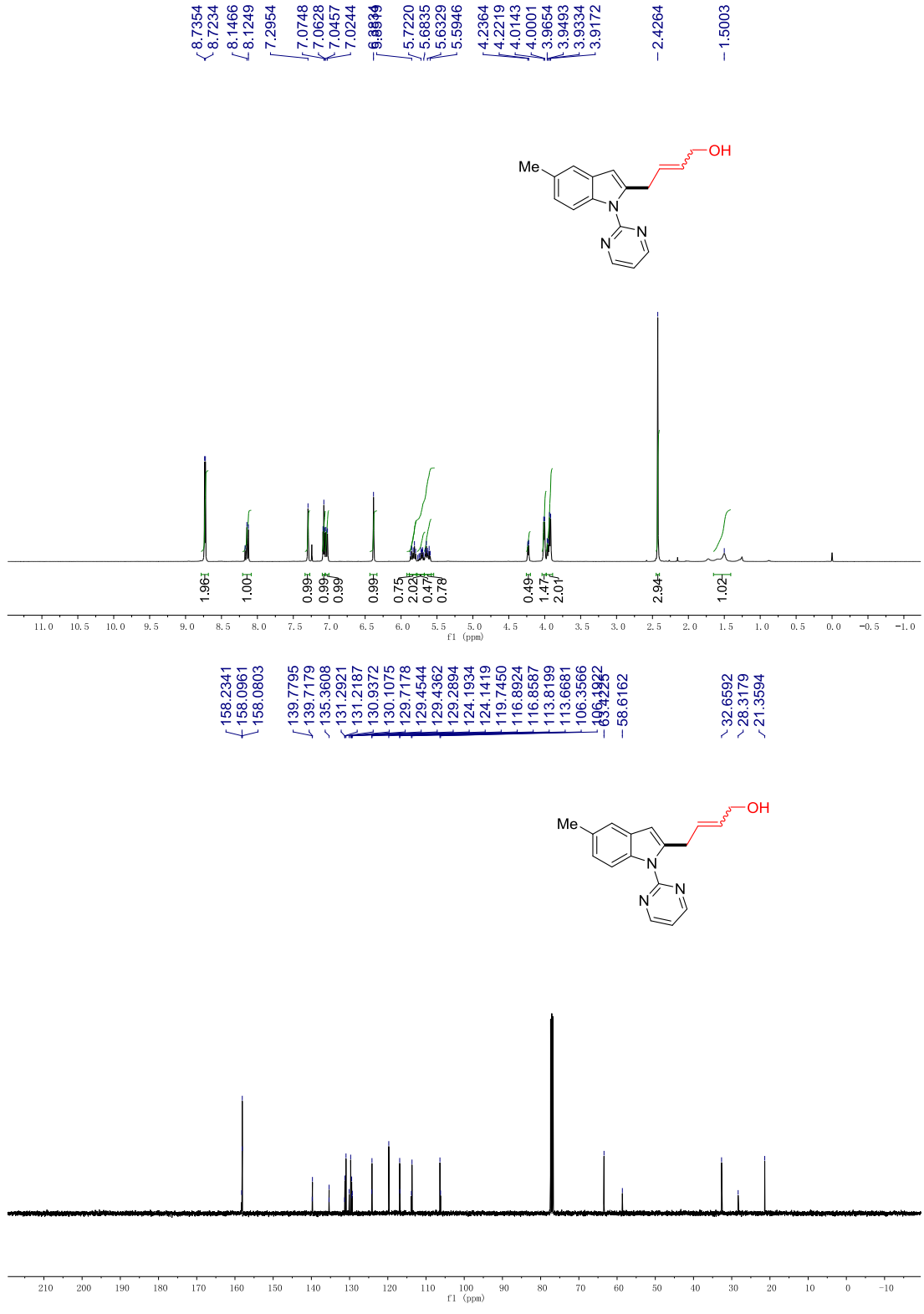
5e


8.7798
8.7753
8.7742
8.7683
8.7635
8.3837
7.9352
7.9162
7.1724
7.1632
7.1581
7.1511
5.8122
5.7271
5.6770
5.6422
5.6100
4.2533
4.2419
4.0230
4.0101
3.9920
3.9645
3.9623
3.9427
1.9511
COOMe
OH
N
N
N
1.99
1.00
1.00
1.12
1.99
0.73
0.58
0.73
0.57
1.46
5.03
1.27
f1 (ppm)
167.8829
158.2986
157.7703
142.1390
137.7566
131.4901
129.1615
124.8463
121.9272
120.5917
118.3086
117.7233
106.8351
63.2833
58.5660
51.8293
32.4487
28.1004
COOMe
OH
f1 (ppm)

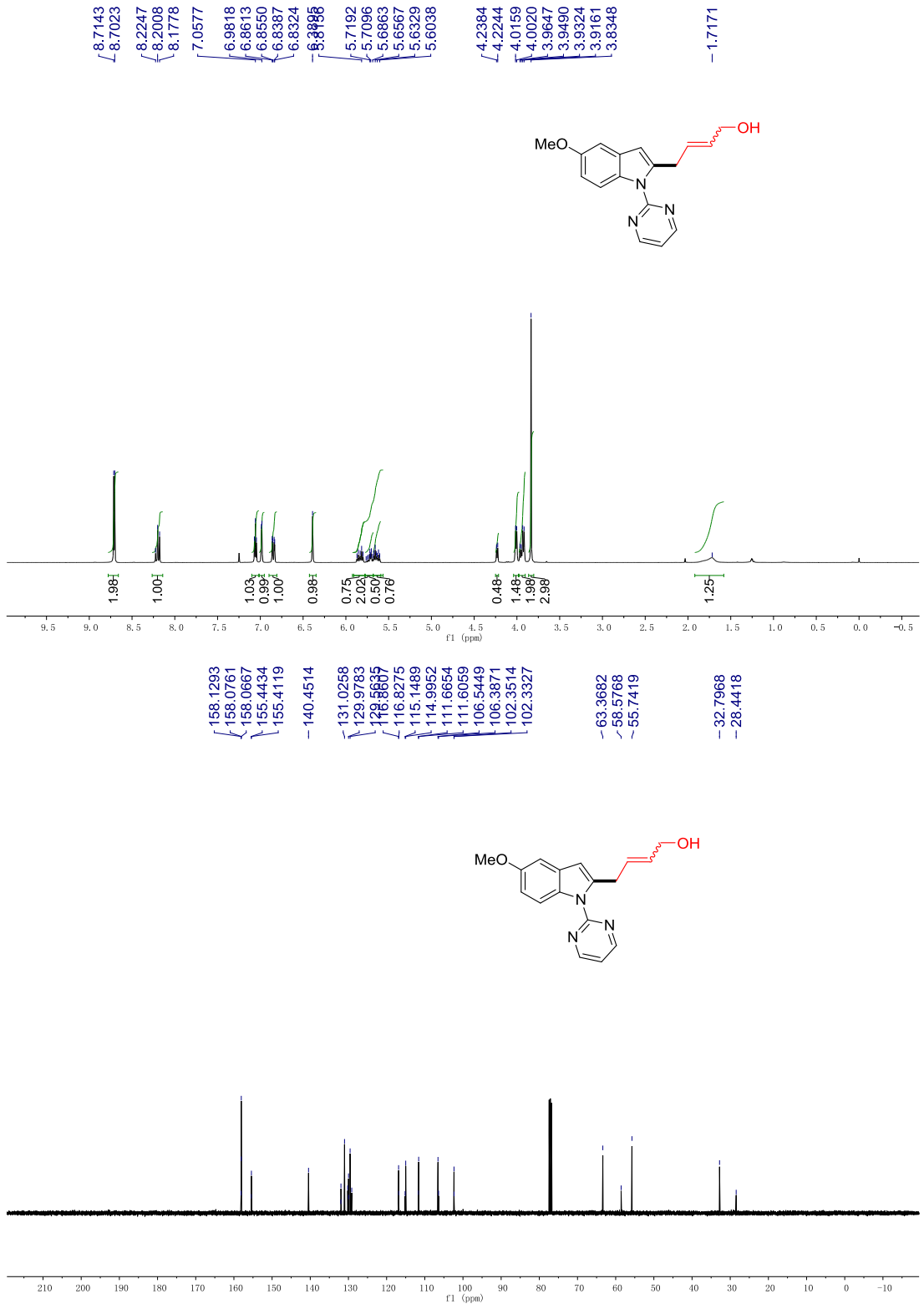
5f


8.7614
8.7494
8.1559
8.1489
8.1280
7.1441
7.1321
7.0805
7.0404
6.5219
5.7863
5.7101
5.6511
5.5983
4.2372
4.2249
4.0242
4.0103
3.9516
3.9379
3.9204
3.9041
1.6931
Br
OH
N
N
N
2.02
1.00
1.00
1.01
1.01
1.01
0.74
0.59
0.74
0.54
1.44
2.02
1.19
f1 (ppm)
158.2899
157.8405
140.6864
140.6608
137.3009
137.2777
131.4963
130.6034
129.6646
129.6526
128.7873
128.4709
124.7454
124.6888
123.6475
123.5988
117.7262
117.6752
113.6997
113.0395
112.8885
106.0845
105.9586
63.2941
58.5665
32.4672
28.1269
Br
OH
N
N
N
f1 (ppm)

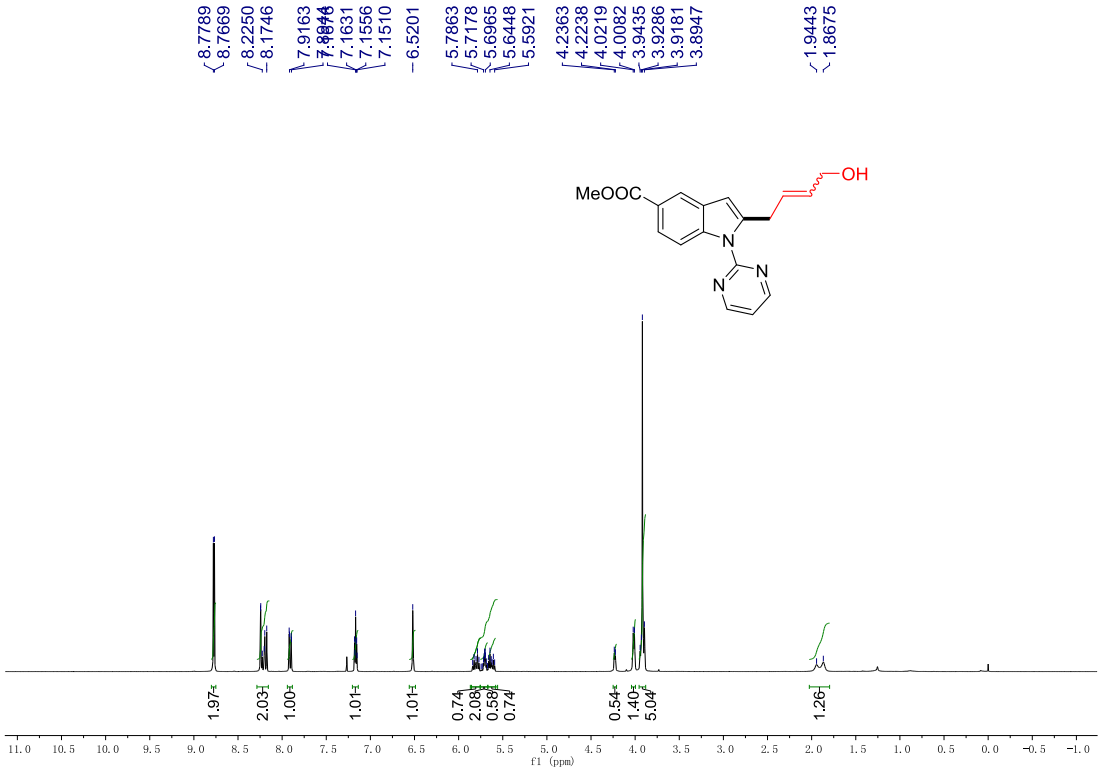
5g

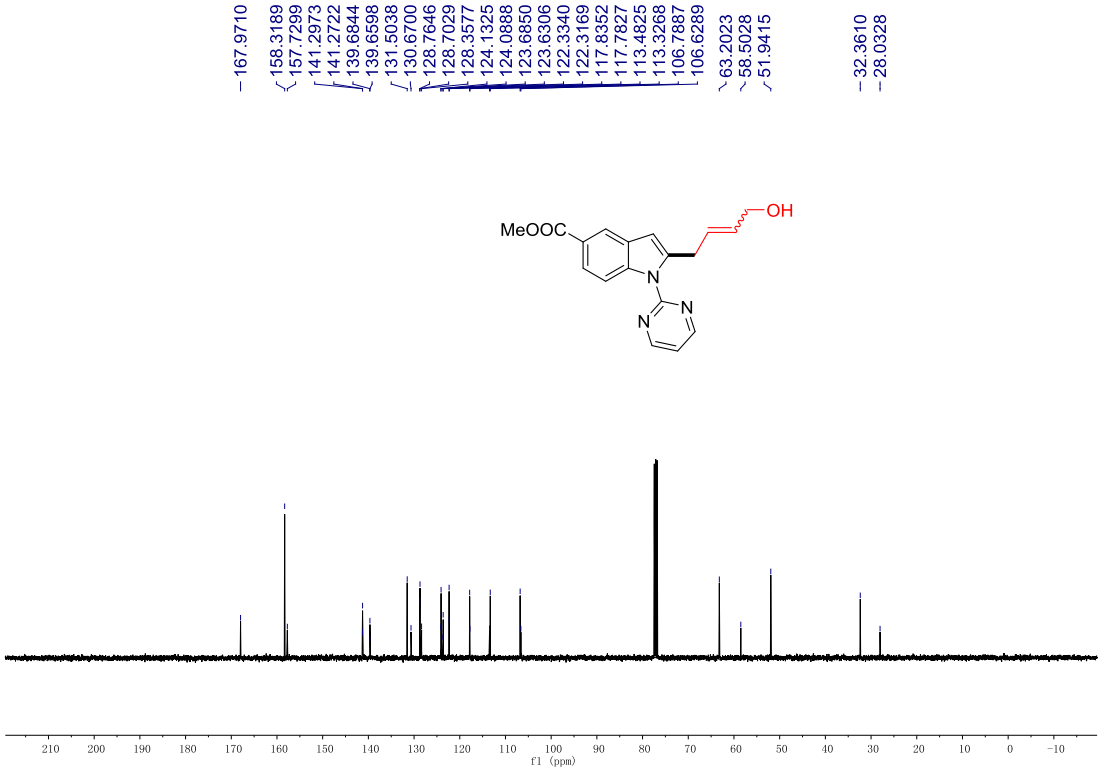

8.7354
8.7234
8.1466
8.1249
7.2954
7.0748
7.0628
7.0457
7.0244
5.7220
5.6835
5.6329
5.5946
4.2364
4.2219
4.0143
4.0001
3.9654
3.9493
3.9334
3.9172
2.4264
1.5003
Me
OH
N
N
N
1.96
1.00
0.99
0.99
0.99
0.99
0.75
2.02
0.47
0.78
0.49
1.47
2.01
2.94
1.02
f1 (ppm)
158.2341
158.0961
158.0803
139.7795
139.7179
135.3608
131.2921
131.2187
130.9372
130.1075
129.7178
129.4544
129.4362
129.2894
124.1934
124.1419
119.7450
116.8924
116.8587
113.8199
113.6681
106.3566
58.6162
32.6592
28.3179
21.3594
f1 (ppm)

5h

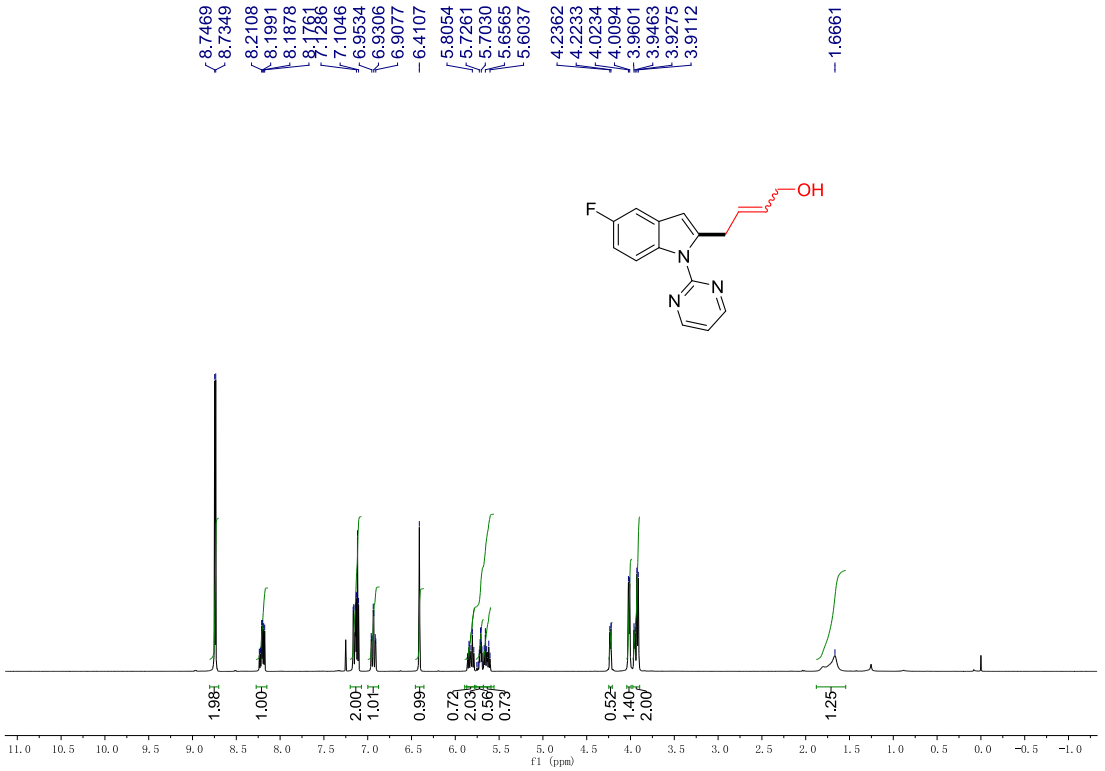

8.7143
8.7023
8.2247
8.2008
8.1778
7.0577
6.9818
6.8613
6.8550
6.8387
6.8324
6.3895
6.3758
5.7192
5.7096
5.6863
5.6567
5.6329
5.6038
4.2384
4.2244
4.0159
4.0020
3.9647
3.9490
3.9324
3.9161
3.8348
1.7171
MeO
OH
N
N
N
1.98
1.00
1.03
0.99
1.00
0.98
0.75
2.02
0.50
0.76
0.48
1.48
1.98
2.98
1.25
f1 (ppm)
158.1293
158.0761
158.0667
155.4434
155.4119
140.4514
131.0258
129.9783
116.8275
115.1489
114.9952
111.6654
111.6059
106.5449
106.3871
102.3514
102.3327
63.3682
58.5768
55.7419
32.7968
28.4418
MeO
OH
N
N
N
f1 (ppm)

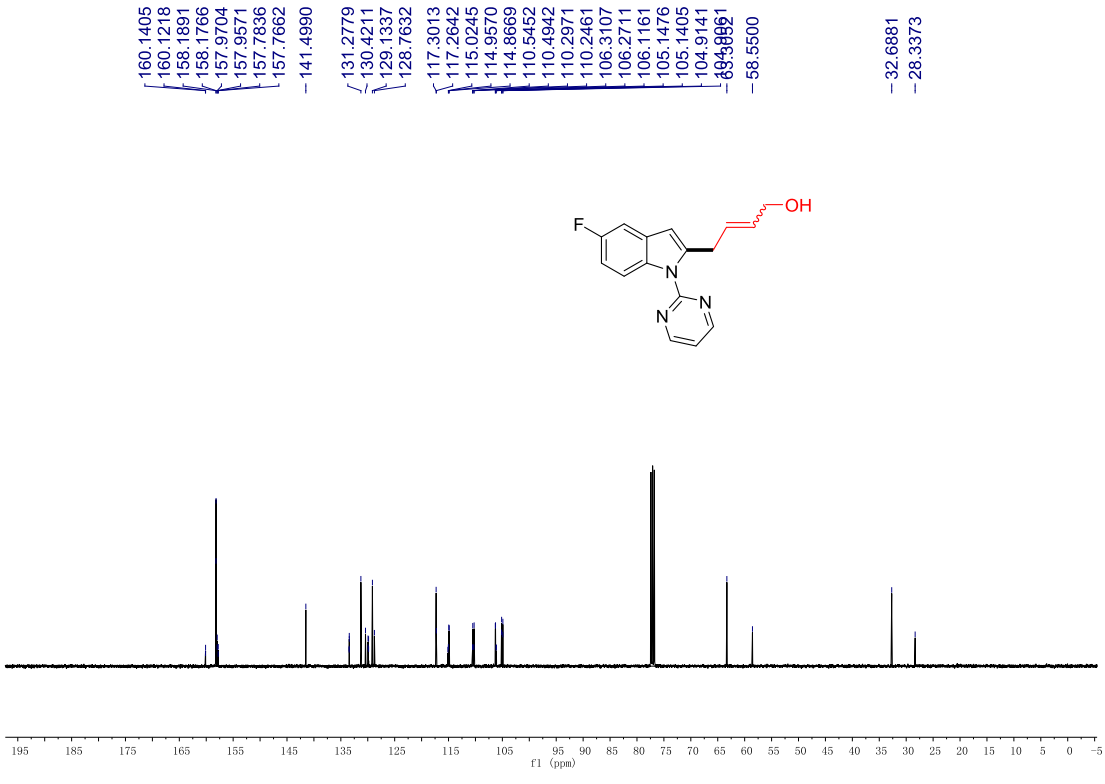
5i


8.7789
8.7669
8.2250
8.1746
7.9163
7.1631
7.1556
7.1510
6.5201
5.7863
5.7178
5.6965
5.6448
5.5921
4.2363
4.2238
4.0219
4.0082
3.9435
3.9286
3.9181
3.8947
1.9443
1.8675
MeOOC
OH
N
N
N
1.97
2.03
1.00
1.01
1.01
0.74
2.08
0.58
0.74
0.54
1.40
5.04
1.26
f1 (ppm)

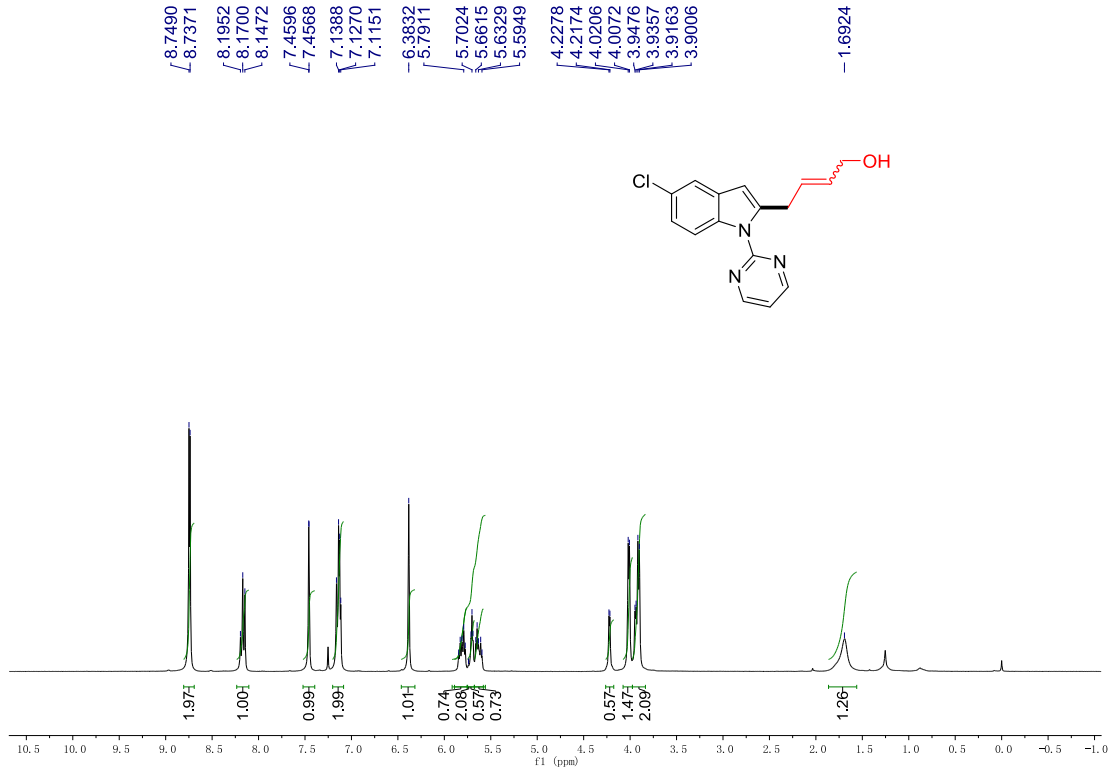

167.9710
158.3189
157.7299
141.2973
141.2722
139.6844
139.6598
131.5038
130.6700
128.7646
128.7029
128.3577
124.1325
124.0888
123.6850
123.6306
122.3340
122.3169
117.8352
117.7827
113.4825
113.3268
106.7887
106.6289
63.2023
58.5028
51.9415
32.3610
28.0328
MeOOC
OH
N
N
N
f1 (ppm)

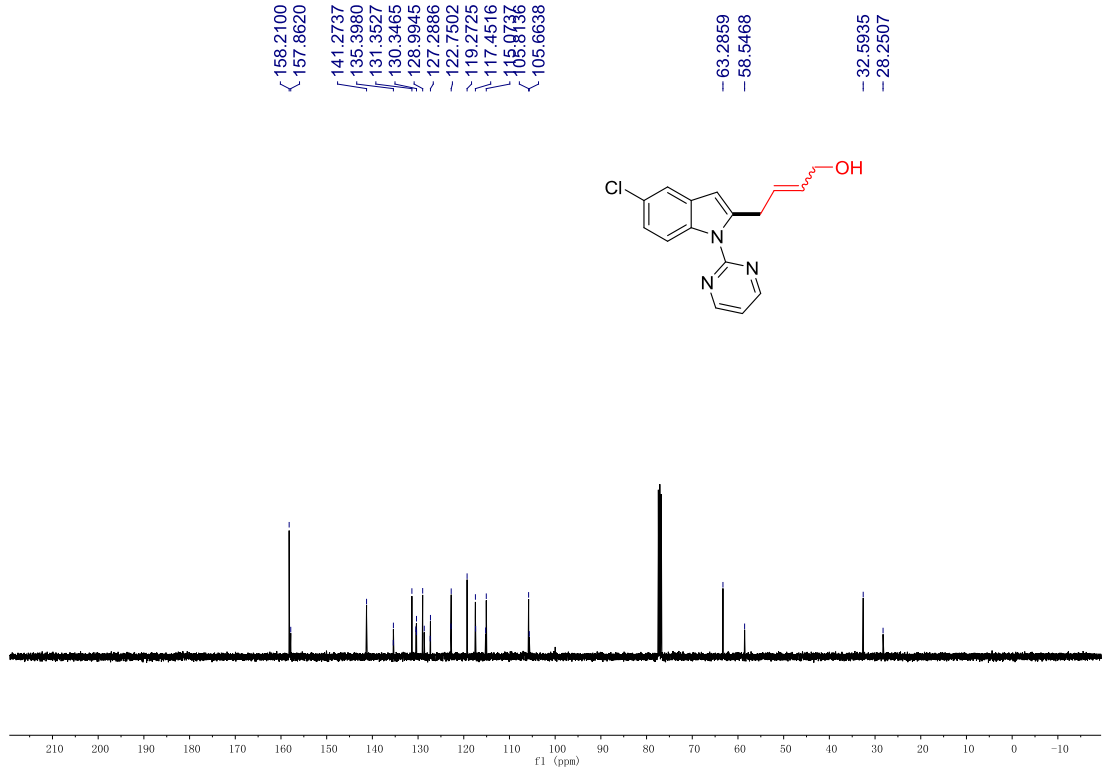
5j


8.7469
8.7349
8.2108
8.1991
8.1878
7.1286
7.1046
6.9534
6.9306
6.9077
6.4107
5.8054
5.7261
5.7030
5.6565
5.6037
4.2362
4.2233
4.0234
4.0094
3.9601
3.9463
3.9275
3.9112
1.6661
F
OH
N
N
N
1.98
1.00
2.00
1.01
0.99
0.72
2.03
0.56
0.73
0.52
1.40
2.00
1.25
f1 (ppm)

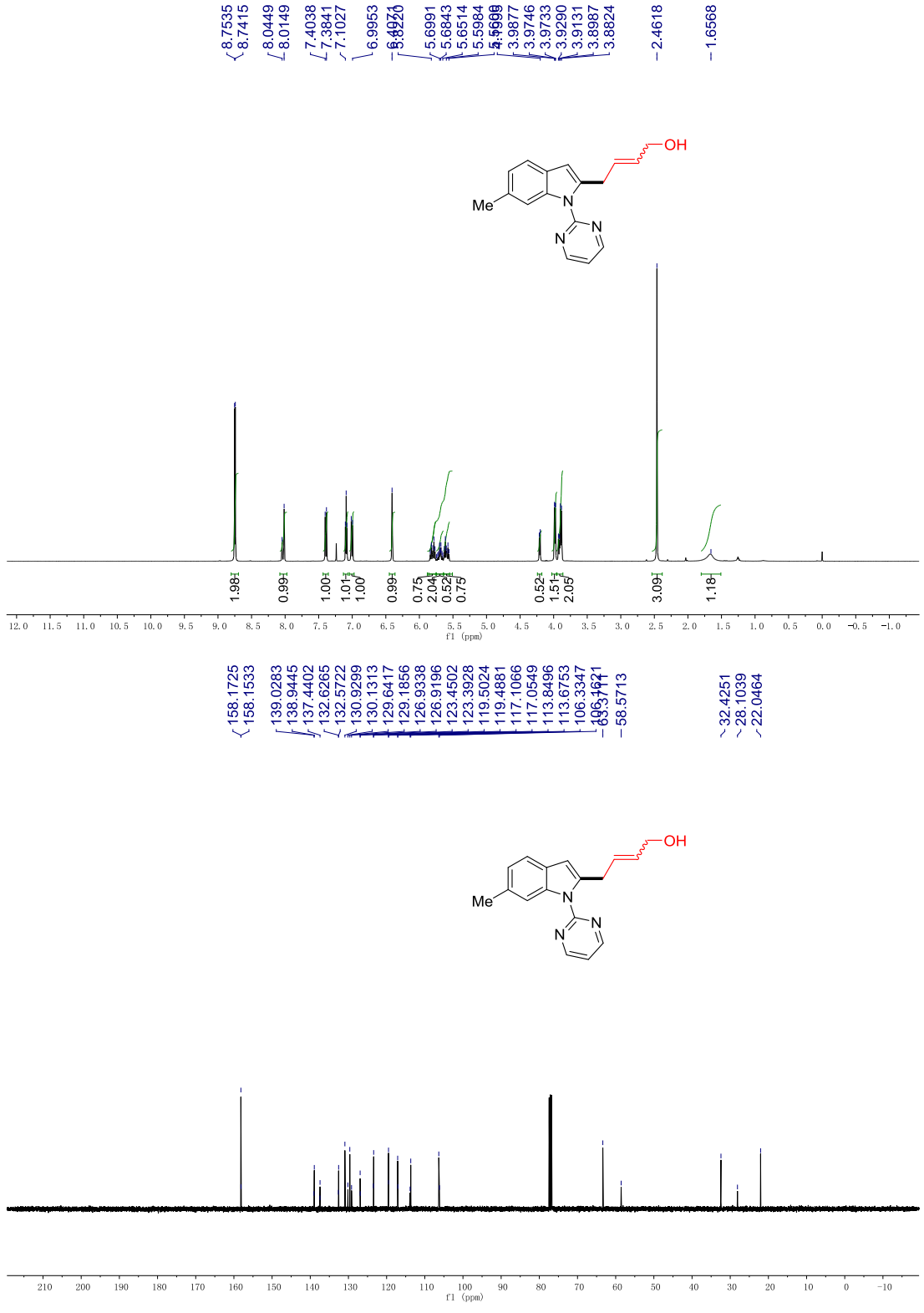

160.1405
160.1218
158.1891
158.1766
157.9704
157.9571
157.7836
157.7662
141.4990
131.2779
130.4211
129.1337
128.7632
117.3013
117.2642
115.0245
114.9570
114.8669
110.5452
110.4942
110.2971
110.2461
106.3107
106.2711
106.1161
105.1476
105.1405
104.9141
83.3082
58.5500
32.6881
28.3373
F
OH
N
N
N
f1 (ppm)

5k

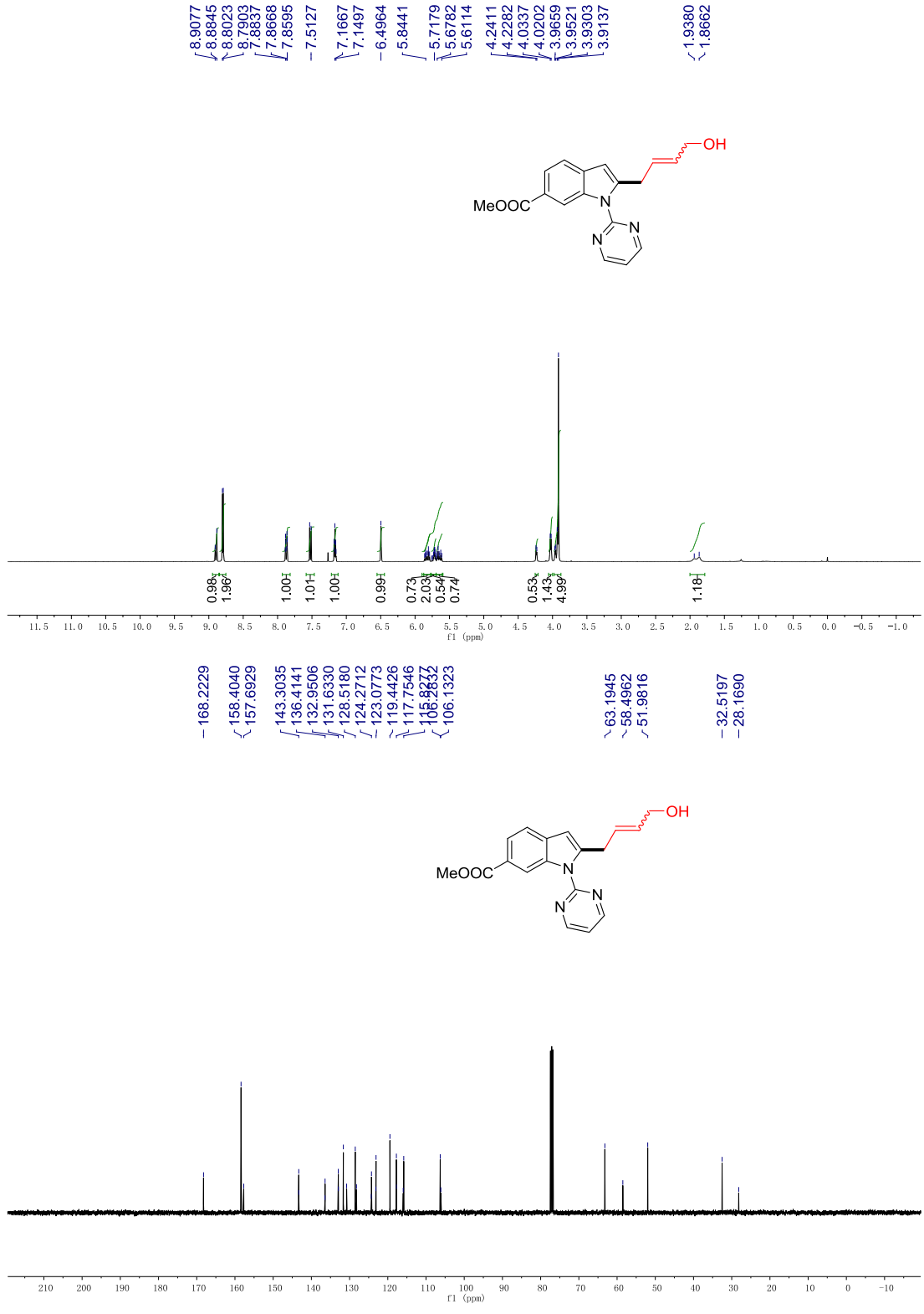

8.7490
8.7371
8.1952
8.1700
8.1472
7.4596
7.4568
7.1388
7.1270
7.1151
6.3832
5.7911
5.7024
5.6615
5.6329
5.5949
4.2278
4.2174
4.0206
4.0072
3.9476
3.9357
3.9163
3.9006
1.6924
Cl
OH
N
N
N
1.97
1.00
0.99
1.99
1.01
0.74
2.08
0.57
0.73
0.57
1.47
2.09
1.26
f1 (ppm)


158.2100
157.8620
141.2737
135.3980
131.3527
130.3465
128.9945
127.2886
122.7502
119.2725
117.4516
105.8136
105.6638
63.2859
58.5468
32.5935
28.2507
Cl
OH
N
N
N
f1 (ppm)

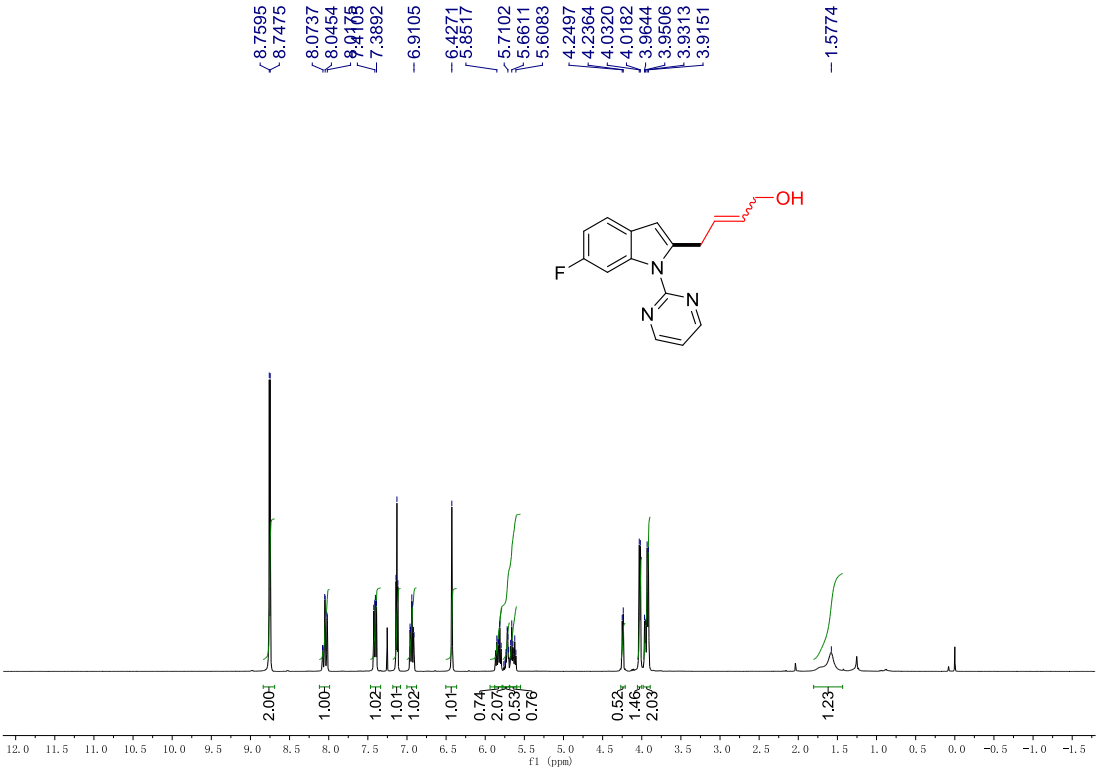
5l

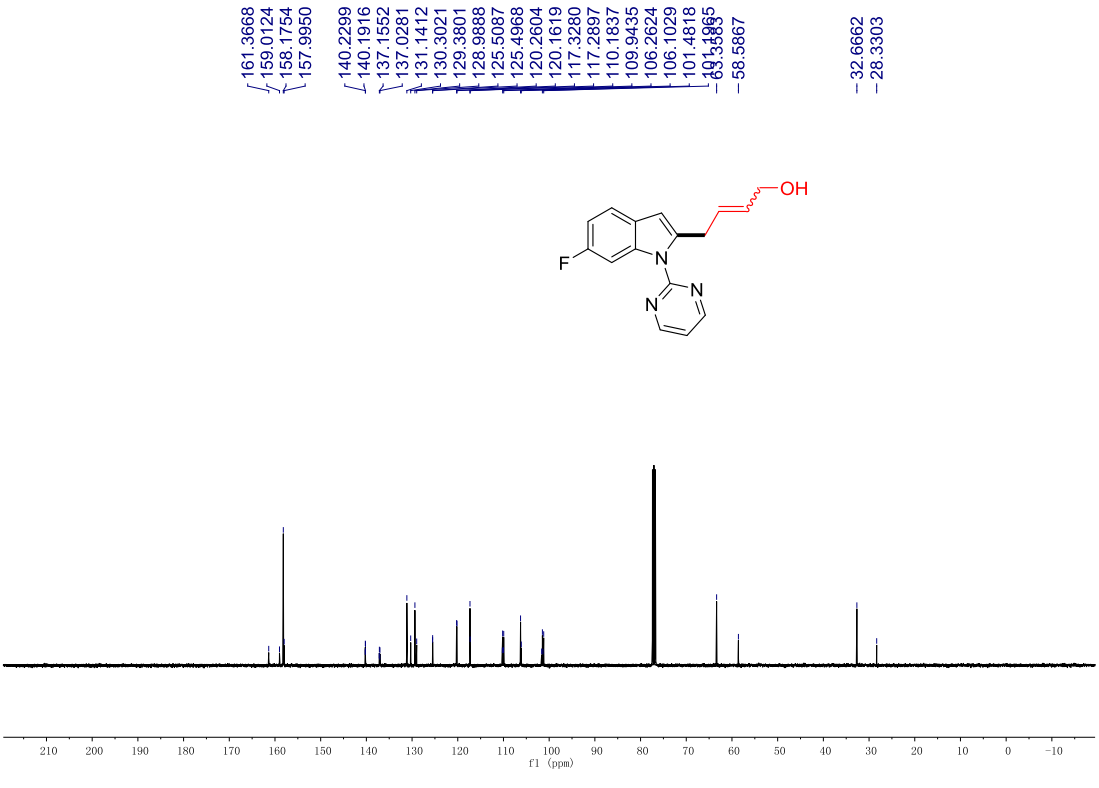

8.7535
8.7415
8.0449
8.0149
7.4038
7.3841
7.1027
6.9953
6.4071
6.3220
5.6991
5.6843
5.6514
5.5984
4.1598
3.9877
3.9746
3.9733
3.9290
3.9131
3.8987
3.8824
2.4618
1.6568
OH
Me
N
N
N
1.98
0.99
1.00
1.01
1.00
0.99
0.75
2.04
0.52
0.75
0.52
1.51
2.05
3.09
1.18
f1 (ppm)
158.1725
158.1533
139.0283
138.9445
137.4402
132.6265
132.5722
130.9299
130.1313
129.6417
129.1856
126.9338
126.9196
123.4502
123.3928
119.5024
119.4881
117.1066
117.0549
113.8496
113.6753
106.3347
106.1621
83.3741
58.5713
32.4251
28.1039
22.0464
OH
Me
N
N
N
f1 (ppm)

5m

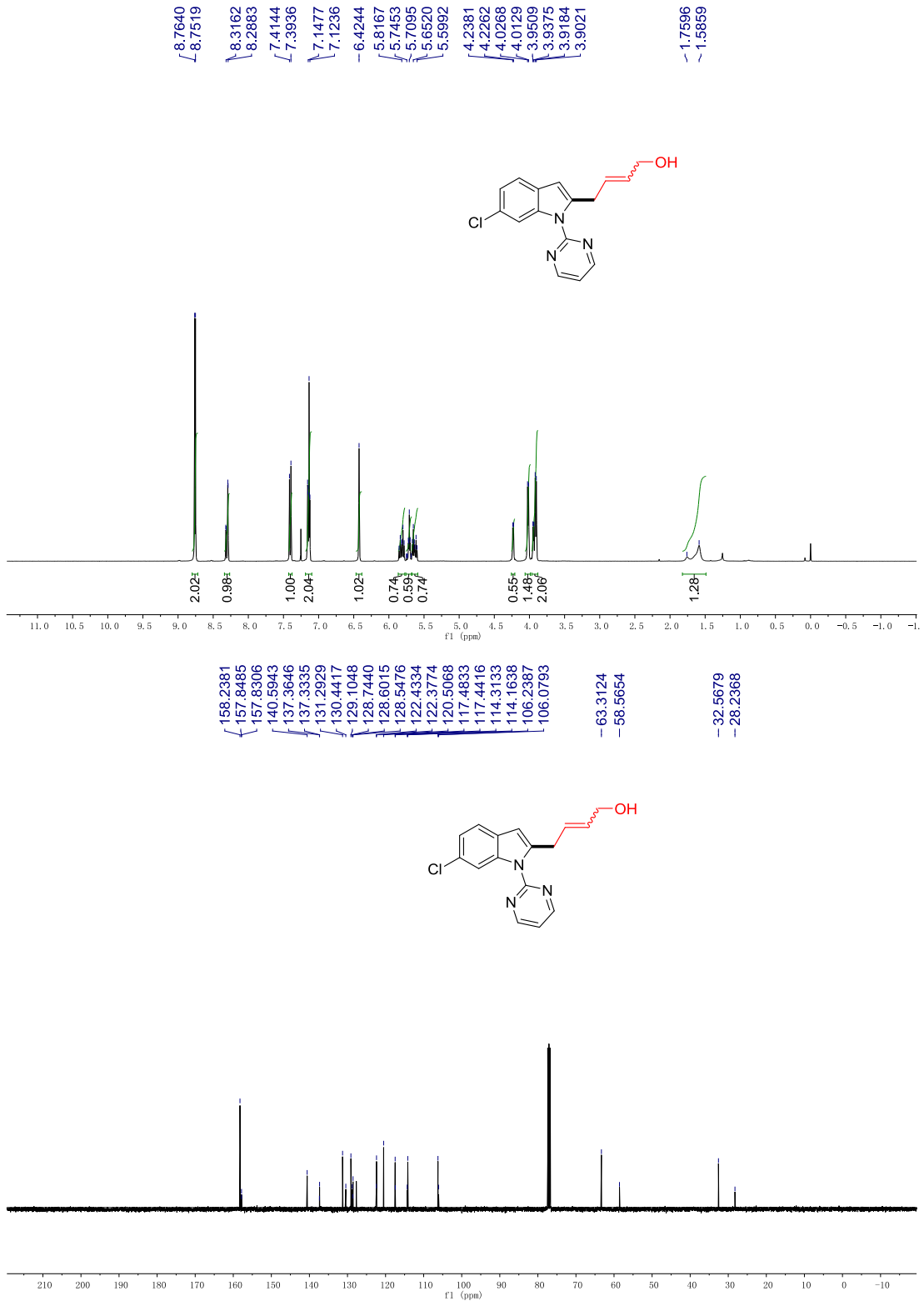

8.9077
8.8845
8.8023
8.7903
7.8837
7.8668
7.8595
7.5127
7.1667
7.1497
6.4964
5.8441
5.7179
5.6782
5.6114
4.2411
4.2282
4.0337
4.0202
3.9659
3.9521
3.9303
3.9137
1.9380
1.8662
OH
MeOOC
N
N
N
0.98
1.96
1.00
1.01
1.00
0.99
0.73
2.03
0.54
0.74
0.53
1.43
4.99
1.18
f1 (ppm)
168.2229
158.4040
157.6929
143.3035
136.4141
132.9506
131.6330
128.5180
124.2712
123.0773
119.4426
117.7546
115.8837
106.2832
106.1323
63.1945
58.4962
51.9816
32.5197
28.1690
OH
MeOOC
N
N
N
f1 (ppm)

5n

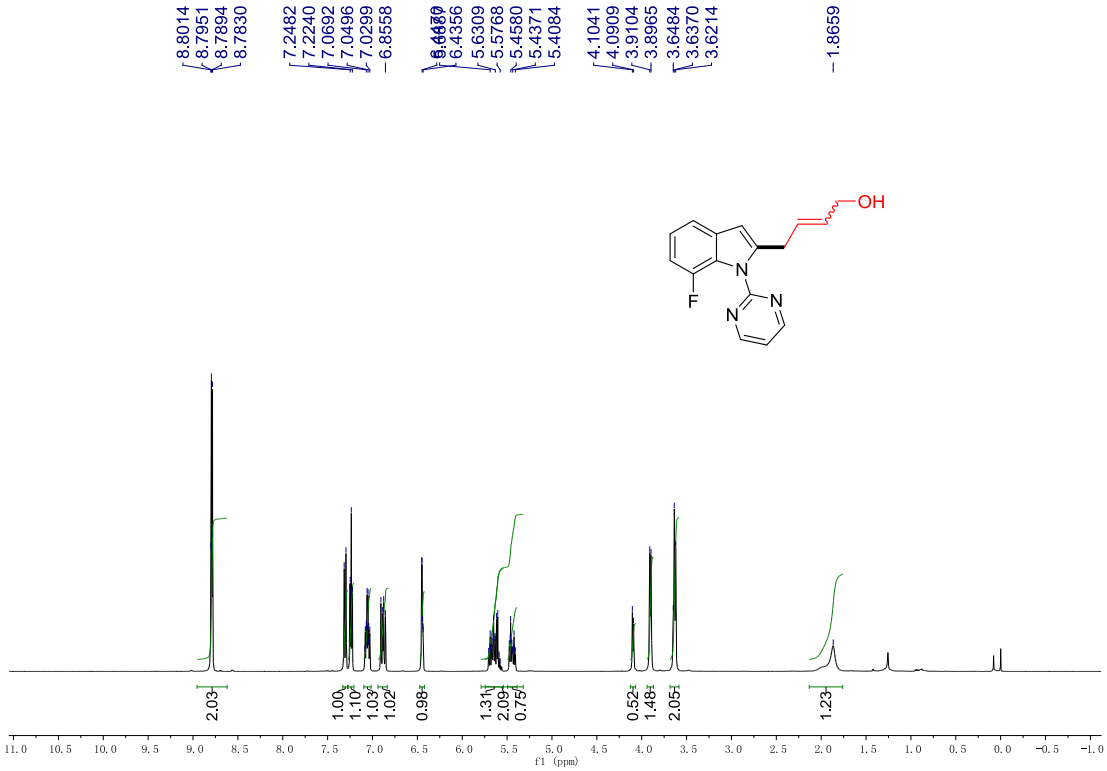

8.7595
8.7475
8.0737
8.0454
7.4105
7.3892
6.9105
6.4271
5.8517
5.7102
5.6611
5.6083
4.2497
4.2364
4.0320
4.0182
3.9644
3.9506
3.9313
3.9151
1.5774
OH
F
N
N
N
2.00
1.00
1.02
1.01
1.02
1.01
0.74
2.07
0.53
0.76
0.52
1.46
2.03
1.23
f1 (ppm)

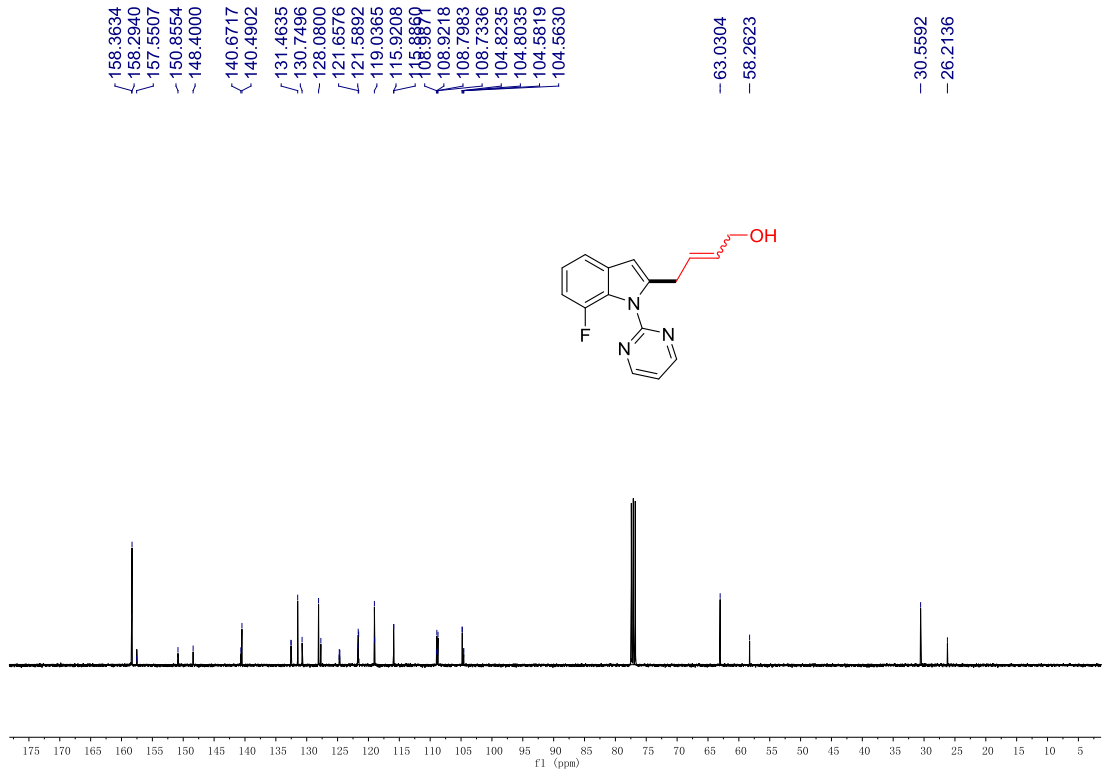

161.3668
159.0124
158.1754
157.9950
140.2299
140.1916
137.1552
137.0281
131.1412
130.3021
129.3801
128.9888
125.5087
125.4968
120.2604
120.1619
117.3280
117.2897
110.1837
109.9435
106.2624
106.1029
101.4818
58.5867
32.6662
28.3303
OH
F
N
N
N
f1 (ppm)

5o


8.7640
8.7519
8.3162
8.2883
7.4144
7.3936
7.1477
7.1236
6.4244
5.8167
5.7453
5.7095
5.6520
5.5992
4.2381
4.2262
4.0268
4.0129
3.9509
3.9375
3.9184
3.9021
1.7596
1.5859
OH
Cl
N
N
N
2.02
0.98
1.00
2.04
1.02
0.74
0.59
0.74
0.55
1.48
2.06
1.28
f1 (ppm)
158.2381
157.8485
157.8306
140.5943
137.3646
137.3335
131.2929
130.4417
129.1048
128.7440
128.6015
128.5476
122.4334
122.3774
120.5068
117.4833
117.4416
114.3133
114.1638
106.2387
106.0793
63.3124
58.5654
32.5679
28.2368
OH
Cl
N
N
N
f1 (ppm)

5p

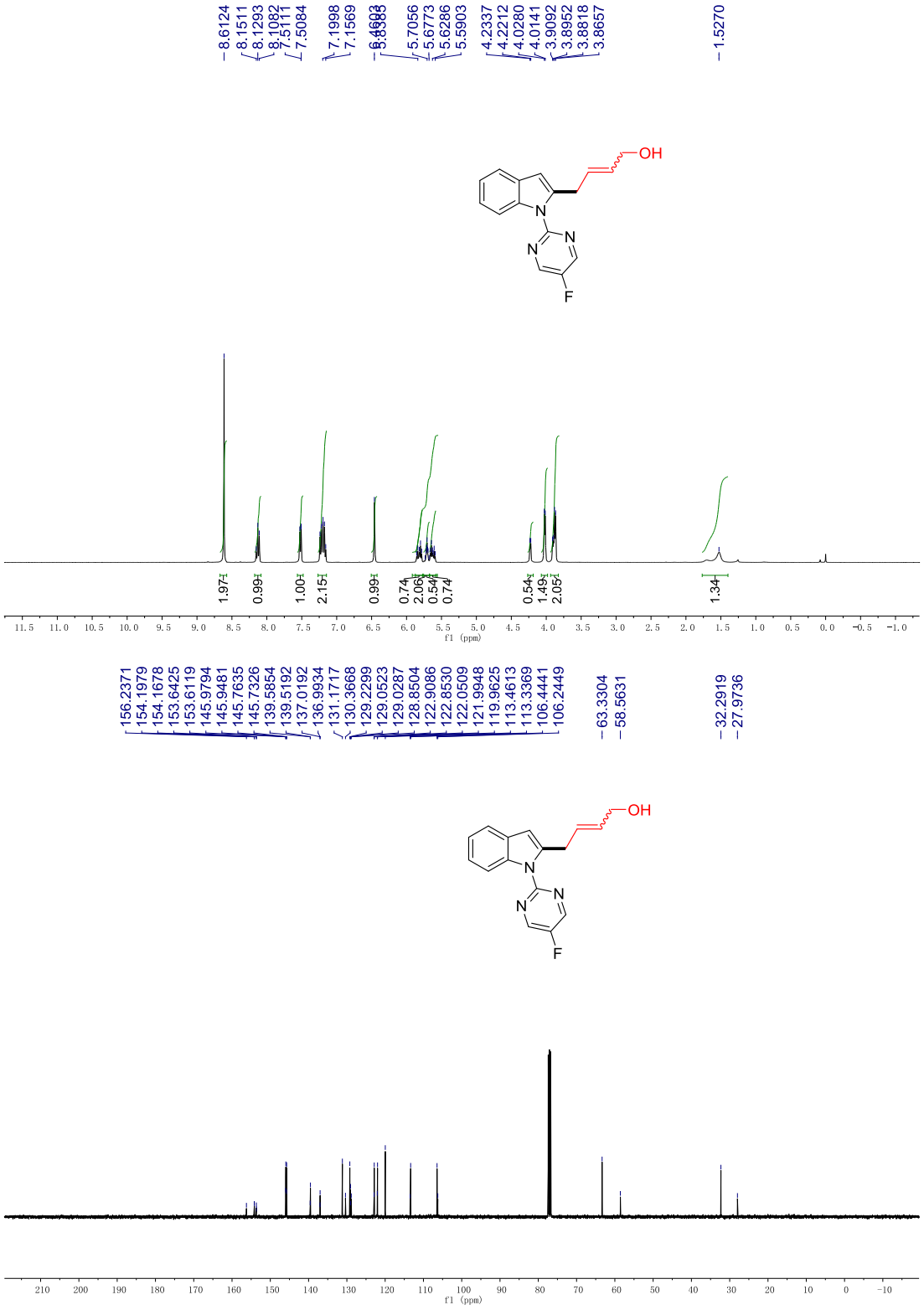

8.8014
8.7951
8.7894
8.7830
7.2482
7.2240
7.0692
7.0496
7.0299
6.8558
6.4356
5.6309
5.5768
5.4580
5.4371
5.4084
4.1041
4.0909
3.9104
3.8965
3.6484
3.6370
3.6214
1.8659
OH
N
F
N
N
2.03
1.00
1.10
1.03
1.02
0.98
1.31
2.09
0.75
0.52
1.48
2.05
1.23
f1 (ppm)


158.3634
158.2940
157.5507
150.8554
148.4000
140.6717
140.4902
131.4635
130.7496
128.0800
121.6576
121.5892
119.0365
115.9208
108.9218
108.7983
108.7336
104.8235
104.8035
104.5819
104.5630
63.0304
58.2623
30.5592
26.2136
OH
N
F
N
N
f1 (ppm)

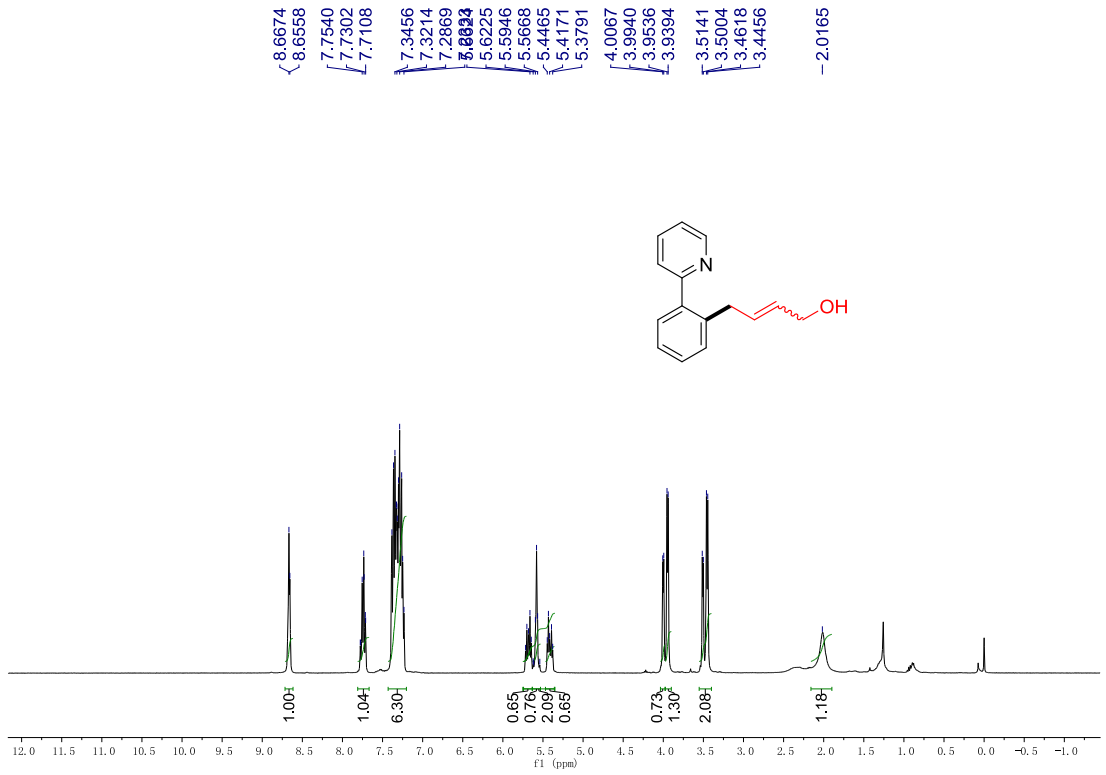
5q

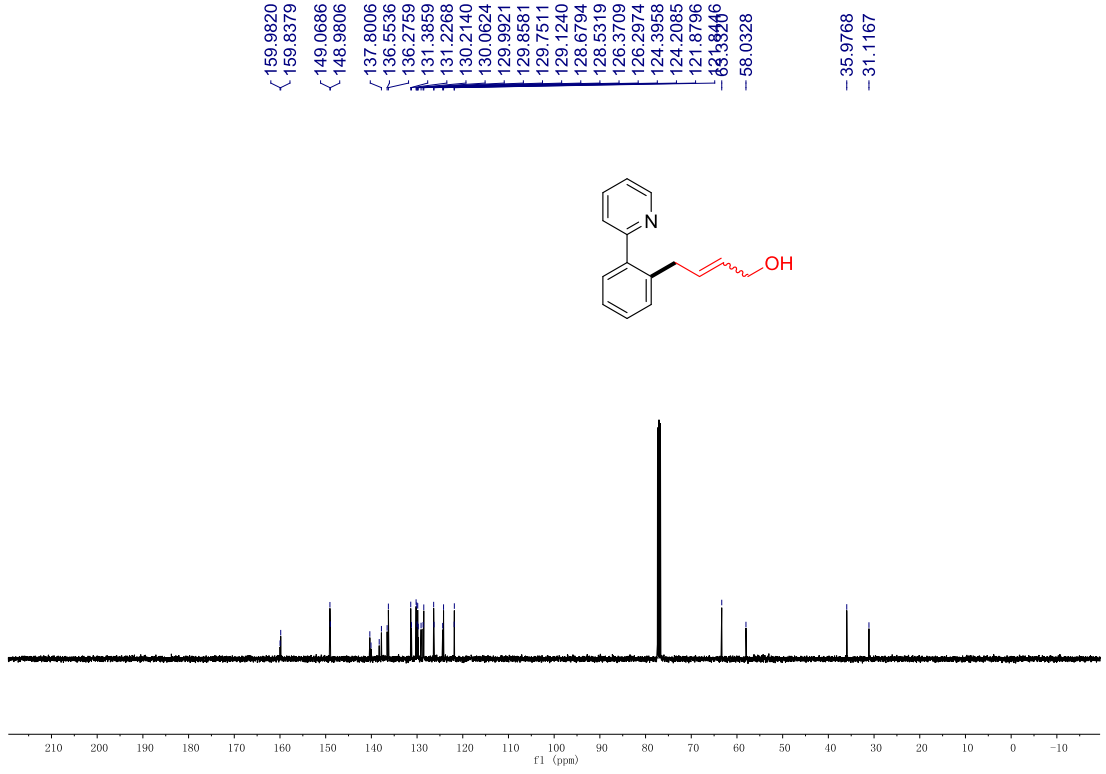

8.8088
8.7976
8.7857
7.2375
7.1234
7.1048
7.0858
7.0191
7.0009
6.4205
6.4076
5.6011
5.5532
5.5114
5.3525
5.3142
4.0351
4.0224
3.8587
3.8450
3.4693
3.4532
2.2691
2.2516
2.2344
1.9255
0.9581
0.9394
0.9206
OH
Et
N
N
1.98
1.00
1.10
1.02
1.02
0.98
1.25
2.05
0.77
0.49
1.54
2.05
2.06
1.20
3.13
f1 (ppm)
159.1080
158.5365
158.4086
139.7316
131.0621
129.6952
128.3480
127.9891
122.9709
121.4757
119.4401
119.4265
118.1251
104.2354
103.9629
63.0270
58.1864
30.6840
26.2352
25.7374
13.9606
f1 (ppm)

5r

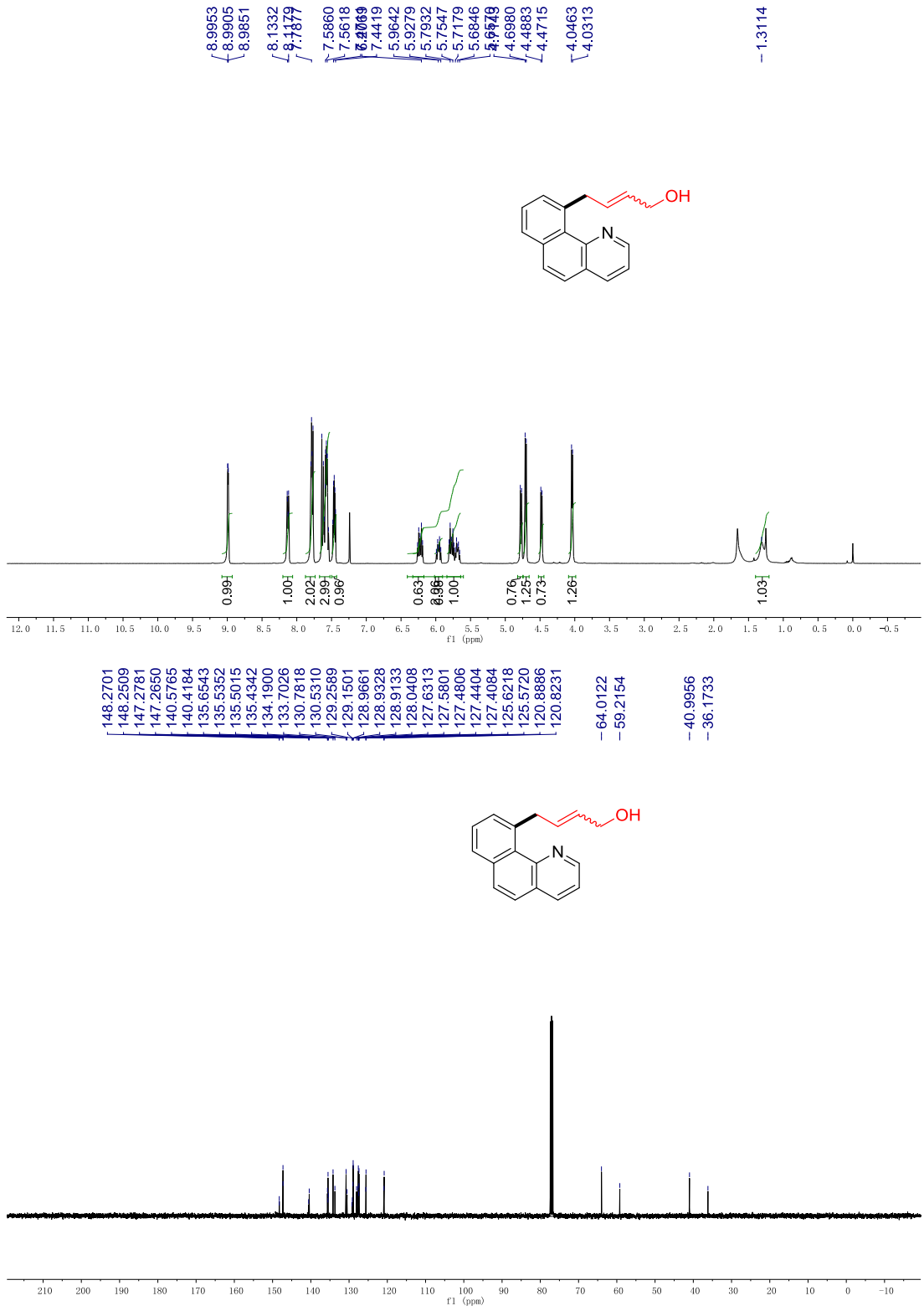

8.6124
8.1511
8.1293
8.1082
7.5111
7.5084
7.1998
7.1569
5.7056
5.6773
5.6286
5.5903
4.2337
4.2212
4.0280
4.0141
3.9092
3.8952
3.8818
3.8657
1.5270
OH
N
N
N
F
1.97
0.99
1.00
2.15
0.99
0.74
2.06
0.54
0.74
0.54
1.49
2.05
1.34
f1 (ppm)
156.2371
154.1979
154.1678
153.6425
153.6119
145.9794
145.9481
145.7635
145.7326
139.5854
139.5192
137.0192
136.9934
131.1717
130.3668
129.2299
129.0523
129.0287
128.8504
122.9086
122.8530
122.0509
121.9948
119.9625
113.4613
113.3369
106.4441
106.2449
63.3304
58.5631
32.2919
27.9736
OH
N
N
N
F
f1 (ppm)

7a

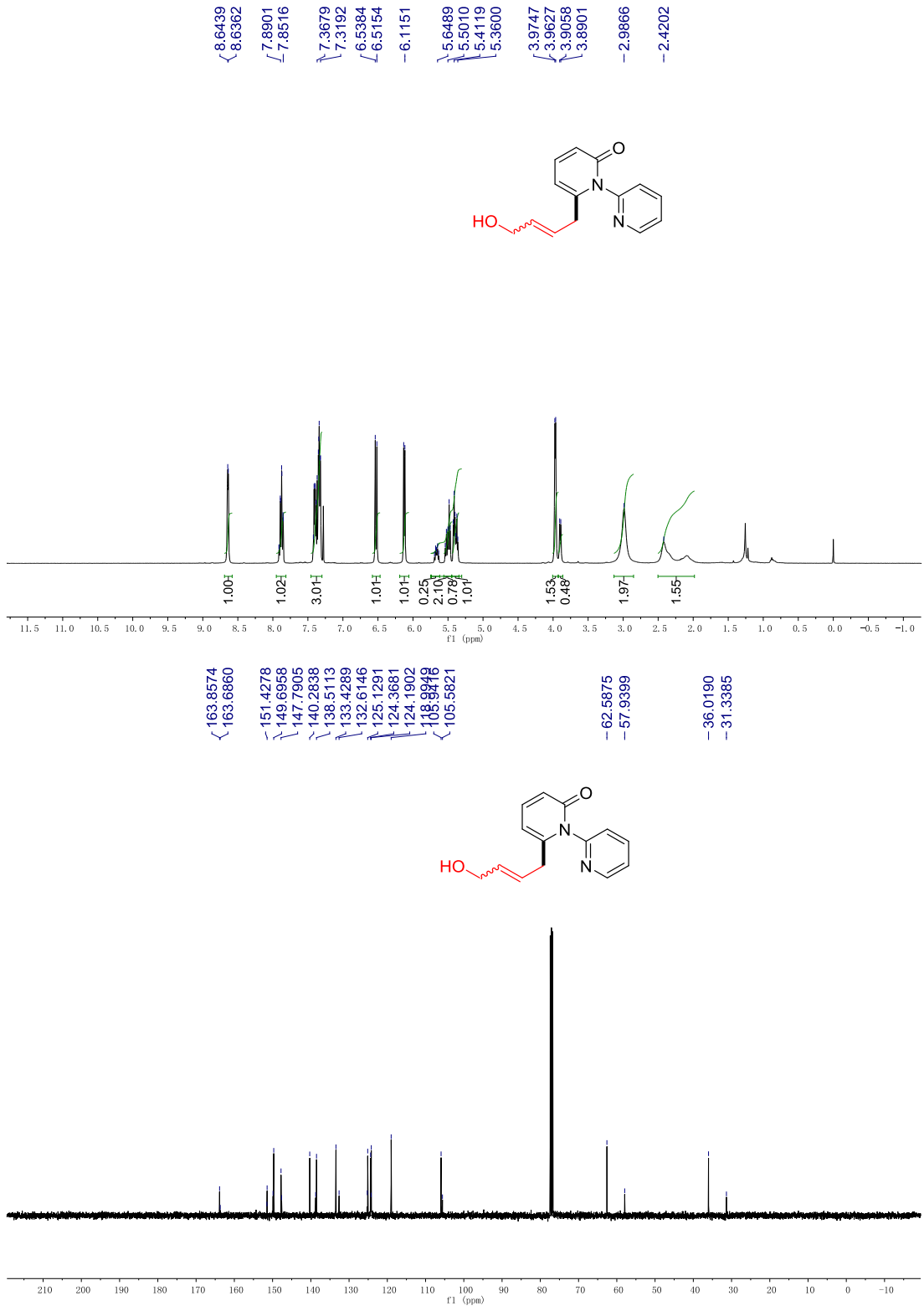

8.6674
8.6558
7.7540
7.7302
7.7108
7.3456
7.3214
7.2869
5.6225
5.5946
5.5668
5.4465
5.4171
5.3791
4.0067
3.9940
3.9536
3.9394
3.5141
3.5004
3.4618
3.4456
2.0165
N
OH
1.00
1.04
6.30
0.65
0.76
2.09
0.65
0.73
1.30
2.08
1.18
f1 (ppm)


159.9820
159.8379
149.0686
148.9806
137.8006
136.5536
136.2759
131.3859
131.2268
130.2140
130.0624
129.9921
129.8581
129.7511
129.1240
128.6794
128.5319
126.3709
126.2974
124.3958
124.2085
121.8796
58.0328
35.9768
31.1167
N
OH
f1 (ppm)

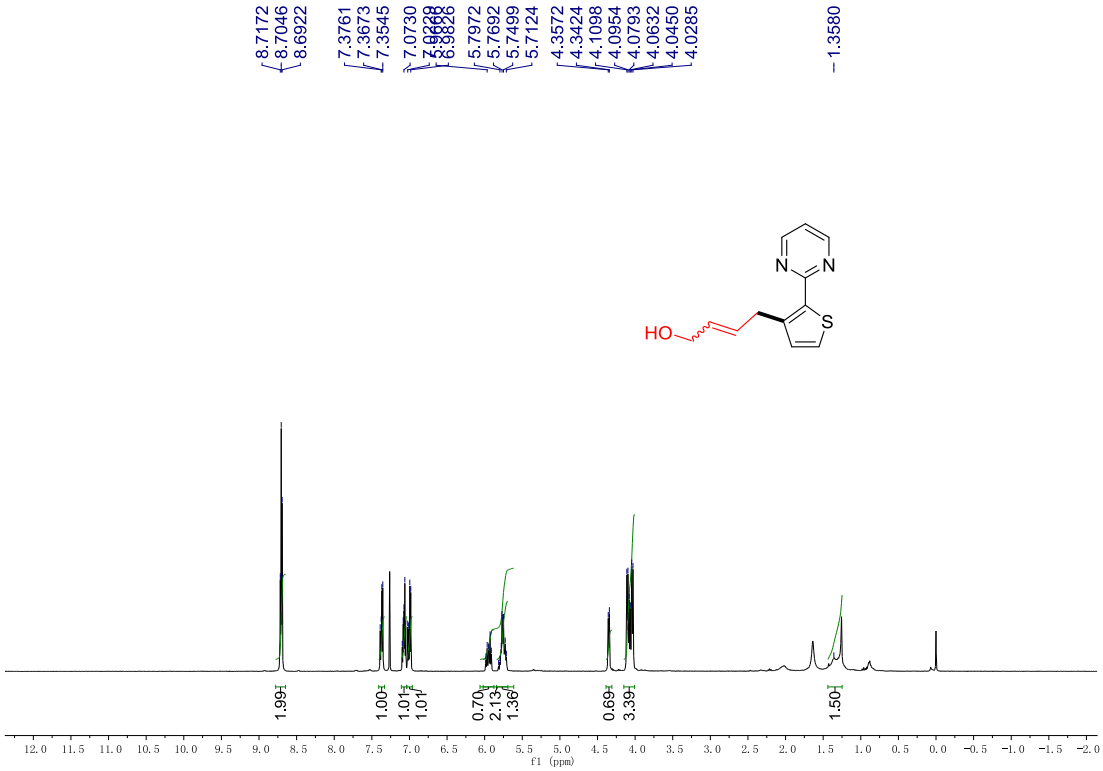
7b

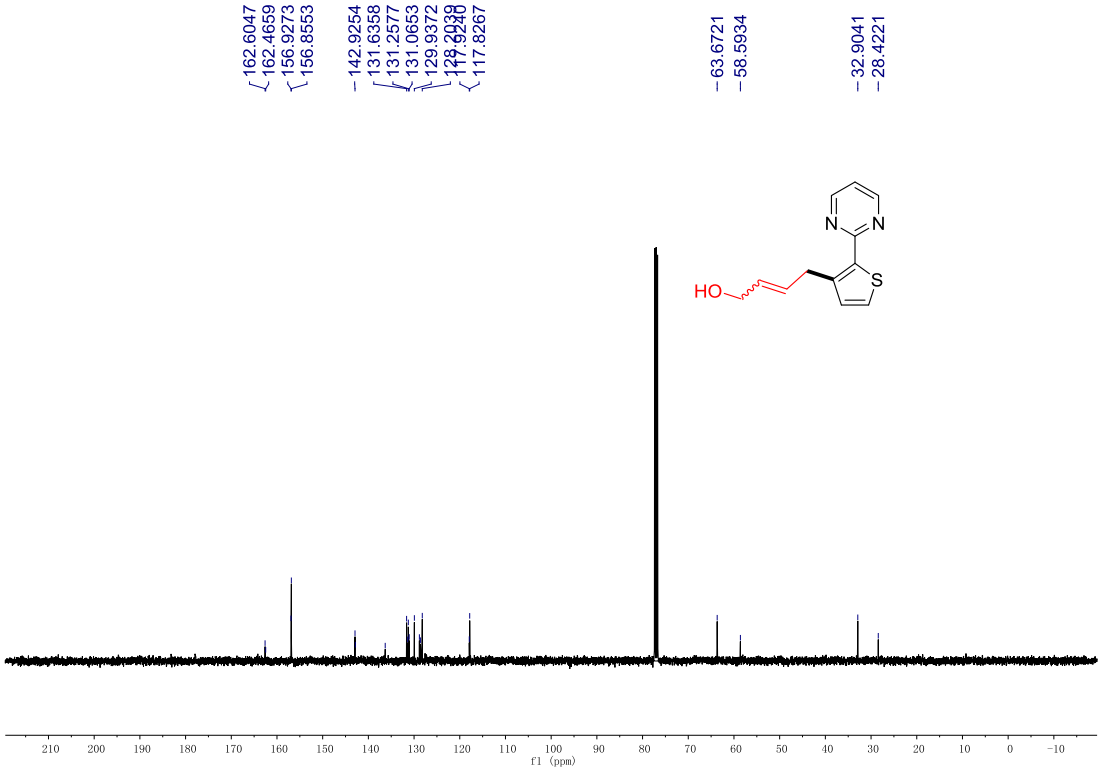

8.9953
8.9905
8.9851
8.1332
8.1179
7.7877
7.5860
7.5618
7.4419
5.9642
5.9279
5.7932
5.7547
5.7179
5.6846
4.6980
4.4883
4.4715
4.0463
4.0313
1.3114
OH
N
0.99
1.00
2.02
2.99
0.98
0.63
1.00
0.76
1.25
0.73
1.26
1.03
f1 (ppm)
148.2701
148.2509
147.2781
147.2650
140.5765
140.4184
135.6543
135.5352
135.5015
135.4342
134.1900
133.7026
130.7818
130.5310
129.2589
129.1501
128.9661
128.9328
128.9133
128.0408
127.6313
127.5801
127.4806
127.4404
127.4084
125.6218
125.5720
120.8886
120.8231
64.0122
59.2154
40.9956
36.1733
OH
N
f1 (ppm)

7c

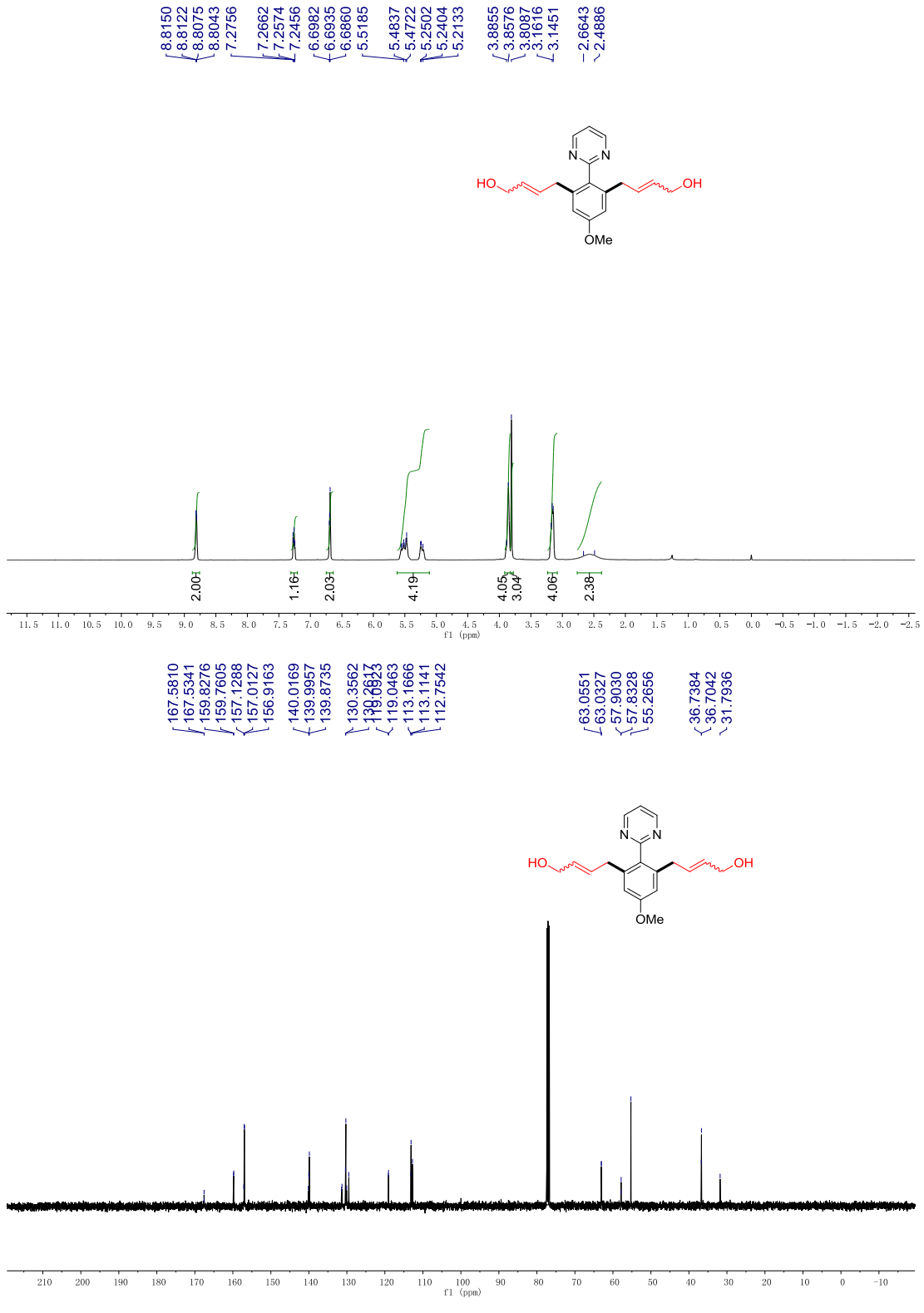

8.6439
8.6362
7.8901
7.8516
7.3679
7.3192
6.5384
6.5154
6.1151
5.6489
5.5010
5.4119
5.3600
3.9747
3.9627
3.9058
3.8901
2.9866
2.4202
O
N
N
HO
1.00
1.02
3.01
1.01
1.01
0.25
2.10
0.78
1.07
1.53
0.48
1.97
1.55
f1 (ppm)
163.8574
163.6860
151.4278
149.6958
147.7905
140.2838
138.5113
133.4289
132.6146
125.1291
124.3681
124.1902
105.5821
62.5875
57.9399
36.0190
31.3385
f1 (ppm)

7d

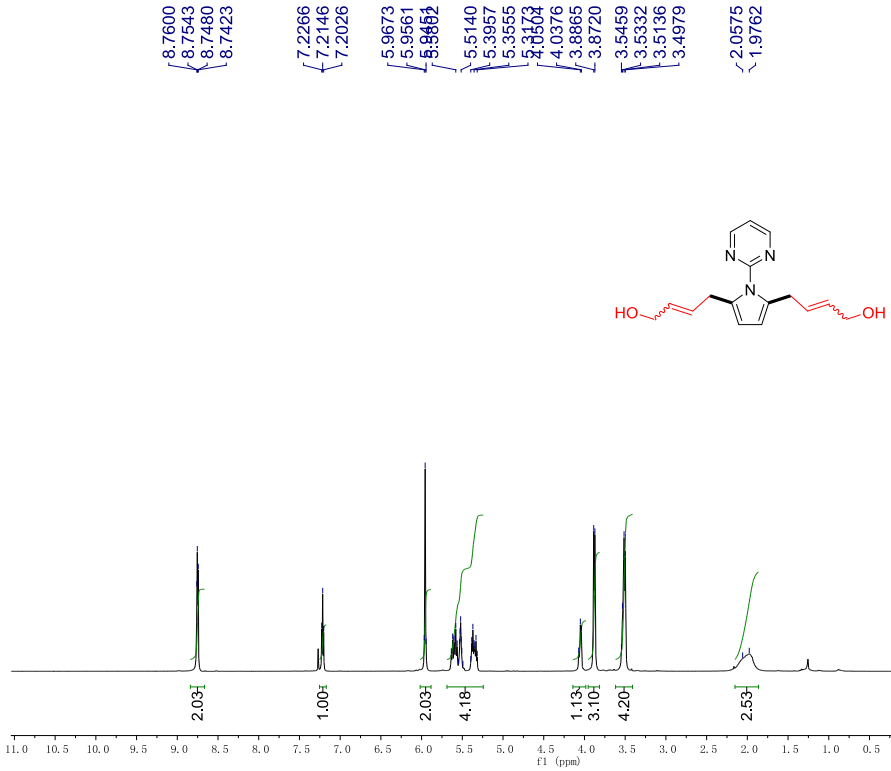

8.7172
8.7046
8.6922
7.3761
7.3673
7.3545
7.0730
5.7972
5.7692
5.7499
5.7124
4.3572
4.3424
4.1098
4.0954
4.0793
4.0632
4.0450
4.0285
1.3580
N
N
HO
S
1.99
1.00
1.01
1.01
0.70
2.13
1.38
0.69
3.39
1.50
f1 (ppm)

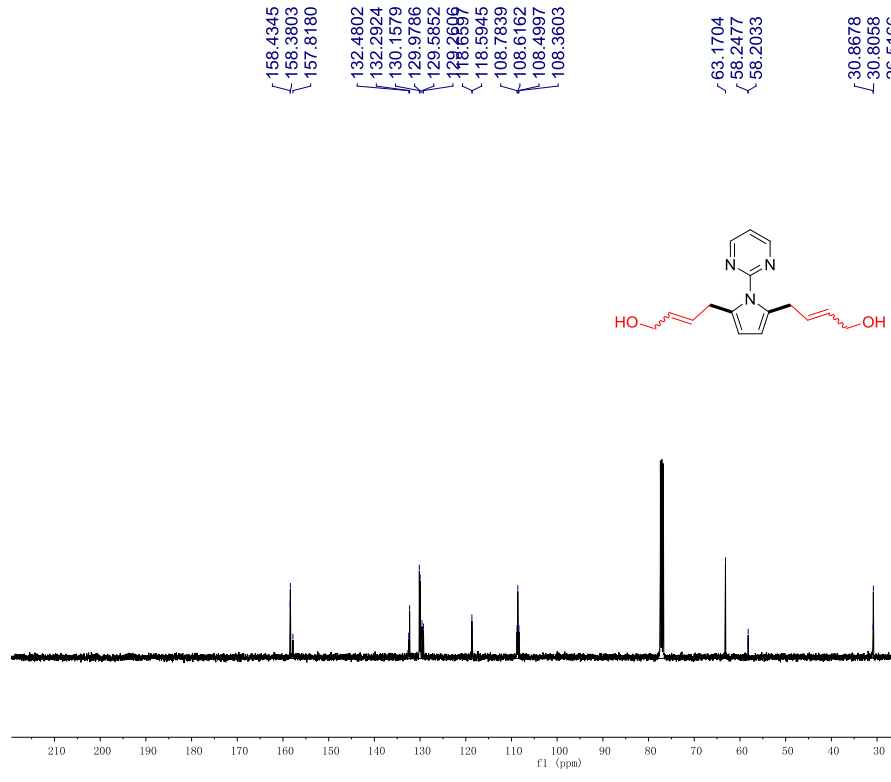

162.6047
162.4659
156.9273
156.8553
142.9254
131.6358
131.2577
131.0653
129.9372
117.8267
63.6721
58.5934
32.9041
28.4221
N
N
HO
S
f1 (ppm)

7e


8.8150
8.8122
8.8075
8.8043
7.2756
7.2662
7.2574
7.2456
6.6982
6.6935
6.6860
5.5185
5.4837
5.4722
5.2502
5.2404
5.2133
3.8855
3.8576
3.8087
3.1616
3.1451
2.6643
2.4886
HO
OH
OMe
2.00
1.16
2.03
4.19
4.05
3.04
4.06
2.38
f1 (ppm)
167.5810
167.5341
159.8276
159.7605
157.1288
157.0127
156.9163
140.0169
139.9957
139.8735
130.3562
130.2617
130.0923
119.0463
113.1666
113.1141
112.7542
63.0551
63.0327
57.9030
57.8328
55.2656
36.7384
36.7042
31.7936
HO
OH
OMe
f1 (ppm)

7f


8.7600
8.7543
8.7480
8.7423
7.2266
7.2146
7.2026
5.9673
5.9561
5.5140
5.3957
5.3555
4.0376
3.8865
3.8720
3.5459
3.5332
3.5136
3.4979
2.0575
1.9762
HO
OH
2.03
1.00
2.03
4.18
1.13
3.10
4.20
2.53
f1 (ppm)


158.4345
158.3803
157.8180
132.4802
132.2924
130.1579
129.9786
129.5852
118.5945
108.7839
108.6162
108.4997
108.3603
63.1704
58.2477
58.2033
30.8678
30.8058
26.5166
26.4513
HO
OH
f1 (ppm)