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Supporting Information for

Diastereoselective Synthesis of Functionalized Tetrahydropyridazines Containing Indole Scaffolds *via* Inverse-Electron-Demand Aza-Diels–Alder Reaction

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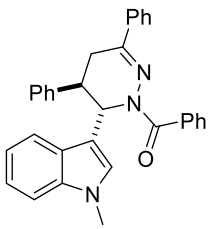
I. General remarks

^{1}H NMR spectra were recorded on a Bruker 400 MHz spectrometer in $CDCl_3$. Chemical shifts are reported in ppm with the internal TMS signal at 0.0 ppm as a standard. The data are reported as (s = single, d = double, t = triple, q = quarte, m = multiple or unresolved, brs = broad single, coupling constant(s) in Hz, integration). ^{13}C NMR spectra were recorded on a Bruker 100 MHz spectrometer in $CDCl_3$. Chemical shifts are reported in ppm with the internal chloroform signal at 77.0 ppm as a standard. Commercially obtained reagents were used without further purification. Solvents were purified prior to use according to the standard methods. Unless otherwise noted, all reactions were carried out under nitrogen atmosphere. All reactions were monitored by TLC with silica gel coated plates. Enantiomeric ratios were determined by chiral-phase HPLC analysis in comparison with authentic racemic materials using a chiralpak IE column. High Resolution Mass Spectra were recorded using ESI-TOF technique. 3-Vinylindoles,[1] azoalkenes,[2] were prepared according to the literature procedure.

II. General procedure for the inverse electron-demand aza-Diels–Alder reaction

A flame dried Schlenck tube was cooled to room temperature and filled with N_2. 3-vinylindoles (0.28 mmol), the azoalkene generating *in situ* from benzohydrazide (0.20 mmol), Na_2CO_3 (0.48 mmol) and CH_3CN (2.0 mL) were added into the Schlenck tube and filled with N_2 at room temperature. TLC analysis indicated completion of the reaction after about 30 h. Then the reaction mixture was concentrated *in vacuo* to obtain the crude product. The crude product was purified by flash silica gel chromatography to afford the product.

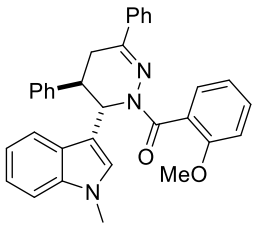


***Trans*-(6-(1-methyl-1*H*-indol-3-yl)-3,5-diphenyl-5,6-dihydropyridazin-1(4*H*)-yl)(phenyl)-methanone (3a):**

Yield (87%); 81 mg; White solid; m.p. 239-241 ºC; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.82 (d, *J* =

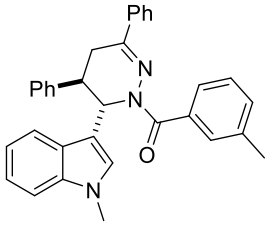
7.8 Hz, 1H), 7.69-7.66 (m, 4H), 7.47 – 7.39 (m, 4H), 7.38 – 7.33 (m, 6H), 7.30 – 7.25 (m, 3H), 7.23 – 7.21 (m, 1H), 6.75 (s, 1H), 6.37 (s, 1H), 4.02 (d, *J* = 7.2 Hz, 1H), 3.66 (s, 3H), 2.95 (d, *J* = 18.3 Hz, 1H), 2.83 (dd, *J* = 18.3, 7.0 Hz, 1H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 170.3, 146.4, 142.3, 137.7, 137.1, 135.2, 130.3, 129.9, 129.4, 128.9, 128.5, 127.4, 127.2, 126.9, 126.1, 125.5, 125.2, 122.0, 119.4, 118.9, 113.2, 109.7, 52.1, 38.5, 32.8, 24.7. HRMS (ESI-TOF) Calcd. For $C_{32}H_{28}N_3O$ ([M+H]$^+$): 470.2227, found: 470.2212.

opt-3a: Yield (81%); 75 mg; $[\alpha]^{20}_D$ = -27.2 (*c* 1.0, $CHCl_3$); >20:1 dr, it was determined by the crude ^{1}H NMR analysis. The product was analyzed by HPLC to determine the enantiomeric excess: 93% ee (Chiralpak IE, *i*-propanol/hexane = 40/60, flow rate 1.2 mL/min, λ = 230 nm); t_r = 28.7 and 34.0 min.



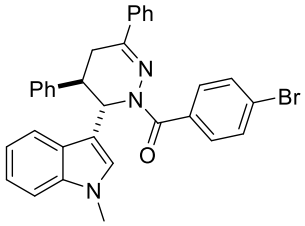
***Trans*-(2-methoxyphenyl)(6-(1-methyl-1*H*-indol-3-yl)-3,5-diphenyl-5,6-dihydropyridazin-1(4*H*)-yl)methanone (3b):**

Yield (84%); 83 mg; White solid; m.p. 189-190 ºC; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.79 (d, *J* = 9.3 Hz, 1H), 7.47 – 7.46 (m, 1H), 7.45-7.43 (m, 1H), 7.41 – 7.37 (m, 3H), 7.36 – 7.25 (m, 9H), 7.25 – 7.19 (m, 1H), 7.00-6.96 (m, 2H), 6.89 (s, 1H), 6.40 (s, 1H), 4.00 (d, *J* = 7.0 Hz, 1H), 3.79 (s, 3H), 3.69 (s, 3H), 2.84 (d, *J* = 18.1 Hz, 1H), 2.74 (dd, *J* = 18.1, 7.0 Hz, 1H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 170.4, 156.0, 145.4, 142.6, 137.9, 137.4, 130.2, 129.1, 128.8, 128.4, 128.2, 127.4, 127.2, 127.1, 126.7, 125.34, 125.31, 121.9, 120.4, 119.3, 119.0, 113.5, 110.5, 109.7, 55.5, 51.3, 38.3, 32.9, 25.0. HRMS (ESI-TOF) Calcd. For $C_{33}H_{30}N_3O_2$ ([M+H]$^+$): 500.2333, found: 500.2322.



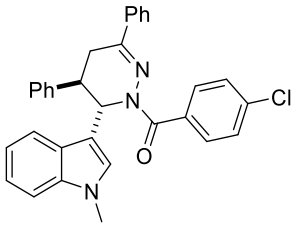
***Trans*-(6-(1-methyl-1*H*-indol-3-yl)-3,5-diphenyl-5,6-dihydropyridazin-1(4*H*)-yl)(*m*-tolyl)-methanone (3c):**

Yield (86%); 83 mg; White solid; m.p. 168-170 ºC; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.88 (d, *J* = 7.8 Hz, 1H), 7.73 (t, *J* = 3.7 Hz, 2H), 7.58 (s, 1H), 7.54 (d, *J* = 7.0 Hz, 1H), 7.44 – 7.38 (m, 7H), 7.37 – 7.27 (m, 6H), 6.81 (s, 1H), 6.43 (s, 1H), 4.07 (d, *J* = 7.2 Hz, 1H), 3.70 (s, 3H), 2.98 (d, *J* = 18.3 Hz, 1H), 2.88 (dd, *J* = 18.2, 6.9 Hz, 1H), 2.45 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 170.4, 146.1, 142.3, 137.6, 137.1, 137.0, 135.1, 130.9, 130.5, 129.3, 128.8, 128.4, 127.13, 127.10, 126.9, 126.0, 125.5, 125.2, 122.0, 119.3, 118.9, 113.2, 109.6, 52.0, 38.4, 32.7, 24.7, 21.4. HRMS (ESI-TOF) Calcd. For $C_{33}H_{30}N_3O$ ([M+H]$^{+}$): 484.2383, found: 484.2375.



***Trans*-(4-bromophenyl)(6-(1-methyl-1*H*-indol-3-yl)-3,5-diphenyl-5,6-dihydropyridazin-1(4*H*)-yl)methanone (3d):**

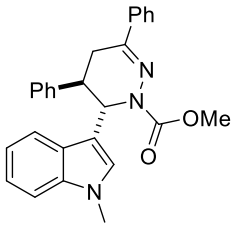
Yield (81%); 89 mg; White solid; m.p. 190-192 ºC; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.81 (d, *J* = 7.9 Hz, 1H), 7.67 (dd, *J* = 7.9, 2.9 Hz, 2H), 7.55 (s, 4H), 7.41 – 7.33 (m, 7H), 7.32 – 7.25 (m, 3H), 7.23 – 7.20 (m, 1H), 6.73 (s, 1H), 6.34 (s, 1H), 4.00 (d, *J* = 7.3 Hz, 1H), 3.66 (s, 3H), 2.96 (d, *J* = 18.4 Hz, 1H), 2.84 (dd, *J* = 18.3, 7.0 Hz, 1H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 169.3, 147.1, 142.2, 137.7, 136.9, 134.0, 131.7, 130.7, 129.6, 129.0, 128.7, 127.3, 126.9, 126.0, 125.6, 125.2, 124.9, 122.1, 119.5, 118.9, 113.1, 109.8, 52.3, 38.5, 32.9, 24.7. HRMS (ESI-TOF) Calcd. For $C_{32}H_{26}BrN_3ONa$ ([M+Na]$^{+}$): 570.1151, found: 570.1136.



***Trans*-(4-chlorophenyl)(6-(1-methyl-1*H*-indol-3-yl)-3,5-diphenyl-5,6-dihydropyridazin-1(4*H*)-yl)methanone (3e):**

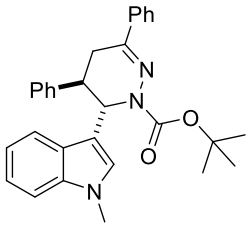
Yield (82%); 82 mg; White solid; m.p. 210-212 ºC; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.73 (d, *J* = 7.6 Hz, 1H), 7.59 (dd, *J* = 7.6, 2.9 Hz, 2H), 7.55 (d, *J* = 8.3 Hz, 2H), 7.31 – 7.26 (m, 9H), 7.25 – 7.16

(m, 3H), 7.13 – 7.10 (m, 1H), 6.65 (s, 1H), 6.27 (s, 1H), 3.92 (d, *J* = 7.3 Hz, 1H), 3.57 (s, 3H), 2.88 (d, *J* = 18.3 Hz, 1H), 2.75 (dd, *J* = 18.4, 7.0 Hz, 1H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 169.1, 146.9, 142.1, 137.6, 136.9, 136.4, 133.5, 131.5, 129.5, 128.9, 128.6, 127.6, 127.2, 126.8, 125.9, 125.5, 125.2, 122.1, 119.4, 118.8, 113.0, 109.7, 52.3, 38.4, 32.8, 24.7. HRMS (ESI-TOF) Calcd. For $C_{32}H_{27}ClN_3O$ ([M+H]$^+$): 504.1837, found: 504.1825.



***Trans*-methyl 6-(1-methyl-1*H*-indol-3-yl)-3,5-diphenyl-5,6-dihydropyridazine-1(4*H*)-carboxylate (3f):**

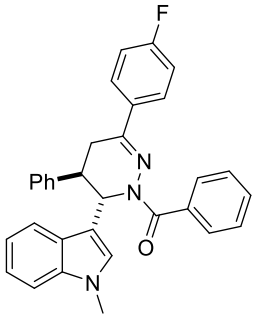
Yield (86%); 72 mg; White solid; m.p. 220-222 ºC; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.89 (dd, *J* = 7.9, 1.8 Hz, 2H), 7.78 (d, *J* = 7.9 Hz, 1H), 7.46 – 7.40 (m, 3H), 7.36 – 7.27 (m, 7H), 7.25 – 7.20 (m, 1H), 6.83 (s, 1H), 5.99 (s, 1H), 3.87 (d, *J* = 7.2 Hz, 1H), 3.81 (s, 3H), 3.70 (s, 3H), 2.88 (d, *J* = 18.3 Hz, 1H), 2.77 (dd, *J* = 18.3, 7.1 Hz, 1H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 155.2, 147.1, 142.5, 137.52, 137.46, 129.3, 128.9, 128.5, 127.1, 126.9, 125.9, 125.6, 125.1, 122.0, 119.3, 118.7, 114.1, 109.7, 53.8, 53.7, 38.7, 32.8, 24.5. HRMS (ESI-TOF) Calcd. For $C_{27}H_{26}N_3O_2$ ([M+H]$^+$): 424.2020, found: 424.2010.



***Trans-tert*-butyl 6-(1-methyl-1*H*-indol-3-yl)-3,5-diphenyl-5,6-dihydropyridazine-1(4*H*)-carboxylate (3g):**

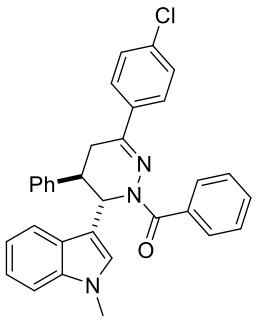
Yield (84%); 78 mg; White solid; m.p. 159-160 ºC; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.93 (d, *J* = 8.0 Hz, 2H), 7.77 (d, *J* = 7.2 Hz, 1H), 7.46 – 7.39 (m, 3H), 7.38 – 7.28 (m, 7H), 7.24 (d, *J* = 7.9 Hz, 1H), 6.86 (s, 1H), 5.96 (s, 1H), 3.86 (d, *J* = 6.8 Hz, 1H), 3.70 (s, 3H), 2.83 (d, *J* = 18.2 Hz, 1H), 2.79 (dd, *J* = 17.7, 6.2 Hz, 1H), 1.43 (s, 9H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 153.4, 146.1, 142.9,

137.6, 137.4, 129.0, 128.7, 128.3, 126.93, 126.88, 126.0, 125.5, 125.2, 121.8, 119.2, 118.6, 114.4, 109.6, 81.3, 53.4, 38.8, 32.7, 28.1, 24.4. HRMS (ESI-TOF) Calcd. For $C_{30}H_{32}N_3O_2$ ($[M+H]^+$): 466.2489, found: 466.2481.



***Trans*-(3-(4-fluorophenyl)-6-(1-methyl-1*H*-indol-3-yl)-5-phenyl-5,6-dihydropyridazin-1(4*H*)-yl)-(phenyl)methanone (3h):**

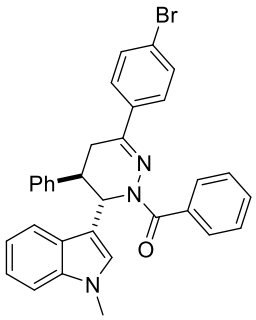
Yield (80%); 78 mg; White solid; m.p. 217-218 ºC; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.81 (d, *J* = 7.9 Hz, 1H), 7.66 – 7.61 (m, 4H), 7.47 – 7.41 (m, 3H), 7.36 (d, *J* = 5.0 Hz, 4H), 7.30 – 7.26 (m, 3H), 7.23 – 7.18 (m, 1H), 7.02 (t, *J* = 8.6 Hz, 2H), 6.74 (s, 1H), 6.36 (s, 1H), 4.01 (d, *J* = 7.0 Hz, 1H), 3.67 (s, 3H), 2.90 (d, *J* = 18.2 Hz, 1H), 2.80 (dd, *J* = 18.2, 6.9 Hz, 1H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 170.3, 163.5 (d, *J* = 248.2 Hz), 145.4, 142.2, 137.7, 135.2, 133.3 (d, *J* = 3.1 Hz), 130.3, 129.9, 129.0, 127.5, 127.4, 127.3, 126.9, 126.0, 125.2, 122.1, 119.4, 119.0, 115.5 (d, *J* = 21.6 Hz), 113.1, 109.7, 52.1, 38.4, 32.9, 24.8. HRMS (ESI-TOF) Calcd. For $C_{32}H_{27}FN_3O$ ($[M+H]^+$): 488.2133, found: 488.2122.



***Trans*-(3-(4-chlorophenyl)-6-(1-methyl-1*H*-indol-3-yl)-5-phenyl-5,6-dihydropyridazin-1(4*H*)-yl)-(phenyl)methanone (3i):**

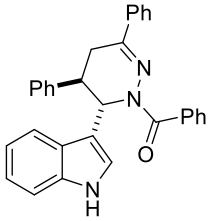
Yield (78%); 78 mg; White solid; m.p. 229-230 ºC; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.81 (d, *J* = 7.9 Hz, 1H), 7.65 (d, *J* = 7.4 Hz, 2H), 7.58 (d, *J* = 8.8 Hz, 2H), 7.49 – 7.38 (m, 3H), 7.35 – 7.33 (m,

4H), 7.32 – 7.24 (m, 5H), 7.15-7.13 (m, 1H), 6.73 (s, 1H), 6.36 (s, 1H), 4.01 (d, *J* = 7.1 Hz, 1H), 3.66 (s, 3H), 2.89 (d, *J* = 18.2 Hz, 1H), 2.79 (dd, *J* = 18.2, 6.9 Hz, 1H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 170.3, 145.2, 142.1, 137.7, 135.5, 135.3, 135.1, 130.3, 129.8, 128.9, 128.7, 127.4, 127.3, 126.8, 126.7, 125.9, 125.1, 122.1, 119.4, 118.9, 113.1, 109.7, 52.1, 38.3, 32.8, 24.6. HRMS (ESI-TOF) Calcd. For $C_{32}H_{27}ClN_3O$ ($[M+H]^+$): 504.1837, found: 504.1826.



***Trans*-(3-(4-bromophenyl)-6-(1-methyl-1*H*-indol-3-yl)-5-phenyl-5,6-dihydropyridazin-1(4*H*)-yl)(phenyl)methanone (3j):**

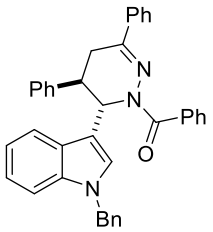
Yield (84%); 92 mg; White solid; m.p. 238-240 ºC; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.81 (d, *J* = 7.8 Hz, 1H), 7.64 (d, *J* = 7.4 Hz, 2H), 7.53 – 7.46 (m, 6H), 7.41 (t, *J* = 7.3 Hz, 2H), 7.36 – 7.35 (m, 4H), 7.31 – 7.28 (m, 2H), 7.23 – 7.19 (m, 1H), 6.73 (s, 1H), 6.36 (s, 1H), 4.01 (d, *J* = 7.1 Hz, 1H), 3.68 (s, 3H), 2.89 (d, *J* = 18.2 Hz, 1H), 2.79 (dd, *J* = 18.3, 6.9 Hz, 1H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 170.4, 145.3, 142.1, 137.7, 136.0, 135.1, 131.7, 130.4, 129.9, 129.0, 127.5, 127.3, 127.0, 126.8, 126.0, 125.2, 123.7, 122.1, 119.4, 118.9, 113.1, 109.7, 52.2, 38.4, 32.9, 24.6. HRMS (ESI-TOF) Calcd. For $C_{32}H_{27}BrN_3O$ ($[M+H]^+$): 548.1332, found: 548.1316.



***Trans*-(6-(1*H*-indol-3-yl)-3,5-diphenyl-5,6-dihydropyridazin-1(4*H*)-yl)(phenyl)methanone (3k):**

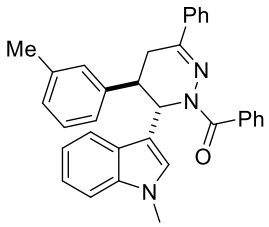
Yield (80%); 72 mg; White solid; m.p. 182-183 ºC; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.23 (s, 1H), 7.82 (d, *J* = 8.8 Hz, 1H), 7.66 – 7.62 (m, 4H), 7.50 – 7.40 (m, 3H), 7.40 – 7.32 (m, 7H), 7.31 – 7.27 (m, 2H), 7.24 – 7.18 (m, 2H), 6.80 (d, *J* = 1.5 Hz, 1H), 6.40 (s, 1H), 4.01 (d, *J* = 5.4 Hz, 1H), 2.94 (d, *J* =

18.3 Hz, 1H), 2.78 (dd, *J* = 18.3, 7.1 Hz, 1H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 170.4, 146.5, 142.2, 137.0, 136.9, 135.2, 130.2, 129.8, 129.4, 128.9, 128.5, 127.4, 127.2, 126.8, 125.5, 124.7, 122.3, 121.5, 119.7, 118.6, 114.6, 111.6, 52.1, 38.3, 24.7. HRMS (ESI-TOF) Calcd. For $C_{31}H_{26}N_3O$ ([M+H]$^+$): 456.2070, found: 456.2061.



***Trans*-(6-(1-benzyl-1*H*-indol-3-yl)-3,5-diphenyl-5,6-dihydropyridazin-1(4*H*)-yl)(phenyl)methanone (3l):**

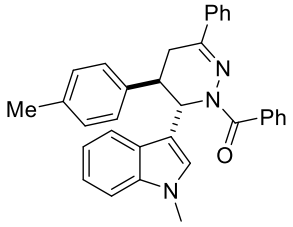
Yield (83%); 90 mg; White solid; m.p. 160-161 ºC; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.84 – 7.82 (m, 1H), 7.67 – 7.59 (m, 4H), 7.47 – 7.30 (m, 10H), 7.27 – 7.21 (m, 3H), 7.20 – 7.14 (m, 4H), 6.99 – 6.94 (m, 2H), 6.86 (s, 1H), 6.41 (s, 1H), 5.23 – 5.10 (m, 2H), 4.02 (d, *J* = 7.3 Hz, 1H), 2.92 (d, *J* = 18.3 Hz, 1H), 2.80 (dd, *J* = 18.3, 7.1 Hz, 1H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 170.3, 146.6, 142.2, 137.2, 137.1, 135.2, 130.2, 129.8, 129.3, 128.9, 128.6, 128.4, 127.5, 127.3, 127.2, 126.9, 126.5, 125.7, 125.5, 125.4, 122.2, 119.6, 119.0, 113.8, 110.2, 52.0, 50.0, 38.5, 24.9. HRMS (ESI-TOF) Calcd. For $C_{38}H_{32}N_3O$ ([M+H]$^+$): 546.2540, found: 546.2530.



***Trans*-(6-(1-methyl-1*H*-indol-3-yl)-3-phenyl-5-(*m*-tolyl)-5,6-dihydropyridazin-1(4*H*)-yl)-(phenyl)methanone (3m):**

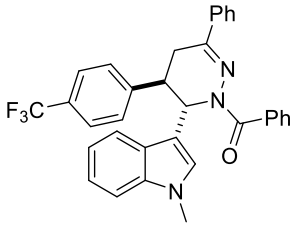
Yield (84%); 80 mg; White solid; m.p. 148-150 ºC; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.82 (d, *J* = 7.8 Hz, 1H), 7.70 – 7.65 (m, 4H), 7.49 – 7.38 (m, 3H), 7.35 – 7.21 (m, 8H), 7.13-7.05 (m, 2H), 6.74 (s, 1H), 6.34 (s, 1H), 3.97 (d, *J* = 7.2 Hz, 1H), 3.64 (s, 3H), 2.91 (d, *J* = 18.3 Hz, 1H), 2.81 (dd, *J* = 18.3, 7.0 Hz, 1H), 2.35 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 170.3, 146.5, 142.3, 138.4, 137.6, 137.1, 135.3, 130.2, 129.9, 129.3, 128.7, 128.4, 127.94, 127.91, 127.3, 126.0, 125.5, 125.2, 123.5,

122.0, 119.3, 118.9, 113.2, 109.6, 52.1, 38.4, 32.7, 24.9, 21.6. HRMS (ESI-TOF) Calcd. For $C_{33}H_{30}N_3O$ ($[M+H]^+$): 484.2383, found: 484.2375.



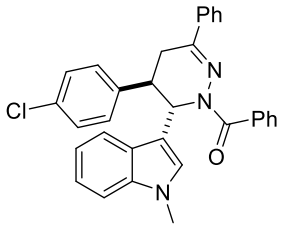
***Trans*-(6-(1-methyl-1*H*-indol-3-yl)-3-phenyl-5-(*p*-tolyl)-5,6-dihydropyridazin-1(4*H*)-yl)-(phenyl)methanone (3n):**

Yield (89%); 85 mg; White solid; m.p. 190-191 ºC; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.81 (d, *J* = 7.8 Hz, 1H), 7.70 – 7.64 (m, 4H), 7.45 – 7.39 (m, 3H), 7.33 – 7.19 (m, 8H), 7.14 (d, *J* = 7.9 Hz, 2H), 6.74 (s, 1H), 6.35 (s, 1H), 3.97 (d, *J* = 7.4 Hz, 1H), 3.62 (s, 3H), 2.90 (d, *J* = 18.3 Hz, 1H), 2.80 (dd, *J* = 18.3, 7.0 Hz, 1H), 2.30 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 170.3, 146.4, 139.2, 137.6, 137.1, 136.7, 135.2, 130.2, 129.9, 129.5, 129.3, 128.4, 127.3, 126.7, 126.0, 125.5, 125.2, 121.9, 119.3, 118.9, 113.2, 109.6, 52.1, 38.0, 32.7, 24.8, 21.0. HRMS (ESI-TOF) Calcd. For $C_{33}H_{30}N_3O$ ($[M+H]^+$): 484.2383, found: 484.2373.



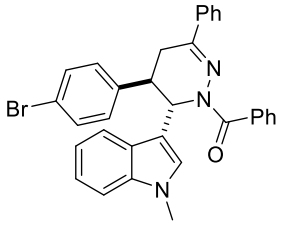
***Trans*-(6-(1-methyl-1*H*-indol-3-yl)-3-phenyl-5-(4-(trifluoromethyl)phenyl)-5,6-dihydropyridazin-1(4*H*)-yl)(phenyl)methanone (3o):**

Yield (80%); 85 mg; White solid; m.p. 189-191 ºC; ^{1}H NMR (400 MHz, Chloroform-d) δ 7.79 (d, *J* = 7.9 Hz, 1H), 7.71 – 7.65 (m, 4H), 7.61– 7.56 (m, 2H), 7.51 – 7.40 (m, 5H), 7.38 – 7.25 (m, 5H), 7.24 – 7.19 (m, 1H), 6.77 (s, 1H), 6.39 (s, 1H), 4.06 (d, *J* = 6.5 Hz, 1H), 3.66 (s, 3H), 2.93 (d, *J* = 18.2 Hz, 1H), 2.86 (dd, *J* = 18.3, 6.5 Hz, 1H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 170.3, 146.3, 145.9, 137.7, 136.8, 134.9, 130.4, 129.9, 129.5 (q, *J* = 32.4 Hz), 128.6, 127.5, 127.4, 126.1, 125.9 (q, *J* = 3.7 Hz), 125.5, 125.1, 124.0 (q, *J* = 270.0 Hz), 122.1, 119.5, 118.7, 112.7, 109.8, 51.6, 38.4, 32.8, 24.6. HRMS (ESI-TOF) Calcd. For $C_{33}H_{27}F_3N_3O$ ($[M+H]^+$): 538.2101, found: 538.2087.



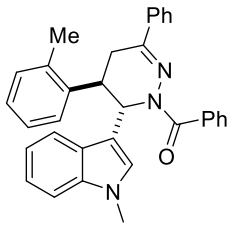
***Trans*-(5-(4-chlorophenyl)-6-(1-methyl-1*H*-indol-3-yl)-3-phenyl-5,6-dihydropyridazin-1(4*H*)-yl)-(phenyl)methanone (3p):**

Yield (80%); 80 mg; White solid; m.p. 174-176 ºC; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.78 (d, *J* = 7.9 Hz, 1H), 7.71 – 7.63 (m, 4H), 7.50 – 7.39 (m, 3H), 7.34 – 7.30 (m, 4H), 7.29 – 7.17 (m, 6H), 6.73 (s, 1H), 6.34 (s, 1H), 3.97 – 3.94 (m, 1H), 3.64 (s, 3H), 2.88 (d, *J* = 18.3 Hz, 1H), 2.81 (dd, *J* = 18.3, 6.5 Hz, 1H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 169.3, 145.0, 139.7, 136.6, 135.9, 134.0, 131.9, 129.4, 128.9, 128.5, 128.0, 127.5, 127.3, 126.4, 125.0, 124.5, 124.1, 121.1, 118.4, 117.8, 111.8, 108.7, 50.9, 36.9, 31.8, 23.7. HRMS (ESI-TOF) Calcd. For $C_{32}H_{27}ClN_3O$ ([M+H]$^+$): 504.1837, found: 504.1826.



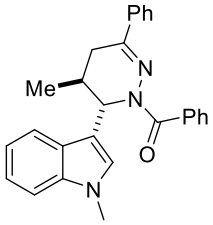
***Trans*-(5-(4-bromophenyl)-6-(1-methyl-1*H*-indol-3-yl)-3-phenyl-5,6-dihydropyridazin-1(4*H*)-yl)(phenyl)methanone (3q):**

Yield (78%); 85 mg; White solid; m.p. 184-185 ºC; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.77 (d, *J* = 5.3 Hz, 1H), 7.69 – 7.64 (m, 4H), 7.47 – 7.41 (m, 5H), 7.35 – 7.21 (m, 7H), 7.20 (dd, *J* = 6.6, 1.6 Hz, 1H), 6.74 (s, 1H), 6.35 (s, 1H), 3.96 (d, *J* = 4.5 Hz, 1H), 3.64 (s, 3H), 2.88 (d, *J* = 16.5 Hz, 1H), 2.81 (dd, *J* = 18.3, 6.5 Hz, 1H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 170.2, 146.0, 141.2, 137.6, 136.8, 135.0, 131.9, 130.4, 129.9, 129.5, 128.6, 128.5, 127.4, 126.0, 125.4, 125.1, 122.0, 121.0, 119.4, 118.7, 112.8, 109.7, 51.8, 38.0, 32.8, 24.6. HRMS (ESI-TOF) Calcd. For $C_{32}H_{27}BrN_3O$ ([M+H]$^+$): 548.1332, found: 548.1320.



***Trans*-(6-(1-methyl-1*H*-indol-3-yl)-3-phenyl-5-(*o*-tolyl)-5,6-dihydropyridazin-1(4*H*)-yl)-(phenyl)methanone (3r):**

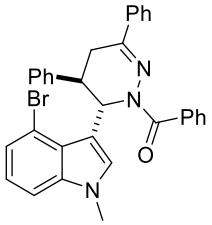
Yield (72%); 69 mg; White solid; m.p. 194-196 ºC; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.79 (d, *J* = 7.9 Hz, 1H), 7.62 (dd, *J* = 10.4, 6.6 Hz, 4H), 7.36 (dt, *J* = 14.2, 7.0 Hz, 3H), 7.30 – 7.19 (m, 6H), 7.17 – 7.06 (m, 4H), 6.71 (s, 1H), 6.17 (s, 1H), 4.10 (d, *J* = 6.7 Hz, 1H), 3.59 (s, 3H), 2.84 (dd, *J* = 18.4, 6.7 Hz, 1H), 2.77 (d, *J* = 18.3 Hz, 1H), 2.63 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 170.4, 147.3, 140.7, 137.6, 137.1, 135.6, 135.3, 131.0, 130.3, 130.0, 129.4, 128.5, 127.4, 127.2, 126.7, 126.6, 125.6, 125.4, 125.3, 121.9, 119.4, 119.1, 113.4, 109.7, 50.4, 34.9, 32.9, 25.4, 20.6. HRMS (ESI-TOF) Calcd. For $C_{33}H_{30}N_3O$ ([M+H]$^+$): 484.2383, found: 484.2373.



***Trans*-5-methyl-6-(1-methyl-1*H*-indol-3-yl)-3-phenyl-5,6-dihydropyridazin-1(4*H*)-yl)(phenyl)-methanone (3s):**

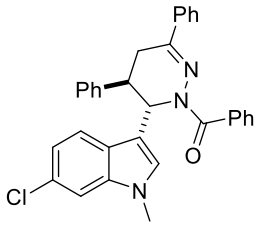
Yield (82%); 66 mg; White solid; m.p. 153-155 ºC; 1.5:1 dr; major: ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.83 (s, 1H), 7.74 (d, *J* = 6.6 Hz, 2H), 7.62 – 7.57 (m, 2H), 7.44 – 7.39 (m, 3H), 7.33 – 7.29 (m, 3H), 7.20 (s, 1H), 7.16 – 7.09 (m, 2H), 6.69 (s, 1H), 6.07 (s, 1H), 3.62 (s, 3H), 2.74 (d, *J* = 19.3 Hz, 1H), 2.38 (dd, *J* = 17.4, 5.7 Hz, 2H), 1.26 (d, *J* = 6.8 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 170.6, 146.8, 137.6, 136.5, 135.4, 130.0, 129.9, 129.1, 128.3, 127.4, 126.6, 125.5, 125.4, 121.8, 119.4, 119.0, 113.6, 109.5, 50.0, 32.7, 27.9, 26.6, 18.9. minor: ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.76 (s, 1H), 7.62 – 7.58 (m, 2H), 7.57 (s, 1H), 7.39 (t, *J* = 7.9 Hz, 3H), 7.29 – 7.26 (m, 2H), 7.18 (dd, *J* = 8.0, 3.6 Hz, 4H), 7.11 (d, *J* = 8.4 Hz, 1H), 6.66 (s, 1H), 6.14 (s, 1H), 3.57 (s, 3H), 2.74 (d, *J* = 17.0 Hz, 1H), 2.45 (dd, *J* = 17.8, 6.1 Hz, 2H), 0.98 (d, *J* = 6.4 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 169.5, 145.6, 137.6, 137.2, 135.6, 130.2, 129.9, 129.1, 128.4, 127.9, 127.2, 125.7, 125.3, 121.6, 119.6, 119.1,

111.5, 109.2, 52.1, 32.7, 28.1, 27.5, 18.4. HRMS (ESI-TOF) Calcd. For $C_{27}H_{25}N_3ONa$ ($[M+Na]^+$): 430.1890, found: 430.1881.



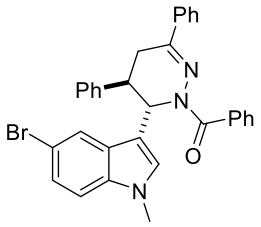
***Trans*-(6-(4-bromo-1-methyl-1*H*-indol-3-yl)-3,5-diphenyl-5,6-dihydropyridazin-1(4*H*)-yl)(phenyl)methanone (3t):**

Yield (78%); 85 mg; White solid; m.p. 236-237 ºC; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.62 – 7.58 (m, 4H), 7.40 – 7.32 (m, 5H), 7.28 – 7.22 (m, 6H), 7.14 (d, *J* = 5.4 Hz, 2H), 7.00 (t, *J* = 7.9 Hz, 1H), 6.85 (s, 1H), 6.71 (s, 1H), 4.08 (d, *J* = 6.7 Hz, 1H), 3.54 (s, 3H), 2.89 (d, *J* = 18.2 Hz, 1H), 2.74 (dd, *J* = 18.2, 6.9 Hz, 1H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 170.1, 146.4, 142.1, 138.8, 137.1, 135.2, 130.3, 130.0, 129.3, 128.7, 128.5, 127.6, 127.4, 127.03, 127.01, 125.5, 124.3, 123.9, 122.8, 114.7, 113.9, 108.8, 50.6, 38.8, 33.1, 24.8. HRMS (ESI-TOF) Calcd. For $C_{32}H_{26}BrN_3ONa$ ($[M+Na]^+$): 570.1151, found: 570.1141.



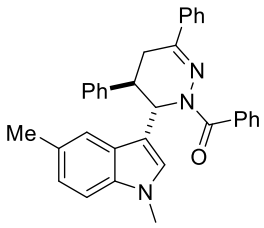
***Trans*-(6-(6-chloro-1-methyl-1*H*-indol-3-yl)-3,5-diphenyl-5,6-dihydropyridazin-1(4*H*)-yl)(phenyl)methanone (3u):**

Yield (78%); 78 mg; White solid; m.p. 206-208 ºC; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.71 – 7.65 (m, 5H), 7.50 – 7.39 (m, 3H), 7.37 – 7.32 (m, 7H), 7.30 – 7.25 (m, 2H), 7.18 – 7.15 (m, 1H), 6.75 (s, 1H), 6.31 (s, 1H), 3.94 (d, *J* = 7.5 Hz, 1H), 3.62 (s, 3H), 2.96 (d, *J* = 18.3 Hz, 1H), 2.81 (dd, *J* = 18.3, 7.1 Hz, 1H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 170.4, 146.4, 142.1, 138.1, 137.0, 135.1, 130.4, 130.0, 129.5, 129.0, 128.6, 128.3, 127.5, 127.3, 126.9, 126.8, 125.6, 123.8, 120.1, 119.8, 113.6, 109.8, 51.9, 38.6, 33.0, 24.7. HRMS (ESI-TOF) Calcd. For $C_{32}H_{27}ClN_3O$ ($[M+H]^+$): 504.1837, found: 504.1830.



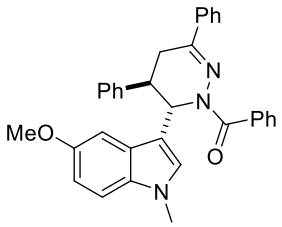
***Trans*-(6-(5-bromo-1-methyl-1*H*-indol-3-yl)-3,5-diphenyl-5,6-dihydropyridazin-1(4*H*)-yl)(phenyl)methanone (3v):**

Yield (83%); 90 mg; White solid; m.p. 246-248 ºC; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.92 (s, 1H), 7.68 – 7.66 (m, 4H), 7.49 – 7.33 (m, 11H), 7.28 – 7.25 (m, 1H), 7.16 (d, *J* = 8.7 Hz, 1H), 6.74 (s, 1H), 6.29 (s, 1H), 3.94 (d, *J* = 7.4 Hz, 1H), 3.63 (s, 3H), 2.97 (d, *J* = 18.4 Hz, 1H), 2.80 (dd, *J* = 18.3, 7.1 Hz, 1H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 170.3, 146.4, 141.9, 137.0, 136.4, 135.0, 130.4, 130.0, 129.5, 129.0, 128.6, 127.5, 127.4, 127.3, 126.90, 126.88, 125.6, 125.0, 121.5, 112.94, 112.88, 111.3, 51.8, 38.4, 33.0, 24.8. HRMS (ESI-TOF) Calcd. For $C_{32}H_{27}BrN_3O$ ([M+H]$^+$): 548.1332, found: 548.1319.



***Trans*-(6-(1,5-dimethyl-1*H*-indol-3-yl)-3,5-diphenyl-5,6-dihydropyridazin-1(4*H*)-yl)-(phenyl)-methanone (3w):**

Yield (74%); 71 mg; White solid; m.p. 192-194 ºC; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.67 (t, *J* = 6.8 Hz, 4H), 7.58 (s, 1H), 7.47 – 7.36 (m, 6H), 7.35 – 7.32 (m, 4H), 7.25 (t, *J* = 7.1 Hz, 1H), 7.18 (d, *J* = 8.3 Hz, 1H), 7.09 (d, *J* = 6.9 Hz, 1H), 6.70 (s, 1H), 6.35 (s, 1H), 4.00 (d, *J* = 7.2 Hz, 1H), 3.61 (s, 3H), 2.94 (d, *J* = 18.2 Hz, 1H), 2.83 (dd, *J* = 18.3, 6.9 Hz, 1H), 2.52 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 170.2, 146.2, 142.3, 137.1, 136.1, 135.2, 130.2, 129.9, 129.3, 128.9, 128.53, 128.45, 127.3, 127.1, 126.9, 126.0, 125.5, 125.4, 123.6, 118.5, 112.6, 109.4, 52.0, 38.2, 32.8, 24.7, 21.6. HRMS (ESI-TOF) Calcd. For $C_{33}H_{30}N_3O$ ([M+H]$^+$): 484.2383, found: 484.2375.



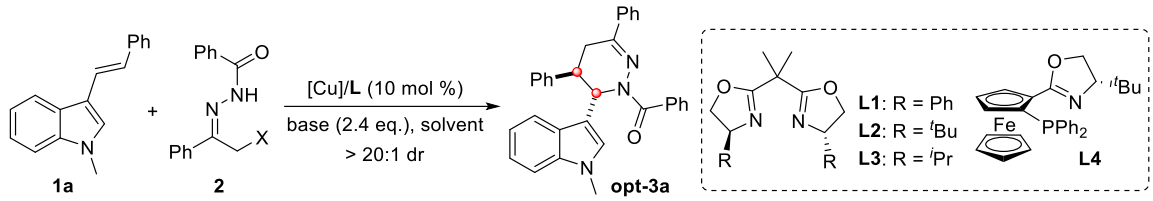
***Trans*-6-(5-methoxy-1-methyl-1*H*-indol-3-yl)-3,5-diphenyl-5,6-dihydropyridazin-1(4*H*)-yl)-(phenyl)methanone (3x):**

Yield (80%); 79 mg; White solid; m.p. 192-194 ºC; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.69 – 7.65 (m, 4H), 7.50 – 7.39 (m, 4H), 7.37 – 7.32 (m, 7H), 7.23 – 7.22 (m, 1H), 7.19 (d, *J* = 8.8 Hz, 1H), 6.94 – 6.92 (m, 1H), 6.74 (s, 1H), 6.32 (s, 1H), 3.96 (d, *J* = 7.1 Hz, 1H), 3.89 (s, 3H), 3.64 (s, 3H), 2.96 (d, *J* = 18.3 Hz, 1H), 2.86 (dd, *J* = 18.3, 6.9 Hz, 1H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 170.4, 154.0, 146.4, 142.4, 137.1, 135.3, 133.1, 130.3, 130.0, 129.4, 129.0, 128.5, 127.4, 127.2, 127.0, 126.9, 126.6, 125.5, 112.8, 112.1, 110.5, 101.1, 56.1, 52.0, 38.5, 33.0, 24.9. HRMS (ESI-TOF) Calcd. For $C_{33}H_{30}N_3O_2$ ([M+H]$^+$): 500.2333, found: 500.2320.

III. Optimization reaction conditions for the asymmetric IEDDA cyclization

As shown in Table S1, a series of chiral oxazoline ligands was firstly examined in the Cu-catalyzed inverse-electron-demand aza-Diels-Alder (IEDDA) reaction between *in situ* generated azoalkene and 3-vinylindole **1a** in the presence of Na_2CO_3, and ligand **L3** could deliver the desired product **opt-3a** with the best result in 72% yield and 75% ee (entry 3). Subsequently, the solvent effect was investigated in the Cu(OTf)$_2$/**L3** catalytic system, this transformation was proceeded smoothly in several solvents, such as THF, MeCN and DCE (entries 5-7), and high yield and good enantioselectivity was given in MeCN (entry 6, 96% yield, 89% ee). It was found that another metal precursor $Cu(MeCN)_4BF_4$ also can provide similar reaction result with Cu(OTf)$_2$ (entry 9 *vs* entry 6, 93% yield, 89% ee). In addition, when the azoalkene was generated *in situ* from (*Z*)-*N*′-(2-chloro-1-phenylethylidene)benzohydrazide in the presence of Na_2CO_3, good yield and better enantioselectivity was afforded (entry 10, 81% yield, 93% ee). Some bases, such as $NaHCO_3$, K_2CO_3 and K_3PO_4, were also inspected into this asymmetric cycloaddition reaction, poor to good reaction results could be provided (entries 11-13, 32-82% yields, 15%-89% ee).

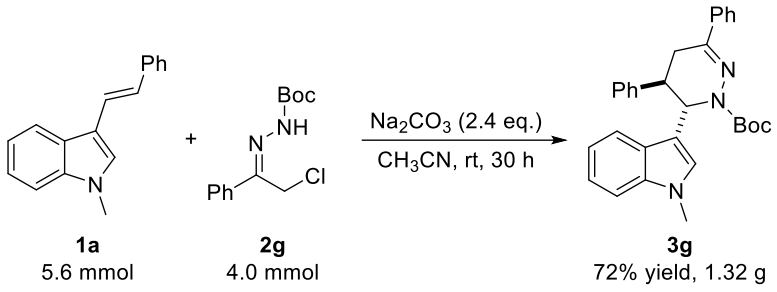
Table S1. Optimization reaction conditions for the asymmetric IEDDA cyclization.[a]



entry	ligand	[Cu]	X	base	solvent	yield (%)[b]	ee (%)[c]
1	**L1**	$Cu(OTf)_2$	Br	Na_2CO_3	DCM	75	21
2	**L2**	$Cu(OTf)_2$	Br	Na_2CO_3	DCM	76	30
3	**L3**	$Cu(OTf)_2$	Br	Na_2CO_3	DCM	72	75
4	**L4**	$Cu(OTf)_2$	Br	Na_2CO_3	DCM	57	19
5	**L3**	$Cu(OTf)_2$	Br	Na_2CO_3	THF	75	0
6	**L3**	$Cu(OTf)_2$	Br	Na_2CO_3	MeCN	96	89
7	**L3**	$Cu(OTf)_2$	Br	Na_2CO_3	DCE	91	31
8	**L3**	$(CuOTf•1/2Ph)_2$	Br	Na_2CO_3	MeCN	67	73
9	**L3**	$Cu(MeCN)_4BF_4$	Br	Na_2CO_3	MeCN	93	89
10	**L3**	$Cu(OTf)_2$	Cl	Na_2CO_3	MeCN	81	93
11	**L3**	$Cu(OTf)_2$	Cl	$NaHCO_3$	MeCN	82	89
12	**L3**	$Cu(OTf)_2$	Cl	K_2CO_3	MeCN	76	73
13	**L3**	$Cu(OTf)_2$	Cl	K_3PO_4	MeCN	32	15

[a] Reaction conditions: **1a** (0.14 mmol), **2a (**0.10 mmol), [Cu] (0.010 mmol), ligand (0.012 mmol), base (0.24 mmol) in 1 mL solvent at room temperature for 24 h. The dr value was determined by the crude ^1H NMR analysis. [b] Yield was obtained after chromatographic purification. [c] The ee value was determined by HPLC analysis.

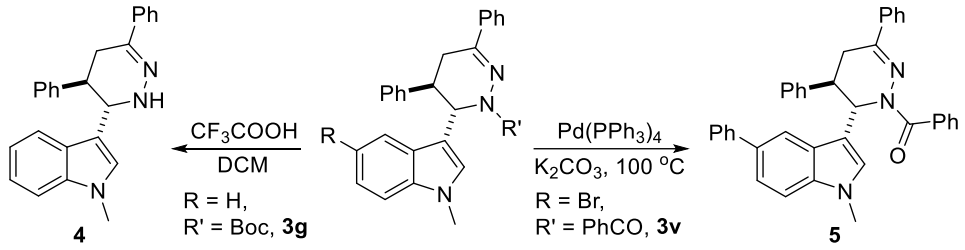
IV. Gram-scale inverse-electron-demand aza-Diels-Alder reaction



A flame dried Schlenck tube was cooled to room temperature and filled with N_2. 3-vinylindole **1a** (5.6 mmol), the azoalkene generating *in situ* from benzohydrazide **2g** (4.0 mmol), Na_2CO_3 (9.6 mmol) and CH_3CN (40 mL) were added into the Schlenck tube and filled with N_2 at room temperature. TLC analysis indicated completion of the reaction after about 30 h. Then the reaction mixture was

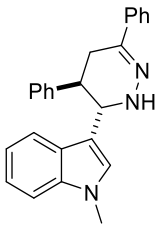
concentrated *in vacuo* to obtain the crude product. The crude product was purified by flash silica gel chromatography to afford the product **3g** in 72% yield (1.32 g).

V. Synthetic transformation



To a solution of **3g** (0.2 mmol) in 1 mL CH_2Cl_2 was added CF_3COOH (0.6 mmol) at room temperature, and the corresponding mixture was stirred at this temperature until the reaction completed (monitoring by TLC). The solvent was removed under reduced pressure and the residue was purified by column chromatography (PE:EA = 3:1) on silica gel to afford desired compound **4** in 62% yield.

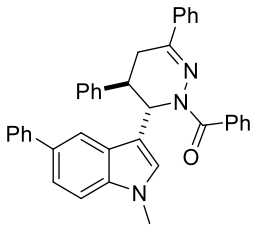
To a solution of **3v** (0.10 mmol) in THF/H_2O (4:1 v/v) was added $Pd(PPh_3)_4$ (0.01 mmol), phenylboronic acid (0.20 mmol) and K_2CO_3 (20.7 mg, 0.15 mmol). The resulting mixture was stirred at 100 ℃ for 24 h under argon atmosphere. After the completion of the reaction which was indicated by TLC, water (5 mL) was added to the reaction mixture, which was then extracted with ethyl acetate (3 ×5 mL). The combined organic layers were dried and concentrated under the reduced pressure to give a residue. Finally, the residue was purified by preparative thin layer chromatography (PE:DCM = 1:1) on silica gel to afford pure product **5** in 80% yield.



***Trans*-3-(4,6-diphenyl-2,3,4,5-tetrahydropyridazin-3-yl)-1-methyl-1H-indole (4):**

Yield (62%); 45 mg; Yellow liquid; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.74 (d, *J* = 7.1 Hz, 2H), 7.68 (d, *J* = 7.9 Hz, 1H), 7.36 (t, *J* = 7.3 Hz, 2H), 7.29 (t, *J* = 8.0 Hz, 2H), 7.19 – 7.15 (m, 4H), 7.12 – 7.04 (m, 4H), 6.83 (s, 1H), 4.57 (d, *J* = 9.7 Hz, 1H), 3.61 (s, 3H), 3.06 (dd, *J* = 18.2, 6.4 Hz, 1H), 2.91

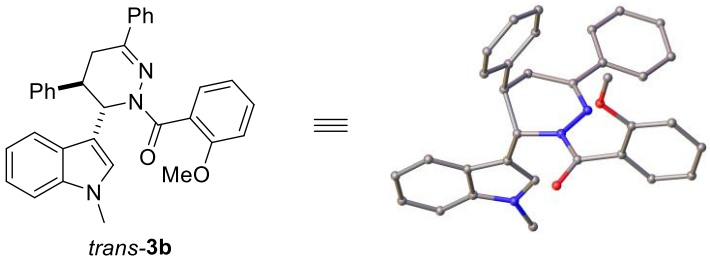
(dd, *J* = 18.2, 10.0 Hz, 1H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 143.7, 143.0, 138.1, 137.0, 128.5, 128.4, 127.9, 127.69, 127.65, 126.61, 126.60, 124.5, 121.6, 119.6, 119.1, 112.7, 109.3, 55.4, 43.1, 32.7, 32.0. HRMS (ESI-TOF) Calcd. For $C_{25}H_{24}N_3$ ([M+H]$^+$): 366.1965, found: 366.1957.



***Trans*-(6-(1-methyl-5-phenyl-1H-indol-3-yl)-3,5-diphenyl-5,6-dihydropyridazin-1(4H)-yl)(phenyl)methanone (5):**

Yield (80%); 44 mg; White solid; m.p. 214-216 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.98 (s, 1H), 7.69 (d, *J* = 6.9 Hz, 6H), 7.54 – 7.38 (m, 7H), 7.38 – 7.31 (m, 8H), 7.28 – 7.25 (m, 1H), 6.79 (s, 1H), 6.42 (s, 1H), 4.03 (d, *J* = 7.1 Hz, 1H), 3.69 (s, 3H), 2.97 (d, *J* = 18.3 Hz, 1H), 2.87 (dd, *J* = 18.3, 6.9 Hz, 1H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 170.4, 146.4, 142.5, 142.2, 137.3, 137.1, 135.2, 133.1, 130.4, 130.0, 129.4, 129.0, 128.8, 128.6, 127.6, 127.4, 127.3, 126.9, 126.8, 126.5, 125.7, 125.6, 122.1, 117.5, 113.7, 110.0, 52.0, 38.6, 33.0, 24.9. HRMS (ESI-TOF) Calcd. For $C_{38}H_{32}N_3O$ ([M+H]$^+$): 546.2467, found: 546.2520.

VI. The configuration determination of *trans*-3b



trans-**3b**

In a 10 mL oven-dried glass sample vial, 40 mg pure **3b** and 1.0 mL CH_2Cl_2 were added, and then 3 mL *n*-hexane was slowly added to the solution, which was sealed with perforated paper at room temperature to grow crystals.[3]

Bond precision: C-C = 0.0077 Å Wavelength = 0.71073

Cell: a = 10.973(3) b = 27.895(9) c = 9.090(3)

alpha = 90 beta = 112.891(6) gamma = 90

Temperature: 200 K

	Calculated	Reported
Volume	2563.3(14)	2563.3(14)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C33 H29 N3 O2	C33 H29 N3 O2
Sum formula	C33 H29 N3 O2	C33 H29 N3 O2
Mr	499.59	499.59
Dx,g cm-3	1.295	1.295
Z	4	4
Mu (mm-1)	0.081	0.081
F000	1056.0	1056.0
F000’	1056.41	
h,k,lmax	13,33,10	13,33,10
Nref 4514		4384
Tmin,Tmax	0.994, 0.996	0.511, 0.745
Tmin’	0.992	

Correction method = # Reported T Limits: Tmin = 0.511 Tmax = 0.745

AbsCorr = MULTI-SCAN

Data completeness = 0.971 Theta(max) = 25.000

R(reflections) = 0.1067(3111) wR2(reflections) = 0.2845(4384)

S = 1.193 Npar = 345

VII. Reference

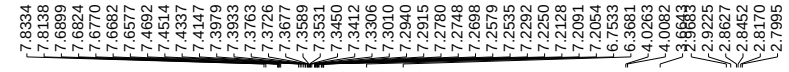
1. Gao H.-Y.; Wu X.-X.; Zhang J.-L. Gold(I)-Catalyzed, Highly Diastereoselective, Tandem Heterocyclizations/[3+2] Cycloadditions: Synthesis of Highly Substituted Cyclopenta[c]furans. *Chem. Eur. J.* **2011**, *17*, 2838.

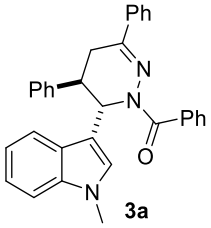
2. Chen J.-R.; Dong W.-R.; M. Candy; Pan F.-F.; M. Jörres; C. Bolm. Enantioselective Synthesis of

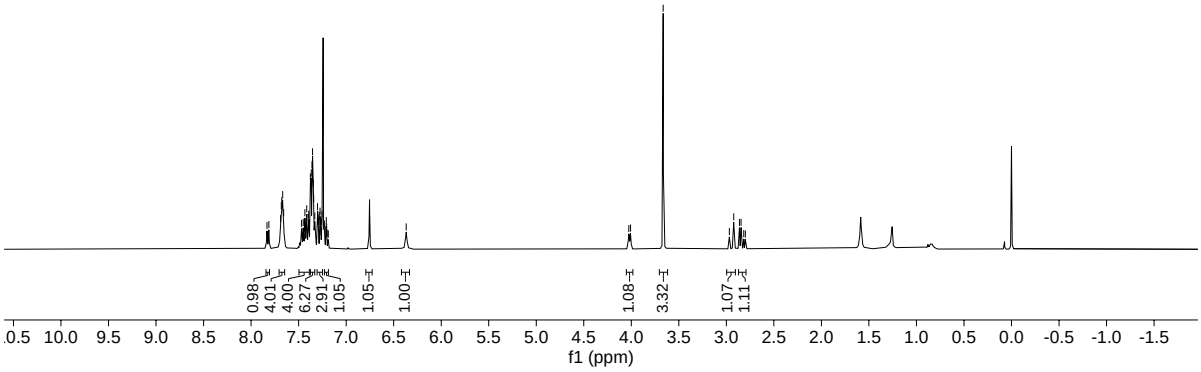
Dihydropyrazoles by Formal [4+1] Cycloaddition of in Situ-Derived Azoalkenes and Sulfur Ylides. *J. Am. Chem. Soc.* **2012**, *134*, 6924.

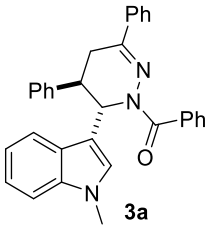
3. CCDC 2077849 (**3b**) contains the supplementary crystallographic data for this paper.

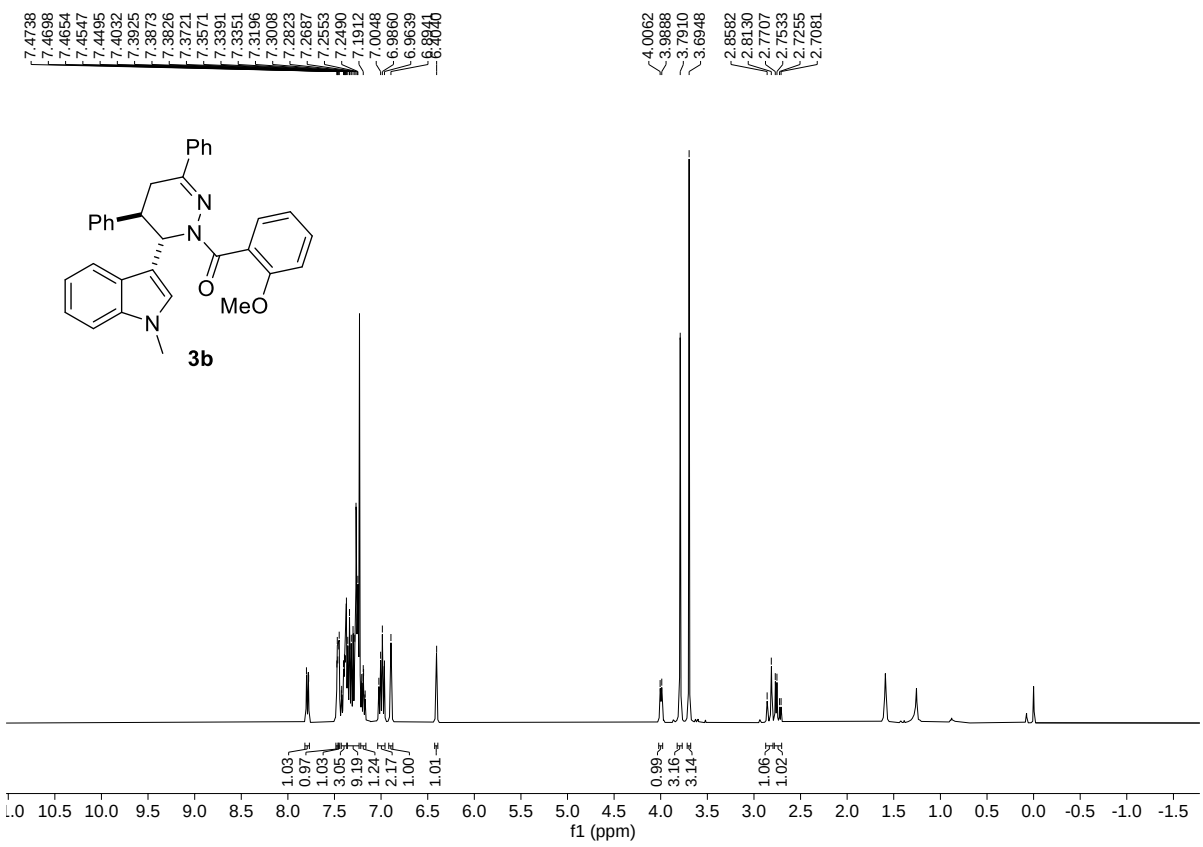
VIII. ^{1}H NMR and ^{13}C NMR spectra







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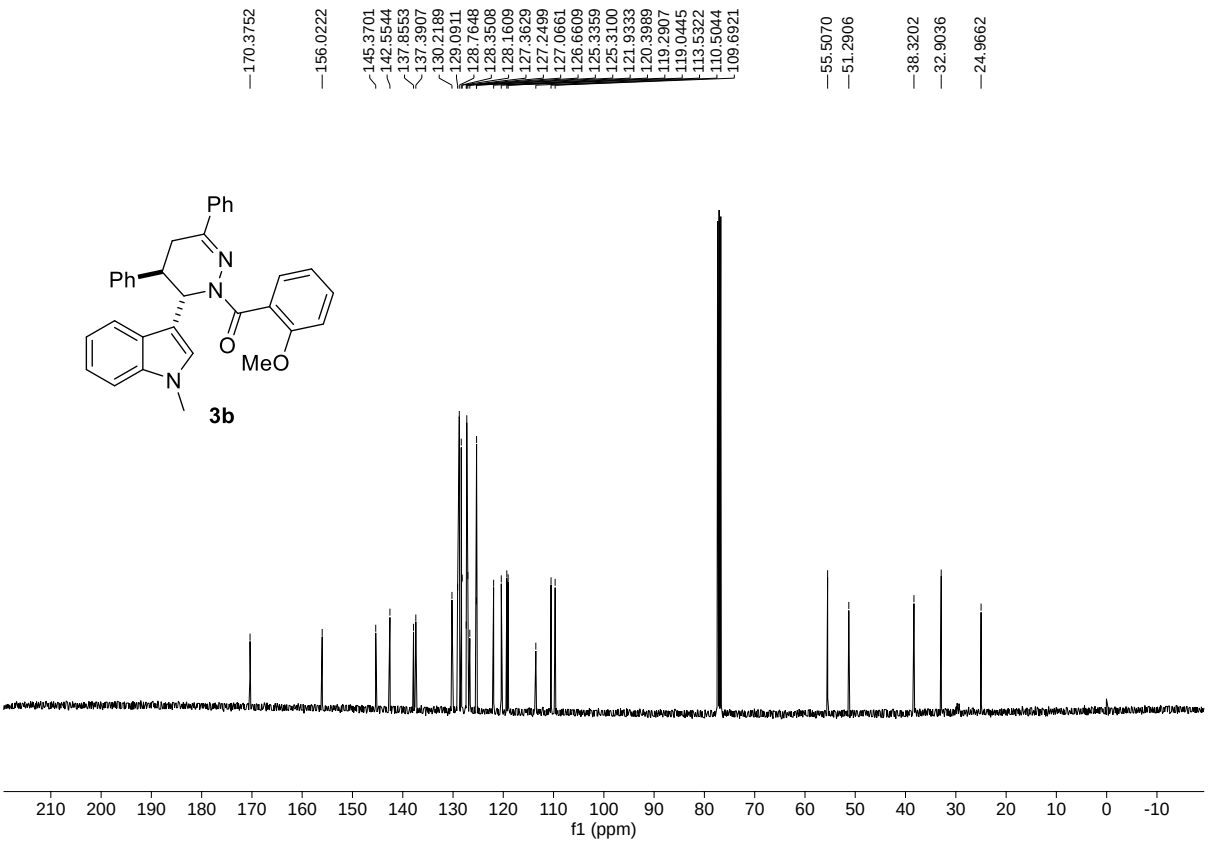
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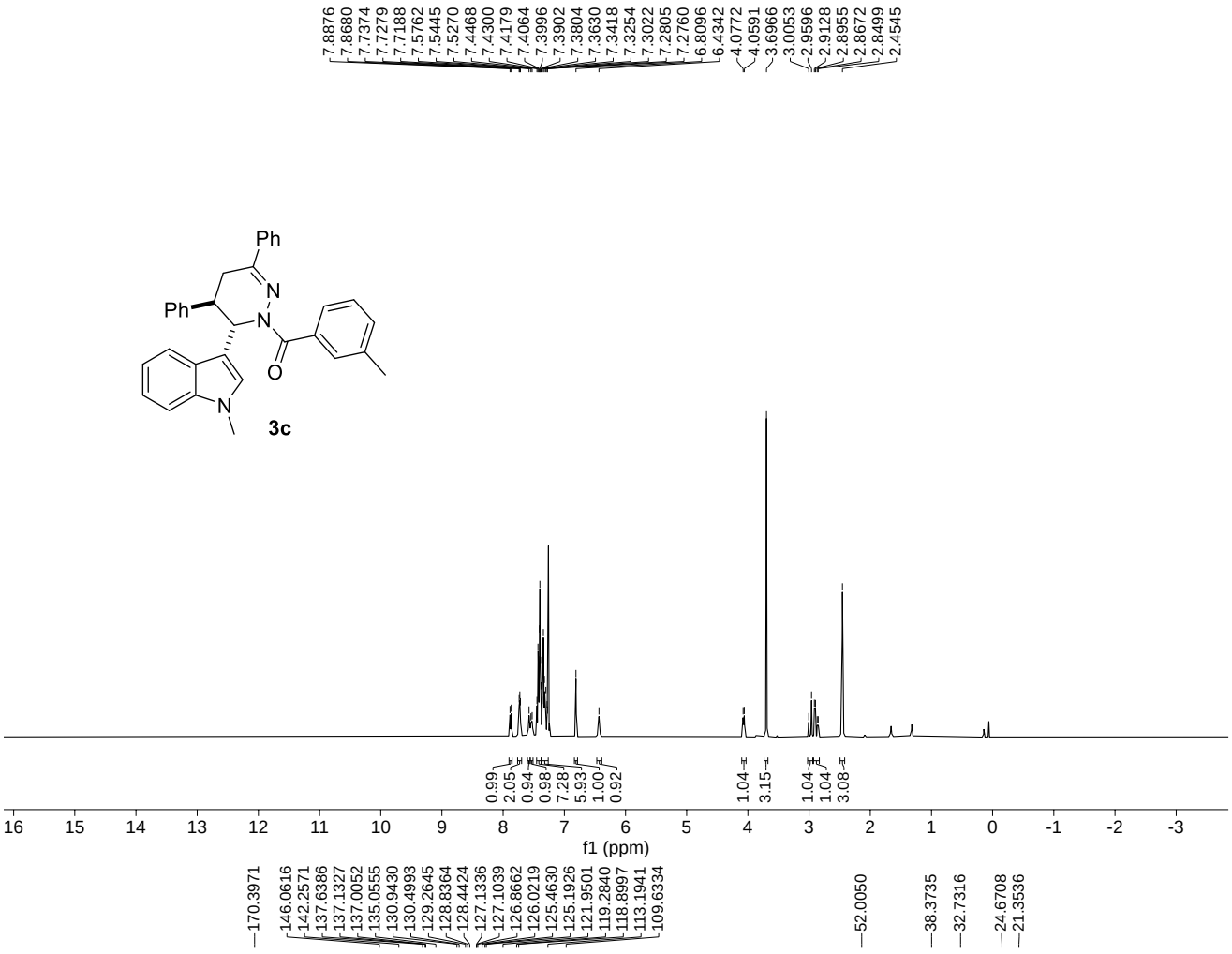
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1.04
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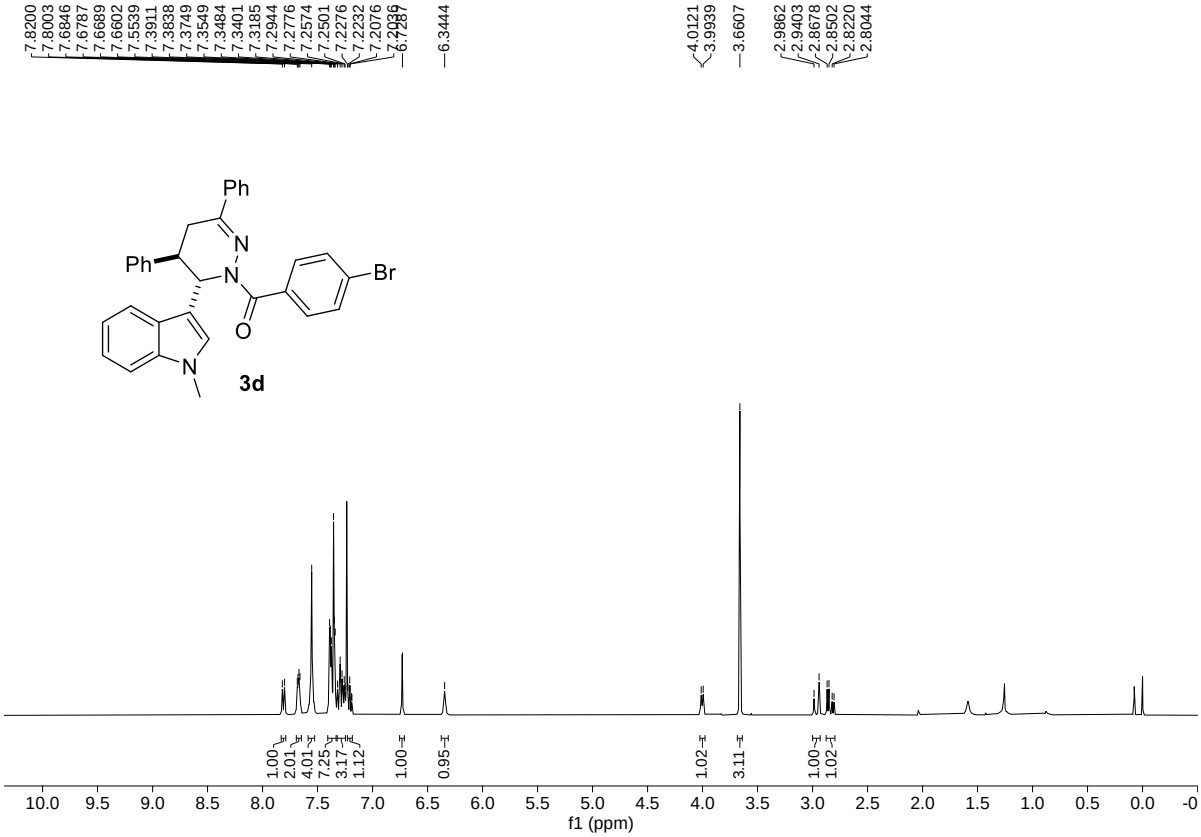
3c
f1 (ppm)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1.02
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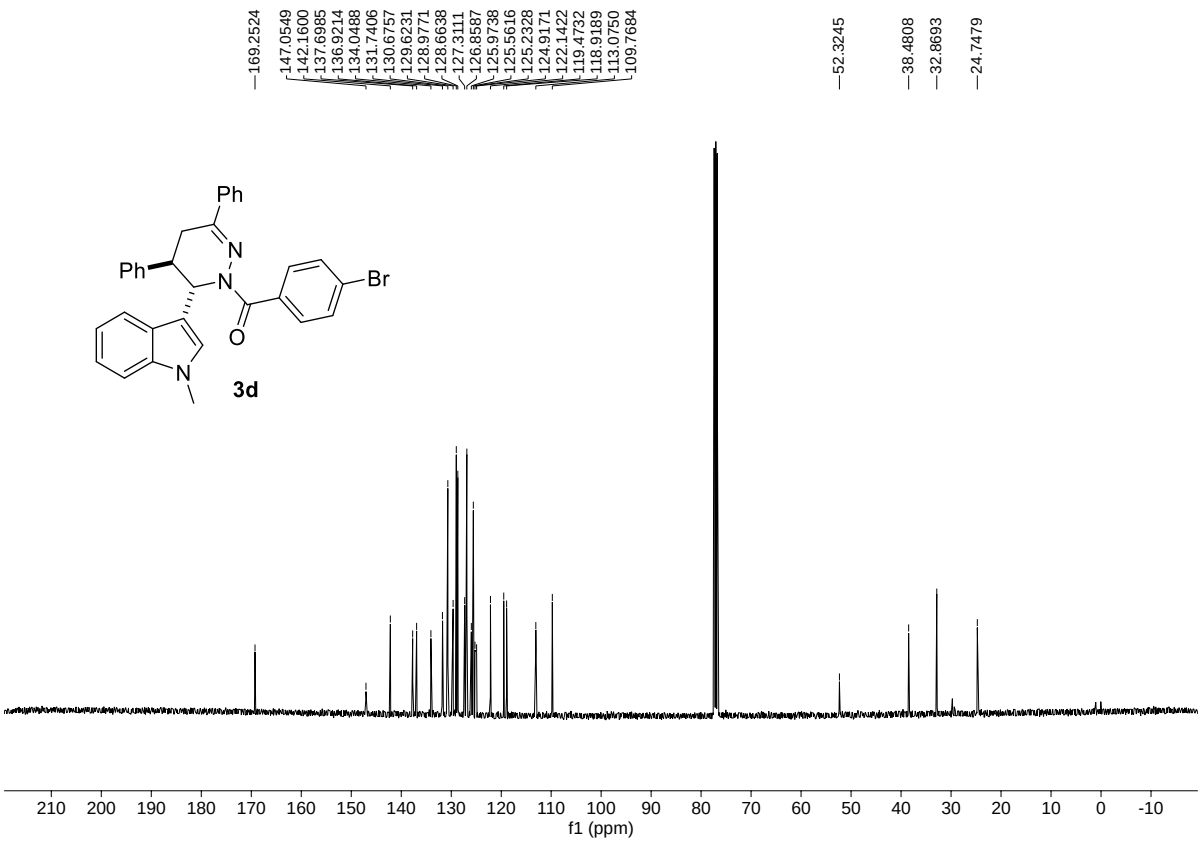
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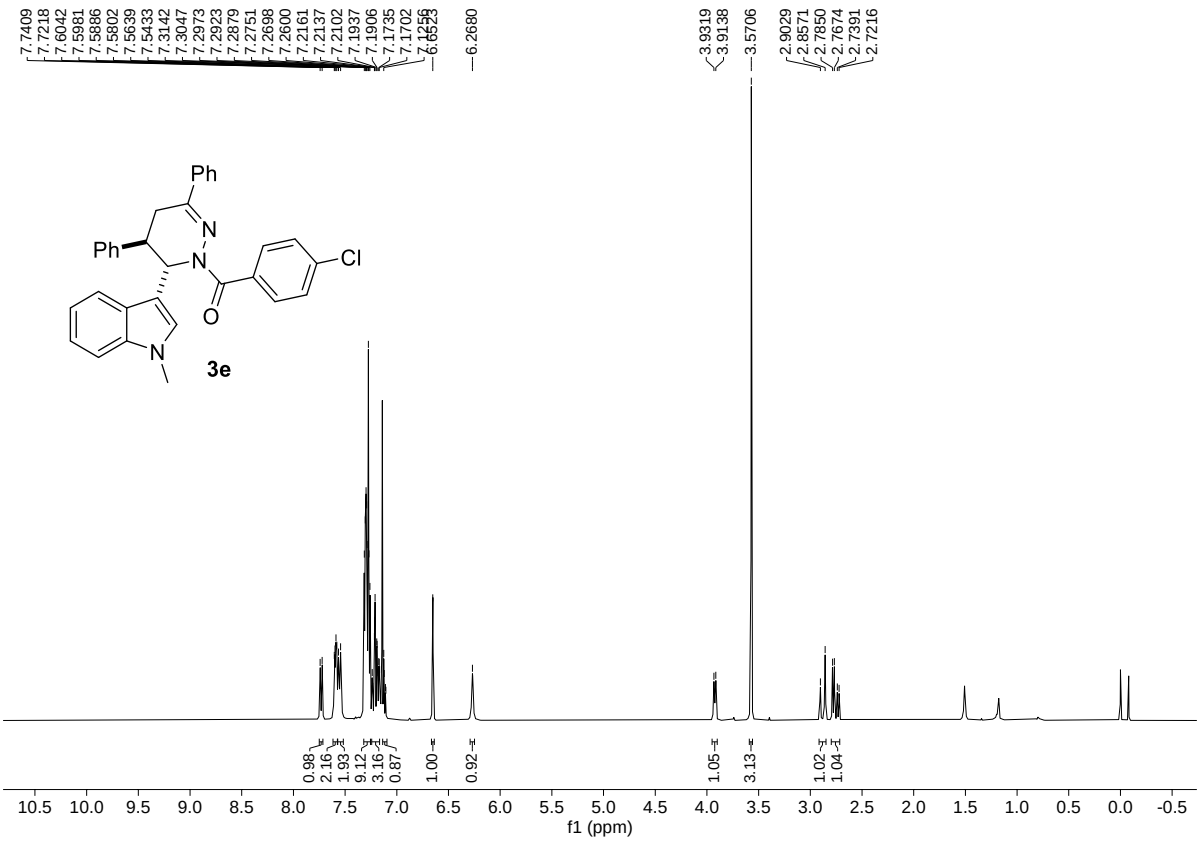
f1 (ppm)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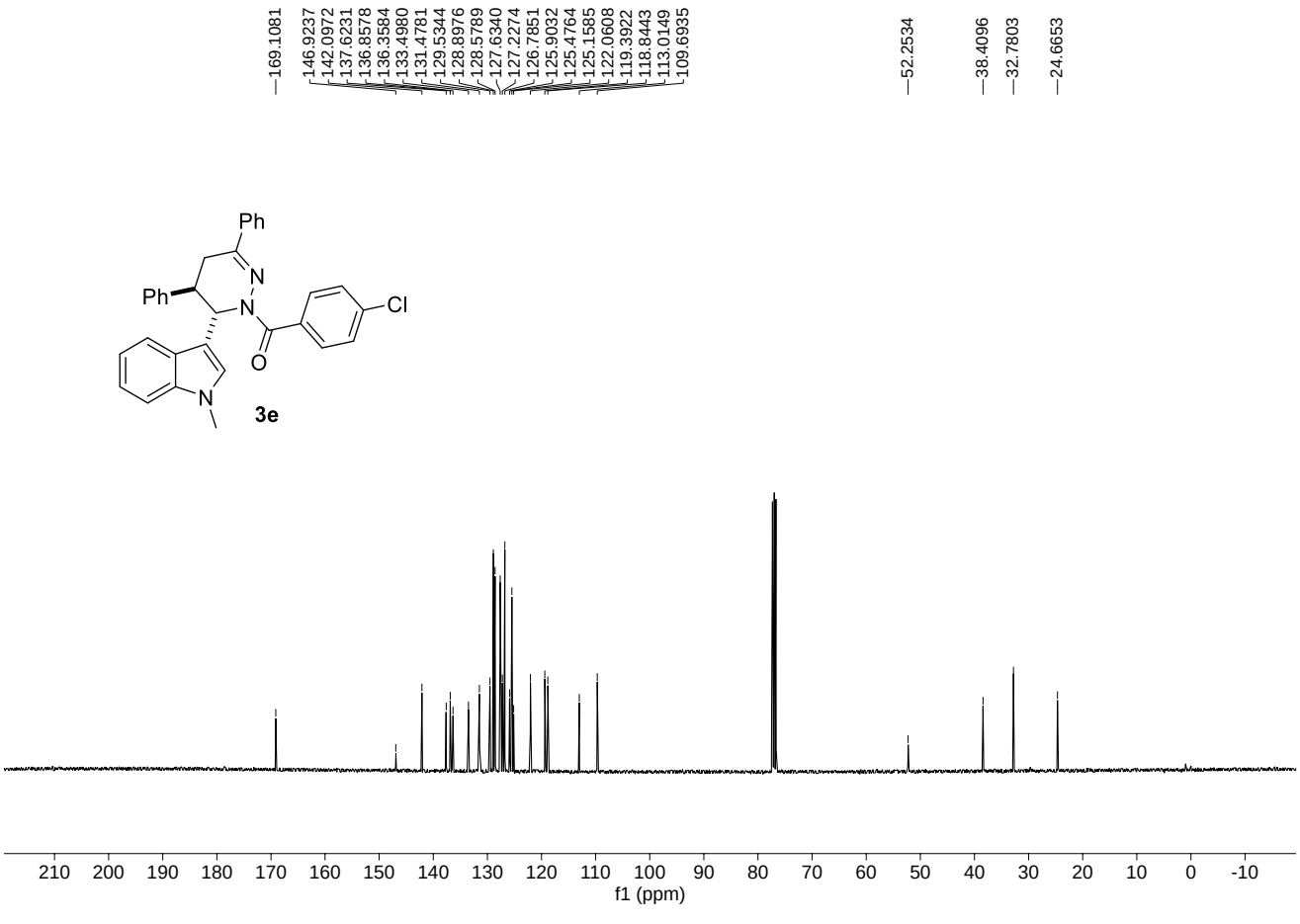
f1 (ppm)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f1 (ppm)


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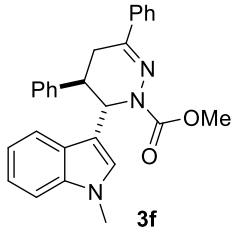
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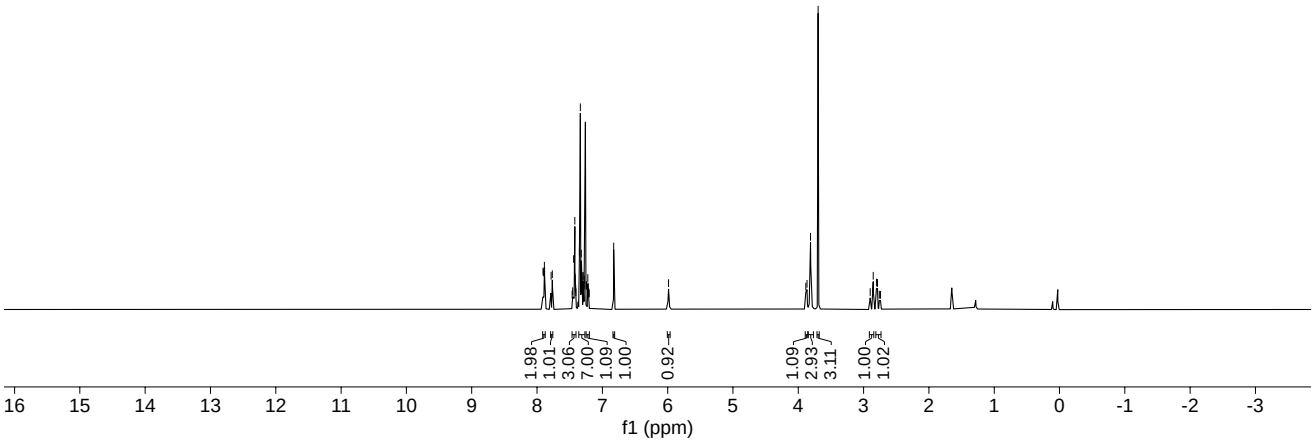
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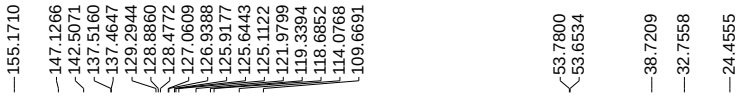
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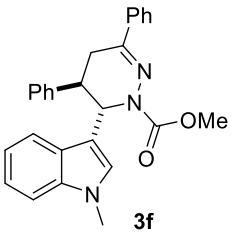
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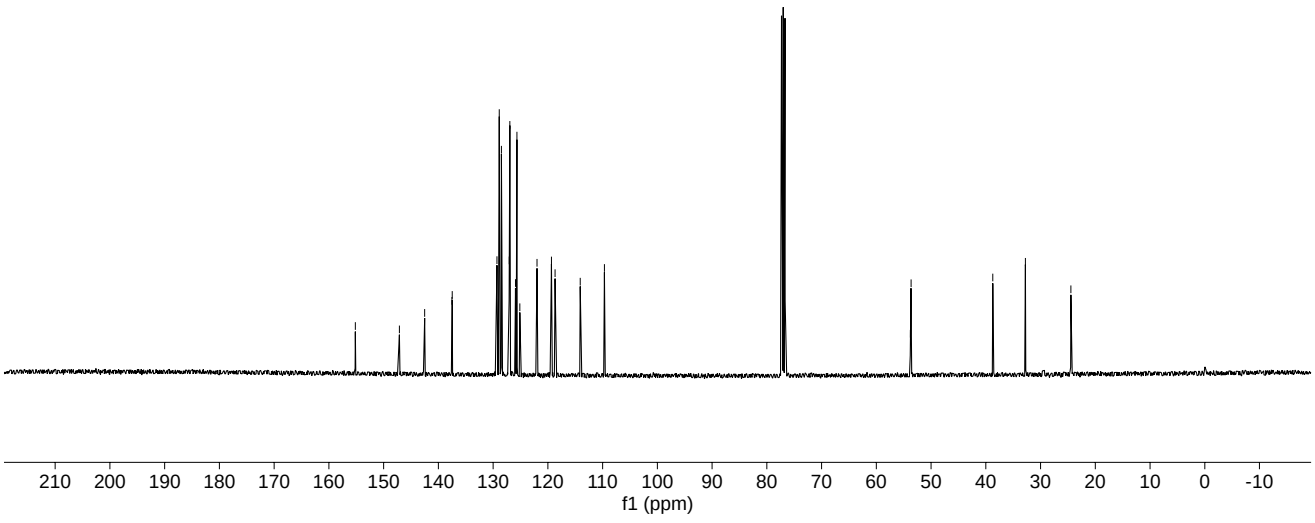
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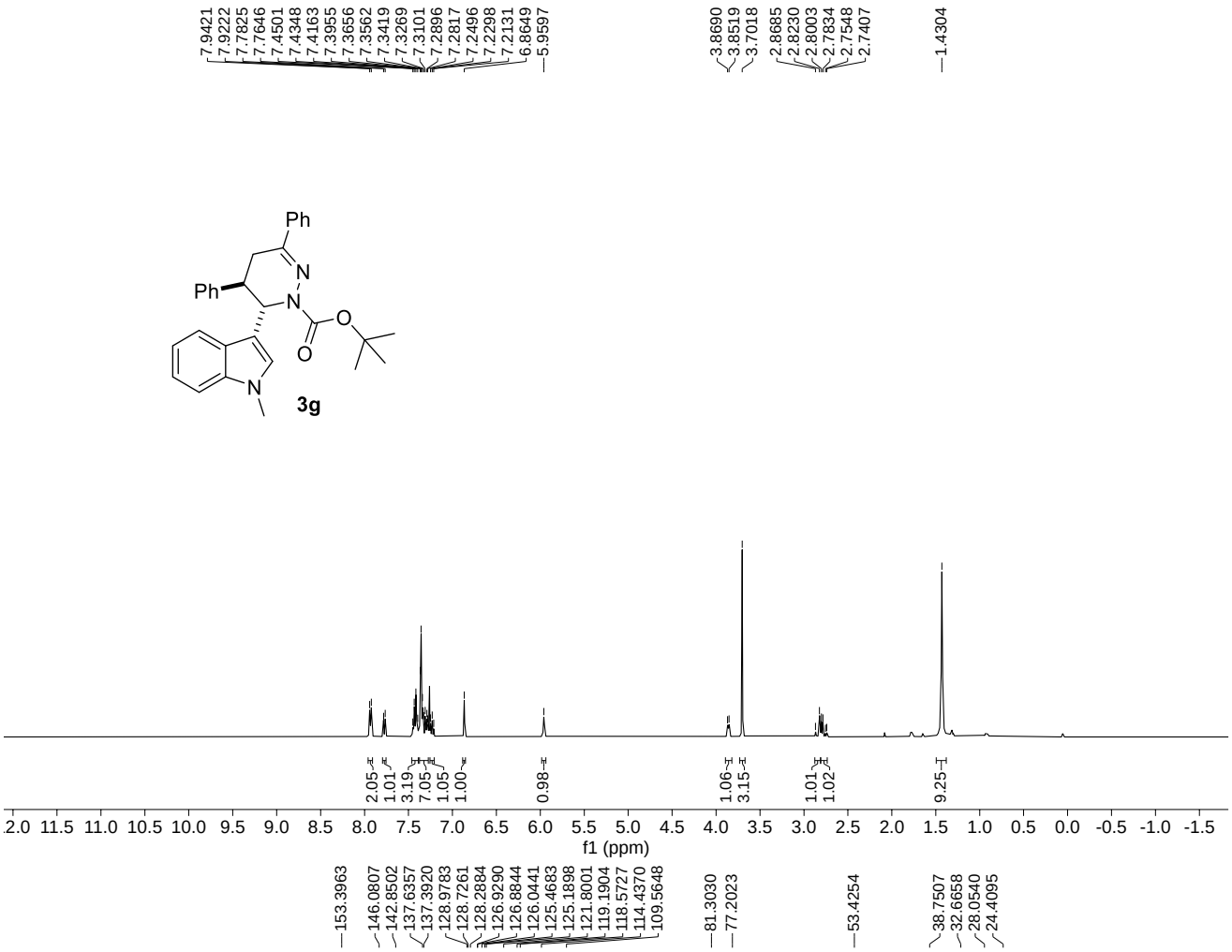
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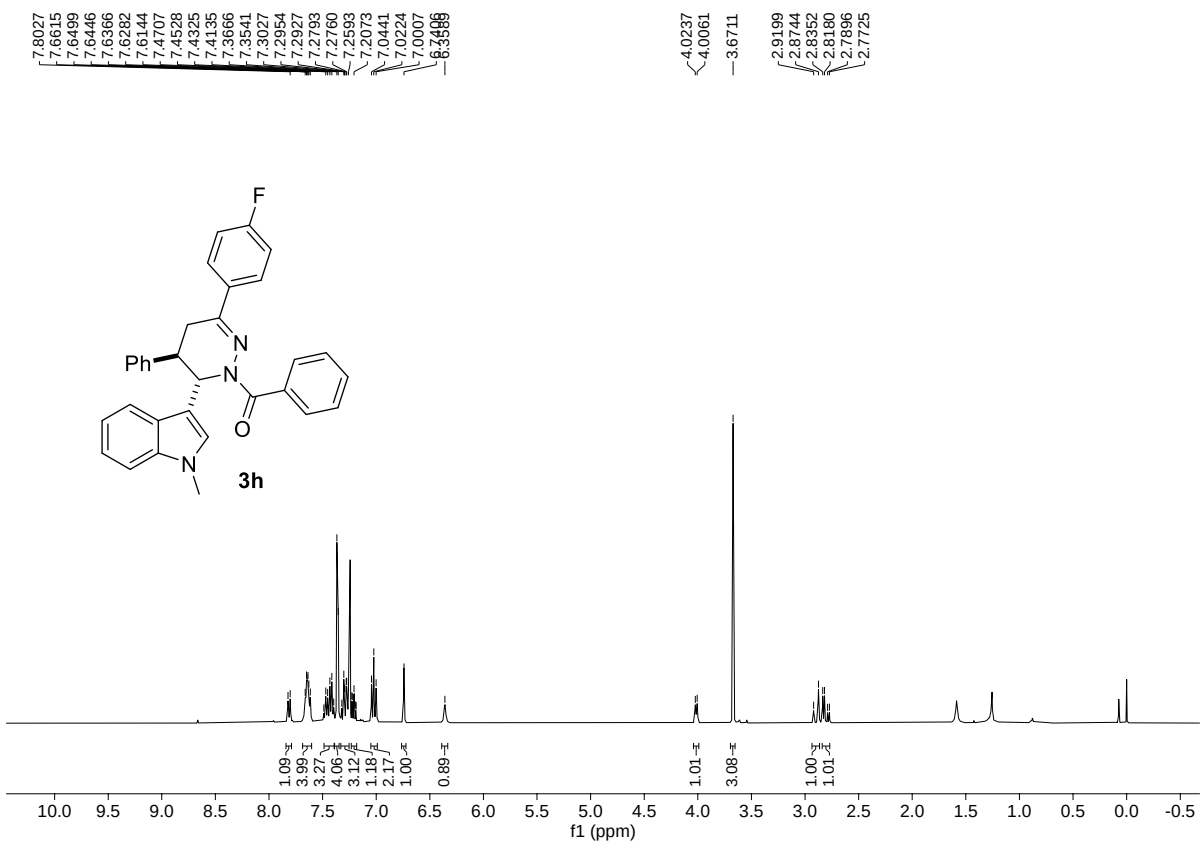
32.6658
28.0540
24.4095
Ph
N
Ph
N
O
O
N
3g
f1 (ppm)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7.6144
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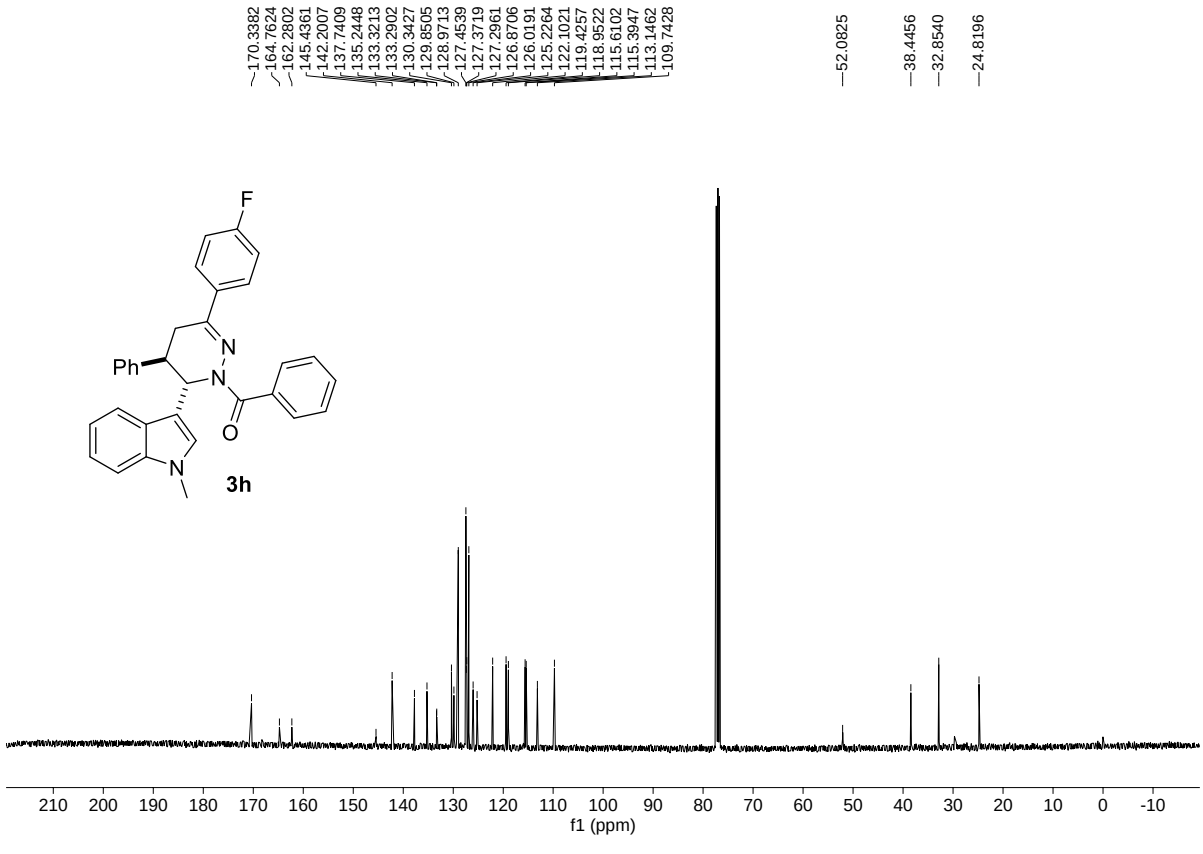
7.4325
7.4135
7.3666
7.3541
7.3027
7.2954
7.2927
7.2793
7.2760
7.2593
7.2073
7.0441
7.0224
7.0007
6.7496
6.3589
4.0237
4.0061
3.6711
2.9199
2.8744
2.8352
2.8180
2.7896
2.7725
F
Ph
N
N
O
N
3h
1.09
3.99
3.27
4.06
3.12
1.18
2.17
1.00
0.89
1.01
3.08
1.00
1.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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162.2802
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142.2007
137.7409
135.2448
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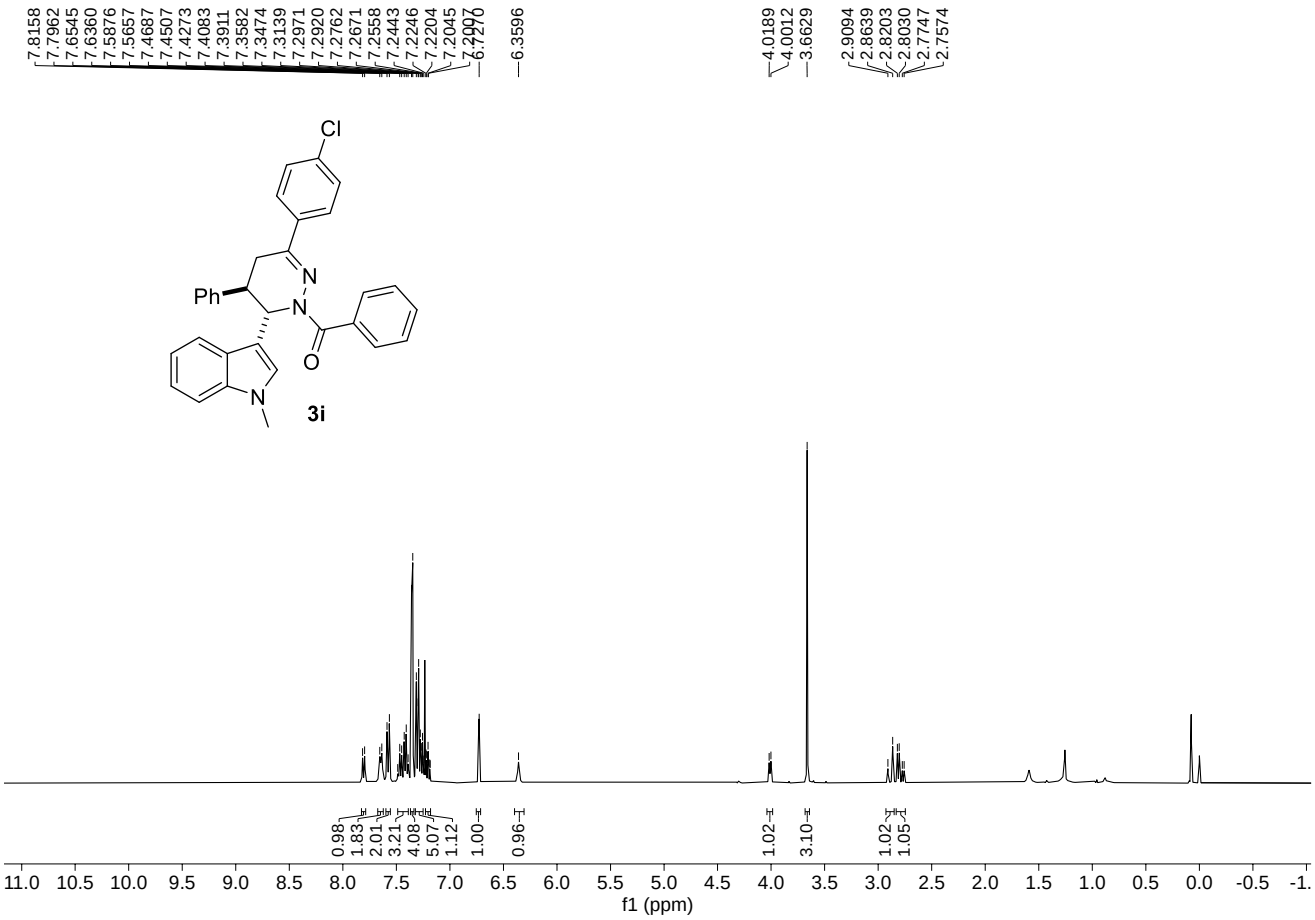
133.2902
130.3427
129.8505
128.9713
127.4539
127.3719
127.2961
126.8706
126.0191
125.2264
122.1021
119.4257
118.9522
115.6102
115.3947
113.1462
109.7428
52.0825
38.4456
32.8540
24.8196
F
Ph
N
N
O
N
3h
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.8158
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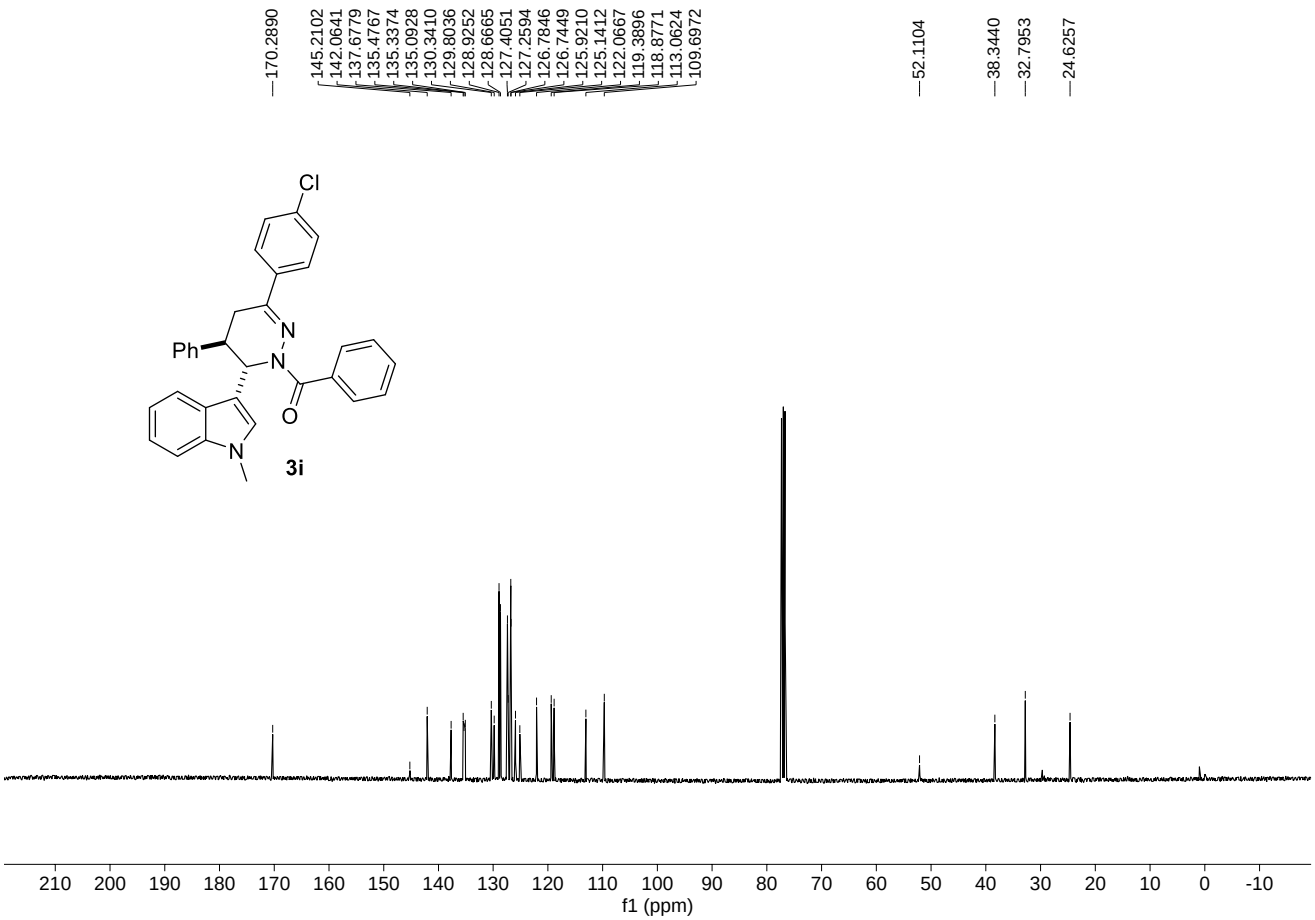
7.5876
7.5657
7.4687
7.4507
7.4273
7.4083
7.3911
7.3582
7.3474
7.3139
7.2971
7.2920
7.2762
7.2671
7.2558
7.2443
7.2246
7.2204
7.2045
7.1907
7.1720
6.3596
4.0189
4.0012
3.6629
2.9094
2.8639
2.8203
2.8030
2.7747
2.7574
Cl
Ph
N
N
O
N
3i
0.98
1.83
2.01
3.21
4.08
5.07
1.12
1.00
0.96
1.02
3.10
1.02
1.05
11.0 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.
f1 (ppm)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127.2594
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126.7449
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125.1412
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119.3896
118.8771
113.0624
109.6972
52.1104
38.3440
32.7953
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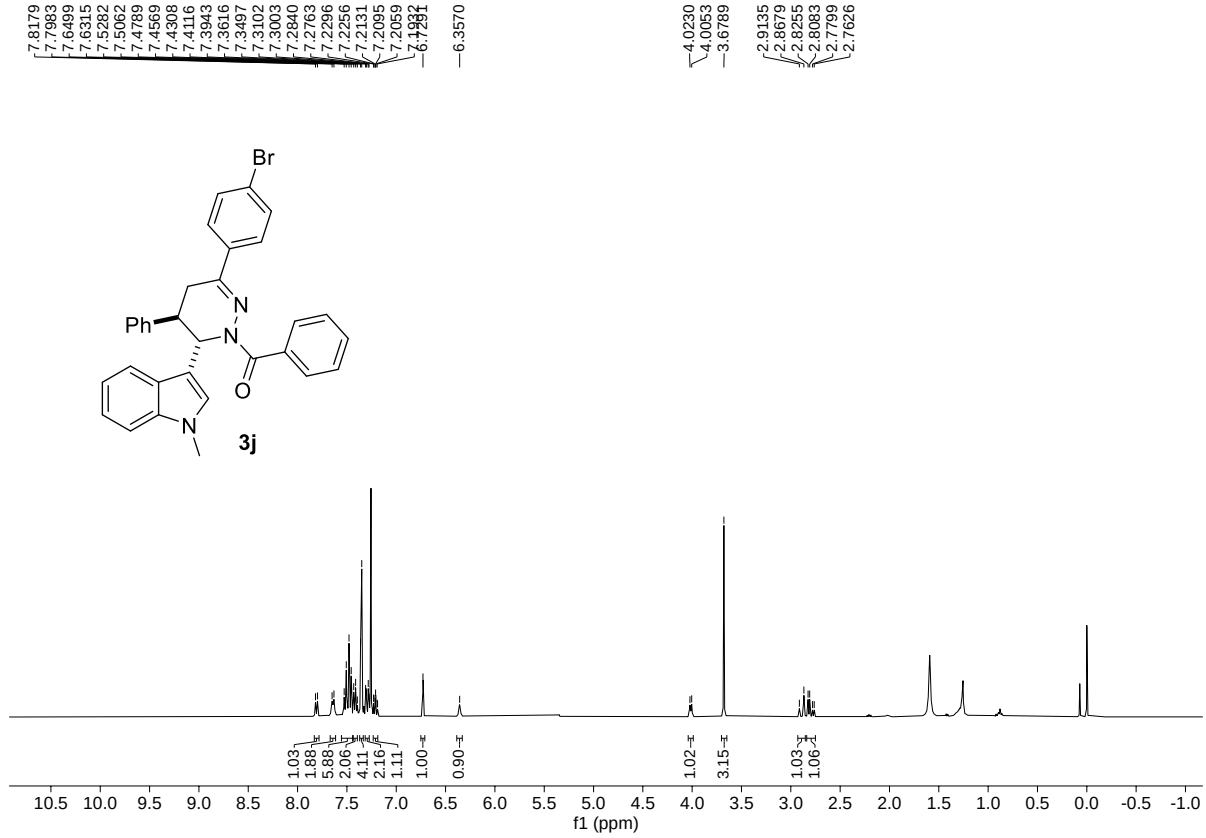
Cl
Ph
N
N
O
N
3i
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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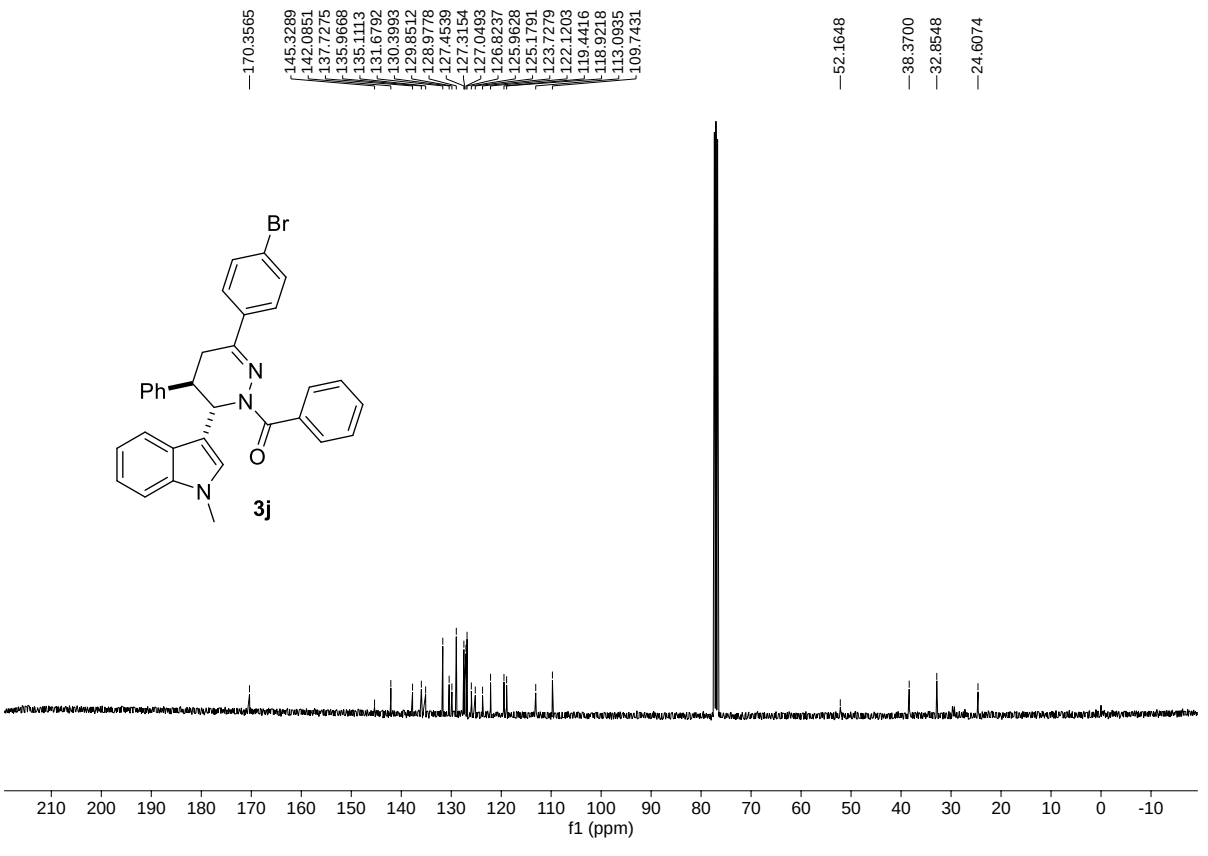
7.3943
7.3616
7.3497
7.3102
7.3003
7.2840
7.2763
7.2296
7.2256
7.2131
7.2095
7.2059
6.7291
6.3570
4.0230
4.0053
3.6789
2.9135
2.8679
2.8255
2.8083
2.7799
2.7626
Br
N
Ph
N
O
N
3j
1.03
1.88
5.88
2.06
4.11
2.16
1.11
1.00
0.90
1.02
3.15
1.03
1.06
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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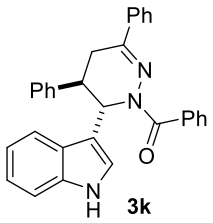
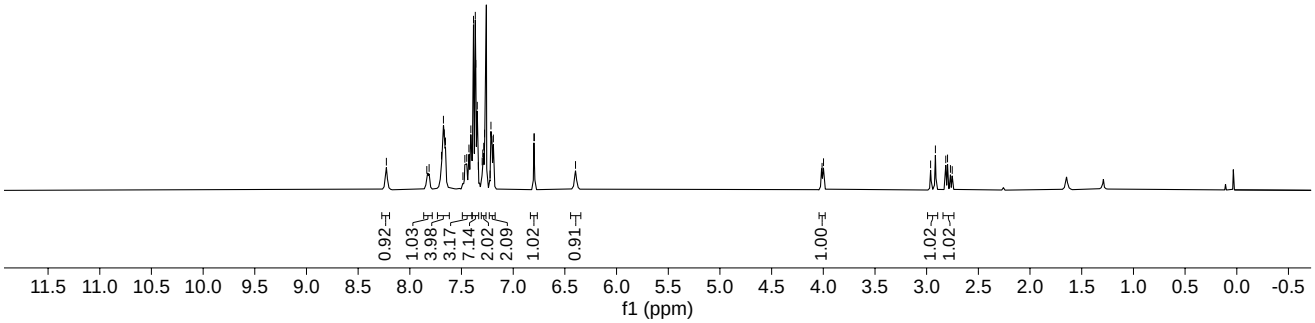
127.4539
127.3154
127.0493
126.8237
125.9628
125.1791
123.7279
122.1203
119.4416
118.9218
113.0935
109.7431
52.1648
38.3700
32.8548
24.6074
Br
N
Ph
N
O
N
3j
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.2273
7.8358
7.8138
7.6934
7.6746
7.6665
7.6552
7.4863
7.4676
7.4496
7.4278
7.4098
7.3843
7.3667
7.3615
7.3529
7.3480
7.3375
7.2998
7.2947
7.2853
7.2766
7.2231
7.2152
7.2055
7.1923
6.7992
6.7956
6.3967
4.0121
3.9985
2.9616
2.9158
2.8157
2.7980
2.7700
2.7522


Ph
N
Ph
N
Ph
O
N
H
3k


0.92
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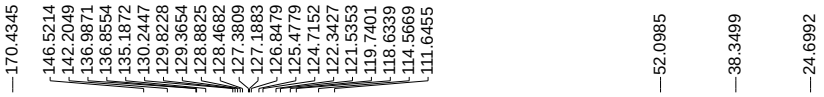
3.98
3.17
7.14
2.02
2.09
1.02
0.91
1.00
1.02
1.02
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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130.2447
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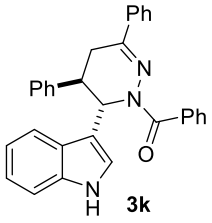
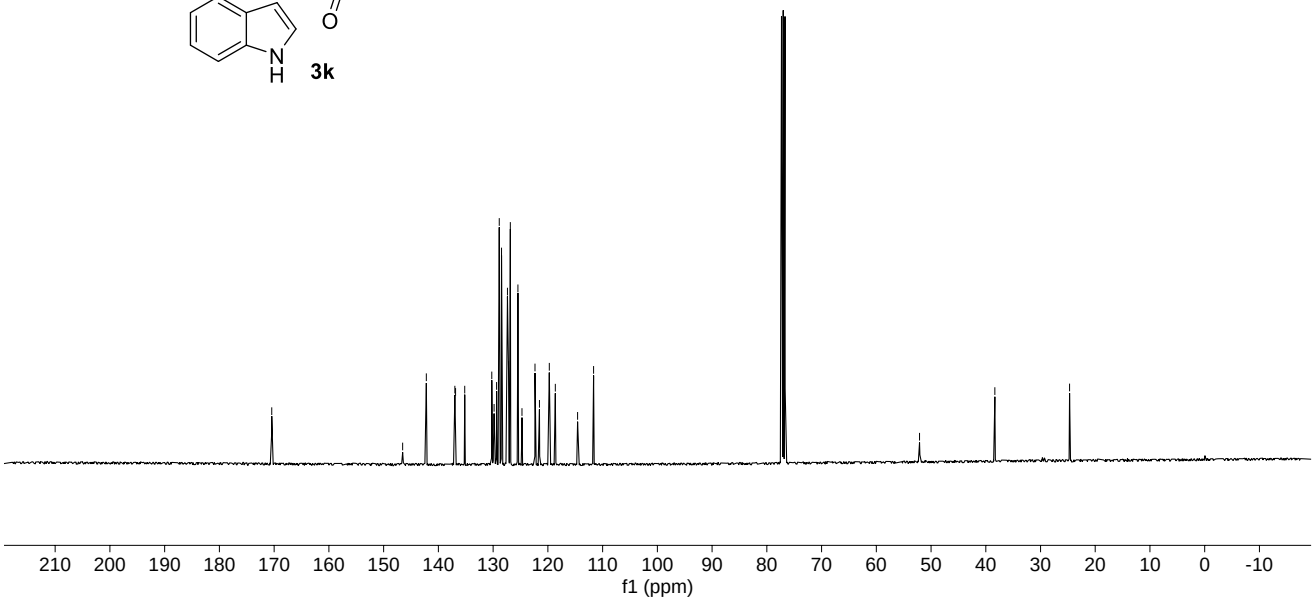
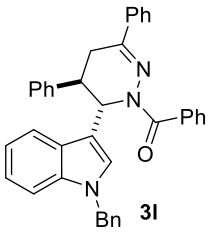
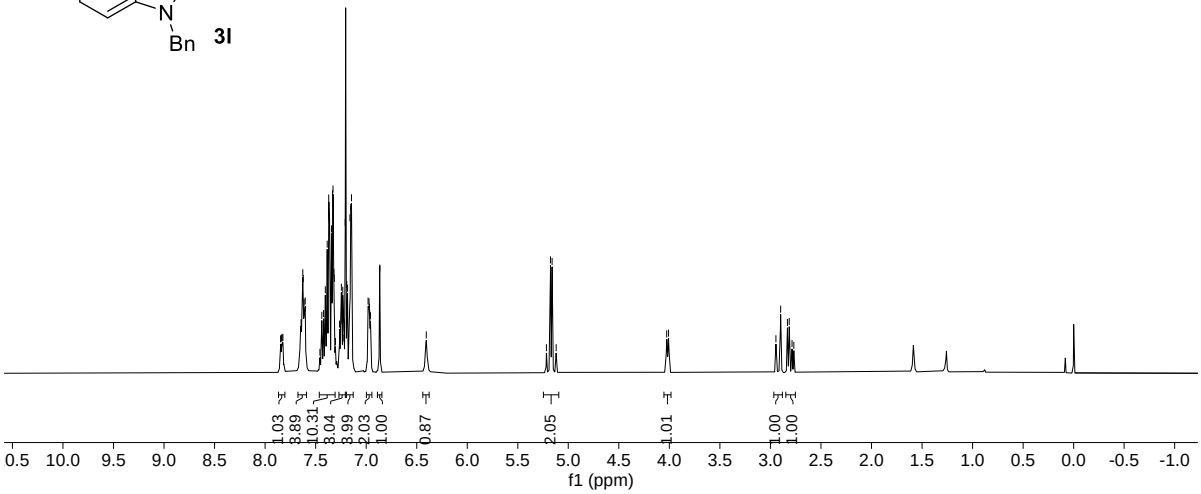
128.8825
128.4682
127.3809
127.1883
126.8479
125.4779
124.7152
122.3427
121.5353
119.7401
118.6339
114.5669
111.6455
52.0985
38.3499
24.6992

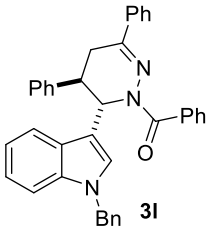

Ph
N
Ph
N
Ph
O
N
H
3k


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



3l





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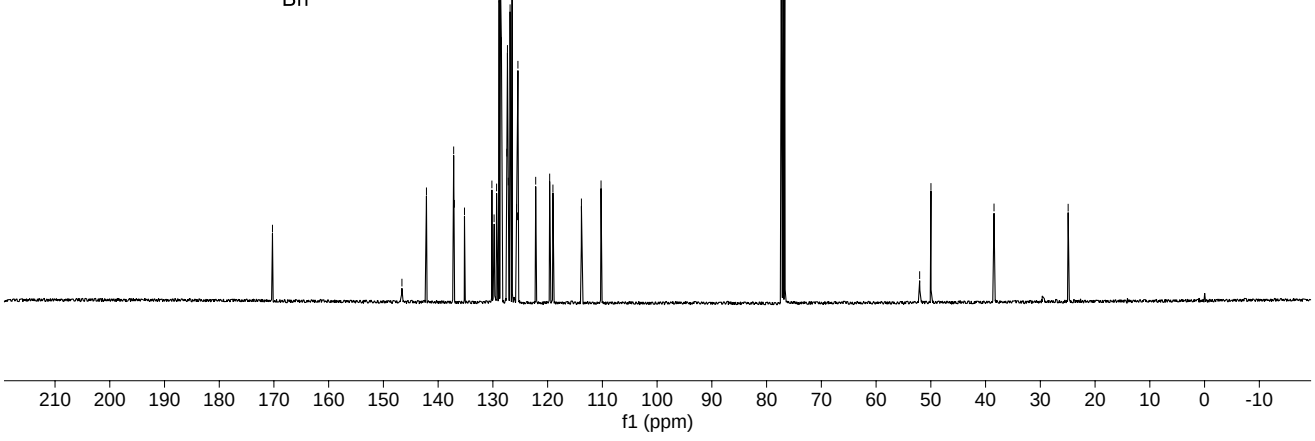

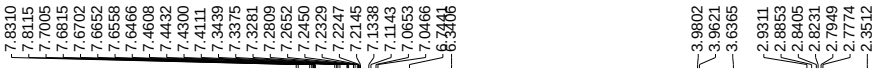
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7.6702
7.6652
7.6558
7.6466
7.4608
7.4432
7.4300
7.4111
7.3439
7.3375
7.3281
7.2809
7.2652
7.2450
7.2329
7.2247
7.2145
7.1338
7.1143
7.0653
7.0466
6.3441
6.3406
3.9802
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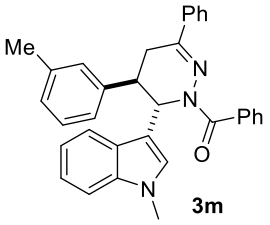
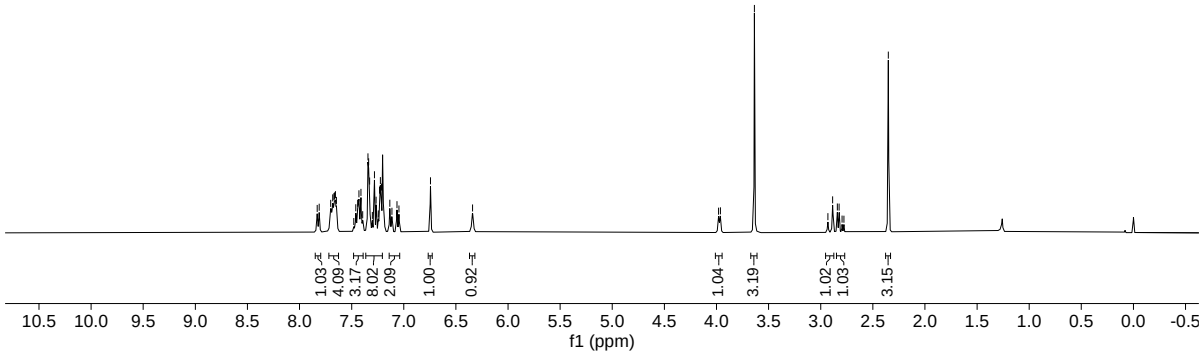
3.6365
2.9311
2.8853
2.8405
2.8231
2.7949
2.7774
2.3512


Ph
Me
N
N
Ph
O
N
3m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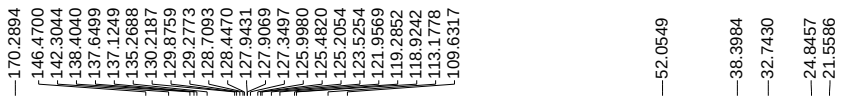
4.09
3.17
8.02
2.09
1.00
0.92
1.04
3.19
1.02
1.03
3.15
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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128.4470
127.9431
127.9069
127.3497
125.9980
125.4820
125.2054
123.5254
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118.9242
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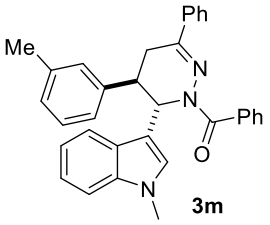
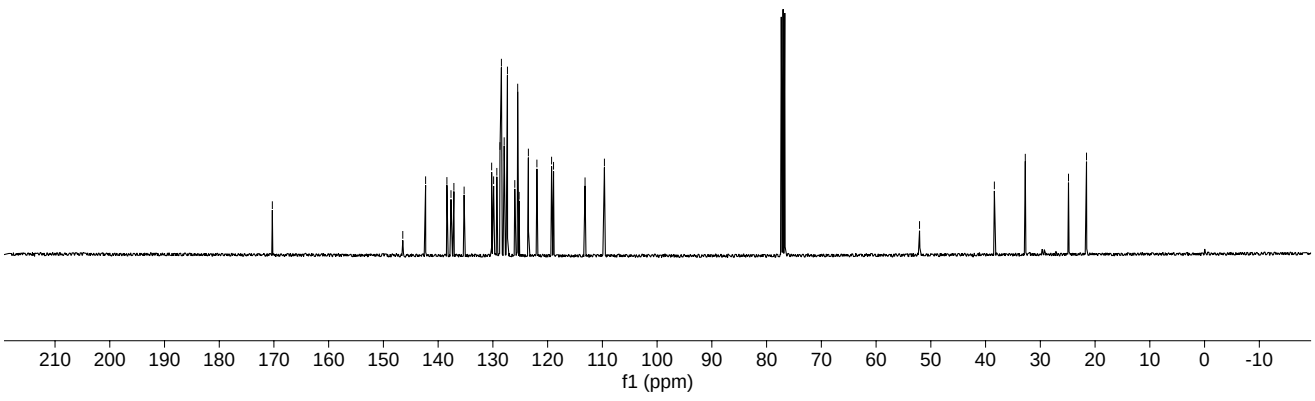
109.6317
52.0549
38.3984
32.7430
24.8457
21.5586


Ph
Me
N
N
Ph
O
N
3m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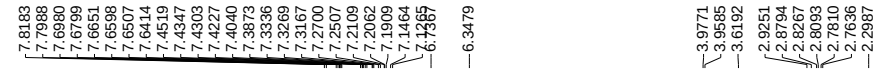
f1 (ppm)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7.6507
7.6414
7.4519
7.4347
7.4303
7.4227
7.4040
7.3873
7.3336
7.3269
7.3167
7.2700
7.2507
7.2109
7.2062
7.1909
7.1464
6.7367
6.3479
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2.8267
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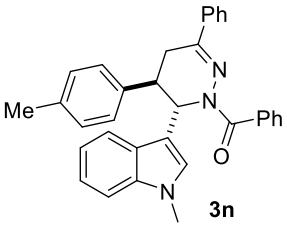
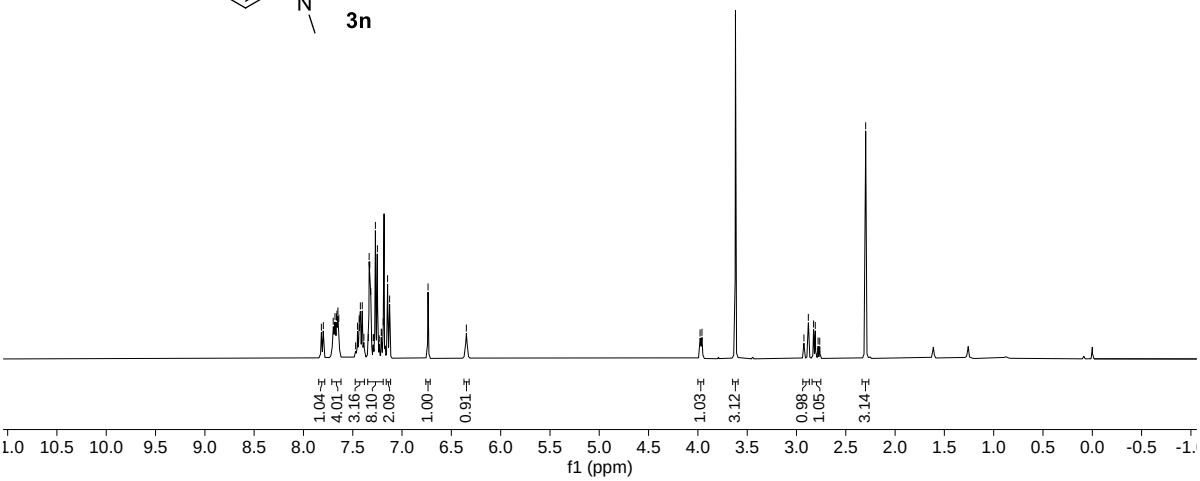
2.7810
2.7636
2.2987


Ph
N
N
Me
Ph
O
N

3n


1.04
4.01
3.16
8.10
2.09
1.00
0.91
1.03
3.12
0.98
1.05
3.14
f1 (ppm)


170.2516
146.3686
139.1968
137.6189
137.0953
136.6747
135.2261
130.1922
129.9045
129.4698
129.2597
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127.3158
126.6880
125.9562
125.4575
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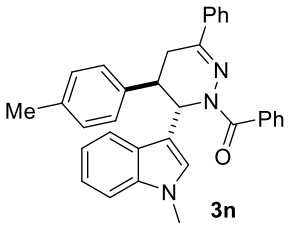
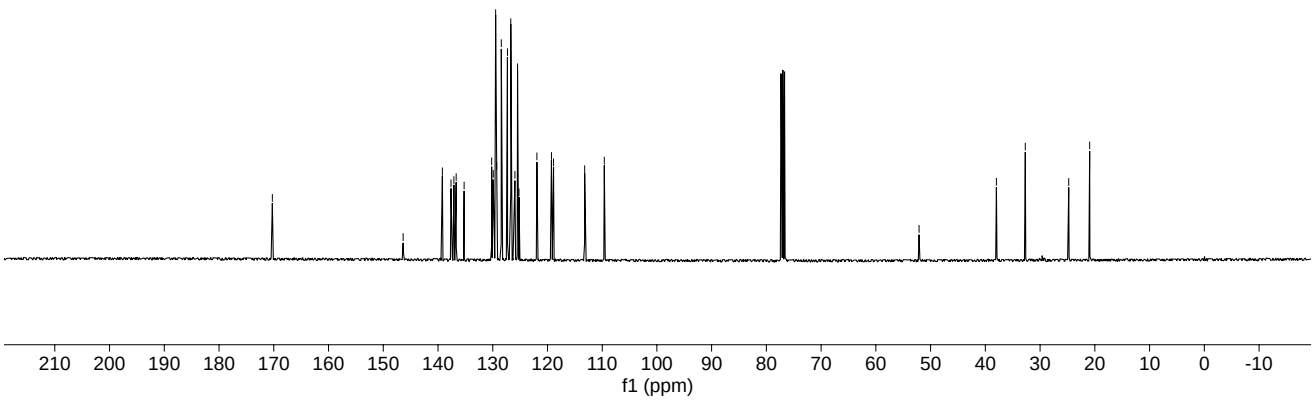
32.7067
24.7756
20.9492


Ph
N
N
Me
Ph
O
N

3n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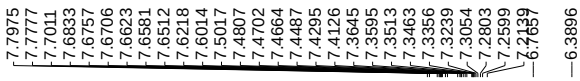
f1 (ppm)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7.6014
7.5017
7.4807
7.4702
7.4664
7.4487
7.4295
7.4126
7.3645
7.3595
7.3513
7.3463
7.3356
7.3239
7.3054
7.2803
7.2599
7.2139
6.7857
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2.8926
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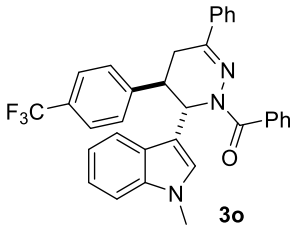
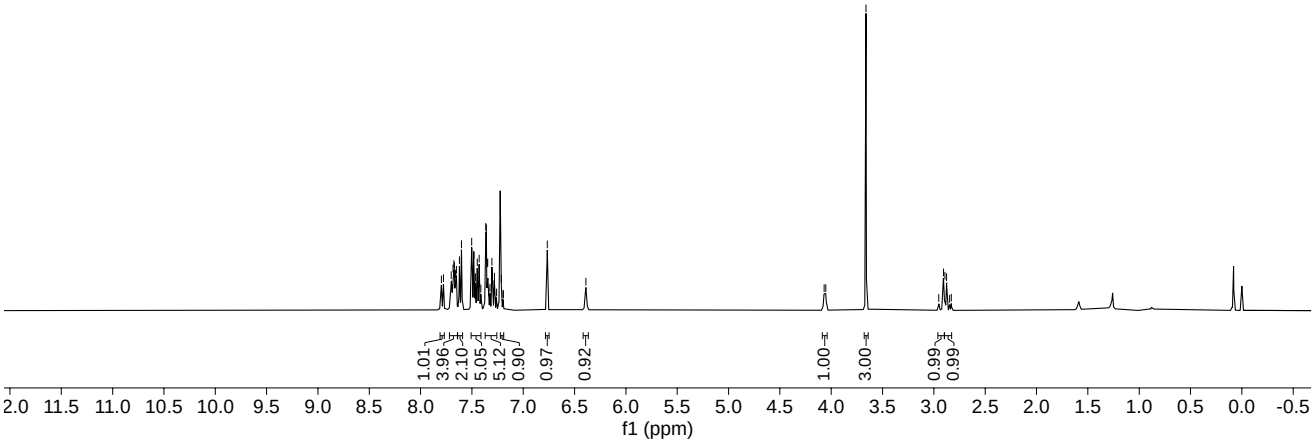
2.8468
2.8306


Ph
N
N
Ph
O
F3C
N

3o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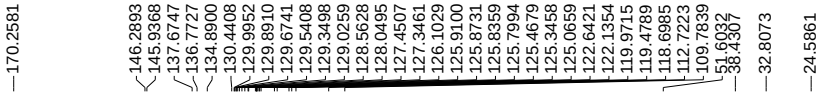
2.10
5.05
5.12
0.90
0.97
0.92
1.00
3.00
0.99
0.99
2.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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125.9100
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125.8359
125.7994
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125.3458
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122.6421
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119.9715
119.4789
118.6985
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109.7839
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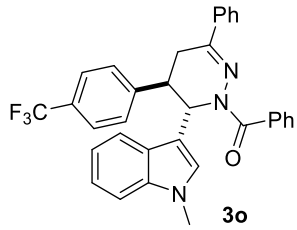
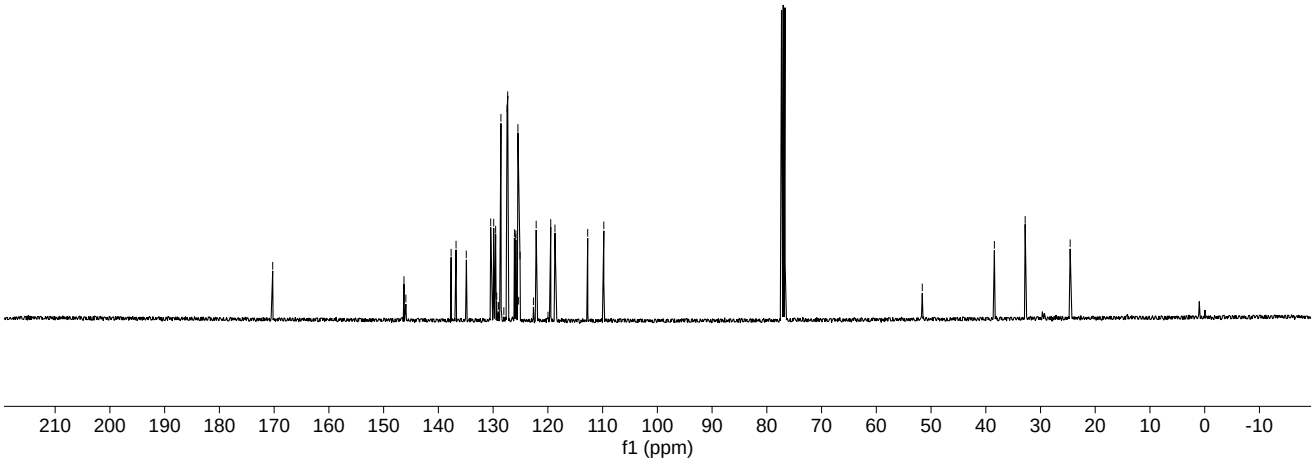
38.4307
32.8073
24.5861


Ph
N
N
Ph
O
F3C
N

3o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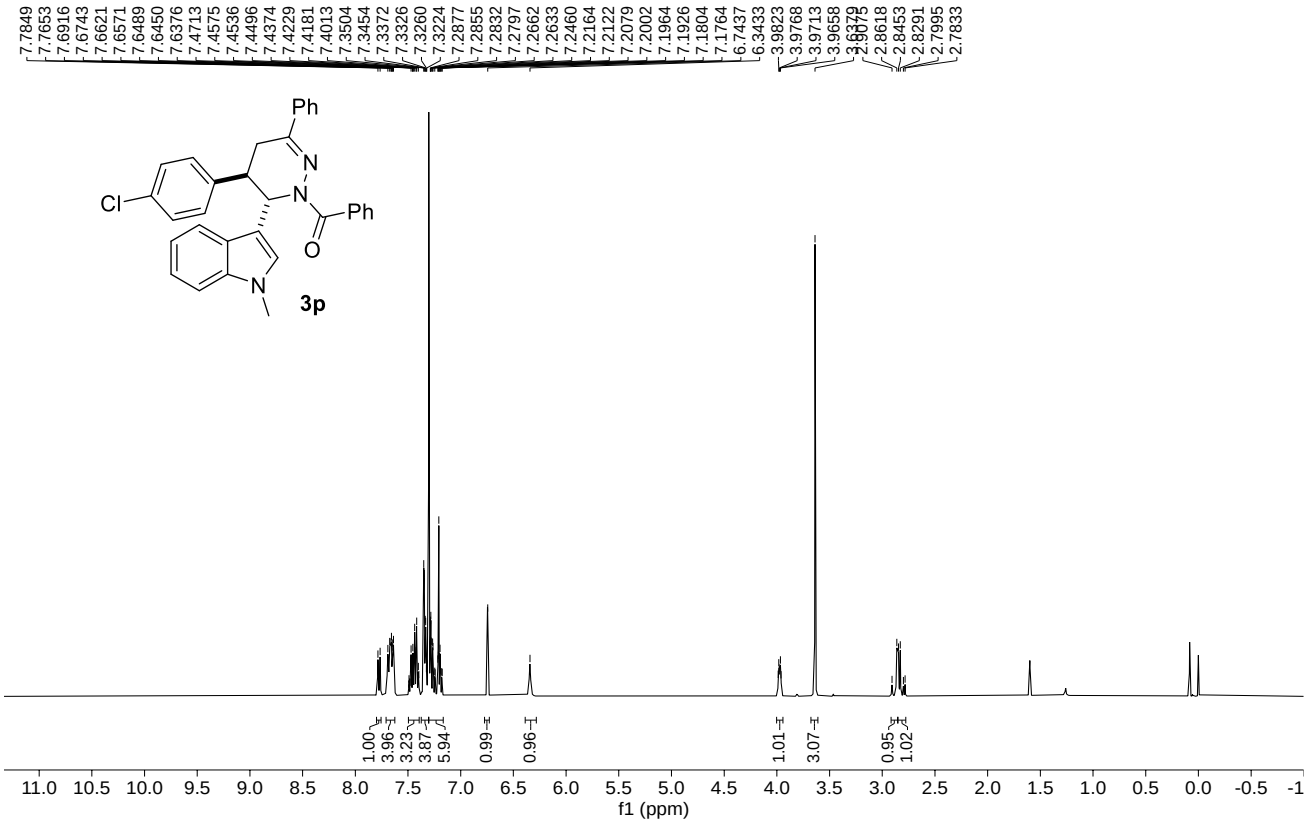
f1 (ppm)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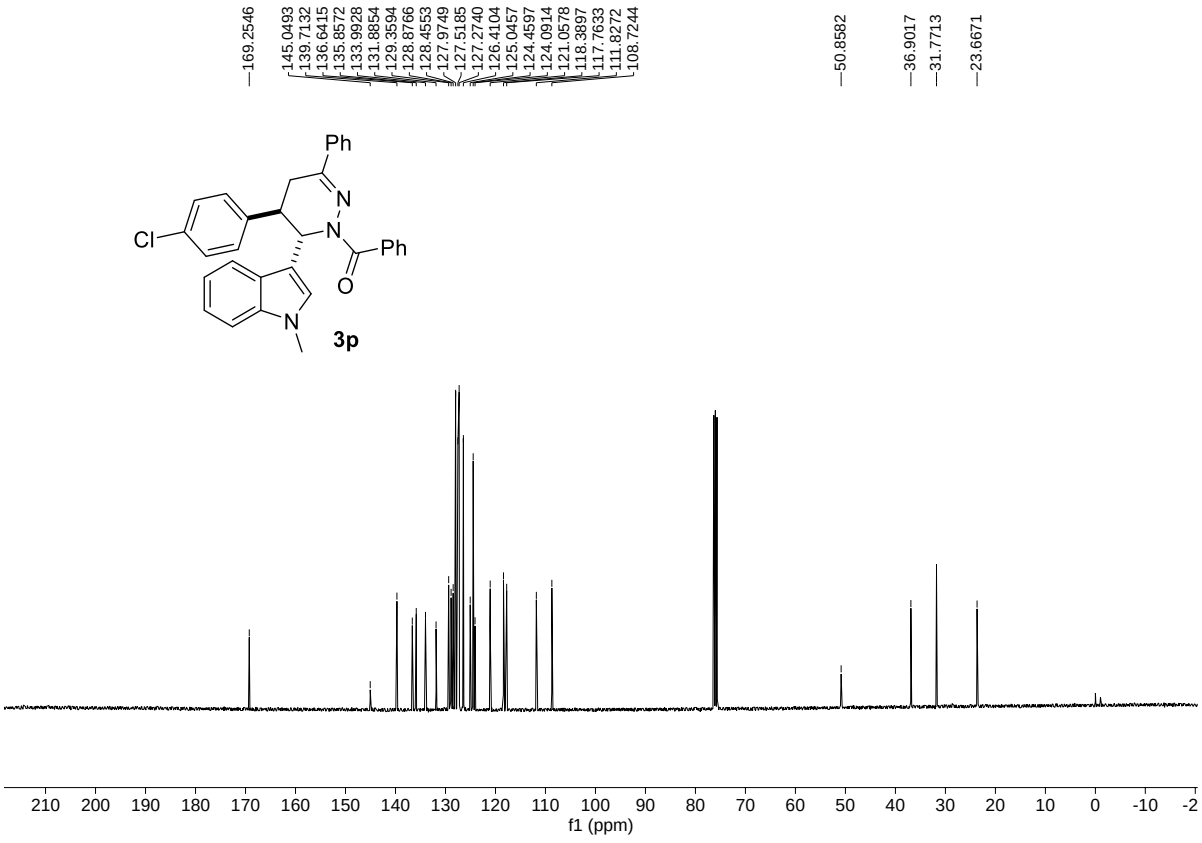
7.4536
7.4496
7.4374
7.4229
7.4181
7.4013
7.3504
7.3454
7.3372
7.3326
7.3260
7.3224
7.2877
7.2855
7.2832
7.2797
7.2662
7.2633
7.2460
7.2164
7.2122
7.2079
7.2002
7.1964
7.1926
7.1804
7.1764
6.7437
6.3433
3.9823
3.9768
3.9713
3.9658
2.8618
2.8453
2.8291
2.7995
2.7833
Ph
N
N
Ph
Cl
O
N
3p
1.00
3.96
3.23
3.87
5.94
0.99
0.96
1.01
3.07
0.95
1.02
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
f1 (ppm)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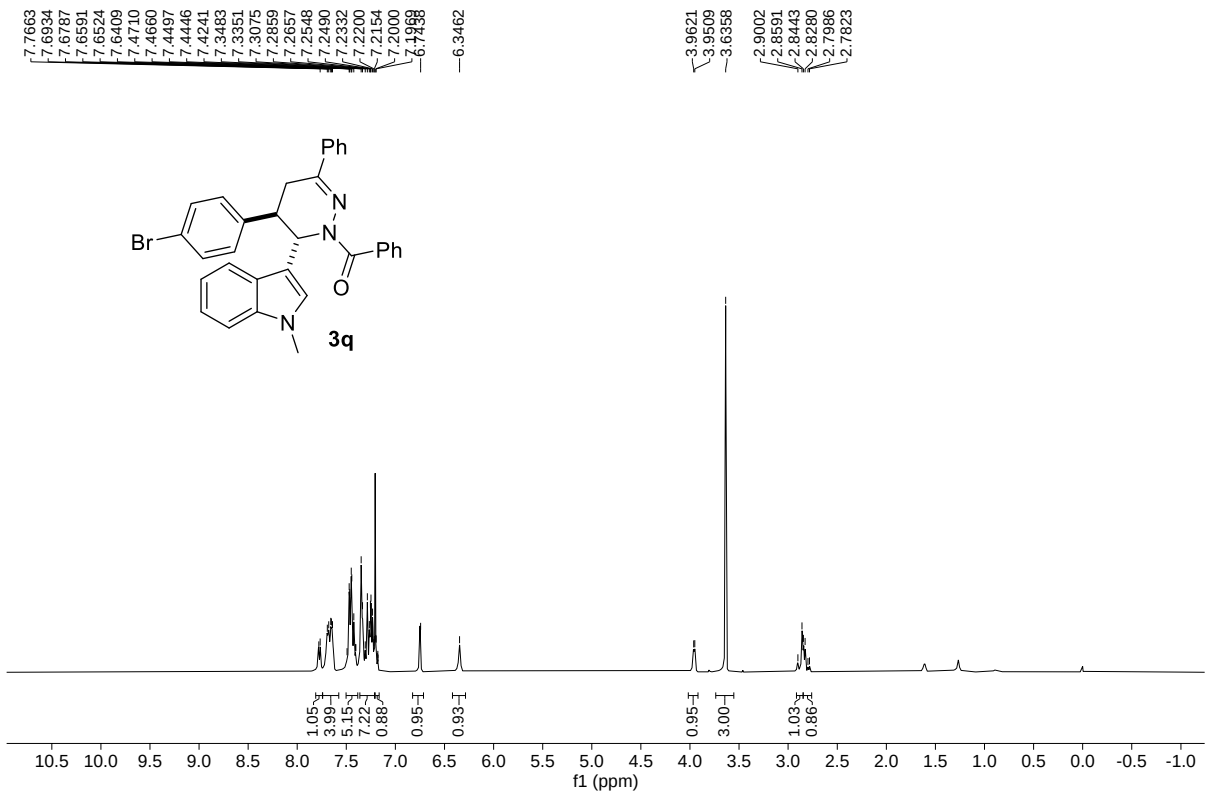
128.8766
128.4553
127.9749
127.5185
127.2740
126.4104
125.0457
124.4597
124.0914
121.0578
118.3897
117.7633
111.8272
108.7244
50.8582
36.9017
31.7713
23.6671
Ph
N
N
Ph
Cl
O
N
3p
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -2
f1 (ppm)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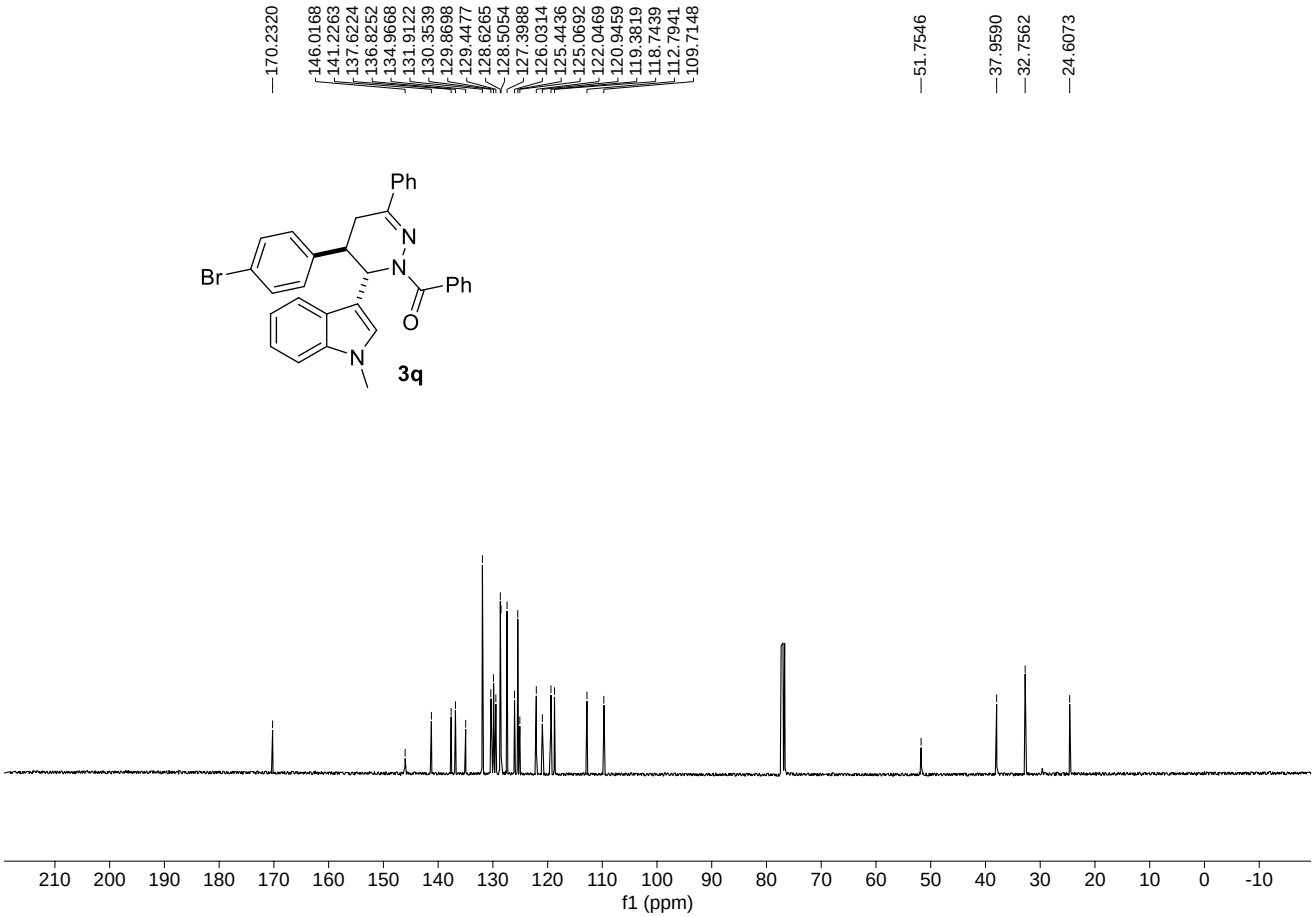
7.6524
7.6409
7.4710
7.4660
7.4497
7.4446
7.4241
7.3483
7.3351
7.3075
7.2859
7.2657
7.2548
7.2490
7.2332
7.2200
7.2154
7.2000
6.3462
3.9621
3.9509
3.6358
2.9002
2.8591
2.8443
2.8280
2.7986
2.7823
Ph
N
N
Br
Ph
O
N
3q
1.05
3.99
5.15
7.22
0.88
0.95
0.93
0.95
3.00
1.03
0.86
10.5 10.0 9.5 9.0 8.5 8.0 7.5 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
f1 (ppm)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129.8698
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128.6265
128.5054
127.3988
126.0314
125.4436
125.0692
122.0469
120.9459
119.3819
118.7439
112.7941
109.7148
51.7546
37.9590
32.7562
24.6073
Ph
N
N
Br
Ph
O
N
3q
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.8019
7.7821
7.6403
7.6169
7.6074
7.5977
7.3996
7.3819
7.3653
7.3470
7.2900
7.2845
7.2765
7.2724
7.2218
7.2122
7.1928
7.1588
7.1377
7.1338
7.1176
7.1008
7.0861
7.0785
6.7088
6.1704
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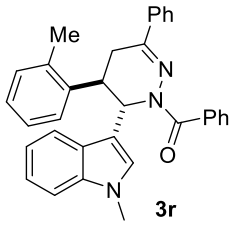
2.8508
2.8215
2.8048
2.7910
2.7452
2.6270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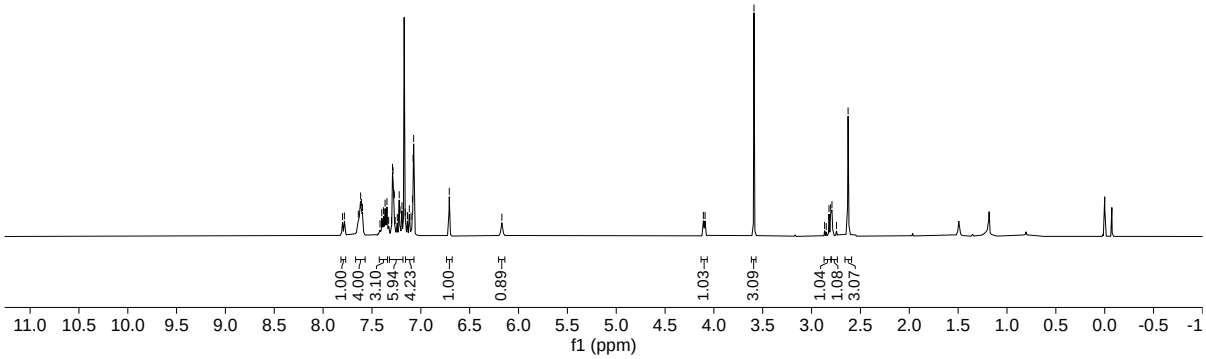
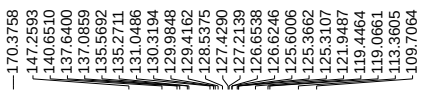
Me
N
N
Ph
O
N

3r


1.00
4.00
3.10
5.94
4.23
1.00
0.89
1.03
3.09
1.04
1.08
3.07
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
f1 (ppm)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128.5375
127.4290
127.2139
126.6538
126.6246
125.6006
125.3662
125.3107
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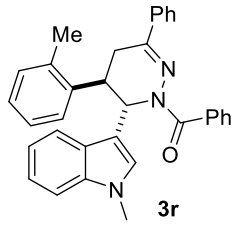
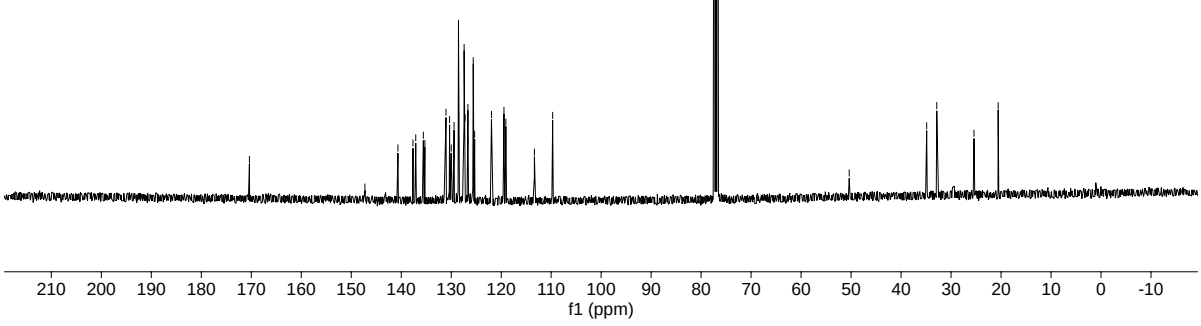
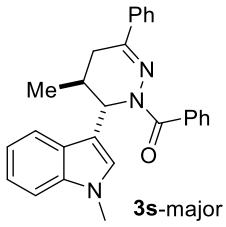
119.0661
113.3605
109.7064
50.3746
34.8774
32.8591
25.4091
20.5681

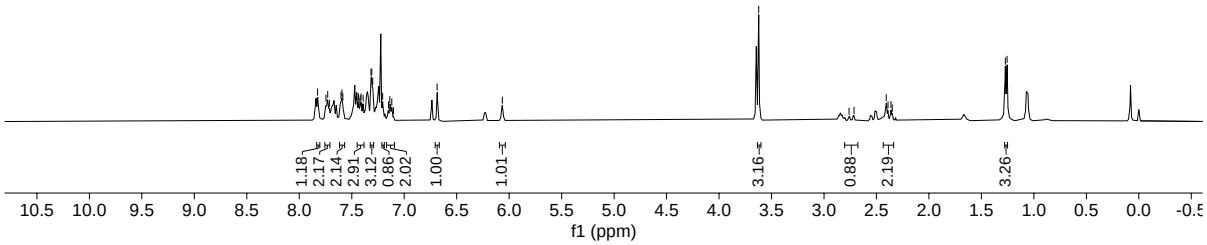

Ph
Me
N
N
Ph
O
N

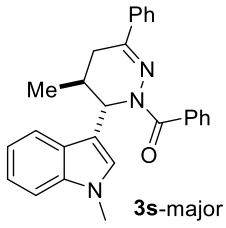
3r


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

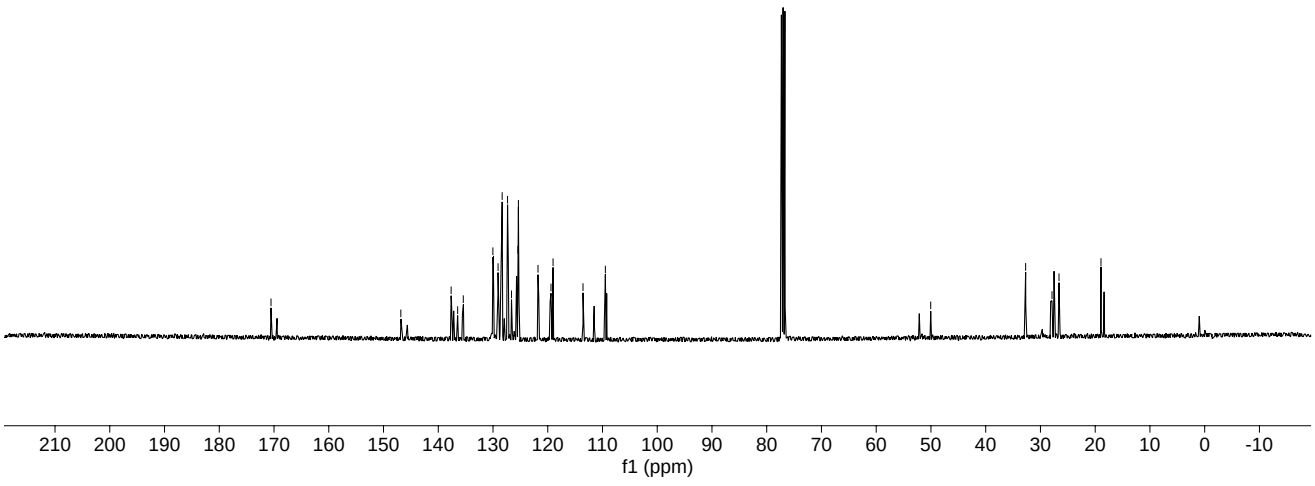


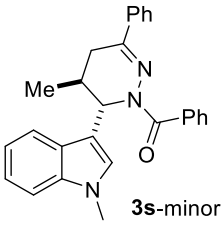
3s-major



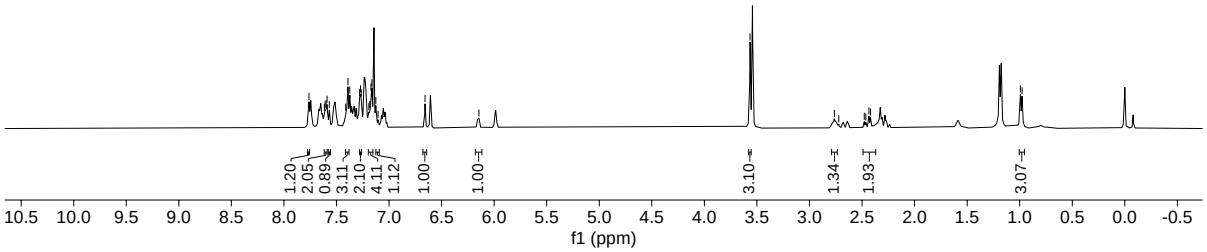


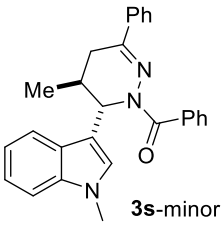
3s-major



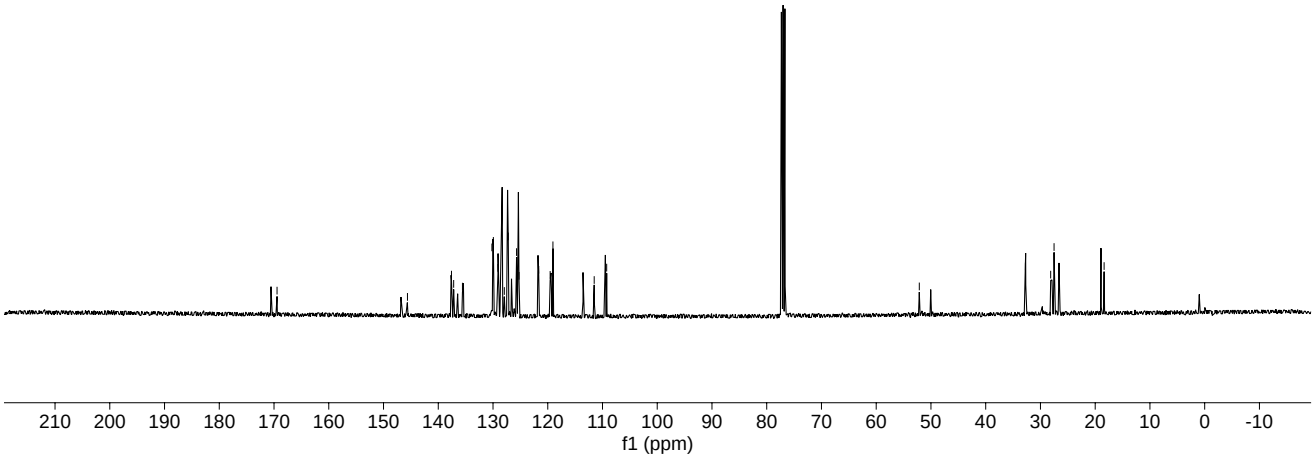


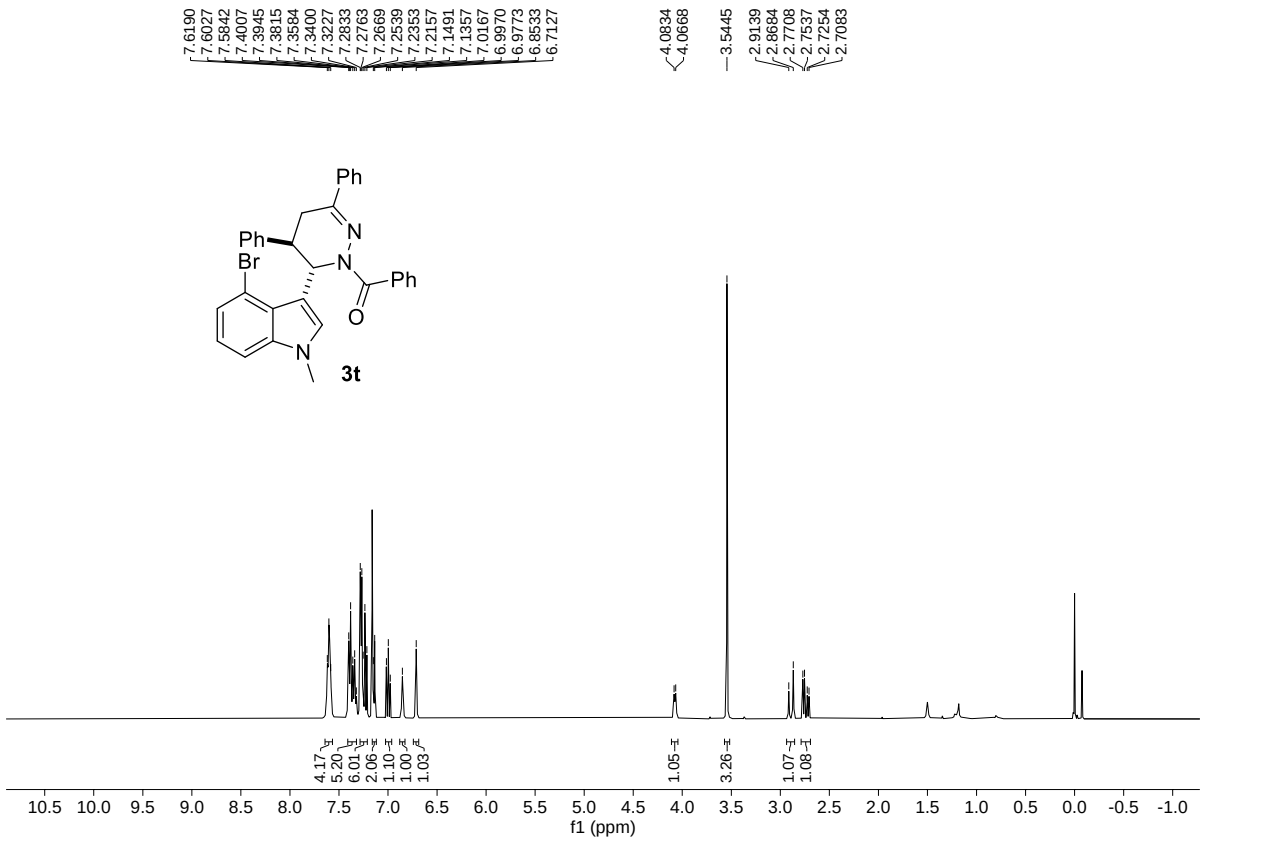
3s-minor





3s-minor

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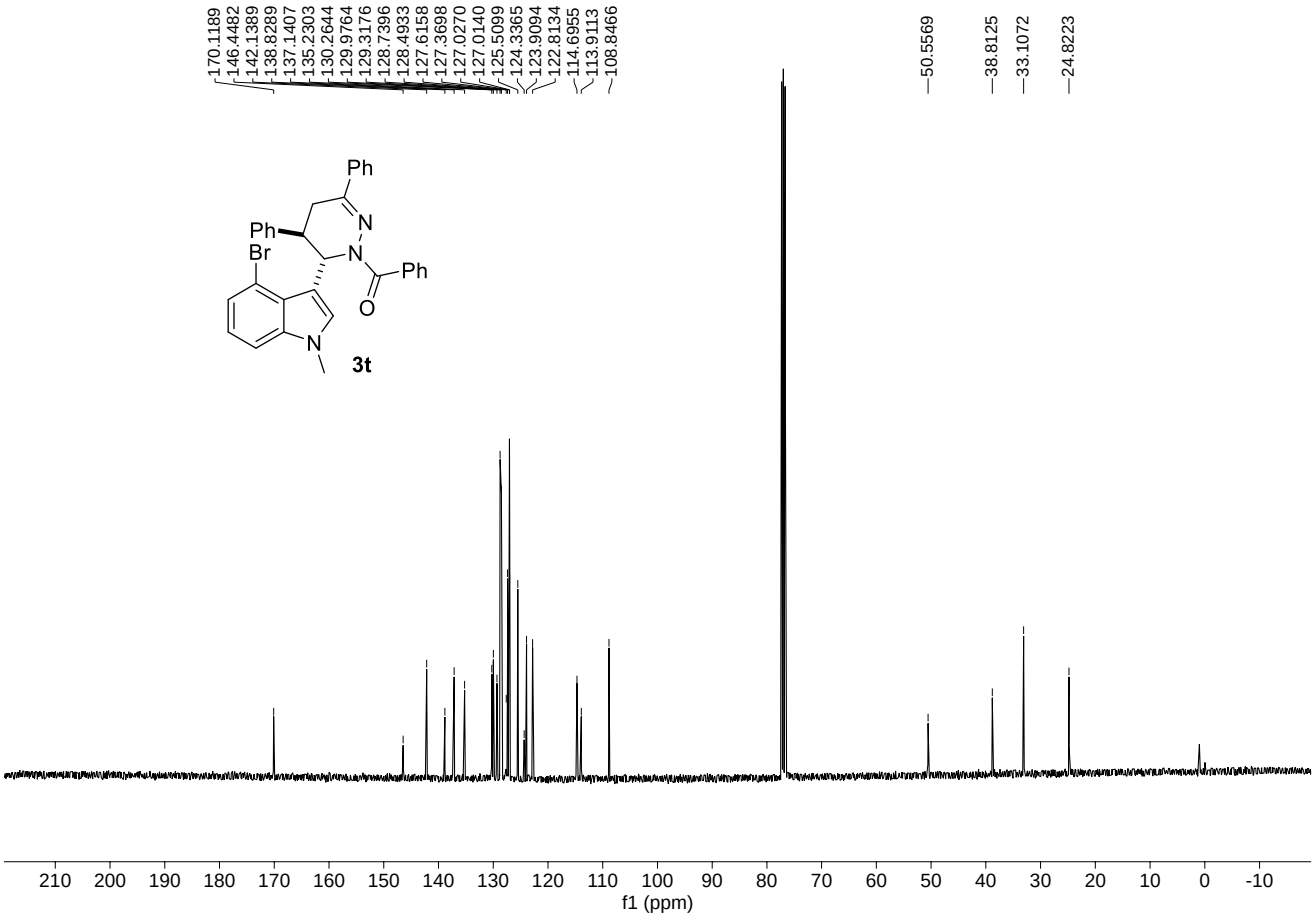
7.3227
7.2833
7.2763
7.2669
7.2539
7.2353
7.2157
7.1491
7.1357
7.0167
6.9970
6.9773
6.8533
6.7127
4.0834
4.0668
3.5445
2.9139
2.8684
2.7708
2.7537
2.7254
2.7083
Ph
Ph
Br
N
N
Ph
O
N
3t
4.17
5.20
6.01
2.06
1.10
1.00
1.03
1.05
3.26
1.07
1.08
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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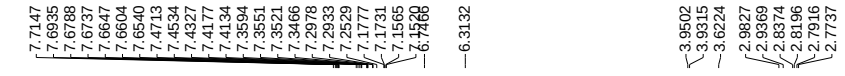
142.1389
138.8289
137.1407
135.2303
130.2644
129.9764
129.3176
128.7396
128.4933
127.6158
127.3698
127.0270
127.0140
125.5099
124.3365
123.9094
122.8134
114.6955
113.9113
108.8466
50.5569
38.8125
33.1072
24.8223
Ph
Ph
Br
N
N
Ph
O
N
3t
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.6737
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7.6540
7.4713
7.4534
7.4327
7.4177
7.4134
7.3594
7.3551
7.3521
7.3466
7.2978
7.2933
7.2529
7.1777
7.1731
7.1565
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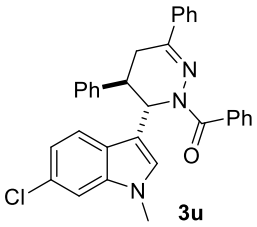
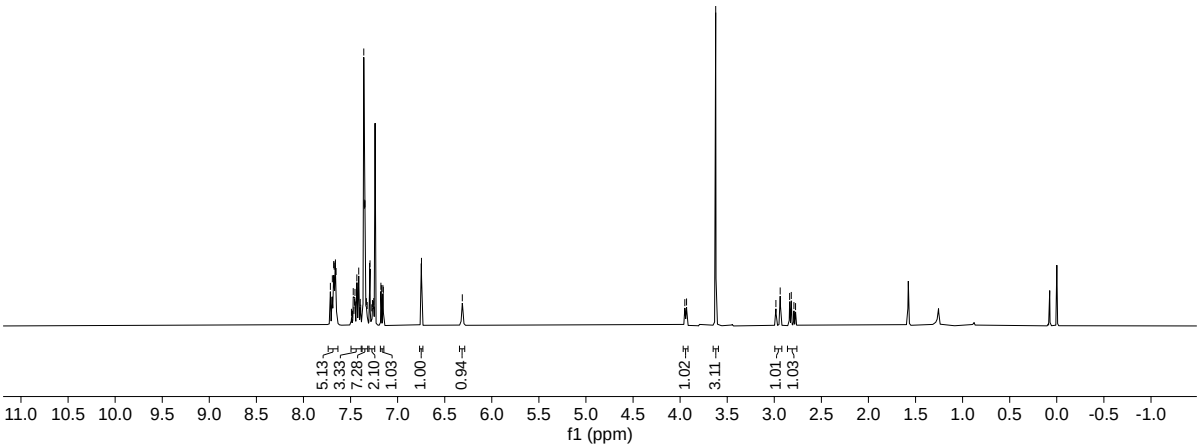
2.9827
2.9369
2.8374
2.8196
2.7916
2.7737


Ph
N
Ph
N
Ph
O
Cl
N

3u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3.33
7.28
2.10
1.03
1.00
0.94
1.02
3.11
1.01
1.03
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
f1 (ppm)


170.3818
146.4229
142.0624
138.0990
136.9990
135.0671
130.4283
129.9808
129.4958
128.9863
128.5723
128.2560
127.4579
127.3441
126.8772
126.8267
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120.1417
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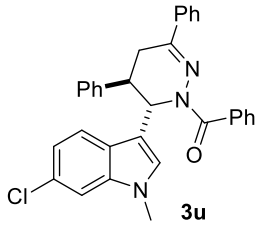
109.7989
51.9234
38.6271
32.9502
24.7385


Ph
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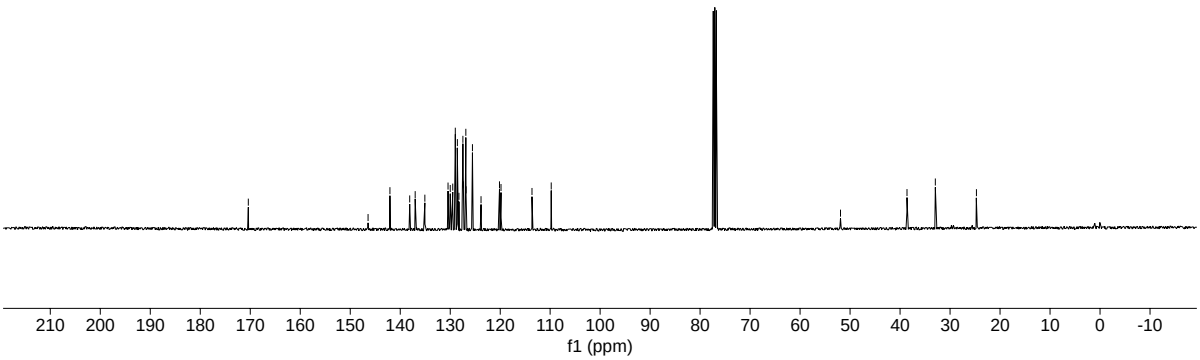
Ph
N
Ph
O
Cl
N

3u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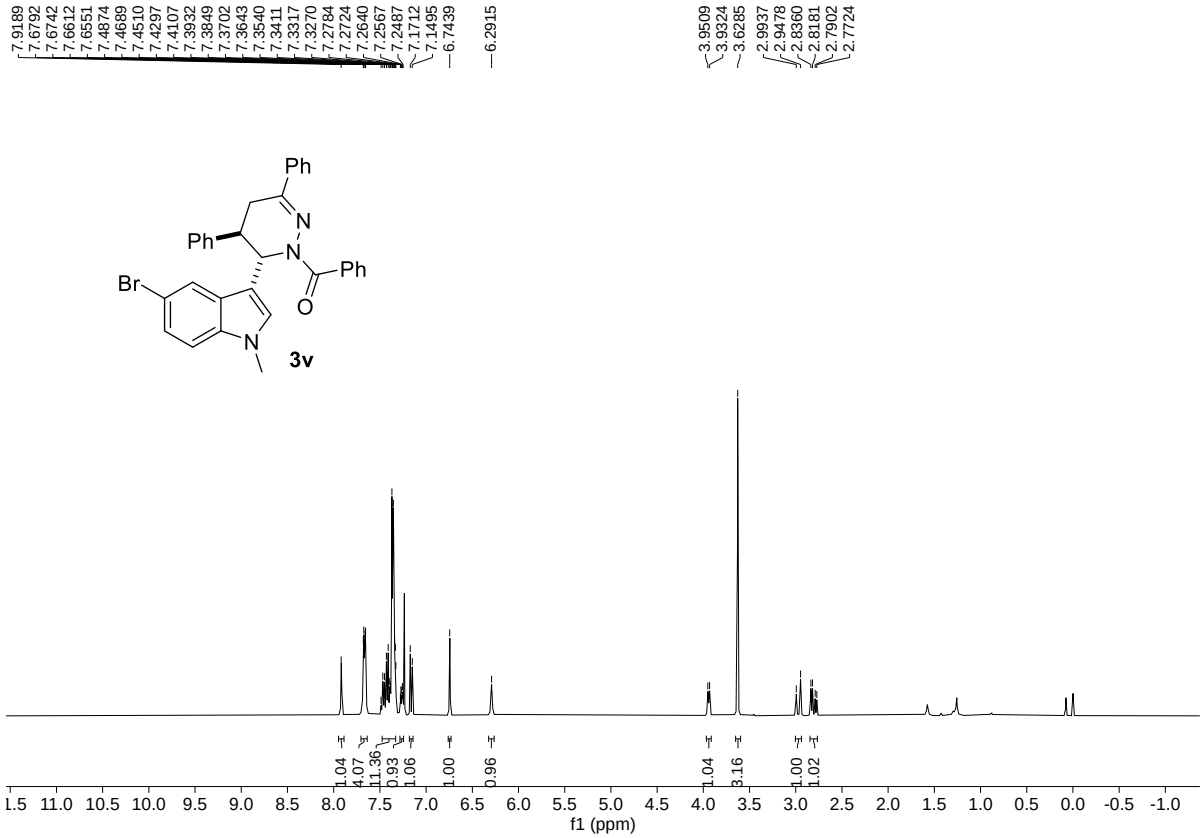
f1 (ppm)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7.4689
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7.4297
7.4107
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7.3849
7.3702
7.3643
7.3540
7.3411
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7.3270
7.2784
7.2724
7.2640
7.2567
7.2487
7.1712
7.1495
6.7439
6.2915
3.9509
3.9324
3.6285
2.9937
2.9478
2.8360
2.8181
2.7902
2.7724
Ph
N
Ph
N
Ph
Br
O
N
3v
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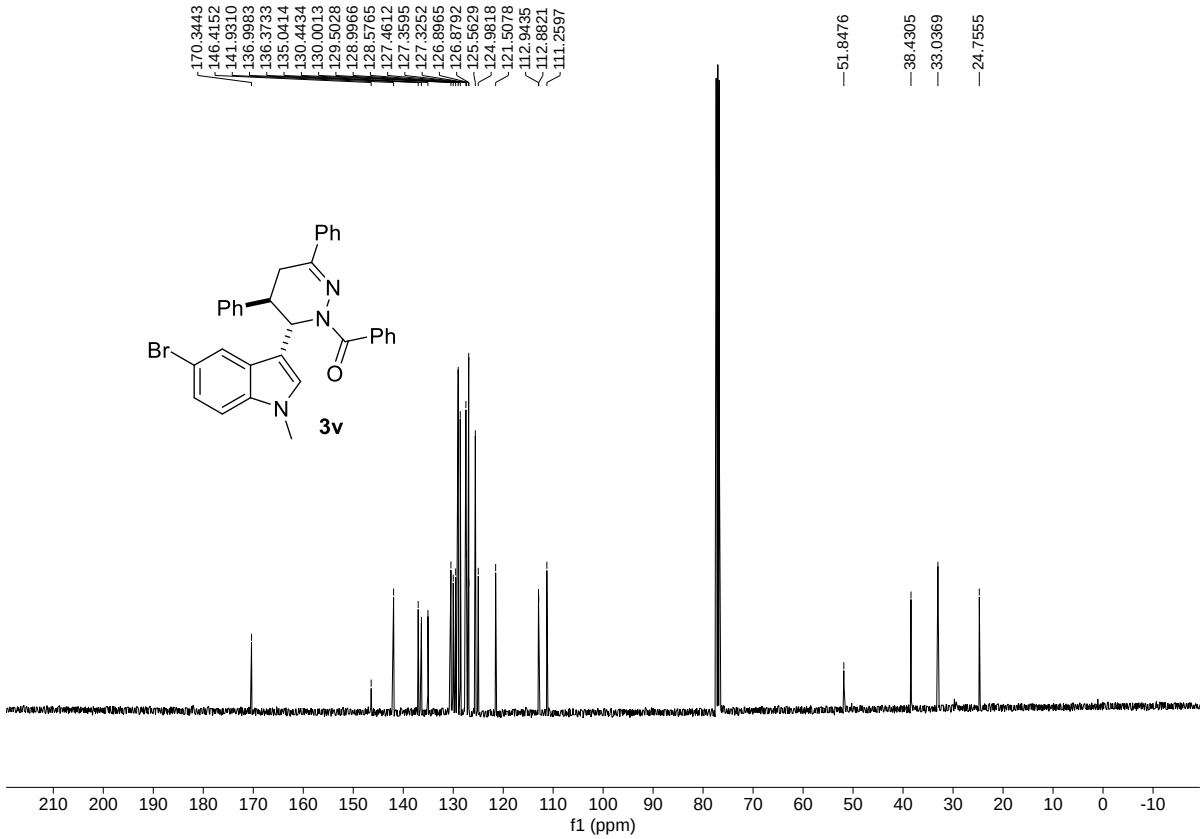
0.93
1.06
1.00
0.96
1.04
3.16
1.00
1.02
f1 (ppm)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136.3733
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127.4612
127.3595
127.3252
126.8965
126.8792
125.5629
124.9818
121.5078
112.9435
112.8821
111.2597
51.8476
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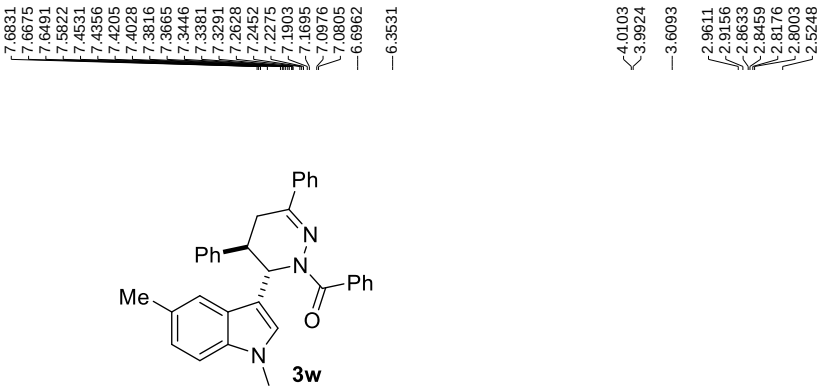
33.0369
24.7555
Ph
N
Ph
N
Ph
Br
O
N
3v
f1 (ppm)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7.3381
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7.2628
7.2452
7.2275
7.1903
7.1695
7.0976
7.0805
6.6962
6.3531
4.0103
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2.9611
2.9156
2.8633
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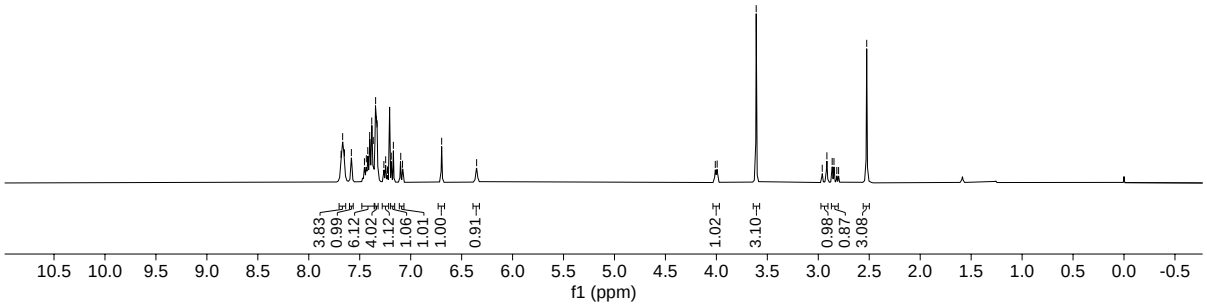
2.8176
2.8003
2.5248

Ph
N
Ph
N
Ph
Me
O
N
3w


3.83
0.99
6.12
4.02
1.12
1.06
1.01
1.00
0.91
1.02
3.10
0.98
0.87
3.08
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
f1 (ppm)


170.2381
146.2246
142.2621
137.1010
136.0893
135.2355
130.1970
129.8945
129.2864
128.8451
128.5330
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126.8589
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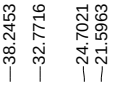
109.3565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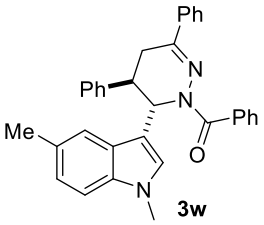
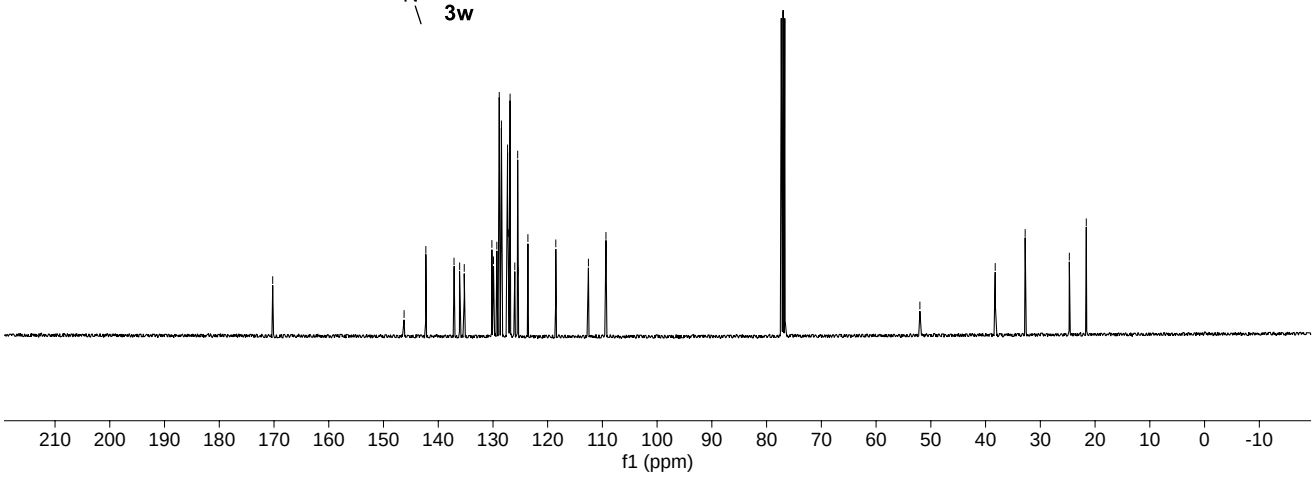
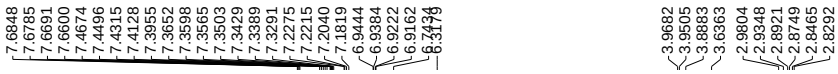
24.7021
21.5963


Ph
N
Ph
N
Ph
Me
O
N
3w


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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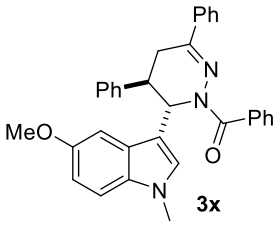
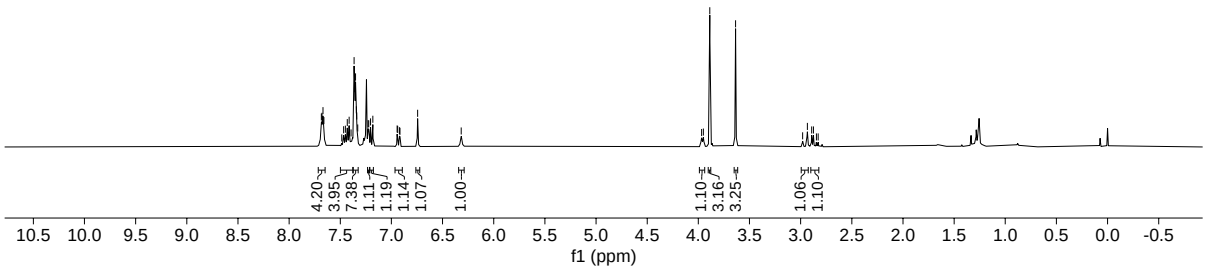
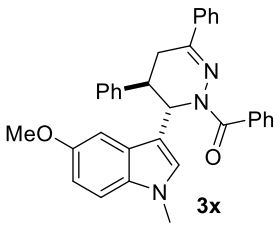
7.6785
7.6691
7.6600
7.4674
7.4496
7.4315
7.4128
7.3955
7.3652
7.3598
7.3565
7.3503
7.3429
7.3389
7.3291
7.2275
7.2215
7.2040
7.1819
6.9444
6.9384
6.9222
6.9162
6.7434
6.7179
3.9682
3.9505
3.8883
3.6363
2.9804
2.9348
2.8921
2.8749
2.8465
2.8292


Ph
N
Ph
N
Ph
MeO
O
N

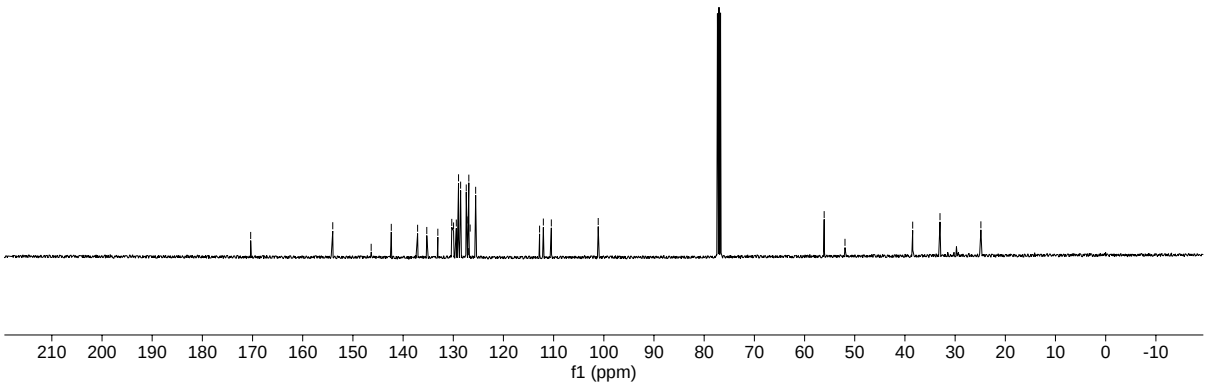
3x

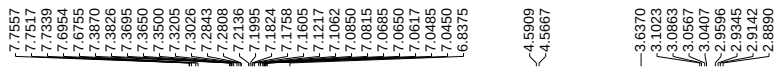

4.20
3.95
7.38
1.11
1.19
1.14
1.07
1.00
1.10
3.16
3.25
1.06
1.10
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


170.3664
154.0201
146.3676
142.3517
137.1186
135.2700
133.0869
130.2943
129.9567
129.3971
128.9626
128.5331
127.4147
127.2386
127.0000
126.9029
126.6408
125.5414
112.8101
112.0545
110.4713
101.1190
56.0906
51.9541
38.4554
33.0086
24.8538


Ph
N
Ph
N
Ph
MeO
O
N

3x


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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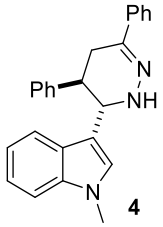
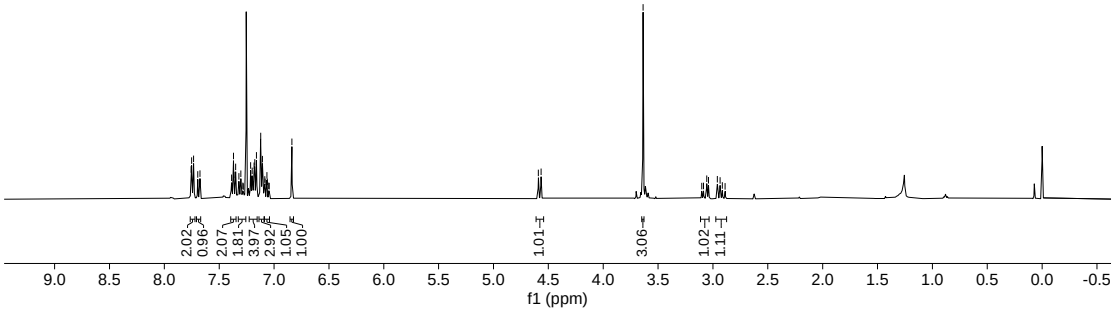
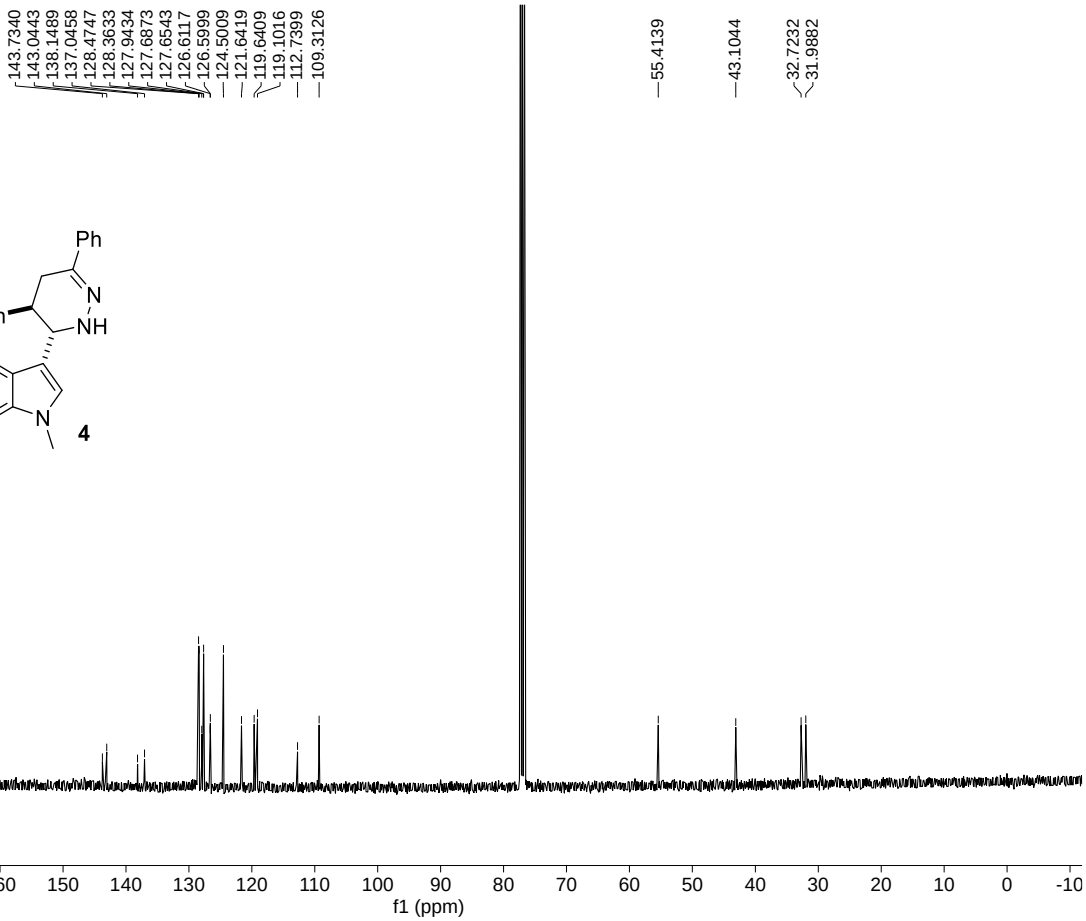
7.7517
7.7339
7.6954
7.6755
7.3870
7.3826
7.3695
7.3650
7.3500
7.3205
7.3026
7.2843
7.2808
7.2136
7.1995
7.1824
7.1758
7.1605
7.1217
7.1062
7.0850
7.0815
7.0685
7.0650
7.0617
7.0485
7.0450
6.8375
4.5909
4.5667
3.6370
3.1023
3.0863
3.0567
3.0407
2.9596
2.9345
2.9142
2.8890


Ph
N
Ph
NH
N

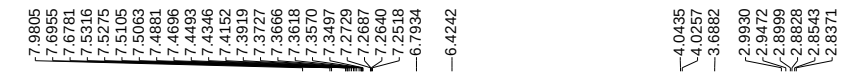
4

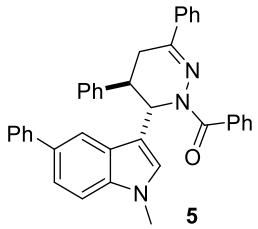

2.02
0.96
2.07
1.81
3.97
2.92
1.05
1.00
1.01
3.06
1.02
1.11
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


143.7340
143.0443
138.1489
137.0458
128.4747
128.3633
127.9434
127.6873
127.6543
126.6117
126.5999
124.5009
121.6419
119.6409
119.1016
112.7399
109.3126
55.4139
43.1044
32.7232
31.9882
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

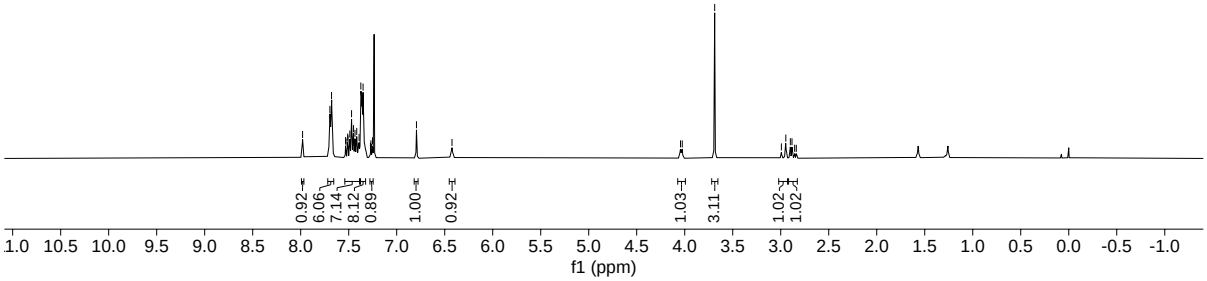
Ph
N
Ph
NH
N

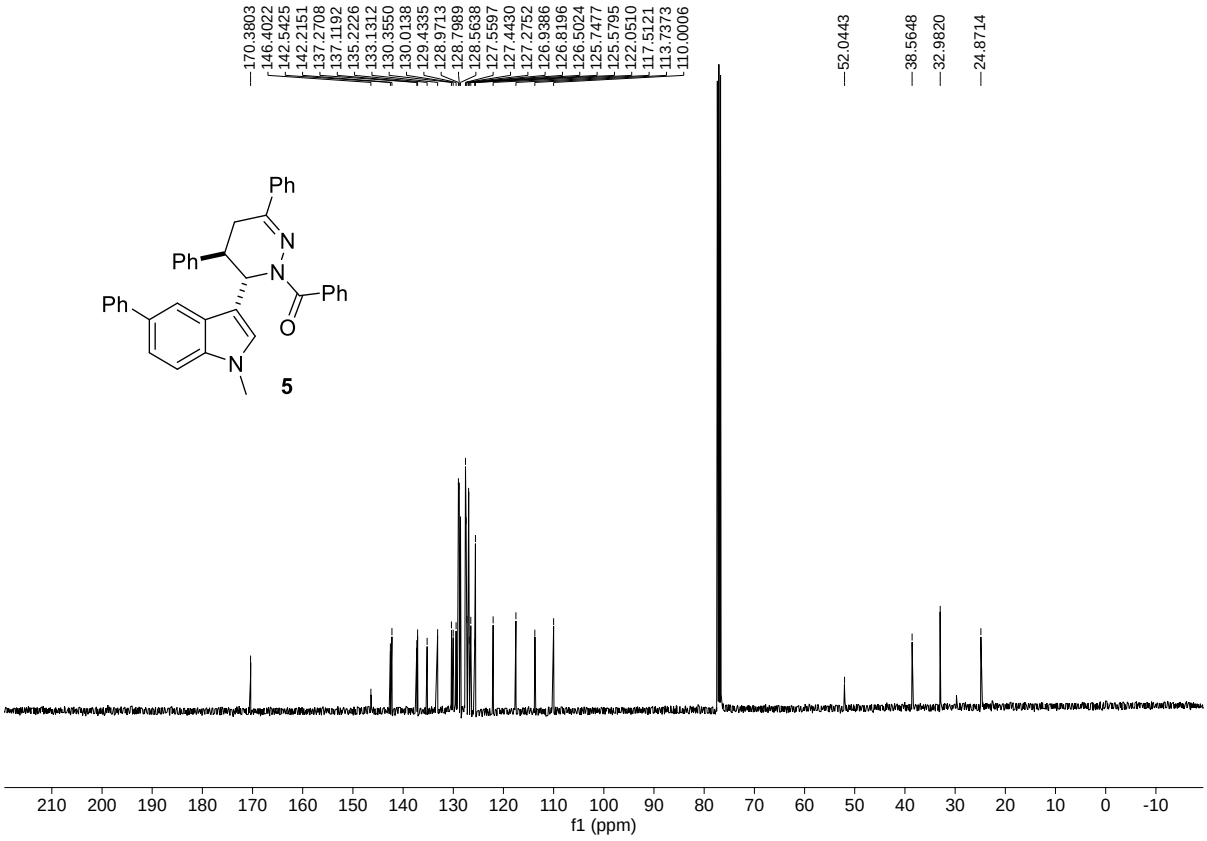
4


7.9805
7.6955
7.6781
7.5316
7.5275
7.5105
7.5063
7.4881
7.4696
7.4493
7.4346
7.4152
7.3919
7.3727
7.3666
7.3618
7.3570
7.3497
7.2729
7.2687
7.2640
7.2518
6.7934
6.4242
4.0435
4.0257
3.6882
2.9930
2.9472
2.8999
2.8828
2.8543
2.8371


Ph
N
Ph
N
Ph
Ph
O
N

5

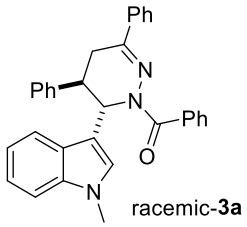

0.92
6.06
7.14
8.12
0.89
1.00
0.92
1.03
3.11
1.02
1.02
f1 (ppm)


170.3803
146.4022
142.5425
142.2151
137.2708
137.1192
135.2226
133.1312
130.3550
130.0138
129.4335
128.9713
128.7989
128.5638
127.5597
127.4430
127.2752
126.9386
126.8196
126.5024
125.7477
125.5795
122.0510
117.5121
113.7373
110.0006
52.0443
38.5648
32.9820
24.8714
f1 (ppm)

Ph
N
Ph
N
Ph
Ph
O
N

5

IX. HPLC spectra



racemic-**3a**

Data File E:\DATA\CTT\CTT\CTT-3A 2021-01-25 19-46-02\CTT-3a1.D
Sample Name: ctt-3a-rac

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Acq. Operator    : SYSTEM                    Seq. Line :   2
Acq. Instrument  : 1260                      Location :   31
Injection Date   : 1/25/2021 7:54:09 PM          Inj :    1
                                          Inj Volume : 15.000 µl
Acq. Method      : E:\DATA\CTT\CTT\CTT-3A 2021-01-25 19-46-02\IE-60-40-1.2mL-15ul-allnm-40min.
                   M
Last changed     : 1/25/2021 7:46:02 PM by SYSTEM
Analysis Method  : E:\DATA\CTT\CTT\CTT-3A 2021-01-25 19-46-02\IE-60-40-1.2mL-15ul-allnm-40min.
                   M (Sequence Method)
Last changed     : 1/28/2021 7:38:02 PM by SYSTEM
                   (modified after loading) (Current integration events modified)
Additional Info  : Peak(s) manually integrated
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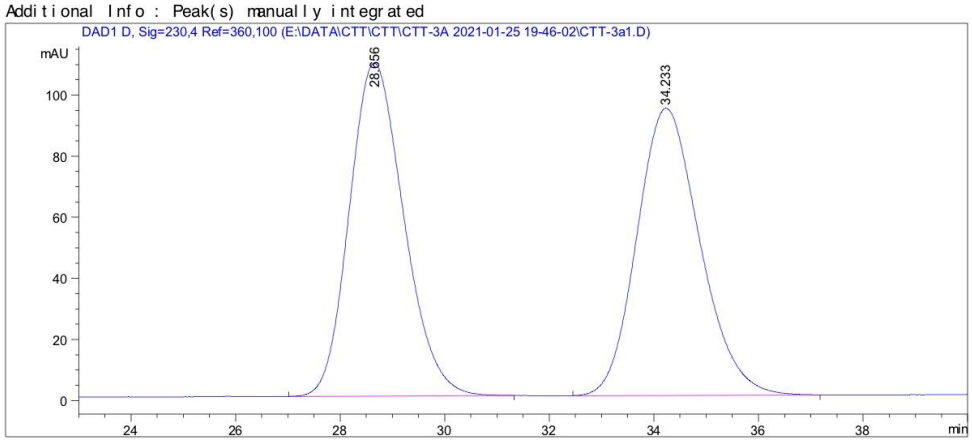


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==================================================
                Area Percent Report
==================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Do not use Multiplier & Dilution Factor with ISTDs

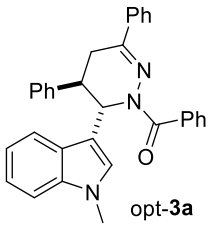

Signal 1: DAD1 D, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]      [min]    [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  28.656 BB    1.1053 7886.20508  109.09609  50.0699
   2  34.233 BB    1.2156 7864.18555   94.04229  49.9301

Totals :                  1.57504e4   203.13838

==================================================
                *** End of Report ***

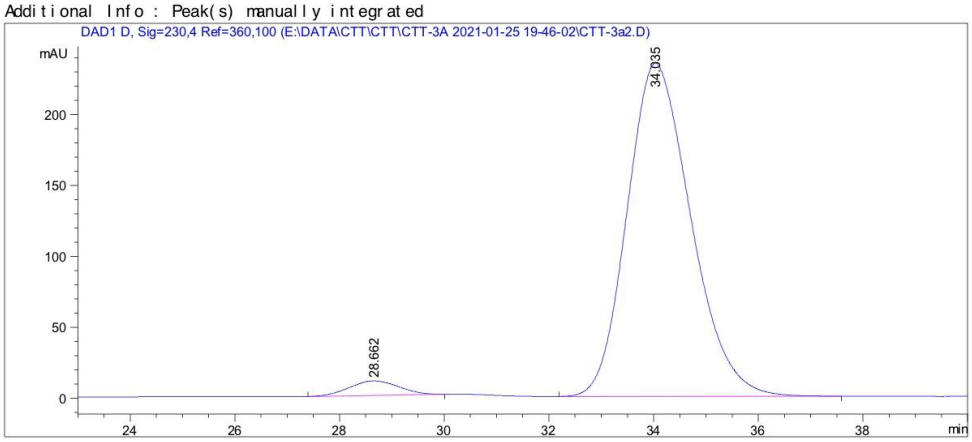
1260 1/28/2021 7:38:45 PM SYSTEM                  Page   1 of 1
```



opt-**3a**

Data File E:\DATA\CTT\CTT\CTT-3A 2021-01-25 19-46-02\CTT-3a2.D
Sample Name: ctt-3a-opt

Acq. Operator	: SYSTEM	Seq. Line	: 3
Acq. Instrument	: 1260	Location	: 32
Injection Date	: 1/25/2021 8:35:07 PM	Inj	: 1
		Inj Volume	: 15.000 µl
Acq. Method	: E:\DATA\CTT\CTT\CTT-3A 2021-01-25 19-46-02\IE-60-40-1.2mL-15ul-allnm-40min.M		
Last changed	: 1/25/2021 7:46:02 PM by SYSTEM		
Analysis Method	: E:\DATA\CTT\CTT\CTT-3A 2021-01-25 19-46-02\IE-60-40-1.2mL-15ul-allnm-40min.M (Sequence Method)		
Last changed	: 1/28/2021 7:38:02 PM by SYSTEM (modified after loading) (Current integration events modified)		
Additional Info	: Peak(s) manually integrated		



Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 D, Sig=230,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	28.662	BB	0.7849	674.79413	10.21168	3.2908
2	34.035	BB	1.2690	1.98307e4	234.87126	96.7092
Totals :				2.05055e4	245.08294	

*** End of Report ***