Electronic Supplementary Information (ESI)

Photocatalytic Prins-like indole addition between tryptophol C2 with aldehydes and ketones

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Contents

1. General experiment

1.1 Materials and Experiments

Photocatalysis experiments were performed in an argon or oxygen atmosphere. Chemical reagents (including purified water) were obtained from commercial suppliers (*Sigma-Aldrich, Adamas,* Shanghai Titan Technology Co., LTD, Adamas et al.) and used without further purification. Reactions were monitored by thin-layer chromatography (TLC) on a 0.25 mm silica gel GF254 plate (Merck Silica gel 60-F254) using UV light as a visualizing agent and an ethanolic solution of phosphomolybdic acid and cerium sulfate and heat as a developing agent. Silica gel (300-400 mesh) was used for normal flash column chromatography. Indole and its related derivate products were isolated by column chromatography with neutral alumina (Al_2O_3, Merck KGaA, 70–230 mesh, and pH = 6.8–7.8). Ethyl acetate and petroleum ether were used as the eluent solvents. Yields refer to chromatographically and spectroscopically homogeneous materials unless otherwise noted. LED lights (including every 5W 10W 20W blue LEDs with different wavenumbers) were purchased from the Changchun Institute of Optics, Fine Mechanics and Physics, Chinese Academy of Sciences, and Changchun Changguang Chenpu Technology Co., LTD.

1.2 Characterizations and Analysis

^{1}H-NMR, and **^{13}C-NMR** were recorded with Bruker Advance (400 and 500 MHz) spectrometers. All chemical shifts were reported as δ values in parts per million (ppm) and coupling constants (*J*) in Hz. Tetramethylsilane (TMS) was used as the internal standard for $CDCl_3$ (7.26 ppm for ^{1}H, 77.00 ppm for ^{13}C).

X-ray crystal structure: Single block crystals of **target molecules** were used as supplied. A suitable crystal with dimensions 0.20 × 0.15 × 0.10 mm^3 was selected and mounted on a Bruker APEX-II CCD diffractometer.

Mass spectra: **(1)** ***HR-MS (ESI)*** was taken on AB QSTAR Pulsar mass spectrometer or Agilent LC/MSD TOF mass spectrometer. HR-MS data were recorded via electron impact mass spectrometry using a time-of-flight analyzer. ***(2) GC–MS*** was performed on a Hewlett-Packard 6890 N gas chromatograph (equipped with the same HP-5MS capillary column) under identical operating conditions used in Mass Spectral Library by R. P. Adams (Adams, 2007).

1.3 Photocatalysis experiments device

The reaction was carried out as follows: a one, two or three-neck reaction quartz flask was fitted with a magnetic stirring bar. Septa capped the other two necks for injections and an atmosphere line. Following evacuation in a vacuum and flushing with argon or oxygen three times, the reaction vessel was charged with a solution of reactants. The reaction conditions were 25 °C and used an argon or oxygen balloon atmosphere, with water or other organic reagents as the solvent.

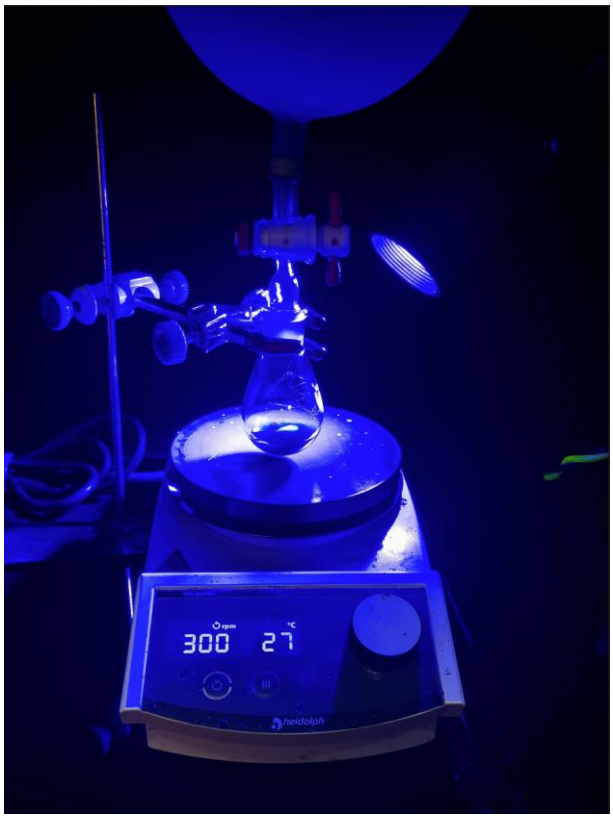


Figure S1. Photocatalysis experiment device.

2. Photocatalysis experiments

2.1 General photocatalytic synthesis

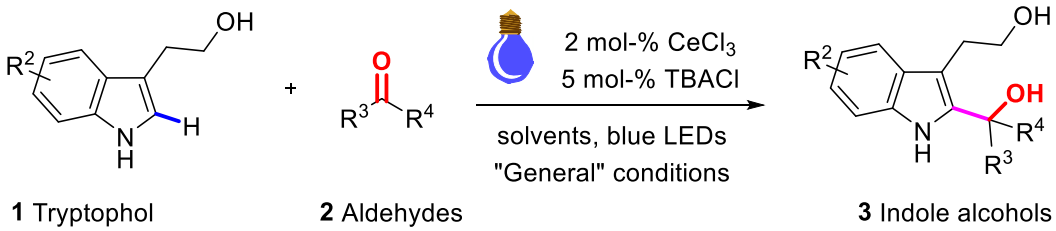


Figure S2. Photocatalytic synthesis of radical Aldol reaction

In an oven-dried quartz flask (50 mL) equipped with a stir bar, tryptophol (250 mg, 1.6 mmol, 1.0 equiv.), aldehydes (1.0 equiv.), cerium (III) chloride (19.11 mg, 0.08 mmol, 0.05 equiv.), tetrabutylammonium chloride (43.09 mg, 0.16 mmol, 0.1 equiv.), 2,2,2-trichloro-ethanol (23.18 mg, 0.16 mmol, 0.1 equiv.) and dichloromethane (DCM, 20.0 mL) were combined and added. The reaction was conducted under an argon atmosphere using an Ar balloon. The reaction mixture was stirred and illuminated by blue LED lights under room temperature for 15 h cooling by a fan. TLC, UV light as a visualizing agent, the reaction was monitored, and an ethanolic solution of phosphomolybdic acid, cerium sulfate, and heat as a developing agent. When the reactant material was no longer decreased, the solution was extracted with DCM (6×10 mL) and H_2O (3×10 mL). The combined organic layer was dried with Na_2SO_4 and filtered. The solvent was removed with a rotary evaporator. The pure product was obtained by flash chromatography on neutral alumina (Al_2O_3, Merck KGaA, 70–230 mesh, and pH = 6.8–7.8) using ethyl acetate and petroleum ether (1:15, vol/vol) as the eluent solvents. The target product was obtained. All the products' isolated yields were calculated by column chromatography.

2.2 Data and NMR spectra products.

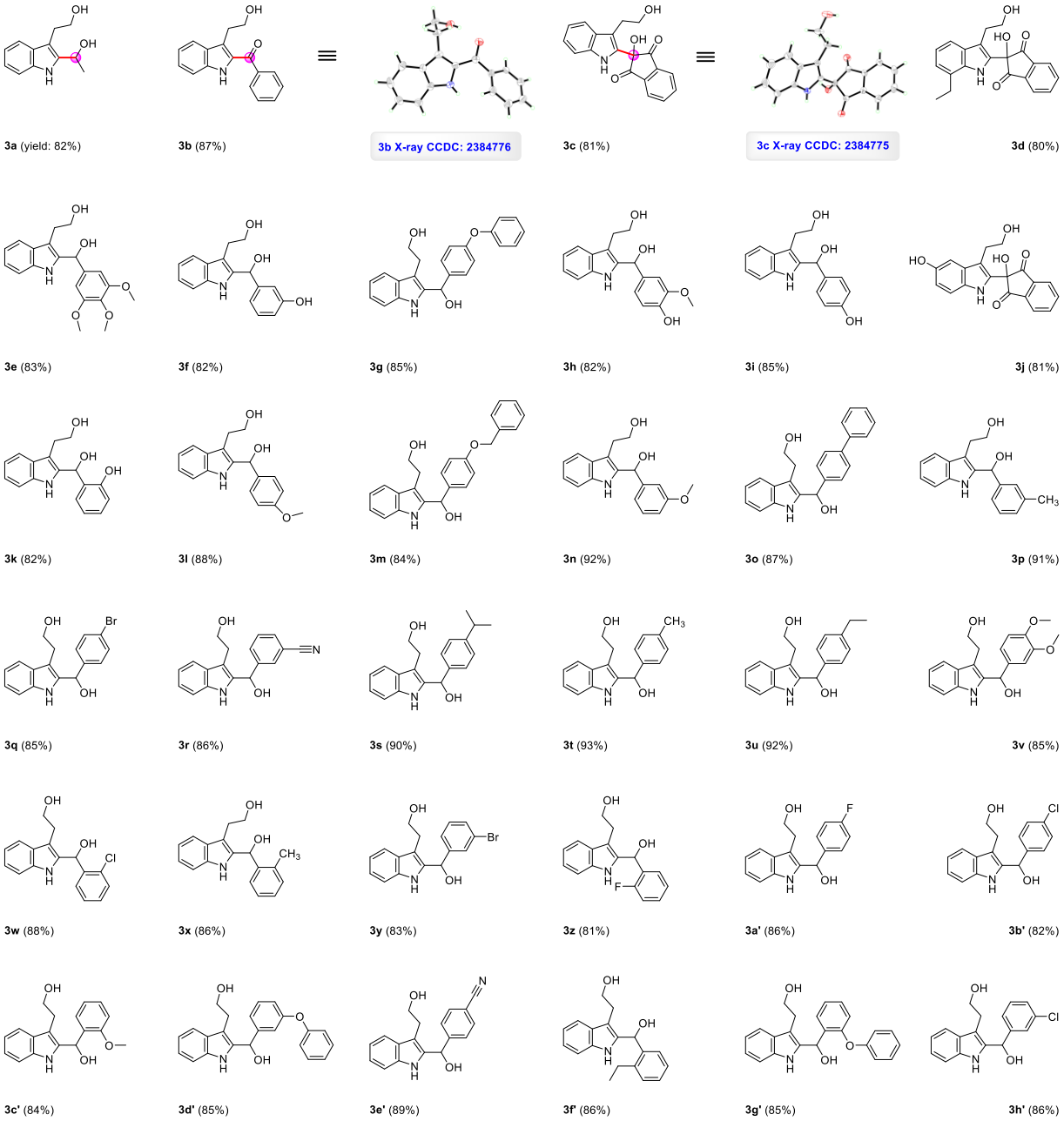
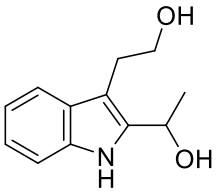
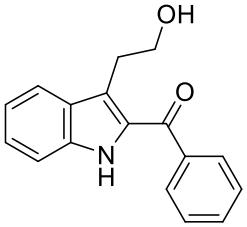


Figure S3. Products of indole intermolecular reaction with aldehydes and ketones.



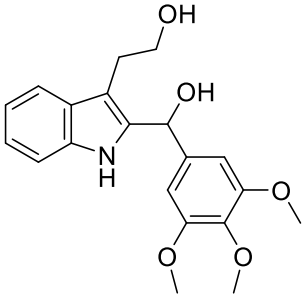
Name: 1-(3-(2-hydroxyethyl)-1H-indol-2-yl)ethan-1-ol

TLC: Petroleum ether/EtOAc = 5/1, R_f = 0.5, Yield: 80%, **^{1}H NMR (**500 MHz, $CDCl_3$) δ ppm: 1.79-1.81 (d, 1H, J = 7.45 Hz), 2.87-2.93 (ss, 0.5H, J = 32.55 Hz), 3.07-3.10 (m, 2H), 3.88-3.92 (m, 2H), 4.88-4.92 (q, 0.5H, J = 22.2 Hz), 7.07-7.15 (m, 2H), 7.23-7.26 (t, 1H, J = 16.25 Hz), 7.50-7.51 (d, 1H, J = 7.7 Hz). **^{13}C NMR (**125 MHz, $CDCl_3$) δ ppm: 20.0, 27.4, 30.1, 62.6, 107.7, 110.9, 118.3, 119.5, 121.7, 128.5, 135.6, 138.3. **HRMS (ESI$^+$):** calculated for $C_{12}H_{16}NO_2$, $[M+H]^+$ 206.7716, found 206.7609.



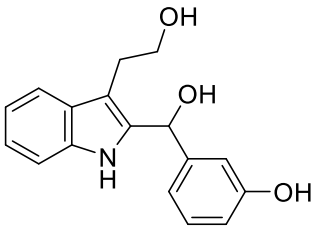
Name: (3-(2-hydroxyethyl)-1H-indol-2-yl)(phenyl)methanone

TLC: Petroleum ether/EtOAc = 8/1, R_f = 0.6, Yield:87%, **^{1}H NMR (**500 MHz, $CDCl_3$) δ ppm: 3.20-3.21 (d, 1H, J = 5.25 Hz), 3.78 (s, 1H), 7.185-7.19 (d, 1H, J =2.35 Hz), 7.38 (s, 2H), 7.48 (s, 2H), 7.58-7.69 (m, 4H), 8.94-8.97 (d, 1H, J = 17.4 Hz). **^{13}C NMR (**125 MHz, $CDCl_3$) δ ppm: 28.2, 63.5, 112.4, 120.7, 120.8, 121.0, 121.1, 122.8, 126.6, 127.1, 128.0, 128.6, 128.7, 128.9, 129.2, 129.3, 132.0, 132.5, 136.8, 138.5. **HRMS (ESI$^+$):** calculated for $C_{17}H_{16}NO_2$, $[M+H]^+$ 266.1176, found 266.1170.



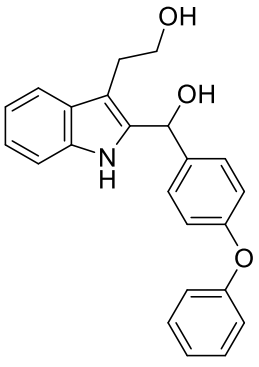
Name: 2-(2-(hydroxy(3,4,5-trimethoxyphenyl)methyl)-1H-indol-3-yl)ethan-1-ol

TLC: Petroleum ether/EtOAc = 15/1, R_f = 0.8, Yield: 83%, **^{1}H NMR (**500 MHz, $CDCl_3$) δ ppm: 1.58 (s, 1H), 2.80-2.83 (d, 1H, *J* = 15.25 Hz), 3.11-3.17 (m, 1H), 3.79 (s, 6H), 3.83 (s, 3H), 3.97-4.02 (t, 1H, *J* = 11 Hz), 4.37-4.40 (q,1H, *J* = 16.25 Hz), 5.72 (s, 1H), 6.57 (s, 2H), 7.12-7.19 (m, 2H), 7.29-7.31 (d,1H, *J* = 7.9Hz), 7.56-7.57 (d,1H, *J* = 7.55 Hz), 7.84(s, 1H). **^{13}C NMR (**125 MHz, $CDCl_3$) δ ppm: 22.3, 56.1, 60.8, 65.5, 105.4, 108.7, 111.1, 118.3, 119.6, 122.0, 127.1, 133.6, 135.1, 136.1, 153.5. **HRMS (ESI$^+$):** calculated for $C_{20}H_{24}NO_5$, $[M+H]^+$ 358.1649, found 358.1657.



Name: 3-(hydroxy(3-(2-hydroxyethyl)-1H-indol-2-yl)methyl)phenol

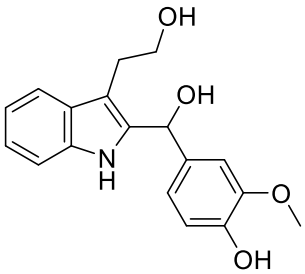
TLC: Petroleum ether/EtOAc = 12/1, R_f = 0.8, Yield: 82%, **^{1}H NMR** (500 MHz, MeOD) δ ppm: 2.82-2.85 (d, 1H, J = 15.15 Hz), 2.97-3.02 (m, 1H), 3.33 (s, 1H), 3.95-3.97 (m, 1H), 4.19-4.22 (m, 1H), 4.63 (s, 1H), 5.79 (s, 1H), 6.77-6.80 (t, 2H, *J* = 12.75 Hz), 6.86-6.87 (d, 1H, *J* = 7.55 Hz), 7.00-7.03 (t, 1H, *J* = 14.8 Hz), 7.05-7.08 (t, 1H, *J* = 14.95 Hz), 7.20-7.23 (t, 1H, *J* = 15.55 Hz), 7.25-7.27 (d, 1H, *J* = 8.05 Hz), 7.47-7.49 (d, 1H, *J* =7.75 Hz). **^{13}C NMR (**125 MHz, MeOD) δ ppm: 25.9, 67.5, 79.9, 111.2, 114.6, 119.1, 121.3, 122.4, 130.6, 133.1, 137.1, 140.6, 145.3, 161.2. **HRMS (ESI$^+$):** calculated for $C_{17}H_{18}NO_3$, $[M+H]^+$ 284.1281, found 284.1273.



Name: 2-(2-(hydroxy(4-phenoxyphenyl)methyl)-1H-indol-3-yl)ethan-1-ol

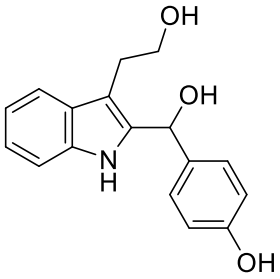
TLC: Petroleum ether/EtOAc = 15/1, R_f = 0.8, Yield: 85%, **^{1}H NMR (**500 MHz, $CDCl_3$) δ ppm: 2.80-2.84 (m, 1H), 3.06-3.12 (m, 1H), 3.95-4.00 (m, 1H), 4.30-4.34 (m, 1H), 5.77 (s, 1H), 6.98-7.02 (m, 4H), 7.09-7.16 (m, 3H), 7.23-7.24 (d, 1H, *J* = 4.15 Hz), 7.31-7.34 (m, 4H), 7.51 (s, 1H), 7.54-7.56 (d, 1H, *J* = 7.35 Hz). **^{13}C NMR (**125 MHz, $CDCl_3$) δ ppm: 22.3, 64.9, 75.6,

109.0, 111.0, 118.4, 118.9, 119.1, 119.7, 122.0, 123.6, 127.0, 129.8, 130.1, 133.6, 134.2, 136.1, 156.9, 158.0. **HRMS (ESI$^+$):** calculated for $C_{23}H_{22}NO_3$, $[M+H]^+$ 360.1594, found 360.1588



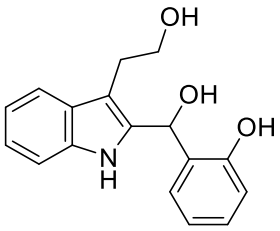
Name: 4-(hydroxy(3-(2-hydroxyethyl)-1H-indol-2-yl)methyl)-2-methoxyphenol

TLC: Petroleum ether/EtOAc = 12/1, R_f = 0.8, Yield: 82%, **^{1}H NMR (**500 MHz, $CDCl_3$) δ ppm: 2.78-2.83 (m, 1H), 3.08-3.15 (m, 1H), 3.82 (s, 3H), 3.96-4.01 (m, 1H), 4.33-4.37 (m, 1H), 5.70-5.72 (d, 1H, J = 12.9 Hz), 6.84-6.844 (d,1H, J =1.6 Hz), 6.88-6.92 (m, 2H), 7.11-7.18 (m, 2H), 7.24-7.26 (d, 1H, J = 6.95 Hz), 7.48 (s, 1H), 7.54-7.56 (d, 1H, J = 8.3 Hz). **^{13}C NMR (**125 MHz, $CDCl_3$) δ ppm: 22.3, 56.0, 65.2, 108.7, 110.5, 111.1, 114.2, 118.3, 119.7, 121.7, 121.9, 127.1, 131.4, 134.0, 136.0, 146.3, 147.0. **HRMS (ESI$^+$):** calculated for $C_{18}H_{20}NO_4$, $[M+H]^+$ 314.1837, found 314.1829.



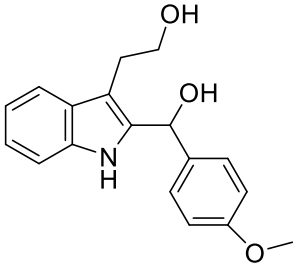
Name: 4-(hydroxy(3-(2-hydroxyethyl)-1H-indol-2-yl)methyl)phenol

TLC: Petroleum ether/EtOAc = 12/1, R_f = 0.6, Yield: 85%, **^{1}H NMR (**500 MHz, $CDCl_3$) δ ppm: 2.81-2.84 (d, 1H, J = 15.45 Hz), 3.07-3.12 (m, 1H), 3.97-4.01 (m, 1H), 4.30-4.32 (m, 1H), 5.77 (s, 1H), 6.75-6.77 (d, 1H, J = 8.25 Hz), 6.92-6.94 (d, 2H, J = 8.4 Hz), 7.11-7.18 (m, 1H), 7.54-7.56 (d, 1H, J = 7.3 Hz), 7.68 (s, 1H), 7.76-7.78 (d, 2H, J = 8.4 Hz), 9.78 (s, 1H). **HRMS (ESI$^+$):** calculated for $C_{17}H_{18}NO_3$, $[M+H]^+$ 284.1280, found 284.1286.



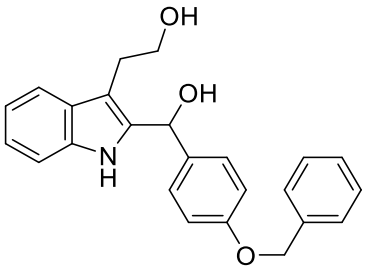
Name: 2-(hydroxy(3-(2-hydroxyethyl)-1H-indol-2-yl)methyl)phenol

TLC: Petroleum ether/EtOAc = 15/1, R_f = 0.8, Yield: 82%, **^{1}H NMR (**500 MHz, $CDCl_3$) δ ppm: 3.25 (s, 2H), 3.94 (s, 2H), 6.93-6.96 (t, 1H, J = 14.8 Hz), 7.07-7.08 (d, 1H, J = 8.3 Hz), 7.17 (s, 1H), 7.34 (s, 2H), 7.50-7.53 (t, 1H, J =15.2 Hz), 7.69-7.71 (d, 1H,J = 7.95 Hz), 7.77-7.78 (d, 1H, J = 8.3 Hz), 8.77 (s, 1H), 11.51 (s, 1H,). **HRMS (ESI$^+$):** calculated for $C_{17}H_{18}NO_3$, $[M+H]^+$ 284.1281, found 284.1289.



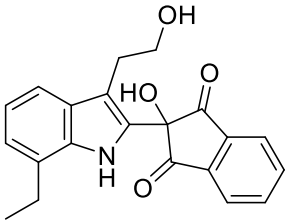
Name: 2-(2-(hydroxy(4-methoxyphenyl)methyl)-1H-indol-3-yl)ethan-1-ol

TLC: Petroleum ether/EtOAc = 15/1, R_f = 0.8, Yield: 88%, **^{1}H NMR (**500 MHz, $CDCl_3$) δ ppm: 2.80-2.85(m, 1H), 3.07-3.13 (m, 1H), 3.81 (s, 3H), 3.96-4.01 (m, 1H), 4.29-4.33 (m, 1H), 5.76 (s, 1H), 6.89-6.92 (d, 2H,J = 14.25 Hz), 7.12-7.18 (m, 1H), 7.23-7.25 (d, 2H, J = 7.25 Hz), 7.28-7.30 (d, 2H,J = 8.6 Hz), 7.49 (s, 1H), 7.56-7.57(d, 1H, J =7.25 Hz). **^{13}C NMR (**125 MHz, $CDCl_3$) δ ppm: 22.4, 55.4, 64.8, 75.7, 108.9, 111.0, 114.2, 118.4, 119.7, 121.9, 127.1, 129.9, 131.6, 133.9, 136.0, 160.1. **HRMS (ESI$^+$):** calculated for $C_{18}H_{20}NO_3$, $[M+H]^+$ 298.1438, found 298.1432.



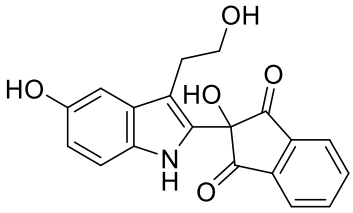
Name: 2-(2-((4-(benzyloxy)phenyl)(hydroxy)methyl)-1H-indol-3-yl)ethan-1-ol

TLC: Petroleum ether/EtOAc = 15/1, R_f = 0.8, Yield: 84%, **^{1}H NMR (**500 MHz, $CDCl_3$) δ ppm: 1.56 (s, 2H), 2.79-2.83 (m, 1H), 3.05-3.12(m, 1H), 3.95-4.00 (m, 1H), 4.28-4.32 (m, 1H), 5.07 (s, 2H), 5.75 (s, 1H), 6.96-6.97 (d, 2H, *J* = 8.7 Hz), 7.12-7.17 (m, 2H), 7.22-7.24(d, 1H, *J* = 7.3 Hz), 7.27-7.29 (d, 2H, *J* = 8.65 Hz), 7.32-7.33 (d, 1H, *J* = 7.15 Hz), 7.36-7.39 (t, 2H, *J* = 14.8 Hz), 7.41-7.43 (d, 2H, *J* = 7.1 Hz), 7.45 (s, 1H), 7.54-7.56 (d, 1H, *J* =7.3 Hz). **HRMS (ESI$^+$):** calculated for $C_{24}H_{24}NO_3$, $[M+H]^+$ 374.1751, found 374.1761.



Name: 2-(7-ethyl-3-(2-hydroxyethyl)-1H-indol-2-yl)-2-hydroxy-1H-indene-1,3(2H)-dione

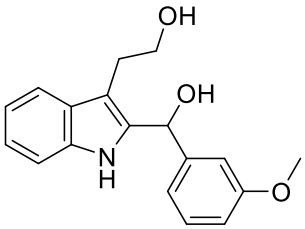
TLC: Petroleum ether/EtOAc = 6/1, R_f = 0.6, Yield: 80%, **^{1}H NMR (**500 MHz, MeOD) δ ppm: 1.30-1.33 (t, 3H, *J* = 15.1 Hz), 2.65-2.68 (t, 2H, *J* = 15.45 Hz), 2.87-2.92 (q, 2H, *J* = 22.7 Hz), 3.31-3.33 (t, 2H, *J* = 9.3 Hz), 6.92-6.96 (q, 2H, *J* = 19.65 Hz), 7.28-7.30(q, 1H, *J* = 9.05 Hz), 8.03-8.05 (q, 2H, *J* = 8.8 Hz), 8.11-8.13 (q, 2H, *J* = 8.8 Hz). **^{13}C NMR (**125 MHz, MeOD) δ ppm: 13.1, 13.3, 23.5, 27.5, 61.6, 76.1, 110.0, 115.8, 119.3, 121.0, 124.0, 126.8, 128.3, 128.4, 134.6, 136.9, 140.6, 197.7. **HRMS (ESI$^+$):** calculated for $C_{21}H_{20}NO_4$, $[M+H]^+$ 350.1387, found 350.1379.



Name: 2-hydroxy-2-(5-hydroxy-3-(2-hydroxyethyl)-1H-indol-2-yl)-1H-indene-1,3(2H)-dione

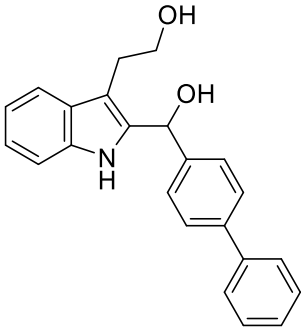
TLC: Petroleum ether/EtOAc = 5/1, R_f = 0.5, Yield: 81%, **^{1}H NMR (**500 MHz, MeOD) δ ppm: 3.26-3.29 (q, 1H, *J* = 14.65 Hz), 3.34 (m, 1H), 3.78-3.82 (m, 1H), 3.86-3.92 (m, 1H), 3.74-3.98(m, 1H), 6.56-6.57(d,1H, *J* = 8.65 Hz), 7.17(s,1H), 7.25-7.27 (d, 1H, *J* = 8.7 Hz), 7.53-7.56 (t, 1H, *J* = 15.8 Hz), 7.71-7.73 (d, 1H, *J* = 7.7 Hz), 7.80-7.83 (m, 1H), 7.97-7.98 (d, 1H, *J* = 7.85 Hz). **^{13}C NMR (**125 MHz, MeOD) δ ppm: 28.5, 64.2, 104.4, 108.1, 111.9, 112.3, 114.3, 122.8,

124.,5 125.0, 130.2, 133.4, 134.8, 135.9, 149.4, 151.5, 200.3. **HRMS (ESI$^+$):** calculated for $C_{19}H_{16}NO_5$, $[M+H]^+$ 338.1023, found 338.1031.



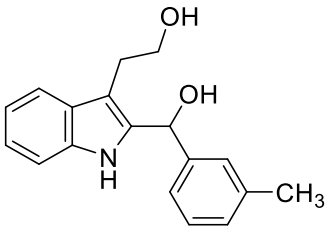
Name: 2-(2-(hydroxy(3-methoxyphenyl)methyl)-1H-indol-3-yl)ethan-1-ol

TLC: Petroleum ether/EtOAc = 15/1, R_f = 0.5, Yield: 92%, **^{1}H NMR (**500 MHz, $CDCl_3$) δ ppm: 2.80-2.83(q, 1H, *J* =15 Hz), 3.10-3.11(dt, 1H, *J*=50 Hz), 3.77(s, 3H), 3.96-4.01(m, 1H), 4.32-4.36(m, 1H), 4.36-4.37(m, 1H), 5.77(s, 1H), 6.89-6.92(m, 2H), 6.96-6.98(d, 1H, *J*=10 Hz), 7.11-7.17(m, 2H), 7.23-7.25(t, 1H, *J*=10 Hz), 7.28-7.31(t, 1H, *J*=10 Hz), 7.40-7.47(m, 1H), 7.54-7.55(t, 1H, J=5 Hz). **^{13}C NMR (**125 MHz, $CDCl_3$) δ ppm: 22.3, 55.3, 65.1, 76.2, 108.6, 111.0, 113.5, 114.7, 118.4, 119.7, 120.6, 121.9, 130.0, 133.6, 135.3, 136.1, 141.0. **HRMS (ESI$^+$):** calculated for $C_{18}H_{20}NO_3$, $[M+H]^+$ 298.1438, found 298.1426.



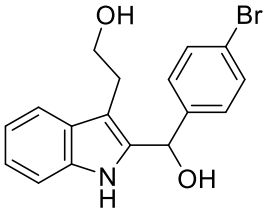
Name: 2-(2-([1,1'-biphenyl]-4-yl(hydroxy)methyl)-1H-indol-3-yl)ethan-1-ol

TLC: Petroleum ether/EtOAc = 15/1, R_f = 0.5., Yield: 87%, **^{1}H NMR (**500 MHz, $CDCl_3$) δ ppm: 2.86-2.87(m, 1H), 3.12-3.13(dt, 1H, *J*=2 Hz), 4.01-4.05(m, 1H), 4.34-4.37(m, 1H), 5.86(s, 1H), 7.13-7.19(m, 2H), 7.26(s, 1H), 7.36-7.37(d, 1H, *J*=7.5 Hz), 7.44-7.46(t, 4H, *J*=8.5 Hz), 7.57-7.61(m, 5H). **^{13}C NMR (**125 MHz, $CDCl_3$) δ ppm: 22.3, 64.9, 108.9, 111.0, 118.4, 119.7, 122.0, 127.0, 127.2, 127.5, 127.6, 128.8, 128.9, 133.6, 136.1, 138.4, 141.9. **HRMS (ESI$^+$):** calculated for $C_{23}H_{22}NO_2$, $[M+H]^+$ 344.1645, found 344.1639.



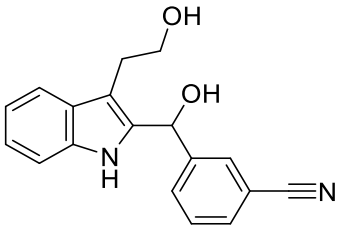
Name: 2-(2-(hydroxy(m-tolyl)methyl)-1H-indol-3-yl)ethan-1-ol

TLC: Petroleum ether/EtOAc = 15/1, R_f = 0.5, Yield: 91%, **^{1}H NMR (**500 MHz, $CDCl_3$) δ ppm: 2.28-2.29(t, 3H, *J* =8.5 Hz), 2.75-2.78(d, 1H, *J*=15.5 Hz), 3.02-3.08(m, 1H), 3.89-3.94(m, 1H), 4.25-4.28(m, 1H), 5.66-5.67(d, 1H, *J*=1.5 Hz), 7.09-7.13(m, 6H), 7.16-7.23(m, 1H), 7.45(s, 1H), 7.51(s, 1H). **^{13}C NMR (**125 MHz, $CDCl_3$) δ ppm: 21.5, 22.4, 64.9, 76.9, 77.2, 77.4, 108.7, 111.1, 118.4, 119.7, 121.9, 125.7, 127.1, 128.7, 129.1, 129.8, 133.8, 136.1, 138.7, 139.5. **HRMS (ESI$^+$):** calculated for $C_{18}H_{20}NO_2$, $[M+H]^+$ 282.1489, found 282.1481.



Name: 2-(2-((4-bromophenyl)(hydroxy)methyl)-1H-indol-3-yl)ethan-1-ol

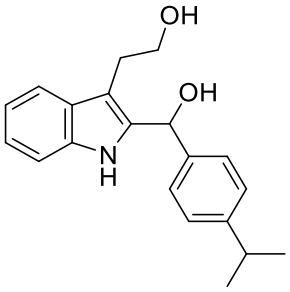
TLC: Petroleum ether/EtOAc = 15/1, R_f = 0.5, Yield: 85%, **^{1}H NMR (**500 MHz, $CDCl_3$) δ ppm: 2.80-2.83(m, 1H), 2.79-2.84(m, 1H), 3.04-3.10(m, 1H), 3.95-3.99(m, 1H), 3.99-4.10(d, 1H, *J*=56.5 Hz), 4.26-4.29(m, 1H), 5.74(s, 1H), 7.12-7.17(m, 2H), 7.22-7.24(q, 3H, , *J*=8.5 Hz), 7.44-7.53(m, 2H), 7.54-7.55(d, 1H, , *J*=7.5 Hz). **^{13}C NMR (**125 MHz, $CDCl_3$) δ ppm: 22.3, 64.8, 75.4, 109.0, 111.1, 118.4, 119.8, 122.2, 123.0, 126.9, 130.1, 131.9, 132.9, 136.1, 138.6. **HRMS (ESI$^+$):** calculated for $C_{17}H_{17}BrNO_2$, $[M+H]^+$ 346.0437, found 346.0428.



Name: 3-(hydroxy(3-(2-hydroxyethyl)-1H-indol-2-yl)methyl)benzonitrile

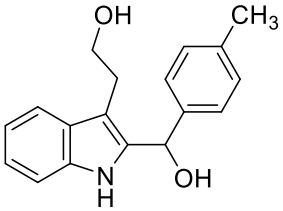
TLC: Petroleum ether/EtOAc = 10/1, R_f = 0.5, Yield: 86%, **^{1}H NMR (**500 MHz, $CDCl_3$) δ ppm: 2.84-2.88(m, 1H), 3.07-3.13(m, 1H), 3.97-4.01(m, 1H), 4.27-4.31(m, 1H), 5.84-5.85(t, 1H, *J*=3 Hz), 7.14-7.21(m, 1H), 7.26-7.29(m, 2H), 7.49-7.75(m, 1H), 7.56-7.58(d, 1H, *J*=8 Hz), 7.63-

7.69(m, 3H). **^{13}C NMR (**125 MHz, $CDCl_3$) δ ppm: 29.7, 64.8, 75.1, 109.5, 111.1, 113.0, 118.4, 118.6, 120.0, 122.5, 126.8, 129.7, 131.9, 132.0, 132.5, 132.7, 136.2, 141.3. **HRMS (ESI$^+$):** calculated for $C_{18}H_{17}N_2O_2$, $[M+H]^+$ 293.1285, found 293.1290.



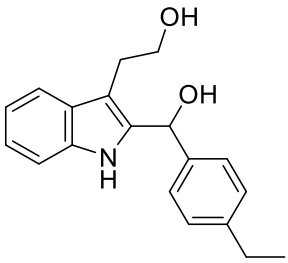
Name: 2-(2-(hydroxy(4-isopropylphenyl)methyl)-1H-indol-3-yl)ethan-1-ol

TLC: Petroleum ether/EtOAc = 15/1, R_f = 0.5, Yield: 90%, **^{1}H NMR (**500 MHz, $CDCl_3$) δ ppm: 1.24-1.2924(m, 6H), 1.54(s, 1H), 2.79-2.85(m, 1H), 2.89-2.94(m, 1H), 3.06-3.13(m, 1H), 3.96-4.00(m, 1H), 4.30-4.34(m, 1H), 5.77-5.78(d, 1H, *J*=3.5 Hz), 7.12-7.17(m, 2H), 7.22-7.29(m, 3H), 7.22-7.25(m, 2H), 7.54(s, 1H), 7.55-7.56(d, 1H, *J*=7 Hz). **^{13}C NMR (**125 MHz, $CDCl_3$) δ ppm: 22.4, 23.9, 23.9, 33.9, 64.9, 75.9, 108.9, 110.9, 118.3, 119.6, 121.9, 126.9, 127.1, 128.5, 133.8, 136.0, 136.8, 149.8. **HRMS (ESI$^+$):** calculated for $C_{20}H_{24}NO_2$, $[M+H]^+$ 310.1802, found 310.1796.



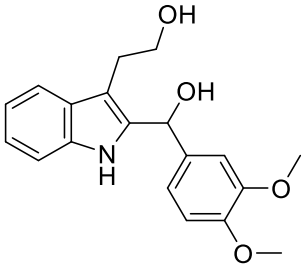
Name: 2-(2-(hydroxy(p-tolyl)methyl)-1H-indol-3-yl)ethan-1-ol

TLC: Petroleum ether/EtOAc = 15/1, R_f = 0.5, Yield: 93%, **^{1}H NMR (**500 MHz, $CDCl_3$) δ ppm: 2.33(s, 3H), 2.76-2.80(m, 1H), 3.04-3.05(m, 1H), 3.90-3.95(m, 1H), 4.24-4.27(m, 1H), 5.70(s, 1H), 7.09-7.12(m, 2H), 7.14-7.15(m, 3H), 7.20-7.22(m, 2H), 7.44(s, 1H), 7.52-7.53(m, 1H). **^{13}C NMR (**125 MHz, $CDCl_3$) δ ppm: 21.3, 22.4, 64.7, 76.9, 77.2, 77.4, 108.8, 111.1, 118.4, 119.7, 121.9, 127.1, 128.5, 129.5, 133.9, 136.1, 136.6, 138.8. **HRMS (ESI$^+$):** calculated for $C_{18}H_{20}NO_2$, $[M+H]^+$ 282.1489, found 282.1480.



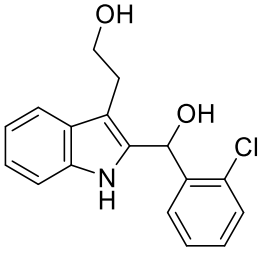
Name: 2-(2-((4-ethylphenyl)(hydroxy)methyl)-1H-indol-3-yl)ethan-1-ol

TLC: Petroleum ether/EtOAc = 15/1, R_f = 0.5, Yield: 92%, **^{1}H NMR (**500 MHz, $CDCl_3$) δ ppm: 1.21-1.24(t, 3H, *J*=15 Hz), 2.62-2.66(q, 2H, *J*=23 Hz), 2.78-2.81(m, 1H), 3.04-3.10(m, 1H), 3.92-3.97(m, 1H), 4.26-4.30(m, 1H), 5.73(s, 1H), 7.10-7.26(m, 7H), 7.53(s, 1H), 7.53-7.54(d, 1H, *J*=6.5 Hz). **^{13}C NMR (**125 MHz, $CDCl_3$) δ ppm: 15.6, 22.4, 28.7, 64.8, 75.9, 108.8, 111.0, 118.3, 119.6, 121.9, 127.1, 128.3, 128.6, 133.9, 136.0, 136.7, 145.2. **HRMS (ESI$^+$):** calculated for $C_{19}H_{22}NO_2$, $[M+H]^+$ 296.1645, found 296.1655.



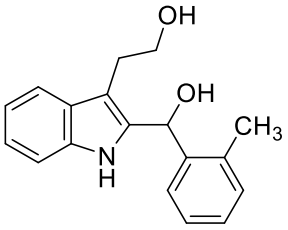
Name: 2-(2-((3,4-dimethoxyphenyl)(hydroxy)methyl)-1H-indol-3-yl)ethan-1-ol

TLC: Petroleum ether/EtOAc = 15/1, R_f = 0.5, Yield: 85%, **^{1}H NMR (**500 MHz, $CDCl_3$) δ ppm: 2.79-2.84(m, 1H), 3.08-3.15(m, 1H), 3.82(s, 3H), 3.89(s, 3H), 3.97-4.01(m, 1H), 4.31-4.37(m, 1H), 5.74-5.75(t, 1H, *J*=3.5 Hz), 6.85-6.88(q, 2H, *J*=16.5 Hz), 6.92-6.94(m, 1H), 7.13-7.17(m, 2H), 7.25-7.49(m, 2H), 7.55(s, 1H), 7.55-7.57(d,1H, *J*=7.5Hz). **^{13}C NMR (**125 MHz, $CDCl_3$) δ ppm: 22.3, 55.9, 55.9, 65.2, 76.2, 108.8, 110.9, 111.1, 111.2, 118.3, 119.7, 120.9, 121.9, 127.1, 131.9, 133.9, 136.0, 149.4, 149.6. **HRMS (ESI$^+$):** calculated for $C_{19}H_{22}NO_4$, $[M+H]^+$ 328.1543, found 328.1539.



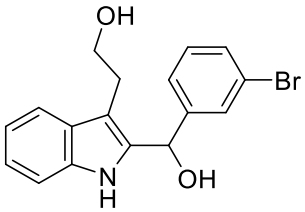
Name: 2-(2-((2-chlorophenyl)(hydroxy)methyl)-1H-indol-3-yl)ethan-1-ol

TLC: Petroleum ether/EtOAc = 11/1, R_f = 0.5, Yield: 88%, **^{1}H NMR (**500 MHz, $CDCl_3$) δ ppm: 2.81-2.86(m, 1H), 3.06-3.09(m, 1H), 3.99-4.04(m, 1H), 4.32-4.36(m, 1H), 6.34(s, 1H), 7.10-7.17(m, 2H), 7.20-7.29(m, 3H), 7.33-7.35(dd, 1H), 7.53-7.55(m, 1H), 7.64(s, 1H). **^{13}C NMR (**125 MHz, $CDCl_3$) δ ppm: 22.3, 64.9, 72.0, 108.9, 111.0, 118.3, 119.3, 122.1, 126.8, 127.4, 129.7, 129.8, 129.9, 132.9, 133.1, 135.9, 137.5. **HRMS (ESI$^+$):** calculated for $C_{17}H_{17}ClNO_2$, $[M+H]^+$ 302.0942, found 302.0931.



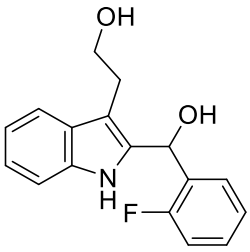
Name: 2-(2-(hydroxy(o-tolyl)methyl)-1H-indol-3-yl)ethan-1-ol

TLC: Petroleum ether/EtOAc = 15/1, R_f = 0.5, Yield: 86%, **^{1}H NMR (**500 MHz, $CDCl_3$) δ ppm: 2.40(s, 3H), 2.82-2.85(m, 1H), 3.03-3.05(m, 1H), 3.94-3.99(m, 1H), 4.24-4.27(m, 1H), 5.99-5.997(t, 1H, *J*=3.5 Hz), 7.12-7.15(m, 4H), 7.21-7.25(m, 3H), 7.47(s, 1H), 7.54-7.55(m, 1H). **^{13}C NMR (**125 MHz, $CDCl_3$) δ ppm: 19.0, 22.4, 64.6, 73.9,109.1, 111.0, 118.3, 119.7, 121.9, 126.1, 127.1, 128.9, 129.4, 131.2, 133.5, 136.0, 137.1, 137.7. **HRMS (ESI$^+$):** calculated for $C_{18}H_{20}NO_2$, $[M+H]^+$ 282.1489, found 282.1475.



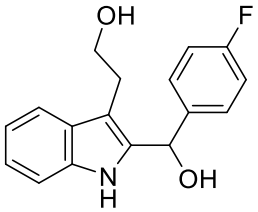
Name: 2-(2-((3-bromophenyl)(hydroxy)methyl)-1H-indol-3-yl)ethan-1-ol

TLC: Petroleum ether/EtOAc = 11/1, R_f = 0.5, Yield: 83%, **^{1}H NMR (**500 MHz, $CDCl_3$) δ ppm: 2.78-2.83(m, 1H), 3.04-3.10(m, 1H), 3.92-3.97(m, 1H), 3.94-3.99(m, 1H), 4.25-4.29(m, 1H), 5.71(s, 1H), 7.11-7.17(m, 2H), 7.21-7.24(t, 2H, *J*=15 Hz), 7.28-7.29(d, 1H, *J*=8 Hz), 7.47-7.50(m, 3H), 7.54-7.55(d, 1H, *J*=7.5 Hz). **^{13}C NMR (**125 MHz, $CDCl_3$) δ ppm: 22.3, 64.9, 75.4, 109.0, 111.1, 118.5, 119.8, 122.2, 122.9, 126.9, 127.1, 130.4, 131.4. 132.8, 136.2, 141.9. **HRMS (ESI$^+$):** calculated for $C_{17}H_{17}BrNO_2$, $[M+H]^+$ 346.0437, found 346.0440



Name: 2-(2-((2-fluorophenyl)(hydroxy)methyl)-1H-indol-3-yl)ethan-1-ol

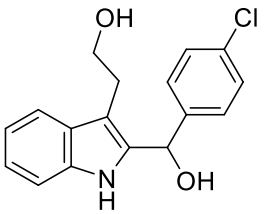
TLC: Petroleum ether/EtOAc = 10/1, R_f = 0.5, Yield: 81%, **^{1}H NMR (**500 MHz, $CDCl_3$) δ ppm: 2.81-2.85(m, 1H), 3.06-3.12(m, 1H), 3.96-4.01(m, 1H), 4.29-4.33(m, 1H), 5.79(s, 1H), 7.05-7.08(m, 2H), 7.12-7.19(m, 2H), 7.25-7.26(m, 2H), 7.34-7.37(m, 2H), 7.42(s, 1H), 7.55-7.56(d, 1H, *J*=7.5 Hz). **^{13}C NMR (**125 MHz, $CDCl_3$) δ ppm: 22.3, 64.9, 75.4, 109.1, 111.0, 115.7, 115.8, 118.4, 119.8, 122.1, 126.9, 130.3, 130.3, 133.3, 135.4, 135.4, 136.1. **HRMS (ESI$^+$):** calculated for $C_{17}H_{17}FNO_2$, $[M+H]^+$ 286.1238, found 286.1245.



Name: 2-(2-((4-fluorophenyl)(hydroxy)methyl)-1H-indol-3-yl)ethan-1-ol

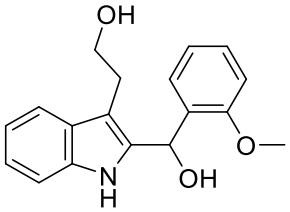
TLC: Petroleum ether/EtOAc = 10/1, R_f = 0.5, Yield: 86%, **^{1}H NMR (**500 MHz, $CDCl_3$) δ ppm: 2.79-2.84(m, 1H), 3.05-3.11(m, 1H), 3.94-3.99(m, 1H), 4.27-4.31(m, 1H), 5.77(s, 1H), 7.03-7.07(m, 2H), 7.11-7.18(m, 2H), 7.23-7.24(m, 1H), 7.31-7.35(m, 2H), 7.43(s, 1H), 7.54-7.56(d, 1H, *J*=7.5 Hz). **^{13}C NMR (**125 MHz, $CDCl_3$) δ ppm: 22.3, 64.9, 75.4, 109.0, 111.0, 115.7, 115.8, 118.4, 119.8, 122.1, 126.9, 130.3, 130.4, 133.3, 135.4, 135.4, 136.1. **HRMS (ESI$^+$):** calculated for $C_{17}H_{17}FNO_2$, $[M+H]^+$ 286.1238, found 286.1240.

The signal at δ_C 164.06-162.09 ppm (d, $^1J_{C\text{-}F}$ = 246.25 Hz) corresponds to the CF carbon, the signal at δ_C 115.83, 115.66 (d, $^2J_{C\text{-}F}$ = 21.25 Hz) corresponds to the adjacent CH carbon.



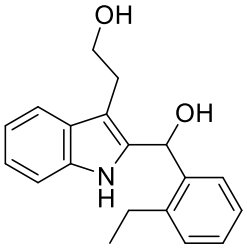
Name: 2-(2-((4-chlorophenyl)(hydroxy)methyl)-1H-indol-3-yl)ethan-1-ol

TLC: Petroleum ether/EtOAc = 15/1, R_f = 0.5, Yield: 82%, **^{1}H NMR (**500 MHz, $CDCl_3$) δ ppm: 2.33(s, 3H), 2.76-2.81(m, 1H), 3.02-3.08(m, 1H), 3.90-3.95(m, 1H), 4.24-4.28(m, 1H), 5.70(s, 1H), 7.09-7.16(m, 5H), 7.20-7.22(d, 2H, *J*=8 Hz), 7.52(s, 1H), 7.53-7.534(d, 1H, *J*=3 Hz). **^{13}C NMR (**125 MHz, $CDCl_3$) δ ppm: 21.2, 22.3, 64.6, 75.9, 108.7, 110.9, 118.3, 119.6, 121.8, 127.0, 128.4, 129.4, 133.8, 135.9, 136.5, 138.7. **HRMS (ESI$^+$):** calculated for $C_{17}H_{17}ClNO_2$, $[M+H]^+$ 302.0942, found 302.0937.



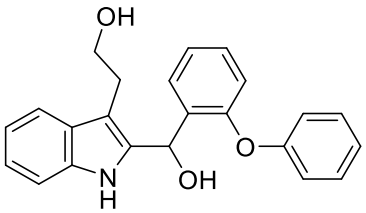
Name: 2-(2-(hydroxy(2-methoxyphenyl)methyl)-1H-indol-3-yl)ethan-1-ol

TLC: Petroleum ether/EtOAc = 15/1, R_f = 0.5, Yield: 84%, **^{1}H NMR (**500 MHz, $CDCl_3$) δ ppm: 2.76-2.81(m, 1H), 3.01-3.06(m, 1H), 3.94(s, 3H), 3.95-4.00(m, 1H), 4.31-4.34(m, 1H), 6.28(s, 1H), 6.90-6.92(t, 1H, *J*=14.5 Hz), 6.96-6.98(d, 1H, *J*=8 Hz), 7.06-7.11(m, 2H), 7.12-7.20(dd, 1H), 7.28-7.31(m, 2H), 7.50-7.52(t, 1H, *J*=8.5 Hz), 7.88(s, 1H). **^{13}C NMR (**125 MHz, $CDCl_3$) δ ppm: 22.4, 55.7, 64.8, 69.3, 108.1, 110.9, 118.1, 119.3, 121.1, 121.6, 126.9, 128.5, 128.5, 129.3, 134.2, 135.7. **HRMS (ESI$^+$):** calculated for $C_{18}H_{20}NO_3$, $[M+H]^+$ 298.1438, found 298.1440



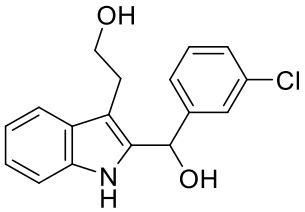
Name: 2-(2-((2-ethylphenyl)(hydroxy)methyl)-1H-indol-3-yl)ethan-1-ol

TLC: Petroleum ether/EtOAc = 15/1, R_f = 0.5, Yield: 86%, **^{1}H NMR (**500 MHz, $CDCl_3$) δ ppm: 1.20-1.23(m, 3H), 2.75-2.81(m, 3H), 2.96-2.99(m, 3H), 3.85-3.89(m, 1H), 4.15-4.17(m, 1H), 5.97(s, 1H), 7.01-7.06(m, 5H), 7.23-7.24(t, 2H, *J*=5 Hz), 7.47-7.50(m, 2H). **^{13}C NMR (**125 MHz, $CDCl_3$) δ ppm: 16.2, 22.5, 25.6, 64.5, 73.1, 76.1, 109.2, 111.2, 118.4, 119.7, 121.9, 126.2, 127.2, 129.2, 129.5, 129.7, 133.9, 136.2, 136.7, 143.9. **HRMS (ESI$^+$):** calculated for $C_{19}H_{22}NO_2$, $[M+H]^+$ 296.1645, found 296.1439.



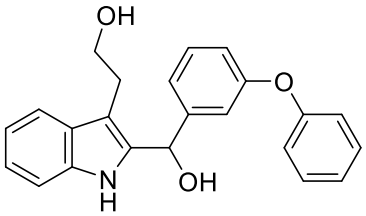
Name: 2-(2-(hydroxy(2-phenoxyphenyl)methyl)-1H-indol-3-yl)ethan-1-ol

TLC: Petroleum ether/EtOAc = 15/1, R_f = 0.5, Yield: 85%, **^{1}H NMR (**500 MHz, $CDCl_3$) δ ppm: 2.72-2.77(m, 1H), 3.89-3.94(m, 1H), 4.31-4.35(m, 1H), 6.22(s, 1H), 6.99-7.13(m, 8H), 7.20-7.27(m, 2H), 7.31-7.34(m, 2H), 7.46-7.51(m, 2H), 7.98(s, 1H). **^{13}C NMR (**125 MHz, $CDCl_3$) δ ppm: 22.4, 65.2, 69.8, 108.3, 111.1, 118.0, 118.3, 119.6, 119.7, 121.9, 123.4, 124.6, 126.9, 129.1, 129.6, 130.0, 131.9, 133.9, 135.9. **HRMS (ESI$^+$):** calculated for $C_{23}H_{22}NO_3$, $[M+H]^+$ 360.1594, found 360.1601.



Name: 2-(2-((3-chlorophenyl)(hydroxy)methyl)-1H-indol-3-yl)ethan-1-ol

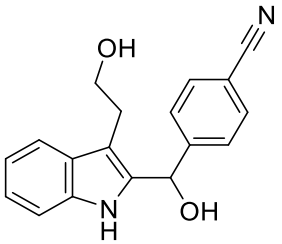
TLC: Petroleum ether/EtOAc = 10/1, R_f = 0.5, Yield: 86%, **^{1}H NMR (**500 MHz, $CDCl_3$) δ ppm: 2.79-2.84(m, 1H), 3.05-3.11(m, 1H), 3.93-3.98(m, 1H), 4.27-4.31(s, 1H), 7.11-7.18(m, 2H), 7.22-7.26(m, 2H), 7.28-7.30(d, 1H, *J*=7.5 Hz), 7.31-7.36(m, 2H), 7.46(s, 1H), 7.54-7.57(m, 1H). **^{13}C NMR (**125 MHz, $CDCl_3$) δ ppm: 22.2, 64.9, 75.5, 109.0, 111.1, 118.5, 119.8, 122.2, 126.5, 126.9, 128.5, 129.1, 130.1, 132.8, 134.8, 136.1, 141.6. **HRMS (ESI$^+$):** calculated for $C_{17}H_{17}ClNO_2$, $[M+H]^+$ 302.0942, found 302.0947.



Name: 2-(2-(hydroxy(3-phenoxyphenyl)methyl)-1H-indol-3-yl)ethan-1-ol

TLC: Petroleum ether/EtOAc = 15/1, R_f = 0.5, Yield: 85%, **^{1}H NMR (**500 MHz, $CDCl_3$) δ ppm: 2.79-2.84(m, 1H), 3.06-3.12(m, 1H), 3.96-4.01(m, 1H), 4.32-4.36(m, 1H), 5.77-5.774(d, 1H, *J*=1.5 Hz), 6.97-7.02(m, 3H), 7.09-7.18(m, 5H), 7.26-7.27(q, 3H, *J*=9 Hz), 7.32-7.35(m, 3H),

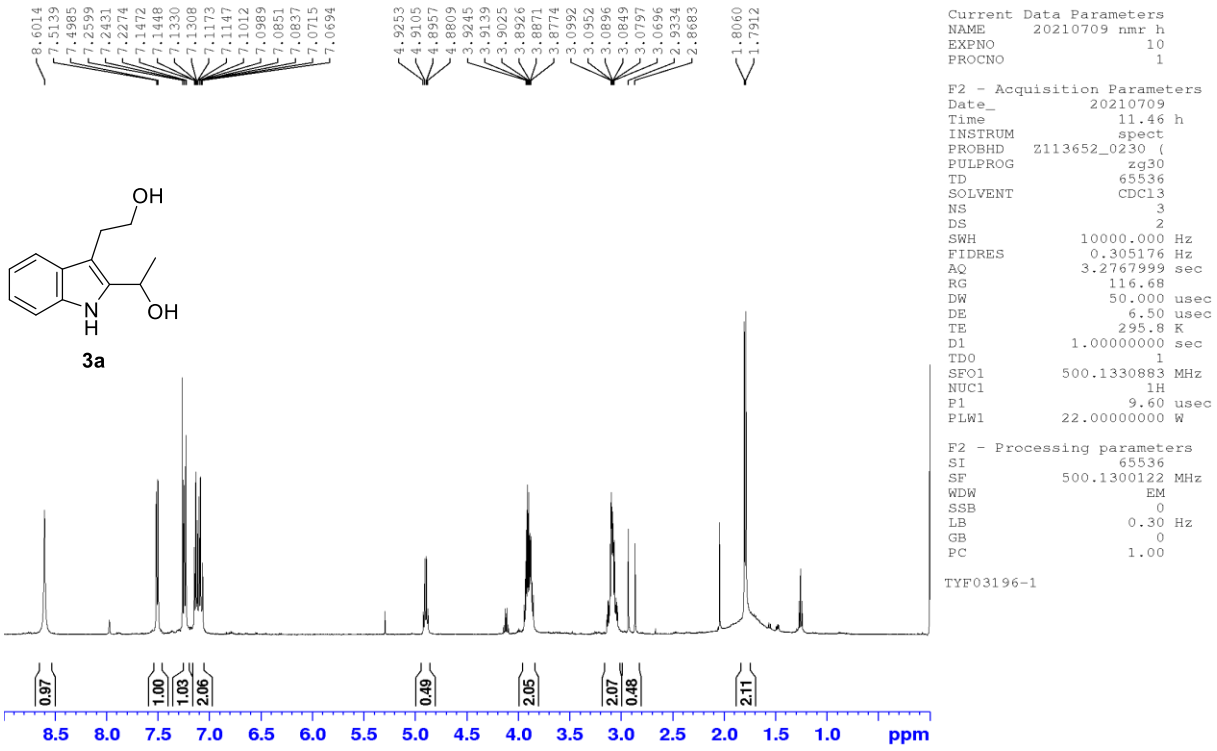
7.47(s, 1H), 7.54-7.55(d, 1H, *J*=7.5 Hz). **^{13}C NMR (**125 MHz, $CDCl_3$) δ ppm: 22.3, 65.0, 75.8, 108.8, 110.0, 118.4, 118.9, 119.0, 119.7, 122.1, 123.5, 127.0, 129.8, 130.1, 133.3, 136.1, 141.6. **HRMS (ESI$^+$):** calculated for $C_{23}H_{22}NO_2$, $[M+H]^+$ 360.1594, found 360.1589.



Name: 4-(hydroxy(3-(2-hydroxyethyl)-1H-indol-2-yl)methyl)benzonitrile

TLC: Petroleum ether/EtOAc = 13/1, R_f = 0.5, Yield: 89%, **^{1}H NMR (**500 MHz, $CDCl_3$) δ ppm:2.82-2.87(m, 1H), 3.06-3.12(m, 1H), 3.96-4.01(m, 1H), 4.27-4.31(m, 1H), 5.85(S, 1H), 7.12-7.20(m, 2H), 7.25-7.27(d, 1H, *J*=7.5 Hz), 7.50-7.51(d, 3H, *J*=8.5 Hz), 7.56-7.57(d, 1H, *J*=2.5 Hz), 7.65-7.67(d, 2H, *J*=8 Hz). **^{13}C NMR (**125 MHz, $CDCl_3$) δ ppm: 22.2, 29.7, 64.9, 75.3, 109.3, 111.1, 112.7, 118.5, 118.5, 119.9, 122.5, 126.8, 129.0, 132.1, 132.7, 136.2, 144.8. **HRMS (ESI$^+$):** calculated for $C_{18}H_{17}N_2O_3$, $[M+H]^+$ 293.1285, found 293.1280.

^{1}H-NMR (500 MHz, $CDCl_3$)

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Current Data Parameters
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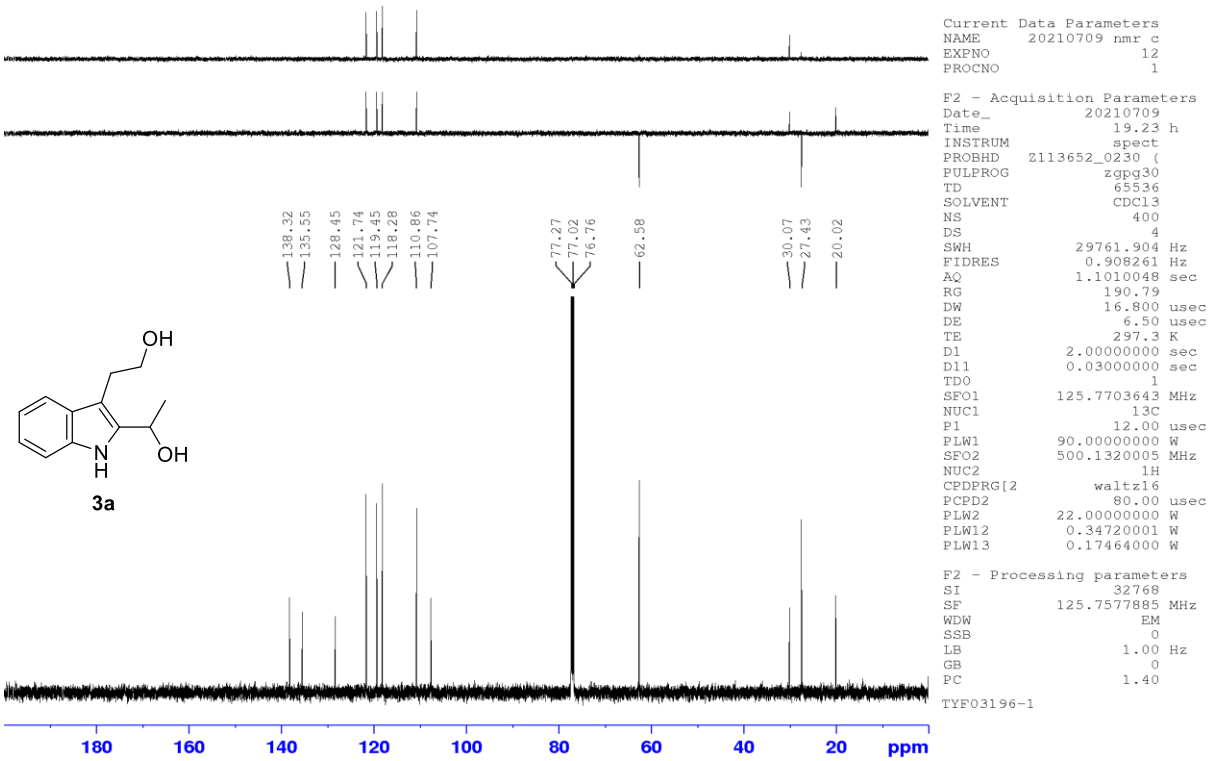
EXPNO               10
PROCNO               1

F2 - Acquisition Parameters
Date_          20210709
Time             11.46 h
INSTRUM          spect
PROBHD   Z113652_0230 (
PULPROG          zg30
TD              65536
SOLVENT          CDCl3
NS                   3
DS                   2
SWH          10000.000 Hz
FIDRES           0.305176 Hz
AQ           3.2767999 sec
RG              116.68
DW               50.000 usec
DE                6.50 usec
TE              295.8 K
D1           1.00000000 sec
TD0                  1
SFO1         500.1330883 MHz
NUC1                 1H
P1                9.60 usec
PLW1        22.00000000 W

F2 - Processing parameters
SI                65536
SF           500.1300122 MHz
WDW                  EM
SSB                  0
LB                0.30 Hz
GB                   0
PC                1.00

TYF03196-1
```

^{13}C-NMR (125 MHz, $CDCl_3$)

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Current Data Parameters
NAME      20210709 nmr c
EXPNO               12
PROCNO               1

F2 - Acquisition Parameters
Date_          20210709
Time             19.23 h
INSTRUM          spect
PROBHD   Z113652_0230 (
PULPROG         zgpg30
TD              65536
SOLVENT          CDCl3
NS                 400
DS                   4
SWH          29761.904 Hz
FIDRES           0.908261 Hz
AQ           1.1010048 sec
RG              190.79
DW               16.800 usec
DE                6.50 usec
TE              297.3 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1
SFO1         125.7703643 MHz
NUC1                13C
P1               12.00 usec
PLW1        90.00000000 W
SFO2         500.1320005 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2            80.00 usec
PLW2        22.00000000 W
PLW12        0.34720001 W
PLW13        0.17464000 W

F2 - Processing parameters
SI                32768
SF           125.7577885 MHz
WDW                  EM
SSB                  0
LB                1.00 Hz
GB                   0
PC                1.40

TYF03196-1
```
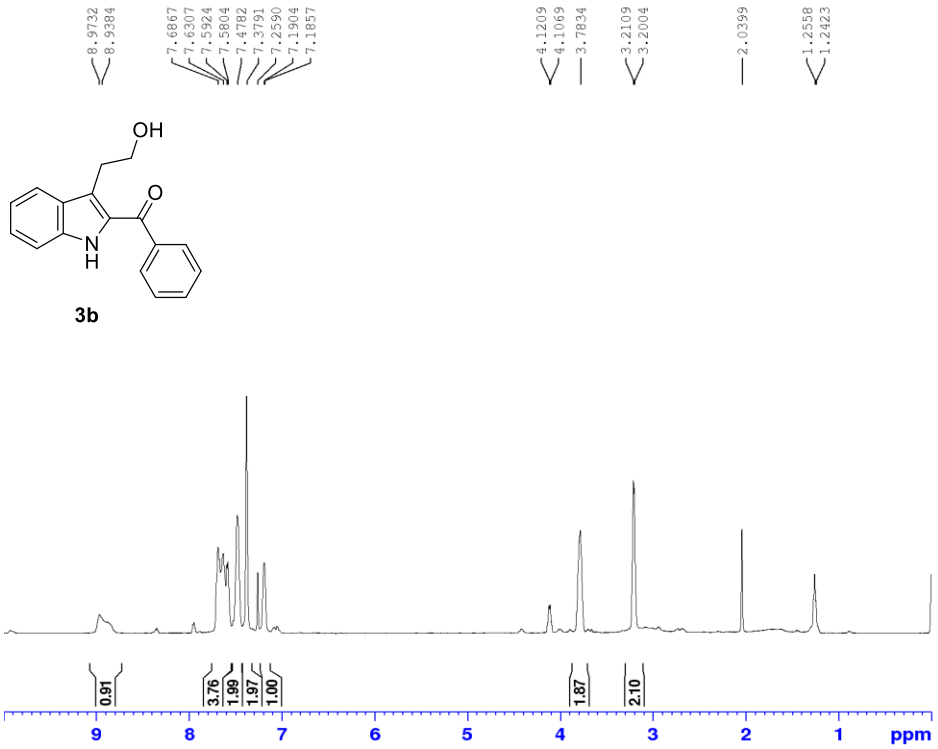

H-NMR (500 MHz, $CDCl_3$)

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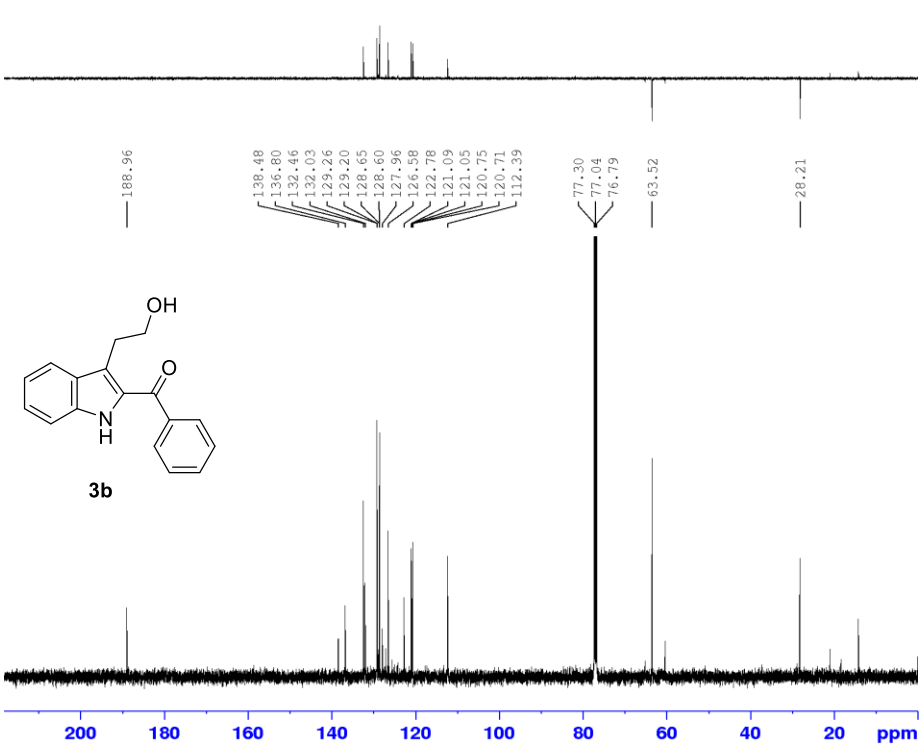
Current Data Parameters
NAME      20211203-1 nmr h
EXPNO                 70
PROCNO                 1

F2 - Acquisition Parameters
Date_           20211203
Time              14.57 h
INSTRUM             spect
PROBHD   Z113652_0230 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     3
DS                     2
SWH            10000.000 Hz
FIDRES             0.305176 Hz
AQ              3.2767999 sec
RG                 95.16
DW                 50.000 usec
DE                 13.89 usec
TE                 294.5 K
D1              1.00000000 sec
TD0                    1
SFO1           500.1330883 MHz
NUC1                  1H
P0                  3.33 usec
P1                 10.00 usec
PLW1           25.23200035 W

F2 - Processing parameters
SI                 65536
SF            500.1300127 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00

YX01107-1
```

^{13}C-NMR (150 MHz, $CDCl_3$)

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Current Data Parameters
NAME      20211203 nm c
EXPNO                 70
PROCNO                 1

F2 - Acquisition Parameters
Date_           20211203
Time              16.52 h
INSTRUM             spect
PROBHD   Z113652_0230 (
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   324
DS                     4
SWH            29761.904 Hz
FIDRES             0.908261 Hz
AQ              1.1010048 sec
RG                 190.79
DW                 16.800 usec
DE                  6.50 usec
TE                 296.0 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                    1
SFO1           125.7703643 MHz
NUC1                  13C
P0                  3.33 usec
P1                 10.00 usec
PLW1           102.87999725 W
SFO2           500.1320005 MHz
NUC2                  1H
CPDPRG[2          waltz65
PCPD2              80.00 usec
PLW2           25.23200035 W
PLW12           0.39425001 W
PLW13           0.19831000 W

F2 - Processing parameters
SI                 32768
SF            125.7577885 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40

YX01107-1
```
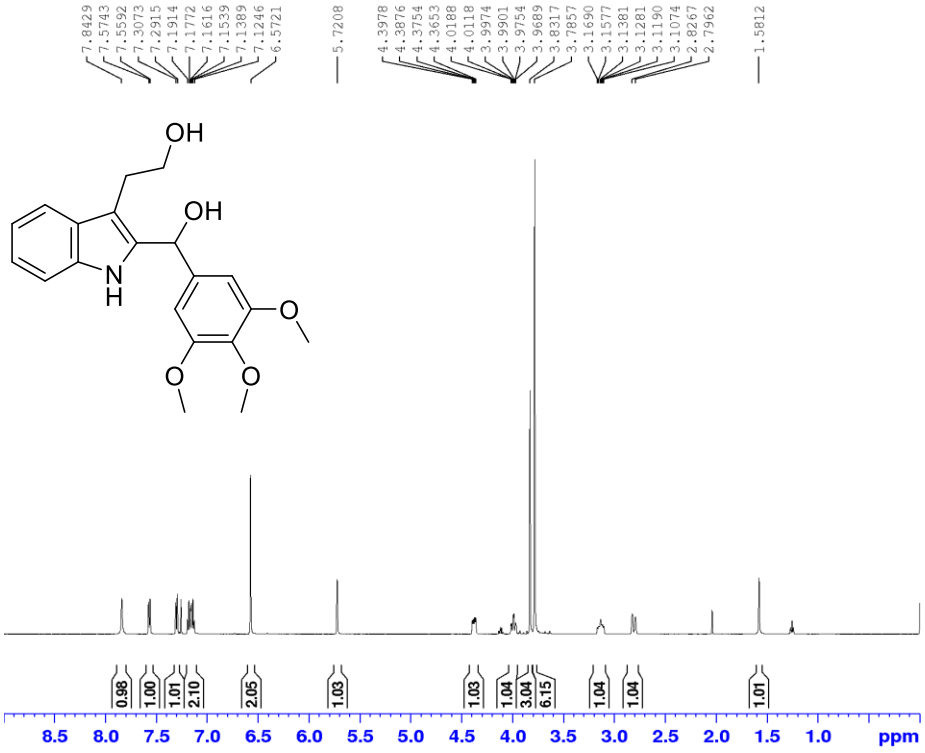

^{1}H-NMR (500 MHz, $CDCl_3$)

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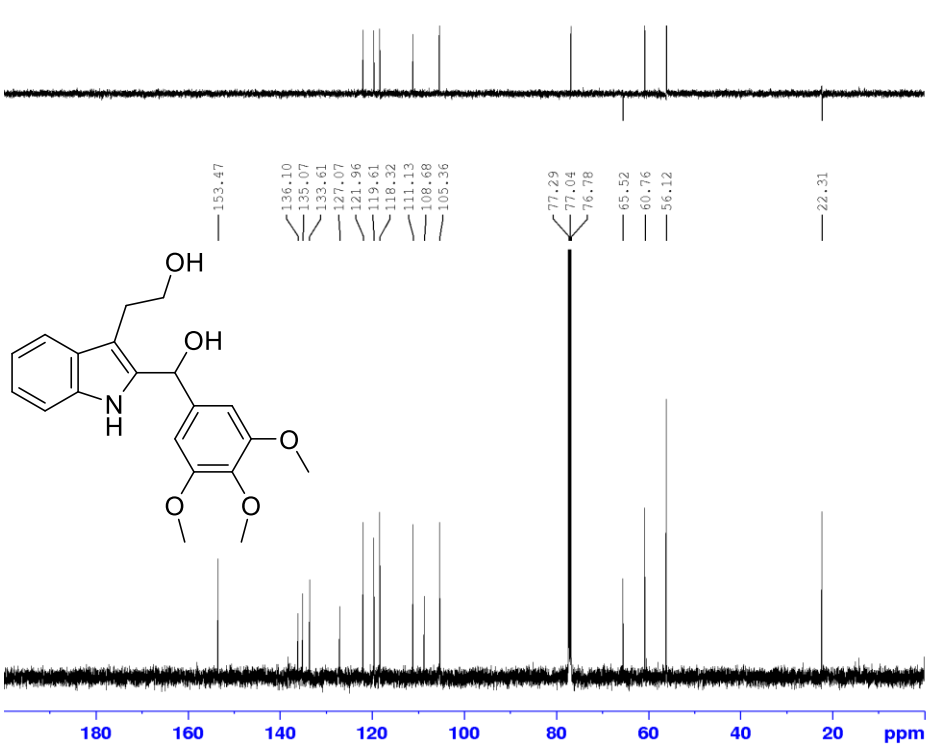
Current Data Parameters
NAME      20220420 hnm h
EXPNO                70
PROCNO                1

F2 - Acquisition Parameters
Date_          20220420
Time             16.38 h
INSTRUM           spect
PROBHD   Z113652_0230 (
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                   3
DS                   2
SWH          10000.000 Hz
FIDRES           0.305176 Hz
AQ             3.2767999 sec
RG                116.68
DW                50.000 usec
DE                13.89 usec
TE                296.2 K
D1           1.00000000 sec
TD0                  1
SFO1         500.1330883 MHz
NUC1                 1H
P0                3.33 usec
P1               10.00 usec
PLW1         25.23200035 W

F2 - Processing parameters
SI                65536
SF           500.1300142 MHz
WDW                  EM
SSB                  0
LB                0.30 Hz
GB                   0
PC                1.00

YX01129-1
```

^{13}C-NMR (150 MHz, $CDCl_3$)

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Current Data Parameters
NAME      20220421 nmr c
EXPNO                21
PROCNO                1

F2 - Acquisition Parameters
Date_          20220421
Time             16.48 h
INSTRUM           spect
PROBHD   Z113652_0230 (
PULPROG          zgpg30
TD               65536
SOLVENT          CDCl3
NS                 132
DS                   4
SWH          29761.904 Hz
FIDRES           0.908261 Hz
AQ             1.1010048 sec
RG                190.79
DW                16.800 usec
DE                 6.50 usec
TE                296.5 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1
SFO1         125.7703643 MHz
NUC1                 13C
P0                3.33 usec
P1               10.00 usec
PLW1        102.87999725 W
SFO2         500.1320005 MHz
NUC2                 1H
CPDPRG[2         waltz65
PCPD2             80.00 usec
PLW2         25.23200035 W
PLW12         0.39425001 W
PLW13         0.19831000 W

F2 - Processing parameters
SI                32768
SF           125.7577885 MHz
WDW                  EM
SSB                  0
LB                1.00 Hz
GB                   0
PC                1.40

YX01129-1
```
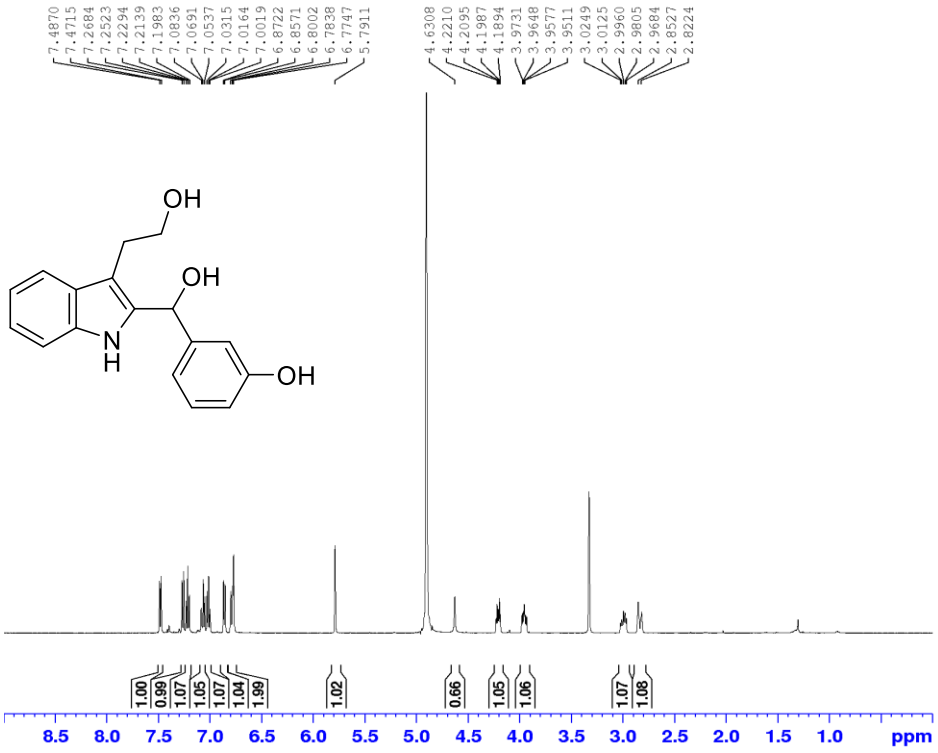

^{1}H-NMR (500 MHz, MeOD)

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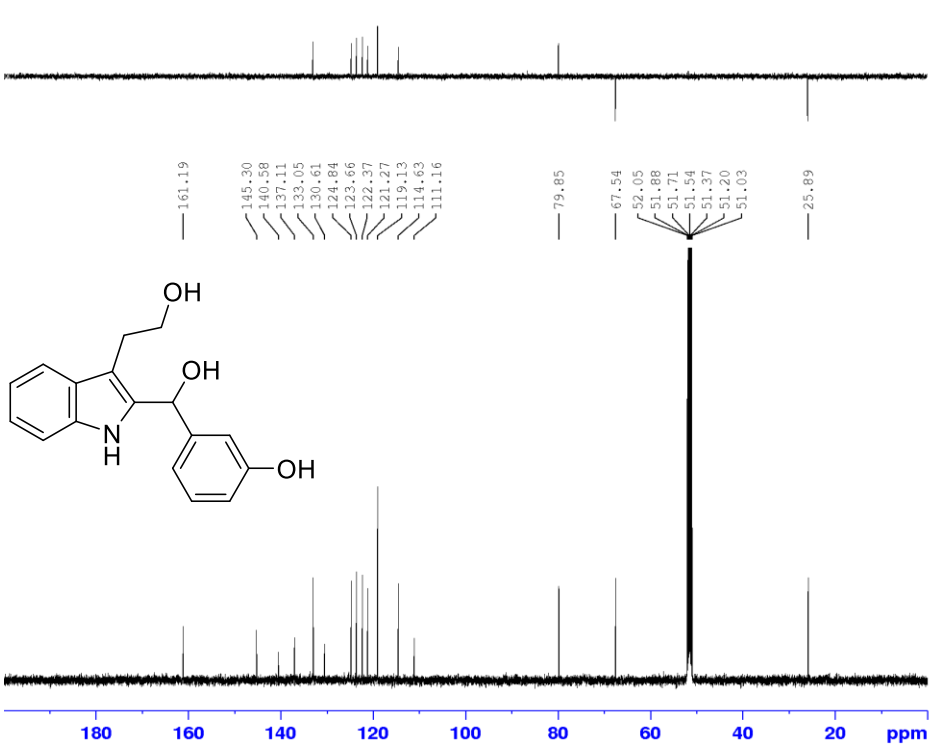
Current Data Parameters
NAME      20220420 hnm h
EXPNO                100
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220420
Time              16.49 h
INSTRUM            spect
PROBHD   Z113652_0230 (
PULPROG             zg30
TD                 65536
SOLVENT             MeOD
NS                     3
DS                     2
SWH            10000.000 Hz
FIDRES         0.305176 Hz
AQ             3.2767999 sec
RG                108.03
DW                50.000 usec
DE                13.89 usec
TE                296.0 K
D1            1.00000000 sec
TD0                    1
SFO1          500.1330883 MHz
NUC1                  1H
P0                  3.33 usec
P1                 10.00 usec
PLW1          25.23200035 W

F2 - Processing parameters
SI                 65536
SF            500.1300000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00

YX01131-1
```

^{13}C-NMR (125 MHz, MeOD)

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Current Data Parameters
NAME      20220421 nmr c
EXPNO                 71
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220421
Time              19.48 h
INSTRUM            spect
PROBHD   Z113652_0230 (
PULPROG           zgpg30
TD                 65536
SOLVENT             CDCl3
NS                   420
DS                     4
SWH            29761.904 Hz
FIDRES         0.908261 Hz
AQ             1.1010048 sec
RG                190.79
DW                16.800 usec
DE                 6.50 usec
TE                296.9 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1
SFO1          125.7703643 MHz
NUC1                  13C
P0                  3.33 usec
P1                 10.00 usec
PLW1         102.87999725 W
SFO2          500.1320005 MHz
NUC2                  1H
CPDPRG[2          waltz65
PCPD2              80.00 usec
PLW2          25.23200035 W
PLW12          0.39425001 W
PLW13          0.19831000 W

F2 - Processing parameters
SI                 32768
SF            125.7577885 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40

YX01131-1
```
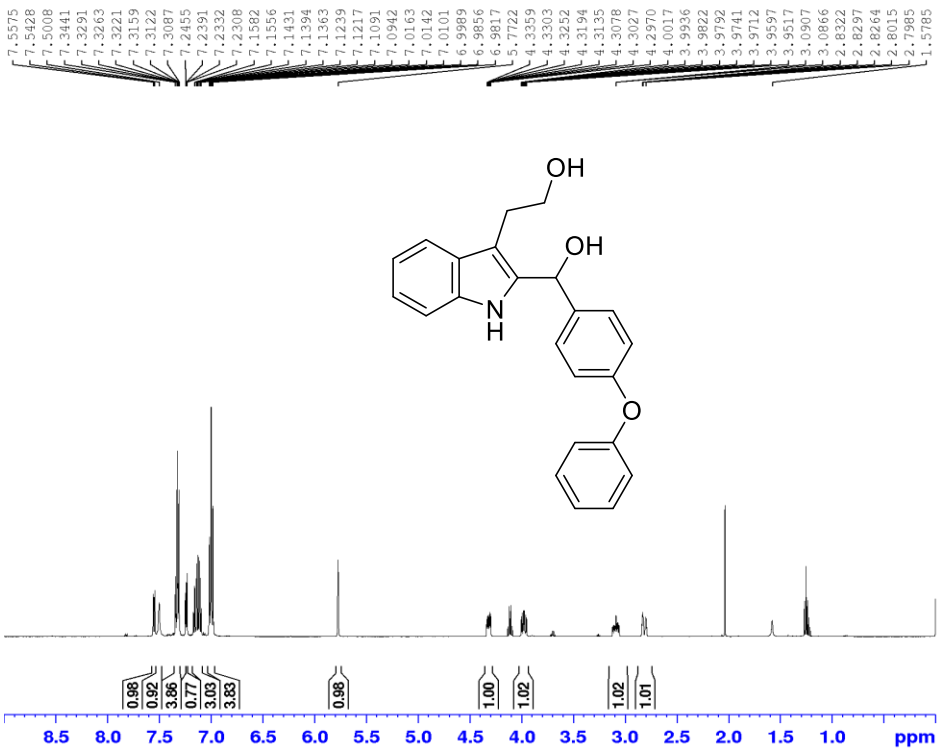
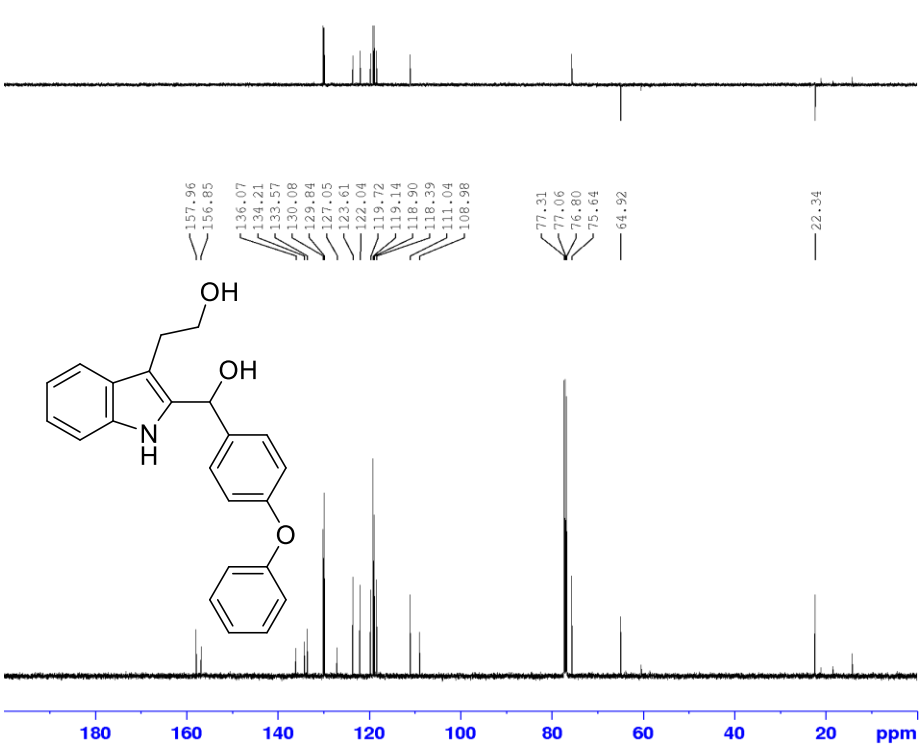

^{1}H-NMR (500 MHz, $CDCl_3$)



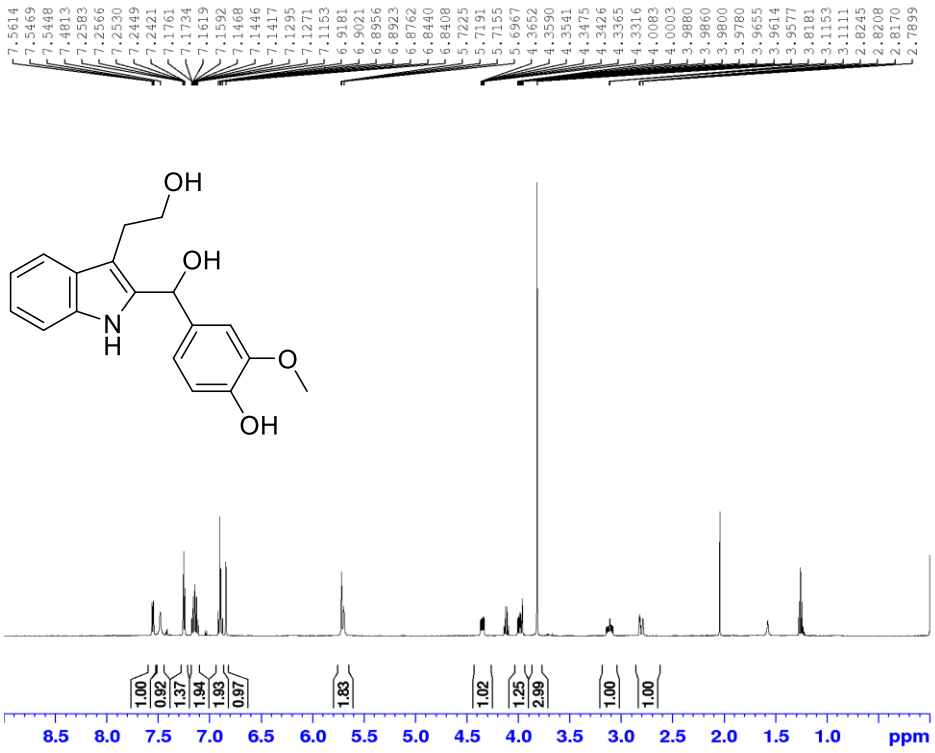

```
Current Data Parameters
NAME      20220505 nmr h
EXPNO                10
PROCNO                1

F2 - Acquisition Parameters
Date_          20220505
Time              17.49 h
INSTRUM           spect
PROBHD    Z113652_0230 (
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                   3
DS                   2
SWH          10000.000 Hz
FIDRES           0.305176 Hz
AQ           3.2767999 sec
RG                76.76
DW                50.000 usec
DE                13.89 usec
TE                295.5 K
D1           1.00000000 sec
TD0                  1
SFO1         500.1330883 MHz
NUC1                 1H
P0                3.33 usec
P1               10.00 usec
PLW1         25.23200035 W

F2 - Processing parameters
SI                65536
SF           500.1300225 MHz
WDW                  EM
SSB                  0
LB                0.30 Hz
GB                   0
PC                1.00

YX01135-1
```

^{13}C-NMR (125 MHz, $CDCl_3$)



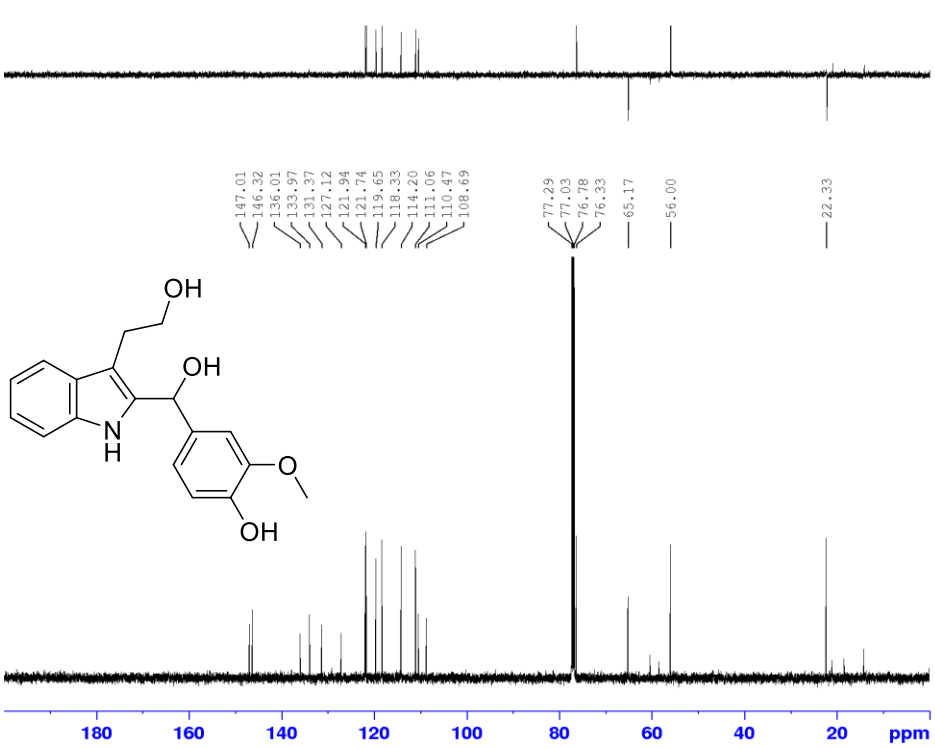

```
Current Data Parameters
NAME      20220505 nmr c
EXPNO                12
PROCNO                1

F2 - Acquisition Parameters
Date_          20220507
Time              2.16 h
INSTRUM           spect
PROBHD    Z113652_0230 (
PULPROG          zgpg30
TD               65536
SOLVENT          CDCl3
NS                 110
DS                   4
SWH          29761.904 Hz
FIDRES           0.908261 Hz
AQ           1.1010048 sec
RG                190.79
DW                16.800 usec
DE                 6.50 usec
TE                296.6 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1
SFO1         125.7703643 MHz
NUC1                 13C
P0                3.33 usec
P1               10.00 usec
PLW1        102.87999725 W
SFO2         500.1320005 MHz
NUC2                 1H
CPDPRG[2          waltz65
PCPD2             80.00 usec
PLW2         25.23200035 W
PLW12         0.39425001 W
PLW13         0.19831000 W

F2 - Processing parameters
SI                32768
SF           125.7577885 MHz
WDW                  EM
SSB                  0
LB                1.00 Hz
GB                   0
PC                1.40

YX01135-1
```

^{1}H-NMR (500 MHz, $CDCl_3$)




```
Current Data Parameters
NAME      20220505 nmr h
EXPNO                20
PROCNO                1

F2 - Acquisition Parameters
Date_          20220505
Time              17.53 h
INSTRUM           spect
PROBHD   Z113652_0230 (
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                   3
DS                   2
SWH          10000.000 Hz
FIDRES           0.305176 Hz
AQ             3.2767999 sec
RG               116.68
DW                50.000 usec
DE                13.89 usec
TE                295.5 K
D1            1.00000000 sec
TD0                  1
SFO1         500.1330883 MHz
NUC1                 1H
P0                3.33 usec
P1               10.00 usec
PLW1         25.23200035 W

F2 - Processing parameters
SI                65536
SF           500.1300156 MHz
WDW                  EM
SSB                  0
LB                0.30 Hz
GB                   0
PC                1.00

YX01138-1
```

^{13}C-NMR (125 MHz, $CDCl_3$)

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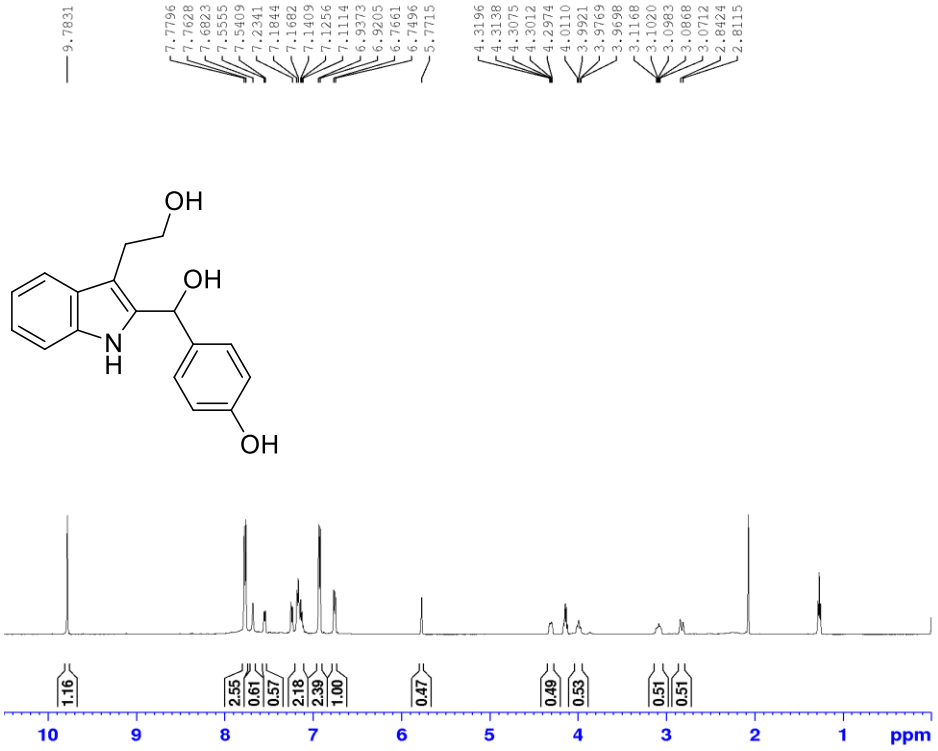
Current Data Parameters
NAME      20220505 nmr c
EXPNO                22
PROCNO                1

F2 - Acquisition Parameters
Date_          20220507
Time              2.30 h
INSTRUM           spect
PROBHD   Z113652_0230 (
PULPROG          zgpg30
TD               65536
SOLVENT          CDCl3
NS                 180
DS                   4
SWH          29761.904 Hz
FIDRES           0.908261 Hz
AQ             1.1010048 sec
RG               190.79
DW                16.800 usec
DE                 6.50 usec
TE                296.7 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                  1
SFO1         125.7703643 MHz
NUC1                13C
P0                3.33 usec
P1               10.00 usec
PLW1        102.87999725 W
SFO2         500.1320005 MHz
NUC2                 1H
CPDPRG[2         waltz65
PCPD2             80.00 usec
PLW2         25.23200035 W
PLW12         0.39425001 W
PLW13         0.19831000 W

F2 - Processing parameters
SI                32768
SF           125.7577885 MHz
WDW                  EM
SSB                  0
LB                1.00 Hz
GB                   0
PC                1.40

YX01138-1
```

^{1}H-NMR (500 MHz, $CDCl_3$)



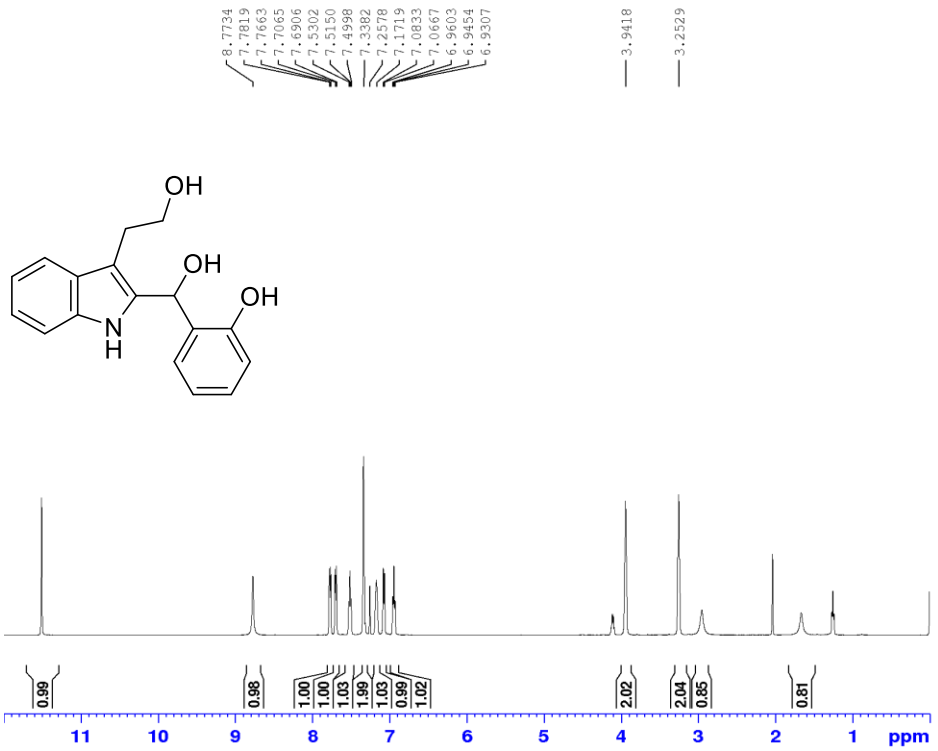

```
Current Data Parameters
NAME      20211223 nmr h
EXPNO                80
PROCNO                1

F2 - Acquisition Parameters
Date_          20211223
Time              17.40 h
INSTRUM           spect
PROBHD   Z113652_0230 (
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                   3
DS                   2
SWH          10000.000 Hz
FIDRES           0.305176 Hz
AQ           3.2767999 sec
RG                69.86
DW               50.000 usec
DE               13.89 usec
TE               294.7 K
D1           1.00000000 sec
TD0                  1
SFO1         500.1330883 MHz
NUC1                 1H
P0                3.33 usec
P1               10.00 usec
PLW1        25.23200035 W

F2 - Processing parameters
SI                65536
SF           500.1300165 MHz
WDW                  EM
SSB                  0
LB                0.30 Hz
GB                   0
PC                1.00

YX01116-1
```

^{1}H-NMR (500 MHz, $CDCl_3$)



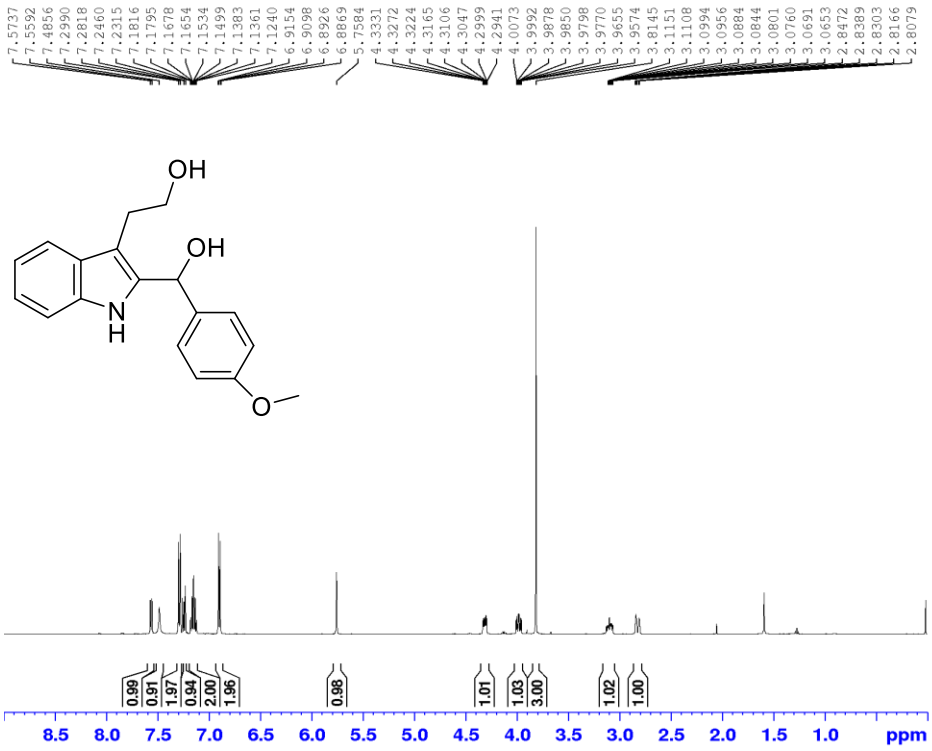

```
Current Data Parameters
NAME      20211209 nmr h
EXPNO                20
PROCNO                1

F2 - Acquisition Parameters
Date_          20211209
Time              10.39 h
INSTRUM           spect
PROBHD   Z113652_0230 (
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                   3
DS                   2
SWH          10000.000 Hz
FIDRES           0.305176 Hz
AQ           3.2767999 sec
RG                108.03
DW               50.000 usec
DE               13.89 usec
TE               295.2 K
D1           1.00000000 sec
TD0                  1
SFO1         500.1330883 MHz
NUC1                 1H
P0                3.33 usec
P1               10.00 usec
PLW1        25.23200035 W

F2 - Processing parameters
SI                65536
SF           500.1300141 MHz
WDW                  EM
SSB                  0
LB                0.30 Hz
GB                   0
PC                1.00

YX01110-2
```

^{1}H-NMR (500 MHz, $CDCl_3$)



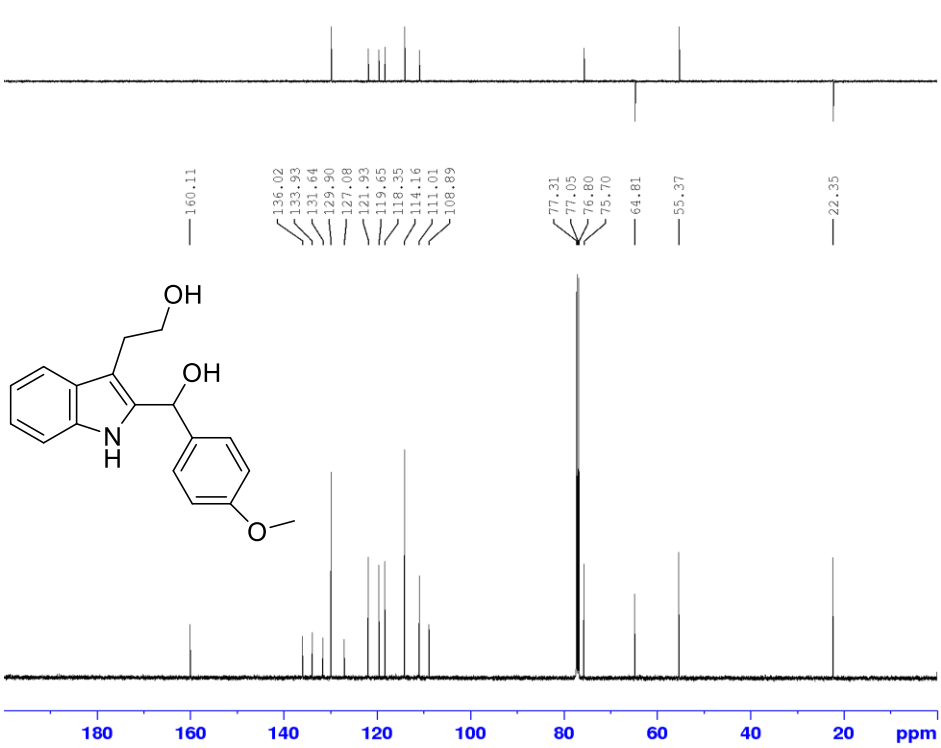

```
Current Data Parameters
NAME      20220407 nmr h
EXPNO                20
PROCNO                1

F2 - Acquisition Parameters
Date_           20220407
Time              16.13 h
INSTRUM           spect
PROBHD   Z113652_0230 (
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                   2
DS                   2
SWH           10000.000 Hz
FIDRES        0.305176 Hz
AQ            3.2767999 sec
RG                95.16
DW               50.000 usec
DE               13.89 usec
TE               293.3 K
D1           1.00000000 sec
TD0                  1
SFO1         500.1330883 MHz
NUC1                 1H
P0                3.33 usec
P1               10.00 usec
PLW1         25.23200035 W

F2 - Processing parameters
SI               65536
SF           500.1300124 MHz
WDW                 EM
SSB                  0
LB                0.30 Hz
GB                   0
PC                1.00

YX01128-1
```

^{13}C-NMR (125 MHz, $CDCl_3$)



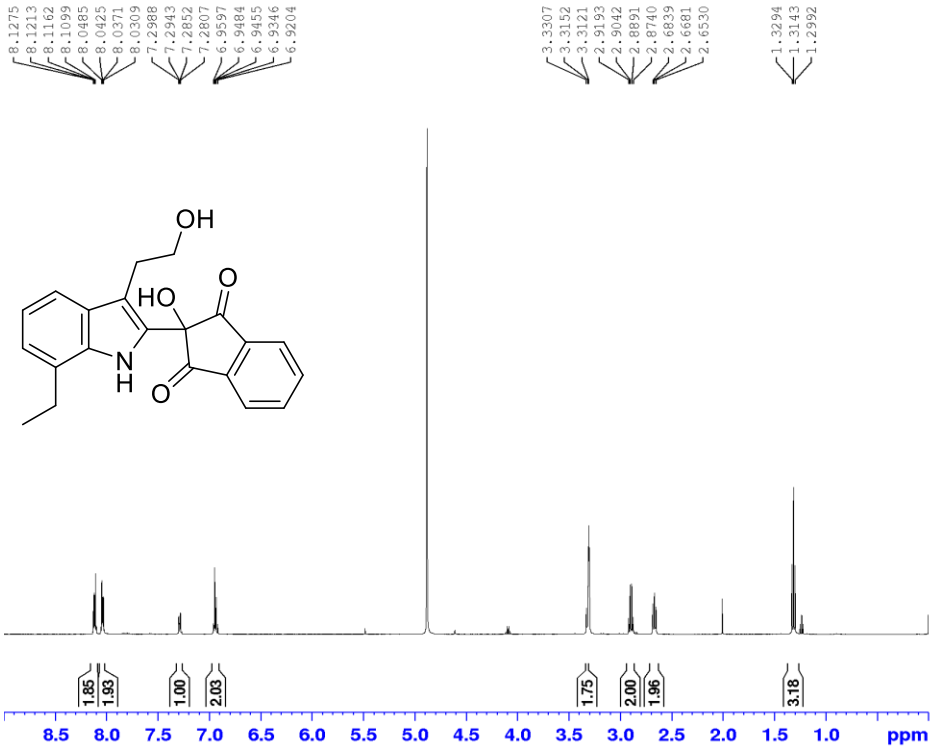

```
Current Data Parameters
NAME      20220407 nmr c
EXPNO                22
PROCNO                1

F2 - Acquisition Parameters
Date_           20220408
Time              0.17 h
INSTRUM           spect
PROBHD   Z113652_0230 (
PULPROG          zgpg30
TD               65536
SOLVENT          CDCl3
NS                 280
DS                   4
SWH           29761.904 Hz
FIDRES        0.908261 Hz
AQ            1.1010048 sec
RG               190.79
DW               16.800 usec
DE                6.50 usec
TE               294.5 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1
SFO1         125.7703643 MHz
NUC1                13C
P0                3.33 usec
P1               10.00 usec
PLW1        102.87999725 W
SFO2         500.1320005 MHz
NUC2                 1H
CPDPRG[2         waltz65
PCPD2             80.00 usec
PLW2         25.23200035 W
PLW12         0.39425001 W
PLW13         0.19831000 W

F2 - Processing parameters
SI               32768
SF           125.7577885 MHz
WDW                 EM
SSB                  0
LB                1.00 Hz
GB                   0
PC                1.40

YX01128-1
```

^{1}H-NMR (500 MHz, MeOD)



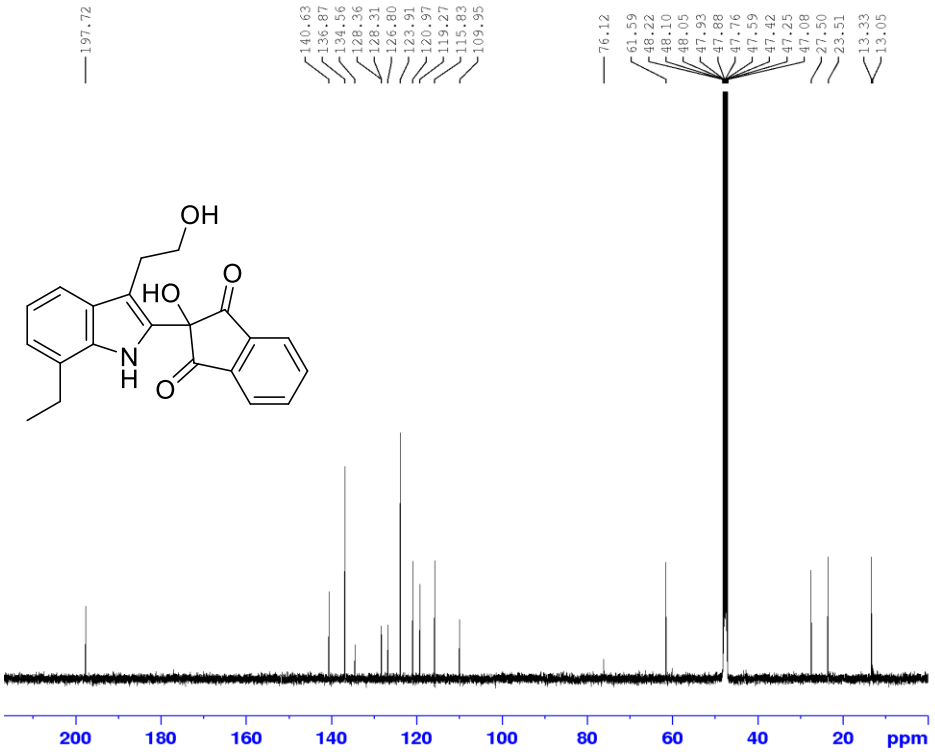

```
Current Data Parameters
NAME                  YX01145-1
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20230407
Time                      10.54 h
INSTRUM                  Avance
PROBHD          Z151574_0127 (
PULPROG                   zg30
TD                       65536
SOLVENT                   MeOD
NS                          16
DS                           2
SWH                  10000.000 Hz
FIDRES                0.305176 Hz
AQ                    3.2767999 sec
RG                          101
DW                       50.000 usec
DE                       11.14 usec
TE                       294.7 K
D1                    1.00000000 sec
TD0                           1
SFO1                500.1330883 MHz
NUC1                         1H
P0                        2.67 usec
P1                        8.00 usec
PLW1                25.47599983 W

F2 - Processing parameters
SI                        65536
SF                  500.1300115 MHz
WDW                          EM
SSB                           0
LB                         0.30 Hz
GB                            0
PC                         1.00

YX01145-1
```

^{13}C-NMR (125 MHz, MeOD)



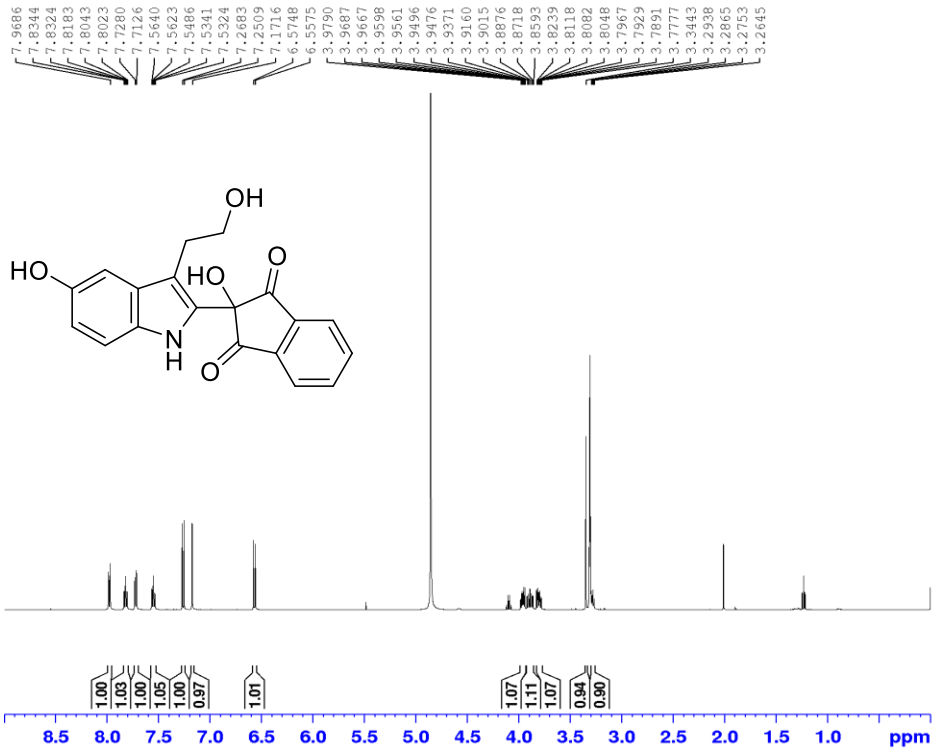

```
Current Data Parameters
NAME                  YX01145-1
EXPNO                         2
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20230410
Time                      16.58 h
INSTRUM                  Avance
PROBHD          Z151574_0127 (
PULPROG                 zgpg30
TD                       65536
SOLVENT                   MeOD
NS                         1024
DS                            4
SWH                  30120.482 Hz
FIDRES                0.919204 Hz
AQ                    1.0878977 sec
RG                          101
DW                       16.600 usec
DE                        6.50 usec
TE                       298.0 K
D1                    2.00000000 sec
D11                   0.03000000 sec
TD0                           1
SFO1                125.7703643 MHz
NUC1                         13C
P0                        3.00 usec
P1                        9.00 usec
PLW1               113.54000092 W
SFO2                500.1320005 MHz
NUC2                         1H
CPDPRG[2                waltz65
PCPD2                    80.00 usec
PLW2                25.47599983 W
PLW12                0.25476000 W
PLW13                0.12814000 W

F2 - Processing parameters
SI                        32768
SF                  125.7577885 MHz
WDW                          EM
SSB                           0
LB                         1.00 Hz
GB                            0
PC                         1.40

YX01145-1
```

^{1}H-NMR (500 MHz, MeOD)



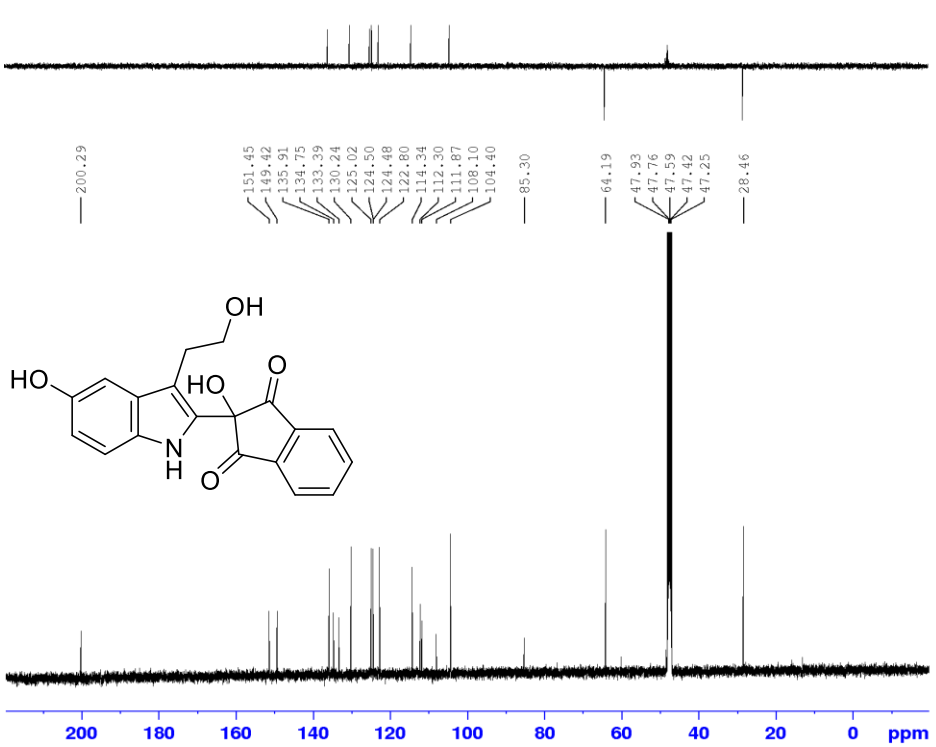

```
Current Data Parameters
NAME                  YX01149-1
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20230421
Time                      17.03 h
INSTRUM                  Avance
PROBHD    Z151574_0127 (
PULPROG                   zg30
TD                       65536
SOLVENT                   MeOD
NS                          16
DS                           2
SWH                  10000.000 Hz
FIDRES                0.305176 Hz
AQ                    3.2767999 sec
RG                          101
DW                       50.000 usec
DE                       11.14 usec
TE                       298.0 K
D1                    1.00000000 sec
TD0                           1
SFO1                500.1330883 MHz
NUC1                        1H
P0                        2.67 usec
P1                        8.00 usec
PLW1                25.47599983 W

F2 - Processing parameters
SI                        65536
SF                  500.1300117 MHz
WDW                          EM
SSB                           0
LB                         0.30 Hz
GB                            0
PC                         1.00

YX01149-1
```

^{13}C-NMR (125 MHz, MeOD)



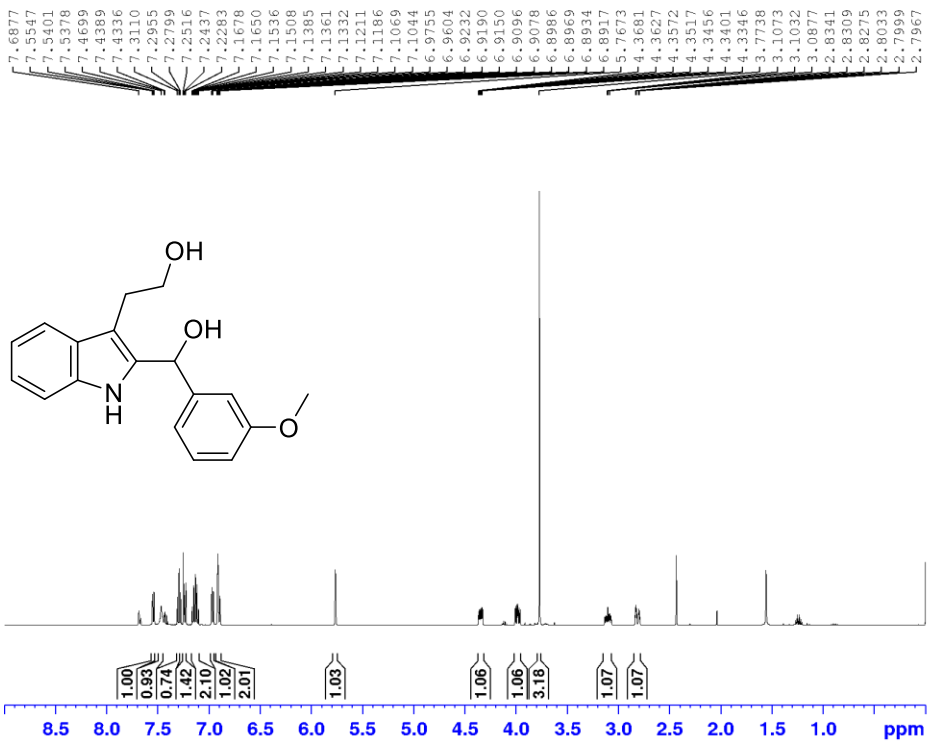

```
Current Data Parameters
NAME                  YX01149-1
EXPNO                         2
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20230422
Time                      19.45 h
INSTRUM                  Avance
PROBHD    Z151574_0127 (
PULPROG                 zgpg30
TD                       65536
SOLVENT                   MeOD
NS                         1024
DS                            4
SWH                  30120.482 Hz
FIDRES                0.919204 Hz
AQ                    1.0878977 sec
RG                          101
DW                       16.600 usec
DE                        6.50 usec
TE                       298.0 K
D1                    2.00000000 sec
D11                   0.03000000 sec
TD0                           1
SFO1                125.7703643 MHz
NUC1                        13C
P0                        3.00 usec
P1                        9.00 usec
PLW1               113.54000092 W
SFO2                500.1320005 MHz
NUC2                        1H
CPDPRG[2                waltz65
PCPD2                    80.00 usec
PLW2                25.47599983 W
PLW12                0.25476000 W
PLW13                0.12814000 W

F2 - Processing parameters
SI                        32768
SF                  125.7577885 MHz
WDW                          EM
SSB                           0
LB                         1.00 Hz
GB                            0
PC                         1.40

YX01149-1
```

^{1}H-NMR (500 MHz, $CDCl_3$)



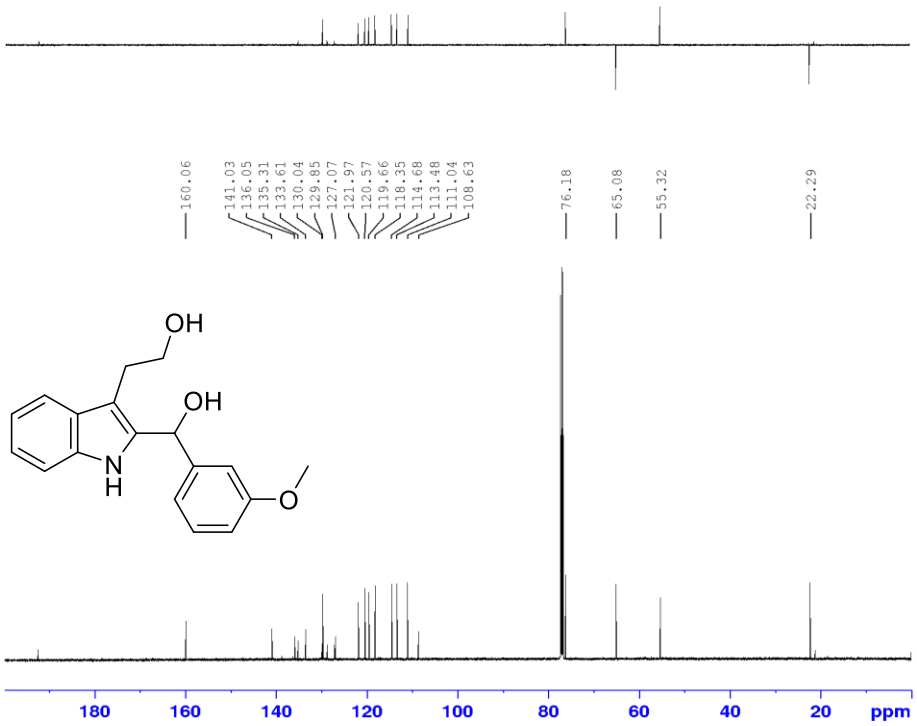

```
Current Data Parameters
NAME                  LYL01022
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20230621
Time                     17.54 h
INSTRUM                 Avance
PROBHD    Z151574_0127 (
PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                          16
DS                           2
SWH                 10000.000 Hz
FIDRES                0.305176 Hz
AQ                    3.2767999 sec
RG                         101
DW                      50.000 usec
DE                      11.14 usec
TE                      298.0 K
D1                  1.00000000 sec
TD0                          1
SFO1                500.1330883 MHz
NUC1                        1H
P0                       2.67 usec
P1                       8.00 usec
PLW1                25.47599983 W

F2 - Processing parameters
SI                       65536
SF                  500.1300156 MHz
WDW                         EM
SSB                          0
LB                        0.30 Hz
GB                           0
PC                        1.00


LYL01022
```

^{13}C-NMR (125 MHz, $CDCl_3$)



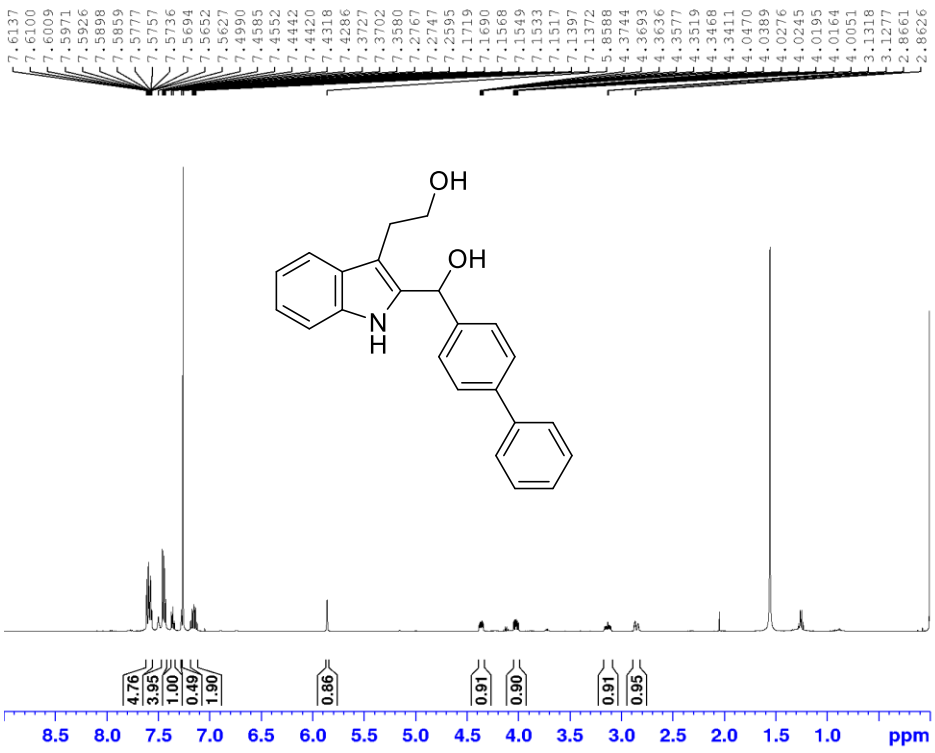

```
Current Data Parameters
NAME                  LYL01022
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20230622
Time                     15.53 h
INSTRUM                 Avance
PROBHD    Z151574_0127 (
PULPROG                zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                       1024
DS                          4
SWH                 30120.482 Hz
FIDRES                0.919204 Hz
AQ                    1.0878977 sec
RG                         101
DW                      16.600 usec
DE                       6.50 usec
TE                      298.0 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                          1
SFO1                125.7703643 MHz
NUC1                        13C
P0                       3.00 usec
P1                       9.00 usec
PLW1                113.54000092 W
SFO2                500.1320005 MHz
NUC2                        1H
CPDPRG[2                waltz65
PCPD2                    80.00 usec
PLW2                25.47599983 W
PLW12                0.25476000 W
PLW13                0.12814000 W

F2 - Processing parameters
SI                       32768
SF                  125.7577885 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40


LYL01022
```

^{1}H-NMR (500 MHz, $CDCl_3$)



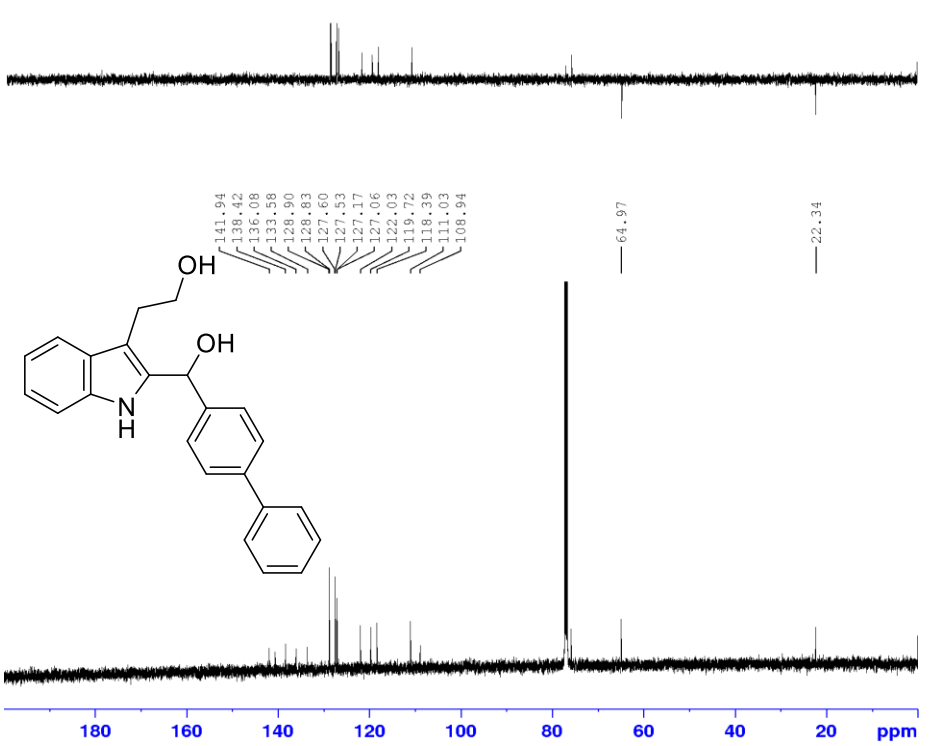

```
Current Data Parameters
NAME              LYL01023
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_              20230704
Time                 10.39 h
INSTRUM              Avance
PROBHD    Z151574_0127 (
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH               10000.000 Hz
FIDRES                0.305176 Hz
AQ                    3.2767999 sec
RG                      101
DW                     50.000 usec
DE                     11.14 usec
TE                     298.0 K
D1                1.00000000 sec
TD0                       1
SFO1              500.1330883 MHz
NUC1                      1H
P0                     2.67 usec
P1                     8.00 usec
PLW1             25.47599983 W

F2 - Processing parameters
SI                    65536
SF              500.1300117 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00


LYL01023
```

^{13}C-NMR (125 MHz, $CDCl_3$)



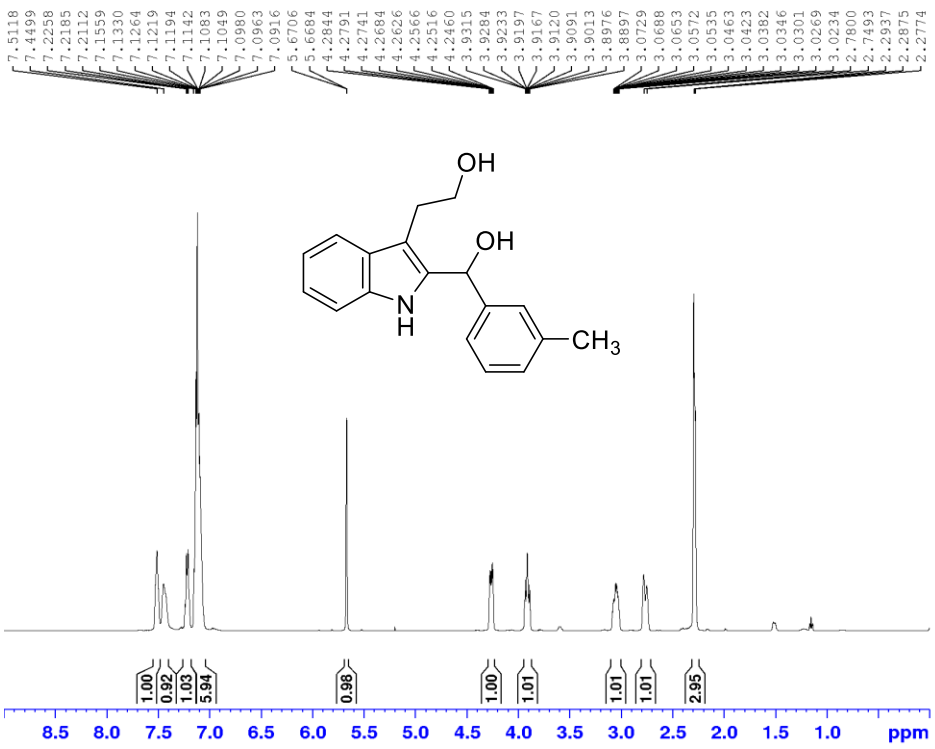

```
Current Data Parameters
NAME              LYL01023
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_              20230704
Time                 16.40 h
INSTRUM              Avance
PROBHD    Z151574_0127 (
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     1280
DS                        4
SWH               30120.482 Hz
FIDRES                0.919204 Hz
AQ                    1.0878977 sec
RG                      101
DW                     16.600 usec
DE                      6.50 usec
TE                     298.0 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                       1
SFO1              125.7703643 MHz
NUC1                      13C
P0                     3.00 usec
P1                     9.00 usec
PLW1             113.54000092 W
SFO2              500.1320005 MHz
NUC2                      1H
CPDPRG[2             waltz65
PCPD2                 80.00 usec
PLW2             25.47599983 W
PLW12             0.25476000 W
PLW13             0.12814000 W

F2 - Processing parameters
SI                    32768
SF              125.7577885 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40


LYL01023
```

^{1}H-NMR (500 MHz, $CDCl_3$)



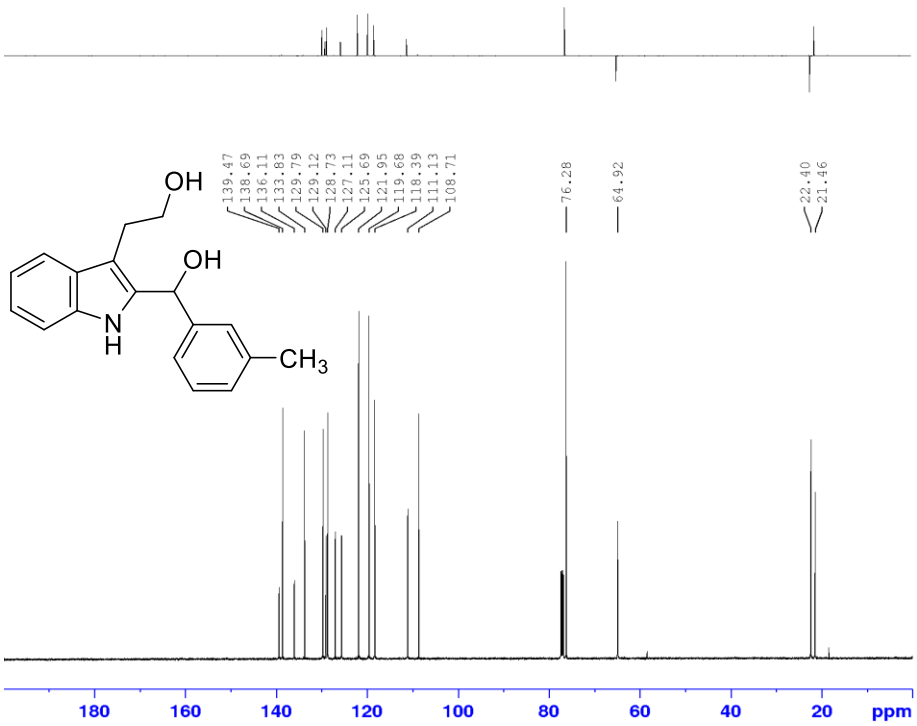

```
Current Data Parameters
NAME                  LYL01024
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20230619
Time                     16.54 h
INSTRUM                  Avance
PROBHD    Z151574_0127 (
PULPROG                   zg30
TD                       65536
SOLVENT                  CDCl3
NS                          16
DS                           2
SWH                  10000.000 Hz
FIDRES                0.305176 Hz
AQ                    3.2767999 sec
RG                      45.2174
DW                       50.000 usec
DE                       11.14 usec
TE                       298.0 K
D1                  1.00000000 sec
TD0                          1
SFO1                500.1330883 MHz
NUC1                        1H
P0                       2.67 usec
P1                       8.00 usec
PLW1                25.47599983 W

F2 - Processing parameters
SI                       65536
SF                  500.1300630 MHz
WDW                         EM
SSB                          0
LB                        0.30 Hz
GB                           0
PC                        1.00


LYL01024
```

^{13}C-NMR (125 MHz, $CDCl_3$)



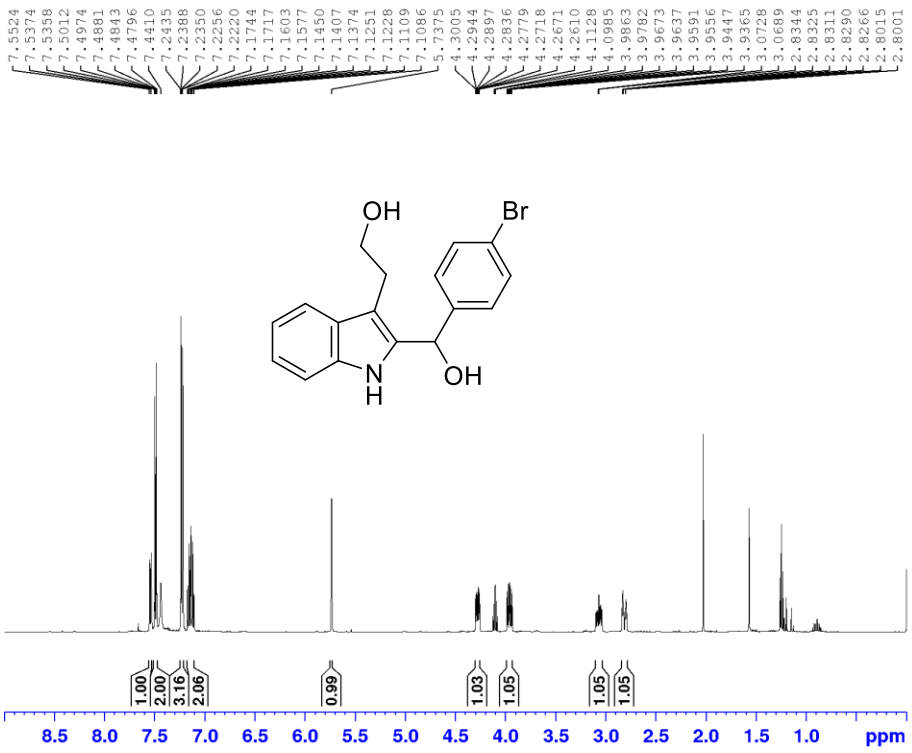

```
Current Data Parameters
NAME                  LYL01024
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20230619
Time                     22.10 h
INSTRUM                  Avance
PROBHD    Z151574_0127 (
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                        1024
DS                           4
SWH                  30120.482 Hz
FIDRES                0.919204 Hz
AQ                    1.0878977 sec
RG                         101
DW                       16.600 usec
DE                        6.50 usec
TE                       298.0 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                          1
SFO1                125.7703643 MHz
NUC1                        13C
P0                       3.00 usec
P1                       9.00 usec
PLW1                113.54000092 W
SFO2                500.1320005 MHz
NUC2                        1H
CPDPRG[2                waltz65
PCPD2                    80.00 usec
PLW2                25.47599983 W
PLW12                0.25476000 W
PLW13                0.12814000 W

F2 - Processing parameters
SI                       32768
SF                  125.7577885 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40


LYL01024
```

^{1}H-NMR (500 MHz, $CDCl_3$)



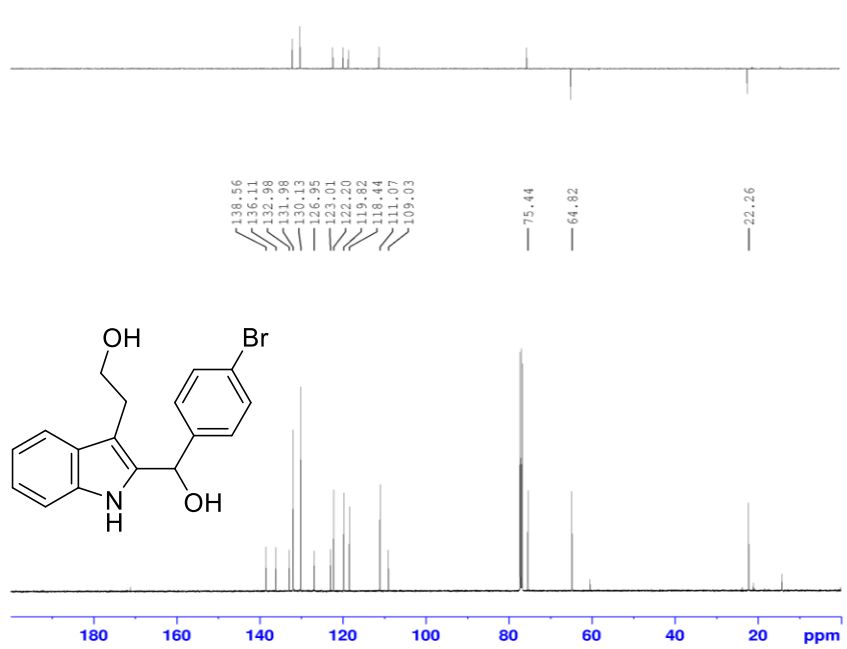

```
Current Data Parameters
NAME                  LYL01027
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20230707
Time                     15.29 h
INSTRUM                 Avance
PROBHD    Z151574_0127 (
PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                         16
DS                          2
SWH                 10000.000 Hz
FIDRES                0.305176 Hz
AQ                    3.2767999 sec
RG                        101
DW                     50.000 usec
DE                     11.14 usec
TE                     298.0 K
D1                  1.00000000 sec
TD0                          1
SFO1                500.1330883 MHz
NUC1                        1H
P0                     2.67 usec
P1                     8.00 usec
PLW1                25.47599983 W

F2 - Processing parameters
SI                       65536
SF                  500.1300214 MHz
WDW                         EM
SSB                          0
LB                        0.30 Hz
GB                           0
PC                        1.00


LYL01027
```

^{13}C-NMR (125 MHz, $CDCl_3$)



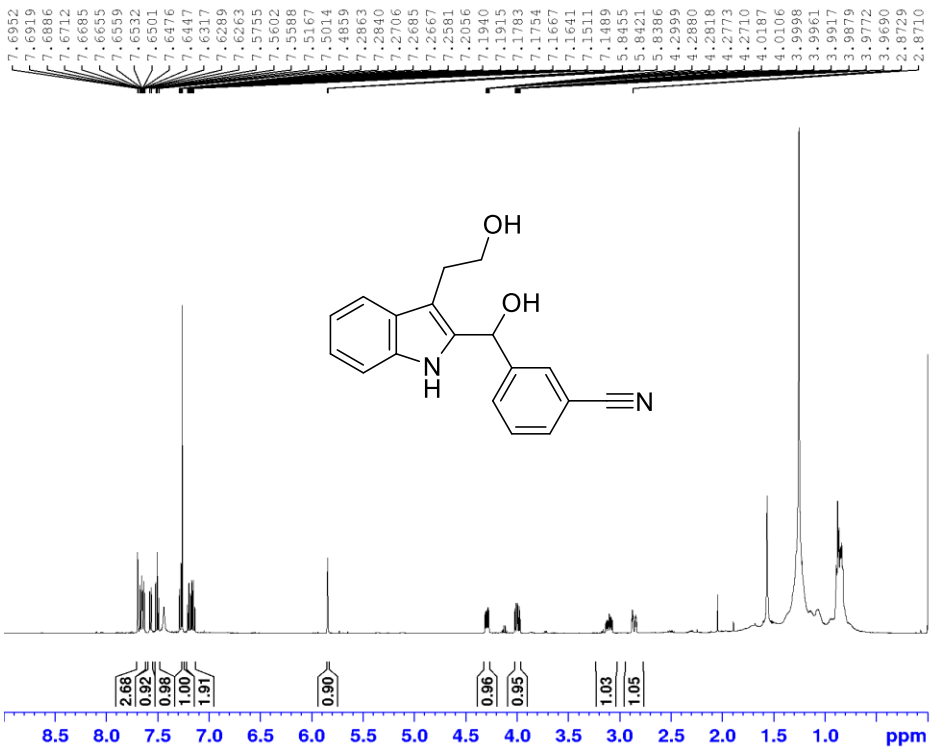

```
Current Data Parameters
NAME                  LYL01027
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20230707
Time                     17.40 h
INSTRUM                 Avance
PROBHD    Z151574_0127 (
PULPROG                zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                         512
DS                           4
SWH                30120.482 Hz
FIDRES             0.919204 Hz
AQ                    1.0878977 sec
RG                        101
DW                     16.600 usec
DE                      6.50 usec
TE                     298.0 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                          1
SFO1                125.7703643 MHz
NUC1                        13C
P0                     3.00 usec
P1                     9.00 usec
PLW1               113.54000092 W
SFO2                500.1320005 MHz
NUC2                        1H
CPDPRG[2                waltz65
PCPD2                  80.00 usec
PLW2                25.47599983 W
PLW12                0.25476000 W
PLW13                0.12814000 W

F2 - Processing parameters
SI                       32768
SF                  125.7577885 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40


LYL01027
```

^{1}H-NMR (500 MHz, $CDCl_3$)



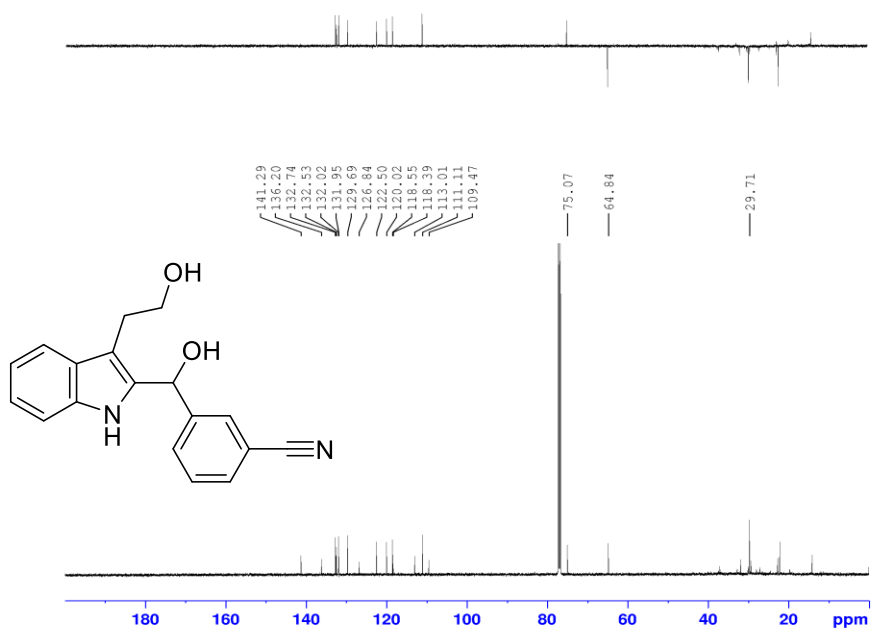

```
Current Data Parameters
NAME                  LYL01028
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20230629
Time                     17.57 h
INSTRUM                 Avance
PROBHD    Z151574_0127 (
PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                         16
DS                          2
SWH                 10000.000 Hz
FIDRES                0.305176 Hz
AQ                    3.2767999 sec
RG                        101
DW                     50.000 usec
DE                     11.14 usec
TE                     298.0 K
D1                  1.00000000 sec
TD0                          1
SFO1               500.1330883 MHz
NUC1                        1H
P0                       2.67 usec
P1                       8.00 usec
PLW1               25.47599983 W

F2 - Processing parameters
SI                       65536
SF                 500.1300124 MHz
WDW                         EM
SSB                          0
LB                        0.30 Hz
GB                           0
PC                        1.00


LYL01028
```

^{13}C-NMR (125 MHz, $CDCl_3$)



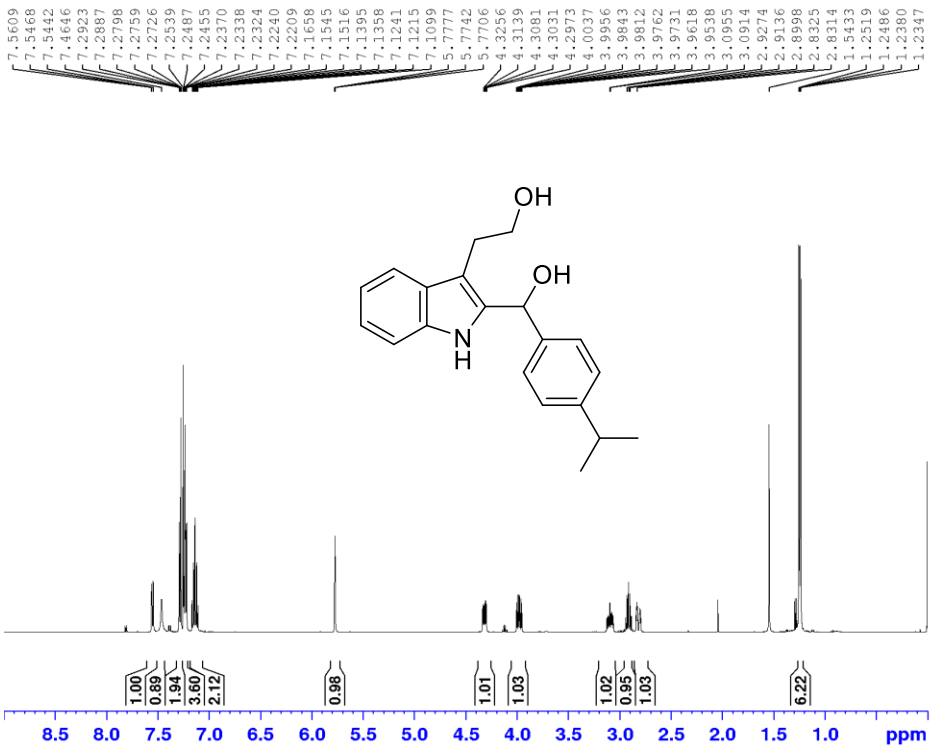

```
Current Data Parameters
NAME                  LYL01028
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20230629
Time                     23.27 h
INSTRUM                 Avance
PROBHD    Z151574_0127 (
PULPROG                zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                       1280
DS                          4
SWH                 30120.482 Hz
FIDRES                0.919204 Hz
AQ                    1.0878977 sec
RG                        101
DW                     16.600 usec
DE                      6.50 usec
TE                     298.0 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                          1
SFO1               125.7703643 MHz
NUC1                        13C
P0                       3.00 usec
P1                       9.00 usec
PLW1               113.54000092 W
SFO2               500.1320005 MHz
NUC2                        1H
CPDPRG[2                waltz65
PCPD2                   80.00 usec
PLW2               25.47599983 W
PLW12               0.25476000 W
PLW13               0.12814000 W

F2 - Processing parameters
SI                       32768
SF                 125.7577885 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40


LYL01028
```

^{1}H-NMR (500 MHz, $CDCl_3$)



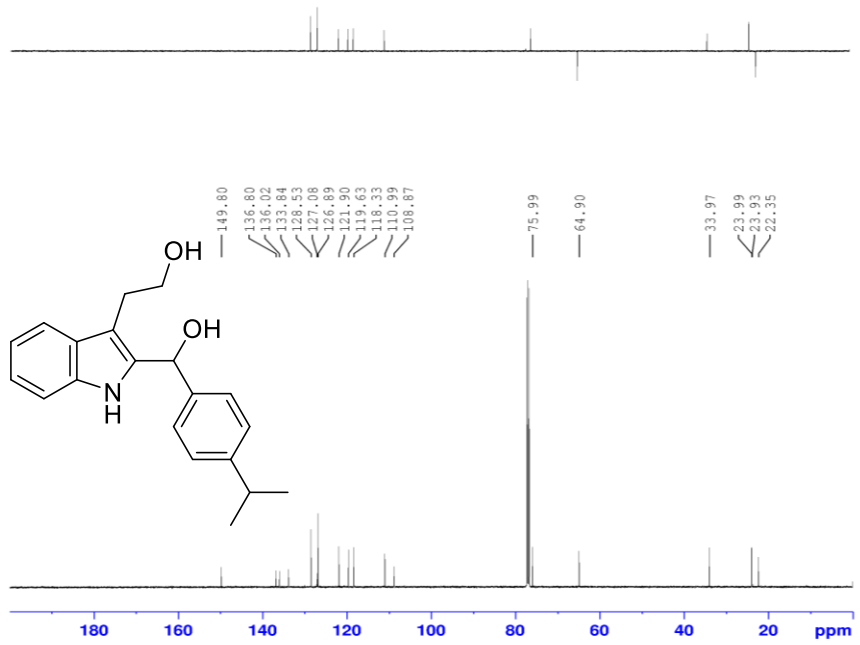

```
Current Data Parameters
NAME                  LYL01029
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20230626
Time                     15.25 h
INSTRUM                  Avance
PROBHD    Z151574_0127 (
PULPROG                  zg30
TD                      65536
SOLVENT                  CDCl3
NS                          16
DS                           2
SWH                  10000.000 Hz
FIDRES               0.305176 Hz
AQ                   3.2767999 sec
RG                         101
DW                      50.000 usec
DE                      11.14 usec
TE                      298.0 K
D1                   1.00000000 sec
TD0                          1
SFO1                 500.1330883 MHz
NUC1                         1H
P0                       2.67 usec
P1                       8.00 usec
PLW1                25.47599983 W

F2 - Processing parameters
SI                       65536
SF                   500.1300145 MHz
WDW                         EM
SSB                          0
LB                        0.30 Hz
GB                           0
PC                        1.00


LYL01029
```

^{13}C-NMR (125 MHz, $CDCl_3$)



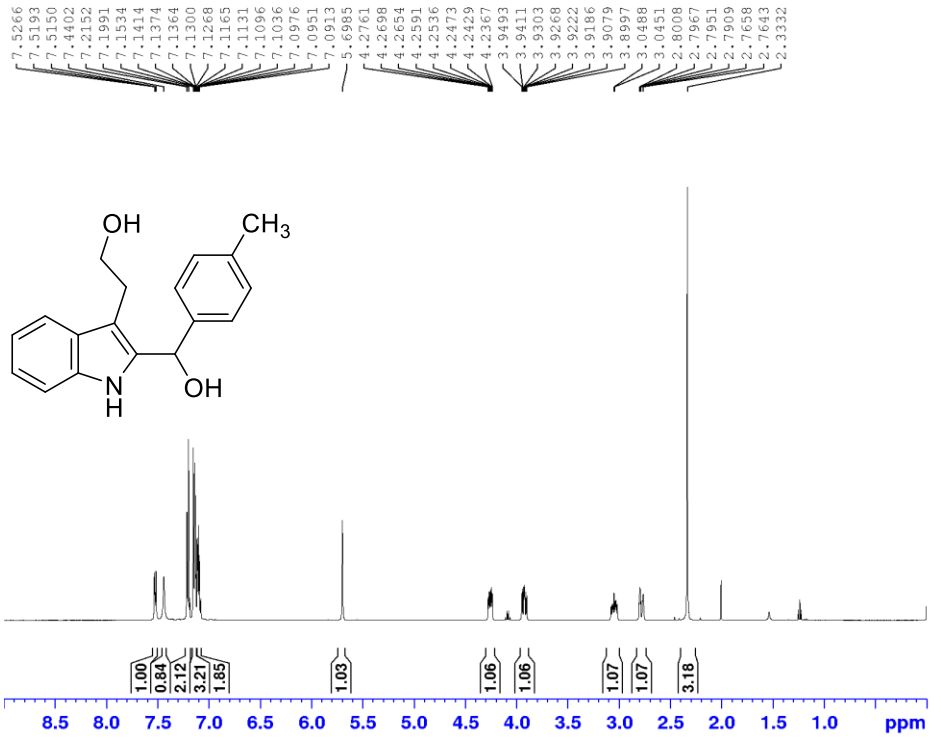

```
Current Data Parameters
NAME                  LYL01029
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20230626
Time                     17.11 h
INSTRUM                  Avance
PROBHD    Z151574_0127 (
PULPROG                 zgpg30
TD                      65536
SOLVENT                  CDCl3
NS                        1024
DS                           4
SWH                  30120.482 Hz
FIDRES               0.919204 Hz
AQ                   1.0878977 sec
RG                         101
DW                      16.600 usec
DE                       6.50 usec
TE                      298.0 K
D1                   2.00000000 sec
D11                  0.03000000 sec
TD0                          1
SFO1                 125.7703643 MHz
NUC1                         13C
P0                       3.00 usec
P1                       9.00 usec
PLW1                113.54000092 W
SFO2                 500.1320005 MHz
NUC2                         1H
CPDPRG[2                waltz65
PCPD2                   80.00 usec
PLW2                25.47599983 W
PLW12                0.25476000 W
PLW13                0.12814000 W

F2 - Processing parameters
SI                       32768
SF                   125.7577885 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40


LYL01029
```

^{1}H-NMR (500 MHz, $CDCl_3$)



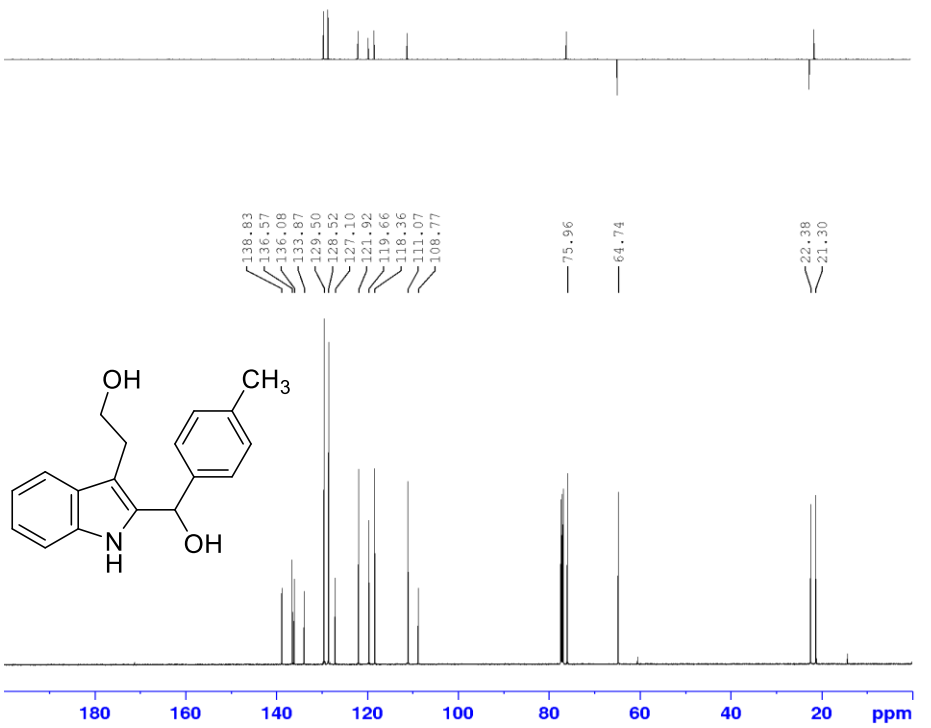

```
Current Data Parameters
NAME          LYL01030-1
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230714
Time               9.41 h
INSTRUM          Avance
PROBHD   Z151574_0127 (
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH           10000.000 Hz
FIDRES        0.305176 Hz
AQ            3.2767999 sec
RG                   52
DW               50.000 usec
DE               11.14 usec
TE                298.0 K
D1           1.00000000 sec
TD0                   1
SFO1        500.1330883 MHz
NUC1                 1H
P0                2.67 usec
P1                8.00 usec
PLW1        25.47599983 W

F2 - Processing parameters
SI                65536
SF          500.1300474 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00


LYL01030-1
```

^{13}C-NMR (125 MHz, $CDCl_3$)



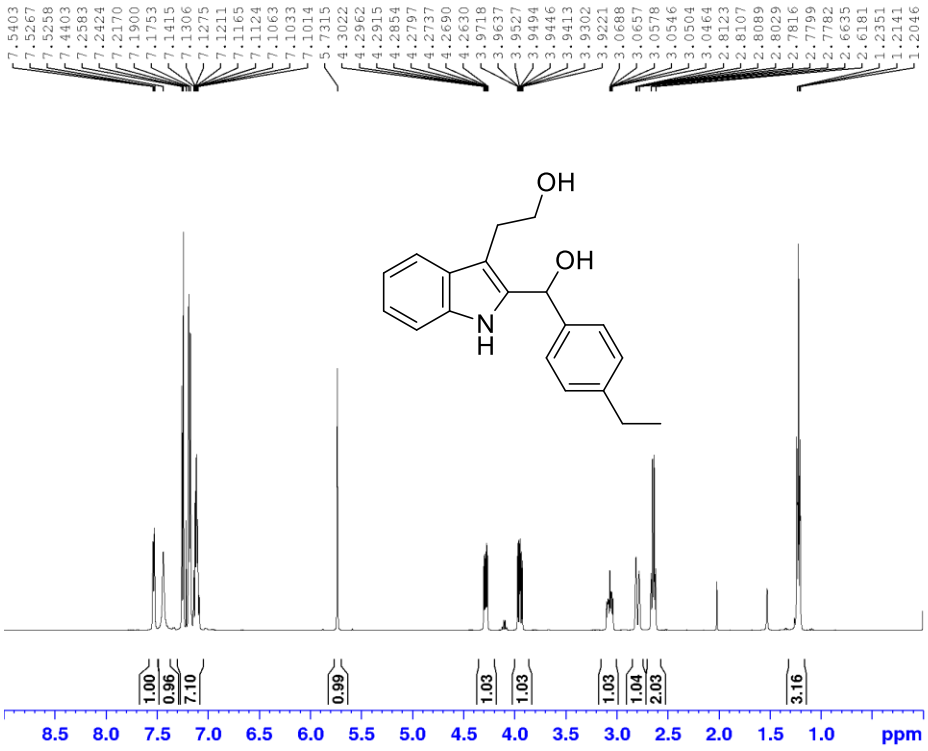

```
Current Data Parameters
NAME          LYL01030-1
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230714
Time              10.36 h
INSTRUM          Avance
PROBHD   Z151574_0127 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           30120.482 Hz
FIDRES        0.919204 Hz
AQ            1.0878977 sec
RG                  101
DW               16.600 usec
DE                6.50 usec
TE                298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1                 13C
P0                3.00 usec
P1                9.00 usec
PLW1       113.54000092 W
SFO2        500.1320005 MHz
NUC2                 1H
CPDPRG[2         waltz65
PCPD2            80.00 usec
PLW2        25.47599983 W
PLW12        0.25476000 W
PLW13        0.12814000 W

F2 - Processing parameters
SI                32768
SF          125.7577885 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40


LYL01030-1
```

^{1}H-NMR (500 MHz, $CDCl_3$)



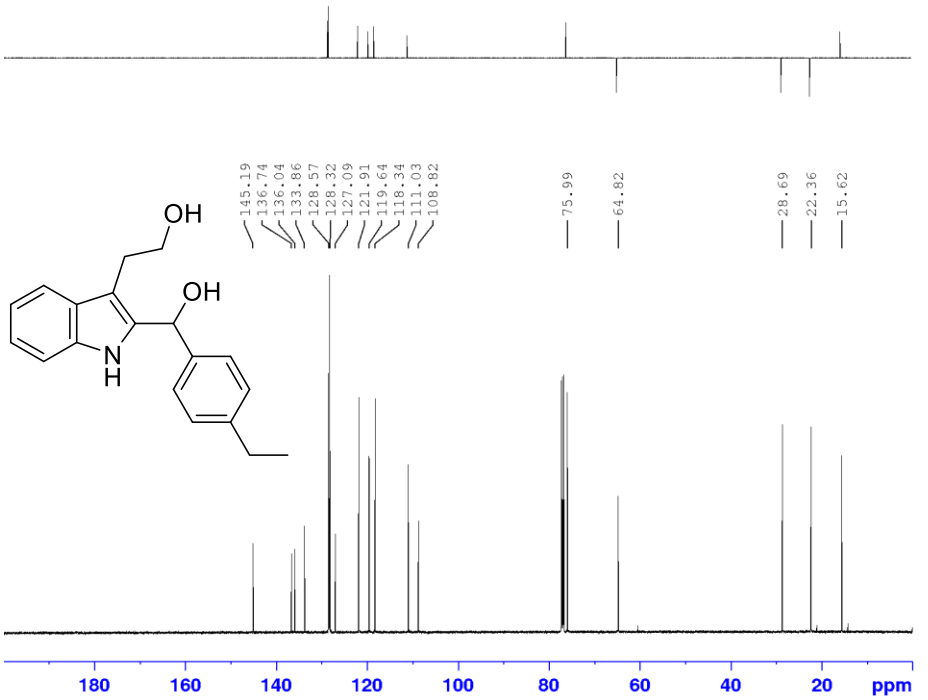

```
Current Data Parameters
NAME          LYL01031-1
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230626
Time              15.29 h
INSTRUM           Avance
PROBHD   Z151574_0127 (
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH           10000.000 Hz
FIDRES        0.305176 Hz
AQ            3.2767999 sec
RG              71.7241
DW              50.000 usec
DE              11.14 usec
TE                298.0 K
D1           1.00000000 sec
TD0                   1
SFO1        500.1330883 MHz
NUC1                1H
P0                2.67 usec
P1                8.00 usec
PLW1        25.47599983 W

F2 - Processing parameters
SI                65536
SF          500.1300327 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00


LYL0100031-1
```

^{13}C-NMR (125 MHz, $CDCl_3$)



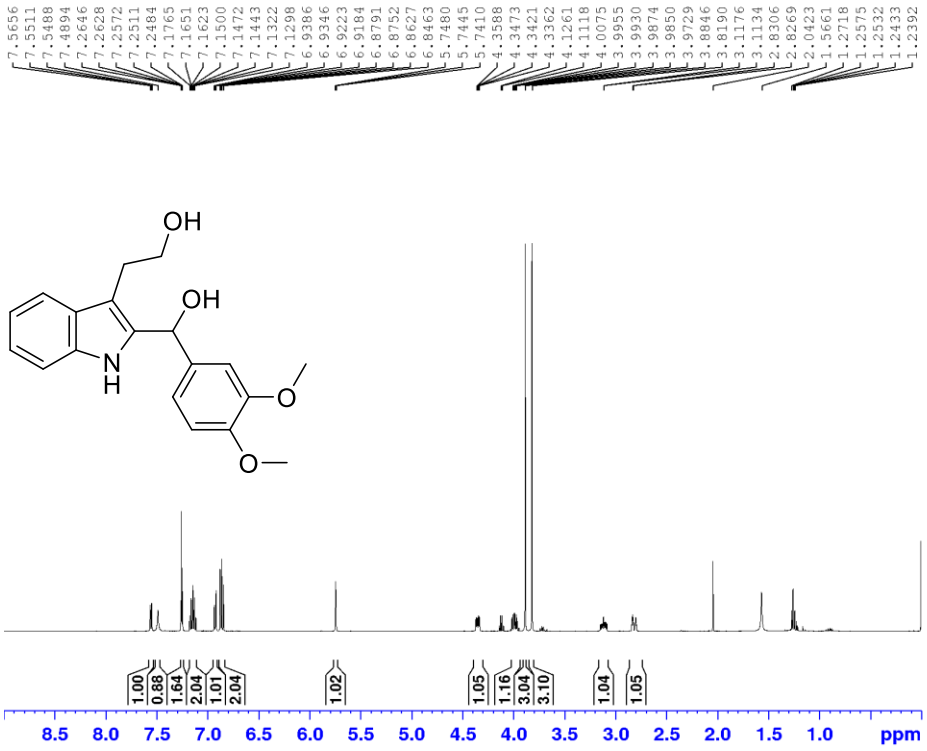

```
Current Data Parameters
NAME          LYL01031-1
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230626
Time              18.23 h
INSTRUM           Avance
PROBHD   Z151574_0127 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           30120.482 Hz
FIDRES        0.919204 Hz
AQ            1.0878977 sec
RG                  101
DW              16.600 usec
DE               6.50 usec
TE                298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1                13C
P0                3.00 usec
P1                9.00 usec
PLW1        113.54000092 W
SFO2        500.1320005 MHz
NUC2                1H
CPDPRG[2        waltz65
PCPD2             80.00 usec
PLW2        25.47599983 W
PLW12        0.25476000 W
PLW13        0.12814000 W

F2 - Processing parameters
SI                32768
SF          125.7577885 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40


LYL01031-1
```

^{1}H-NMR (500 MHz, $CDCl_3$)



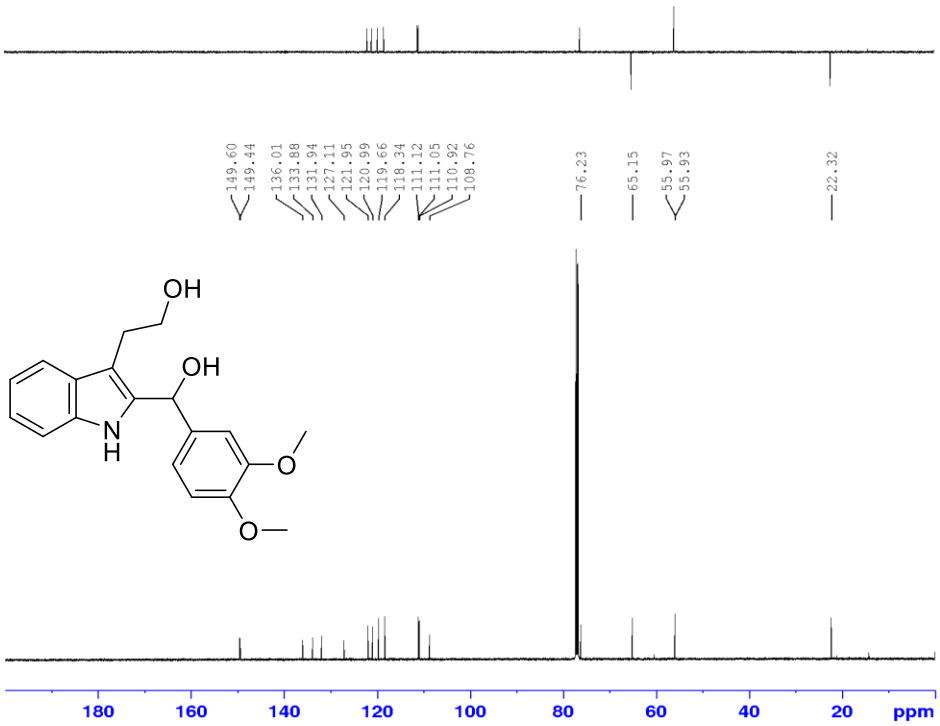

```
Current Data Parameters
NAME                  LYL01032
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20230704
Time                     10.44 h
INSTRUM                 Avance
PROBHD    Z151574_0127 (
PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                          16
DS                           2
SWH                  10000.000 Hz
FIDRES                0.305176 Hz
AQ                    3.2767999 sec
RG                         101
DW                      50.000 usec
DE                      11.14 usec
TE                      298.0 K
D1                   1.00000000 sec
TD0                          1
SFO1                500.1330883 MHz
NUC1                        1H
P0                       2.67 usec
P1                       8.00 usec
PLW1                25.47599983 W

F2 - Processing parameters
SI                       65536
SF                  500.1300127 MHz
WDW                         EM
SSB                          0
LB                        0.30 Hz
GB                           0
PC                        1.00


LYL01032
```

^{13}C-NMR (125 MHz, $CDCl_3$)



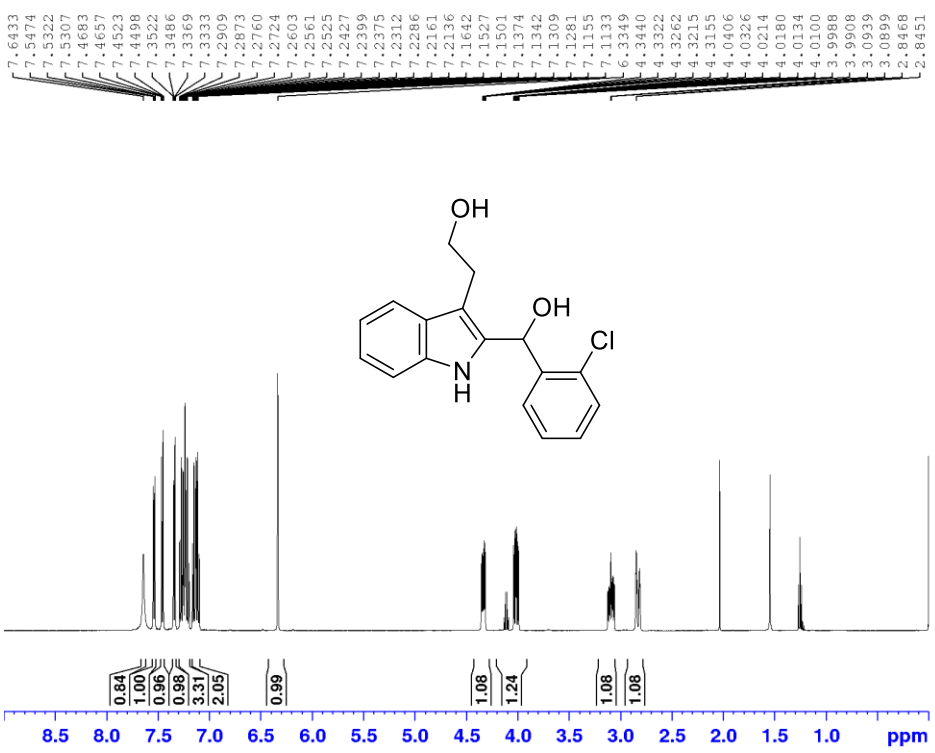

```
Current Data Parameters
NAME                  LYL01032
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20230704
Time                     21.34 h
INSTRUM                 Avance
PROBHD    Z151574_0127 (
PULPROG                zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                       1024
DS                          4
SWH                  30120.482 Hz
FIDRES                0.919204 Hz
AQ                    1.0878977 sec
RG                         101
DW                      16.600 usec
DE                       6.50 usec
TE                      298.0 K
D1                   2.00000000 sec
D11                  0.03000000 sec
TD0                          1
SFO1                125.7703643 MHz
NUC1                        13C
P0                       3.00 usec
P1                       9.00 usec
PLW1               113.54000092 W
SFO2                500.1320005 MHz
NUC2                        1H
CPDPRG[2                waltz65
PCPD2                   80.00 usec
PLW2                25.47599983 W
PLW12                0.25476000 W
PLW13                0.12814000 W

F2 - Processing parameters
SI                       32768
SF                  125.7577885 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40


LYL01032
```

^{1}H-NMR (500 MHz, $CDCl_3$)



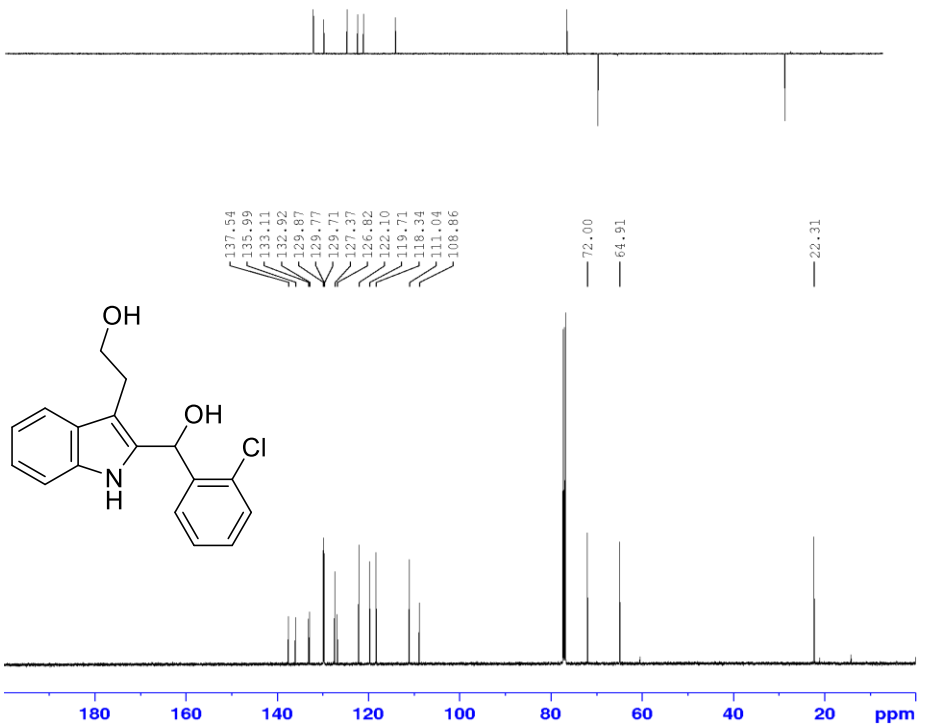

```
Current Data Parameters
NAME                 LYL01034
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_               20230718
Time                   10.56 h
INSTRUM                Avance
PROBHD    Z151574_0127 (
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         2
SWH                10000.000 Hz
FIDRES             0.305176 Hz
AQ                 3.2767999 sec
RG                       101
DW                    50.000 usec
DE                    11.14 usec
TE                    298.0 K
D1                 1.00000000 sec
TD0                         1
SFO1              500.1330883 MHz
NUC1                       1H
P0                     2.67 usec
P1                     8.00 usec
PLW1              25.47599983 W

F2 - Processing parameters
SI                     65536
SF                500.1300200 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00


LYL01034
```

^{13}C-NMR (125 MHz, $CDCl_3$)



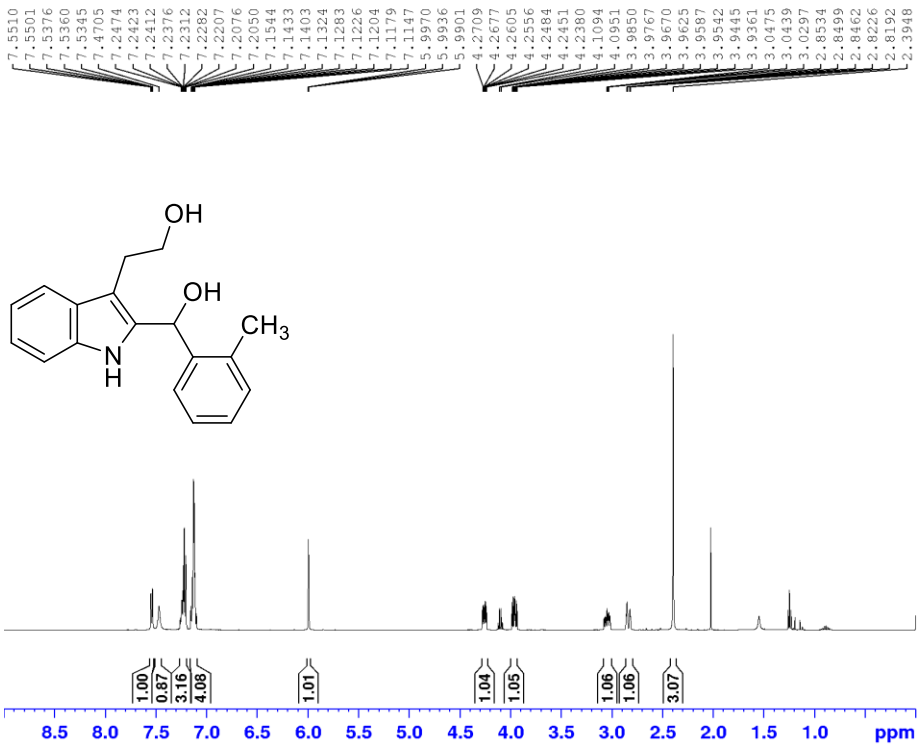

```
Current Data Parameters
NAME                 LYL01034
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_               20230718
Time                   17.13 h
INSTRUM                Avance
PROBHD    Z151574_0127 (
PULPROG                zgpg30
TD                     65536
SOLVENT                CDCl3
NS                       512
DS                         4
SWH                30120.482 Hz
FIDRES             0.919204 Hz
AQ                 1.0878977 sec
RG                       101
DW                    16.600 usec
DE                     6.50 usec
TE                    298.0 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                         1
SFO1              125.7703643 MHz
NUC1                       13C
P0                     3.00 usec
P1                     9.00 usec
PLW1              113.54000092 W
SFO2              500.1320005 MHz
NUC2                       1H
CPDPRG[2              waltz65
PCPD2                  80.00 usec
PLW2              25.47599983 W
PLW12              0.25476000 W
PLW13              0.12814000 W

F2 - Processing parameters
SI                     32768
SF                125.7577885 MHz
WDW                       EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.40


LYL01034
```

^{1}H-NMR (500 MHz, $CDCl_3$)



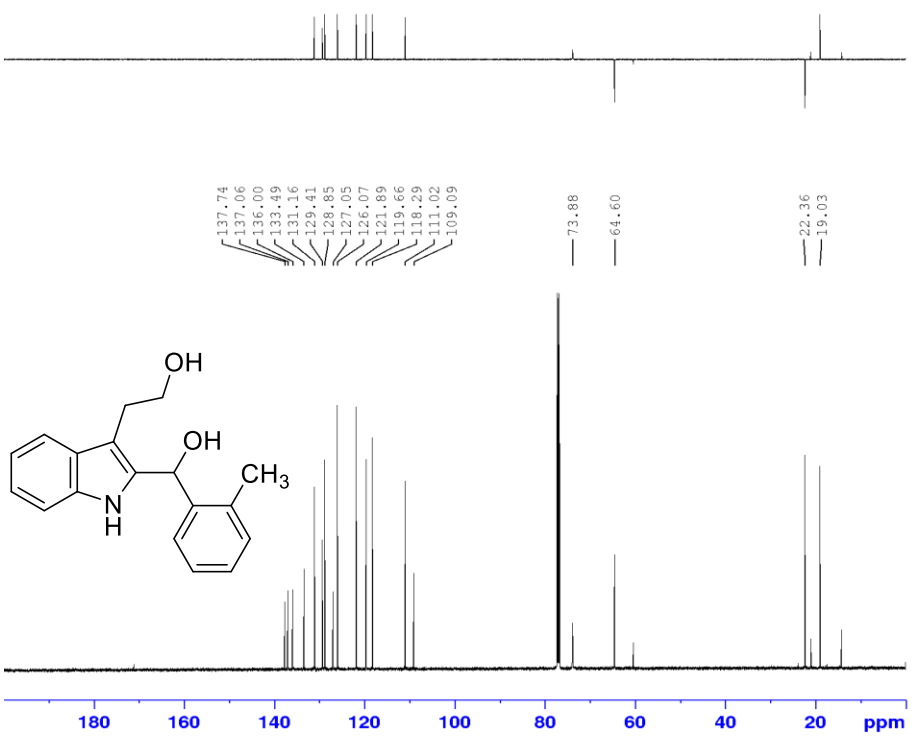

```
Current Data Parameters
NAME          LYL01035-1
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230714
Time              13.25 h
INSTRUM           Avance
PROBHD   Z151574_0127 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           10000.000 Hz
FIDRES        0.305176 Hz
AQ            3.2767999 sec
RG                   101
DW               50.000 usec
DE               11.14 usec
TE                298.0 K
D1            1.00000000 sec
TD0                    1
SFO1         500.1330883 MHz
NUC1                1H
P0                2.67 usec
P1                8.00 usec
PLW1         25.47599983 W

F2 - Processing parameters
SI                 65536
SF           500.1300272 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00


LYL01035-1
```

^{13}C-NMR (125 MHz, $CDCl_3$)



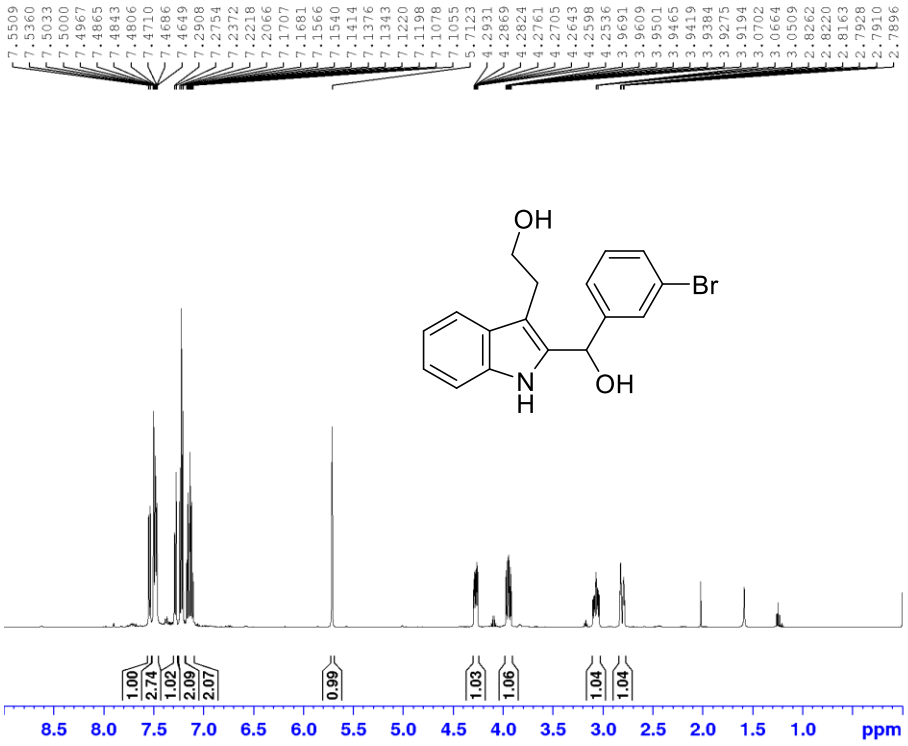

```
Current Data Parameters
NAME          LYL01035-1
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230714
Time              14.20 h
INSTRUM           Avance
PROBHD   Z151574_0127 (
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH           30120.482 Hz
FIDRES        0.919204 Hz
AQ            1.0878977 sec
RG                   101
DW               16.600 usec
DE                6.50 usec
TE                298.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1
SFO1         125.7703643 MHz
NUC1                13C
P0                3.00 usec
P1                9.00 usec
PLW1         113.54000092 W
SFO2         500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz65
PCPD2             80.00 usec
PLW2         25.47599983 W
PLW12         0.25476000 W
PLW13         0.12814000 W

F2 - Processing parameters
SI                 32768
SF           125.7577885 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40


LYL01035-1
```

^{1}H-NMR (500 MHz, $CDCl_3$)



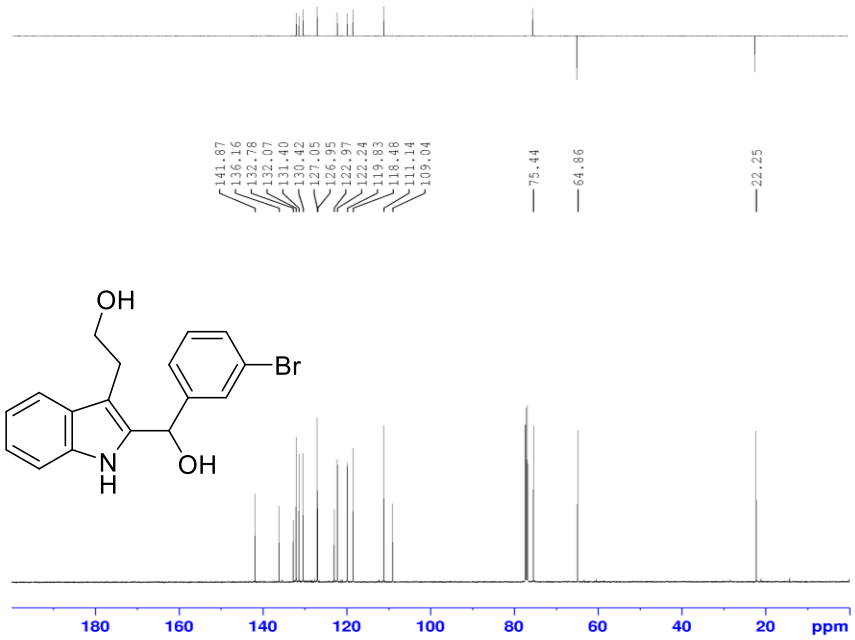

```
Current Data Parameters
NAME                  LYL01038
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20230729
Time                      3.50 h
INSTRUM                 Avance
PROBHD    Z151574_0127 (
PULPROG                   zg30
TD                       65536
SOLVENT                  CDCl3
NS                          16
DS                           2
SWH                  10000.000 Hz
FIDRES                0.305176 Hz
AQ                    3.2767999 sec
RG                       88.0208
DW                       50.000 usec
DE                       11.14 usec
TE                       298.0 K
D1                    1.00000000 sec
TD0                          1
SFO1                500.1330883 MHz
NUC1                        1H
P0                        2.67 usec
P1                        8.00 usec
PLW1                25.47599983 W

F2 - Processing parameters
SI                       65536
SF                  500.1300306 MHz
WDW                         EM
SSB                          0
LB                        0.30 Hz
GB                           0
PC                        1.00


LYL01038
```

^{13}C-NMR (125 MHz, $CDCl_3$)



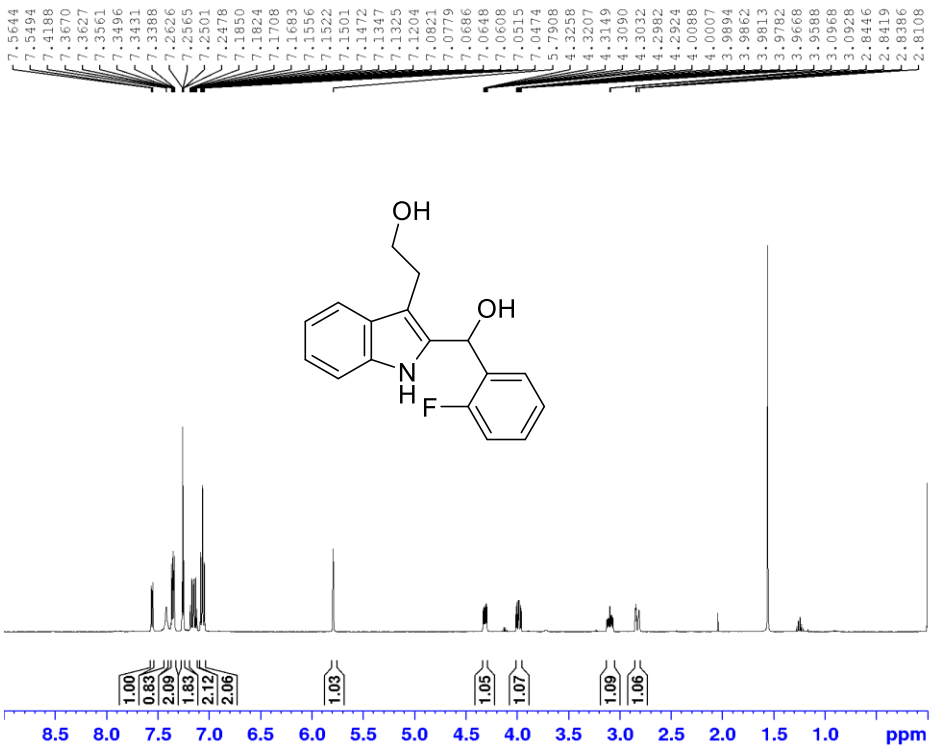

```
Current Data Parameters
NAME                  LYL01038
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20230729
Time                      4.45 h
INSTRUM                 Avance
PROBHD    Z151574_0127 (
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                        1024
DS                           4
SWH                  30120.482 Hz
FIDRES                0.919204 Hz
AQ                    1.0878977 sec
RG                         101
DW                       16.600 usec
DE                        6.50 usec
TE                       298.0 K
D1                    2.00000000 sec
D11                   0.03000000 sec
TD0                          1
SFO1                125.7703643 MHz
NUC1                        13C
P0                        3.00 usec
P1                        9.00 usec
PLW1                113.54000092 W
SFO2                500.1320005 MHz
NUC2                        1H
CPDPRG[2                waltz65
PCPD2                     80.00 usec
PLW2                25.47599983 W
PLW12                0.25476000 W
PLW13                0.12814000 W

F2 - Processing parameters
SI                       32768
SF                  125.7577885 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40


LYL01038
```

^{1}H-NMR (500 MHz, $CDCl_3$)



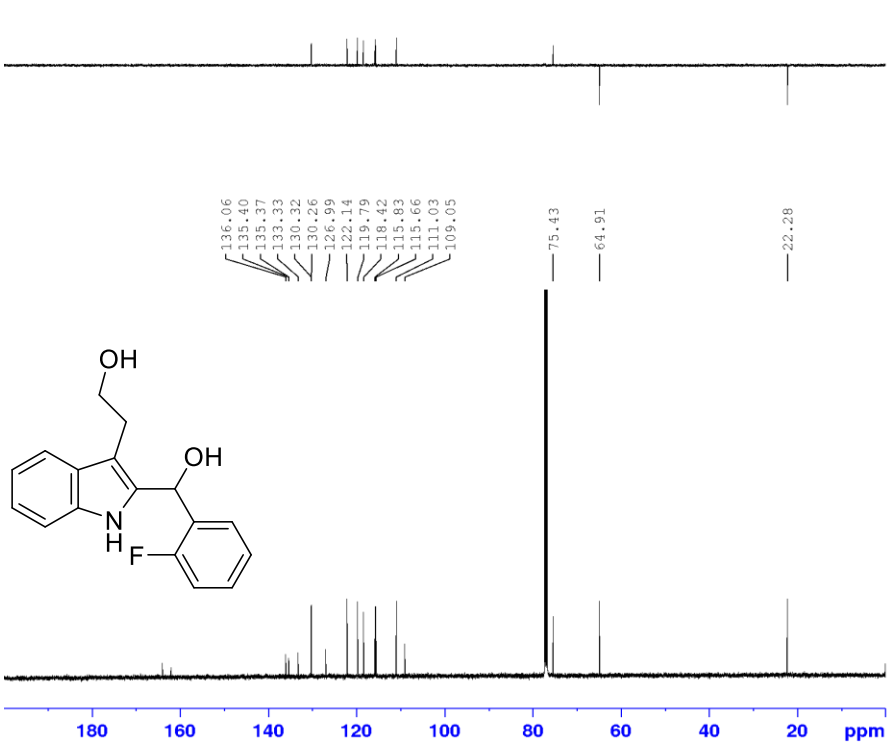

```
Current Data Parameters
NAME                  LYL01040
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20230729
Time                      6.46 h
INSTRUM                 Avance
PROBHD    Z151574_0127 (
PULPROG                   zg30
TD                       65536
SOLVENT                  CDCl3
NS                          16
DS                           2
SWH                  10000.000 Hz
FIDRES                0.305176 Hz
AQ                    3.2767999 sec
RG                         101
DW                      50.000 usec
DE                      11.14 usec
TE                        298.0 K
D1                    1.00000000 sec
TD0                          1
SFO1                500.1330883 MHz
NUC1                        1H
P0                        2.67 usec
P1                        8.00 usec
PLW1                25.47599983 W

F2 - Processing parameters
SI                       65536
SF                  500.1300132 MHz
WDW                         EM
SSB                          0
LB                        0.30 Hz
GB                           0
PC                        1.00


LYL01040
```

^{13}C-NMR (125 MHz, $CDCl_3$)



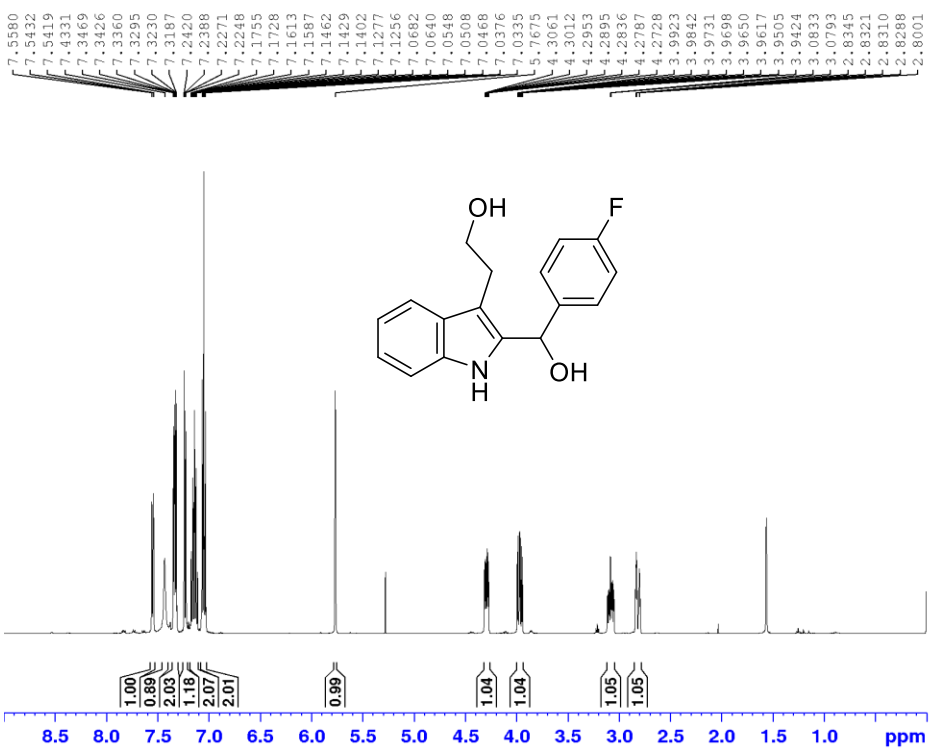

```
Current Data Parameters
NAME                  LYL01040
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20230729
Time                      7.41 h
INSTRUM                 Avance
PROBHD    Z151574_0127 (
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                        1024
DS                           4
SWH                  30120.482 Hz
FIDRES                0.919204 Hz
AQ                    1.0878977 sec
RG                         101
DW                      16.600 usec
DE                       6.50 usec
TE                        298.0 K
D1                    2.00000000 sec
D11                   0.03000000 sec
TD0                          1
SFO1                125.7703643 MHz
NUC1                        13C
P0                        3.00 usec
P1                        9.00 usec
PLW1               113.54000092 W
SFO2                500.1320005 MHz
NUC2                        1H
CPDPRG[2                waltz65
PCPD2                    80.00 usec
PLW2                25.47599983 W
PLW12                0.25476000 W
PLW13                0.12814000 W

F2 - Processing parameters
SI                       32768
SF                  125.7577885 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40


LYL01040
```

^{1}H-NMR (500 MHz, $CDCl_3$)



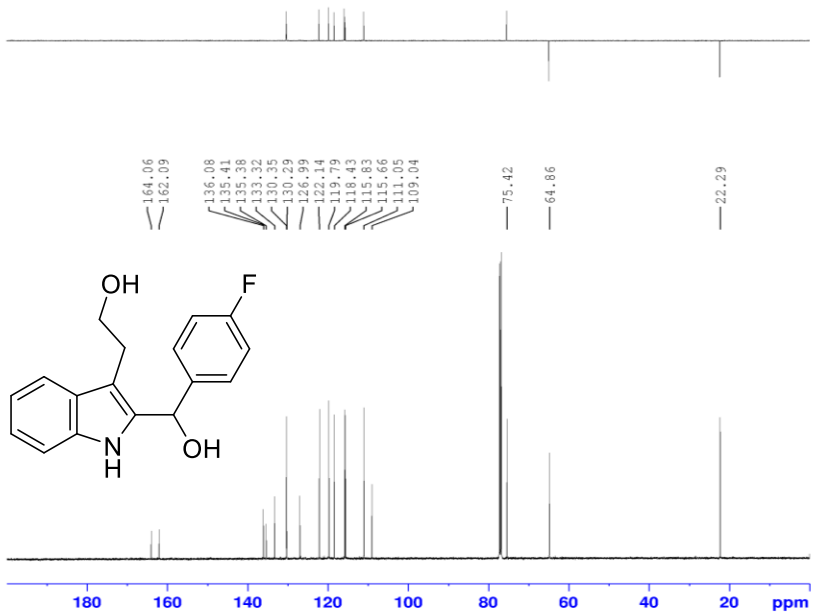

```
Current Data Parameters
NAME       LYL01041-0906
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230906
Time              11.53 h
INSTRUM           Avance
PROBHD    Z151574_0127 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           10000.000 Hz
FIDRES        0.305176 Hz
AQ            3.2767999 sec
RG                   101
DW               50.000 usec
DE               11.14 usec
TE                296.1 K
D1            1.00000000 sec
TD0                    1
SFO1          500.1330883 MHz
NUC1                  1H
P0                 2.67 usec
P1                 8.00 usec
PLW1         25.47599983 W

F2 - Processing parameters
SI                 65536
SF           500.1300220 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00

LYL01041-0906
```

^{13}C-NMR (125 MHz, $CDCl_3$)



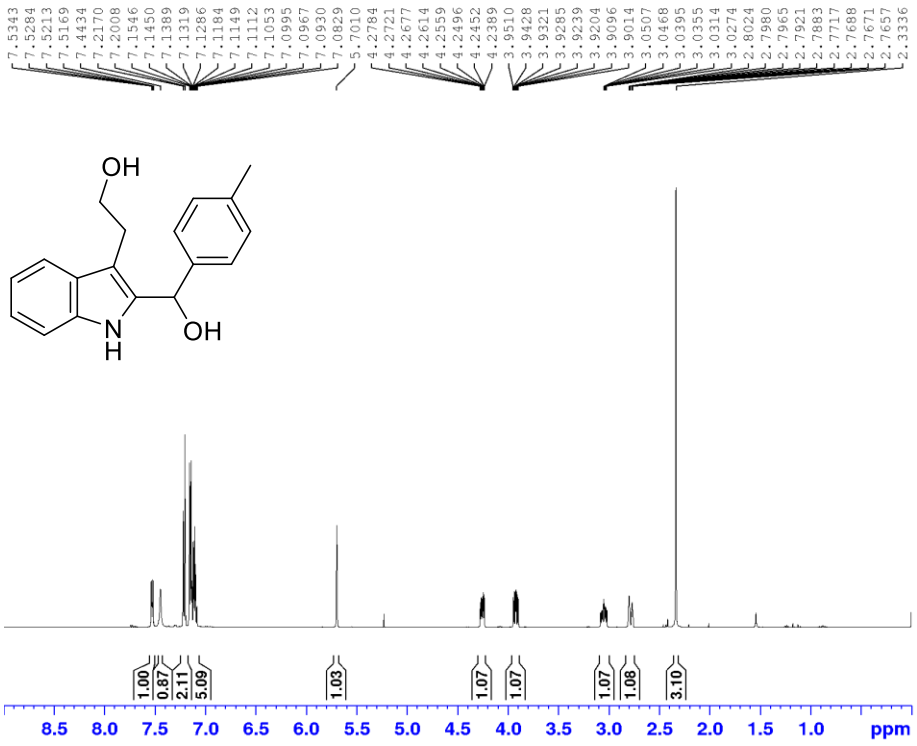

```
Current Data Parameters
NAME       LYL01041-0906
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230906
Time              12.48 h
INSTRUM           Avance
PROBHD    Z151574_0127 (
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH           30120.482 Hz
FIDRES        0.919204 Hz
AQ            1.0878977 sec
RG                   101
DW               16.600 usec
DE                6.50 usec
TE                297.3 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1
SFO1         125.7703643 MHz
NUC1                  13C
P0                 3.00 usec
P1                 9.00 usec
PLW1        113.54000092 W
SFO2         500.1320005 MHz
NUC2                  1H
CPDPRG[2         waltz65
PCPD2             80.00 usec
PLW2         25.47599983 W
PLW12         0.25476000 W
PLW13         0.12814000 W

F2 - Processing parameters
SI                 32768
SF           125.7577885 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40

LYL01041-0906
```

^{1}H-NMR (500 MHz, $CDCl_3$)



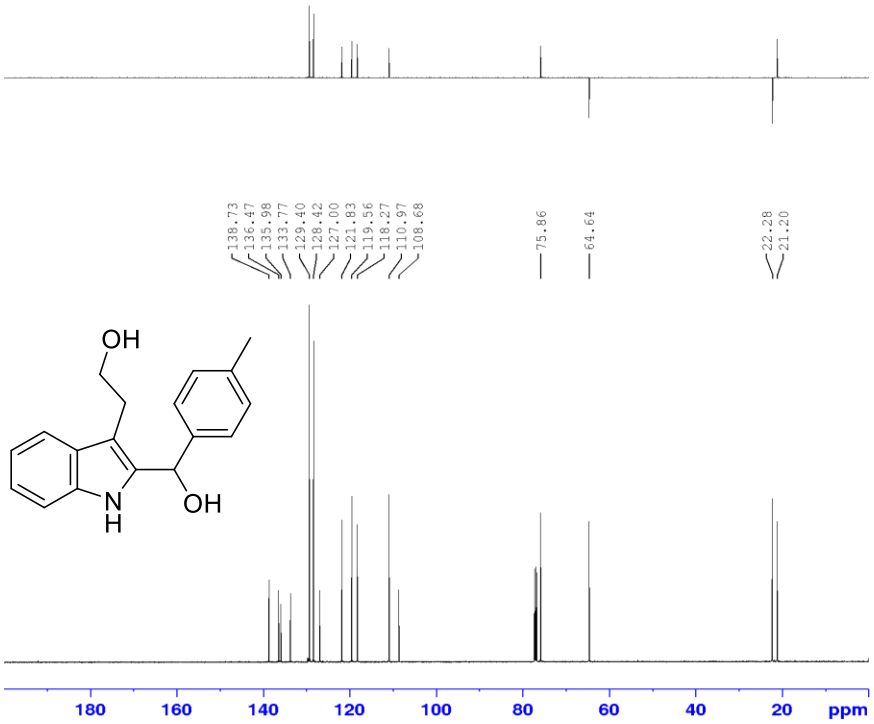

```
Current Data Parameters
NAME              LYL01045
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_              20230814
Time                 4.55 h
INSTRUM              Avance
PROBHD    Z151574_0127 (
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH              10000.000 Hz
FIDRES               0.305176 Hz
AQ                3.2767999 sec
RG                     50.7317
DW                    50.000 usec
DE                    11.14 usec
TE                    296.9 K
D1               1.00000000 sec
TD0                      1
SFO1           500.1330883 MHz
NUC1                     1H
P0                    2.67 usec
P1                    8.00 usec
PLW1           25.47599983 W

F2 - Processing parameters
SI                    65536
SF             500.1300461 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00


LYL01045
```

^{13}C-NMR (125 MHz, $CDCl_3$)



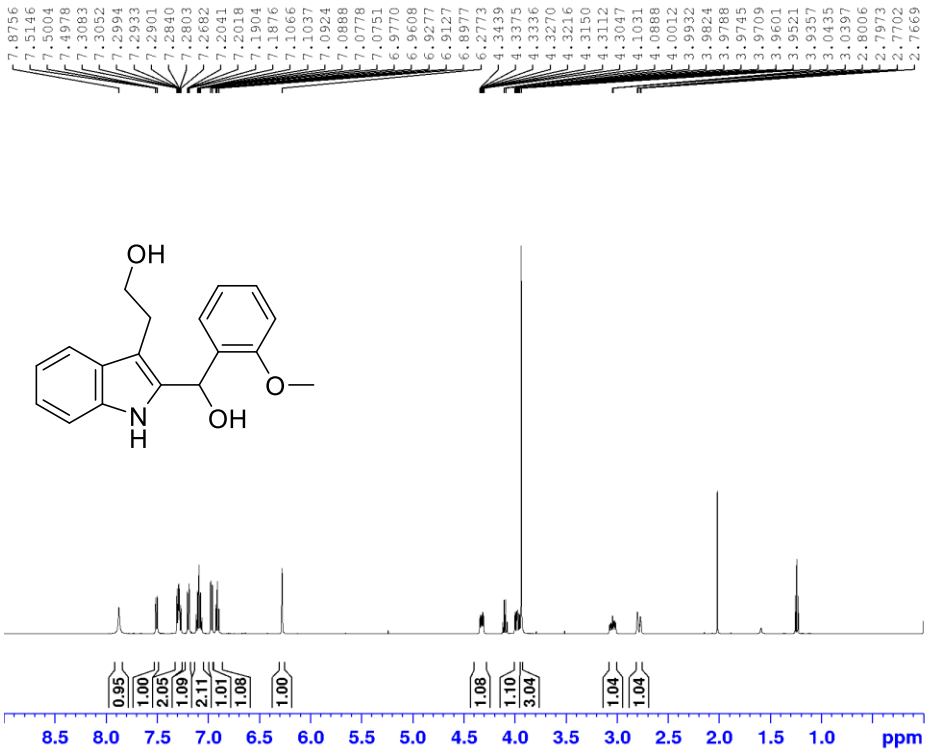

```
Current Data Parameters
NAME              LYL01045
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_              20230814
Time                 5.50 h
INSTRUM              Avance
PROBHD    Z151574_0127 (
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     1024
DS                        4
SWH              30120.482 Hz
FIDRES               0.919204 Hz
AQ                1.0878977 sec
RG                       101
DW                   16.600 usec
DE                    6.50 usec
TE                    298.0 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                      1
SFO1           125.7703643 MHz
NUC1                     13C
P0                    3.00 usec
P1                    9.00 usec
PLW1           113.54000092 W
SFO2           500.1320005 MHz
NUC2                     1H
CPDPRG[2          waltz65
PCPD2                80.00 usec
PLW2           25.47599983 W
PLW12           0.25476000 W
PLW13           0.12814000 W

F2 - Processing parameters
SI                    32768
SF             125.7578006 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40


LYL01045
```

^{1}H-NMR (500 MHz, $CDCl_3$)



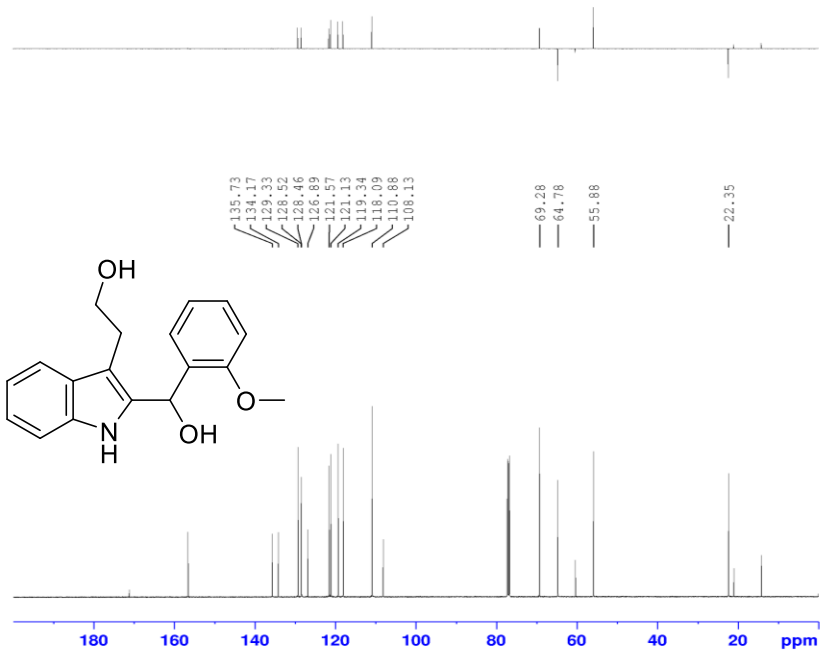

```
Current Data Parameters
NAME                  LYL01046
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20230827
Time                     14.55 h
INSTRUM                 Avance
PROBHD    Z151574_0127 (
PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                         16
DS                          2
SWH                 10000.000 Hz
FIDRES                0.305176 Hz
AQ                    3.2767999 sec
RG                      49.5238
DW                       50.000 usec
DE                       11.14 usec
TE                       295.6 K
D1                   1.00000000 sec
TD0                          1
SFO1                500.1330883 MHz
NUC1                        1H
P0                       2.67 usec
P1                       8.00 usec
PLW1                25.47599983 W

F2 - Processing parameters
SI                       65536
SF                  500.1300389 MHz
WDW                         EM
SSB                          0
LB                        0.30 Hz
GB                           0
PC                        1.00


LYL01046
```

^{13}C-NMR (125 MHz, $CDCl_3$)



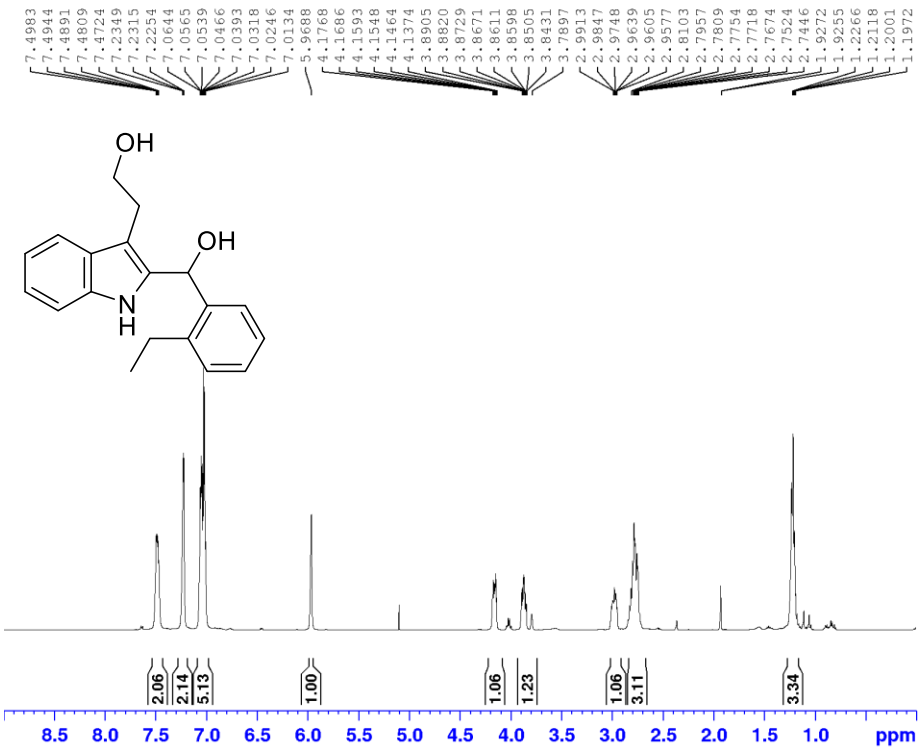

```
Current Data Parameters
NAME                  LYL01046
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20230827
Time                     15.50 h
INSTRUM                 Avance
PROBHD    Z151574_0127 (
PULPROG                zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                       1024
DS                          4
SWH                 30120.482 Hz
FIDRES                0.919204 Hz
AQ                    1.0878977 sec
RG                         101
DW                       16.600 usec
DE                        6.50 usec
TE                       296.7 K
D1                   2.00000000 sec
D11                  0.03000000 sec
TD0                          1
SFO1                125.7703643 MHz
NUC1                        13C
P0                        3.00 usec
P1                        9.00 usec
PLW1                113.54000092 W
SFO2                500.1320005 MHz
NUC2                        1H
CPDPRG[2                waltz65
PCPD2                    80.00 usec
PLW2                25.47599983 W
PLW12                0.25476000 W
PLW13                0.12814000 W

F2 - Processing parameters
SI                       32768
SF                  125.7577987 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40


LYL01046
```

^{1}H-NMR (500 MHz, $CDCl_3$)



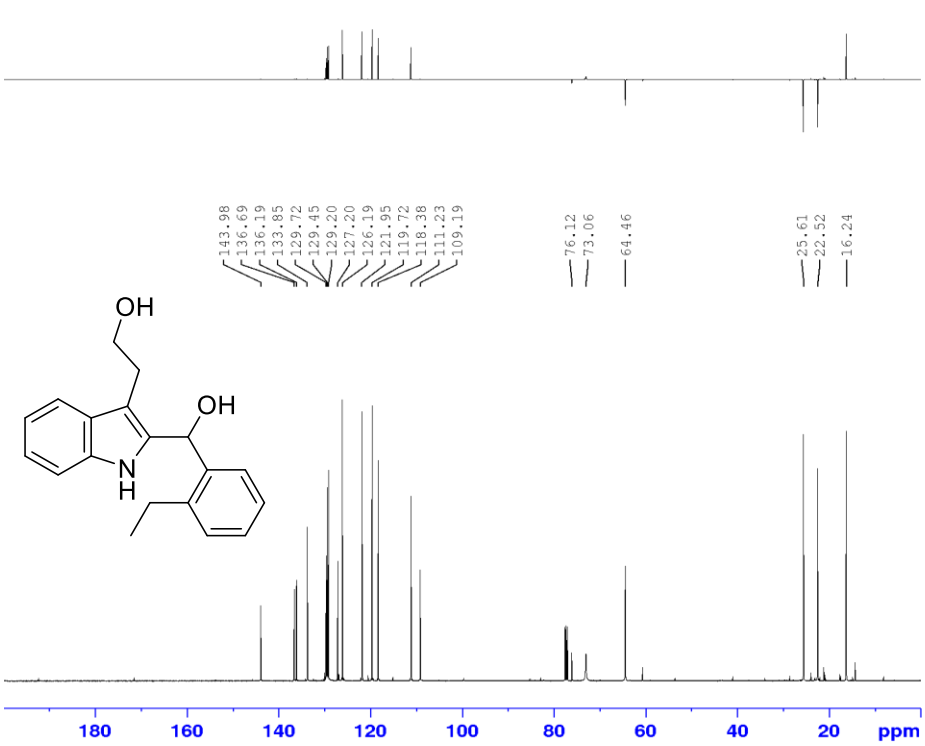

```
Current Data Parameters
NAME             LYL01047
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_             20230814
Time                6.10 h
INSTRUM           Avance
PROBHD    Z151574_0127 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           10000.000 Hz
FIDRES        0.305176 Hz
AQ            3.2767999 sec
RG               16.7782
DW               50.000 usec
DE               11.14 usec
TE                296.9 K
D1            1.00000000 sec
TD0                    1
SFO1         500.1330883 MHz
NUC1                1H
P0                2.67 usec
P1                8.00 usec
PLW1         25.47599983 W

F2 - Processing parameters
SI                 65536
SF            500.1301097 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00


LYL01047
```

^{13}C-NMR (125 MHz, $CDCl_3$)



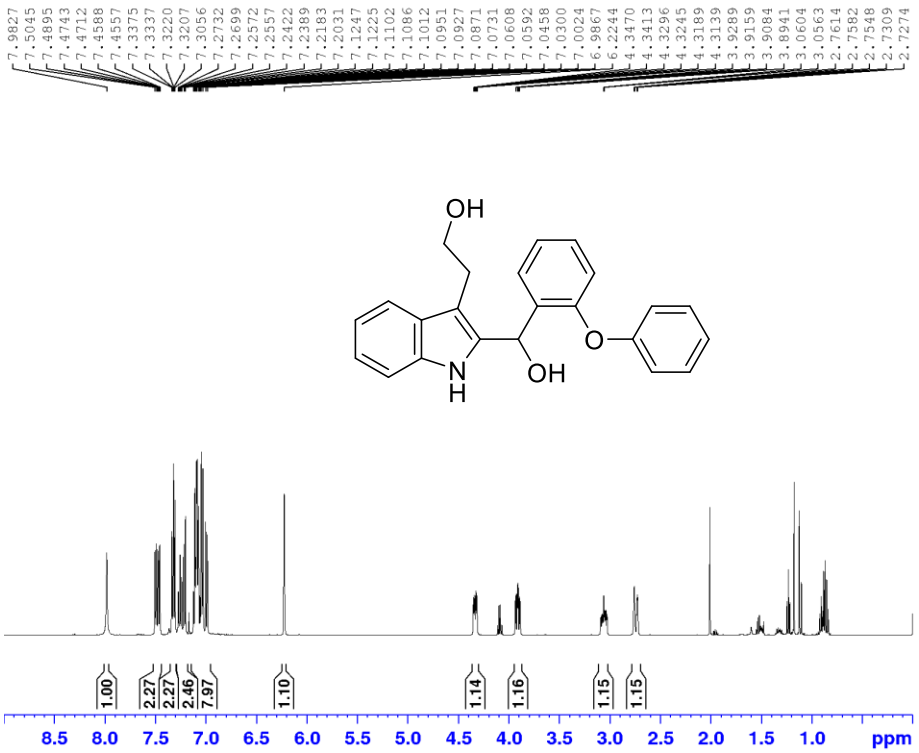

```
Current Data Parameters
NAME             LYL01047
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_             20230814
Time                7.05 h
INSTRUM           Avance
PROBHD    Z151574_0127 (
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH           30120.482 Hz
FIDRES        0.919204 Hz
AQ            1.0878977 sec
RG                   101
DW               16.600 usec
DE                6.50 usec
TE                298.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1
SFO1         125.7703643 MHz
NUC1                13C
P0                3.00 usec
P1                9.00 usec
PLW1         113.54000092 W
SFO2          500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz65
PCPD2             80.00 usec
PLW2         25.47599983 W
PLW12         0.25476000 W
PLW13         0.12814000 W

F2 - Processing parameters
SI                 32768
SF            125.7577885 MHz
WDW                   EM
SSB                    0
LB                1.00 Hz
GB                     0
PC                1.40


LYL01047
```

^{1}H-NMR (500 MHz, $CDCl_3$)



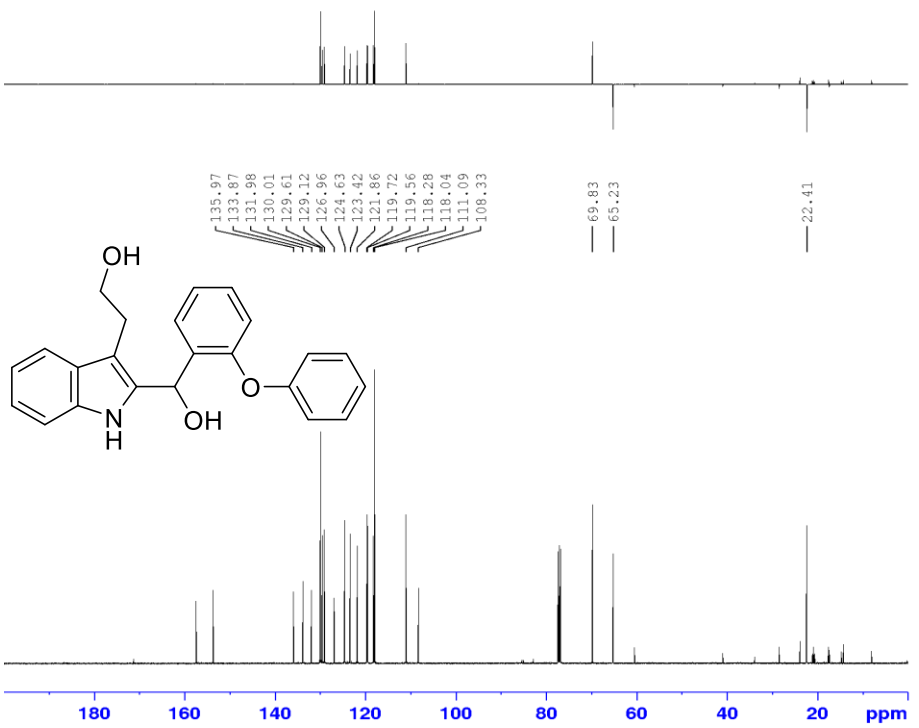

```
Current Data Parameters
NAME                  LYL01051
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20230830
Time                     14.54 h
INSTRUM                 Avance
PROBHD    Z151574_0127 (
PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                         16
DS                          2
SWH                10000.000 Hz
FIDRES             0.305176 Hz
AQ                 3.2767999 sec
RG                         32
DW                     50.000 usec
DE                     11.14 usec
TE                     296.1 K
D1                 1.00000000 sec
TD0                         1
SFO1               500.1330883 MHz
NUC1                       1H
P0                      2.67 usec
P1                      8.00 usec
PLW1               25.47599983 W

F2 - Processing parameters
SI                      65536
SF                 500.1300575 MHz
WDW                        EM
SSB                         0
LB                      0.30 Hz
GB                          0
PC                      1.00


LYL01051
```

^{13}C-NMR (125 MHz, $CDCl_3$)



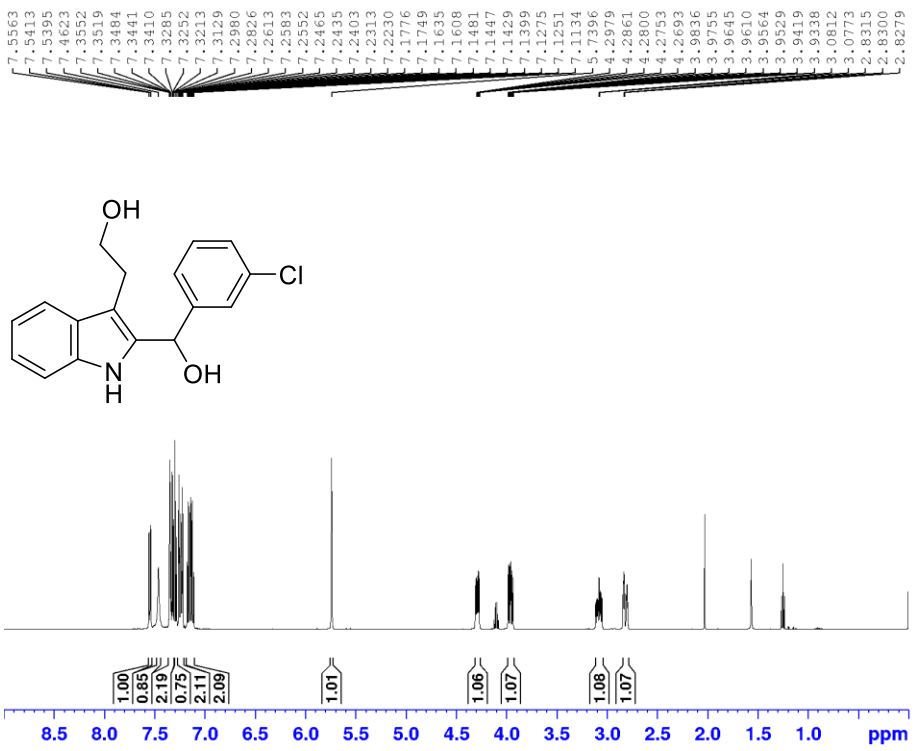

```
Current Data Parameters
NAME                  LYL01051
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20230830
Time                     15.11 h
INSTRUM                 Avance
PROBHD    Z151574_0127 (
PULPROG                zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                         311
DS                           4
SWH                30120.482 Hz
FIDRES             0.919204 Hz
AQ                 1.0878977 sec
RG                         101
DW                     16.600 usec
DE                      6.50 usec
TE                     297.2 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                         1
SFO1               125.7703643 MHz
NUC1                       13C
P0                      3.00 usec
P1                      9.00 usec
PLW1               113.54000092 W
SFO2               500.1320005 MHz
NUC2                       1H
CPDPRG[2                waltz65
PCPD2                  80.00 usec
PLW2               25.47599983 W
PLW12               0.25476000 W
PLW13               0.12814000 W

F2 - Processing parameters
SI                      32768
SF                 125.7577885 MHz
WDW                        EM
SSB                         0
LB                      1.00 Hz
GB                          0
PC                      1.40


LYL01051
```

^{1}H-NMR (500 MHz, $CDCl_3$)



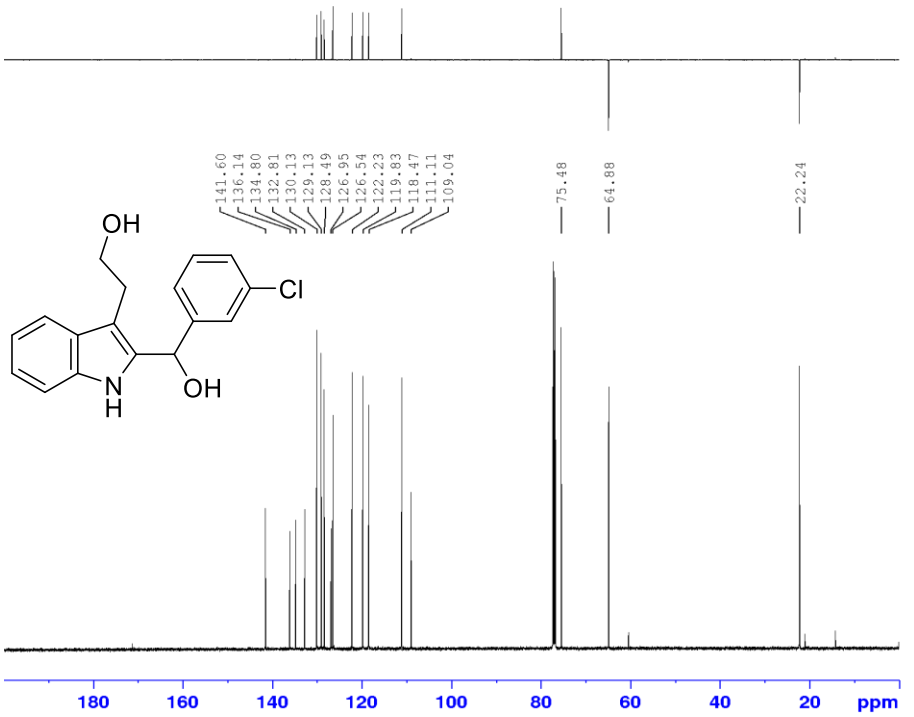

```
Current Data Parameters
NAME              LYL01053
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_            20230906
Time               14.22 h
INSTRUM            Avance
PROBHD    Z151574_0127 (
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH            10000.000 Hz
FIDRES          0.305176 Hz
AQ              3.2767999 sec
RG                    101
DW                 50.000 usec
DE                 11.14 usec
TE                 296.2 K
D1             1.00000000 sec
TD0                     1
SFO1         500.1330883 MHz
NUC1                   1H
P0                  2.67 usec
P1                  8.00 usec
PLW1         25.47599983 W

F2 - Processing parameters
SI                  65536
SF           500.1300257 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00

LYL01053
```

^{13}C-NMR (125 MHz, $CDCl_3$)



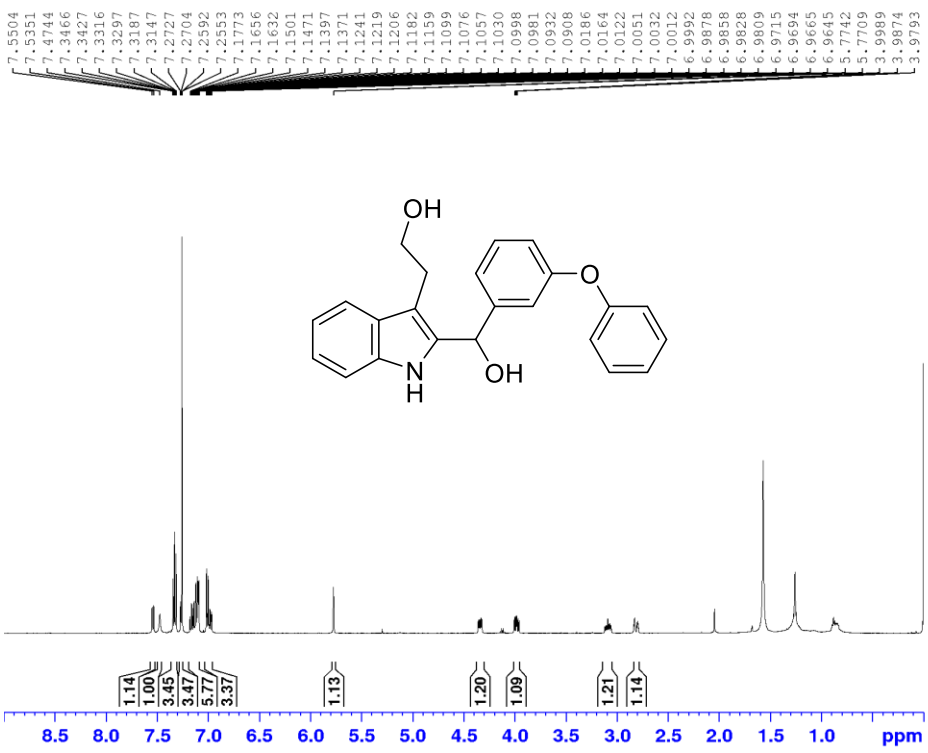

```
Current Data Parameters
NAME              LYL01053
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_            20230906
Time               15.17 h
INSTRUM            Avance
PROBHD    Z151574_0127 (
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                   1024
DS                      4
SWH            30120.482 Hz
FIDRES          0.919204 Hz
AQ              1.0878977 sec
RG                    101
DW                 16.600 usec
DE                  6.50 usec
TE                 297.4 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                     1
SFO1         125.7703643 MHz
NUC1                   13C
P0                  3.00 usec
P1                  9.00 usec
PLW1         113.54000092 W
SFO2         500.1320005 MHz
NUC2                   1H
CPDPRG[2          waltz65
PCPD2              80.00 usec
PLW2         25.47599983 W
PLW12         0.25476000 W
PLW13         0.12814000 W

F2 - Processing parameters
SI                  32768
SF           125.7577885 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40

LYL01053
```

^{1}H-NMR (500 MHz, $CDCl_3$)



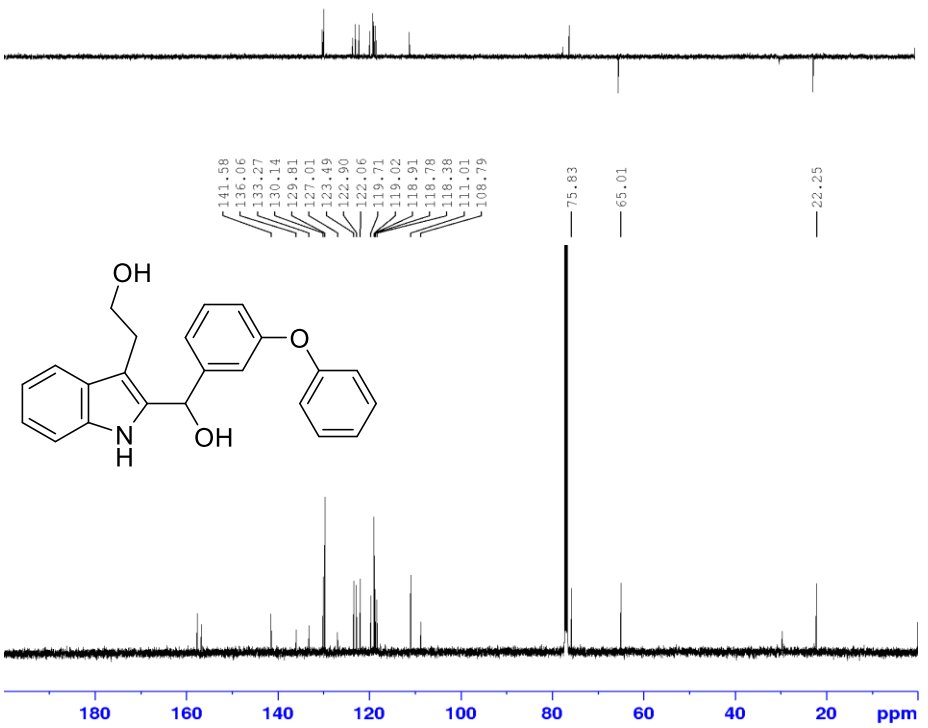

```
Current Data Parameters
NAME                  LYL01060
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20230919
Time                     15.31 h
INSTRUM                 Avance
PROBHD    Z151574_0127 (
PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                         16
DS                          2
SWH                 10000.000 Hz
FIDRES                0.305176 Hz
AQ                    3.2767999 sec
RG                        101
DW                     50.000 usec
DE                     11.14 usec
TE                     296.7 K
D1                  1.00000000 sec
TD0                         1
SFO1               500.1330883 MHz
NUC1                       1H
P0                      2.67 usec
P1                      8.00 usec
PLW1               25.47599983 W

F2 - Processing parameters
SI                      65536
SF                 500.1300125 MHz
WDW                        EM
SSB                         0
LB                       0.30 Hz
GB                          0
PC                       1.00


LYL01060
```

^{13}C-NMR (125 MHz, $CDCl_3$)



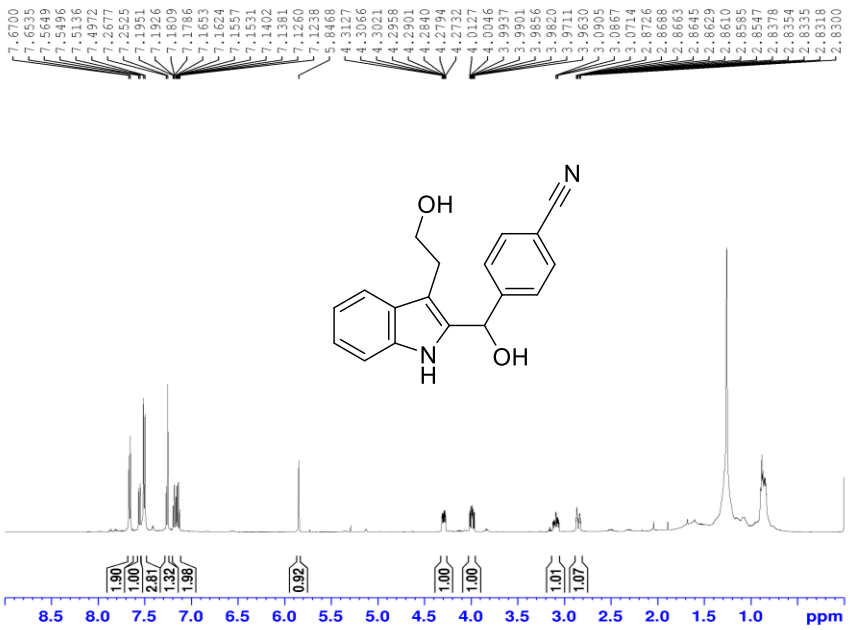

```
Current Data Parameters
NAME                  LYL01060
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20230919
Time                     16.39 h
INSTRUM                 Avance
PROBHD    Z151574_0127 (
PULPROG                zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                        1280
DS                           4
SWH                30120.482 Hz
FIDRES                0.919204 Hz
AQ                    1.0878977 sec
RG                        101
DW                     16.600 usec
DE                      6.50 usec
TE                     297.9 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                         1
SFO1               125.7703643 MHz
NUC1                       13C
P0                      3.00 usec
P1                      9.00 usec
PLW1               113.54000092 W
SFO2               500.1320005 MHz
NUC2                       1H
CPDPRG[2                waltz65
PCPD2                   80.00 usec
PLW2               25.47599983 W
PLW12               0.25476000 W
PLW13               0.12814000 W

F2 - Processing parameters
SI                      32768
SF                 125.7577895 MHz
WDW                        EM
SSB                         0
LB                       1.00 Hz
GB                          0
PC                       1.40


LYL01060
```

^{1}H-NMR (500 MHz, $CDCl_3$)



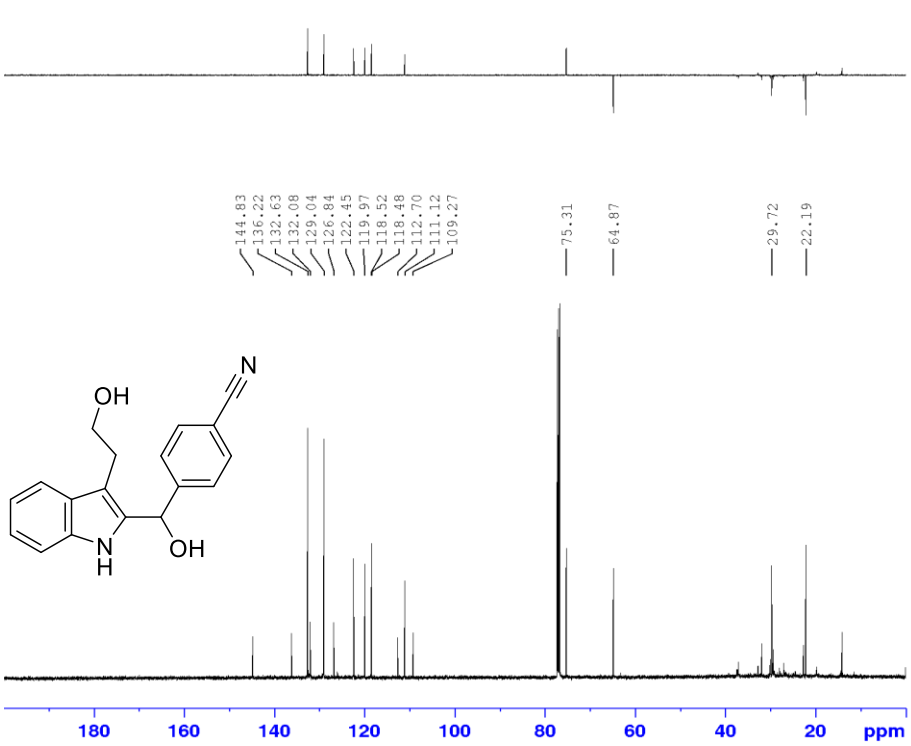

```
Current Data Parameters
NAME                  LYL01059
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_               20230919
Time                  13.49 h
INSTRUM                Avance
PROBHD    Z151574_0127 (
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         2
SWH               10000.000 Hz
FIDRES            0.305176 Hz
AQ                3.2767999 sec
RG                       101
DW                  50.000 usec
DE                  11.14 usec
TE                  296.6 K
D1                1.00000000 sec
TD0                        1
SFO1           500.1330883 MHz
NUC1                      1H
P0                    2.67 usec
P1                    8.00 usec
PLW1           25.47599983 W

F2 - Processing parameters
SI                     65536
SF                500.1300159 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00


LYL01059
```

^{13}C-NMR (125 MHz, $CDCl_3$)



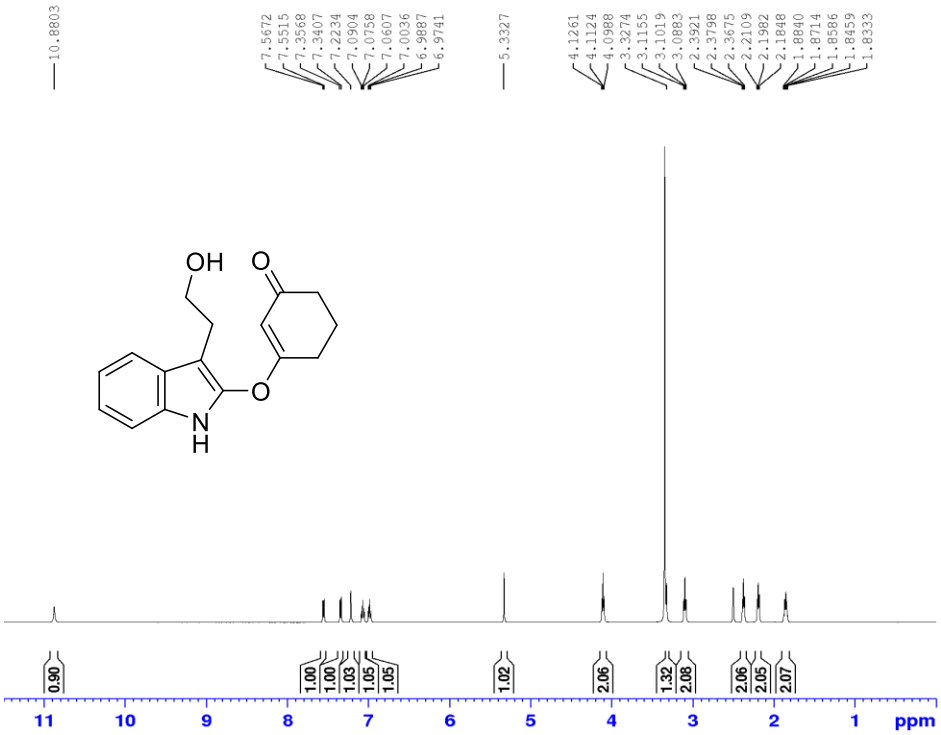

```
Current Data Parameters
NAME                  LYL01059
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_               20230919
Time                  14.58 h
INSTRUM                Avance
PROBHD    Z151574_0127 (
PULPROG                zgpg30
TD                     65536
SOLVENT                CDCl3
NS                      1280
DS                         4
SWH               30120.482 Hz
FIDRES            0.919204 Hz
AQ                1.0878977 sec
RG                       101
DW                  16.600 usec
DE                   6.50 usec
TE                  297.8 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                        1
SFO1           125.7703643 MHz
NUC1                      13C
P0                    3.00 usec
P1                    9.00 usec
PLW1          113.54000092 W
SFO2           500.1320005 MHz
NUC2                      1H
CPDPRG[2              waltz65
PCPD2                80.00 usec
PLW2           25.47599983 W
PLW12           0.25476000 W
PLW13           0.12814000 W

F2 - Processing parameters
SI                     32768
SF                125.7577885 MHz
WDW                       EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.40


LYL01059
```

^{1}H-NMR (500 MHz, DMSO)

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Current Data Parameters
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EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
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Time                      17.19 h
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PROBHD    Z151574_0127 (
PULPROG                   zg30
TD                       65536
SOLVENT                   DMSO
NS                          16
DS                           2
SWH                  10000.000 Hz
FIDRES                0.305176 Hz
AQ                    3.2767999 sec
RG                          101
DW                     50.000 usec
DE                     11.14 usec
TE                     298.0 K
D1                   1.00000000 sec
TD0                           1
SFO1                500.1330883 MHz
NUC1                         1H
P0                        2.67 usec
P1                        8.00 usec
PLW1                25.47599983 W

F2 - Processing parameters
SI                        65536
SF                  500.1300000 MHz
WDW                          EM
SSB                           0
LB                         0.30 Hz
GB                            0
PC                         1.00

YX01155-1
```
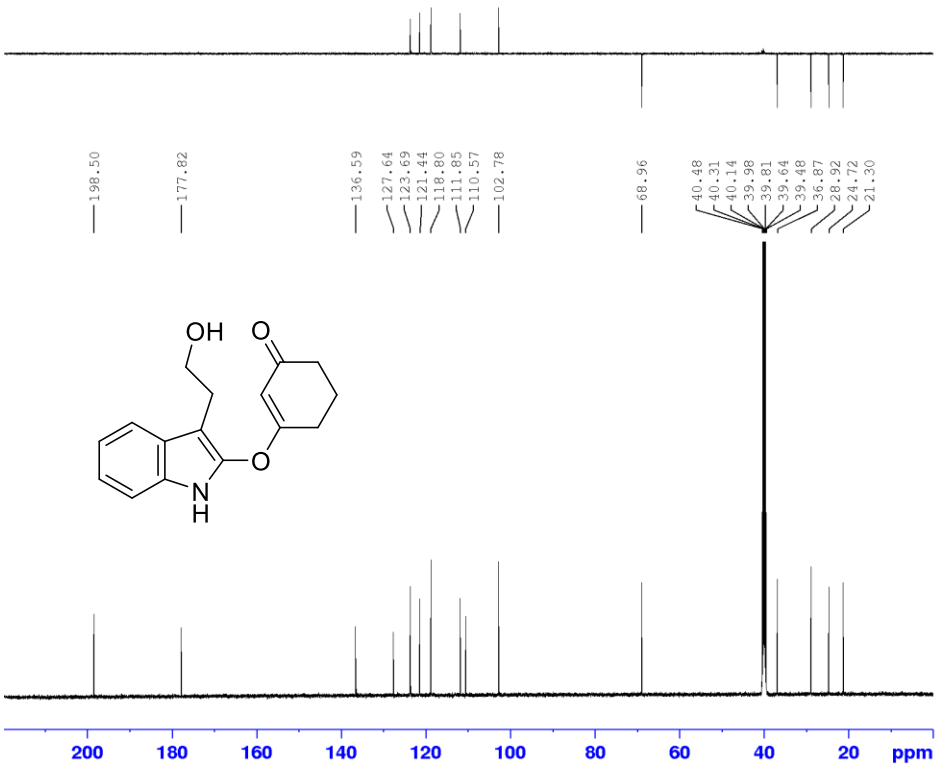

^{13}C-NMR (125 MHz, DMSO)

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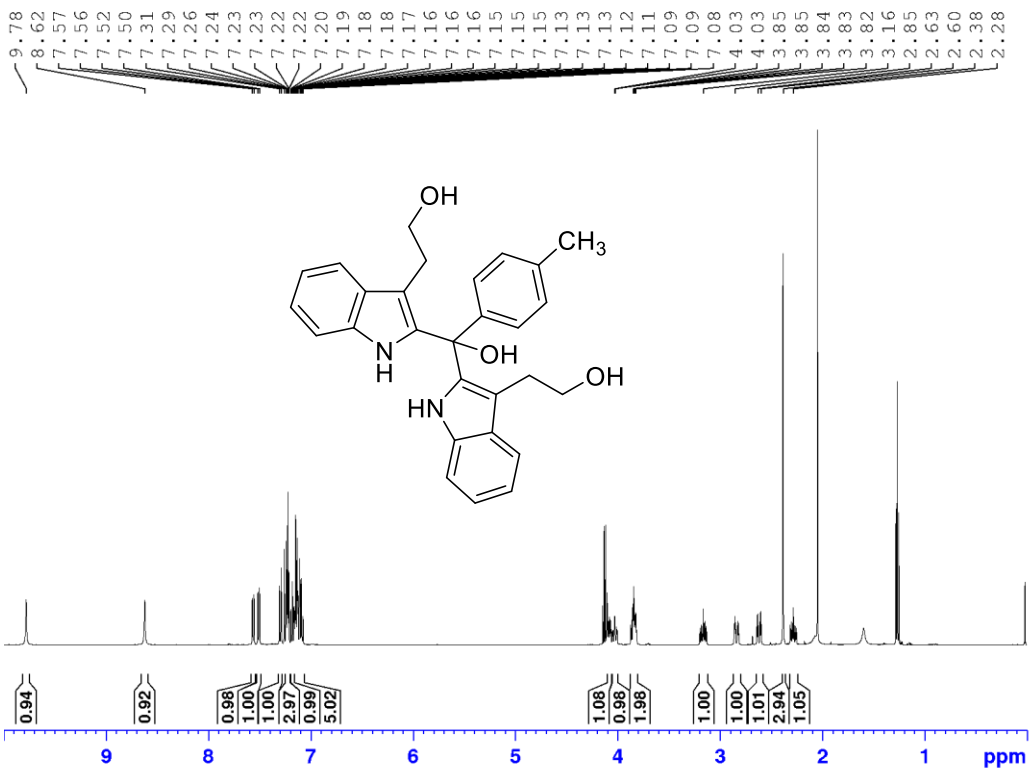
Current Data Parameters
NAME                  YX01155-1
EXPNO                         2
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20230610
Time                       4.34 h
INSTRUM                  Avance
PROBHD    Z151574_0127 (
PULPROG                 zgpg30
TD                       65536
SOLVENT                   DMSO
NS                         1024
DS                            4
SWH                  30120.482 Hz
FIDRES                0.919204 Hz
AQ                    1.0878977 sec
RG                          101
DW                     16.600 usec
DE                      6.50 usec
TE                     298.0 K
D1                   2.00000000 sec
D11                  0.03000000 sec
TD0                           1
SFO1                125.7703643 MHz
NUC1                         13C
P0                        3.00 usec
P1                        9.00 usec
PLW1               113.54000092 W
SFO2                500.1320005 MHz
NUC2                         1H
CPDPRG[2                waltz65
PCPD2                    80.00 usec
PLW2                25.47599983 W
PLW12                0.25476000 W
PLW13                0.12814000 W

F2 - Processing parameters
SI                        32768
SF                  125.7577885 MHz
WDW                          EM
SSB                           0
LB                         1.00 Hz
GB                            0
PC                         1.40

YX01155-1
```

^{1}H-NMR (500 MHz, $CDCl_3$)

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Current Data Parameters
NAME          LYL01030-2
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230714
Time               12.10 h
INSTRUM           Avance
PROBHD   Z151574_0127 (
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH           10000.000 Hz
FIDRES            0.305176 Hz
AQ             3.2767999 sec
RG                  101
DW                50.000 usec
DE                11.14 usec
TE                298.0 K
D1            1.00000000 sec
TD0                    1
SFO1          500.1330883 MHz
NUC1                  1H
P0                 2.67 usec
P1                 8.00 usec
PLW1          25.47599983 W

F2 - Processing parameters
SI                 65536
SF            500.1300114 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```
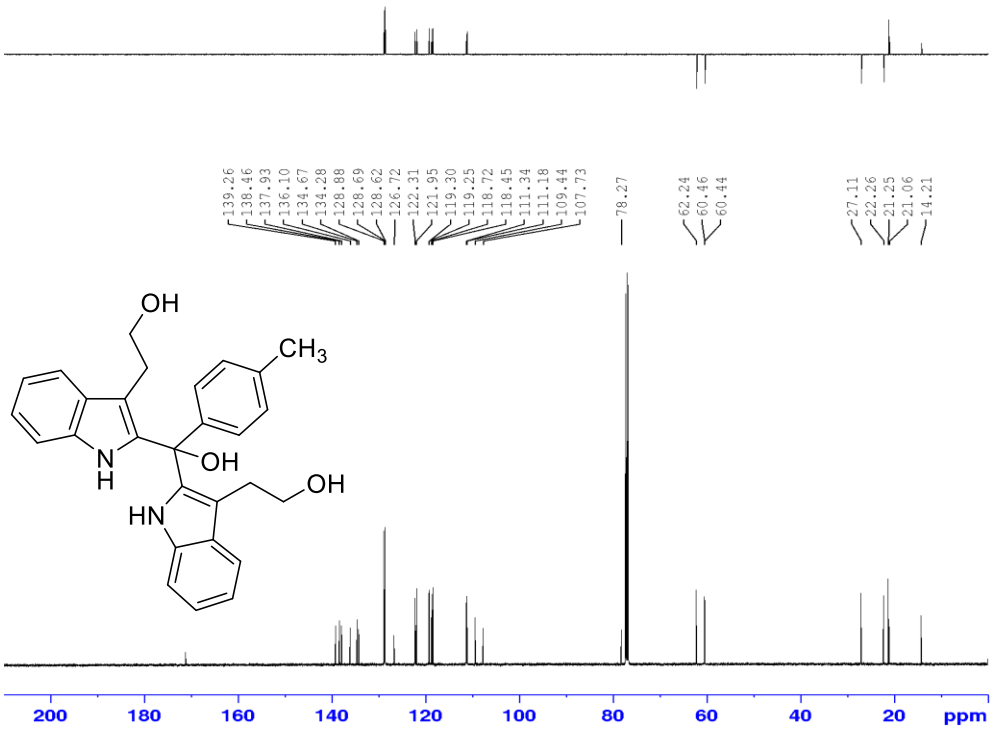

^{13}C-NMR (125 MHz, $CDCl_3$)




```
Current Data Parameters
NAME          LYL01030-2
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230714
Time               13.05 h
INSTRUM           Avance
PROBHD   Z151574_0127 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           30120.482 Hz
FIDRES            0.919204 Hz
AQ             1.0878977 sec
RG                  101
DW                16.600 usec
DE                 6.50 usec
TE                298.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1
SFO1          125.7703643 MHz
NUC1                  13C
P0                 3.00 usec
P1                 9.00 usec
PLW1         113.54000092 W
SFO2          500.1320005 MHz
NUC2                  1H
CPDPRG[2          waltz65
PCPD2             80.00 usec
PLW2          25.47599983 W
PLW12          0.25476000 W
PLW13          0.12814000 W

F2 - Processing parameters
SI                 32768
SF            125.7577885 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40

LYL01030-2
```

3. Computational experiments data

Geometries and Energies for All Optimized Starting Materials, Transition States, Intermediates, and Target Materials

Single Point Energy■,Δ (*E*M06, in Hartree)
Zero-point correction (*E*0, in Hartree)
Thermal correction to Enthalpy (*H*, in Hartree)
Thermal correction to Gibbs Free Energy (*G*, in Hartree)
Sum of electronic and zero-point Energies (*E*M06+*E*0, in Hartree)
Sum of electronic and thermal Enthalpies (*E*M06+*H*, in Hartree)
Sum of electronic and thermal Free Energies (*E*M06+*G*, in Hartree)
■ The single-point energies and solvent effects were computed at the M06/6-31+G(d) level
Δ The single-point energies and solvent effects were computed at the M06/6-311+G(2d,2p) level

Gaussian program 16 was employed for DFT calculations, and /M06-2X/def2-SVP level were used for geometry optimization and frequency calculations. The 6-311+G(2d,p) basis sets were employed in the calculations of triplet-singlet energy gaps. In the model substrate's reaction profile calculations, 6-31G(d,p) basis sets were used. Optimizations were conducted without constraint using the implicit solvation model (SMD)19 in dichloromethane (ε = 8.93). Frequency analyses (at 298.15 K and 1 atm) were carried out to confirm that each structure is a minimum (no imaginary frequency) or a transition state (only one imaginary frequency). The searching for minimal energy crossing points was conducted using a modified version of Harvey's code20 (sobMECP21) interfaced with Gaussian 16. The Gibbs free energies in dichloromethane (ΔG) were discussed throughout this Article unless otherwise specified. The single-point calculations were at M06-2X/def2-TZVP level. The SMD implicit solvent model was used to account for water's solvation effect. The 3D images of the calculated structures and the orbital diagrams were prepared using CYLView22 or VMD.

1 Tryptophol
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.619500	-0.290149	0.005676
2	6	0	-1.485741	0.915736	-0.024440
3	6	0	-2.909779	0.741402	-0.033323
4	6	0	-3.433750	-0.509071	-0.014244
5	6	0	-2.591872	-1.681040	0.015025
6	6	0	-1.239448	-1.583847	0.024749
7	6	0	0.687833	0.103649	0.009428
8	6	0	0.751343	1.608437	-0.018376
9	1	0	-3.545006	1.638685	-0.055652
10	1	0	-4.522510	-0.668000	-0.020552
11	1	0	-3.090159	-2.661960	0.029246
12	1	0	-0.591910	-2.472288	0.047017
13	1	0	1.273614	2.006247	0.888077
14	1	0	-0.998497	3.072654	-0.060908
15	7	0	-0.695068	2.028770	-0.038651
16	6	0	1.951804	-0.775685	0.036791
17	1	0	1.965297	-1.352896	0.937649
18	1	0	1.947575	-1.432683	-0.807742
19	6	0	3.202442	0.121322	-0.016911
20	1	0	3.233689	0.742226	0.853951
21	1	0	3.163249	0.735914	-0.891920
22	8	0	4.374369	-0.696923	-0.061237
23	1	0	5.155188	-0.138436	-0.064968

Rotational constants (GHZ): 2.2183356 0.5197959 0.4239576
Standard basis: 6-31G(d) (6D, 7F)
There are 202 symmetry adapted cartesian basis functions of A symmetry.
There are 202 symmetry adapted basis functions of A symmetry.
202 basis functions, 380 primitive gaussians, 202 cartesian basis functions
43 alpha electrons 43 beta electrons
nuclear repulsion energy 643.9649887180 Hartrees.
NAtoms= 23 NActive= 23 NUniq= 23 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
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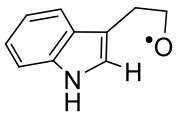
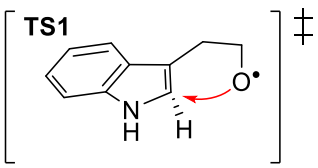
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
Nuclear repulsion after empirical dispersion term = 643.9429154510 Hartrees.



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.559404	-0.290709	0.005266
2	6	0	-1.423360	0.916831	-0.024174
3	6	0	-2.847733	0.745219	-0.032111
4	6	0	-3.374080	-0.504252	-0.012775
5	6	0	-2.534423	-1.677830	0.015837
6	6	0	-1.181809	-1.583222	0.024658
7	6	0	0.748681	0.100589	0.008167
8	6	0	0.815048	1.605256	-0.019564
9	1	0	-3.481260	1.643715	-0.053944
10	1	0	-4.463145	-0.661101	-0.018362
11	1	0	-3.034574	-2.657797	0.030319
12	1	0	-0.535955	-2.472901	0.046422
13	1	0	1.338689	2.001996	0.886568
14	1	0	-0.932019	3.072817	-0.060805
15	7	0	-0.630570	2.028352	-0.038833
16	6	0	2.010988	-0.781160	0.034611
17	1	0	2.023985	-1.358467	0.935416
18	1	0	2.004935	-1.438083	-0.809969
19	6	0	3.263302	0.113459	-0.019865
20	1	0	3.296321	0.734235	0.851024
21	1	0	3.224694	0.728194	-0.894800
22	8	0	4.433633	-0.707019	-0.065042

Rotational constants (GHZ): 2.2184832 0.5347696 0.4338695
Standard basis: 6-31G(d) (6D, 7F)
There are 200 symmetry adapted cartesian basis functions of A symmetry.
There are 200 symmetry adapted basis functions of A symmetry.
200 basis functions, 376 primitive gaussians, 200 cartesian basis functions
43 alpha electrons 42 beta electrons
nuclear repulsion energy 631.1210890369 Hartrees.
NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
Nuclear repulsion after empirical dispersion term = 631.0994529136 Hartrees.



Input orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-0.483721	0.409009	-0.558946
2	6	0	-0.972741	1.111212	0.579850
3	6	0	-2.118431	1.896574	0.527566
4	6	0	-2.780477	1.975963	-0.693982
5	6	0	-2.307720	1.303700	-1.838165
6	6	0	-1.162808	0.526958	-1.785462
7	6	0	0.688283	-0.282103	-0.154831
8	6	0	0.909662	0.057848	1.206991
9	1	0	-2.479239	2.427778	1.403175
10	1	0	-3.682417	2.576947	-0.767292
11	1	0	-2.851800	1.401404	-2.773010
12	1	0	-0.795653	0.009040	-2.667195
13	1	0	1.511939	-0.458437	1.938106
14	1	0	-0.249449	1.169809	2.578025
15	7	0	-0.110645	0.861327	1.626255
16	6	0	1.845227	-0.749398	-0.969534
17	1	0	2.259133	-1.673784	-0.551109
18	1	0	1.586129	-0.922771	-2.017520
19	6	0	2.813856	0.425319	-0.789219
20	1	0	2.532501	1.216385	-1.506574
21	1	0	3.856613	0.140499	-1.008349
22	8	0	2.734169	0.867139	0.542900

Rotational constants (GHZ): 2.0133165 0.7437634 0.6045868
Standard basis: 6-31G(d) (6D, 7F)
200 basis functions, 376 primitive gaussians, 200 cartesian basis functions
43 alpha electrons 42 beta electrons
nuclear repulsion energy 669.6107434781 Hartrees.
NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned off.
Nuclear repulsion after empirical dispersion term = 669.5883129015 Hartrees.
Force inversion solution in PCM.

4. X-ray crystal structure experiments data

Experimental. Single block crystals of **target molecules** were used as supplied. A suitable crystal with dimensions 0.20 × 0.15 × 0.10 mm^3 was selected and mounted on a Bruker APEX-II CCD diffractometer. The crystal was kept at a steady T = 296.15 K during data collection. The structure was solved with the ShelXT 2018/2 solution program using dual methods and by using Olex2 as the graphical interface. The model was refined with ShelXL 2018/3 using full matrix least squares minimisation on $\boldsymbol{F^2}$.

Structure Quality Indicators

Reflections:	d min (Mo) 2θ=55.0°	0.77	I/σ(I)	21.5	Rint	3.41%	Full 50.5° 99% to 55.0°	99.9	
Refinement:	Shift	0.001	Max Peak	0.2	Min Peak	-0.4	GooF	1.039	Flack -.3(5)

A block-shaped crystal with dimensions 0.20 × 0.15 × 0.10 mm^3 was mounted. Data were collected using a Bruker APEX-II CCD diffractometer operating at T = 296.15 K.

Data were measured using *f* and *w* scans using MoK_a radiation. The maximum resolution that was achieved was Q = 27.484 (0.77 Å).

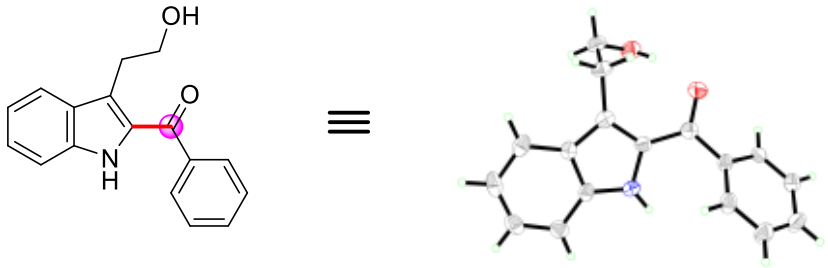
The unit cell was refined using SAINT (Bruker, V8.34A, after 2013) on 4339 reflections, 23% of the observed reflections.

Data reduction, scaling and absorption corrections were performed using SAINT (Bruker, V8.34A, after 2013). The final completeness is 99.80 % out to 27.484° in Q. A multi-scan absorption correction was performed using SADABS-2014/5 (Bruker, 2014/5) was used for absorption correction. wR_2(int) was 0.0371 before and 0.0319 after correction. The Ratio of minimum to maximum transmission is 0.9501. The l/2 correction factor is 0.00150. The absorption coefficient m of this material is 0.099 mm^{-1} at this wavelength (l = 0.71073Å) and the minimum and maximum transmissions are 0.708 and 0.746.

The structure was solved and the space group $P2_12_12_1$ (# 19) determined by the ShelXT 2018/2 structure solution program using using dual methods and refined by full matrix least squares minimisation on $\boldsymbol{F^2}$ using version 2018/3 of ShelXL 2018/3. All non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were calculated geometrically and refined using the riding model. Hydrogen atom positions were calculated geometrically and refined using the riding model.

_exptl_absorpt_process_details: SADABS-2014/5 (Bruker,2014/5) was used for absorption correction.wR_2(int) was 0.0371 before and 0.0319 after correction. The Ratio of minimum to maximum transmission is 0.9501. The l/2 correction factor is 0.00150.

X-ray crystal structure data (1)



3b (87%)

3b X-ray CCDC: 2384776

Figure S4. X-ray crystal structure of **3b** product.

Datablock: a

Bond precision: C-C = 0.0097 A Wavelength=0.71073

Cell:	a=15.269(5)		b=10.765(3)	c=16.567(5)
Temperature:	alpha=90 296 K		beta=90	gamma=90
Volume Space	2723.1(14)		2723.0(14)	
group Hall group	Pna21P2c -	O_2	Pna21P2c-2n	
Moiety formula	2n$C_{17}H_{15}N$		$C_{17}H_{15}NO_2$	
Sum formula	$C_{17}H_{15}N$	O_2	$C_{17}H_{15}NO_2$	
Mr	265.30		265.30	
Dx,g cm-3	1.294		1.294	
Z	8		8	
Mu (mm-1)	0.085		0.085	
F000	1120.0		1120.0	
F000'	1120.50			
h,k,lmax	19,14,21		19,14,21	
Nref	6366[3293]		5800	
Tmin,Tmax	0.985,0.992		0.568,0.746	
Tmin'	0.983			

Correction method= # Reported T Limits: Tmin=0.568 Tmax=0.746 AbsCorr = MULTI-SCAN

Data completeness= 1.76/0.91 Theta(max)= 27.658

R(reflections)= 0.0732(3340)

wR2(reflections)= 0.1984(5800)

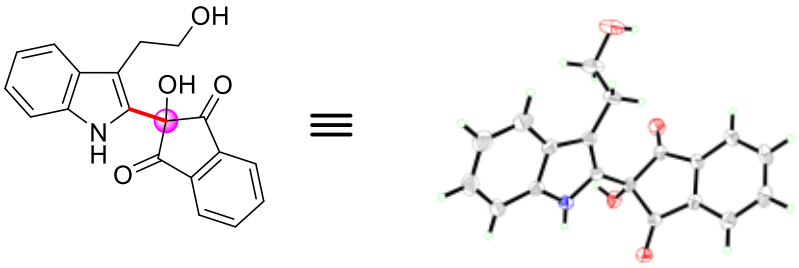
S = 1.102 Npar= 363

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

X-ray crystal structure data (2)



3c (81%)

3c X-ray CCDC: 2384775

Figure S5. X-ray crystal structure of **3c** product

Datablock: a

Bond precision:	C-C = 0.0057 A	Wavelength=0.71073	
Cell:	a=9.8256(7)	b=17.7127(12)	c=18.3028(12)
Temperature:	alpha=90 296 K	beta=90	gamma=90
Volume	3185.4(4)		3185.4(4)
Space group	P 21 21 21		P 21 21 21
Hall group	P 2ac 2ab		P 2ac 2ab
Moiety formula	$2(C_{19}H_{15}NO_4),C_{38}H_{32}N_2O_9$	O	$2(C_{19}H_{15}NO_4), H_2O$
Sum formula			$C_{38}H_{32}N_2O_9$
Mr	660.66	2	660.65
Dx,g cm-3	1.378		1.378
Z	4		4
Mu (mm-1)	0.099		0.099
F000	1384.0		1384.0
F000’	1384.74		
h,k,lmax	12,23,23		12,22,23
Nref	7311[4087]		7245
Tmin,Tmax	0.982,0.990		0.708,0.746
Tmin’	0.980		

Correction method= # Reported T Limits: Tmin=0.708 Tmax=0.746 AbsCorr = MULTI-SCAN

Data completeness= 1.77/0.99

Theta(max)= 27.484 R(reflections)= 0.0525(4914)

wR2(reflections)= 0.1505(7245)

S = 1.039 Npar= 449

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.