

Supplementary Information for

Photoredox catalysed synthesis of amino alcohol

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General Information: Melting points were determined by an open glass capillary method and are uncorrected. All chemicals used were reagent grade and were used as received. IR spectra in KBr/neat were recorded on a Perkin-Elmer 993 IR spectrophotometer. ¹H NMR and ¹³C NMR spectra were recorded on a Bruker AVANCE DPX (400 MHz and 75 MHz) FT spectrometer in CDCl₃ using TMS as an internal reference (chemical shift in δ , ppm). Mass spectra were recorded on JEOL SX-303 (FAB) mass spectrophotometer. Elemental analyses were carried out using a Coleman automatic C, H, N analyser.

General Procedure for the photocatalysed synthesis of substituted amino alcohol (Table 2): A round bottom flask was charged with α , β - unsaturated aldehydes 1(a-l) (1.0 mmol), eosin Y (2 mol%), aminating reagent (1.0 mmol) and CH₃OH (3 mL) and the contents were stirred in open air under irradiation with Luxeon Rebel high power green LEDs [2.50 W, λ = 535 nm] at room temperature for 40-180 min. After the completion of reaction (as indicated by TLC), it was extracted with ethyl acetate (3 $\times$ 5 mL). The organic phase was dried over anhydrous magnesium sulfate and concentrated under reduced pressure to yield the crude product, which was purified by silica gel column chromatography using a mixture of EtOAc-Hexane to give the pure product 2(a-l) in high yields (62-92%) in table 2.

Gram Scale Reaction: A round bottom flask was charged with α , β - unsaturated aldehydes 1 (1.0g), eosin Y (2 mol%), aminating reagent (1.0 equiv.) and CH₃OH (3 mL) and the contents were stirred in open air under irradiation with Luxeon Rebel high power green LEDs [2.50 W, λ = 535 nm] at room temperature for 40-180 min. After the completion of reaction (as indicated by TLC), it was extracted with ethyl acetate (3 $\times$ 5 mL). The organic phase was dried over anhydrous magnesium sulfate and concentrated under reduced pressure to yield the crude product, which was purified by silica gel column chromatography using a mixture of EtOAc-Hexane to give the pure product 2.

(2S,3S,4R)-4-(dibenzylamino)-3-methyl-4-phenylbutan-2-ol (2a): m.p. 220°C, m/z: 331.19; Mol. Wt: 331.46. IR (thin film, cm⁻¹) 2972, 1452, 907, 731, 698; ¹H NMR (400 MHz, CDCl₃): 7.44 – 7.06 (m, 15H), 4.70 (br, s, 1H, -OH, exchangeable with D₂O), 4.44 – 4.01 (m, 1H), 3.59 (d, J = 11.3 Hz, 1H), 2.50 – 2.43 (m, 1H), 0.87 (d, J = 6.5 Hz, 3H), 0.40 (d, J = 6.8 Hz, 3H); ¹³C NMR (101 MHz, CDCl₃): 149.1, 140.5, 129.6, 128.5, 128.1, 125.9, 121.9, 119.1, 71.3, 71.1, 42.9, 22.6, 14.6. Anal. Calcd for C₂₃H₂₅NO: C, 83.34; H, 7.60; N, 4.23. Found: C, 83.32; H, 7.58; N, 4.20.

(2S,3S,4R)-4-(dibenzylamino)-4-(3-methoxyphenyl)-3-methylbutan-2-ol (2b): m.p. 260°C, m/z: 361.20; Mol. Wt: 361.49. IR (thin film, cm⁻¹) 2970, 1492, 1258, 910, 576; ¹H NMR (400 MHz, CDCl₃): 7.40 – 6.91 (m, 14H), 4.70 (br, s, 1H, -OH, exchangeable with D₂O), 4.44 – 4.01 (m, 1H), 3.59 (d, J = 11.3 Hz, 1H), 3.70 (s, 3H, -OCH₃), 2.50 – 2.43 (m, 1H), 0.87 (d, J = 6.5 Hz, 3H), 0.40 (d, J = 6.8 Hz, 3H); ¹³C NMR (101 MHz, CDCl₃): 160.4, 149.1, 141.5, 129.6, 129.5, 121.9, 120.4, 119.1, 113.2, 111.5, 71.3, 55.8, 42.9, 22.6, 14.6. Anal. Calcd for C₂₄H₂₇NO₂: C, 79.74; H, 7.53; N, 3.87. Found: C, 79.72; H, 7.51; N, 3.85.

(2S,3S,4R)-4-(dibenzylamino)-4-(2-fluorophenyl)-3-methylbutan-2-ol (2c): m.p. 230°C, m/z: 349.18; Mol. Wt: 349.45. IR (thin film, cm⁻¹) 2972, 1486, 1452, 750, 699; ¹H NMR (400 MHz, CDCl₃): 7.71 – 7.06 (m, 14H), 4.70 (br, s, 1H, -OH, exchangeable with D₂O), 4.44 – 4.01 (m, 1H), 3.59 (d, *J* = 11.3 Hz, 1H), 2.50 – 2.43 (m, 1H), 0.87 (d, *J* = 6.5 Hz, 3H), 0.40 (d, *J* = 6.8 Hz, 3H); ¹³C NMR (101 MHz, CDCl₃): 160.6, 149.1, 129.6, 127.5, 124.1, 121.9, 119.1, 105.8, 71.3, 64.3, 42.9, 22.6, 14.6. Anal. Calcd for C₂₃H₂₄NFO: C, 79.05; H, 6.92; N, 4.01, F, 5.44. Found: C, 79.03; H, 6.90; N, 4.00, F, 5.41.

(2S,3S,4R)-4-(3-chlorophenyl)-4-(dibenzylamino)-3-methylbutan-2-ol (2d): m.p. 258°C, m/z: 365.15; Mol. Wt: 365.90. IR (thin film, cm⁻¹) 2972, 1453, 907, 733, 698; ¹H NMR (400 MHz, CDCl₃): 7.46 – 7.06 (m, 14H), 4.70 (br, s, 1H, -OH, exchangeable with D₂O), 4.44 – 4.01 (m, 1H), 3.59 (d, *J* = 11.3 Hz, 1H), 2.50 – 2.43 (m, 1H), 0.87 (d, *J* = 6.5 Hz, 3H), 0.40 (d, *J* = 6.8 Hz, 3H); ¹³C NMR (101 MHz, CDCl₃): 149.1, 141.9, 134.1, 129.9, 129.6, 127.9, 126.2, 126.0, 121.9, 119.1, 71.3, 70.6, 42.9, 22.6, 14.6. Anal. Calcd for C₂₃H₂₄NCIO: C, 75.50; H, 6.61; N, 3.83; Cl, 9.69. Found: C, 75.48; H, 6.59; N, 3.81, Cl, 9.67.

(2S,3S,3R)-(dibenzylamino)(phenylmethyl)pentan-2-ol (2e): m.p. 258°C, m/z: 345.21; Mol. Wt: 373.49. IR (thin film, cm⁻¹) 2967, 1493, 1453, 733, 698; ¹H NMR (400 MHz, CDCl₃): 7.40 – 7.06 (m, 15H), 4.70 (br, s, 1H, -OH, exchangeable with D₂O), 4.44 – 4.01 (m, 1H), 3.59 (d, *J* = 11.3 Hz, 1H), 2.25 – 2.05 (m, 1H), 1.60-1.40 (m, 2H), 0.93 (d, *J* = 6.5 Hz, 3H), 0.40 (d, *J* = 6.8 Hz, 3H); ¹³C NMR (101 MHz, CDCl₃): 149.1, 140.5, 129.6, 128.5, 128.1, 125.9, 121.9, 119.1, 68.8, 68.6, 48.6, 22.9, 17.2, 12.2. Anal. Calcd for C₂₄H₂₇NO: C, 83.44; H, 7.88; N, 4.05. Found: C, 83.41; H, 7.86; N, 4.03.

(2S,4R)-4-(dibenzylamino)-4-phenylbutan-2-ol (2f): m.p. 220°C, m/z: 361.20; Mol. Wt: 361.49. IR (thin film, cm⁻¹) 1493, 1452, 1073, 747, 697; ¹H NMR (400 MHz, CDCl₃): 7.40 – 7.06 (m, 15H), 4.70 (br, s, 1H, -OH, exchangeable with D₂O), 4.50 – 4.15 (m, 1H), 3.59 (d, *J* = 11.3 Hz, 1H), 1.96 (dd, *J* = 6.3 Hz, 2H), 0.70 (d, *J* = 6.8 Hz, 3H); ¹³C NMR (101 MHz, CDCl₃): 149.1, 140.5, 129.6, 128.5, 128.1, 125.9, 121.9, 119.1, 72.3, 66.5, 44.7, 23.5. Anal. Calcd for C₂₂H₂₃NO: C, 83.24; H, 7.30; N, 4.41. Found: C, 83.22; H, 7.28; N, 4.38.

(2S,3R)-3-(diphenylamino)-3-(4-(1-hydroxyethyl)phenyl)-2-methylpropan-1-ol (2g): m.p. 275°C, m/z: 389.24; Mol. Wt: 389.54. IR (thin film, cm⁻¹) 3340, 2967, 1453, 1028, 733, 698; ¹H NMR (400 MHz, CDCl₃): 7.40 – 7.06 (m, 14H), 5.00-4.90 (m, 1H), 4.70 (br, s, 2H, -OH, exchangeable with D₂O), 3.10 – 3.40 (dd, 1H, *J* = 10.3 Hz, 1H), 3.60 (d, *J* = 11.3 Hz, 2H), 2.60 – 2.40 (m, 1H), 1.50 (d, *J* = 8.3 Hz, 3H), 0.40 (d, *J* = 6.8 Hz, 3H); ¹³C NMR (101 MHz, CDCl₃): 149.1, 142.9, 141.1, 129.6, 127.2, 125.1, 121.9, 119.1, 73.6, 69.9, 65.5, 38.3, 22.8, 12.1. Anal. Calcd for C₂₄H₂₇NO₂: C, 79.74; H, 7.53; N, 3.87. Found: C, 79.72; H, 7.51; N, 3.85.

(2S,3R)-3-(dibenzylamino)-2-methyl-3-phenylpropan-1-ol (2h): m.p. 218°C, m/z: 317.18; Mol. Wt: 317.43. IR (thin film, cm⁻¹) 3027, 2926, 1452, 908, 729, 697; ¹H NMR (400 MHz, CDCl₃): 7.40 – 7.06 (m, 15H), 4.70 (br, s, 1H, -OH, exchangeable with D₂O), 3.10 – 3.40 (dd, *J* = 10.3 Hz, 1H), 3.60 (d, *J* = 11.3 Hz, 2H), 2.60 – 2.40 (m, 1H), 0.40 (d, *J* = 6.8 Hz, 3H); ¹³C NMR (101 MHz, CDCl₃): 149.1, 142.2, 129.6, 128.5, 127.8, 125.5, 121.9, 119.1, 73.6, 65.5, 38.3, 12.1. Anal. Calcd for C₂₂H₂₃NO: C, 83.24; H, 7.30; N, 4.41. Found: C, 83.22; H, 7.28; N, 4.38.

(2S,3R)-2-cyclopropyl-3-(dibenzylamino)-3-(4-(trifluoromethoxy)phenyl)propan-1-ol (2i): m.p. 310°C, m/z: 427.18; Mol. Wt: 427.47. IR (thin film, cm⁻¹) 1256, 1221, 1163, 748, 699; ¹H NMR (400 MHz, CDCl₃): 7.40 – 6.89 (m, 14H), 4.70 (br, s, 1H, -OH, exchangeable with D₂O), 3.10 – 3.40 (dd, *J* = 10.3 Hz, 2H), 3.59 (d, *J* = 11.3 Hz, 1H), 2.40 – 2.20 (m, 1H), 0.10-1.10 (m, 5H); ¹³C NMR (101 MHz, CDCl₃): 149.1, 144.8, 132.8, 129.7, 129.6, 127.8, 121.9, 119.1, 68.6, 60.5, 48.6,

4.1, 3.2. Anal. Calcd for $C_{25}H_{24}F_3NO_2$: C, 70.25; H, 5.66; N, 3.28; F, 13.33. Found: C, 70.23; H, 5.63; N, 3.26; F, 13.30.

(1R,2S)-3-(3-hydroxy-2-methyl-1-(1-methyl-1H-indol-3-yl)

methyl)(phenyl)amino)propyl)phenol (2j): m.p. 390°C, m/z: 400.22; Mol. Wt: 400.52. IR (thin film, cm^{-1}) 3010, 2915, 1587, 1097, 753; 1H NMR (400 MHz, $CDCl_3$) : 9.30 (br, s, 1H, -OH), 7.54 – 6.35 (m, 14H), 4.70 (br, s, 1H, -OH, exchangeable with D_2O), 4.50 (s, 2H), 3.70 (s, 3H), 3.59 (d, $J = 11.3$ Hz, 2H), 3.10 – 3.40 (dd, $J = 10.3$ Hz, 1H), 2.60 – 2.40 (m, 1H), 0.40 (d, $J = 6.8$ Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ : 156.1, 149.6, 143.6, 137.5, 129.6, 127.7, 126.5, 121.9, 121.7, 119.8, 118.8, 114.3, 114.2, 112.5, 71.4, 65.5, 38.7, 34.0, 12.1. Anal. Calcd for $C_{26}H_{28}N_2O_2$: C, 77.97; H, 7.05; N, 6.99. Found: C, 77.95; H, 7.03; N, 6.96.

(1R,2S)-methyl-2-hydroxy-5-(3-hydroxy-1-(6-methoxypyridin-3-yl)-2-methylpropyl)

(phenyl)amino)methyl)benzoate (2k): m.p. 450°C, m/z: 436.21; Mol. Wt: 436.51. IR (thin film, cm^{-1}) 1676, 1601, 1498, 1204, 751; 1H NMR (400 MHz, $CDCl_3$) : 15.20 (br, s, 1H), 7.78 – 6.58 (m, 11H), 4.70 (br, s, 1H, -OH, exchangeable with D_2O), 4.60 (s, 2H), 3.95 (s, 3H), 3.70 (s, 3H), 3.59 (d, $J = 11.3$ Hz, 2H), 3.10 – 3.40 (dd, $J = 10.3$ Hz, 1H), 2.60 – 2.40 (m, 1H), 0.40 (d, $J = 6.8$ Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ : 169.7, 163.9, 149.6, 146.3, 138.2, 136.2, 130.4, 129.6, 127.4, 121.9, 116.7, 114.3, 111.7, 110.3, 71.1, 65.5, 54.1, 53.5, 51.5, 38.7, 12.1. Anal. Calcd for $C_{25}H_{28}N_2O_5$: C, 68.79; H, 6.47; N, 6.42. Found: C, 68.76; H, 6.45; N, 6.40.

(2S,3R)- 2-methyl-3-phenyl-3-(phenyl(1-phenylethyl)amino)propan-1-ol (2l): m.p. 210°C, m/z: 345.21; Mol. Wt: 345.49. IR (thin film, cm^{-1}) 1493, 1451, 1216, 752, 576; 1H NMR (400 MHz, $CDCl_3$) : 7.36 – 6.80 (m, 15H), 4.70 (br, s, 1H, -OH, exchangeable with D_2O), 4.05–3.98 (m, 1H), 3.60 (d, $J = 11.3$ Hz, 2H), 3.10 – 3.40 (dd, $J = 10.3$ Hz, 1H), 2.60 – 2.40 (m, 1H), 1.10 (d, $J = 6.9$ Hz, 3H), 0.40 (d, $J = 6.8$ Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ : 144.9, 144.7, 138.3, 129.6, 128.5, 127.9, 127.8, 127.0, 125.5, 121.9, 116.8, 68.6, 65.5, 39.0, 12.1. Anal. Calcd for $C_{24}H_{27}NO$: C, 83.44; H, 7.88; N, 4.05. Found: C, 83.42; H, 7.86; N, 4.03.

¹H and ¹³C NMR Spectra of Compounds

Figure S1a: ¹H NMR (400 MHz, CDCl₃) of 4-(dibenzylamino)-3-methyl-4-phenylbutan-2-ol (**2a**)

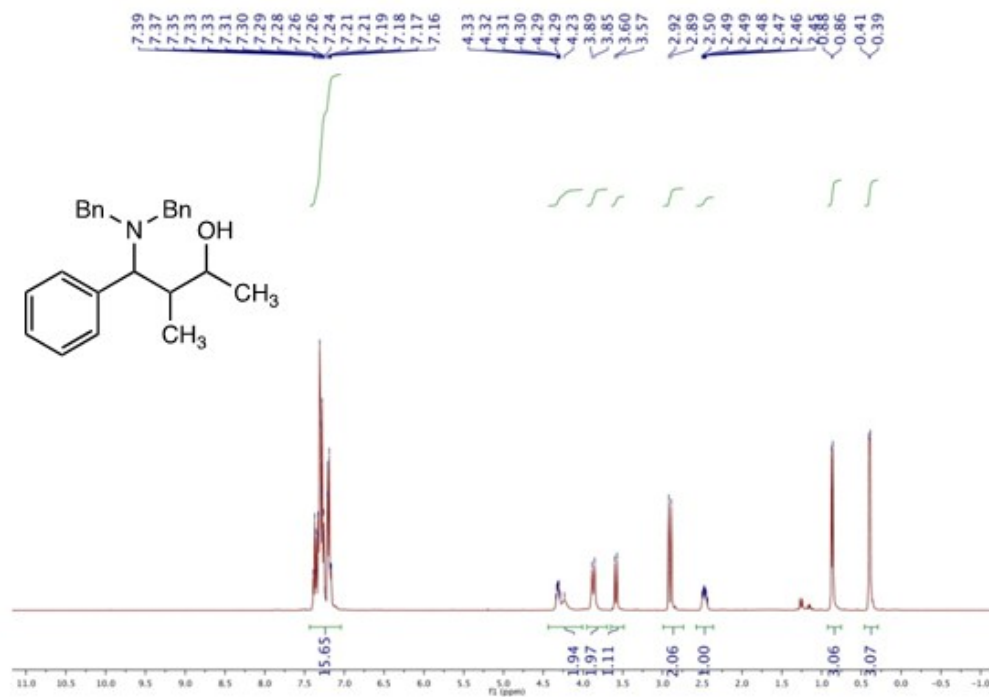


Figure S1b: ¹³C NMR (101 MHz, CDCl₃) of 4-(dibenzylamino)-3-methyl-4-phenylbutan-2-ol (**2a**)

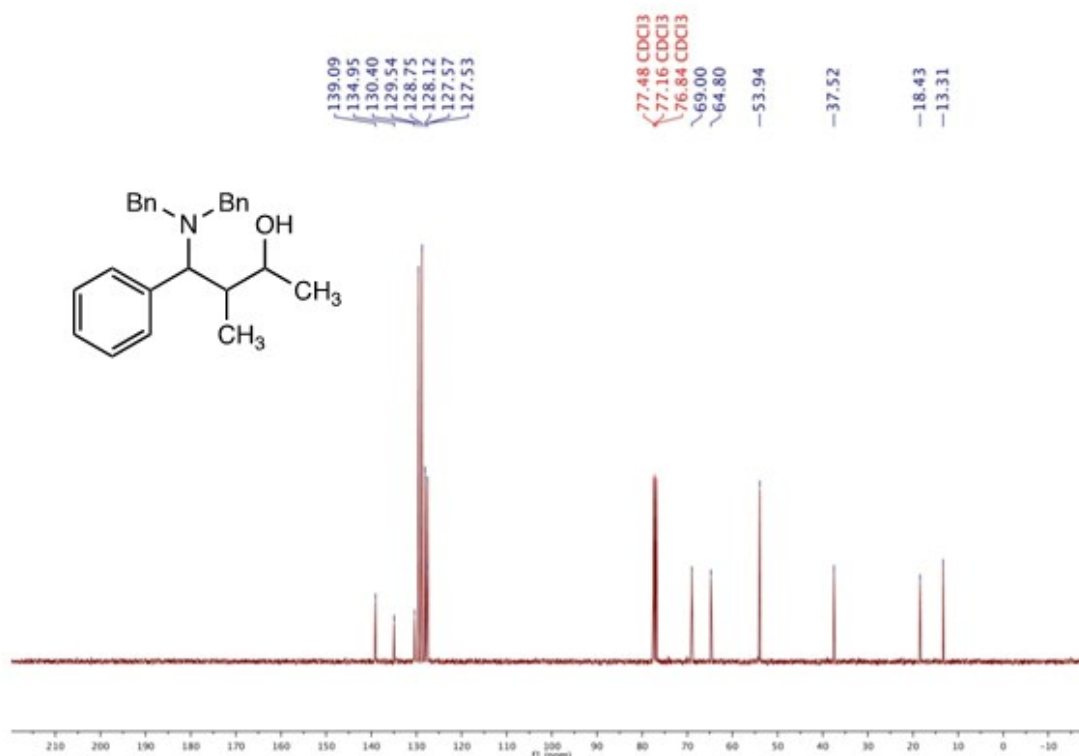


Figure S2a: ^1H NMR (400 MHz, CDCl_3) of 4-(dibenzylamino)-4-(3-methoxyphenyl)-3-methylbutan-2-ol (**2b**)

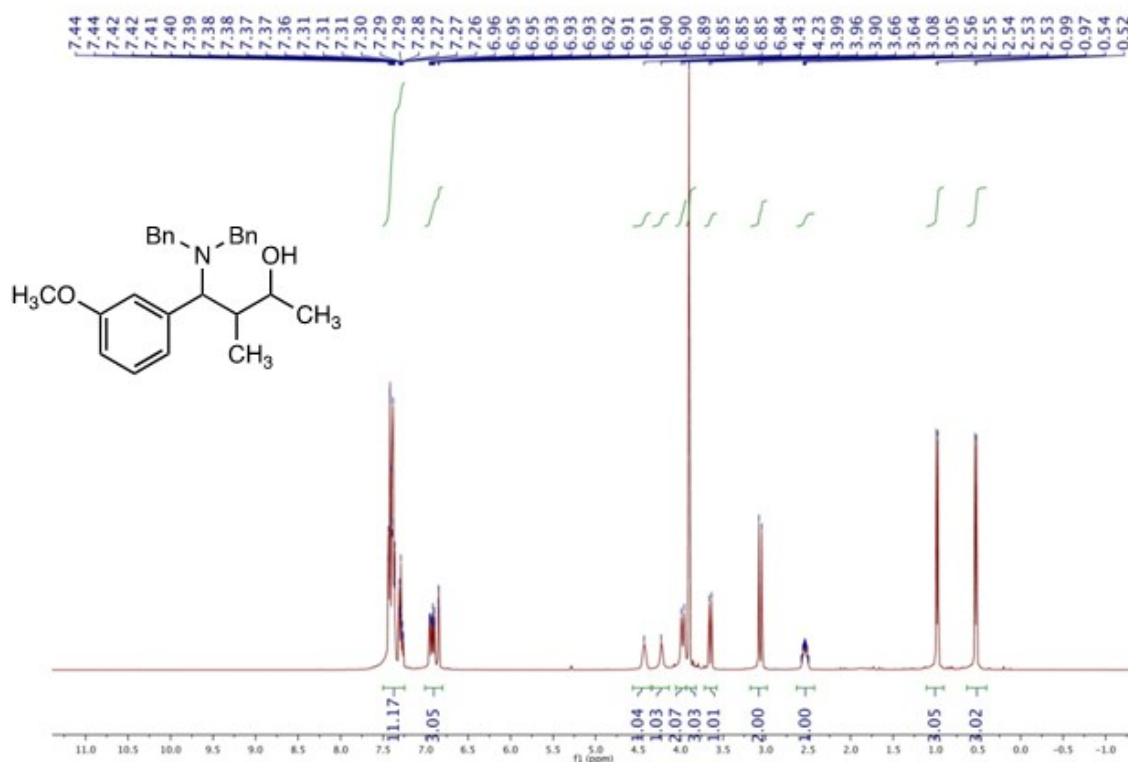


Figure S2b: ^{13}C NMR (101 MHz, CDCl_3) of 4-(dibenzylamino)-4-(3-methoxyphenyl)-3-methylbutan-2-ol (**2b**)

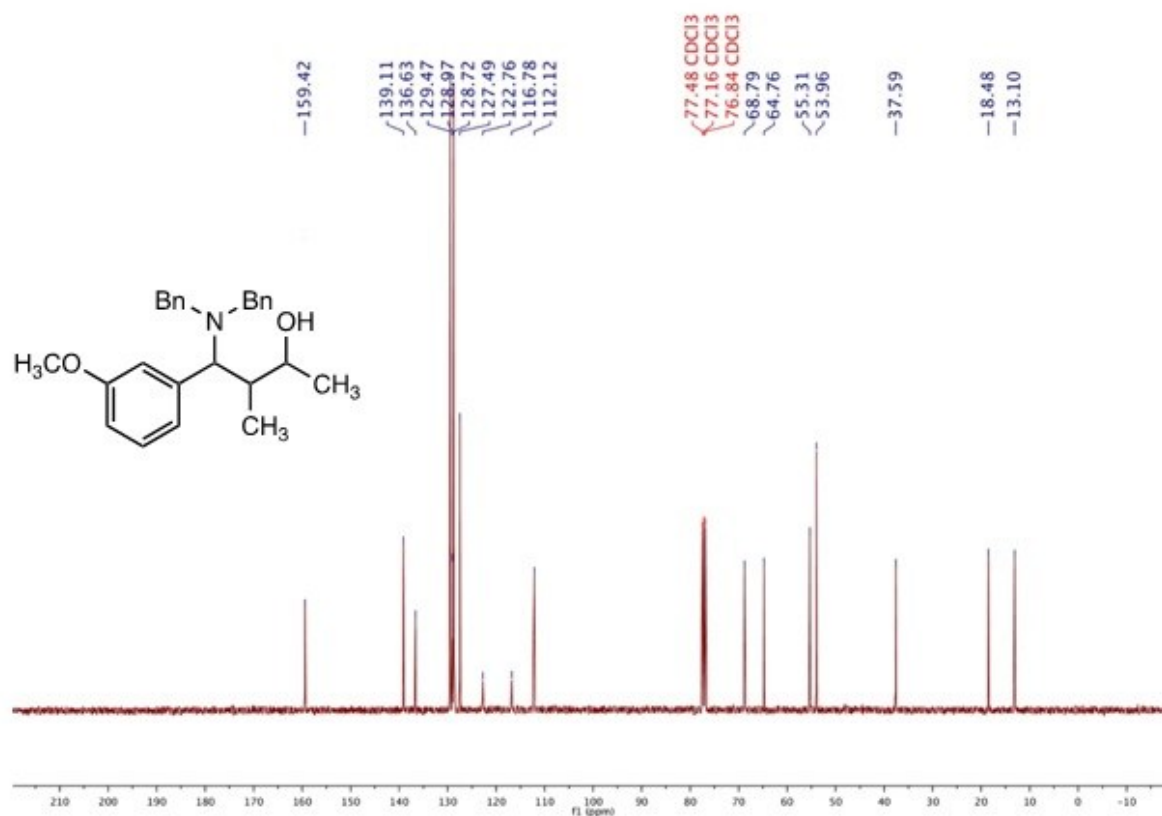


Figure S3a: ^1H NMR (400 MHz, CDCl_3) of 4-(dibenzylamino)-4-(2-fluorophenyl)-3-methylbutan-2-ol (**2c**)

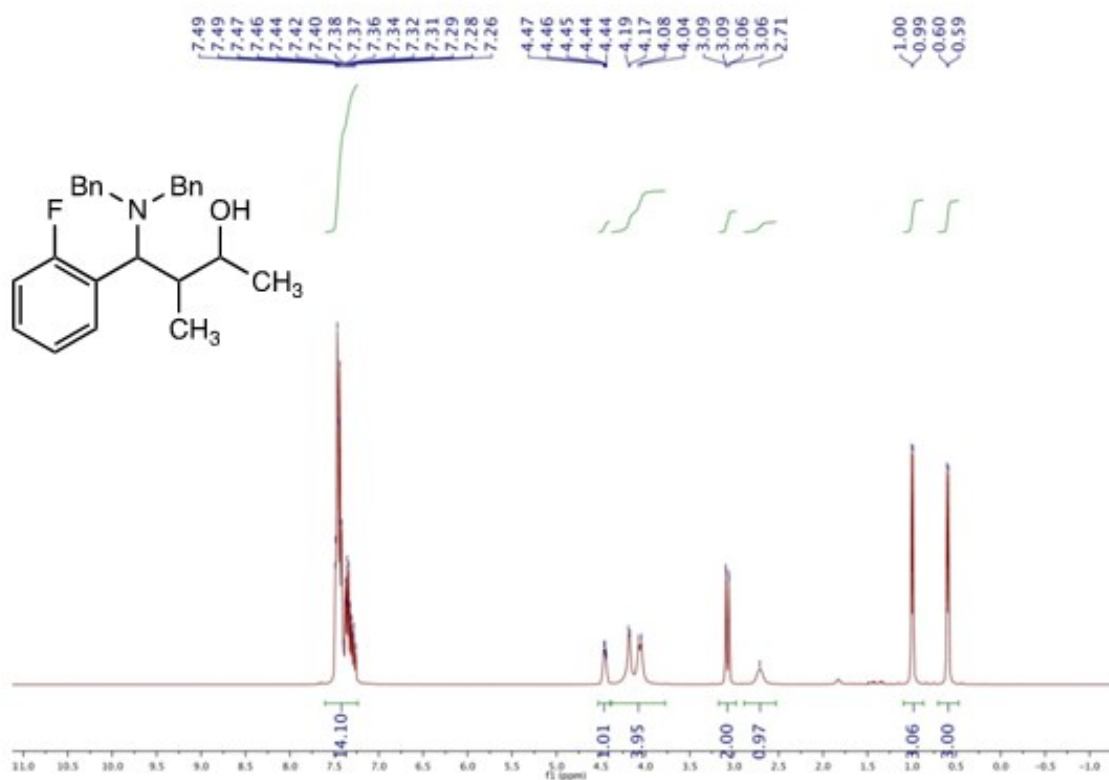


Figure S3b: ^{13}C NMR (101 MHz, CDCl_3) of 4-(dibenzylamino)-4-(2-fluorophenyl)-3-methylbutan-2-ol (**2c**)

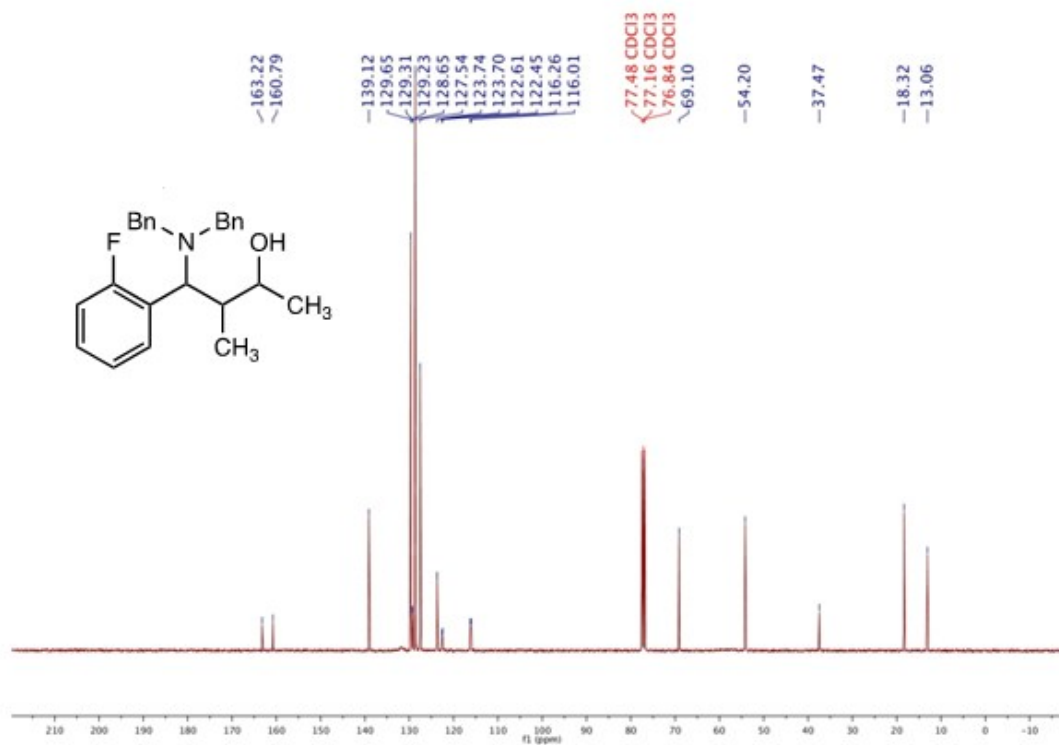


Figure S4a: ^1H NMR (400 MHz, CDCl_3) of 4-(3-chlorophenyl)-4-(dibenzylamino)-3-methylbutan-2-ol (**2d**)

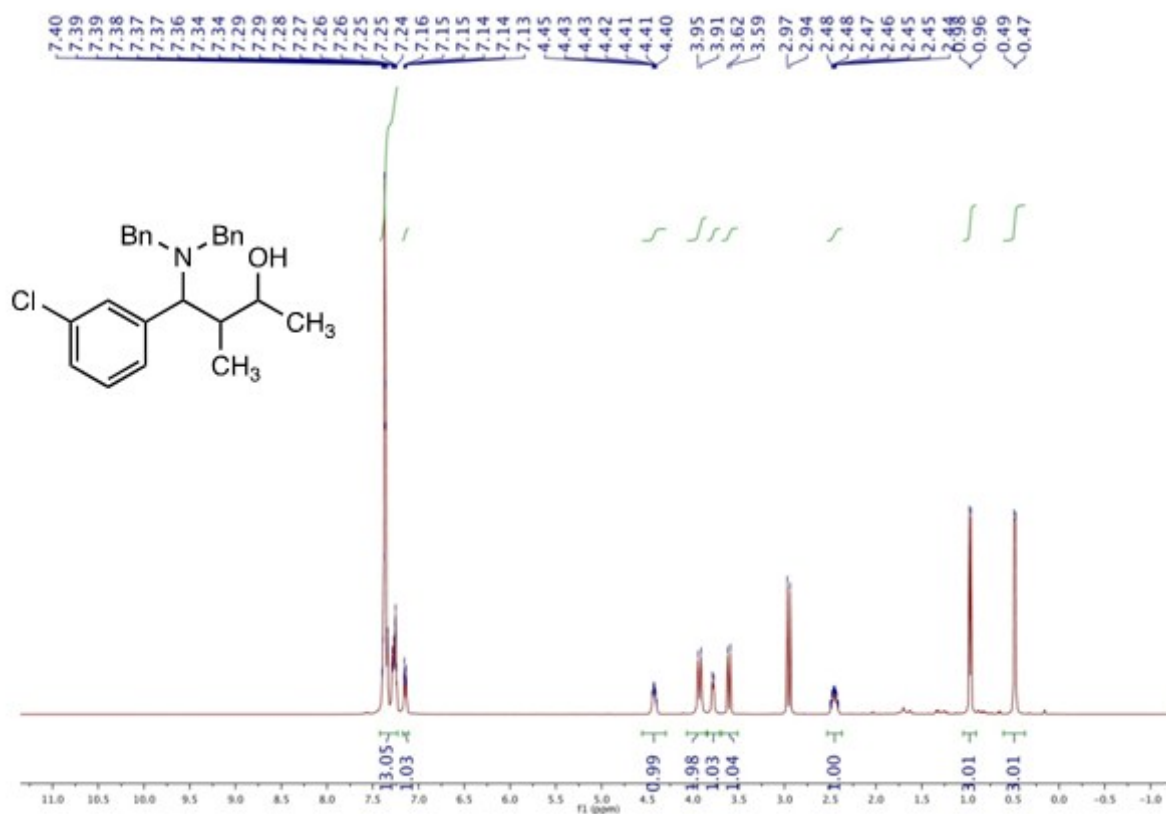


Figure S4b: ^{13}C NMR (101 MHz, CDCl_3) of 4-(3-chlorophenyl)-4-(dibenzylamino)-3-methylbutan-2-ol (**2d**)

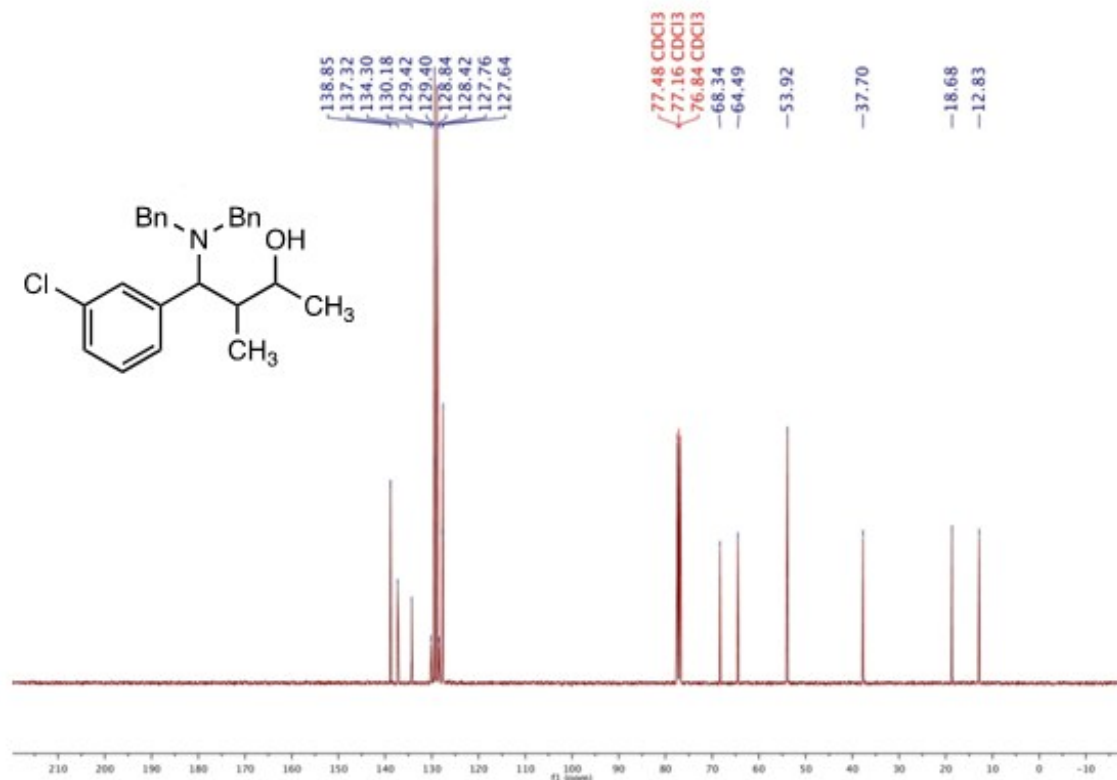


Figure S5a: ^1H NMR (400 MHz, CDCl_3) of 3-(dibenzylamino) phenyl methyl pentan-2-ol (**2e**)

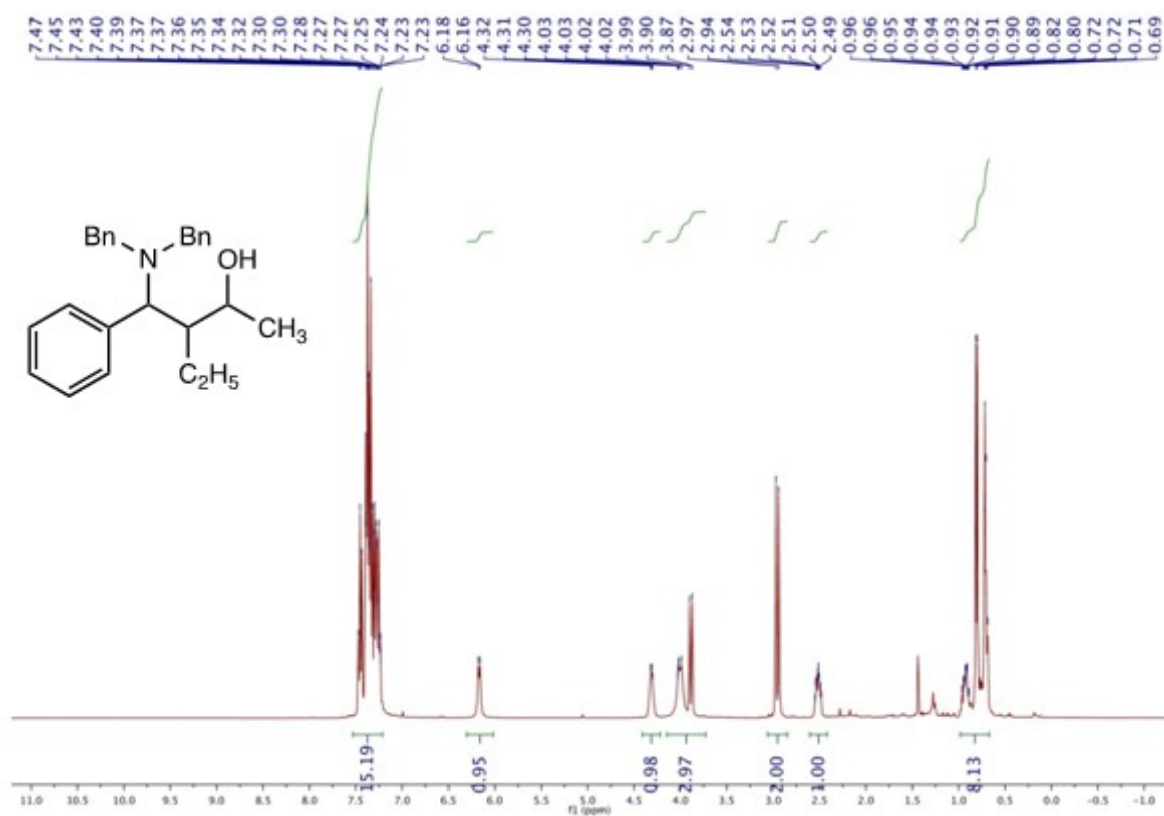


Figure S5b: ^{13}C NMR (101 MHz, CDCl_3) of 3-(dibenzylamino) phenyl methyl pentan-2-ol (**2e**)

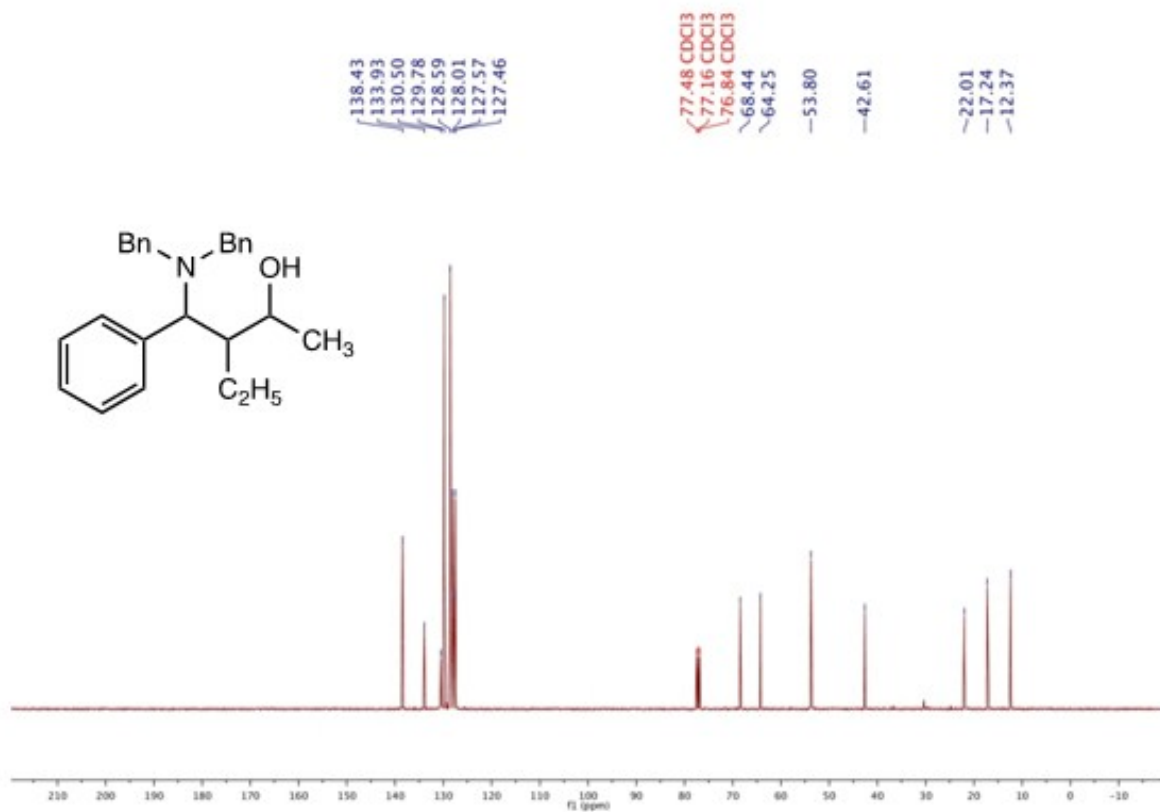


Figure S6a: ^1H NMR (400 MHz, CDCl_3) of 4-(dibenzylamino)-4-phenylbutan-2-ol (**2f**)

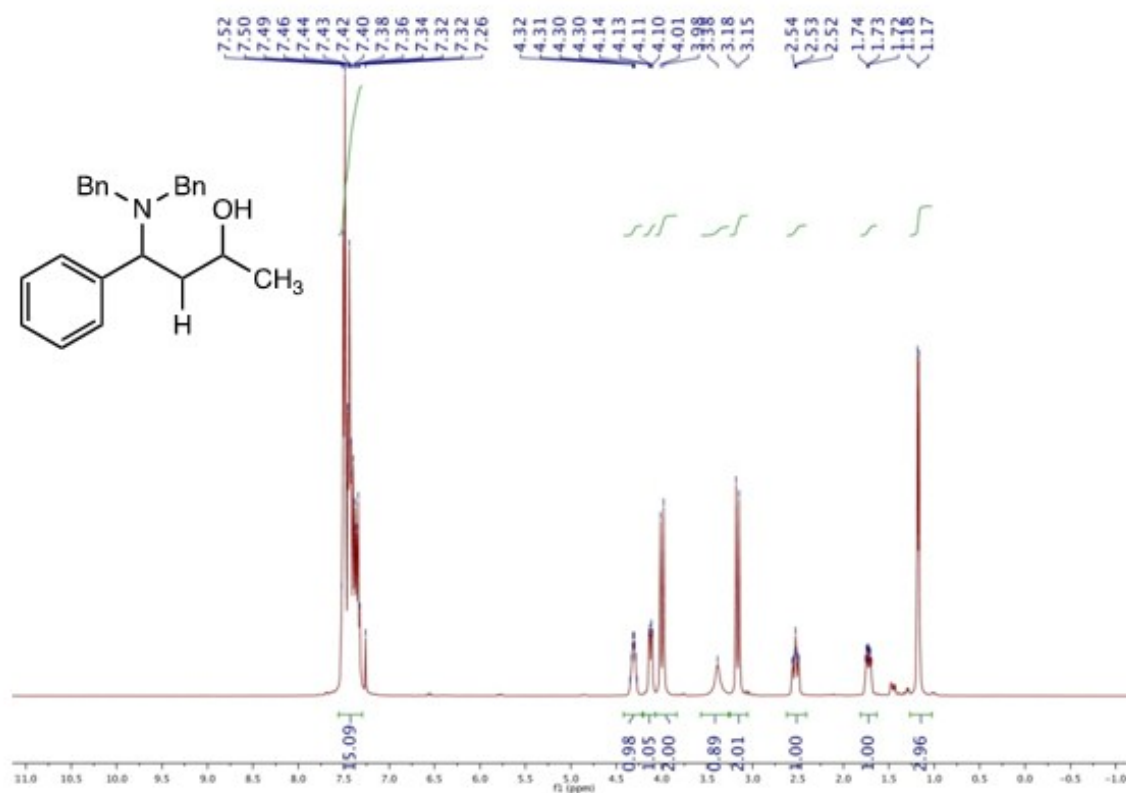


Figure S6b: ^{13}C NMR (101 MHz, CDCl_3) of 4-(dibenzylamino)-4-phenylbutan-2-ol (**2f**)

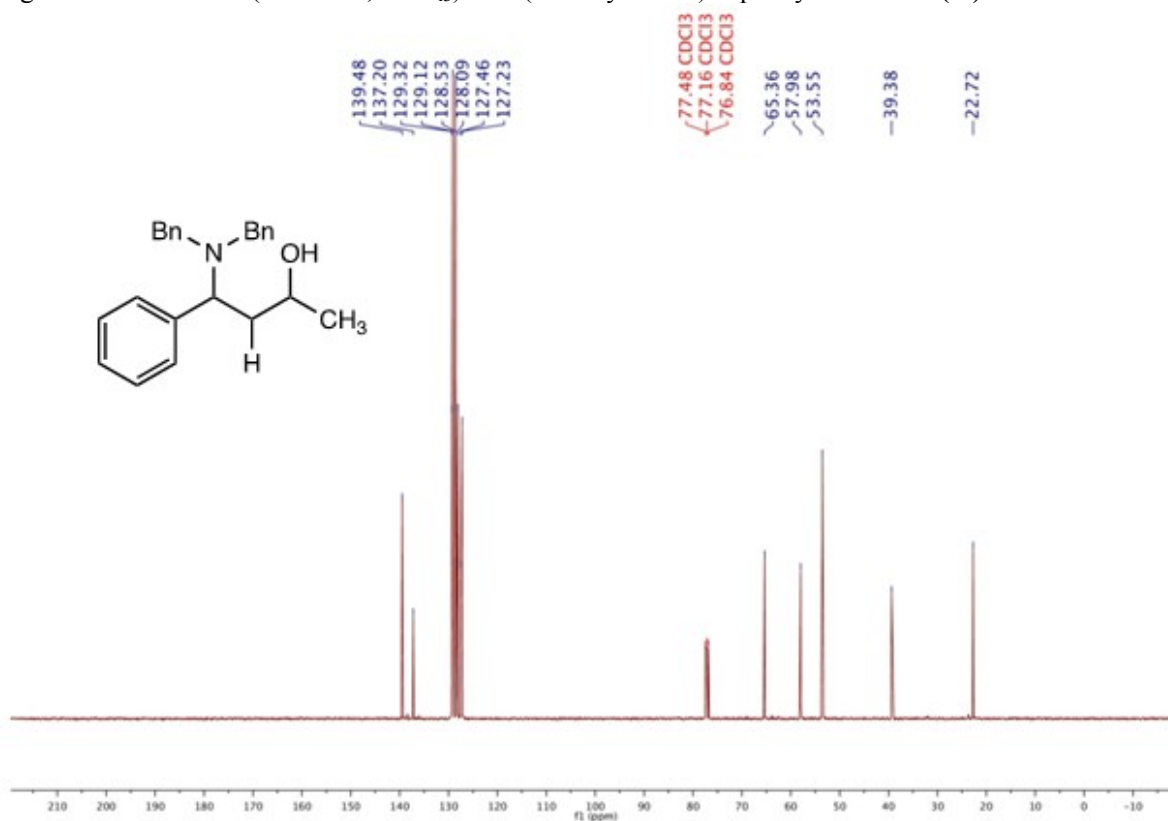


Figure S7a: ^1H NMR (400 MHz, CDCl_3) of 3-(diphenylamino)-3-(4-(1-hydroxyethyl)phenyl)-2-methylpropan-1-ol (**2g**)

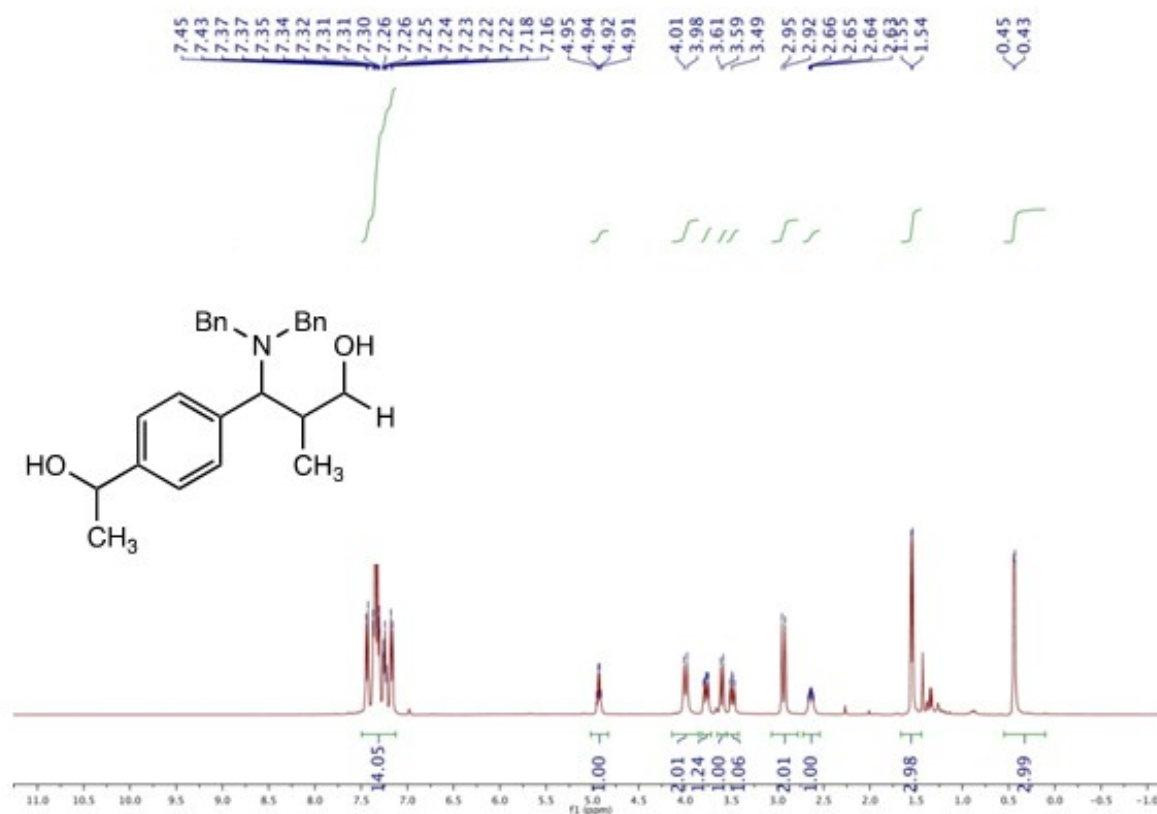


Figure S7b: ^{13}C NMR (101 MHz, CDCl_3) of 3-(diphenylamino)-3-(4-(1-hydroxyethyl)phenyl)-2-methylpropan-1-ol (**2g**)

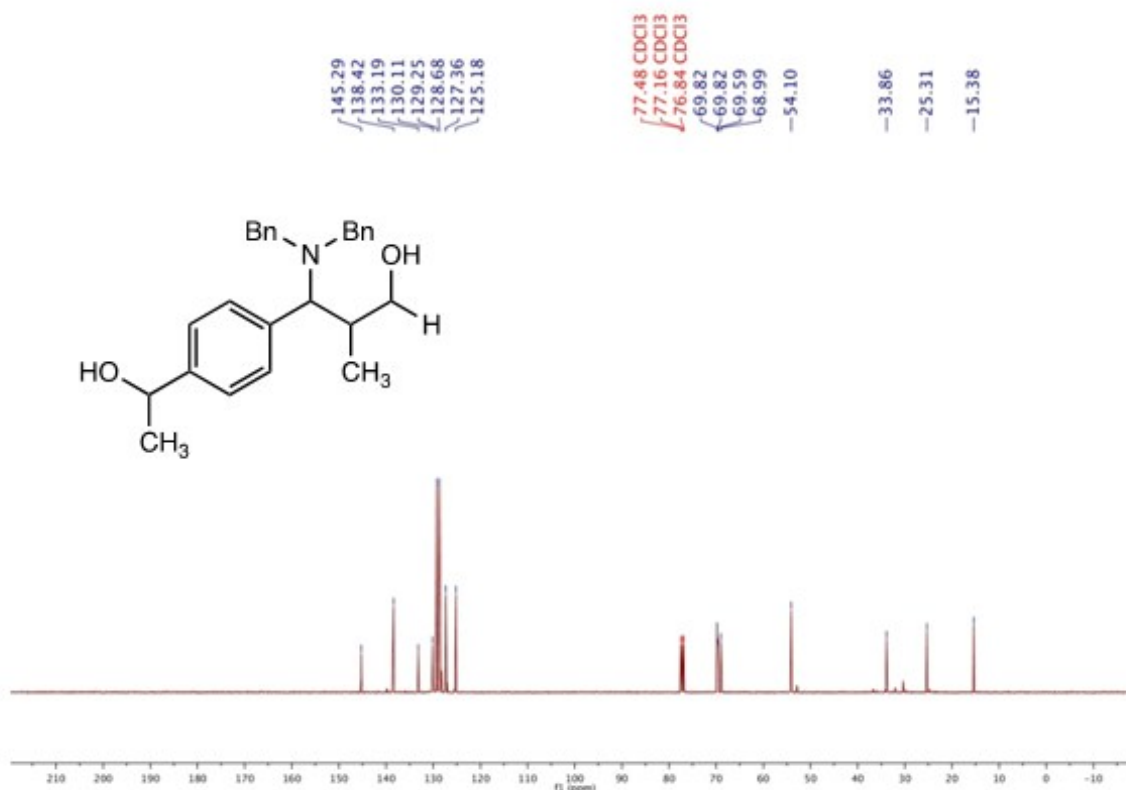


Figure S8a: ^1H NMR (400 MHz, CDCl_3) of 3-(dibenzylamino)-2-methyl-3-phenylpropan-1-ol (**2h**)

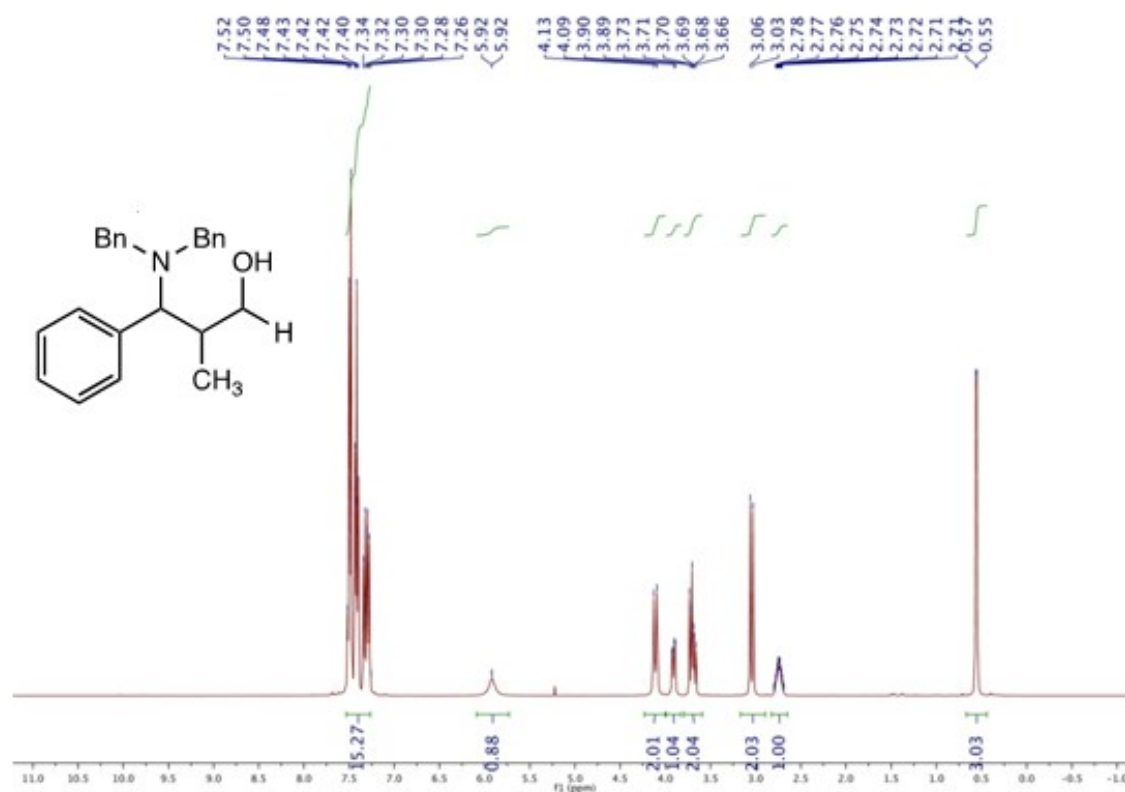


Figure S8b: ^{13}C NMR (101 MHz, CDCl_3) of 3-(dibenzylamino)-2-methyl-3-phenylpropan-1-ol (**2h**)

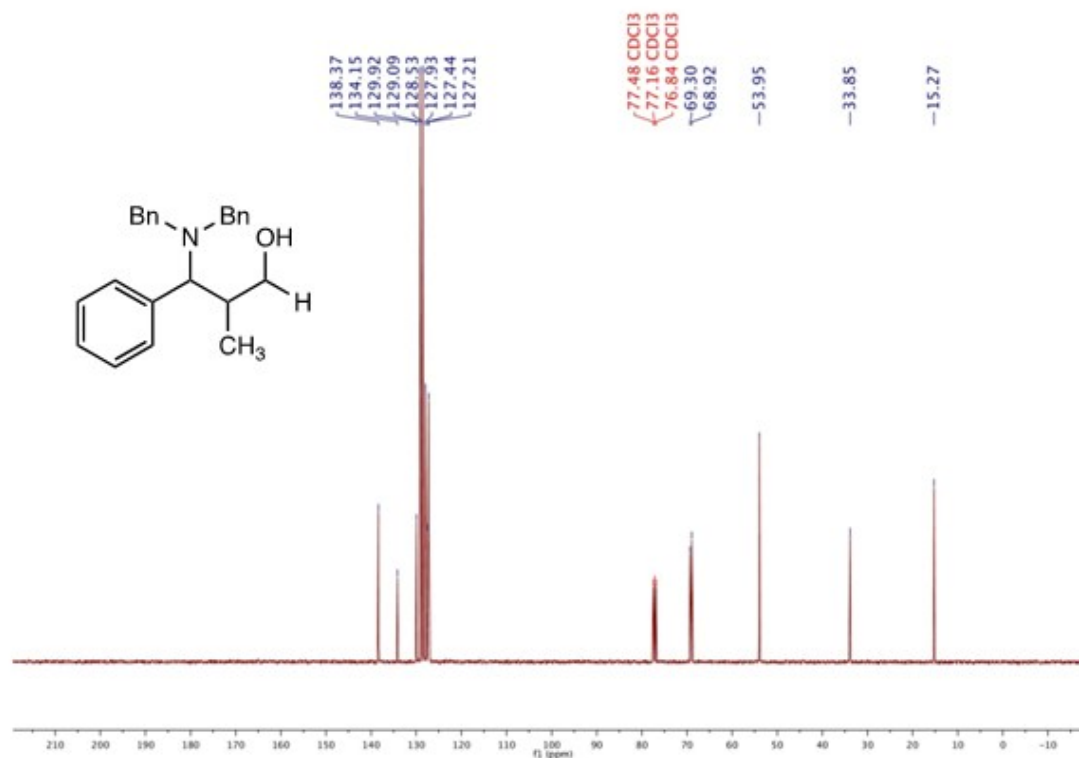


Figure S9a: ^1H NMR (400 MHz, CDCl_3) of 2-cyclopropyl-3-(dibenzylamino)-3-(4-(trifluoromethoxy)phenyl)propan-1-ol (**2i**)

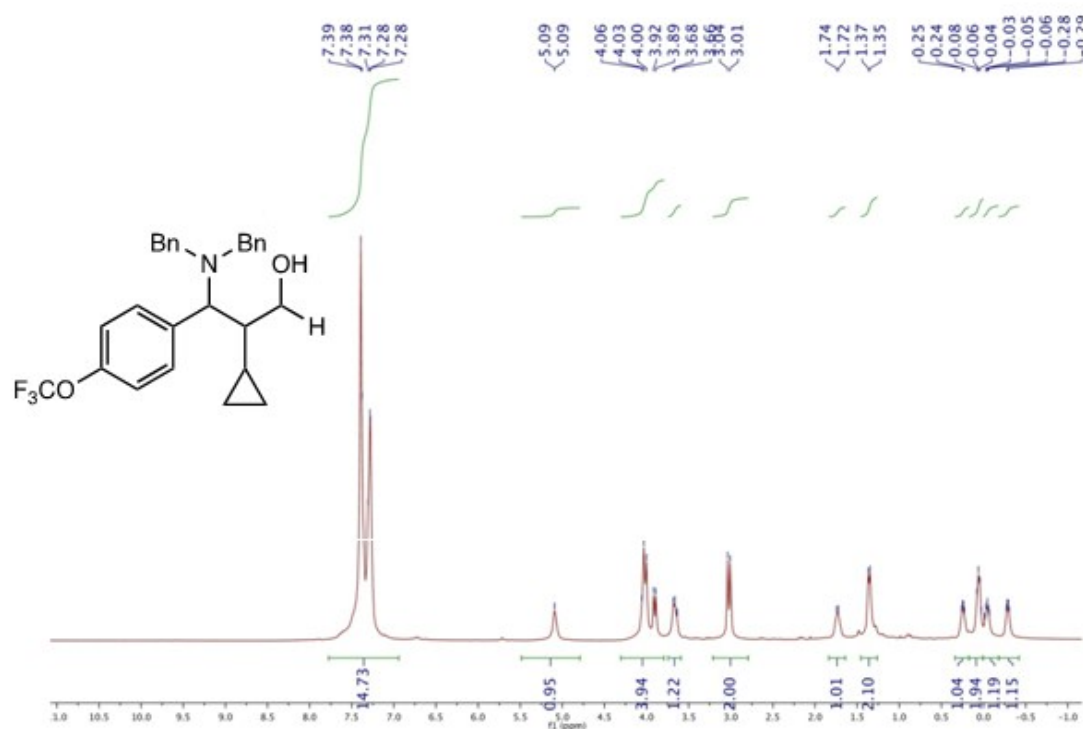


Figure S9b: ^{13}C NMR (101 MHz, CDCl_3) of 2-cyclopropyl-3-(dibenzylamino)-3-(4-(trifluoromethoxy)phenyl)propan-1-ol (**2i**)

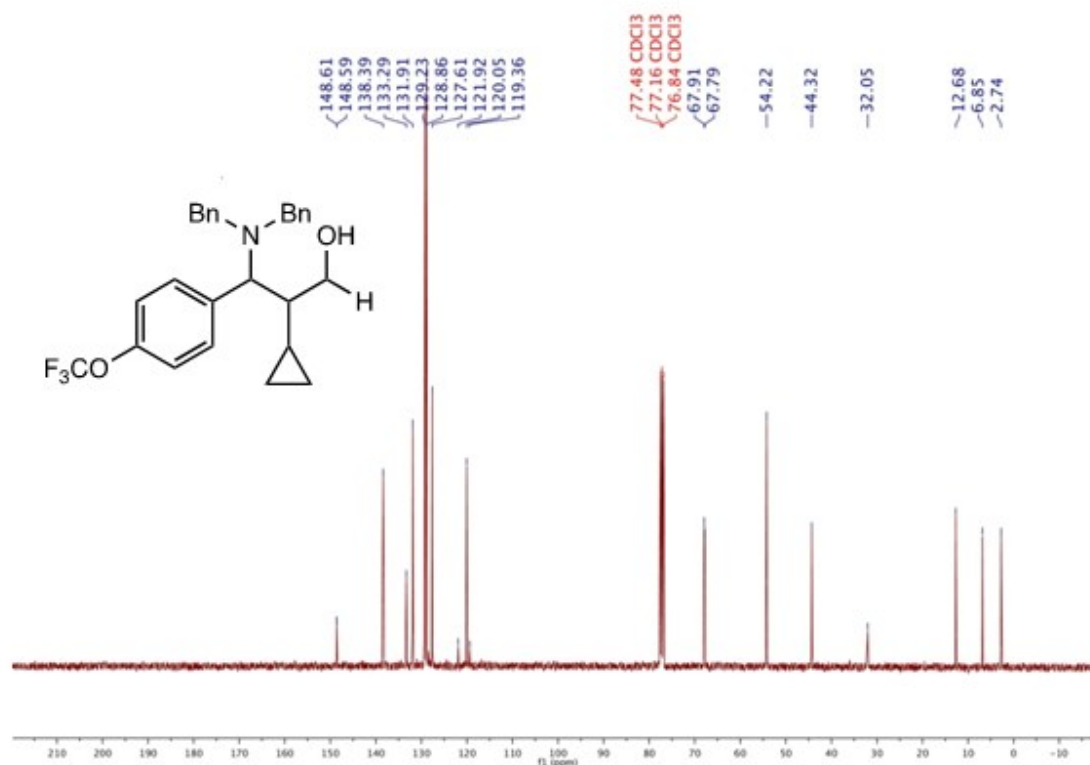


Fig S10a: ^1H NMR (400 MHz, CDCl_3) of 3-(3-hydroxy-2-methyl-1-(1-methyl-1H-indol-3-yl) methyl) (phenyl)amino)propyl)phenol (**2j**)

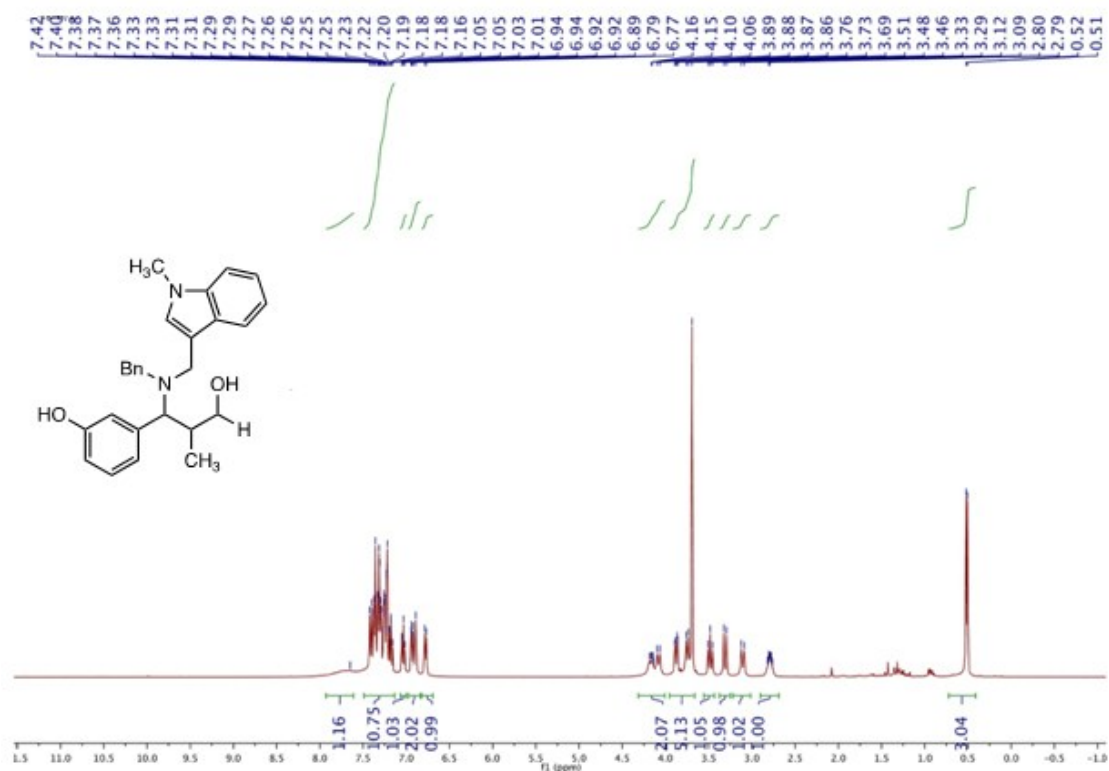


Fig S10b: ^{13}C NMR (101 MHz, CDCl_3) of 3-(3-hydroxy-2-methyl-1-(1-methyl-1H-indol-3-yl) methyl) (phenyl) amino)propyl)phenol (**2j**)

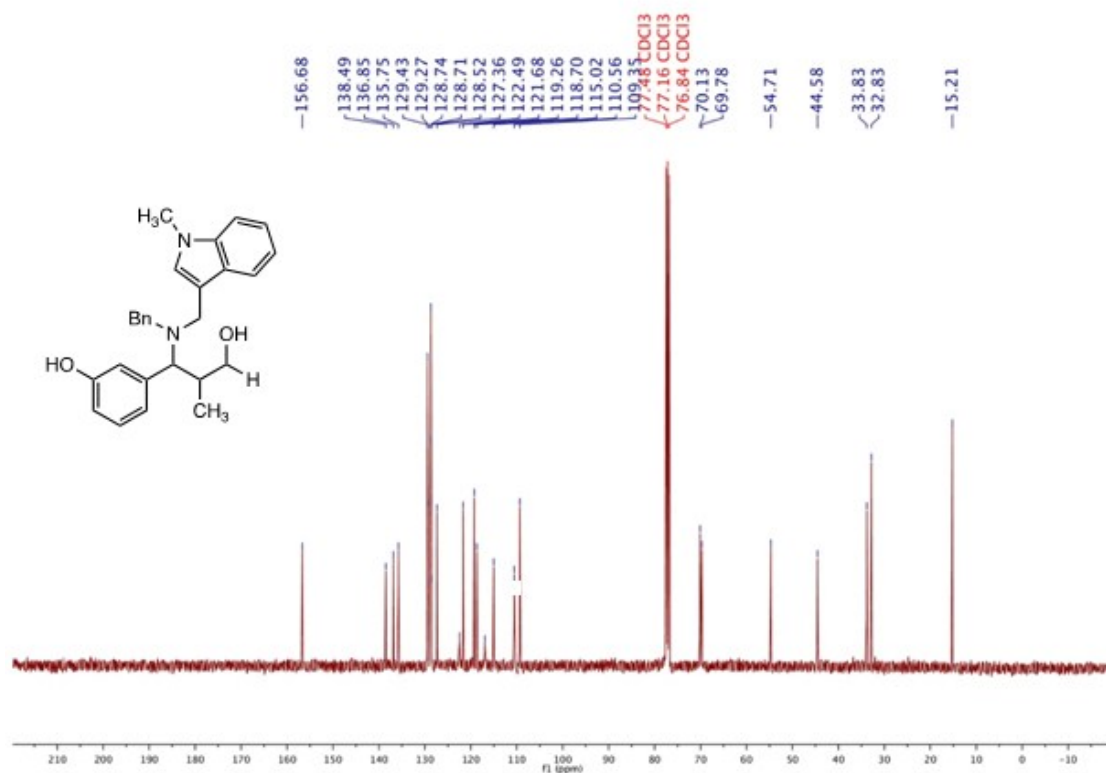


Fig S11a: ^1H NMR (400 MHz, CDCl_3) of methyl 2-hydroxy-5-(3-hydroxy-1-(6-methoxypyridin-3-yl)-2-methylpropyl)(phenyl)amino)benzoate (**2k**)

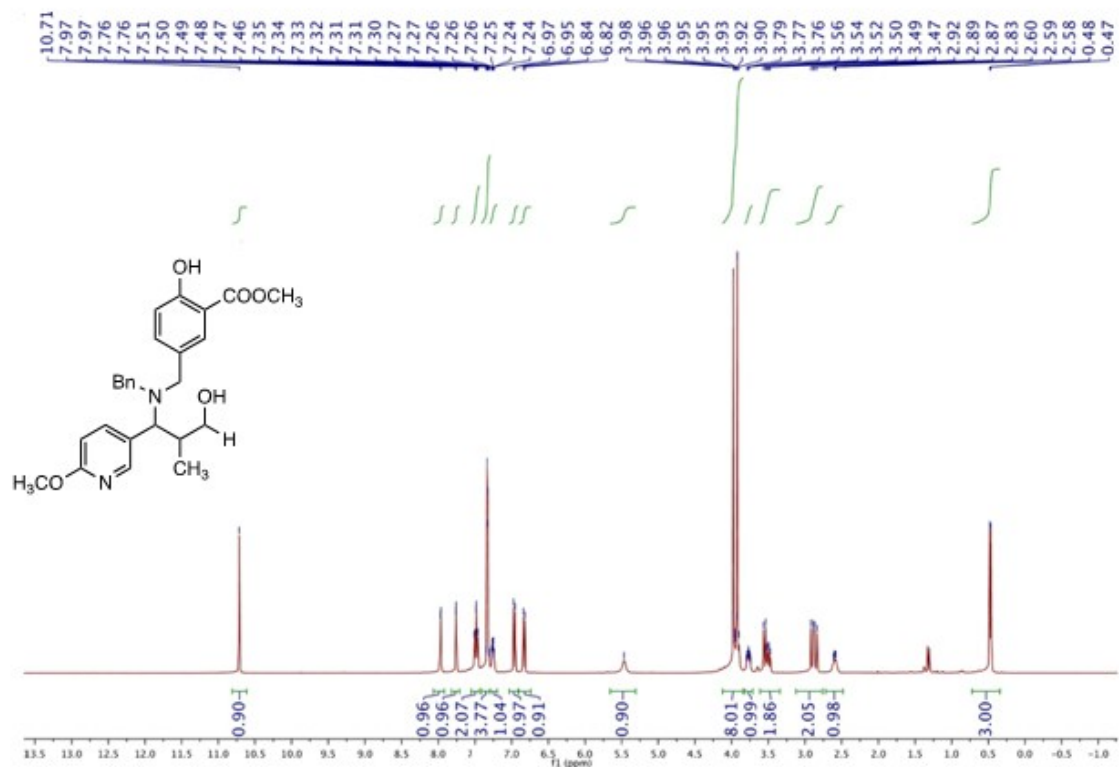


Fig S11b: ^{13}C NMR (101 MHz, CDCl_3) of methyl 2-hydroxy-5-(3-hydroxy-1-(6-methoxypyridin-3-yl)-2-methylpropyl)(phenyl)amino)benzoate (**2k**)

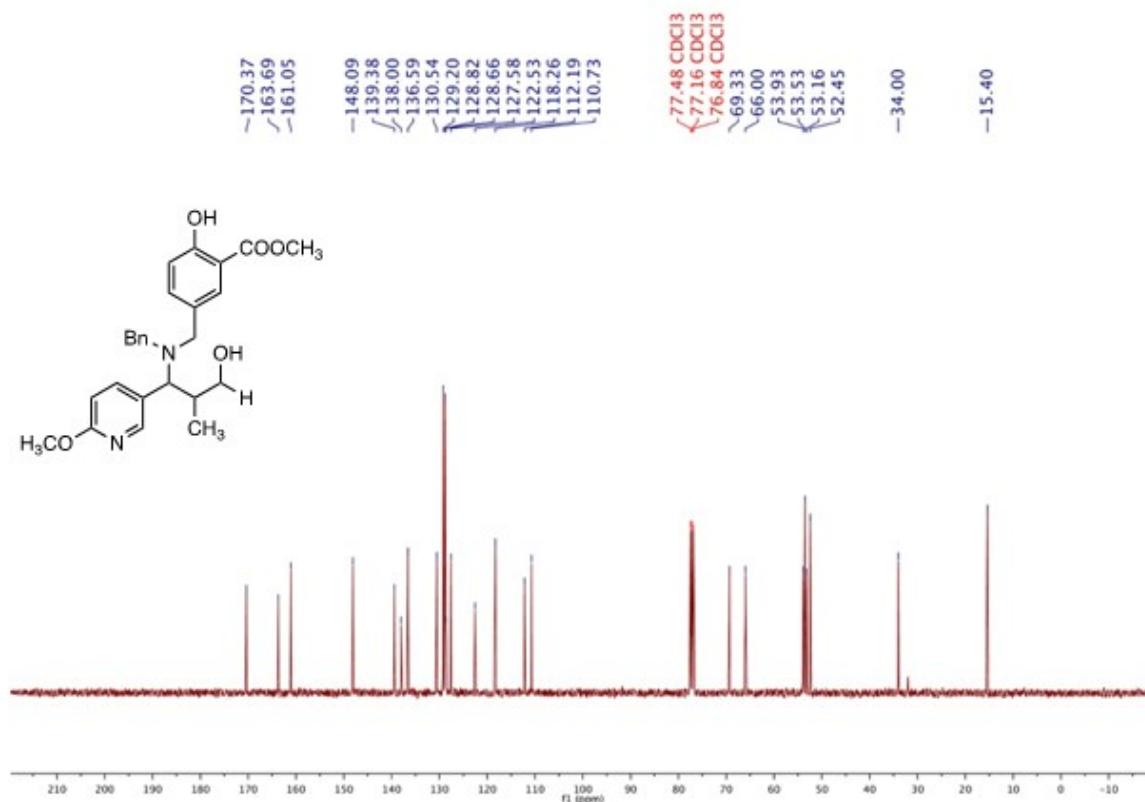


Fig S12a: ^1H NMR (400 MHz, CDCl_3) of 2-methyl-3-phenyl-3-(phenyl(1-phenylethyl)amino)propan-1-ol (**2l**)

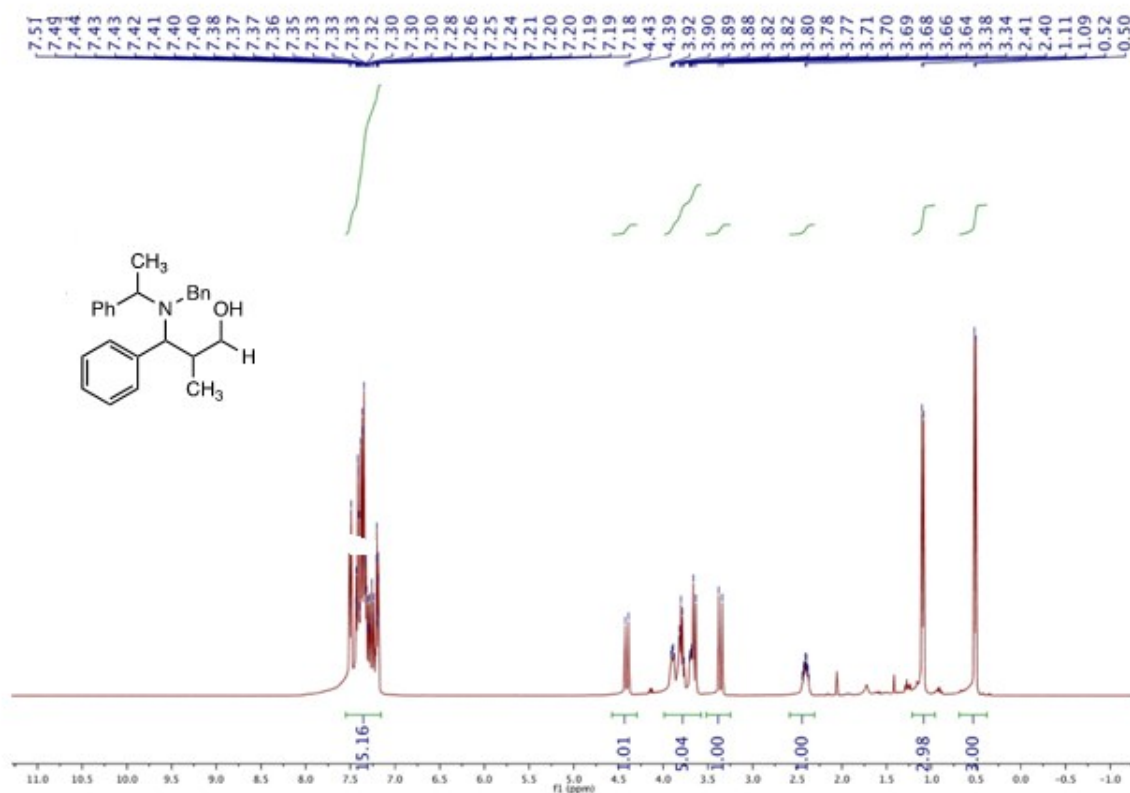


Fig S12b: ^{13}C NMR (101 MHz, CDCl_3) of 2-methyl-3-phenyl-3-(phenyl(1-phenylethyl)amino)propan-1-ol (**2l**)

