Supporting Information

for

Regio- and Stereoselective Ring-Opening of Aziridines: A Click Chemistry Approach to Chiral Amino Alcohols and Triazole-Modified Compounds

Julia Szymańska,[a,b] Marcin Palusiak,[c] Agnieszka J. Rybarczyk-Pirek,[c] Gabriela Wiosna-Sałyga,[d] Michał Rachwalski,[a] Adam M. Pieczonka*[a]

[a]*Department of Organic and Applied Chemistry, Faculty of Chemistry, University of Lodz, Tamka 12, 91-403 Lodz, Poland*

[b]*Doctoral School of Exact and Natural Sciences, University of Lodz, Matejki 21/23, 90-237 Lodz, Poland*

[c]*Department of Physical Chemistry, Faculty of Chemistry, University of Lodz, Pomorska 163/165, 90-236 Lodz, Poland*

[d]*Department of Molecular Physics, Lodz University of Technology, Zeromskiego 114, 90-543, Lodz, Poland*

* Corresponding author:
Adam Pieczonka – *Faculty of Chemistry, University of Lodz, 91-403 Lodz, Poland; https://orcid.org/0000-0001-6526-315X*; Phone: 48-42-6355762; E-mail: adam.pieczonka@chemia.uni.lodz.pl

Content:

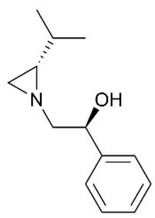
1. General Information

All commercially available chemicals and solvents were used as received. Aziridines were prepared according to the literature procedures [1]. Products were purified by crystallization or column chromatography with silica gel using a solvent mixture of hexane/ethyl acetate or dichloromethane/methanol as eluents. NMR spectra ^{1}H, ^{13}C, ^{19}F, ^{1}H-^{13}C HMQC or ^{1}H-^{13}C HSQC for the solutions in deuterated chloroform ($CDCl_3$) were recorded on a Bruker Avance III or Bruker AvanceNeo spectrometers (^{1}H NMR at 600 MHz, ^{13}C NMR at 151 MHz, and ^{19}F NMR at 565 MHz), using the solvent as an internal standard. The following abbreviations were used to describe the NMR spectra: δ, chemical shift (ppm); *J,* coupling constants (Hz); s, singlet; br.s, broad singlet dd, double-doublet; t, triplet; q, quartet, and m, multiplet. The IR spectra were taken with an Agilent Cary 630 FTIR spectrometer, in neat. Melting points were determined in capillaries with a MPM-H2 apparatus (Laboratory Devices), and are uncorrected. Optical rotations were determined with an Anton Paar MCP 500 polarimeter at the temperatures indicated. High resolution MS (ESI-TOF) measurements were performed with a Finningan MAT 95 spectrometer. Combustion analyses were obtained with a Vario EL III (Elementar Analysensysteme GmbH) instrument. Photophysical studies, including absorption measurements, were registered on Carry 5000 (Varian) spectrometer, photoluminescence spectra were registered on Edinburg Instruments FLS980 spectrofluorometer. The luminescence quantum yields of the SAAs were determined using an integrating sphere with BENFLEC inside coating. Spectral resolution of spectra was equal to 1 nm. Analyzed compounds in diluted solutions were measured in the standard 1 cm path length quartz cuvette. X-ray diffraction data for the investigated compound were measured on a four-circle Oxford Diffraction Supernova Dual diffractometer using a two-dimensional area CCD detector and a low-temperature device Oxford Cryosystem cooler.

2. Synthetic procedures and characterization data

General procedure for synthesis of aziridine alcohols **1a**-**1e**, **2c**-**2e**: A solution of (*R*)- or (*S*)-styrene oxide (1.5 mmol, 171.5 µL), the corresponding aziridine (4.75 mmol), water (5 mL) and triethylamine (1.0 mmol, 150.0 µL) was refluxed for 24 hours. Next, solvent was removed *in vacuo* and the resulting materials were separated by column chromatography (SiO_2, hexane/ethyl acetate 5:5) to give spectroscopically pure aziridine alcohols.

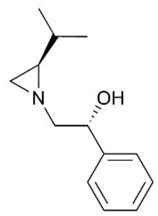
(*S*)-2-((*S*)-2-isopropylaziridin-1-yl)-1-phenylethan-1-ol **(1a)**: [2]



1a

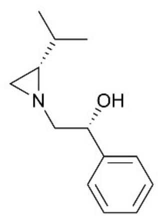
White solid (268.5 mg, 87% yield); mp = 106.5-107.8 °C (hexane/DCM); $[\alpha]^{20}_{D}$ = +98.27 (c 0.0015 in $CHCl_3$). **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.30–7.24 (m, 4H, C$\mathbf{H}_{ar}$), 7.20–7.18 (m, 1H, C$\mathbf{H}_{ar}$), 4.73 (dd, *J* = 3.3 Hz, 9.6 Hz, 1H, C**H**OH), 3.40 (br. s, 1H, O**H**), 2.74 (dd, *J* = 9.6 Hz, 12.0 Hz, 1H, C$\mathbf{H}_2$), 2.02 (dd, *J* = 3.3 Hz, 12.0 Hz, 1H, C$\mathbf{H}_2$), 1.52 (d, *J* = 2.6 Hz, 1H, C$\mathbf{H}_2$), 1.24–1.21 (m, 2H, 2xC**H**), 1.18–1.16 (m, 1H, C$\mathbf{H}_2$), 0.93 (d, *J* = 6.0 Hz, 3H, C$\mathbf{H}_3$), 0.83 (d, *J* = 6.0 Hz, 3H, C$\mathbf{H}_3$). **^{13}C{^{1}H} NMR** (151 MHz, $CDCl_3$): δ 142.0 ($\mathbf{C}_{qar}$), 128.3 (2$\mathbf{C}_{ar}$), 127.5 ($\mathbf{C}_{ar}$), 126.0 (2$\mathbf{C}_{ar}$), 73.0 (**C**HOH), 69.1 (**C**H_2), 46.1 (**C**H), 32.7 (**C**H_2), 31.4 (**C**H), 20.3 (**C**H$_3$), 19.4 (**C**H$_3$). **Anal. Calcd. for $C_{13}H_{19}NO$**: C, 76.06; H, 9.33; N, 6.82; Found: C, 76.09; H, 9.25; N, 6.66. Crystals of **1a** suitable for X-ray measurements were obtained from dichloromethane /hexane (1:1) mixture by slow evaporation of the solvent.

(*R*)-2-((*R*)-2-isopropylaziridin-1-yl)-1-phenylethan-1-ol **(1b)**:



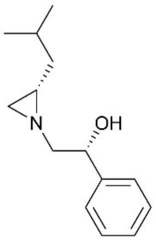
1b White solid (232.2 mg, 75% yield); mp = 106.5-107.8 °C (hexane/DCM); $[\alpha]^{20}_D$ = –98.27 (c 0.0015 in CHCl$_3$). **^{1}H NMR** (600 MHz, CDCl$_3$): δ 7.30–7.25 (m, 4H, C**H**$_{ar}$), 7.20–7.18 (m, 1H, C**H**$_{ar}$), 4.73 (dd, *J* = 3.3 Hz, 9.6 Hz, 1H, C**H**OH), 3.37 (br. s, 1H, O**H**), 2.74 (dd, *J* = 9.6 Hz, 12.0 Hz, 1H, C**H**$_2$), 2.02 (dd, *J* = 3.3 Hz, 12.0 Hz, 1H, C**H**$_2$), 1.52 (d, *J* = 2.9 Hz, 1H, C**H**$_2$), 1.23–1.21 (m, 2H, 2xC**H**), 1.19–1.17 (m, 1H, C**H**$_2$), 0.93 (d, *J* = 6.2 Hz, 3H, C**H**$_3$), 0.83 (d, *J* = 6.2 Hz, 3H, C**H**$_3$). **^{13}C{^{1}H} NMR** (151 MHz, CDCl$_3$): δ 142.0 (**C**$_{qar}$), 128.3 (2**C**$_{ar}$), 127.5 (**C**$_{ar}$), 126.0 (2**C**$_{ar}$), 73.0 (**C**HOH), 69.1 (**C**H$_2$), 46.1 (**C**H), 32.7 (**C**H$_2$), 31.4 (**C**H), 20.3 (**C**H$_3$), 19.4 (**C**H$_3$). **Anal. Calcd. for $C_{13}H_{19}NO$**: C, 76.06; H, 9.33; N, 6.82; Found: C, 76.12; H, 9.33; N, 6.59. Crystals of **1b** suitable for X-ray measurements were obtained from dichloromethane /hexane (1:1) mixture by slow evaporation of the solvent.

(*R*)-2-((*S*)-2-isopropylaziridin-1-yl)-1-phenylethan-1-ol **(1c)**:



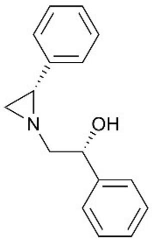
1c Colorless oil (164.2 mg, 53% yield); $[\alpha]^{20}_D$ = –6.71 (c 0.0015 in CHCl$_3$). **^{1}H NMR** (600 MHz, CDCl$_3$): δ 7.30–7.24 (m, 4H, C**H**$_{ar}$), 7.20–7.17 (m, 1H, C**H**$_{ar}$), 4.71 (dd, *J* = 3.0 Hz, 9.8 Hz, 1H, C**H**OH), 3.61 (br. s, 1H, O**H**), 2.71 (dd, *J* = 9.8 Hz, 12.0 Hz, 1H, C**H**$_2$), 1.99 (dd, *J* = 3.0 Hz, 12.0 Hz, 1H, C**H**$_2$), 1.59 (d, *J* = 3.5 Hz, 1H, C**H**$_2$), 1.28 (d, *J* = 6.4 Hz, 1H, C**H**$_2$), 1.22–1.19 (m, 1H, C**H**), 1.14–1.12 (m, 1H, C**H**), 0.99 (d, *J* = 6.6 Hz, 3H, C**H**$_3$), 0.88 (d, *J* = 6.6 Hz, 3H, C**H**$_3$). **^{13}C{^{1}H} NMR** (151 MHz, CDCl$_3$): δ 141.9 (**C**$_{qar}$), 128.3 (2**C**$_{ar}$), 127.5 (**C**$_{ar}$), 126.0 (2**C**$_{ar}$), 73.2 (**C**HOH), 68.8 (**C**H$_2$), 46.7 (**C**H), 33.0 (**C**H$_2$), 31.3 (**C**H), 20.4 (**C**H$_3$), 19.6 (**C**H$_3$). **Anal. Calcd. for $C_{13}H_{19}NO$**: C, 76.06; H, 9.33; N, 6.82; Found: C, 76.00; H, 9.29; N, 6.65.

(*R*)-2-((*S*)-2-isobutylaziridin-1-yl)-1-phenylethan-1-ol **(1d)**:



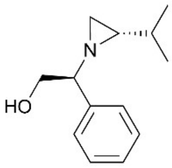
1d White solid (171.2 mg, 52% yield); mp = 71.2-72.5 °C (hexane/DCM); $[\alpha]^{20}_{D}$ = +10.79 (c 0.0015 in $CHCl_3$). **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.30–7.25 (m, 4H, C**H**$_{ar}$), 7.20–7.18 (m, 1H, C**H**$_{ar}$), 4.76 (dd, *J* = 3.4 Hz, 9.3 Hz, 1H, C**H**OH), 3.48 (br. s, 1H, O**H**), 2.63 (dd, *J* = 9.3 Hz, 12.1 Hz, 1H, C**H**$_2$), 2.16 (dd, *J* = 3.4 Hz, 12.1 Hz, 1H, C**H**$_2$), 1.72–1.65 (m, 1H, C**H**), 1.52 (d, *J* = 3.3 Hz, 1H, C**H**$_2$), 1.35–1.27 (m, 3H, C**H**, 2xC**H**$_2$), 1.12–1.08 (m, 1H, C**H**$_2$), 0.89 (d, *J* = 6.6 Hz, 3H, C**H**$_3$), 0.88 (d, *J* = 6.6 Hz, 3H, C**H**$_3$). **^{13}C{^{1}H} NMR** (151 MHz, $CDCl_3$): δ 142.1 (**C**$_{qar}$), 128.3 (2**C**$_{ar}$), 127.5 (**C**$_{ar}$), 126.0 (2**C**$_{ar}$), 73.4 (**C**HOH), 68.6 (**C**H$_2$), 42.2 (**C**H$_2$), 38.2 (**C**H), 34.5 (**C**H$_2$), 27.2 (**C**H), 23.1 (**C**H$_3$), 22.3 (**C**H$_3$). **Anal. Calcd. for $C_{14}H_{21}NO$**: C, 76.67; H, 9.65; N, 6.39; Found: C, 76.71; H, 9.40; N, 6.37. Crystals of **1d** suitable for X-ray measurements were obtained from dichloromethane/hexane (1:1) mixture by slow evaporation of the solvent.

(*R*)-1-phenyl-2-((*S*)-2-phenylaziridin-1-yl)ethan-1-ol **(1e)**:



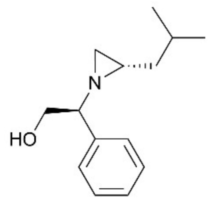
1e Yellow solid (187.9 mg, 52% yield); mp = 63.2-64.5 °C (hexane/DCM); $[\alpha]^{20}_{D}$ = +124.07 (c 0.0015 in $CHCl_3$). **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.29–7.14 (m, 10H, C**H**$_{ar}$), 4.78 (dd, *J* = 3.3 Hz, 9.0 Hz, 1H, C**H**OH), 3.35 (br. s, 1H, O**H**), 2.84 (dd, *J* = 9.0 Hz, 12.0 Hz, 1H, C**H**$_2$), 2.33–2.30 (m, 2H, C**H**, C**H**$_2$), 1.90 (d, *J* = 3.3 Hz, 1H, C**H**$_2$), 1.73 (d, *J* = 6.5 Hz, 1H, C**H**$_2$). **^{13}C{^{1}H} NMR** (151 MHz, $CDCl_3$): δ 141.9 (**C**$_{qar}$), 139.8 (**C**$_{qar}$), 128.4, 127.6, 127.1, 126.1 (10**C**$_{ar}$), 73.2 (**C**HOH), 68.7 (**C**H$_2$), 41.2 (**C**H), 38.1 (**C**H$_2$). **Anal. Calcd. for $C_{16}H_{17}NO$**: C, 80.30; H, 7.16; N, 5.85; Found: C, 80.27; H, 7.15; N, 5.68. Crystals of **1e** suitable for X-ray measurements were obtained from dichloromethane/hexane (1:1) mixture by slow evaporation of the solvent.

(*S*)-2-((*S*)-2-isopropylaziridin-1-yl)-2-phenylethan-1-ol **(2c)**:



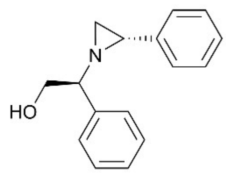
2c Colorless oil (118.1 mg, 38% yield); $[\alpha]^{20}_{D}$ = +105.00 (c 0.0015 in $CHCl_3$). **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.33–7.26 (m, 4H, C**H**$_{ar}$), 7.23–7.19 (m, 1H, C**H**$_{ar}$), 3.81 (dd, *J* = 5.4 Hz, 11.0 Hz, 1H, C**H**$_2$), 3.77 (dd, *J* = 4.3 Hz, 11.0 Hz, 1H, C**H**$_2$), 2.48 (t, *J* = 4.9 Hz, 1H, C**H**OH), 1.93 (br. s, 1H, O**H**), 1.48 (d, *J* = 3.5 Hz, 1H, C**H**$_2$), 1.35–1.32 (m, 1H, C**H**), 1.28–1.23 (m, 1H, C**H**), 1.16 (d, *J* = 6.4 Hz, 1H, C**H**$_2$), 1.04 (d, *J* = 6.7 Hz, 3H, C**H**$_3$), 0.90 (d, *J* = 6.7 Hz, 3H, C**H**$_3$). **^{13}C{^{1}H} NMR** (151 MHz, $CDCl_3$): δ 140.5 (**C**$_{qar}$), 128.4 (2**C**$_{ar}$), 127.8 (**C**$_{ar}$), 127.5 (2**C**$_{ar}$), 75.0 (**C**HOH), 67.1 (**C**H$_2$), 48.1 (**C**H), 31.7 (**C**H), 31.5 (**C**H$_2$), 20.6 (**C**H$_3$), 19.7 (**C**H$_3$). **Anal. Calcd. for $C_{13}H_{19}NO$**: C, 76.06; H, 9.33; N, 6.82; Found: C, 75.91; H, 9.15; N, 6.82.

(*S*)-2-((*S*)-2-isobutylaziridin-1-yl)-2-phenylethan-1-ol **(2d)**:



2d Colorless oil (121.8 mg, 37% yield); $[\alpha]^{20}_D$ = +93.07 (c 0.0015 in $CHCl_3$). **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.31–7.25 (m, 4H, CH_{ar}), 7.22–7.19 (m, 1H, CH_{ar}), 3.80 (dd, *J* = 5.4 Hz, *J* = 11.0 Hz, 1H, CH_2), 3.76 (dd, *J* = 5.4 Hz, *J* = 11.0 Hz, 1H, CH_2), 2.53 (t, *J* = 5.3 Hz 1H, C**H**OH), 2.06 (br. s, 1H, O**H**), 1.76–1.69 (m, 1H, C**H**), 1.65–1.61 (m, 1H, C**H**), 1.51–1.47 (m, 1H, CH_2), 1.42 (d, *J* = 3.6 Hz, 1H, CH_2), 1.21 (d, *J* = 6.4 Hz, 1H, CH_2), 1.14–1.09 (m, 1H, CH_2), 0.92 (d, *J* = 6.6 Hz, 3H, CH_3), 0.91 (d, *J* = 6.6 Hz, 3H, CH_3). **^{13}C{^{1}H} NMR** (151 MHz, $CDCl_3$): δ 140.4 (C_{qar}), 128.4 (2C_{ar}), 127.8 (2C_{ar}), 127.5 (C_{ar}), 75.2 (**C**HOH), 67.3 (CH_2), 42.5 (CH_2), 40.2 (**C**H), 32.4 (CH_2), 27.0 (**C**H), 23.3 (CH_3), 22.3 (CH_3). **Anal. Calcd. for $C_{14}H_{21}NO$**: C, 76.67; H, 9.65; N, 6.39; Found: C, 76.50; H, 9.66; N, 6.34.

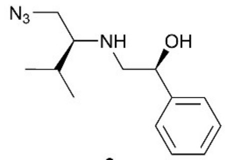
(*S*)-2-phenyl-2-((*S*)-2-phenylaziridin-1-yl)ethan-1-ol **(2e)**:



2e Yellow solid (119.9 mg, 33% yield); mp = 64.6-65.9 °C (hexane/DCM); $[\alpha]^{20}_D$ = +104.29 (c 0.0015 in $CHCl_3$). **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.39–7.37 (m, 2H, CH_{ar}), 7.31–7.28 (m, 2H, CH_{ar}), 7.26–7.16 (m, 6H, CH_{ar}), 3.77 (d, *J* = 5.0 Hz, 2H, CH_2), 2.79 (t, *J* = 5.6 Hz 1H, C**H**OH), 2.65 (dd, *J* = 3.4 Hz, 6.5 Hz, 1H, C**H**), 1.89 (br. s, 1H, O**H**), 1.82 (d, *J* = 3.4 Hz, 1H, CH_2), 1.61 (d, *J* = 6.5 Hz, 1H, CH_2). **^{13}C{^{1}H} NMR** (151 MHz, $CDCl_3$): δ 140.1 (C_{qar}), 139.9 (C_{qar}), 128.5, 128.4, 127.8, 127.7, 127.2, 126.3 (10C_{ar}), 75.3 (**C**HOH), 67.9 (CH_2), 42.8 (**C**H), 35.3 (CH_2). **Anal. Calcd. for $C_{16}H_{17}NO$**: C, 80.30; H, 7.16; N, 5.85; Found: C, 80.35; H, 7.05; N, 5.80.

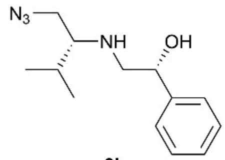
General procedure for synthesis of azides **3a**-**3e**, **4c, 4e, 16**: A solution of appropriate aziridine alcohol **1a-1e, 2c-2e and 15** (1.0 mmol), sodium azide (2.0 mmol, 130.0 mg) and ammonium chloride NH_4Cl (1.0 mmol, 53.5 mg) in methanol (8 mL) was refluxed for 24 hours. After, solvent was removed *in vacuo* and the mixture was extracted with diethyl ether (3 x 10 mL). Combined organic layers were dried over anhydrous $MgSO_4$, filtered, and the solvent was removed under reduced pressure. The products were purified by crystallization (dichloromethane/hexane (1:1) mixture by slow evaporation of the solvent). Compound **16** was purified by column chromatography (SiO_2, dichloromethane/methanol 95:5).

(*S*)-2-(((*S*)-1-azido-3-methylbutan-2-yl)amino)-1-phenylethan-1-ol **(3a)**:



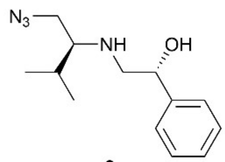
3a Colorless oil (197.1 mg, 79% yield); $[\alpha]^{20}_{D}$ = +47.29 (c 0.0015 in $CHCl_3$). **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.30–7.26 (m, 4H, C**H**$_{ar}$), 7.21–7.18 (m, 1H, C**H**$_{ar}$), 4.59 (dd, *J* = 3.4 Hz, 9.0 Hz, 1H, C**H**OH), 3.33 (dd, *J* = 4.2 Hz, 12.4 Hz, 1H, C**H**$_2$), 3.20 (dd, *J* = 6.5 Hz, 12.4 Hz, 1H, C**H**$_2$), 2.93 (dd, *J* = 3.4 Hz, 12.1 Hz, 1H, C**H**$_2$), 2.58 (dd, *J* = 9.0 Hz, 12.1 Hz, 1H, C**H**$_2$), 2.39–2.37 (m, 1H, C**H**), 1.78–1.72 (m, 1H, C**H**), 0.88 (d, *J* = 6.9 Hz, 3H, C**H**$_3$), 0.85 (d, *J* = 6.9 Hz, 3H, C**H**$_3$). **^{13}C{^{1}H} NMR** (151 MHz, $CDCl_3$): δ 142.3 (**C**$_{qar}$), 128.4 (2**C**$_{ar}$), 127.5 (**C**$_{ar}$), 125.8 (2**C**$_{ar}$), 72.5 (**C**HOH), 63.1 (**C**H), 55.8 (**C**H$_2$), 52.7 (**C**H$_2$), 29.9 (**C**H), 18.9 (**C**H$_3$), 18.7 (**C**H$_3$). **IR** (neat): ν 3358, 3030, 2959, 2095, 1454, 1271, 1059 cm^{-1}. **Anal. Calcd. for $C_{13}H_{20}N_4O$**: C, 62.88; H, 8.12; N, 22.56; Found: C, 62.80; H, 8.09; N, 22.60.

(*R*)-2-(((*R*)-1-azido-3-methylbutan-2-yl)amino)-1-phenylethan-1-ol **(3b)**:



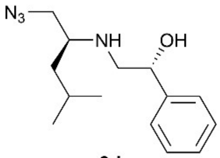
3b Colorless oil (194.3 mg, 78% yield); $[\alpha]^{20}_{D}$ = –47.29 (c 0.0015 in $CHCl_3$). **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.31–7.26 (m, 4H, C**H**$_{ar}$), 7.22–7.18 (m, 1H, C**H**$_{ar}$), 4.60 (dd, *J* = 3.4 Hz, 9.0 Hz, 1H, C**H**OH), 3.34 (dd, *J* = 4.2 Hz, 12.4 Hz, 1H, C**H**$_2$), 3.20 (dd, *J* = 6.5 Hz, 12.4 Hz, 1H, C**H**$_2$), 2.94 (dd, *J* = 3.4 Hz, 12.1 Hz, 1H, C**H**$_2$), 2.58 (dd, *J* = 9.0 Hz, 12.1 Hz, 1H, C**H**$_2$), 2.40–2.37 (m, 1H, C**H**), 1.78–1.73 (m, 1H, C**H**), 0.89 (d, *J* = 6.9 Hz, 3H, C**H**$_3$), 0.85 (d, *J* = 6.9 Hz, 3H, C**H**$_3$). **^{13}C{^{1}H} NMR** (151 MHz, $CDCl_3$): δ 142.2 (**C**$_{qar}$), 128.4 (2**C**$_{ar}$), 127.5 (**C**$_{ar}$), 125.8 (2**C**$_{ar}$), 72.5 (**C**HOH), 63.1 (**C**H), 55.7 (**C**H$_2$), 52.7 (**C**H$_2$), 29.9 (**C**H), 18.9 (**C**H$_3$), 18.7 (**C**H$_3$). **IR** (neat): ν 3358, 3030, 2959, 2095, 1454, 1271, 1059 cm^{-1}. **Anal. Calcd. for $C_{13}H_{20}N_4O$**: C, 62.88; H, 8.12; N, 22.56; Found: C, 62.86; H, 8.10; N, 22.56.

(*R*)-2-(((*S*)-1-azido-3-methylbutan-2-yl)amino)-1-phenylethan-1-ol **(3c)**:



3c White solid (174.9 mg, 70% yield); mp = 45.2-46.7 °C (hexane/DCM); $[\alpha]^{20}_{D}$ = –71.07 (c 0.0015 in $CHCl_3$). **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.30–7.26 (m, 4H, C**H**$_{ar}$), 7.21–7.18 (m, 1H, C**H**$_{ar}$), 4.57 (dd, *J* = 3.6 Hz, 8.8 Hz, 1H, C**H**OH), 3.34 (dd, *J* = 4.4 Hz, 12.5 Hz, 1H, C**H**$_2$), 3.20 (dd, *J* = 6.5 Hz, 12.5 Hz, 1H, C**H**$_2$), 2.88 (dd, *J* = 3.6 Hz, 12.3 Hz, 1H, C**H**$_2$), 2.66 (dd, *J* = 8.8 Hz, 12.3 Hz, 1H, C**H**$_2$), 2.42–2.40 (m, 1H, C**H**), 1.77–1.72 (m, 1H, C**H**), 0.88 (d, *J* = 6.9 Hz, 3H, C**H**$_3$), 0.86 (d, *J* = 6.9 Hz, 3H, C**H**$_3$). **^{13}C{^{1}H} NMR** (151 MHz, $CDCl_3$): δ 142.3 (**C**$_{qar}$), 128.4 (2**C**$_{ar}$), 127.5 (**C**$_{ar}$), 125.8 (2**C**$_{ar}$), 72.1 (**C**HOH), 62.7 (**C**H), 55.3 (**C**H_2), 52.5 (**C**H_2), 29.8 (**C**H), 18.8 (**C**H_3), 18.7 (**C**H_3). **IR** (neat): ν 3287, 3120, 2967, 2833, 2102, 1454, 1267, 1066 cm^{-1}. **Anal. Calcd. for $C_{13}H_{20}N_4O$**: C, 62.88; H, 8.12; N, 22.56; Found: C, 62.87; H, 8.12; N, 22.50. Crystals of **3c** suitable for X-ray measurements were obtained from dichloromethane/hexane (1:1) mixture by slow evaporation of the solvent.

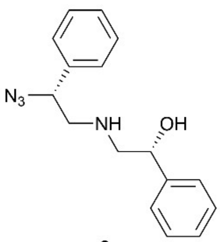
(*R*)-2-(((*S*)-1-azido-4-methylpentan-2-yl)amino)-1-phenylethan-1-ol **(3d)**:



3d

White solid (176.3 mg, 67% yield); mp = 74.2-75.4 °C (hexane/DCM); $[\alpha]^{20}_D$ = –63.79 (c 0.0015 in $CHCl_3$). **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.31–7.27 (m, 4H, C**H**$_{ar}$), 7.22–7.19 (m, 1H, C**H**$_{ar}$), 4.58 (dd, *J* = 3.7 Hz, 8.7 Hz, 1H, C**H**OH), 3.33 (dd, *J* = 4.3 Hz, 12.3 Hz, 1H, C**H**$_2$), 3.18 (dd, *J* = 5.5 Hz, 12.3 Hz, 1H, C**H**$_2$), 2.88 (dd, *J* = 3.7 Hz, 12.2 Hz, 1H, C**H**$_2$), 2.73–2.69 (m, 1H, C**H**), 2.63 (dd, *J* = 8.7 Hz, 12.2 Hz, 1H, C**H**$_2$), 1.66–1.59 (m, 1H, C**H**), 1.31–1.26 (m, 1H, C**H**$_2$), 1.20–1.16 (m, 1H, C**H**$_2$), 0.85 (d, *J* = 2.9 Hz, 3H, C**H**$_3$), 0.84 (d, *J* = 2.9 Hz, 3H, C**H**$_3$). **^{13}C{^{1}H} NMR** (151 MHz, $CDCl_3$): δ 142.3 (**C**$_{qar}$), 128.4 (2**C**$_{ar}$), 127.6 (**C**$_{ar}$), 125.8 (2**C**$_{ar}$), 72.1 (**C**HOH), 55.0 (**C**H), 54.8 (**C**H_2), 54.2 (**C**H_2), 42.1 (**C**H_2), 24.9 (**C**H), 22.9 (**C**H_3), 22.6 (**C**H_3). **IR** (neat): ν 3295, 3071, 2959, 2851, 2095, 1450, 1290, 1059 cm^{-1}. **Anal. Calcd. for $C_{14}H_{22}N_4O$**: C, 64.09; H, 8.45; N, 21.36; Found: C, 64.08; H, 8.40; N, 21.40. Crystals of **3d** suitable for X-ray measurements were obtained from dichloromethane/hexane (1:1) mixture by slow evaporation of the solvent.

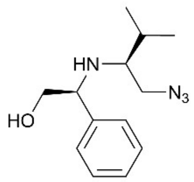
(*R*)-2-(((*R*)-2-azido-2-phenylethyl)amino)-1-phenylethan-1-ol **(3e)**:



3e

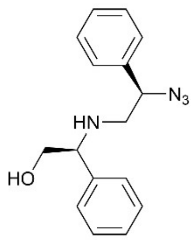
Yellow solid (200.9 mg, 71% yield); mp = 81.2-82.2 °C (hexane/DCM); $[\alpha]^{20}_D$ = –133.43 (c 0.0015 in $CHCl_3$). **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.44–7.41 (m, 2H, C**H**$_{ar}$), 7.39–7.29 (m, 8H, C**H**$_{ar}$), 4.72 (dd, *J* = 3.5 Hz, 8.9 Hz, 1H, C**H**OH), 4.67 (dd, *J* = 5.0 Hz, 8.5 Hz, 1H, C**H**), 3.02 (dd, *J* = 8.5 Hz, 12.6 Hz, 1H, C**H**$_2$), 2.96 (dd, *J* = 3.5 Hz, 12.2 Hz, 1H, C**H**$_2$), 2.91 (dd, *J* = 5.0 Hz, 12.6 Hz, 1H, C**H**$_2$), 2.77 (dd, *J* = 8.9 Hz, 12.2 Hz, 1H, C**H**$_2$). **^{13}C{^{1}H} NMR** (151 MHz, $CDCl_3$): δ 142.2 (**C**$_{qar}$), 137.7 (**C**$_{qar}$), 129.0 (2**C**$_{ar}$), 128.6, 128.4, 127.6, 127.0, 125.8 (8**C**$_{ar}$), 71.9 (**C**HOH), 66.1 (**C**H), 56.7 (**C**H_2), 54.6 (**C**H_2). **IR** (neat): ν 3317, 3056, 2963, 2848, 2102, 1457, 1249, 1062 cm^{-1}. **Anal. Calcd. for $C_{16}H_{18}N_4O$**: C, 68.06; H, 6.43; N, 19.84; Found: C, 68.07; H, 6.40; N, 19.81. Crystals of **3e** suitable for X-ray measurements were obtained from dichloromethane/hexane (1:1) mixture by slow evaporation of the solvent.

(*S*)-2-(((*S*)-1-azido-3-methylbutan-2-yl)amino)-2-phenylethan-1-ol **(4c)**:



4c Colorless oil (199.2 mg, 80% yield); $[\alpha]^{20}_{D}$ = +55.07 (c 0.0015 in $CHCl_3$). **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.30–7.27 (m, 2H, C**H**$_{ar}$), 7.24–7.20 (m, 3H, C**H**$_{ar}$), 3.76 (dd, *J* = 4.5 Hz, 8.9 Hz, 1H, C**H**), 3.58 (dd, *J* = 4.5 Hz, 10.7 Hz, 1H, C**H**$_2$), 3.43 (dd, *J* = 8.9 Hz, 10.7 Hz, 1H, C**H**$_2$), 3.16 (dd, *J* = 4.1 Hz, 12.2 Hz, 1H, C**H**$_2$), 3.04 (dd, *J* = 7.4 Hz, 12.2 Hz, 1H, C**H**$_2$), 2.42–2.39 (m, 1H, C**H**), 1.85–1.82 (m, 1H, C**H**), 0.86–0.84 (m, 6H, 2xC**H**$_3$). **^{13}C{^{1}H} NMR** (151 MHz, $CDCl_3$): δ 140.9 (**C**$_{qar}$), 128.7 (2**C**$_{ar}$), 127.8 (**C**$_{ar}$), 127.2 (2**C**$_{ar}$), 67.1 (**C**H$_2$), 62.6 (**C**H), 59.7 (**C**H), 52.5 (**C**H$_2$), 28.8 (**C**H), 19.0 (**C**H$_3$), 17.5 (**C**H$_3$). **IR** (neat): ν 3351, 3027, 2959, 2874, 2095, 1454, 1267, 1025 cm^{-1}. **Anal. Calcd. for $C_{13}H_{20}N_4O$**: C, 62.88; H, 8.12; N, 22.56; Found: C, 62.86; H, 8.03; N, 22.55.

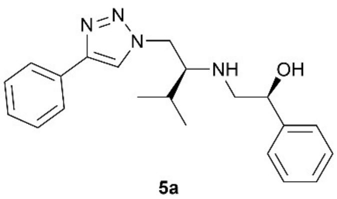
(*S*)-2-(((*R*)-2-azido-2-phenylethyl)amino)-2-phenylethan-1-ol **(4e)**:



4e Yellow solid (226.8 mg, 80% yield); mp = 94.1-95.2 °C (hexane/DCM) $[\alpha]^{20}_{D}$ = –49.21 (c 0.0015 in $CHCl_3$). **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.40–7.33 (m, 5H, C**H**$_{ar}$), 7.31–7.28 (m, 5H, C**H**$_{ar}$), 4.57 (t, *J* = 6.7 Hz, 1H, C**H**), 3.81 (dd, *J* = 4.0 Hz, 8.4 Hz, 1H, C**H**), 3.72 (dd, *J* = 4.0 Hz, 10.8 Hz, 1H, C**H**$_2$), 3.56 (t, *J* = 10.8 Hz, 1H, C**H**$_2$), 2.84 (d, *J* = 6.7 Hz, 2H, C**H**$_2$). **^{13}C{^{1}H} NMR** (151 MHz, $CDCl_3$): δ 140.3 (**C**$_{qar}$), 137.8 (**C**$_{qar}$), 128.9, 128.7, 128.5, 127.8, 127.1, 127.0 (10**C**$_{ar}$), 66.9 (**C**H$_2$), 66.5 (**C**H), 64.9 (**C**H), 52.9 (**C**H$_2$). **IR** (neat): ν 3276, 3064, 2963, 2840, 2095, 1462, 1223, 1028 cm^{-1}. **Anal. Calcd. for $C_{16}H_{18}N_4O$**: C, 68.06; H, 6.43; N, 19.84; Found: C, 68.02; H, 6.31; N, 19.72. Crystals of **4e** suitable for X-ray measurements were obtained from dichloromethane/hexane (1:1) mixture by slow evaporation of the solvent.

General procedure for synthesis of 1,2,3-triazoles **5a**-**5e**, **6c, 6e, 7-14, 17** and **18**: An appropriate azide **3a-3e, 4c, 4e** and **16** (1.0 mmol) was dissolved in methanol (8 mL), then the CuI as a catalyst (0.1 mmol, 19.0 mg) and appropriate acetylene (1.0 mmol) were added. The whole mixture was stirred for 24 hours. After, solvent was removed *in vacuo* and the mixture was extracted with DCM (3 x 10 mL). Combined organic layers were dried over anhydrous $MgSO_4$, filtered, and the solvent was removed under reduced pressure. The products were purified by crystallization (dichloromethane/hexane (1:1) mixture by slow evaporation of the solvent) or by column chromatography (SiO_2, hexane/ethyl acetate in gradient).

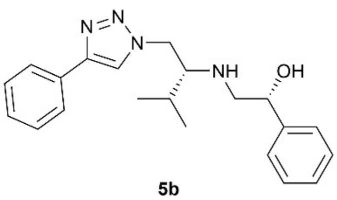
(*S*)-2-(((*S*)-3-methyl-1-(4-phenyl-1*H*-1,2,3-triazol-1-yl)butan-2-yl)amino)-1-phenylethan-1-ol **(5a)**:



5a

Green solid (274.9 mg, 78% yield); mp = 102.4-103.1 °C (hexane/DCM); $[\alpha]^{20}_{D}$ = –3.78 (c 0.0015 in $CHCl_3$). **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.86–7.84 (m, 3H, C**H**$_{ar,}$ C**H**$_{triazole}$), 7.46–7.44 (m, 2H, C**H**$_{ar}$), 7.37–7.31 (m, 5H, C**H**$_{ar}$), 7.28–7.25 (m, 1H, C**H**$_{ar}$), 4.62 (dd, *J* = 3.5 Hz, 8.7 Hz, 1H, C**H**OH), 4.49 (dd, *J* = 4.2 Hz, 13.9 Hz, 1H, C**H**$_2$), 4.32 (dd, *J* = 7.5 Hz, 13.9 Hz, 1H, C**H**$_2$), 2.86–2.83 (m, 2H, C**H**, C**H**$_2$), 2.73 (dd, *J* = 8.7 Hz, 12.0 Hz, 1H, C**H**$_2$), 1.82–1.76 (m, 1H, C**H**), 1.04–1.03 (m, 6H, 2xC**H**$_3$). **^{13}C{^{1}H} NMR** (151 MHz, $CDCl_3$): δ 147.7, 142.1, 130.6 (3**C**$_{qar}$), 128.9, 128.4, 128.2, 127.6, 125.8 (10**C**$_{ar}$), 120.6 (**C**$_{ar\ triazole}$), 72.7 (**C**HOH), 63.7 (**C**H), 55.7 (**C**H$_2$), 51.7 (**C**H$_2$), 29.7 (**C**H), 18.7 (**C**H$_3$), 18.5 (**C**H$_3$). **IR** (neat): ν 3276, 3064, 2963, 2840, 2095, 1462, 1223, 1028 cm^{-1}. **Anal. Calcd. for $C_{21}H_{26}N_4O$**: C, 71.97; H, 7.48; N, 15.99; Found: C, 71.90; H, 7.58; N, 15.77. Crystals of **5a** suitable for X-ray measurements were obtained from dichloromethane/hexane (1:1) mixture by slow evaporation of the solvent.

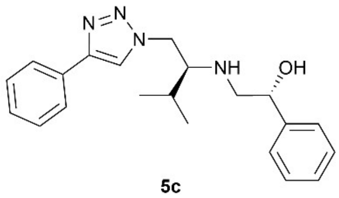
(*R*)-2-(((*R*)-3-methyl-1-(4-phenyl-1*H*-1,2,3-triazol-1-yl)butan-2-yl)amino)-1-phenylethan-1-ol **(5b)**:



5b

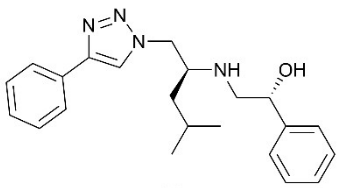
Green solid (264.5 mg, 75% yield); mp = 102.4-103.1 °C (hexane/DCM); $[\alpha]^{20}_{D}$ = +3.78 (c 0.0015 in $CHCl_3$). **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.85–7.84 (m, 3H, C**H**$_{ar,}$ C**H**$_{triazole}$), 7.46–7.43 (m, 2H, C**H**$_{ar}$), 7.37–7.31 (m, 5H, C**H**$_{ar}$), 7.28–7.25 (m, 1H, C**H**$_{ar}$), 4.64 (br. s, 1H, C**H**OH), 4.49 (dd, *J* = 4.1 Hz, 13.9 Hz, 1H, C**H**$_2$), 4.31 (dd, *J* = 7.5 Hz, 13.9 Hz, 1H, C**H**$_2$), 2.85–2.83 (m, 2H, C**H**, C**H**$_2$), 2.73 (dd, *J* = 8.8 Hz, 12.0 Hz, 1H, C**H**$_2$), 1.81–1.76 (m, 1H, C**H**), 1.04 (d, *J* = 1.7 Hz, 3H, C**H**$_3$), 1.03 (d, *J* = 1.7 Hz, 3H, C**H**$_3$). **^{13}C{^{1}H} NMR** (151 MHz, $CDCl_3$): δ 147.7, 142.2, 130.6 (3**C**$_{qar}$), 128.9, 128.4, 128.2, 127.6, 125.8 (10**C**$_{ar}$), 120.6 (**C**$_{ar\ triazole}$), 72.7 (**C**HOH), 63.8 (**C**H), 55.8 (**C**H$_2$), 51.6 (**C**H$_2$), 29.6 (**C**H), 18.7 (**C**H$_3$), 18.6 (**C**H$_3$). **IR** (neat): ν 3295, 2959, 2926, 2870, 1450, 1223, 1025 cm^{-1}. **Anal. Calcd. for $C_{21}H_{26}N_4O$**: C, 71.97; H, 7.48; N, 15.99; Found: C, 71.89; H, 7.37; N, 15.99. Crystals of **5b** suitable for X-ray measurements were obtained from dichloromethane/hexane (1:1) mixture by slow evaporation of the solvent.

(*R*)-2-(((*S*)-3-methyl-1-(4-phenyl-1*H*-1,2,3-triazol-1-yl)butan-2-yl)amino)-1-phenylethan-1-ol **(5c)**:



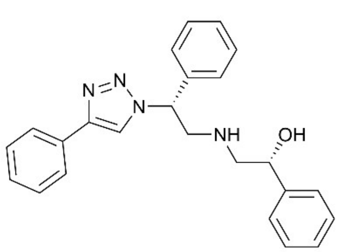
5c White solid (288.6 mg, 82% yield); mp = 127.3-128.4 °C (hexane/DCM); $[\alpha]^{20}_{D}$ = –25.57 (c 0.0015 in $CHCl_3$). **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.85–7.83 (m, 2H, C**H**$_{ar}$), 7.79 (s, 1H, C**H**$_{triazole}$), 7.47–7.44 (m, 2H, C**H**$_{ar}$), 7.38–7.32 (m, 5H, C**H**$_{ar}$), 7.28–7.25 (m, 1H, C**H**$_{ar}$), 4.67 (dd, *J* = 3.7 Hz, 8.3 Hz, 1H, C**H**OH), 4.49 (dd, *J* = 4.4 Hz, 14.0 Hz, 1H, C**H**$_2$), 4.34 (dd, *J* = 7.4 Hz, 14.0 Hz, 1H, C**H**$_2$), 2.95 (dd, *J* = 3.7 Hz, 12.3 Hz, 1H, C**H**$_2$), 2.91–2.88 (m, 1H, C**H**), 2.65 (dd, *J* = 8.3 Hz, 12.3 Hz, 1H, C**H**$_2$), 1.82–1.76 (m, 1H, C**H**), 1.06 (d, *J* = 6.9 Hz, 3H, C**H**$_3$), 1.04 (d, *J* = 6.9 Hz, 3H, C**H**$_3$). **^{13}C{^{1}H} NMR** (151 MHz, $CDCl_3$): δ 147.7, 142.0, 130.6 (3**C**$_{qar}$), 128.8, 128.4, 128.1, 127.6, 125.8 (10**C**$_{ar}$), 120.5 (**C**$_{ar\ triazole}$), 72.3 (**C**HOH), 63.3 (**C**H), 55.3 (**C**H$_2$), 51.6 (**C**H$_2$), 29.7 (**C**H), 18.9 (**C**H$_3$), 18.3 (**C**H$_3$). **IR** (neat): ν 3332, 2959, 2896, 2836, 1465, 1155, 1073 cm^{-1}. **Anal. Calcd. for $C_{21}H_{26}N_4O$**: C, 71.97; H, 7.48; N, 15.99; Found: C, 71.77; H, 7.25; N, 15.80.

(*R*)-2-(((*S*)-4-methyl-1-(4-phenyl-1*H*-1,2,3-triazol-1-yl)pentan-2-yl)amino)-1-phenylethan-1-ol **(5d)**:



5d White solid (233.9 mg, 64% yield); mp = 107.2-108.1 °C (hexane/DCM); $[\alpha]^{20}_{D}$ = –72.43 (c 0.0015 in $CHCl_3$). **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.75–7.74 (m, 2H, C**H**$_{ar}$), 7.68 (s, 1H, C**H**$_{triazole}$), 7.37–7.34 (m, 2H, C**H**$_{ar}$), 7.28–7.24 (m, 5H, C**H**$_{ar}$), 7.21–7.18 (m, 1H, C**H**$_{ar}$), 4.62 (dd, *J* = 3.6 Hz, 8.3 Hz, 1H, C**H**OH), 4.36 (dd, *J* = 4.2 Hz, 13.9 Hz, 1H, C**H**$_2$), 4.24 (dd, *J* = 5.9 Hz, 13.9 Hz, 1H, C**H**$_2$), 3.07–3.03 (m, 1H, C**H**), 2.93 (dd, *J* = 3.6 Hz, 12.1 Hz, 1H, C**H**$_2$), 2.65 (dd, *J* = 8.3 Hz, 12.1 Hz, 1H, C**H**$_2$), 1.74–1.68 (m, 1H, C**H**), 1.24–1.18 (m, 1H, C**H**$_2$), 1.16–1.11 (m, 1H, C**H**$_2$), 0.85 (d, *J* = 6.6 Hz, 3H, C**H**$_3$), 0.84 (d, *J* = 6.6 Hz, 3H, C**H**$_3$). **^{13}C{^{1}H} NMR** (151 MHz, $CDCl_3$): δ 147.6, 142.1, 130.6 (3**C**$_{qar}$), 128.8, 128.5, 128.1, 127.7, 125.8 (10**C**$_{ar}$), 120.7 (**C**$_{ar\ triazole}$), 72.4 (**C**HOH), 55.4 (**C**H), 54.2 (**C**H$_2$), 53.4 (**C**H$_2$), 41.9 (**C**H$_2$), 24.8 (**C**H), 23.0 (**C**H$_3$), 22.4 (**C**H$_3$). **IR** (neat): ν 3123, 2956, 2866, 1439, 1223, 1073, 1051 cm^{-1}. **Anal. Calcd. for $C_{22}H_{28}N_4O$**: C, 72.50; H, 7.74; N, 15.37; Found: C, 72.32; H, 7.98; N, 15.18.

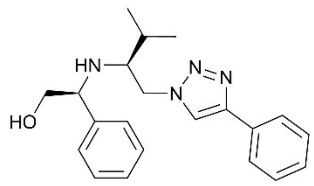
(*R*)-1-phenyl-2-(((*R*)-2-phenyl-2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)ethyl)amino)ethan-1-ol **(5e)**:



5e White solid (262.5 mg, 68% yield); mp = 167.2-168.1 °C (hexane/DCM); $[\alpha]^{20}_{D}$ = –21.21 (c 0.0015 in $CHCl_3$). **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.83–7.82 (m, 2H, C**H**$_{ar}$), 7.74 (s, 1H, C**H**$_{triazole}$), 7.44–7.28 (m, 13H, C**H**$_{ar}$), 5.75 (dd, *J* = 5.1 Hz, 8.7 Hz, 1H, C**H**OH), 4.70 (dd, *J* = 3.4 Hz, 9.1 Hz, 1H, C**H**), 3.91 (dd, *J* = 8.7 Hz, 13.0 Hz, 1H, C**H**$_2$), 3.39 (dd, *J* = 5.1 Hz, 13.0 Hz, 1H, C**H**$_2$), 3.04 (dd, *J* = 3.4 Hz, 12.4 Hz, 1H, C**H**$_2$), 2.79 (dd, *J* = 9.1 Hz, 12.4 Hz, 1H, C**H**$_2$). **^{13}C{^{1}H} NMR** (151 MHz, $CDCl_3$): δ 147.9, 142.0, 137.4, 130.4 (4**C**$_{qar}$), 129.2, 128.9, 128.8, 128.4, 128.2, 127.6, 127.0, 125.8, 125.7 (15**C**$_{ar}$), 119.9

($C_{ar\ triazole}$), 71.9 (**C**HOH), 65.5 (**C**H), 56.9 (**C**H_2), 53.3 (**C**H_2). **IR** (neat): ν 3079, 2952, 2922, 2863, 1465, 1230, 1118, 1062 cm^{-1}. **Anal. Calcd. for $C_{24}H_{24}N_4O$**: C, 74.97; H, 6.29; N, 14.57; Found: C, 74.85; H, 6.38; N, 14.33.

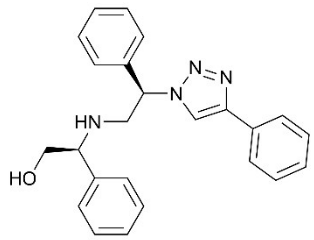
(*S*)-2-(((*S*)-3-methyl-1-(4-phenyl-1*H*-1,2,3-triazol-1-yl)butan-2-yl)amino)-2-phenylethan-1-ol **(6c)**:



6c

Colorless oil (301.9 mg, 86% yield); $[\alpha]^{20}_D$ = +22.93 (c 0.0015 in $CHCl_3$). **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.68–7.66 (m, 2H, CH_{ar}), 7.47 (s, 1H, C$H_{triazole}$), 7.35–7.32 (m, 2H, CH_{ar}), 7.26–7.24 (m, 1H, CH_{ar}), 7.03–7.00 (m, 3H, CH_{ar}), 6.86–6.85 (m, 2H, CH_{ar}), 4.15 (dd, *J* = 4.0 Hz, 13.9 Hz, 1H, CH_2), 4.10 (dd, *J* = 8.9 Hz, 13.9 Hz, 1H, CH_2), 3.72 (dd, *J* = 4.3 Hz, 9.2 Hz, 1H, C**H**OH), 3.53 (dd, *J* = 4.3 Hz, 10.8 Hz, 1H, CH_2), 3.40 (dd, *J* = 9.2 Hz, 10.8 Hz, 1H, CH_2), 2.66–2.63 (m, 1H, C**H**), 1.89–1.86 (m, 1H, C**H**), 0.95 (d, *J* = 7.0 Hz, 3H, CH_3), 0.93 (d, *J* = 7.0 Hz, 3H, CH_3). **^{13}C{^{1}H} NMR** (151 MHz, $CDCl_3$): δ 147.7, 140.4, 130.6 (3C_{qar}), 128.8, 128.6, 128.1, 127.6, 127.2, 125.7 (10C_{ar}), 120.4 ($C_{ar\ triazole}$), 67.0 (**C**H_2), 62.8 (**C**HOH), 60.5 (**C**H), 51.6 (**C**H_2), 28.8 (**C**H), 18.9 (**C**H_3), 17.2 (**C**H_3). **IR** (neat): ν 3328, 2959, 2870, 1465, 1226, 1055, 1025 cm^{-1}. **HRMS** (ESI-TOF): Calcd for $C_{21}H_{26}N_4O$ 350.2107; Found 350.2104.

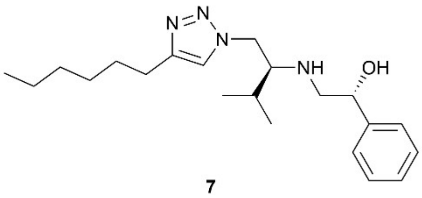
(*S*)-2-phenyl-2-(((*R*)-2-phenyl-2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)ethyl)amino)ethan-1-ol **(6e)**:



6e

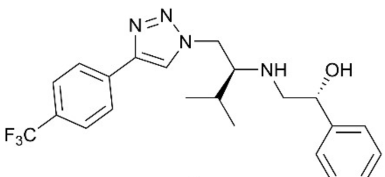
White solid (226.9 mg, 59% yield); mp = 144.2-144.9 °C (hexane/DCM); $[\alpha]^{20}_D$ = +45.07 (c 0.0015 in $CHCl_3$). **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.71–7.70 (m, 2H, CH_{ar}), 7.50 (s, 1H, C$H_{triazole}$), 7.34–7.31 (m, 2H, CH_{ar}), 7.27–7.14 (m, 11H, CH_{ar}), 5.53 (dd, *J* = 5.3 Hz, 8.5 Hz, 1H, C**H**OH), 3.73 (dd, *J* = 4.4 Hz, 8.8 Hz, 1H, C**H**), 3.63 (dd, *J* = 8.5 Hz, 13.1 Hz, 1H, CH_2), 3.57 (dd, *J* = 4.4 Hz, 10.9 Hz, 1H, CH_2), 3.40 (dd, *J* = 8.8 Hz, 10.9 Hz, 1H, CH_2), 3.26 (dd, *J* = 5.3 Hz, 13.1 Hz, 1H, CH_2). **^{13}C{^{1}H} NMR** (151 MHz, $CDCl_3$): δ 147.7, 140.5, 137.5, 130.5 (4C_{qar}), 129.1, 128.8, 128.2, 127.8, 127.1, 126.9, 125.7 (15C_{ar}), 119.9 ($C_{ar\ triazole}$), 66.8 (**C**H_2), 65.7 (**C**HOH), 65.1 (**C**H), 51.8 (**C**H_2). **IR** (neat): ν 3284, 3082, 2933, 2855, 1454, 1226, 1021 cm^{-1}. **Anal. Calcd. for $C_{24}H_{24}N_4O$**: C, 74.97; H, 6.29; N, 14.57; Found: C, 74.87; H, 6.12; N, 14.55. Crystals of **6e** suitable for X-ray measurements were obtained from dichloromethane/hexane (1:1) mixture by slow evaporation of the solvent.

(*R*)-2-(((*S*)-1-(4-hexyl-1*H*-1,2,3-triazol-1-yl)-3-methylbutan-2-yl)amino)-1-phenylethan-1-ol **(7)**:



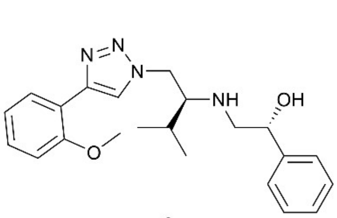
7 Colorless oil (183.8 mg, 51% yield); $[\alpha]^{20}_{D}$ = –22.93 (c 0.0015 in $CHCl_3$). **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.35–7.31 (m, 4H, C**H**$_{ar}$), 7.28–7.26 (m, 2H, C**H**$_{ar,}$ C**H**$_{triazole}$), 4.62 (dd, *J* = 3.5 Hz, 8.5 Hz, 1H, C**H**OH), 4.38 (dd, *J* = 4.4 Hz, 13.9 Hz, 1H, C**H**$_2$), 4.23 (dd, *J* = 7.7 Hz, 13.9 Hz, 1H, C**H**$_2$), 2.86–2.81 (m, 2H, C**H**, C**H**$_2$), 2.70 (t, *J* = 7.7 Hz, 2H, C**H**$_2$), 2.56 (dd, *J* = 8.5 Hz, 12.2 Hz, 1H, C**H**$_2$), 1.77–1.71 (m, 1H, C**H**), 1.68–1.63 (m, 2H, C**H**$_2$), 1.36–1.30 (m, 6H, 3xC**H**$_2$), 1.01–0.99 (m, 6H, 2xC**H**$_3$), 0.90 (t, *J* = 7.0 Hz, 3H, C**H**$_3$). **^{13}C{^{1}H} NMR** (151 MHz, $CDCl_3$): δ 148.4, 142.2 (2**C**$_{qar}$), 128.3, 127.5, 125.8 (5**C**$_{ar}$), 121.5 (**C**$_{ar\ triazole}$), 72.1 (**C**HOH), 63.3 (**C**H), 55.3 (**C**H$_2$), 51.5 (**C**H$_2$), 31.6 (**C**H$_2$), 29.8 (**C**H), 29.5 (**C**H$_2$), 28.9 (**C**H$_2$), 25.7 (**C**H$_2$), 22.6 (**C**H$_2$), 18.8 (**C**H$_3$), 18.3 (**C**H$_3$), 14.1 (**C**H$_3$). **IR** (neat): ν 3325, 2956, 2926, 2855, 1603, 1454, 1215, 1059 cm^{-1}. **Anal. Calcd. for $C_{21}H_{34}N_4O$**: C, 70.35; H, 9.56; N, 15.63; Found: C, 70.37; H, 9.33; N, 15.51.

(*R*)-2-(((*S*)-3-methyl-1-(4-(4-(trifluoromethyl)phenyl)-1*H*-1,2,3-triazol-1-yl)butan-2-yl)amino)-1-phenylethan-1-ol **(8)**:



8 White solid (331.8 mg, 79% yield); mp = 96.2-97.3 °C (hexane/DCM); $[\alpha]^{20}_{D}$ = –53.07 (c 0.0015 in $CHCl_3$). **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.96–7.94 (m, 2H, C**H**$_{ar}$), 7.88 (s, 1H, C**H**$_{triazole}$), 7.71–7.70 (m, 2H, C**H**$_{ar}$), 7.33–7.32 (m, 4H, C**H**$_{ar}$), 7.29–7.28 (m, 1H, C**H**$_{ar}$), 4.69 (dd, *J* = 8.2 Hz, 3.7 Hz, 1H, C**H**OH), 4.51 (dd, *J* = 14.0 Hz, 4.3 Hz, 1H, C**H**$_2$), 4.35 (dd, *J* = 14.0 Hz, 7.5 Hz, 1H, C**H**$_2$), 2.98 (dd, *J* = 12.2 Hz, 3.7 Hz, 1H, C**H**$_2$), 2.90–2.87 (m, 1H, C**H**), 2.64 (dd, *J* = 12.2 Hz, 8.2 Hz, 1H, C**H**$_2$), 1.82–1.77 (m, 1H, C**H**), 1.06 (d, *J* = 6.8 Hz, 3H, C**H**$_3$), 1.04 (d, *J* = 6.8 Hz, 3H, C**H**$_3$). **^{13}C{^{1}H} NMR** (151 MHz, $CDCl_3$): δ 146.3, 142.0, 134.1 (3**C**$_{qar}$), 130.0 (q, $^2J_{C\text{-}F}$ = 33.7 Hz, **C**$_{qar}$), 128.4, 127.7, 125.9 (5**C**$_{ar}$), 125.8 (q, $^3J_{C\text{-}F}$ = 4.4 Hz, 2**C**$_{ar}$), 125.8 (2**C**$_{ar}$), 124.1 (q, $^1J_{C\text{-}F}$ = 271.0 Hz, **C**F$_3$), 121.3 (**C**$_{ar\ triazole}$), 72.4 (**C**HOH), 63.4 (**C**H), 55.3 (**C**H$_2$), 51.7 (**C**H$_2$), 29.7 (**C**H), 18.8 (**C**H$_3$), 18.4 (**C**H$_3$). **^{19}F NMR** (565 MHz, $CDCl_3$): δ –62.6 (s, CF$_3$). **IR** (neat): ν 3377, 2959, 2922, 2851, 1461, 1327, 1111, 1062 cm^{-1}. **Anal. Calcd. for $C_{22}H_{25}F_3N_4O$**: C, 63.15; H, 6.02; N, 13.39; Found: C, 63.33; H, 6.13; N, 13.16.

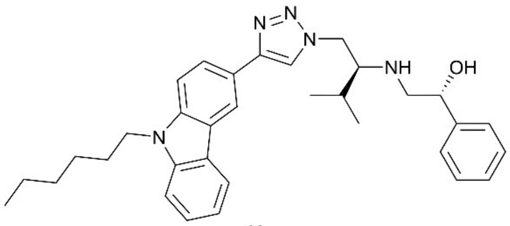
(*R*)-2-(((*S*)-1-(4-(2-methoxyphenyl)-1*H*-1,2,3-triazol-1-yl)-3-methylbutan-2-yl)amino)-1-phenylethan-1-ol **(9)**:



9 Colorless oil (225.3 mg, 59% yield); $[\alpha]^{20}_{D}$ = –44.36 (c 0.0015 in $CHCl_3$). **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.37–8.35 (m, 1H, C**H**$_{ar}$), 8.09 (s, 1H, C**H**$_{triazole}$), 7.35–7.29 (m, 5H, C**H**$_{ar}$), 7.26–7.24 (m, 1H, C**H**$_{ar}$), 7.12–7.09 (m, 1H, C**H**$_{ar}$), 7.01–7.00 (m, 1H, C**H**$_{ar}$), 4.63 (dd, *J* = 3.6 Hz, 8.7 Hz, 1H, C**H**OH), 4.49 (dd, *J* = 4.5 Hz, 14.0 Hz, 1H, C**H**$_2$), 4.33 (dd, *J* = 7.7 Hz, 14.0 Hz, 1H, C**H**$_2$), 3.96 (s, 3H,

OC**H**$_3$), 2.94–2.90 (m, 2H, C**H**, C**H**$_2$), 2.61 (dd, *J* = 8.7 Hz, 12.3 Hz, 1H, C**H**$_2$), 1.84–1.78 (m, 1H, C**H**), 1.05 (d, *J* = 6.9 Hz, 3H, C**H**$_3$), 1.04 (d, *J* = 6.9 Hz, 3H, C**H**$_3$). **^{13}C{^{1}H} NMR** (151 MHz, CDCl$_3$): δ 155.7, 143.1, 142.1 (3**C**$_{qar}$), 128.9, 128.4, 127.7, 127.5, 125.8 (7**C**$_{ar}$), 123.9 (**C**$_{ar\ triazole}$), 121.1 (**C**$_{ar}$), 119.4 (**C**$_{qar}$), 110.8 (**C**$_{ar}$), 72.2 (**C**HOH), 63.3 (**C**H), 55.4 (O**C**H$_3$), 55.3 (**C**H$_2$), 51.5 (**C**H$_2$), 29.7 (**C**H), 18.8 (**C**H$_3$), 18.3 (**C**H$_3$). **IR** (neat): ν 3347, 2959, 2922, 1491, 1465, 1245, 1048 cm^{-1}. HRMS (ESI-TOF): Calcd for $C_{22}H_{28}N_4O_2$ 380.2212; Found 380.2214.

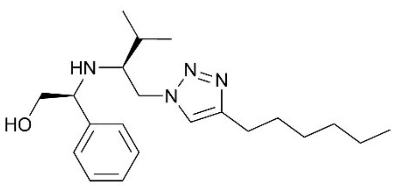
(*R*)-2-(((*S*)-1-(4-(9-hexyl-9*H*-carbazol-3-yl)-1*H*-1,2,3-triazol-1-yl)-3-methylbutan-2-yl)amino)-1-phenylethan-1-ol **(10)**:



10

Yellow oil (337.3 mg, 64% yield); $[\alpha]^{20}_D$ = –30.93 (c 0.0015 in CHCl$_3$). **^{1}H NMR** (600 MHz, CDCl$_3$): δ 8.46–8.45 (m, 1H, C**H**$_{ar}$), 8.04–8.03 (m, 1H, C**H**$_{ar}$), 7.80–7.79 (m, 1H, C**H**$_{ar}$), 7.69 (s, 1H, C**H**$_{triazole}$), 7.39–7.36 (m, 1H, C**H**$_{ar}$), 7.31–7.30 (m, 2H, C**H**$_{ar}$), 7.22–7.11 (m, 6H, C**H**$_{ar}$), 4.54 (dd, *J* = 3.6 Hz, 8.3 Hz, 1H, C**H**OH), 4.34–4.31 (m, 1H, C**H**$_2$), 4.21–4.16 (m, 3H, 2xC**H**$_2$), 2.82–2.77 (m, 2H, C**H**, C**H**$_2$), 2.53 (dd, *J* = 8.4 Hz, 12.2 Hz, 1H, C**H**$_2$), 1.78–1.74 (m, 2H, C**H**$_2$), 1.67–1.65 (m, 1H, C**H**), 1.30–1.26 (m, 2H, C**H**$_2$), 1.21–1.17 (m, 4H, 2xC**H**$_2$), 0.91 (d, *J* = 6.7 Hz, 3H, C**H**$_3$), 0.89 (d, *J* = 6.7 Hz, 3H, C**H**$_3$), 0.77 (t, *J* = 7.1 Hz, 3H, C**H**$_3$). **^{13}C{^{1}H} NMR** (151 MHz, CDCl$_3$): δ 148.8, 142.2, 140.9, 140.4 (4**C**$_{qar}$), 128.4, 127.5, 125.9, 123.8 (7**C**$_{ar}$), 123.2, 122.9, 121.5 (3**C**$_{qar}$), 120.6 (**C**$_{ar}$), 119.8 (**C**$_{ar\ triazole}$), 119.0, 117.8, 109.0, 108.9 (4**C**$_{ar}$), 72.2 (**C**HOH), 63.3 (**C**H), 55.3 (**C**H$_2$), 51.6 (**C**H$_2$), 43.2 (**C**H$_2$), 31.6 (**C**H$_2$), 29.7 (**C**H), 29.0 (**C**H$_2$), 27.0 (**C**H$_2$), 22.6 (**C**H$_2$), 18.9 (**C**H$_3$), 18.3 (**C**H$_3$), 14.0 (**C**H$_3$). **IR** (neat): ν 3332, 2956, 2926, 2855, 1629, 1454, 1327, 1219, 1051 cm^{-1}. **Anal. Calcd. for $C_{33}H_{41}N_5O$**: C, 75.68; H, 7.89; N, 13.37; Found: C, 75.40; H, 7.96; N, 13.17.

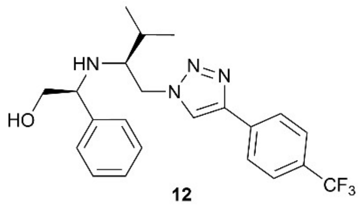
(*S*)-2-(((*S*)-1-(4-hexyl-1*H*-1,2,3-triazol-1-yl)-3-methylbutan-2-yl)amino)-2-phenylethan-1-ol **(11)**:



11

Red oil (234.2 mg, 65% yield); $[\alpha]^{20}_D$ = +28.36 (c 0.0015 in CHCl$_3$). **^{1}H NMR** (600 MHz, CDCl$_3$): δ 7.22–7.19 (m, 3H, C**H**$_{ar}$), 7.04 (s, 1H, C**H**$_{triazole}$), 6.92–6.90 (m, 2H, C**H**$_{ar}$), 4.18–4.14 (m, 2H, C**H**$_2$), 3.77 (dd, *J* = 4.4 Hz, 9.1 Hz, 1H, C**H**OH), 3.60 (dd, *J* = 4.4 Hz, 10.8 Hz, 1H, C**H**$_2$), 3.45 (dd, *J* = 9.1 Hz, 10.8 Hz, 1H, C**H**$_2$), 2.70–2.62 (m, 3H, C**H**, C**H**$_2$), 1.96–1.91 (m, 1H, C**H**), 1.64–1.59 (m, 2H, C**H**$_2$), 1.37–1.28 (m, 6H, 3xC**H**$_2$), 1.02 (d, *J* = 7.0 Hz, 3H, C**H**$_3$), 0.99 (d, *J* = 7.0 Hz, 3H, C**H**$_3$), 0.89 (t, *J* = 7.1 Hz, 3H, C**H**$_3$). **^{13}C{^{1}H} NMR** (151 MHz, CDCl$_3$): δ 148.6, 140.3 (2**C**$_{qar}$), 128.6, 127.6, 127.0 (5**C**$_{ar}$), 121.1 (**C**$_{ar\ triazole}$), 66.9 (**C**H$_2$), 62.4 (**C**HOH), 60.3 (**C**H), 51.1 (**C**H$_2$), 31.6 (**C**H$_2$), 29.4 (**C**H$_2$), 29.0 (**C**H$_2$), 28.6 (**C**H), 25.7 (**C**H$_2$), 22.6 (**C**H$_2$), 18.8 (**C**H$_3$), 17.0 (**C**H$_3$), 14.1 (**C**H$_3$). **IR** (neat): ν 3332, 2956, 2926, 2855, 1551, 1454, 1219, 1055 cm^{-1}. **Anal. Calcd. for $C_{21}H_{34}N_4O$**: C, 70.35; H, 9.56; N, 15.63; Found: C, 70.21; H, 9.49; N, 15.40.

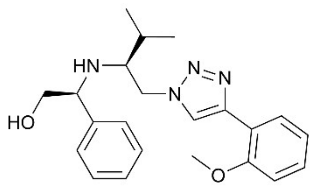
(*S*)-2-(((*S*)-3-methyl-1-(4-(4-(trifluoromethyl)phenyl)-1*H*-1,2,3-triazol-1-yl)butan-2-yl)amino)-2-phenylethan-1-ol **(12)**:



12

White solid (294.4 mg, 70% yield); mp = 104.2-104.9 °C (hexane/DCM); $[\alpha]^{20}_{D}$ = –11.43 (c 0.0015 in $CHCl_3$). **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.87–7.86 (m, 2H, CH_{ar}), 7.69–7.68 (m, 2H, CH_{ar}), 7.59 (s, 1H, C$H_{triazole}$), 7.12–7.09 (m, 3H, CH_{ar}), 6.95–6.93 (m, 2H, CH_{ar}), 4.29–4.21 (m, 2H, CH_2), 3.78 (dd, *J* = 9.0 Hz, 4.4 Hz, 1H, C**H**OH), 3.62 (dd, *J* = 10.8 Hz, 4.4 Hz, 1H, CH_2), 3.50 (dd, *J* = 10.8 Hz, 9.0 Hz, 1H, CH_2), 2.76–2.74 (m, 1H, C**H**), 2.00–1.95 (m, 1H, C**H**), 1.06 (d, *J* = 6.9 Hz, 3H, CH_3), 1.04 (d, *J* = 6.9 Hz, 3H, CH_3). **^{13}C{^{1}H} NMR** (151 MHz, $CDCl_3$): δ 146.4, 140.2, 134.1 (3C_{qar}), 130.0 (q, $^2J_{C-F}$ = 32.6 Hz, C_{qar}), 128.6, 127.7, 127.1 (5C_{ar}), 125.8 (q, $^3J_{C-F}$ = 4.4 Hz, 2C_{ar}), 125.8 (2C_{ar}), 124.1 (q, $^1J_{C-F}$ = 272.2 Hz, CF_3), 121.0 ($C_{ar\ triazole}$), 66.9 (CH_2), 62.9 (**C**HOH), 60.7 (**C**H), 51.7 (CH_2), 29.0 (**C**H), 18.9 (CH_3), 17.2 (CH_3). **^{19}F NMR** (565 MHz, $CDCl_3$): δ –62.6 (s, CF_3). **IR** (neat): ν 3355, 2963, 2922, 2851, 1454, 1323, 1118, 1066 cm^{-1}. **Anal. Calcd. for $C_{22}H_{25}F_3N_4O$**: C, 63.15; H, 6.02; N, 13.39; Found: C, 63.23; H, 6.02; N, 13.39.

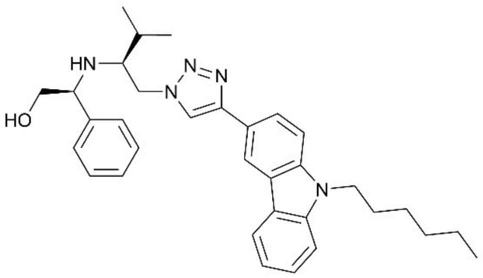
(*S*)-2-(((*S*)-1-(4-(2-methoxyphenyl)-1*H*-1,2,3-triazol-1-yl)-3-methylbutan-2-yl)amino)-2-phenylethan-1-ol **(13)**:



13

Colorless oil (194.9 mg, 51% yield); $[\alpha]^{20}_{D}$ = +13.36 (c 0.0015 in $CHCl_3$). **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.38–8.37 (m, 1H, CH_{ar}), 7.84 (s, 1H, C$H_{triazole}$), 7.37–7.34 (m, 1H, CH_{ar}), 7.14–7.07 (m, 4H, CH_{ar}), 7.01–6.99 (m, 1H, CH_{ar}), 6.94–6.93 (m, 2H, CH_{ar}), 4.31–4.23 (m, 2H, CH_2), 3.91 (s, 3H, OCH_3), 3.82 (dd, *J* = 4.4 Hz, 8.9 Hz, 1H, C**H**OH), 3.63 (dd, *J* = 4.4 Hz, 10.8 Hz, 1H, CH_2), 3.48 (dd, *J* = 9.1 Hz, 10.8 Hz, 1H, CH_2), 2.82–2.79 (m, 1H, C**H**), 2.01–1.96 (m, 1H, C**H**), 1.08 (d, *J* = 6.9 Hz, 3H, CH_3), 1.05 (d, *J* = 6.9 Hz, 3H, CH_3). **^{13}C{^{1}H} NMR** (151 MHz, $CDCl_3$): δ 155.6, 143.3, 140.2 (3C_{qar}), 128.9, 128.5, 127.7, 127.5, 127.0 (7C_{ar}), 123.7 ($C_{ar\ triazole}$), 121.1 (C_{ar}), 119.5 (C_{qar}), 110.8 (C_{ar}), 67.0 (CH_2), 62.6 (**C**HOH), 60.3 (**C**H), 55.3 (OCH_3), 51.2 (CH_2), 28.8 (**C**H), 18.7 (CH_3), 17.2 (CH_3). **IR** (neat): ν 3328, 2956, 2870, 1491, 1465, 1245, 1025 cm^{-1}. HRMS (ESI-TOF): Calcd for $C_{22}H_{28}N_4O_2$ 380.2212; Found 380.2215.

(*S*)-2-(((*S*)-1-(4-(9-hexyl-9*H*-carbazol-3-yl)-1*H*-1,2,3-triazol-1-yl)-3-methylbutan-2-yl)amino)-2-phenylethan-1-ol **(14)**:

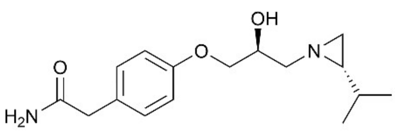


14

Yellow oil (190.1 mg, 36% yield); $[\alpha]^{20}_{D}$ = –24.43 (c 0.0015 in $CHCl_3$). **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.57–8.56 (m, 1H, C**H**$_{ar}$), 8.23–8.22 (m, 1H, C**H**$_{ar}$), 7.96–7.95 (m, 1H, C**H**$_{ar}$), 7.63 (s, 1H, C**H**$_{triazole}$), 7.59–7.51 (m, 3H, C**H**$_{ar}$), 7.36–7.33 (m, 1H, C**H**$_{ar}$), 7.22–7.15 (m, 3H, C**H**$_{ar}$), 7.03–7.02 (m, 2H, C**H**$_{ar}$), 4.41 (t, *J* = 7.3 Hz, 2H, C**H**$_2$), 4.36 (d, *J* = 6.5 Hz, 2H, C**H**$_2$), 3.89 (dd, *J* = 4.4 Hz, 9.1 Hz, 1H, C**H**OH), 3.70 (dd, *J* = 4.4 Hz, 10.8 Hz, 1H, C**H**$_2$), 3.57 (t, *J* = 9.9 Hz, 1H, C**H**$_2$), 2.89–2.86 (m, 1H, C**H**), 2.10–2.07 (m, 1H, C**H**), 2.01–1.96 (m, 2H, C**H**$_2$), 1.53–1.48 (m, 2H, C**H**$_2$), 1.44–1.37 (m, 4H, 2xC**H**$_2$), 1.16 (d, *J* = 6.9 Hz, 3H, C**H**$_3$), 1.13 (d, *J* = 6.9 Hz, 3H, C**H**$_3$), 0.96 (t, *J* = 7.0 Hz, 3H, C**H**$_3$). **^{13}C{^{1}H} NMR** (151 MHz, $CDCl_3$): δ 149.1, 140.9, 140.4, 140.3 (4**C**$_{qar}$), 128.7, 127.7, 127.1, 125.9, 123.8 (7**C**$_{ar}$), 123.1, 122.9, 121.5 (3**C**$_{qar}$), 120.5 (**C**$_{ar}$), 119.4 (**C**$_{ar\ triazole}$), 119.1, 117.8, 108.9 (4**C**$_{ar}$), 66.9 (**C**H$_2$), 62.7 (**C**HOH), 60.5 (**C**H), 51.4 (**C**H$_2$), 43.2 (**C**H$_2$), 31.6 (**C**H$_2$), 29.0 (**C**H$_2$), 28.9 (**C**H), 27.0 (**C**H$_2$), 22.6 (**C**H$_2$), 18.9 (**C**H$_3$), 17.2 (**C**H$_3$), 14.0 (**C**H$_3$). **IR** (neat): ν 3317, 2959, 2926, 2855, 1629, 1454, 1324, 1219, 1055 cm^{-1}. **Anal. Calcd. for $C_{33}H_{41}N_5O$**: C, 75.68; H, 7.89; N, 13.37; Found: C, 75.50; H, 7.64; N, 13.13.

General procedure for synthesis of **15**: Into a flask containing oxirane (1.5 mmol), triethylamine (1.0 mmol, 150.0 µL) and acetonitrile (5 mL), aziridine (4.50 mmol) was carefully added dropwise, and the whole mixture was refluxed for 24 hours. After, solvent was removed *in vacuo* and the product was purified by column chromatography (SiO_2, dichloromethane/methanol 9:1).

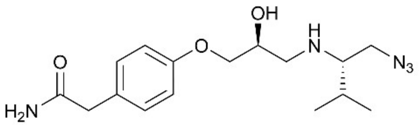
2-(4-((*S*)-2-hydroxy-3-((*S*)-2-isopropylaziridin-1-yl)propoxy)phenyl)acetamide **(15)**:



15

White solid (320.1 mg, 73% yield); mp = 148.2-149.5 °C (hexane /DCM); $[\alpha]^{20}_{D}$ = +9.71 (c 0.0015 in MeOH). **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.18–7.17 (m, 2H, C**H**$_{ar}$), 6.91–6.90 (m, 2H, C**H**$_{ar}$), 5.50 (br.s, 1H, N**H**$_2$), 5.39 (br.s, 1H, N**H**$_2$), 4.14–4.07 (m, 2H, C**H**$_2$, C**H**OH), 4.00 (dd, *J* = 9.3 Hz, 6.1 Hz, 1H, C**H**$_2$), 3.52 (s, 2H, C**H**$_2$), 3.03 (br.s, 1H, O**H**), 2.54 (dd, *J* = 12.0 Hz, 7.1 Hz, 1H, C**H**$_2$), 2.39 (dd, *J* = 5.3 Hz, 12.0 Hz, 1H, C**H**$_2$), 1.59 (s, 1H, C**H**$_2$), 1.27–1.25 (m, 3H, C**H**$_2$, C**H**, C**H**), 1.01 (d, *J* = 6.0 Hz, 3H, C**H**$_3$), 0.91 (d, *J* = 6.0 Hz, 3H, C**H**$_3$). **^{13}C{^{1}H} NMR** (151 MHz, $CDCl_3$): δ 173.9 (**C**=O), 158.2 (**C**$_{qar}$), 130.6 (2**C**$_{ar}$), 127.4 (**C**$_{qar}$), 115.3 (2**C**$_{ar}$), 70.4 (**C**H$_2$), 69.6 (**C**HOH), 63.5 (**C**H$_2$), 46.7 (**C**H), 42.5 (**C**H$_2$), 33.0 (**C**H$_2$), 31.6 (**C**H), 20.6 (**C**H$_3$), 19.6 (**C**H$_3$). **IR** (neat): ν 3343, 3161, 2959, 1633, 1513, 1416, 1245 cm^{-1}. **Anal. Calcd. for $C_{16}H_{24}N_2O_3$**: C, 65.73; H, 8.27; N, 9.58; Found: C, 65.61; H, 8.26; N, 9.76.

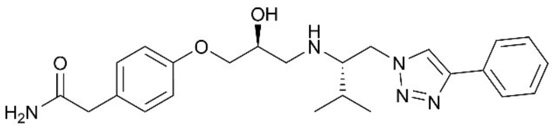
2-(4-((*S*)-3-(((*S*)-1-azido-3-methylbutan-2-yl)amino)-2-hydroxypropoxy)phenyl)acetamide **(16)**:



16

White solid (179.1 mg, 53% yield); mp = 109.7-110.4 °C (hexane /DCM); $[\alpha]^{20}_{D}$ = +0.93 (c 0.0015 in $CHCl_3$). **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.19–7.17 (m, 2H, C**H**$_{ar}$), 6.91–6.90 (m, 2H, C**H**$_{ar}$), 5.57 (br.s, 1H, N**H**$_2$), 5.39 (br.s, 1H, N**H**$_2$), 4.01–3.99 (m, 3H, C**H**$_2$, C**H**OH), 3.52 (s, 2H, C**H**$_2$), 3.42 (dd, *J* = 12.4 Hz, 4.1 Hz, 1H, C**H**$_2$), 3.27 (dd, *J* = 12.4 Hz, 6.7 Hz, 1H, C**H**$_2$), 2.95 (dd, *J* = 12.0 Hz, 3.1 Hz, 1H, C**H**$_2$), 2.77–2.74 (m, 1H, C**H**$_2$), 2.47–2.45 (m, 1H, C**H**), 1.87–1.82 (m, 1H, C**H**), 0.97 (d, *J* = 6.9 Hz, 3H, C**H**$_3$), 0.93 (d, *J* = 6.9 Hz, 3H, C**H**$_3$). **^{13}C{^{1}H} NMR** (151 MHz, $CDCl_3$): δ 174.0 (**C**=O), 158.2 (**C**$_{qar}$), 130.7 (2**C**$_{ar}$), 127.4 (**C**$_{qar}$), 115.3 (2**C**$_{ar}$), 70.5 (**C**H$_2$), 69.0 (**C**HOH), 63.4 (**C**H), 52.8 (**C**H$_2$), 50.3 (**C**H$_2$), 42.5 (**C**H$_2$), 29.9 (**C**H), 19.0 (**C**H$_3$), 18.8 (**C**H$_3$). **IR** (neat): ν 3351, 3168, 2926, 2098, 1636, 1513, 1409, 1241 cm^{-1}. **Anal. Calcd. for $C_{16}H_{25}N_5O_3$**: C, 57.30; H, 7.51; N, 20.88; Found: C, 57.24; H, 7.36; N, 20.75.

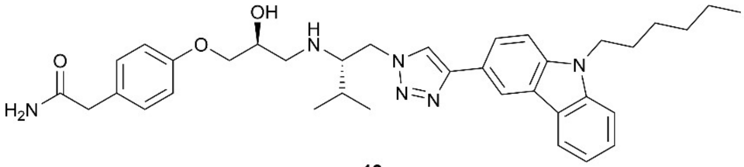
2-(4-((*S*)-2-hydroxy-3-(((*S*)-3-methyl-1-(4-phenyl-1*H*-1,2,3-triazol-1-yl)butan-2-yl)amino)propoxy) phenyl)acetamide **(17)**:



17

Green solid (245.9 mg, 56% yield); mp = 86.7-87.2 °C (hexane/DCM); $[\alpha]^{20}_{D}$ = +2.36 (c 0.0015 in $CHCl_3$). **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.87 (s, 1H, C**H**$_{triazole}$), 7.81–7.80 (m, 2H, C**H**$_{ar}$), 7.41–7.39 (m, 2H, C**H**$_{ar}$), 7.33–7.30 (m, 1H, C**H**$_{ar}$), 7.11–7.10 (m, 2H, C**H**$_{ar}$), 6.81–6.80 (m, 2H, C**H**$_{ar}$), 5.64 (br.s, 1H, N**H**$_2$), 5.47 (br.s, 1H, N**H**$_2$), 4.47 (dd, *J* = 13.9 Hz, 4.1 Hz, 1H, C**H**$_2$), 4.29 (dd, *J* = 13.9 Hz, 7.9 Hz, 1H, C**H**$_2$), 3.91–3.86 (m, 3H, C**H**$_2$, C**H**OH), 3.48 (s, 2H, C**H**$_2$), 2.85–2.82 (m, 1H, C**H**), 2.76 (dd, *J* = 12.0 Hz, 6.4 Hz, 1H, C**H**$_2$), 2.71 (dd, *J* = 12.0 Hz, 3.8 Hz, 1H, C**H**$_2$), 1.83–1.78 (m, 1H, C**H**), 1.03 (d, *J* = 1.4 Hz, 3H, C**H**$_3$), 1.02 (d, *J* = 1.4 Hz, 3H, C**H**$_3$). **^{13}C{^{1}H} NMR** (151 MHz, $CDCl_3$): δ 174.0 (**C**=O), 158.0, 147.7 (3**C**$_{qar}$), 130.7, 130.6, 129.0, 128.3 (5**C**$_{ar}$), 127.4 (**C**$_{qar}$), 125.0 (2**C**$_{ar}$), 120.8 (**C**$_{ar\ triazole}$), 115.2 (2**C**$_{ar}$), 70.4 (**C**H$_2$), 69.2 (**C**HOH), 64.0 (**C**H), 51.9 (**C**H$_2$), 50.4 (**C**H$_2$), 42.5 (**C**H$_2$), 29.9 (**C**H), 18.8 (**C**H$_3$), 18.7 (**C**H$_3$). **IR** (neat): ν 3321, 3176, 2956, 2870, 1662, 1513, 1252, 1036 cm^{-1}. HRMS (ESI-TOF): Calcd for $C_{24}H_{31}N_5O_3$ 437.2427; Found 437.2429.

2-(4-((*S*)-3-(((*S*)-1-(4-(9-hexyl-9*H*-carbazol-3-yl)-1*H*-1,2,3-triazol-1-yl)-3-methylbutan-2-yl)amino)-2-hydroxypropoxy)phenyl)acetamide **(18)**:

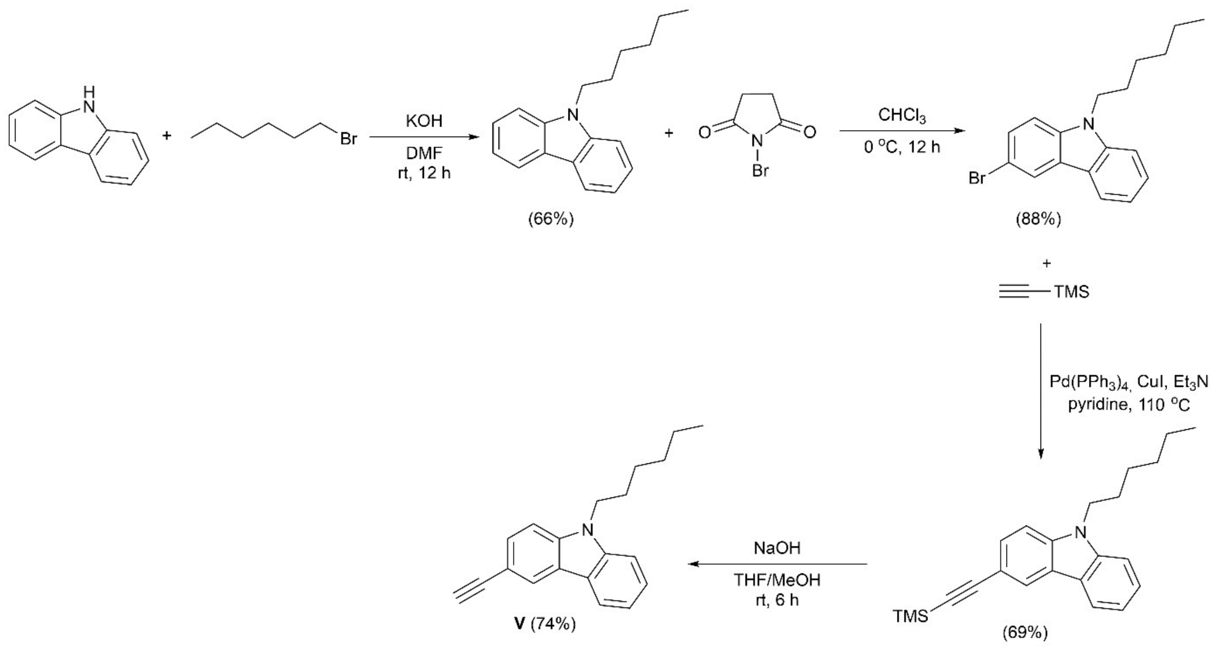


18

Yellow oil (153.9 mg, 25% yield); $[\alpha]^{20}_{D}$ = –10.29 (c 0.0015 in $CHCl_3$). **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.59–8.58 (m, 1H, C**H**$_{ar}$), 8.14–8.13 (m, 1H, C**H**$_{ar}$), 7.95–7.94 (m, 1H, C**H**$_{ar}$), 7.92 (s, 1H, C**H**$_{triazole}$), 7.52–7.49 (m, 1H, C**H**$_{ar}$), 7.46–7.43 (m, 2H, C**H**$_{ar}$), 7.27–7.25 (m, 1H, C**H**$_{ar}$), 7.08–7.06 (m, 2H, C**H**$_{ar}$), 6.83–6.81 (m, 2H, C**H**$_{ar}$), 5.39 (br.s, 1H, N**H**$_2$), 5.33 (br.s, 1H, N**H**$_2$), 4.53 (dd, *J* = 13.9 Hz, 4.1 Hz, 1H, C**H**$_2$), 4.36–4.32 (m, 3H, C**H**$_2$, C**H**$_2$), 3.95–3.92 (m, 2H, C**H**$_2$, C**H**OH), 3.91–3.88 (m, 1H, C**H**$_2$), 3.44 (s, 2H, C**H**$_2$), 2.93–2.90 (m, 1H, C**H**), 2.82–2.75 (m, 2H,

CH_2), 1.91–1.87 (m, 3H, C**H**, C**H**$_2$), 1.43–1.39 (m, 2H, C**H**$_2$), 1.35–1.30 (m, 4H, C**H**$_2$x2), 1.08 (d, *J* = 6.7 Hz, 3H, C**H**$_3$), 1.07 (d, *J* = 6.7 Hz, 3H, C**H**$_3$), 0.87 (t, *J* = 7.1 Hz, 3H, C**H**$_3$). **^{13}C{^{1}H} NMR** (151 MHz, $CDCl_3$): δ 173.8 (**C**=O), 158.0, 148.9, 141.0, 140.5 (4**C**$_{qar}$), 130.6 (2**C**$_{ar}$), 127.4 (**C**$_{qar}$), 126.1, 123.8 (2**C**$_{ar}$), 123.3, 123.0, 121.6 (3**C**$_{qar}$), 120.7, 119.9, 119.2 (3**C**$_{ar}$), 117.9 (**C**$_{ar\ triazole}$), 115.2, 109.1, 109.0 (4**C**$_{ar}$), 70.4 (**C**H$_2$), 69.3 (**C**HOH), 64.1 (**C**H), 52.0 (**C**H$_2$), 50.5 (**C**H$_2$), 43.3 (**C**H$_2$), 42.5 (**C**H$_2$), 31.7 (**C**H$_2$), 30.0 (**C**H), 29.1 (**C**H$_2$), 27.1 (**C**H$_2$), 22.7 (**C**H$_2$), 18.9 (**C**H$_3$), 18.7 (**C**H$_3$), 14.1 (**C**H$_3$). **IR** (neat): ν 3317, 3202, 2926, 2855, 1662, 1513, 1241, 1044 cm^{-1}. HRMS (ESI-TOF): Calcd for $C_{36}H_{46}N_6O_3$ 610.3631; Found 610.3627.

3. 3-Ethynyl-9-hexyl-9*H*-carbazole synthesis



General procedure for synthesis of 3-Ethynyl-9-hexyl-9*H*-carbazole (**V**):

In the first step, KOH (30 mmol, 1.68 g) and DMF (10 mL) were added to a flask containing hexyl bromide (6 mmol, 842 μL), and then carbazole (5 mmol, 836 mg) was added.The entire mixture was stirred for 12 hours at room temperature. After, the mixture was extracted with ethyl acetate (3 x 20 mL). The combined organic layers were dried over anhydrous $MgSO_4$, filtered, and the solvent was removed under reduced pressure, affording 9-hexyl-9*H*-carbazole in 66% yield.

In the next step, the obtained compound (1 eq.) was dissolved in chloroform (10 mL) and cooled to 0 °C, then *N*-Bromosuccinimide (1 eq.) was added in small portions over 30 minutes, maintaining the temperature at around 0 °C. The resulting mixture was stirred at room temperature for 12 hours and the solution was washed with water and the mixture was extracted with DCM (3 x 10 mL). Combined organic layers were dried over anhydrous $MgSO_4$, filtered, and the solvent was removed under reduced pressure, obtaining 9-bromo-9-hexyl-9H-carbazole with a 88% yield.

In the next step, the obtained compound (1 eq.), $Pd(PPh_3)_4$ (0.1 eq), CuI (0.11 eq.) and trimethylsilylacetylene (2.7 eq.) were added to the solution of Et_3N (15 mL) and pyridine (15 mL) under argon. A whole mixture was refluxed for 24 hours in 110 °C. After, obtained solution was washed with

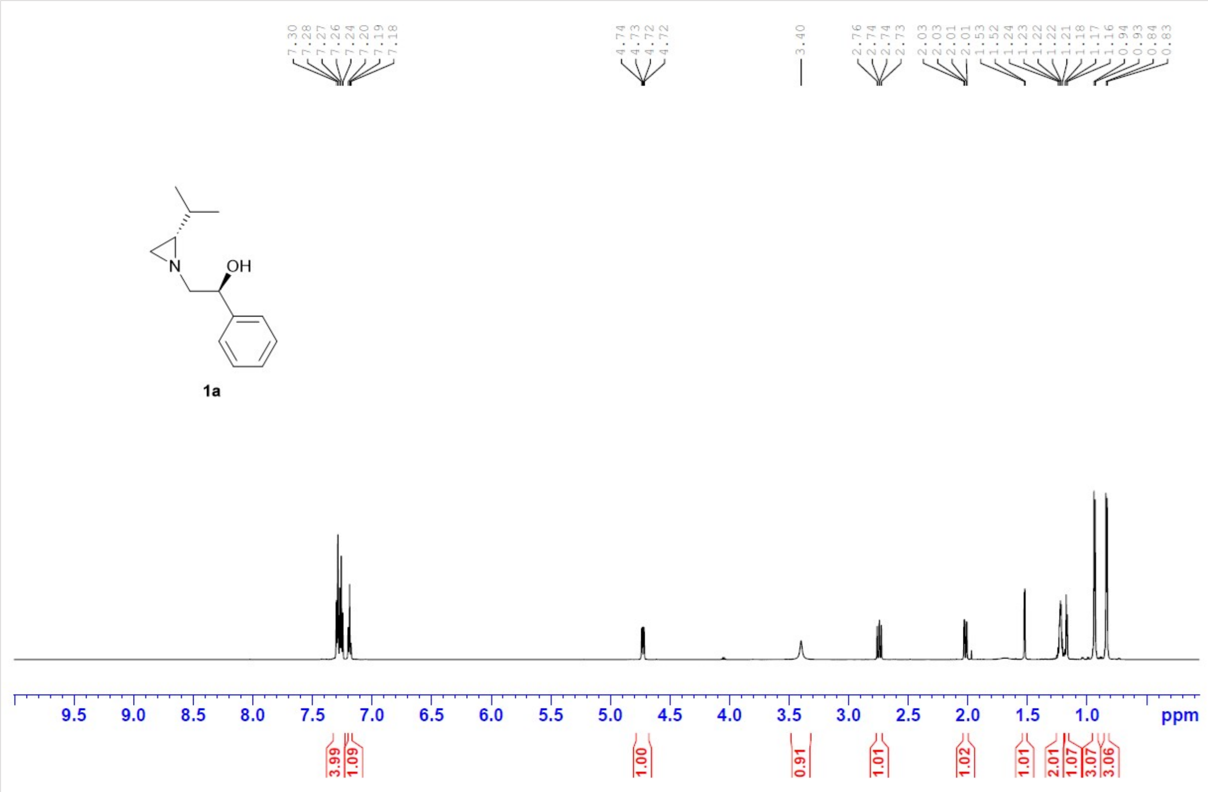
NH_4Cl and extracted with ethyl acetate (3 x 10 mL). Combined organic layers were dried over anhydrous $MgSO_4$, filtered, and the solvent was removed under reduced pressure. The product was purified by column chromatography (SiO_2, hexane/ethyl acetate 98:2), affording 9-hexyl-3-((trimethylsilyl)ethynyl)-9*H*-carbazole in 69% yield.

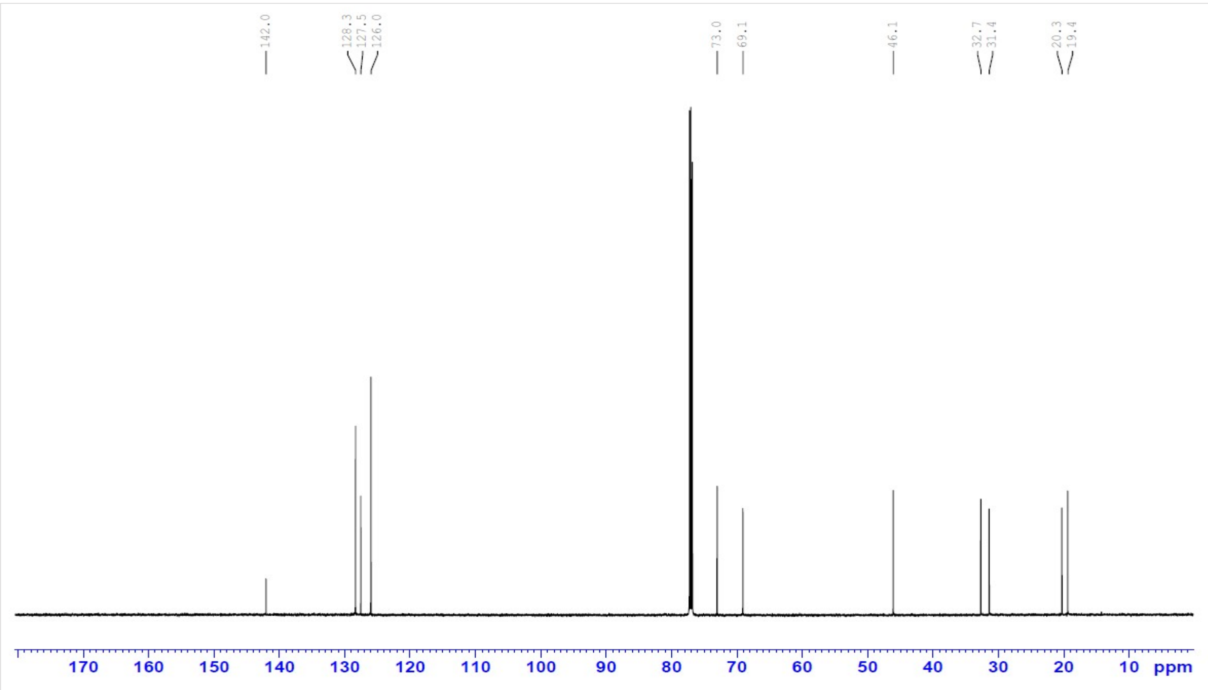
In the final step, the obtained compound (1 eq.) was dissolved in solution THF/MeOH (6.5 mL, 1:2). Then, NaOH was added (3.3 eq in 1 mL H_2O) and the mixture was stirred for 6 hours in room temperature. After, the mixture was extracted with DCM (3 x 10 mL). Combined organic layers were dried over anhydrous $MgSO_4$, filtered, and the solvent was removed under reduced pressure, obtaining 9-bromo-9-hexyl-9H-carbazole with a 88% yield, obtaining 3-Ethynyl-9-hexyl-9*H*-carbazole (**V**) with a 74% yield.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.28–8.27 (m, 1H), 8.09–8.08 (m, 1H), 7.61–7.60 (m, 1H), 7.51–7.48 (m, 1H), 7.42–7.40 (m, 1H), 7.35–7.33 (m, 1H), 7.28–7.25 (m, 1H), 4.28 (t, *J* = 7.3 Hz, 2H), 3.09 (s, 1H), 1.89–1.84 (m, 2H), 1.41–1.36 (m, 2H), 1.34–1.27 (m, 4H), 0.88 (t, *J* = 7.1 Hz, 3H). **^{13}C{^{1}H} NMR** (151 MHz, $CDCl_3$): δ 140.8, 140.3, 129.6, 126.2, 124.7, 122.7, 122.4, 120.5, 119.4, 111.9, 109.0, 108.7, 85.2, 75.1, 43.2, 31.6, 28.9, 27.0, 22.5, 14.0.

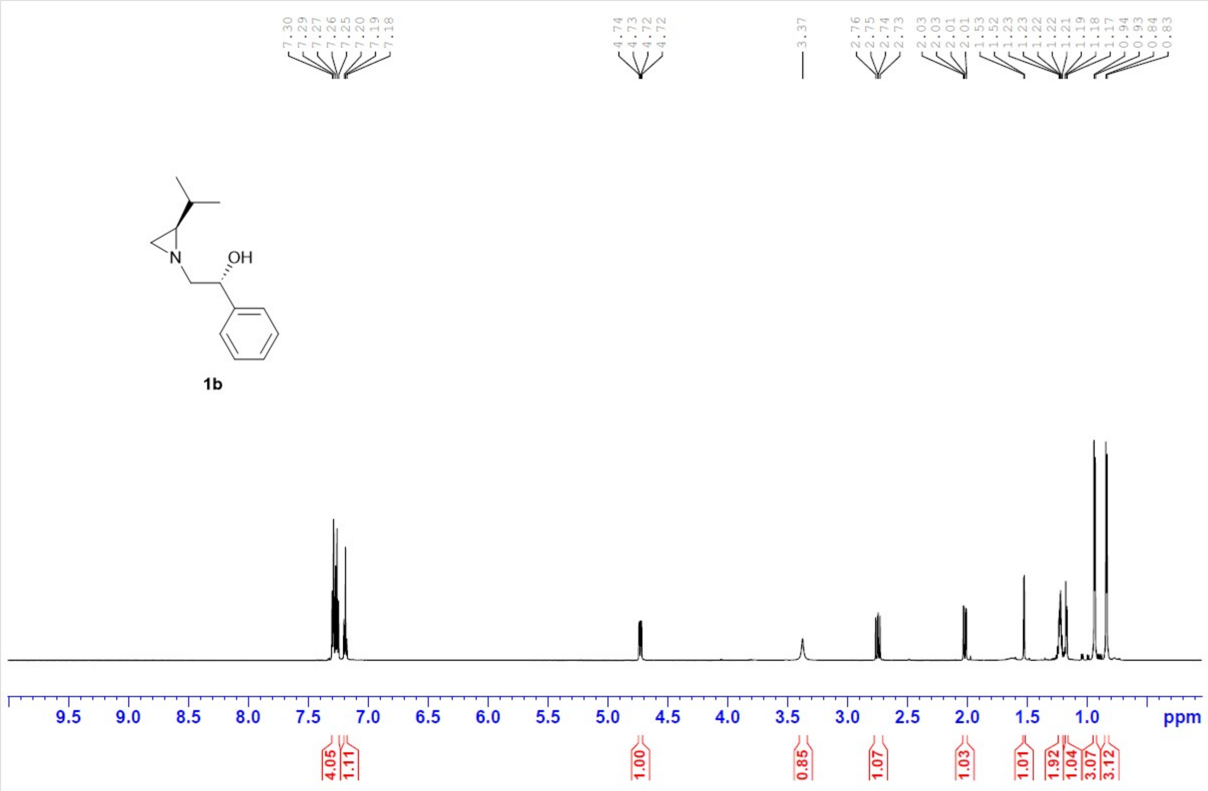
4. Copies of NMR spectra

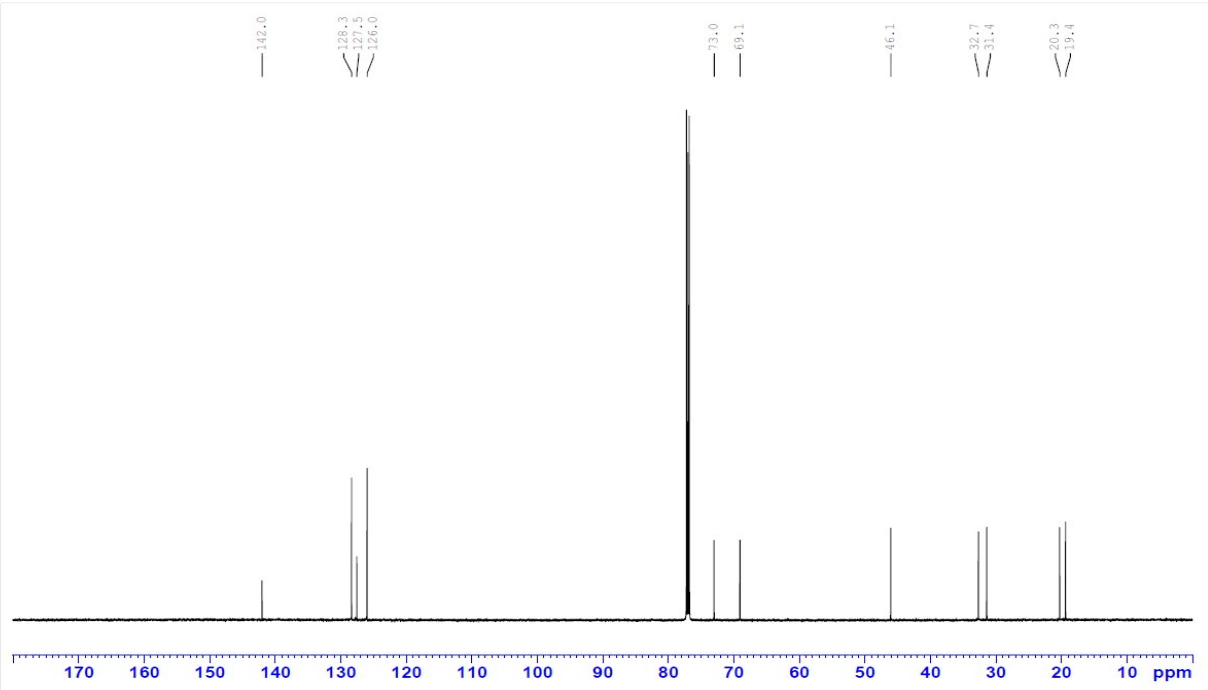
^{1}H NMR (600 MHz, $CDCl_3$) and $^{13}C\{1H\}$ NMR (151 MHz, $CDCl_3$) spectra for compound **1a**.



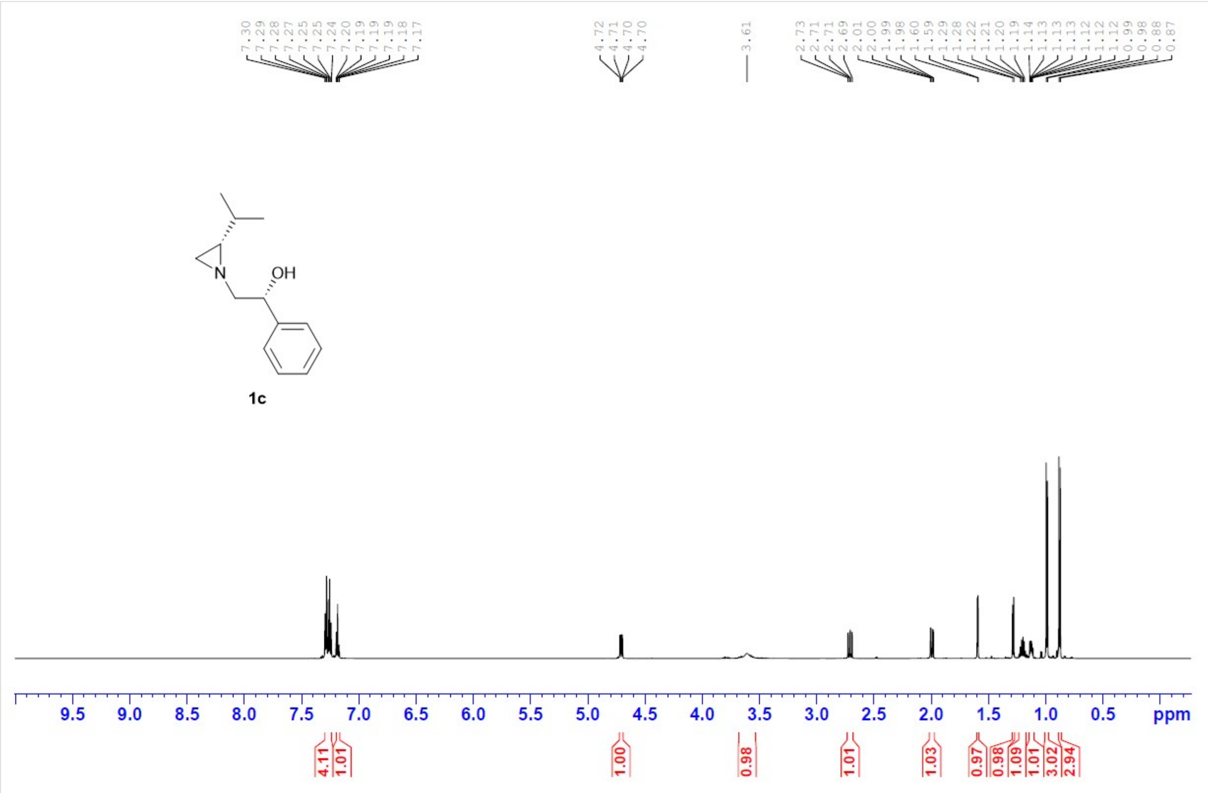


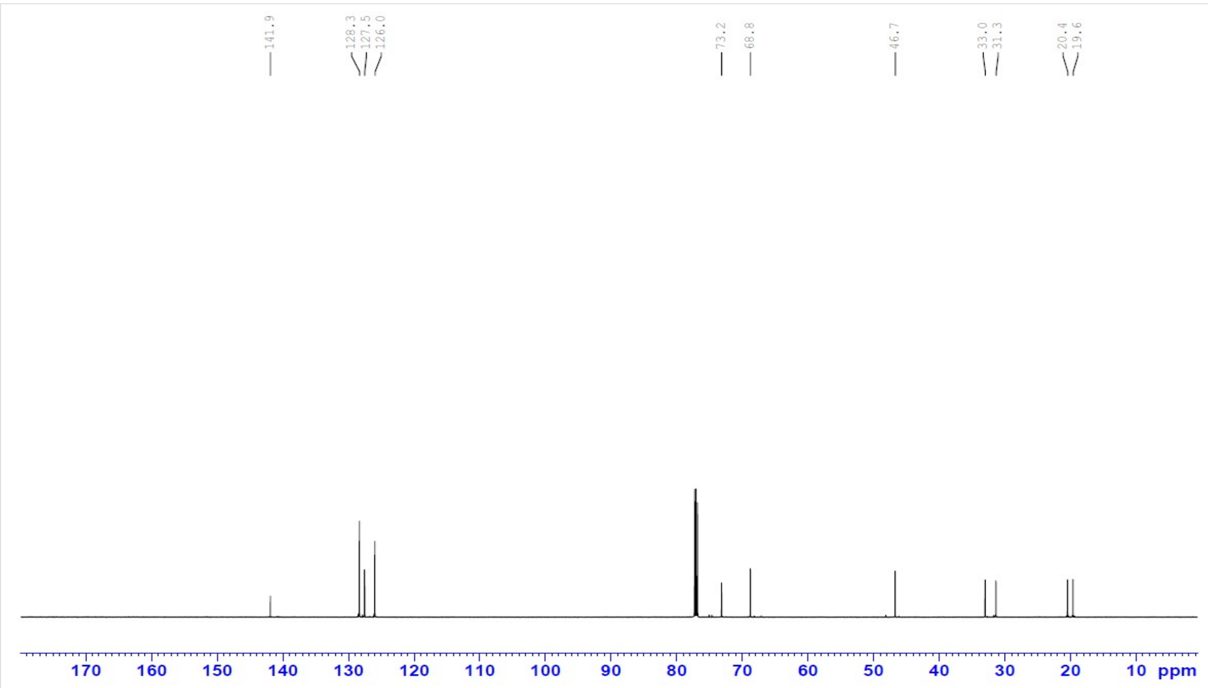
^{1}H NMR (600 MHz, $CDCl_3$) and $^{13}C\{1H\}$ NMR (151 MHz, $CDCl_3$) spectra for compound **1b**.

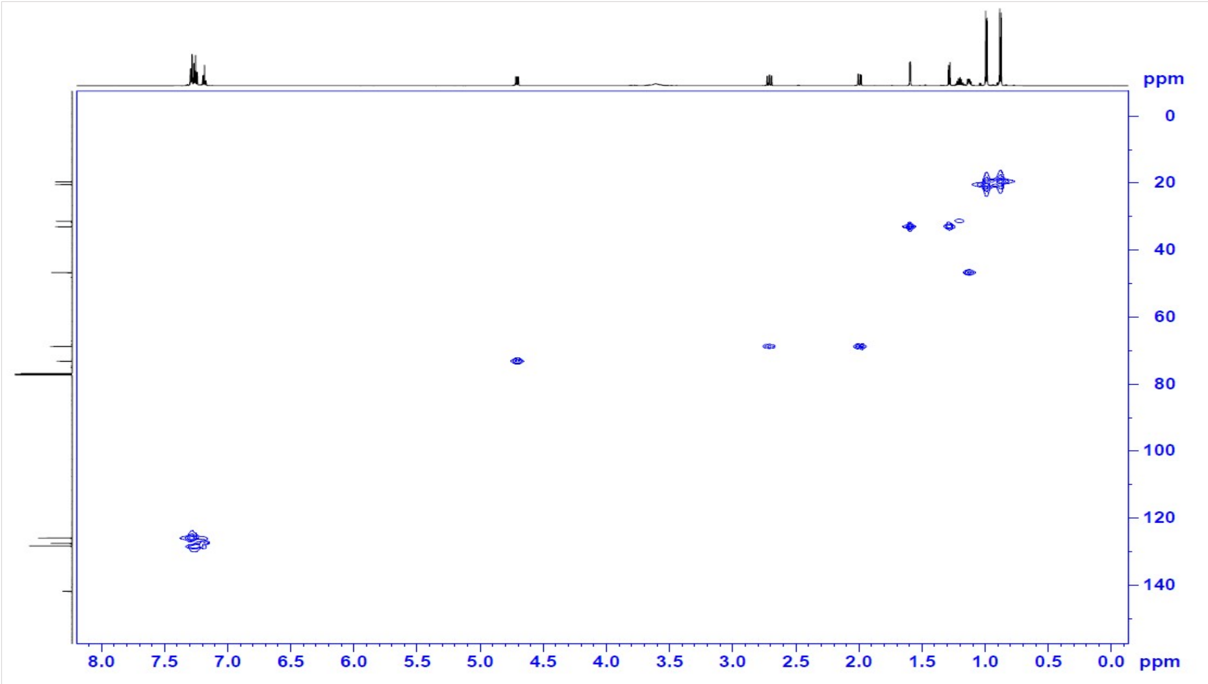




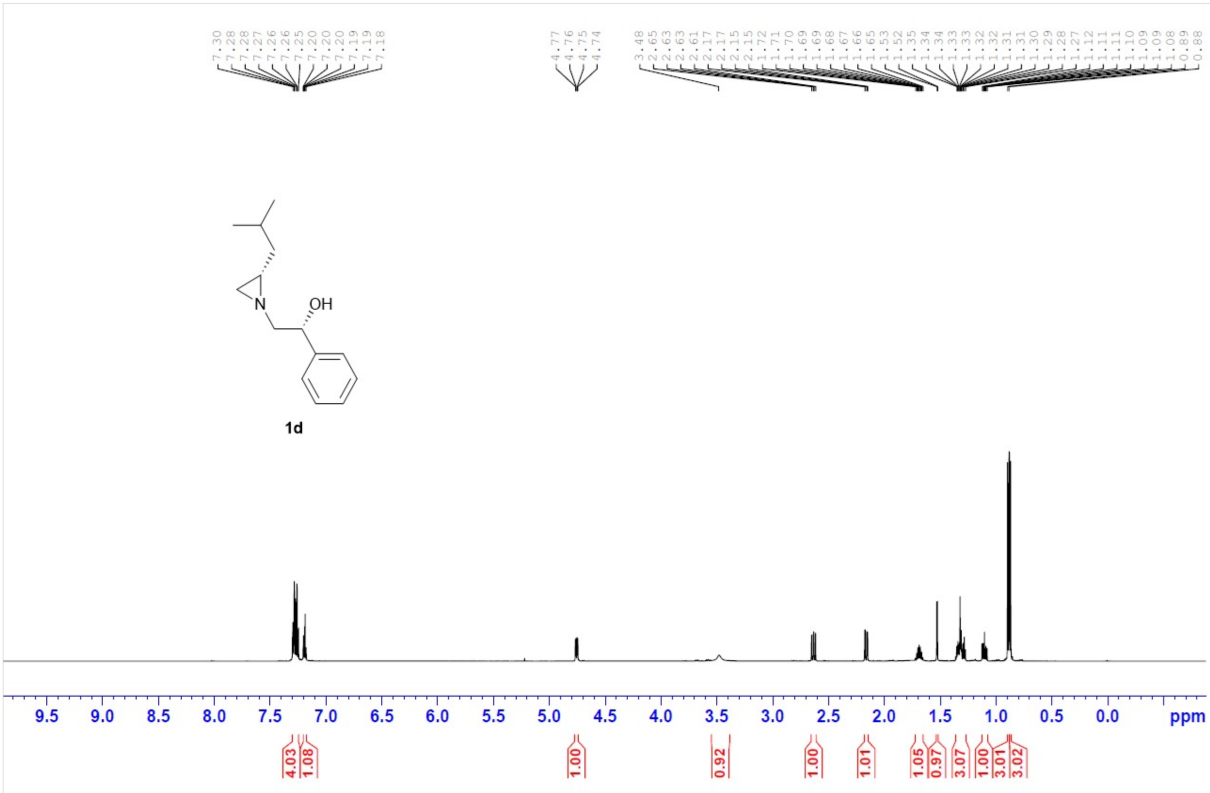
^{1}H NMR (600 MHz, $CDCl_3$), $^{13}C\{1H\}$ NMR (151 MHz, $CDCl_3$) and HMQC ($CDCl_3$) spectra for compound **1c**.

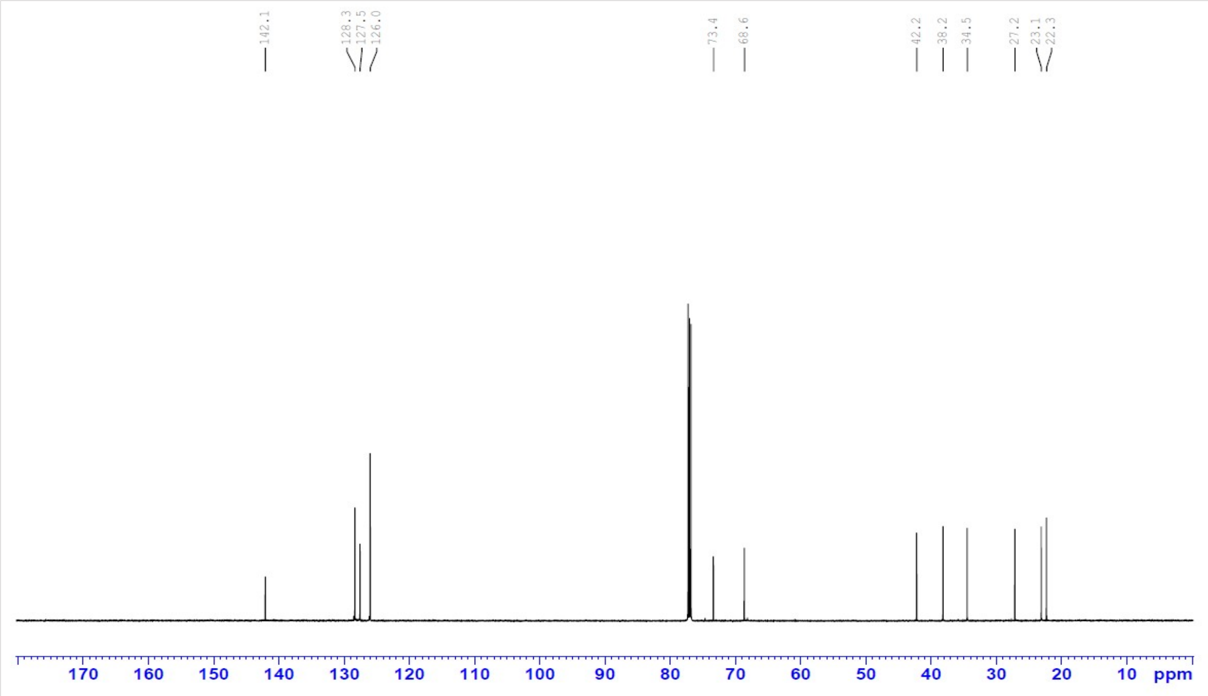




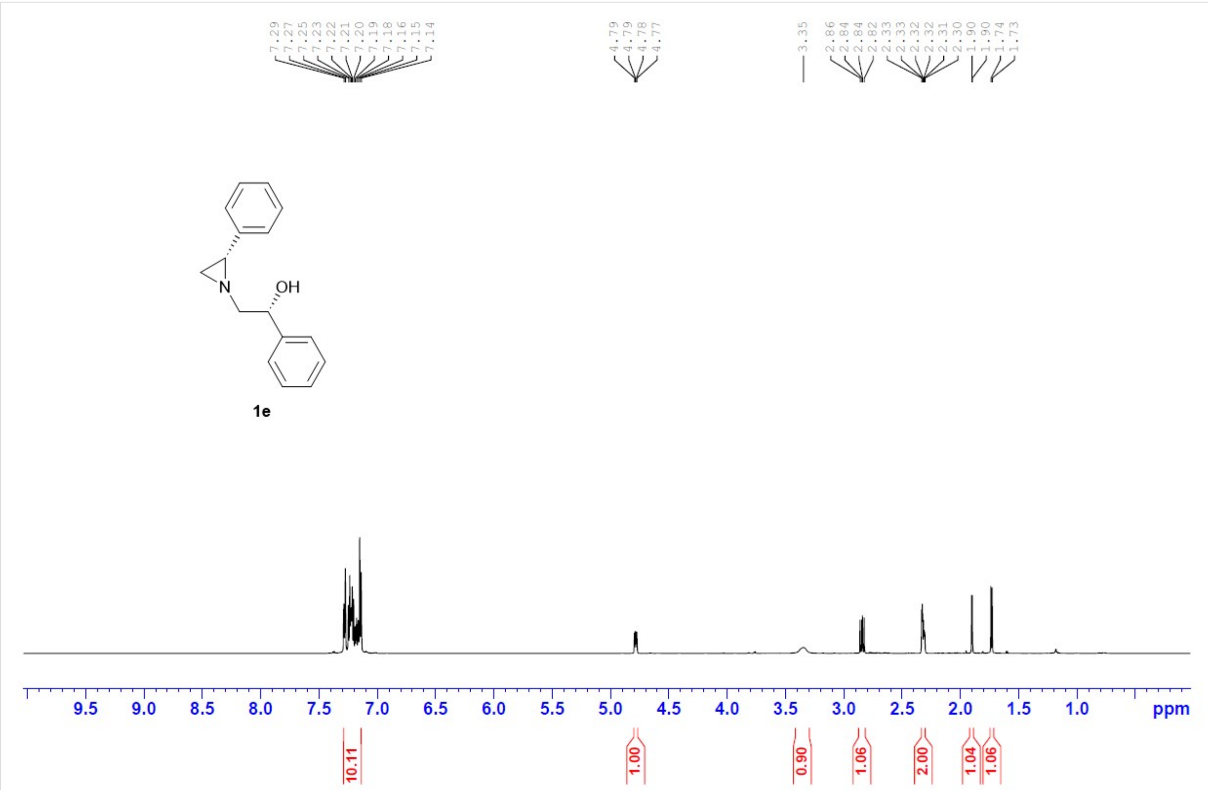


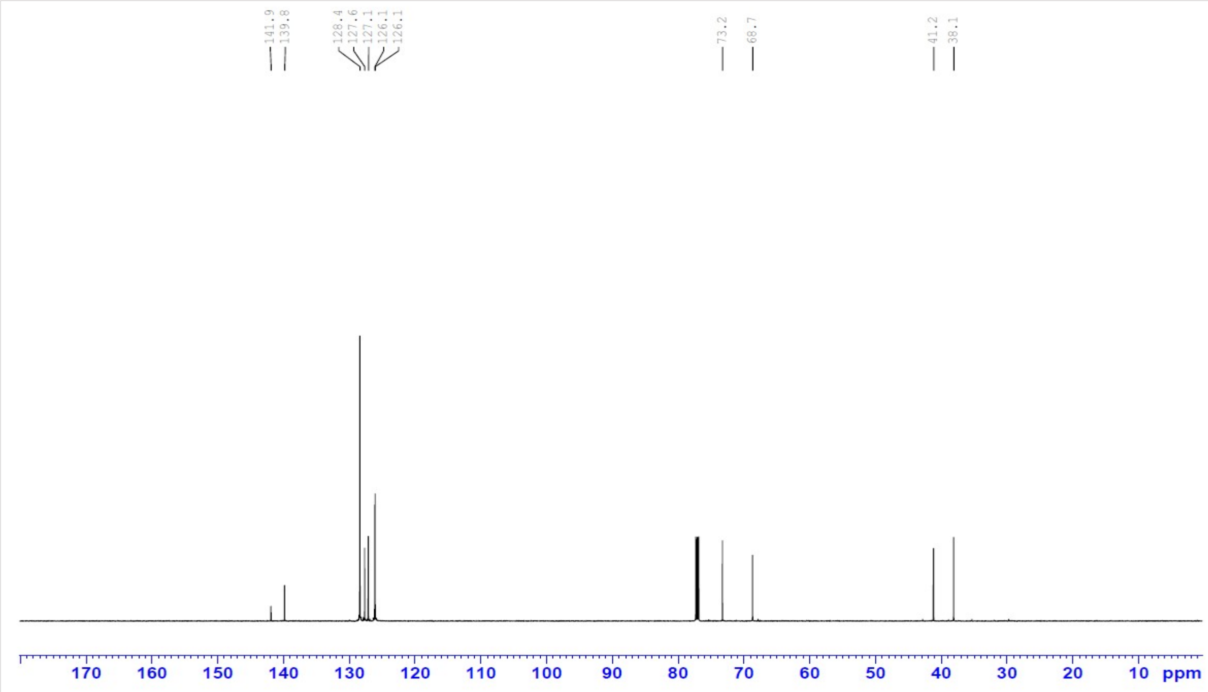
[1]H NMR (600 MHz, $CDCl_3$) and [13]C{1H} NMR (151 MHz, $CDCl_3$) spectra for compound **1d**.

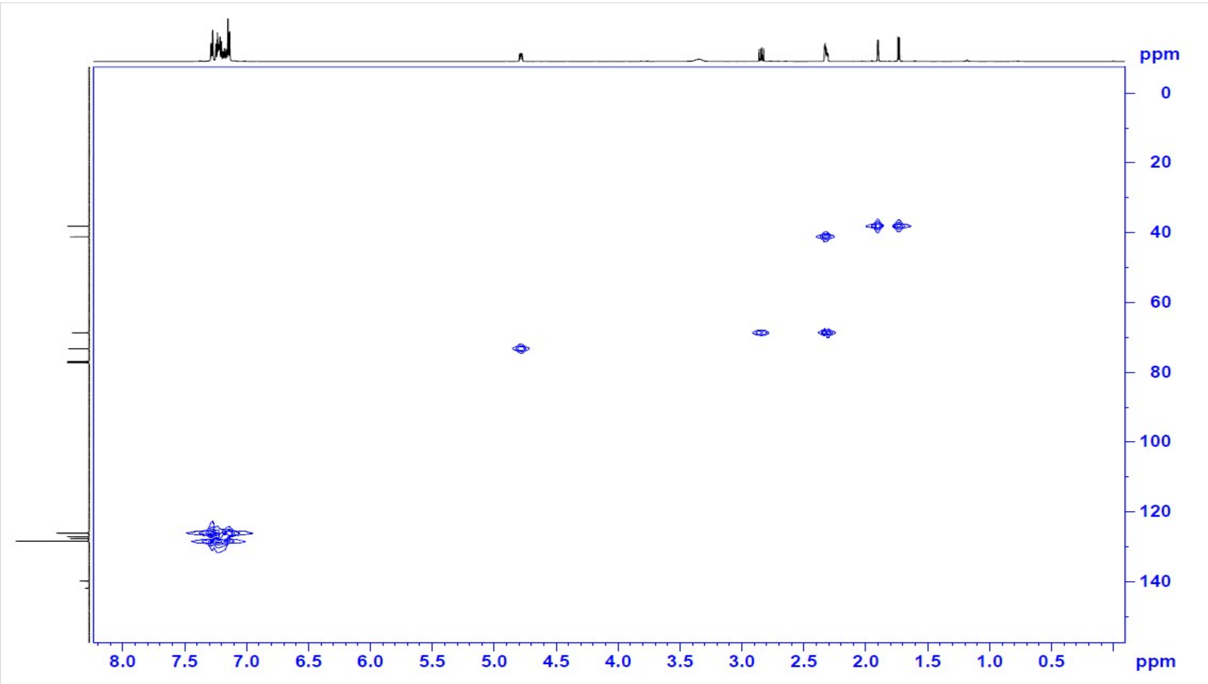




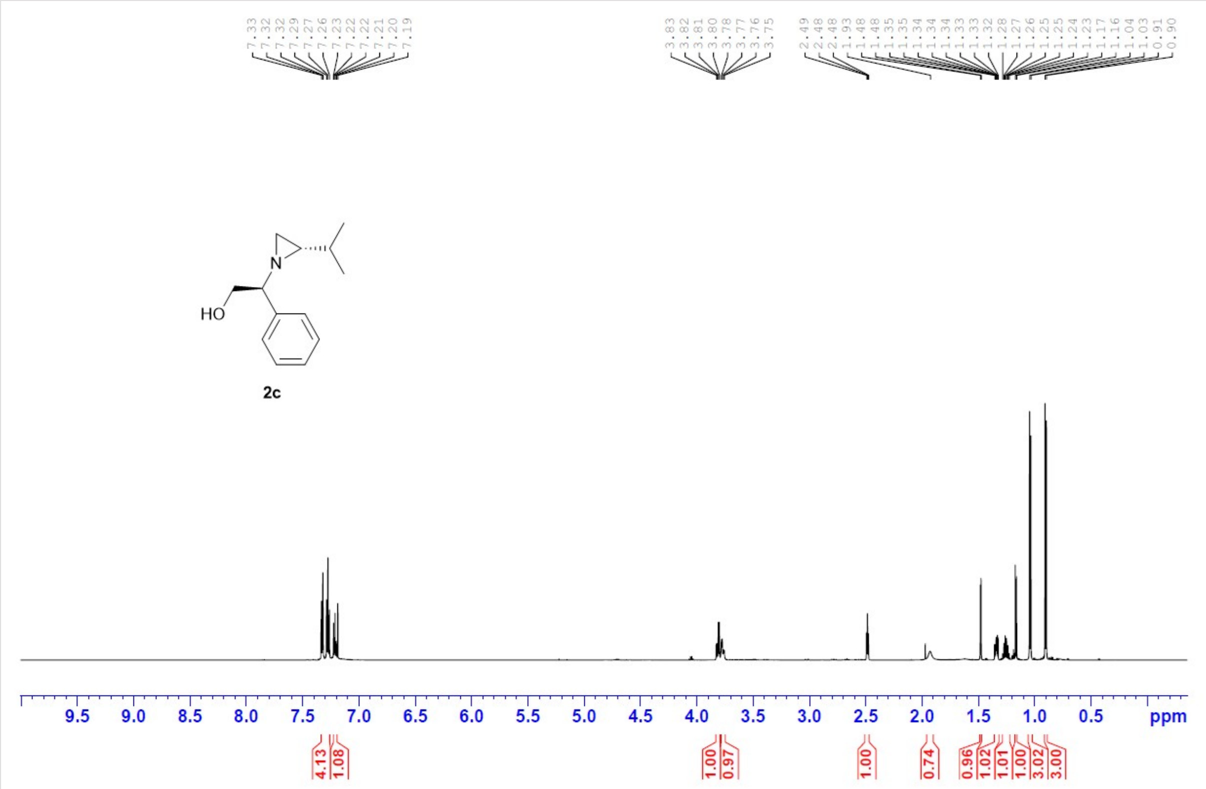
^{1}H NMR (600 MHz, $CDCl_3$), $^{13}C\{1H\}$ NMR (151 MHz, $CDCl_3$) and HMQC ($CDCl_3$) spectra for compound **1e**.

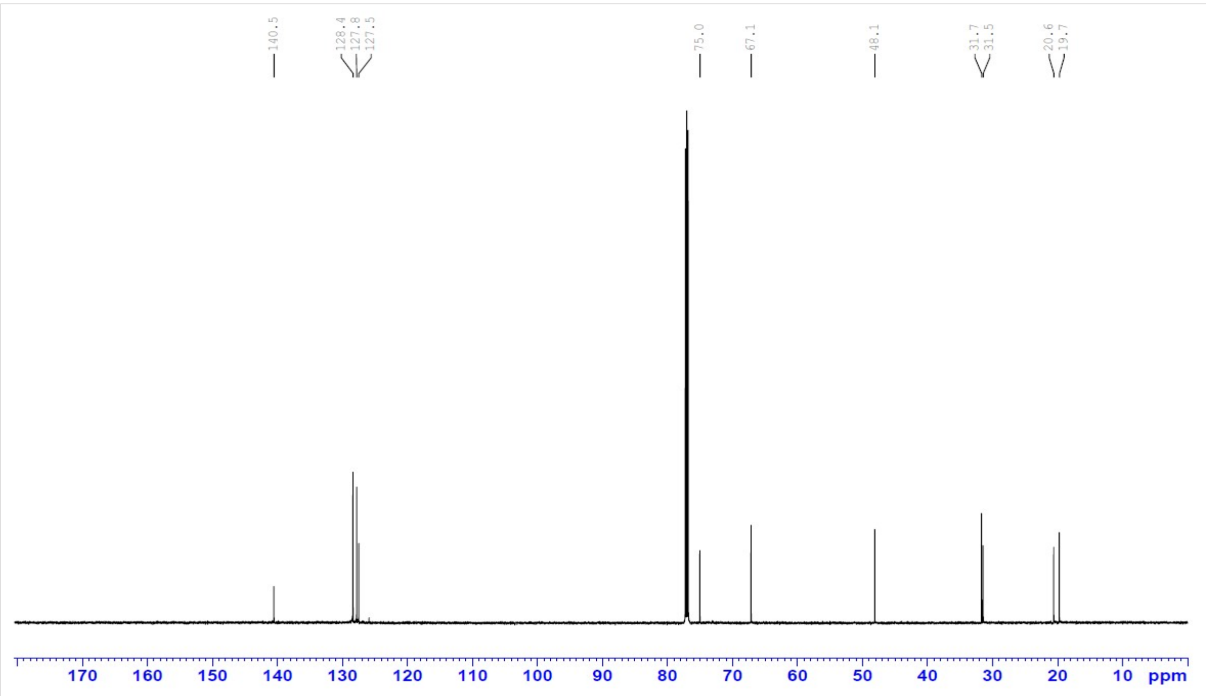


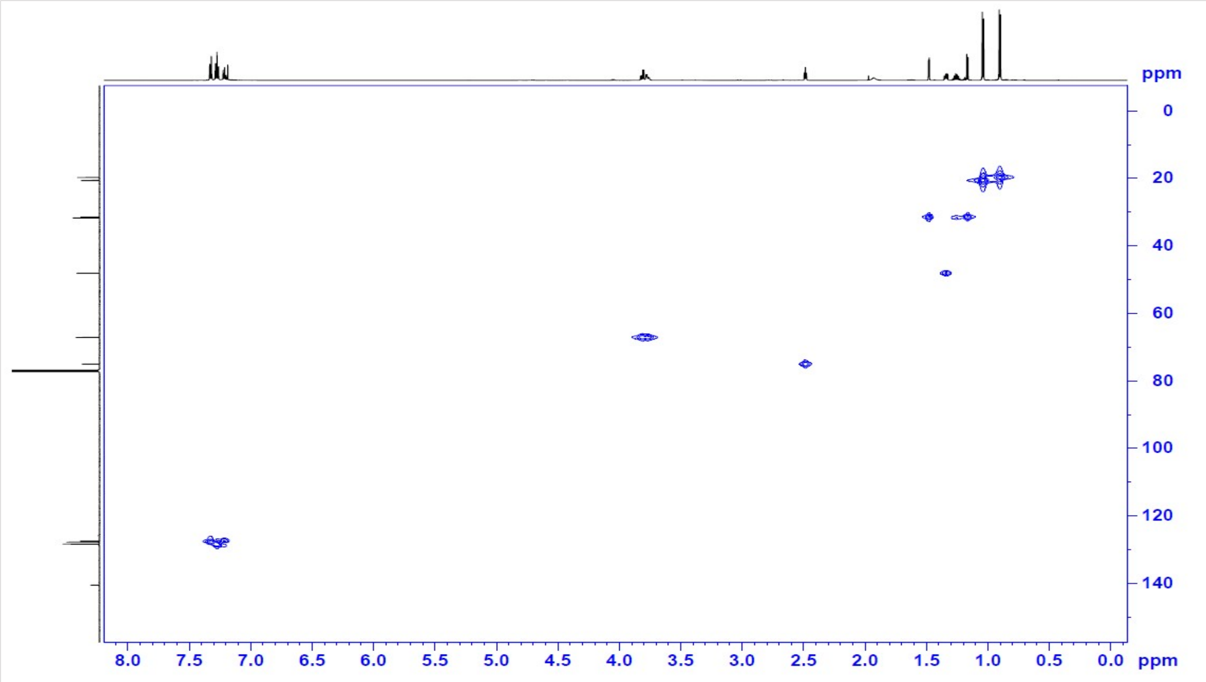

141.9
139.8
128.4
127.6
127.1
126.1
126.1
73.2
68.7
41.2
38.1
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


ppm
0
20
40
60
80
100
120
140
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
ppm

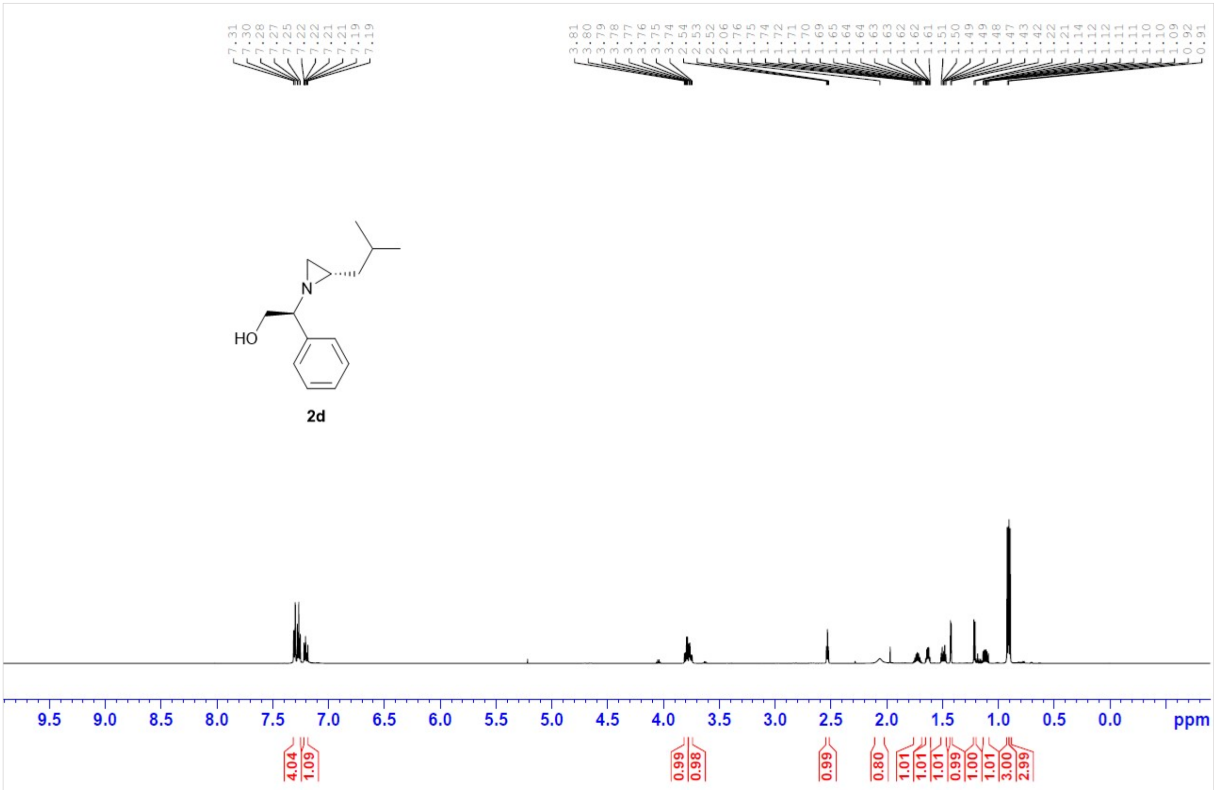
[1]H NMR (600 MHz, $CDCl_3$), [13]C{1H} NMR (151 MHz, $CDCl_3$) and HMQC ($CDCl_3$) spectra for compound **2c**.

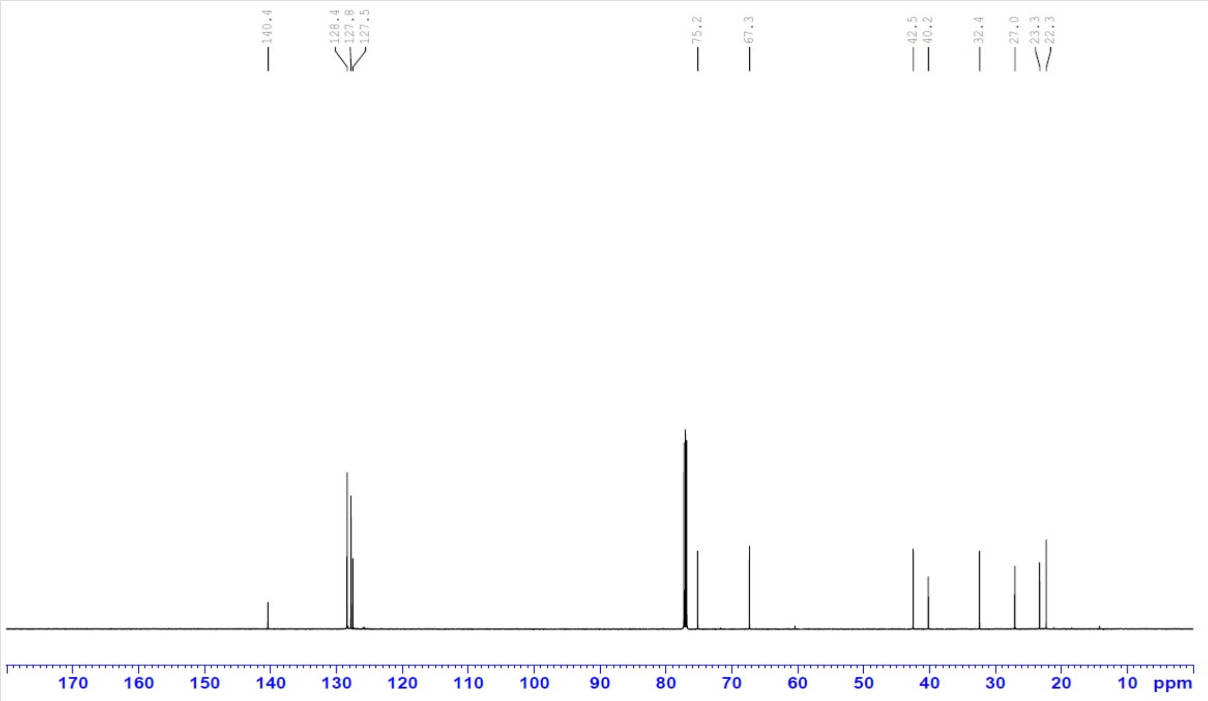




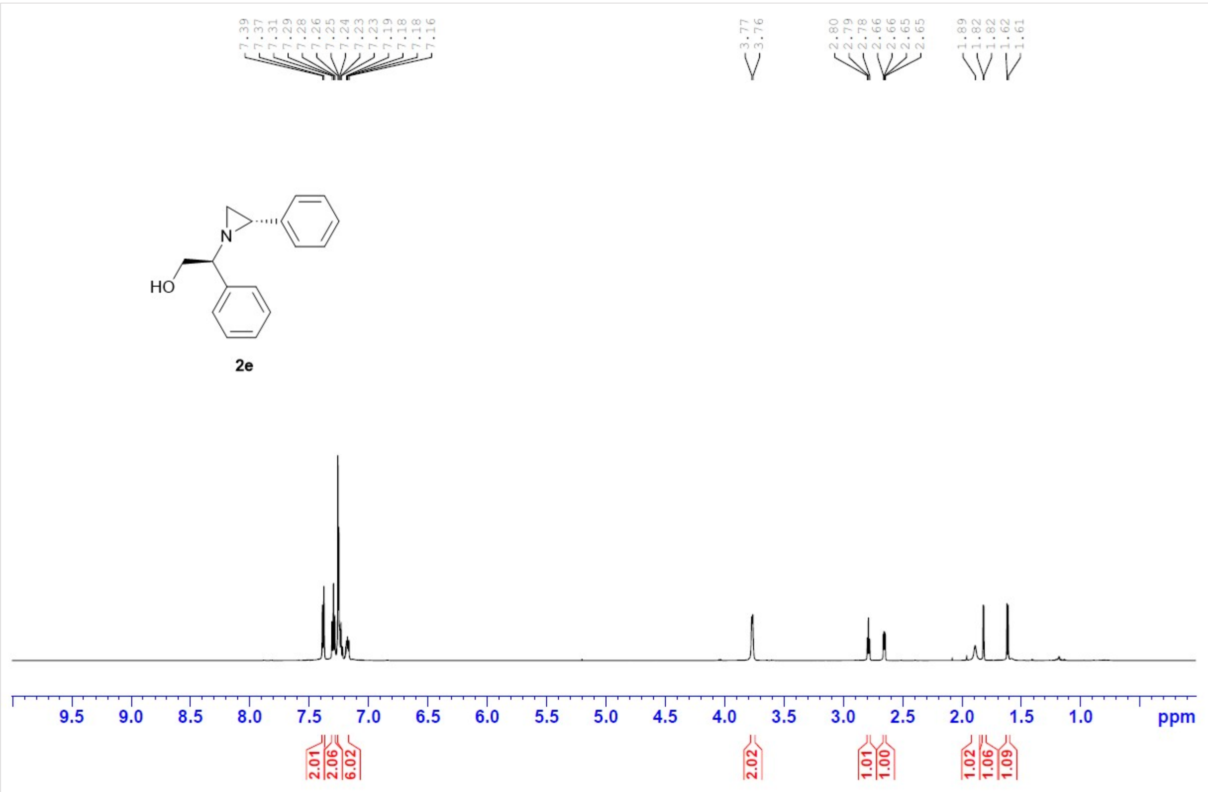


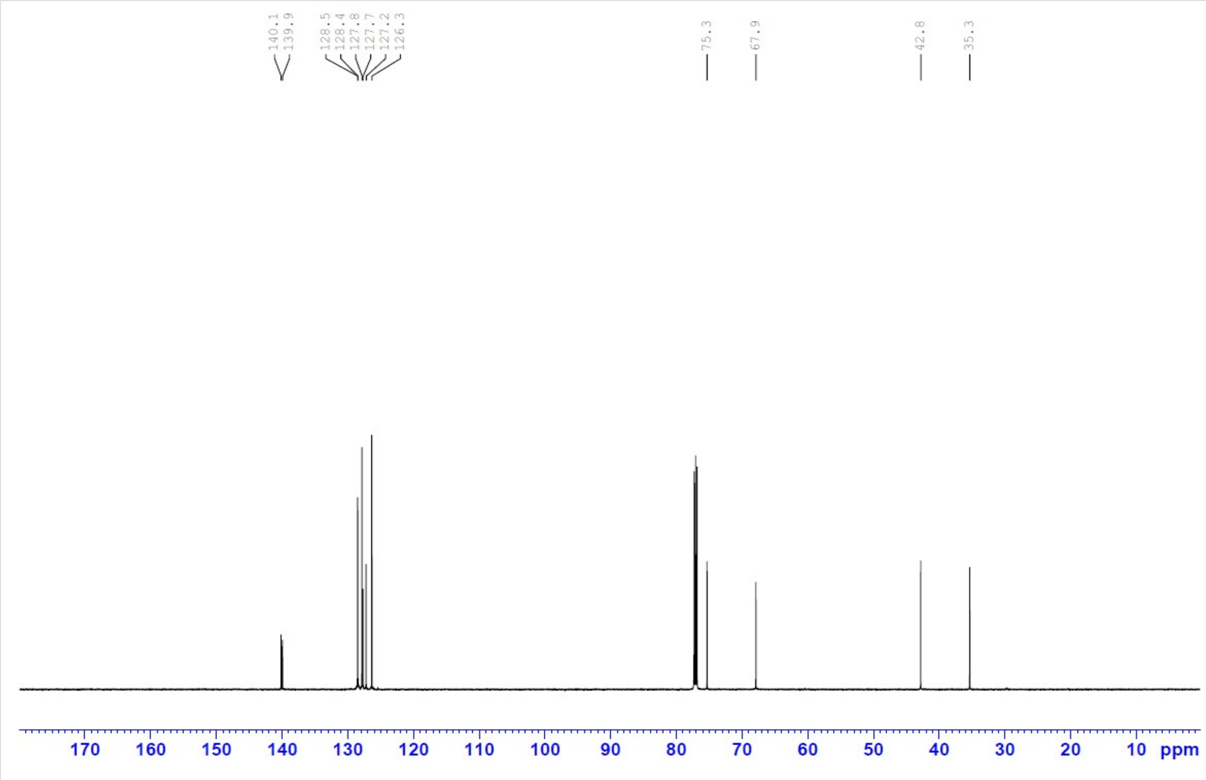
^{1}H NMR (600 MHz, $CDCl_3$) and $^{13}C\{1H\}$ NMR (151 MHz, $CDCl_3$) spectra for compound **2d**.

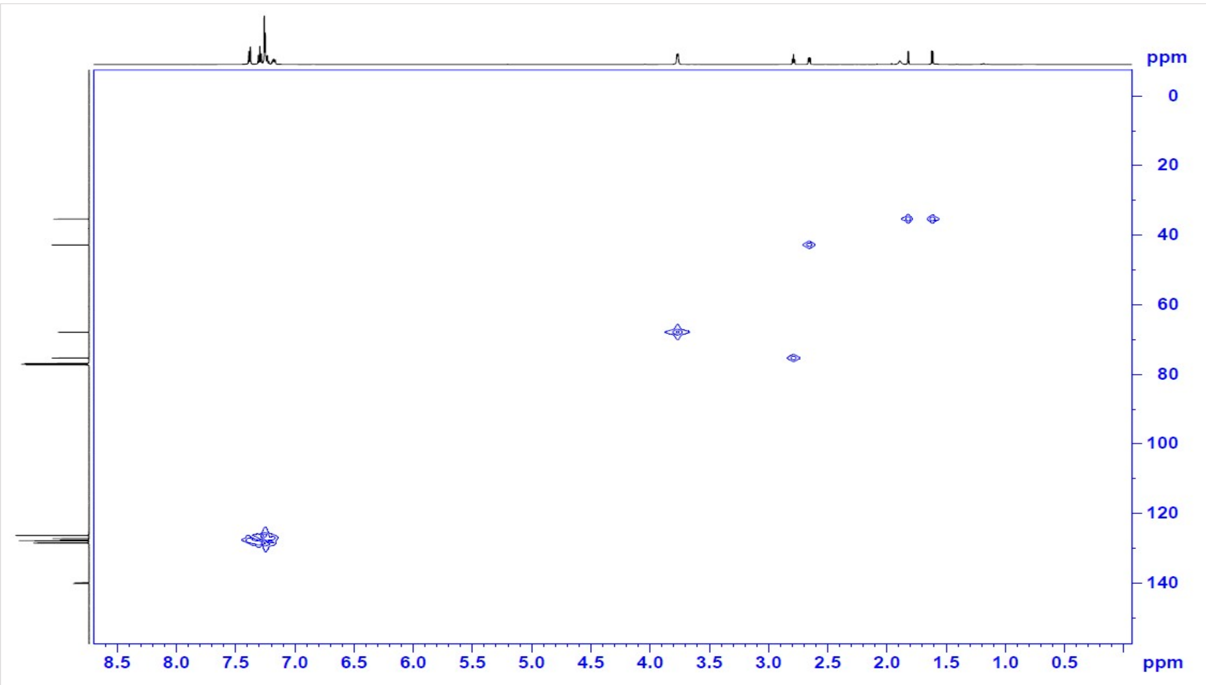




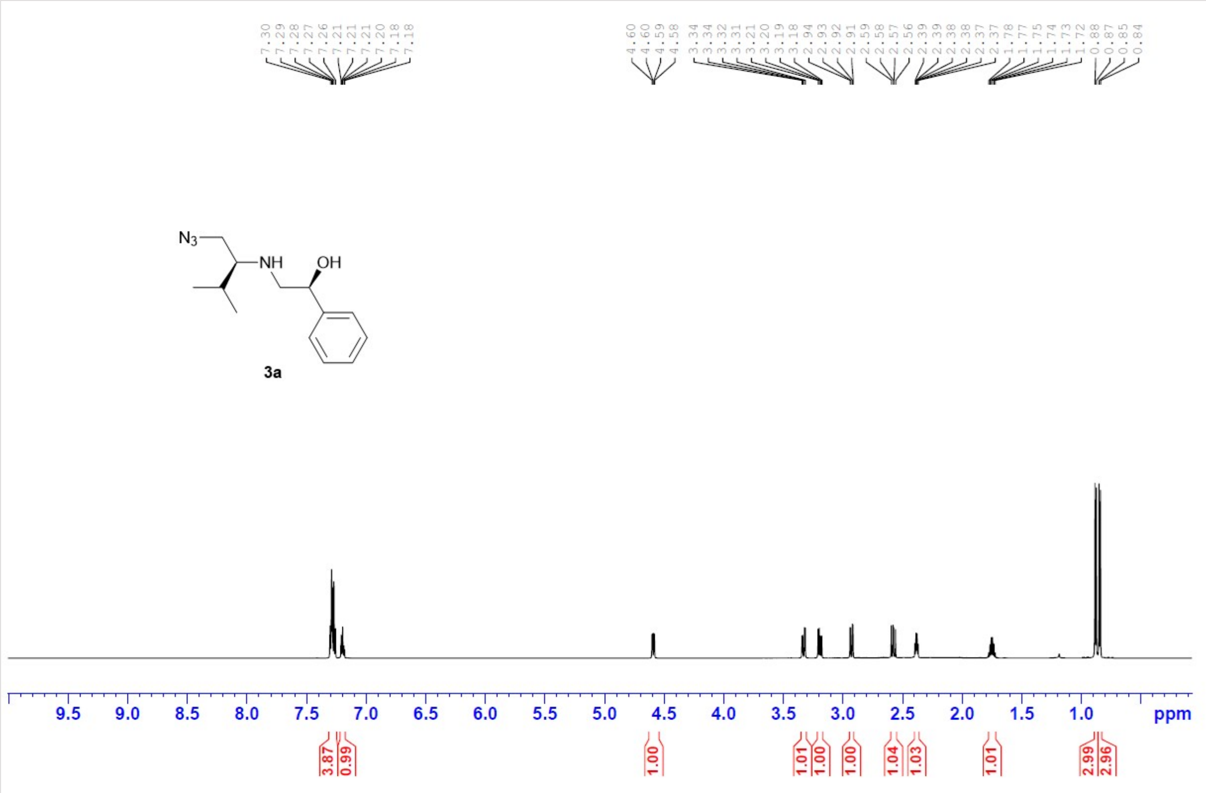
^{1}H NMR (600 MHz, $CDCl_3$), $^{13}C\{1H\}$ NMR (151 MHz, $CDCl_3$) and HMQC ($CDCl_3$) spectra for compound **2e**.

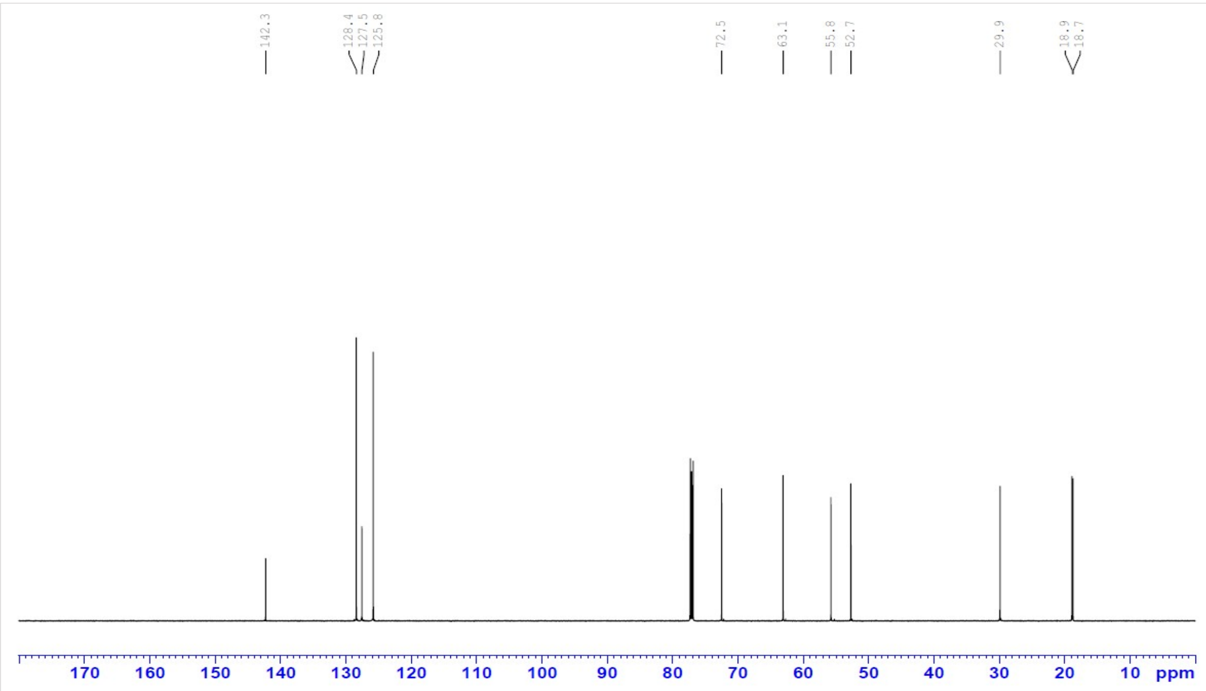


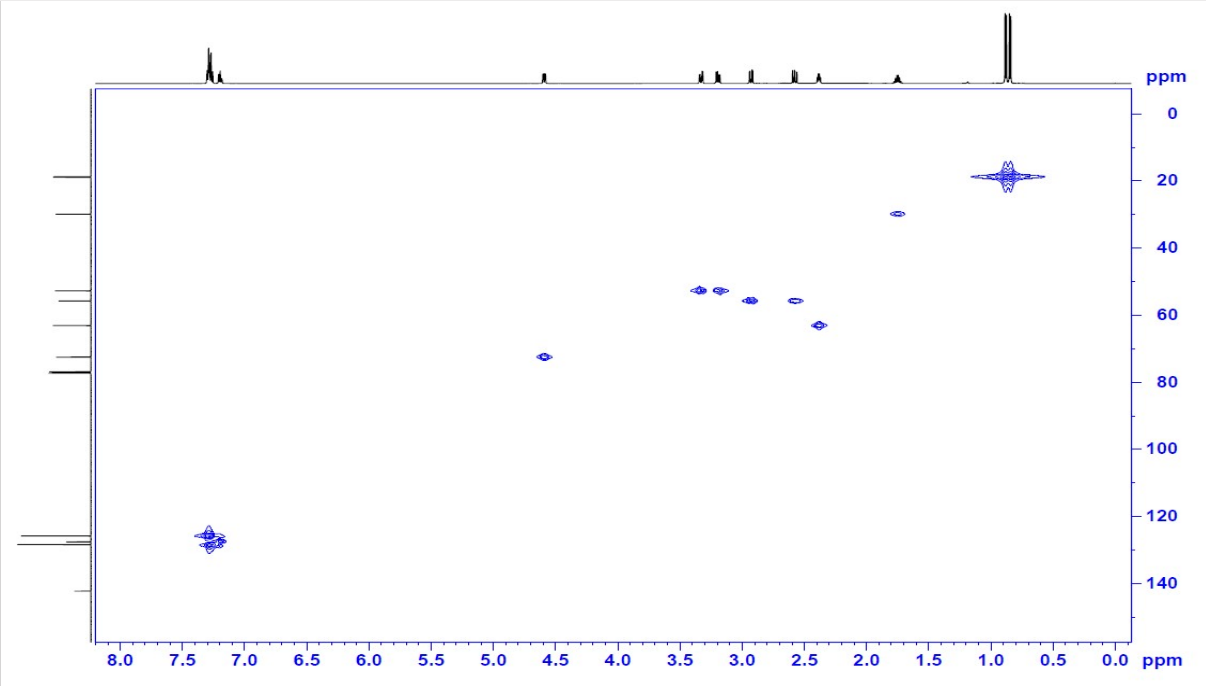

140.1
139.9
128.5
128.4
127.8
127.7
127.2
126.3
75.3
67.9
42.8
35.3
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


ppm
0 20 40 60 80 100 120 140
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

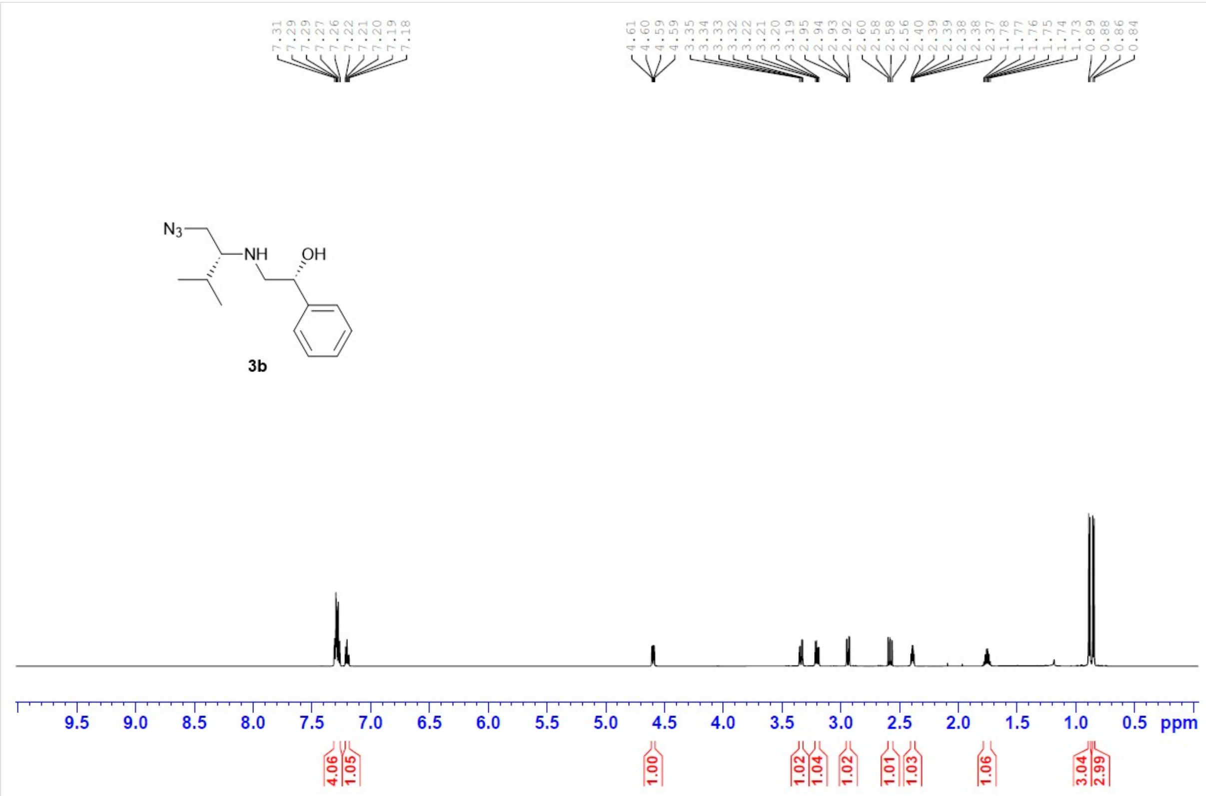
^{1}H NMR (600 MHz, $CDCl_3$), ^{13}C{1H} NMR (151 MHz, $CDCl_3$) and HMQC ($CDCl_3$) spectra for compound **3a**.

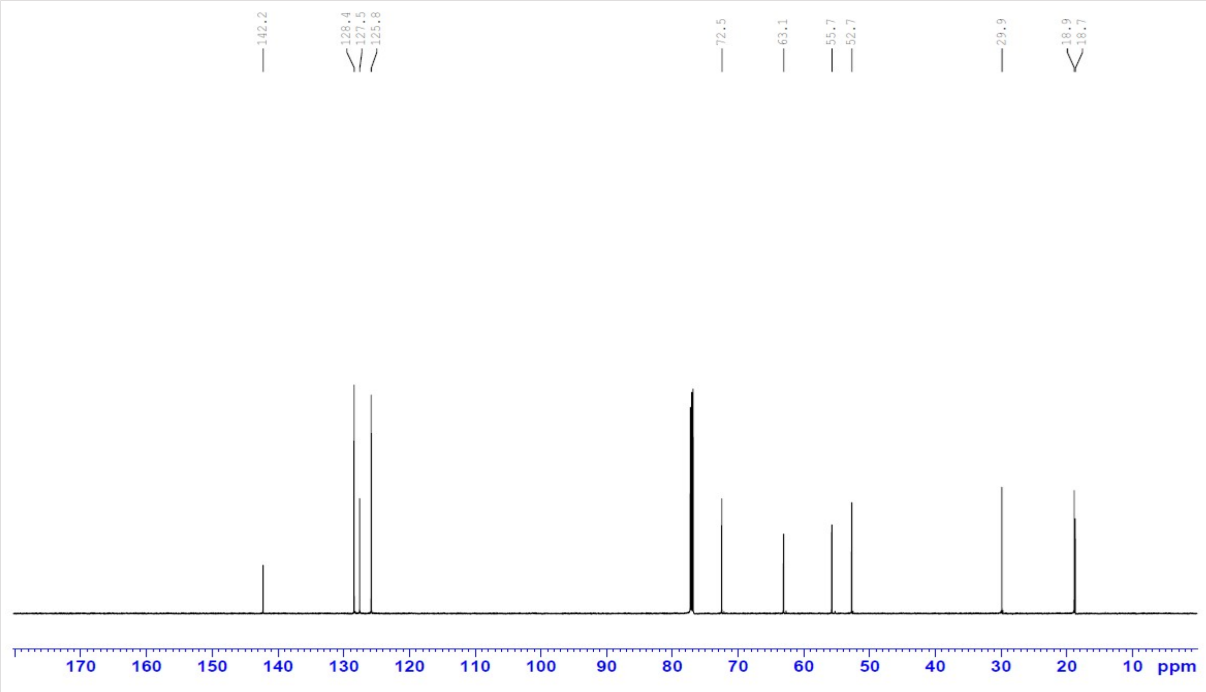




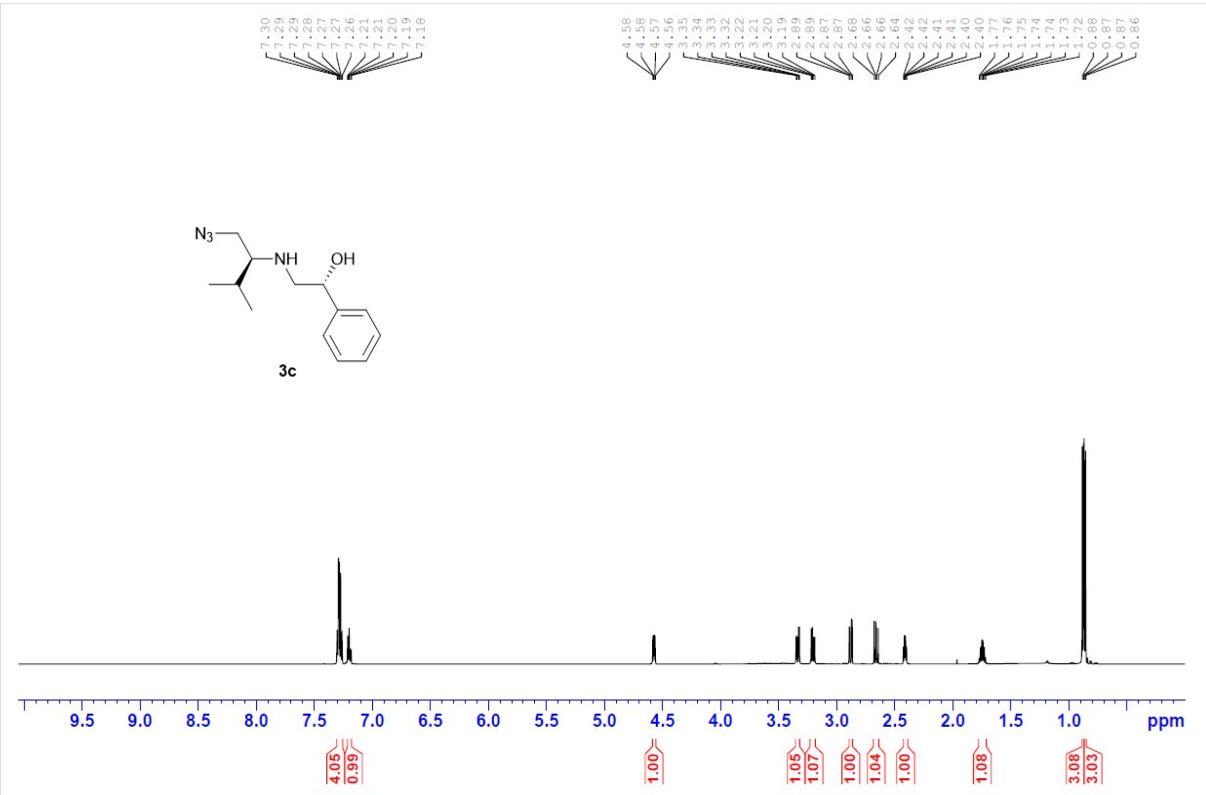


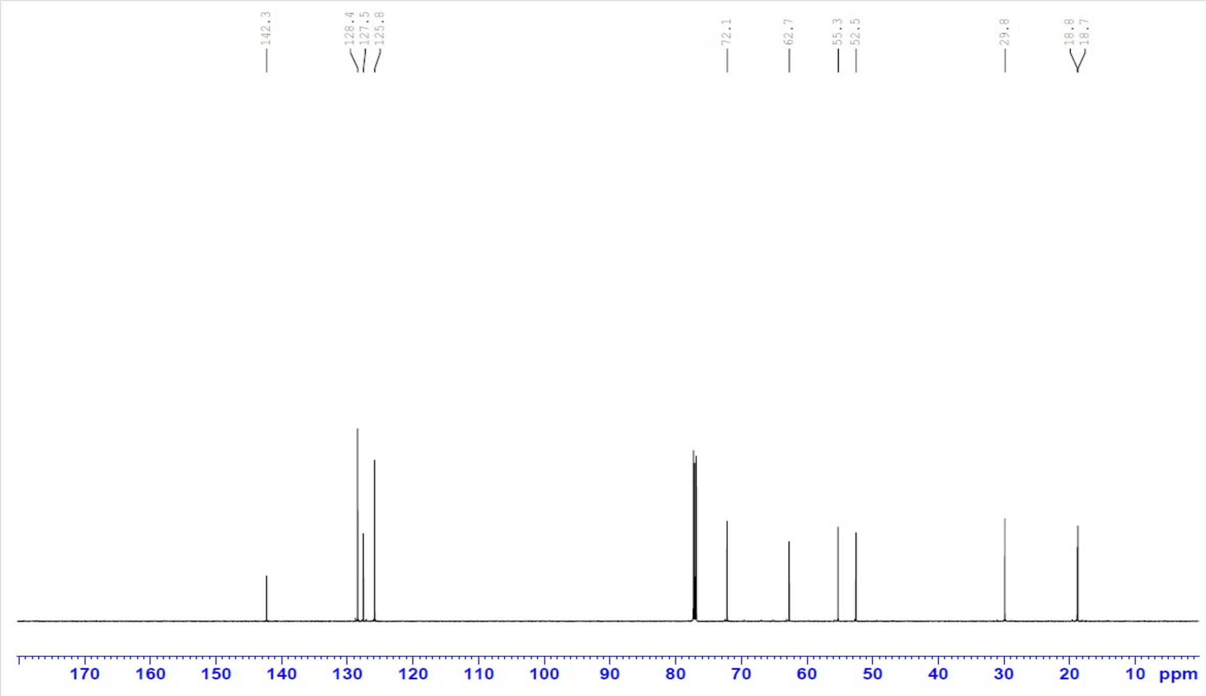
[1]H NMR (600 MHz, $CDCl_3$) and [13]C{1H} NMR (151 MHz, $CDCl_3$) spectra for compound **3b**.



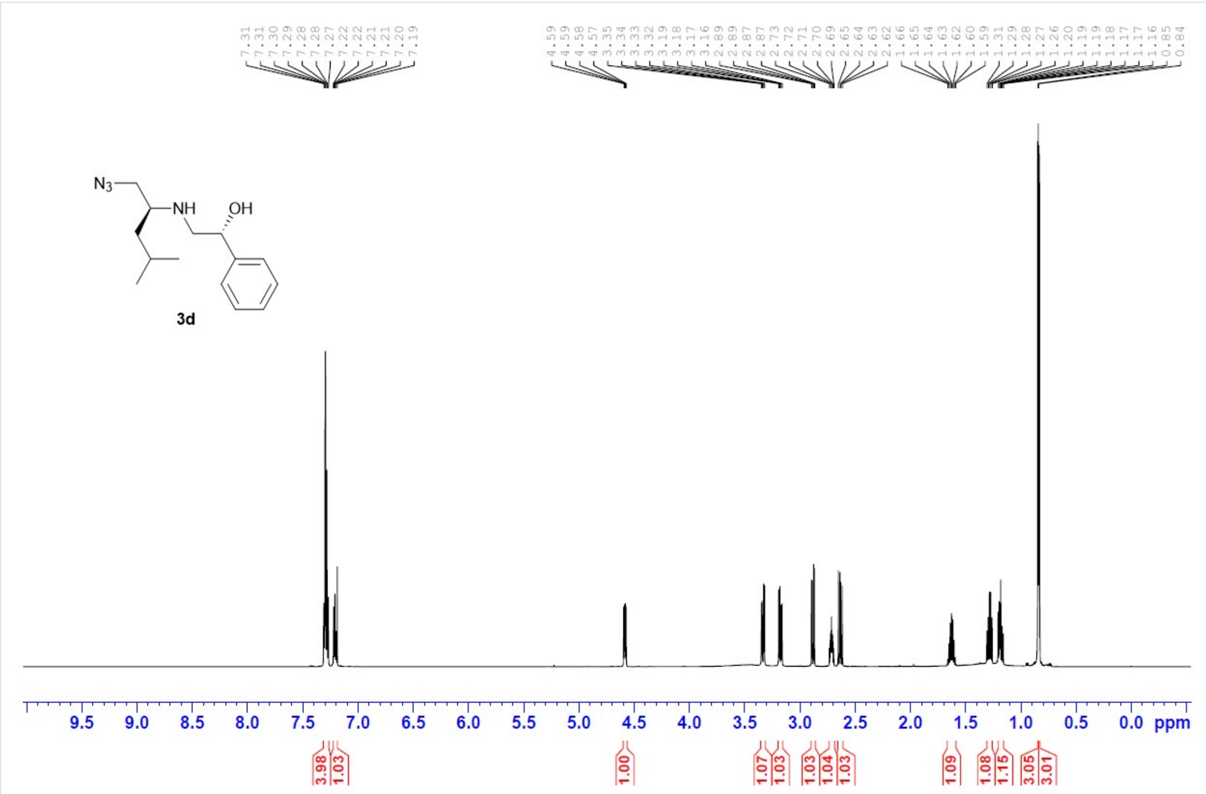


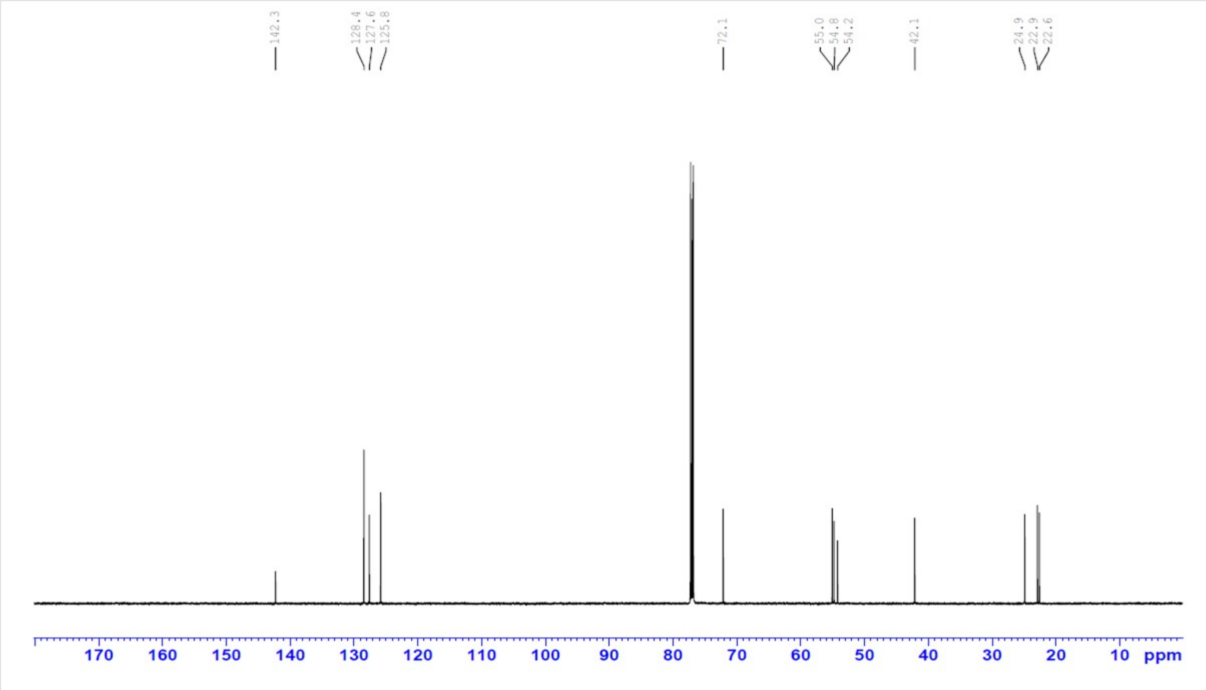
^{1}H NMR (600 MHz, $CDCl_3$) and ^{13}C{1H} NMR (151 MHz, $CDCl_3$) spectra for compound **3c**.



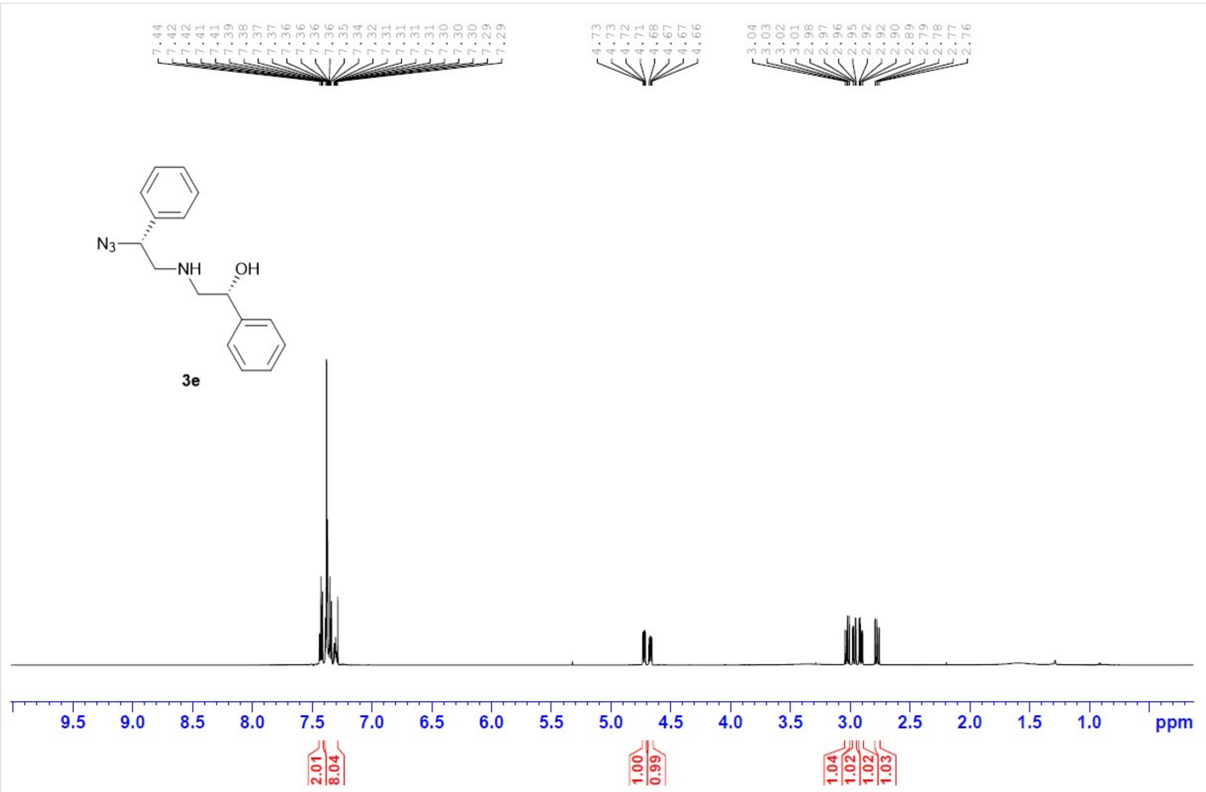


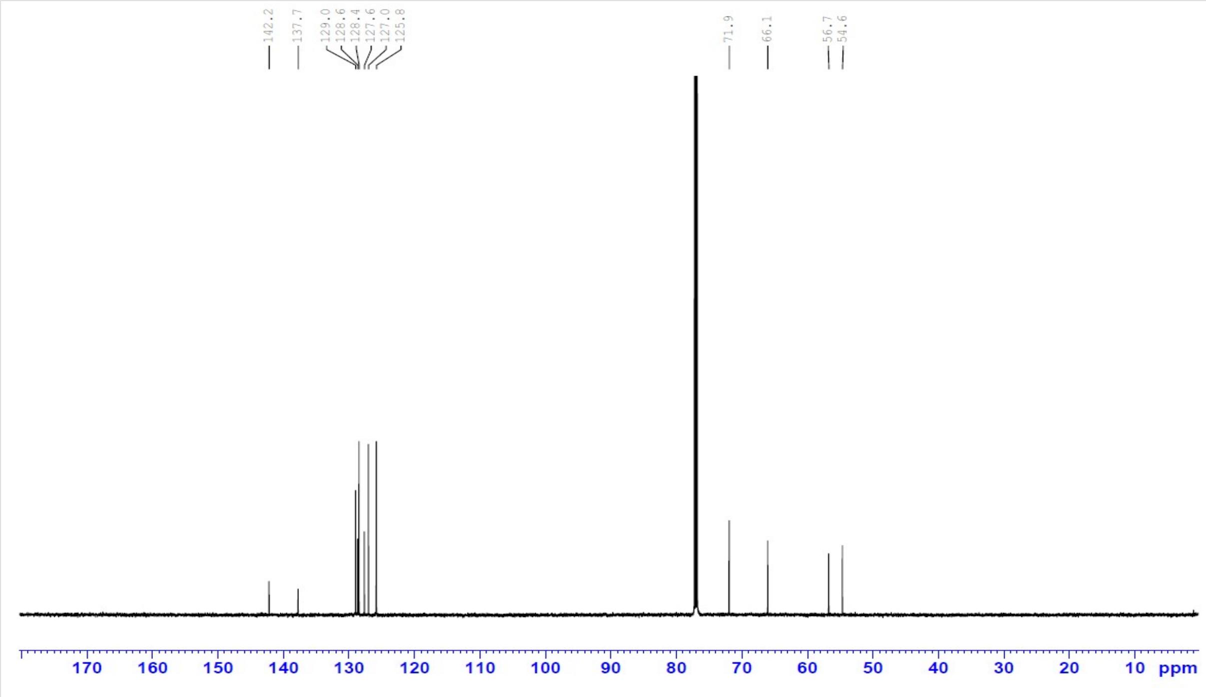
[1]H NMR (600 MHz, $CDCl_3$) and [13]C{1H} NMR (151 MHz, $CDCl_3$) spectra for compound **3d**.

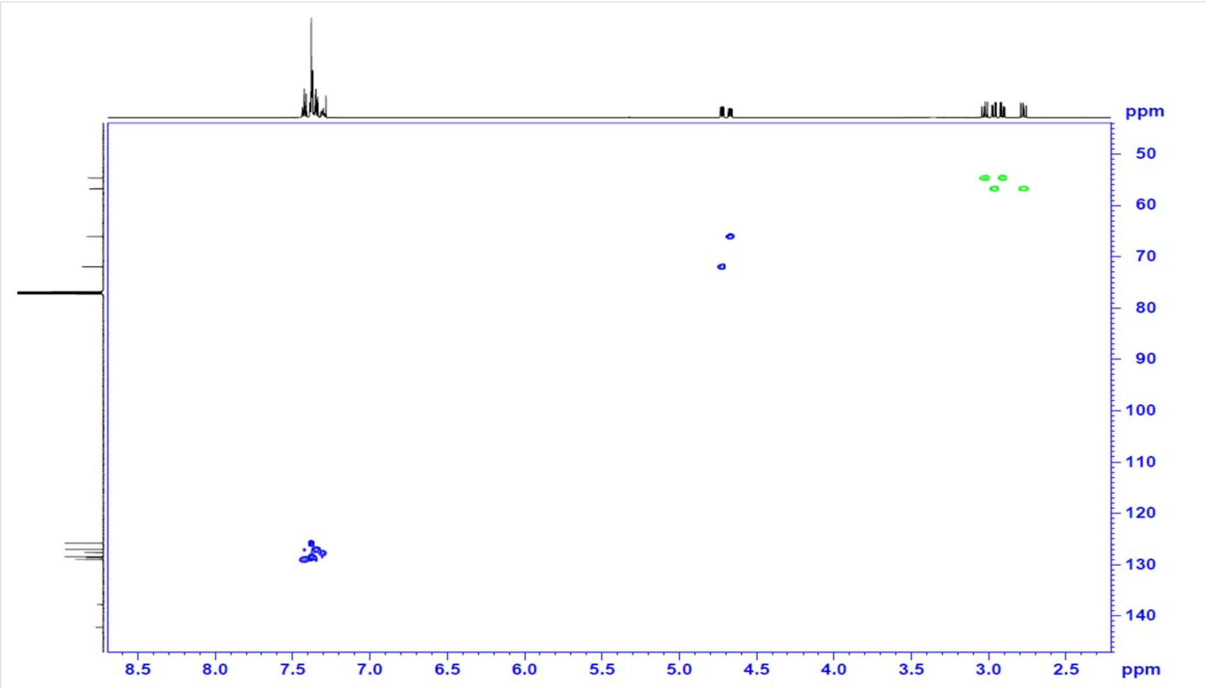




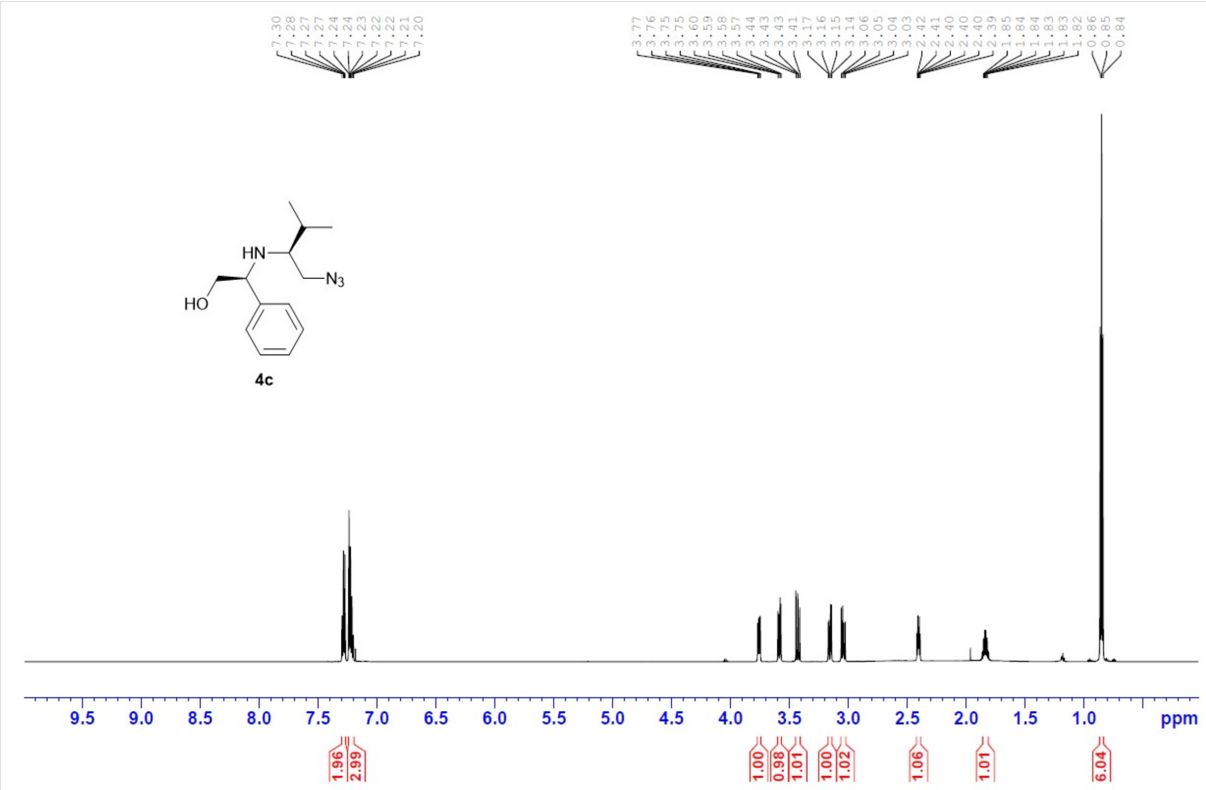
^{1}H NMR (600 MHz, $CDCl_3$), ^{13}C{1H} NMR (151 MHz, $CDCl_3$) and HSQC ($CDCl_3$) spectra for compound **3e**.

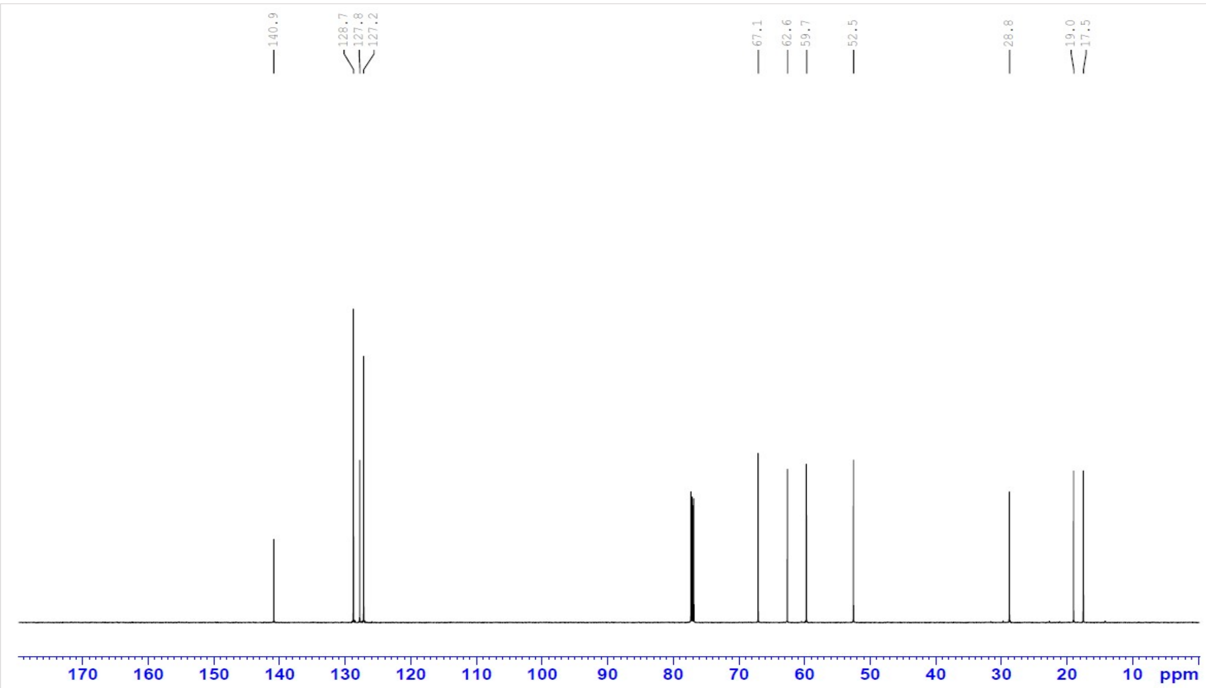


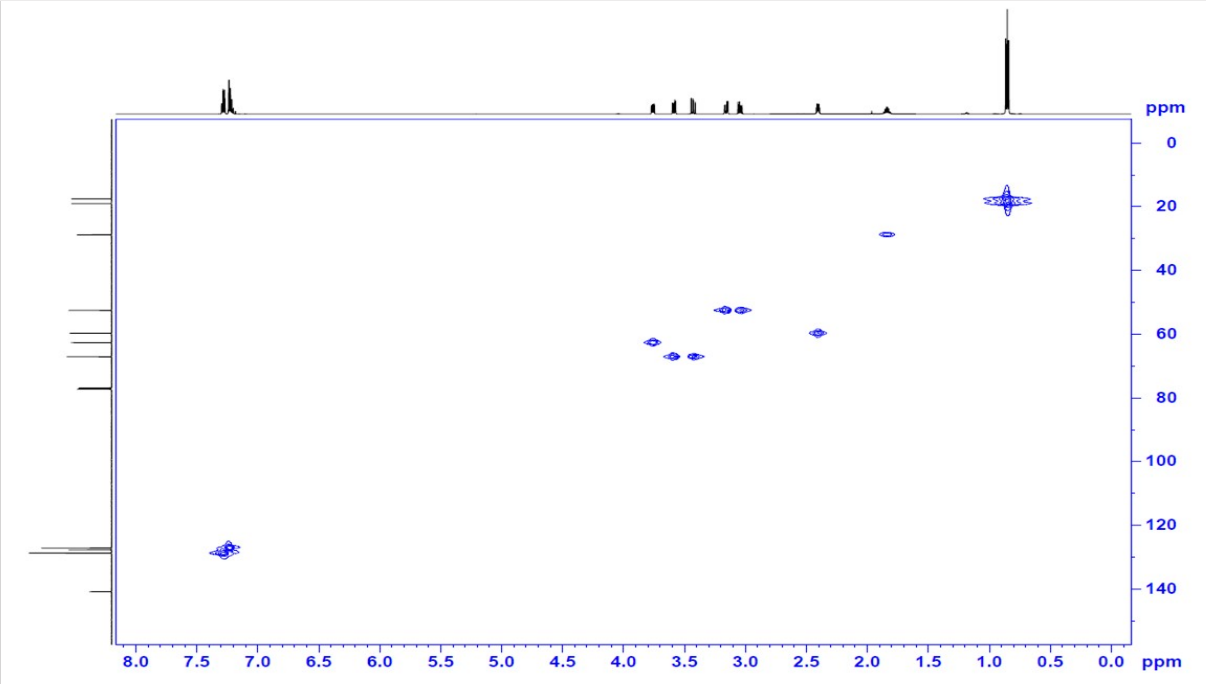

142.2
137.7
129.0
128.6
128.4
127.6
127.0
125.8
71.9
66.1
56.7
54.6
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


ppm
50 60 70 80 90 100 110 120 130 140
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 ppm

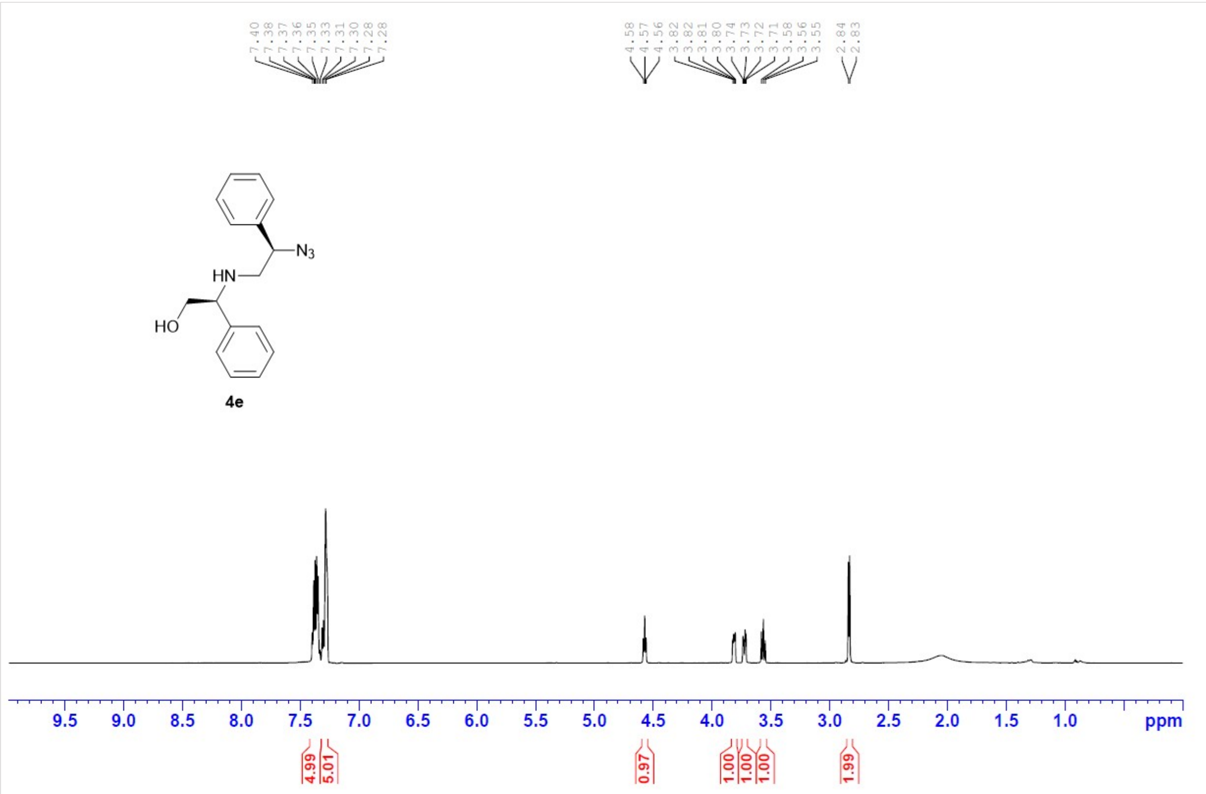
[1]H NMR (600 MHz, $CDCl_3$), [13]C{1H} NMR (151 MHz, $CDCl_3$) and HMQC ($CDCl_3$) spectra for compound **4c**.

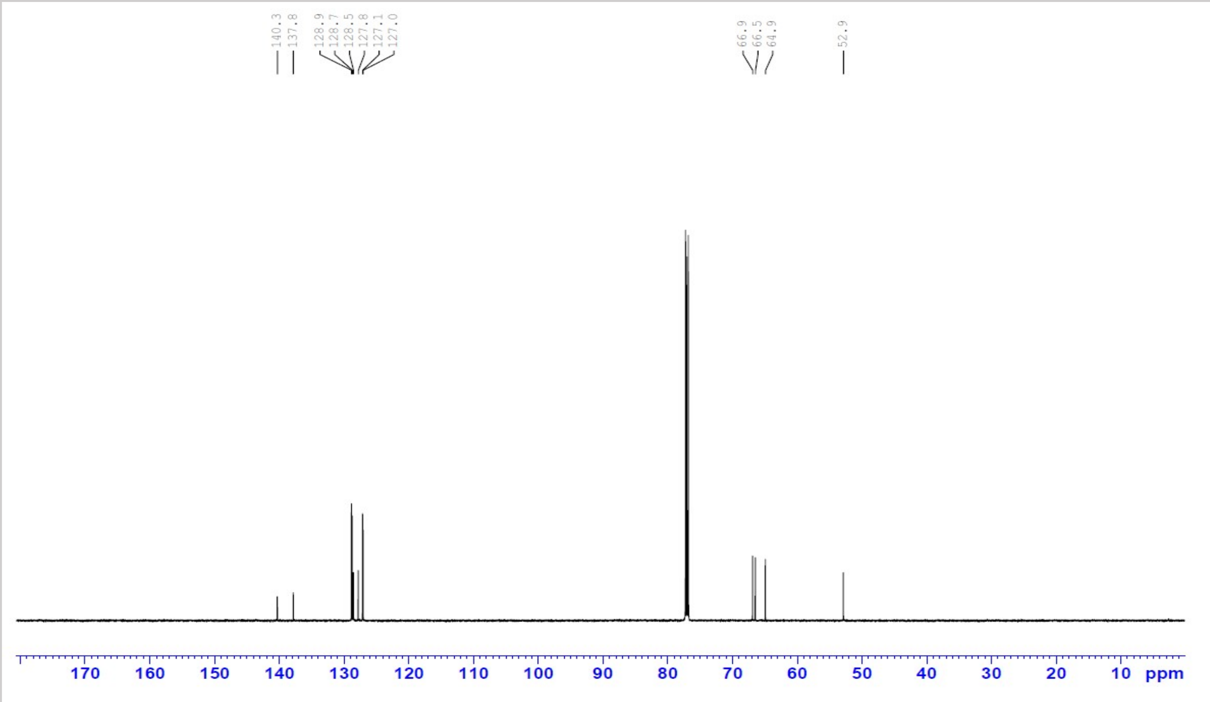


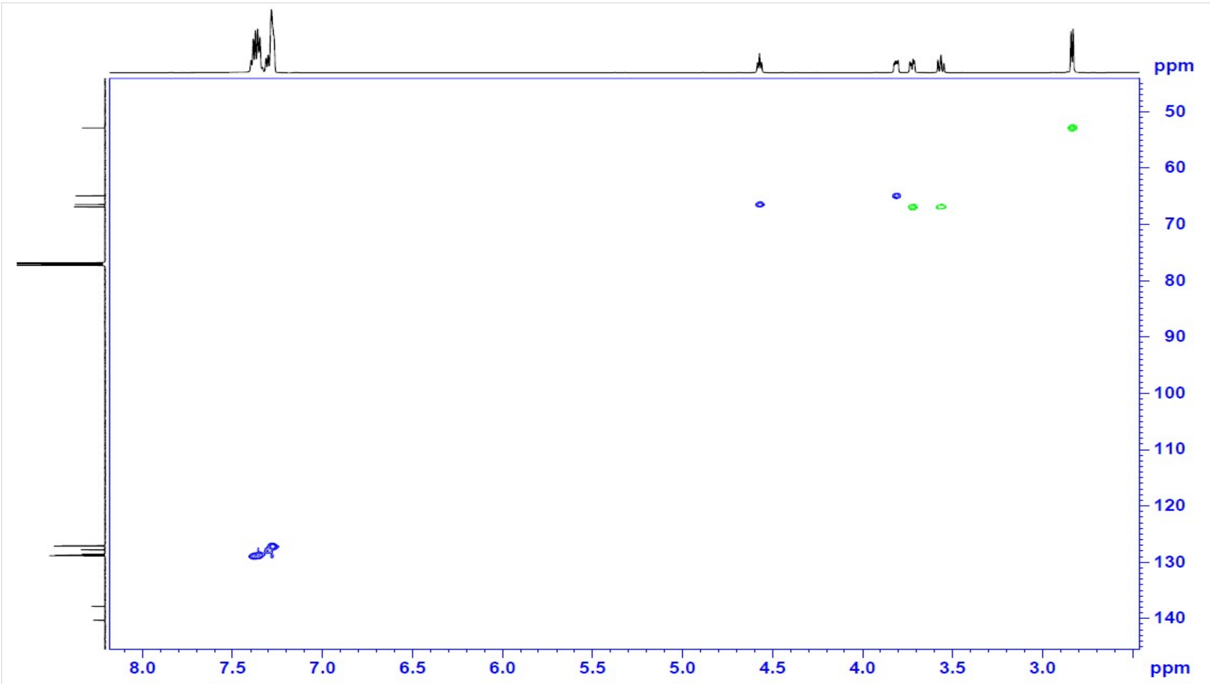




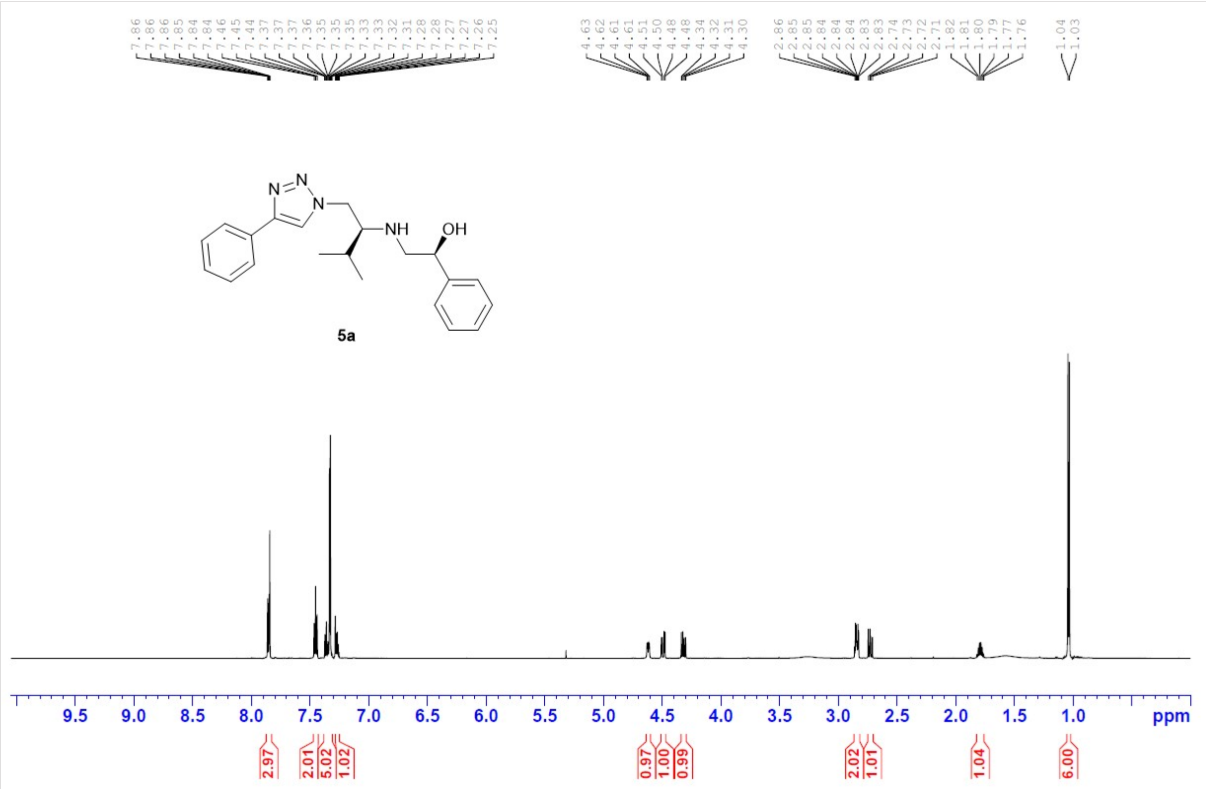
^{1}H NMR (600 MHz, $CDCl_3$), ^{13}C{1H} NMR (151 MHz, $CDCl_3$) and HSQC ($CDCl_3$) spectra for compound **4e**.

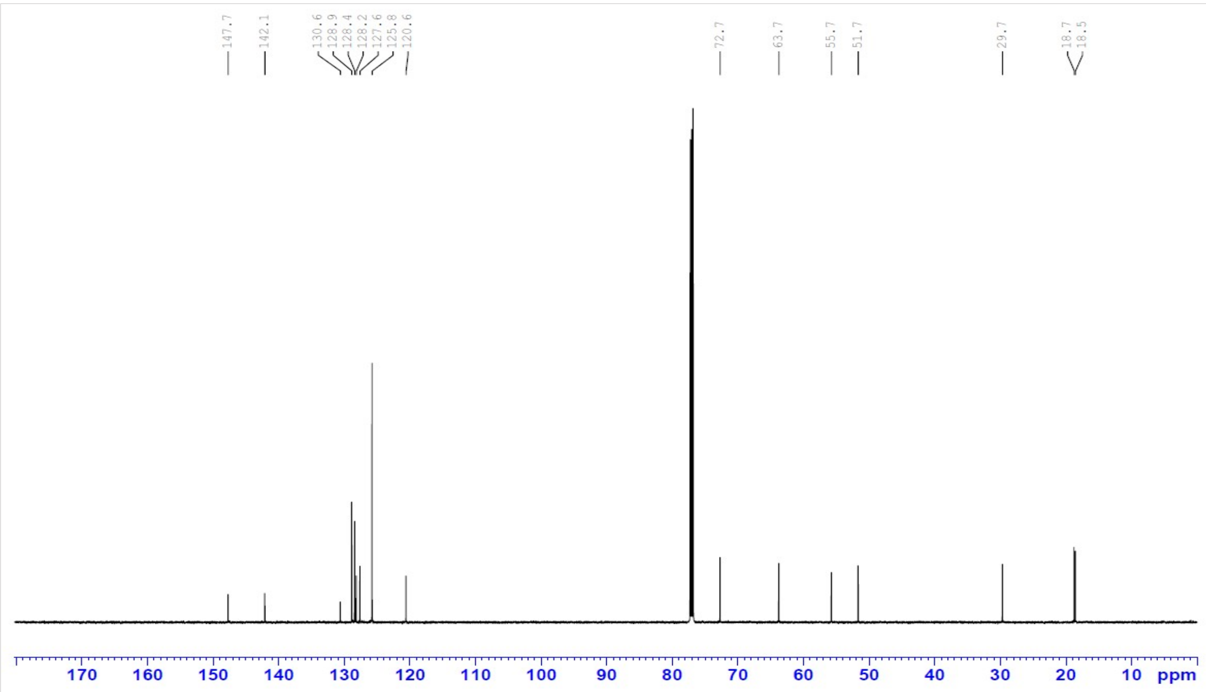


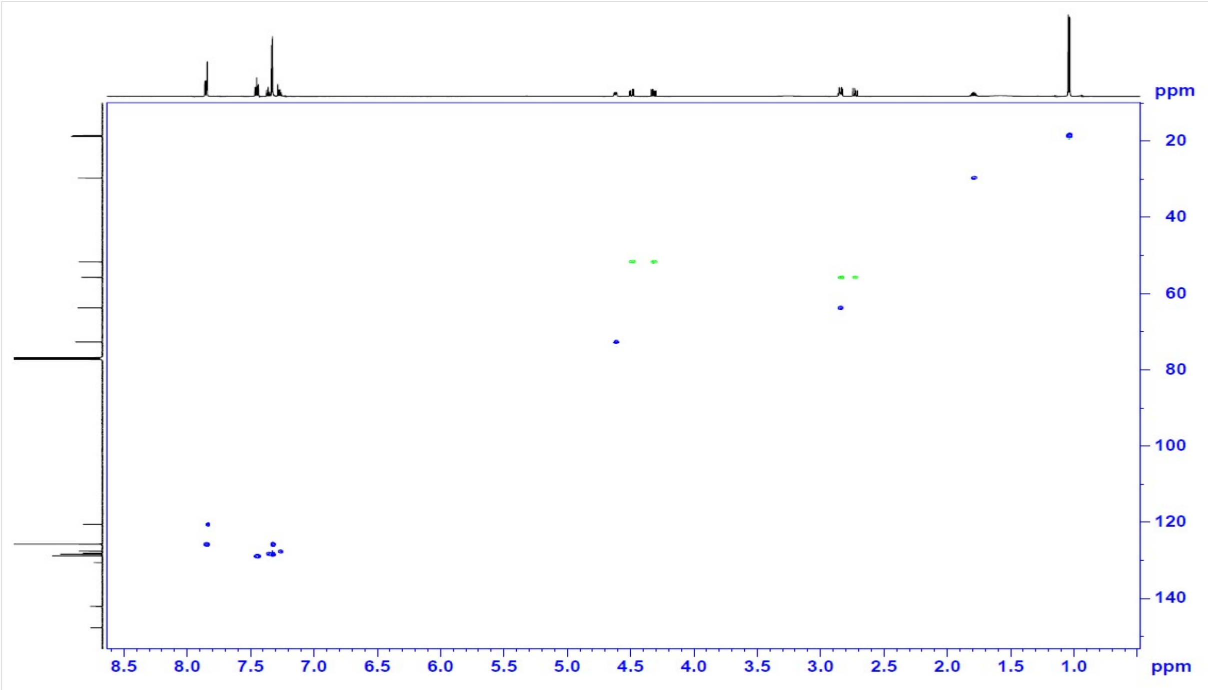

140.3
137.8
128.9
128.7
128.5
127.8
127.1
127.0
66.9
66.5
64.9
52.9
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


ppm
50 60 70 80 90 100 110 120 130 140
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 ppm

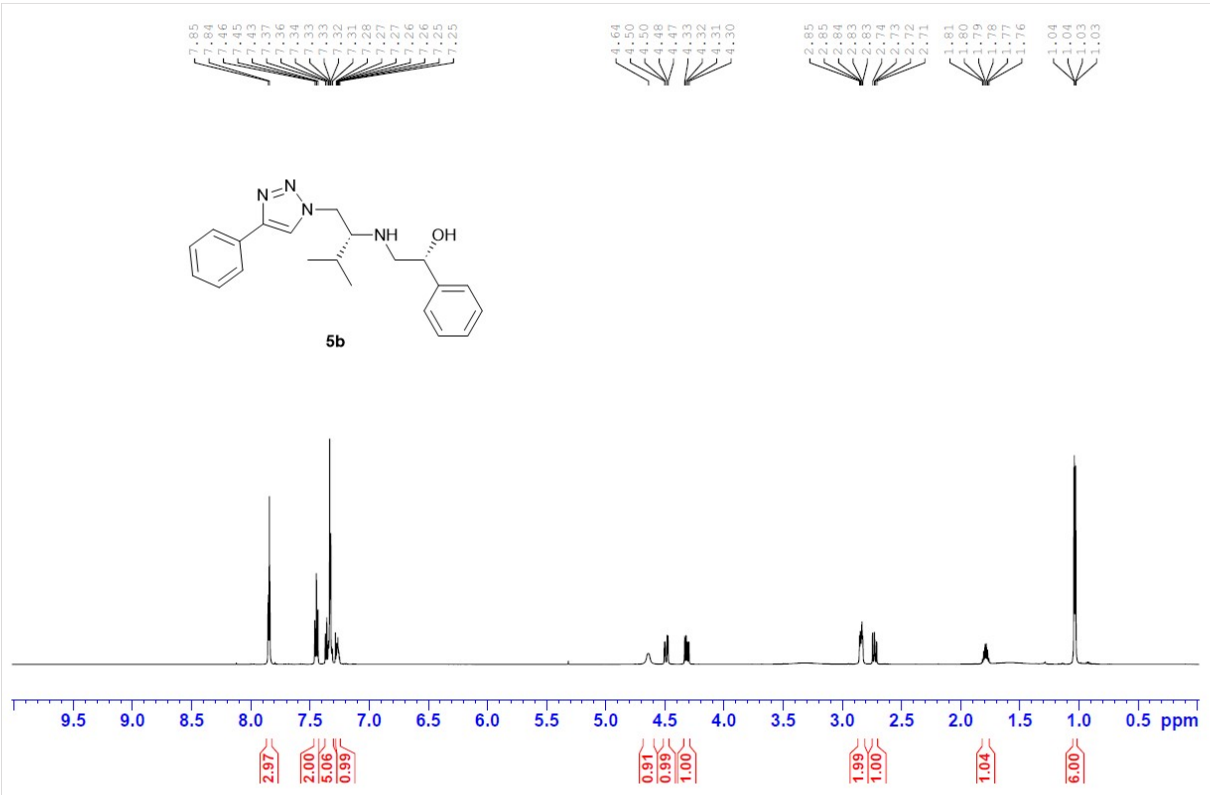
^{1}H NMR (600 MHz, $CDCl_3$), $^{13}C\{1H\}$ NMR (151 MHz, $CDCl_3$) and HSQC ($CDCl_3$) spectra for compound **5a**.

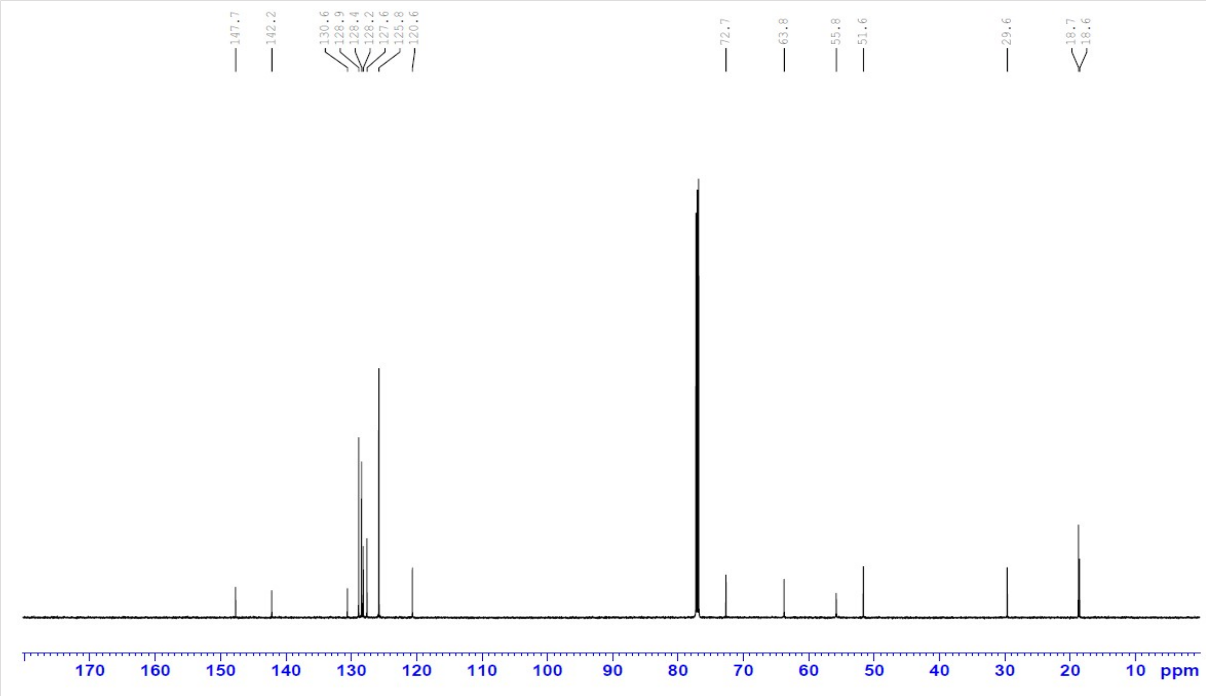




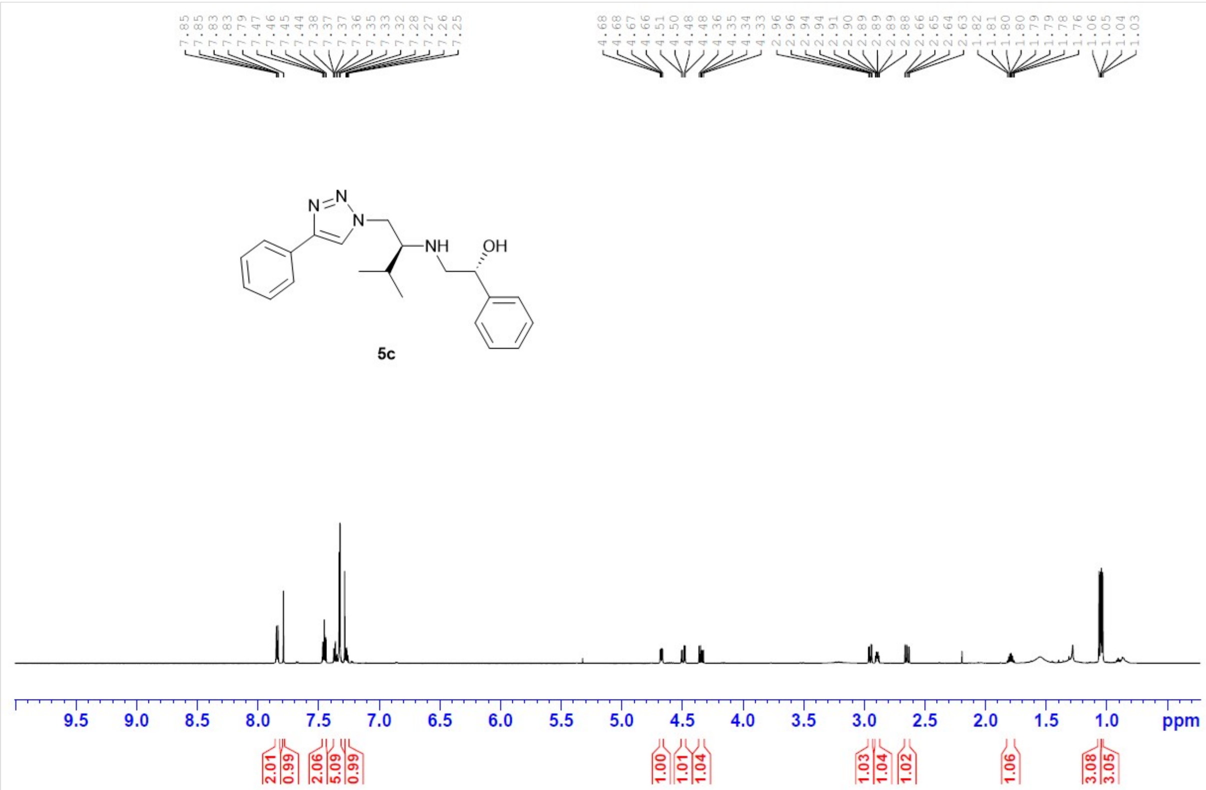


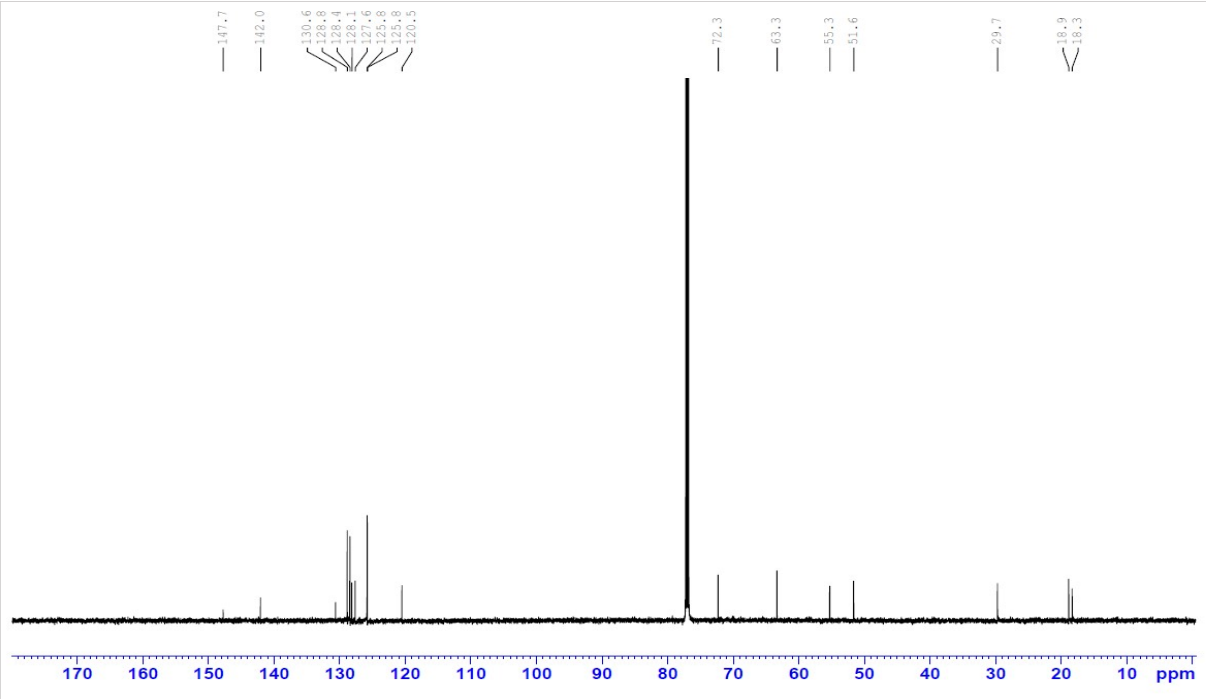
^{1}H NMR (600 MHz, $CDCl_3$) and $^{13}C\{1H\}$ NMR (151 MHz, $CDCl_3$) spectra for compound **5b**.



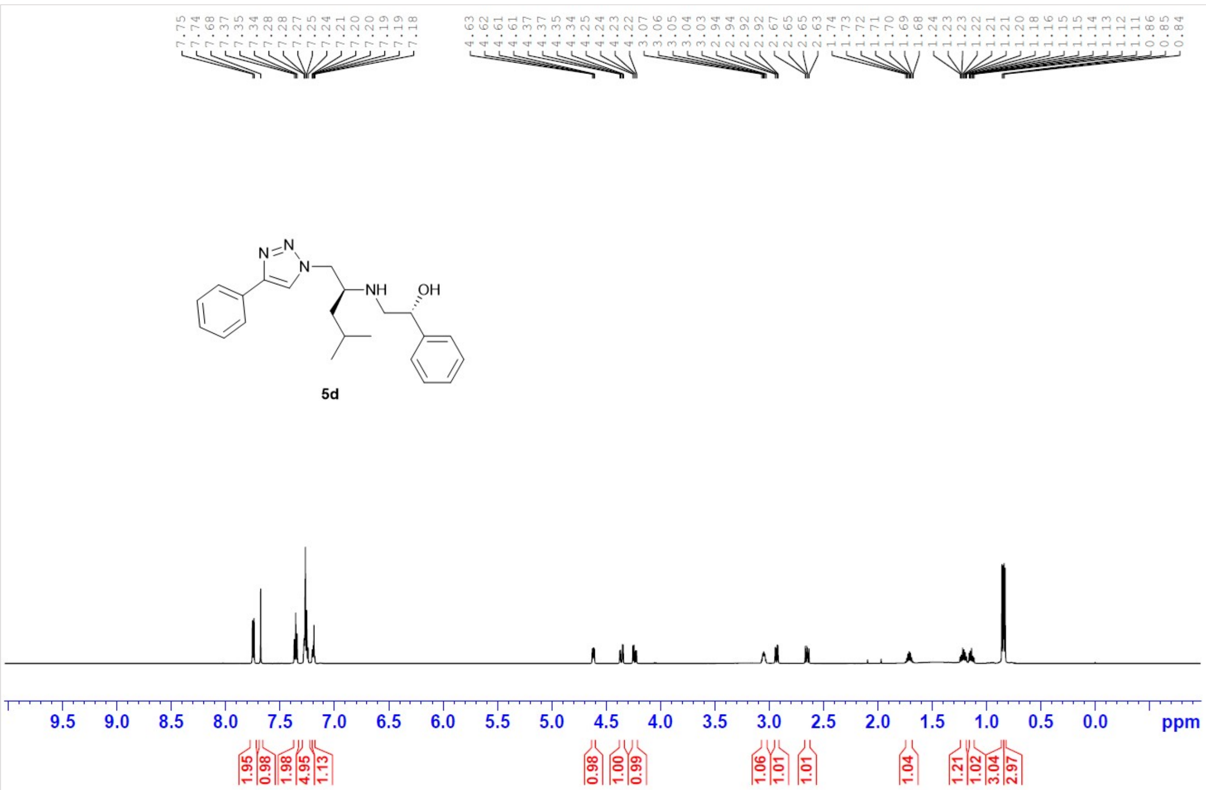


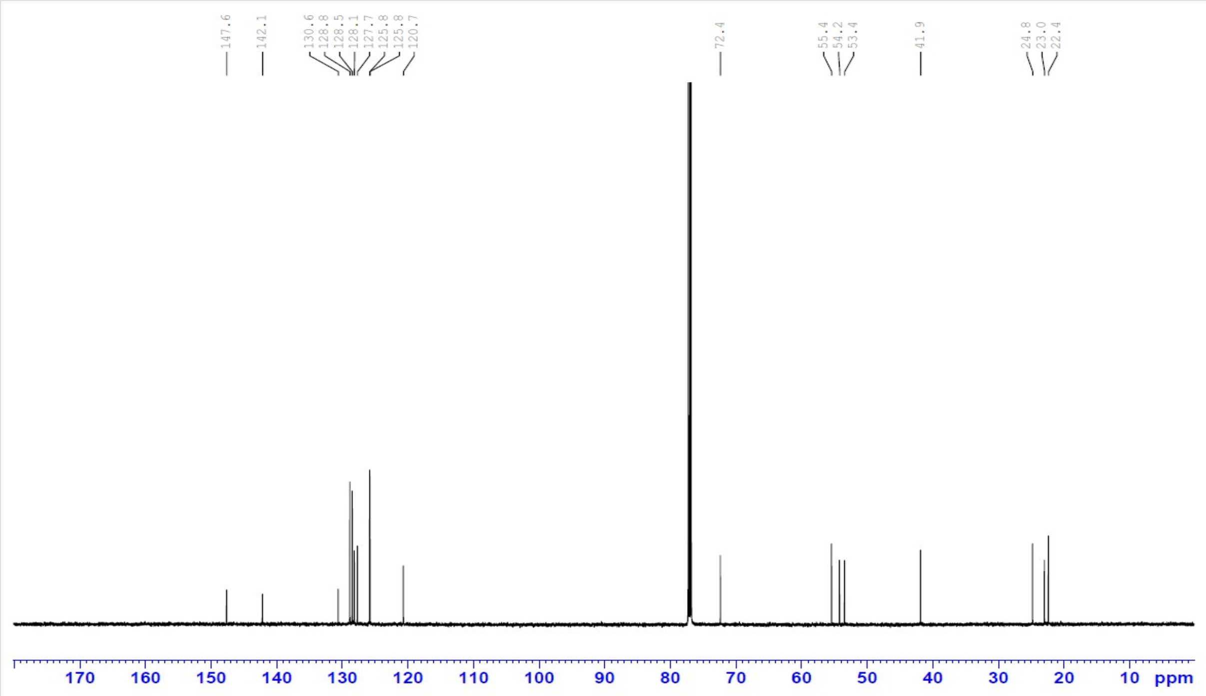
^{1}H NMR (600 MHz, $CDCl_3$) and $^{13}C\{1H\}$ NMR (151 MHz, $CDCl_3$) spectra for compound **5c**.



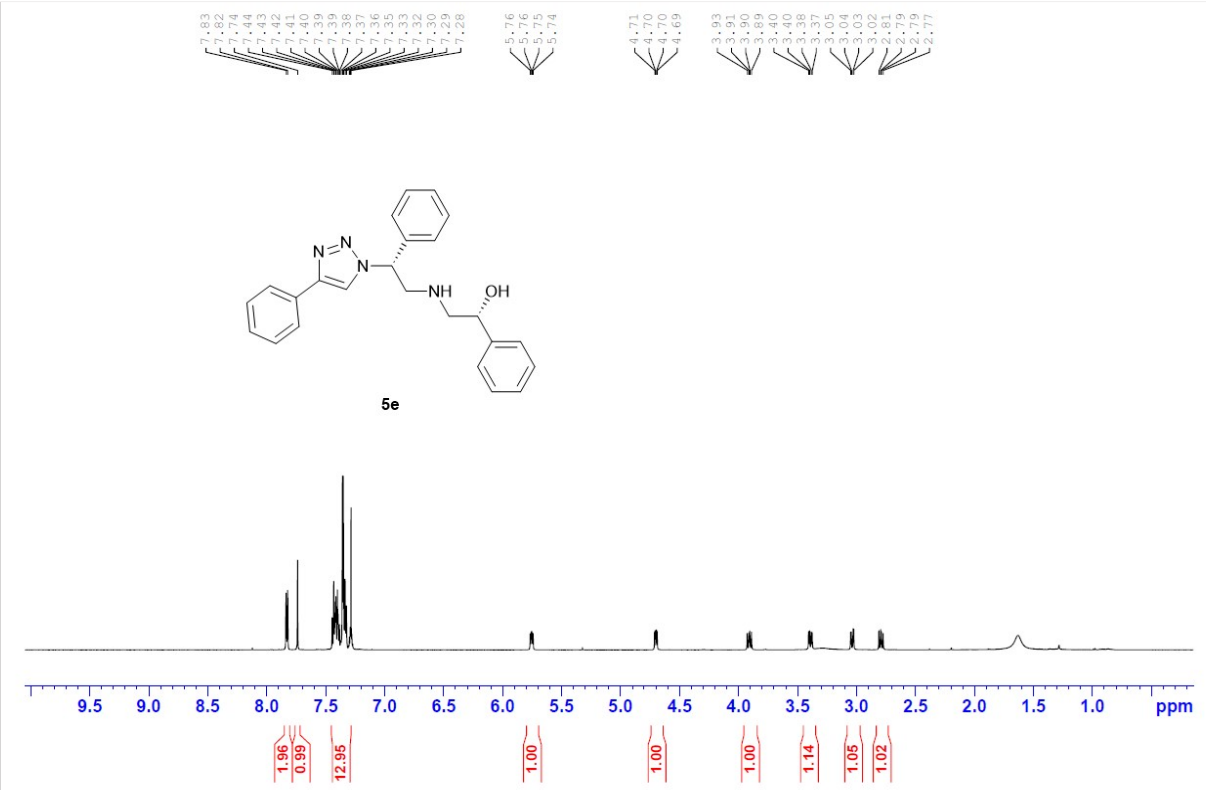


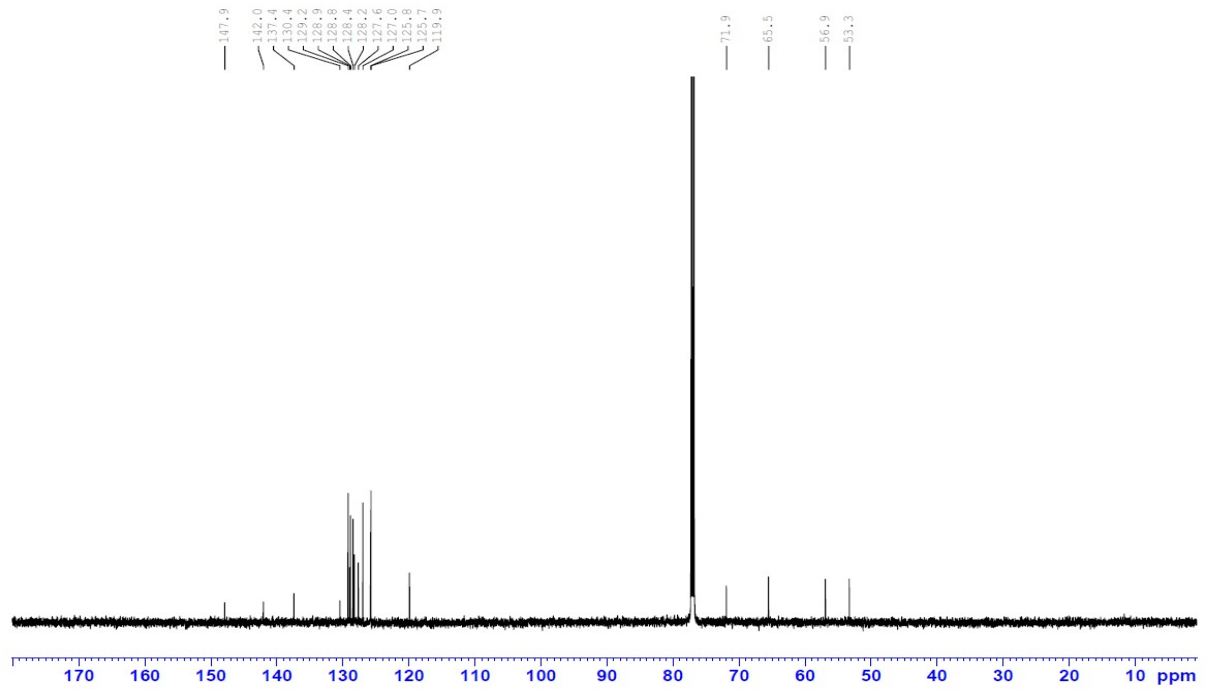
[1]H NMR (600 MHz, $CDCl_3$) and [13]C{1H} NMR (151 MHz, $CDCl_3$) spectra for compound **5d**.

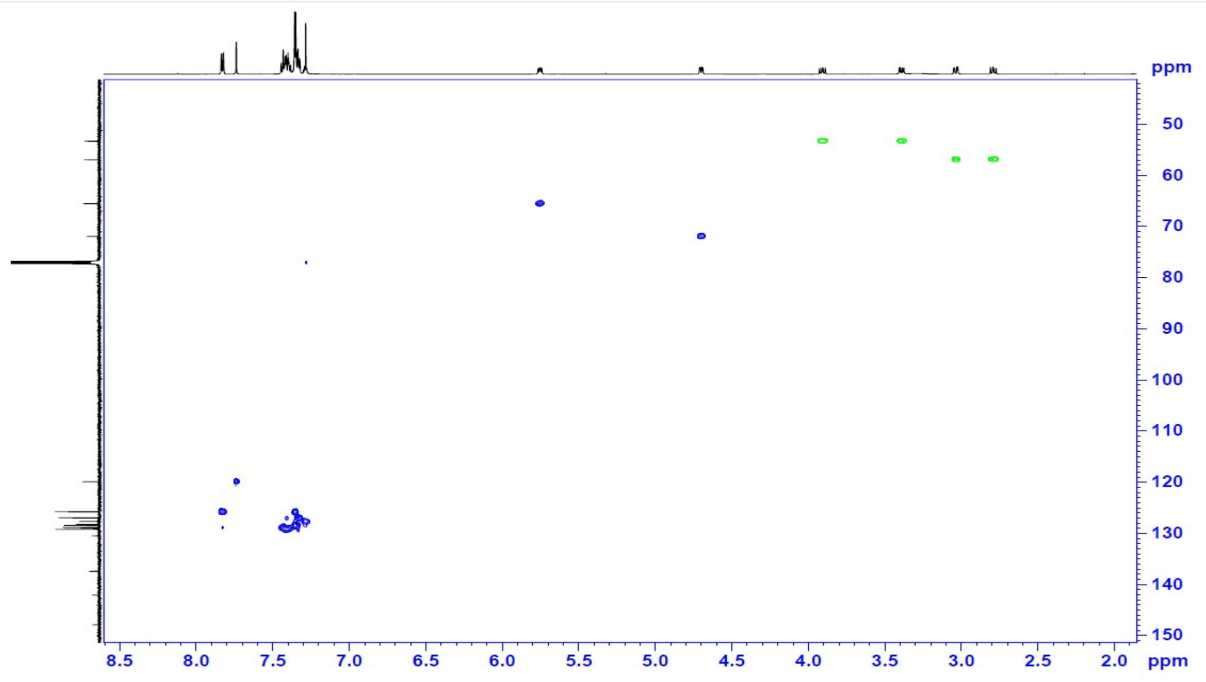




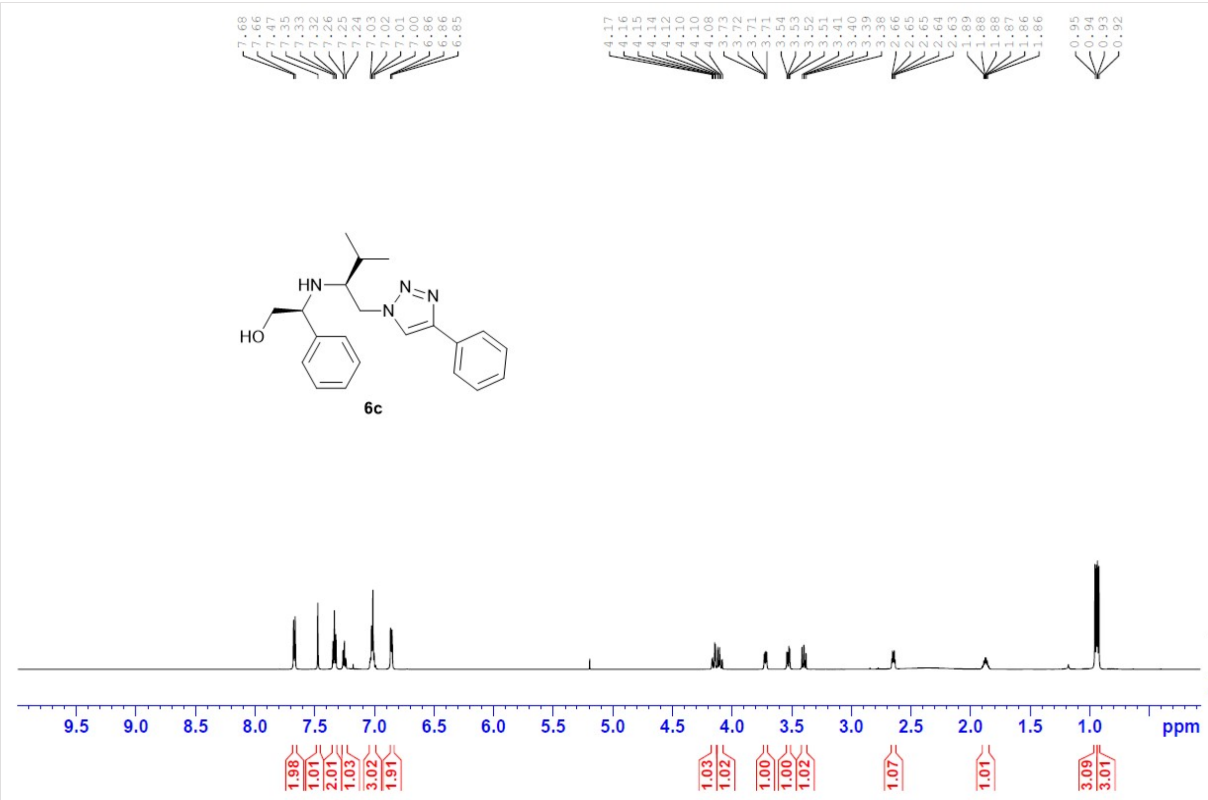
[1]H NMR (600 MHz, $CDCl_3$), [13]C{1H} NMR (151 MHz, $CDCl_3$) and HSQC ($CDCl_3$) spectra for compound **5e**.

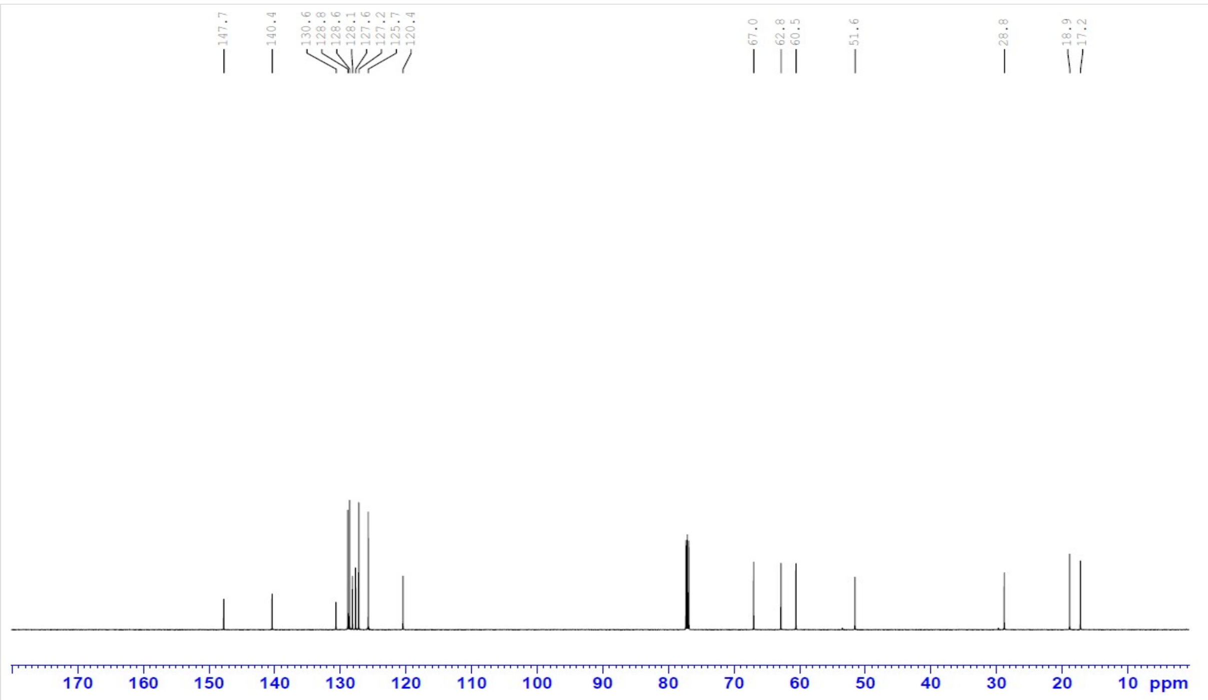


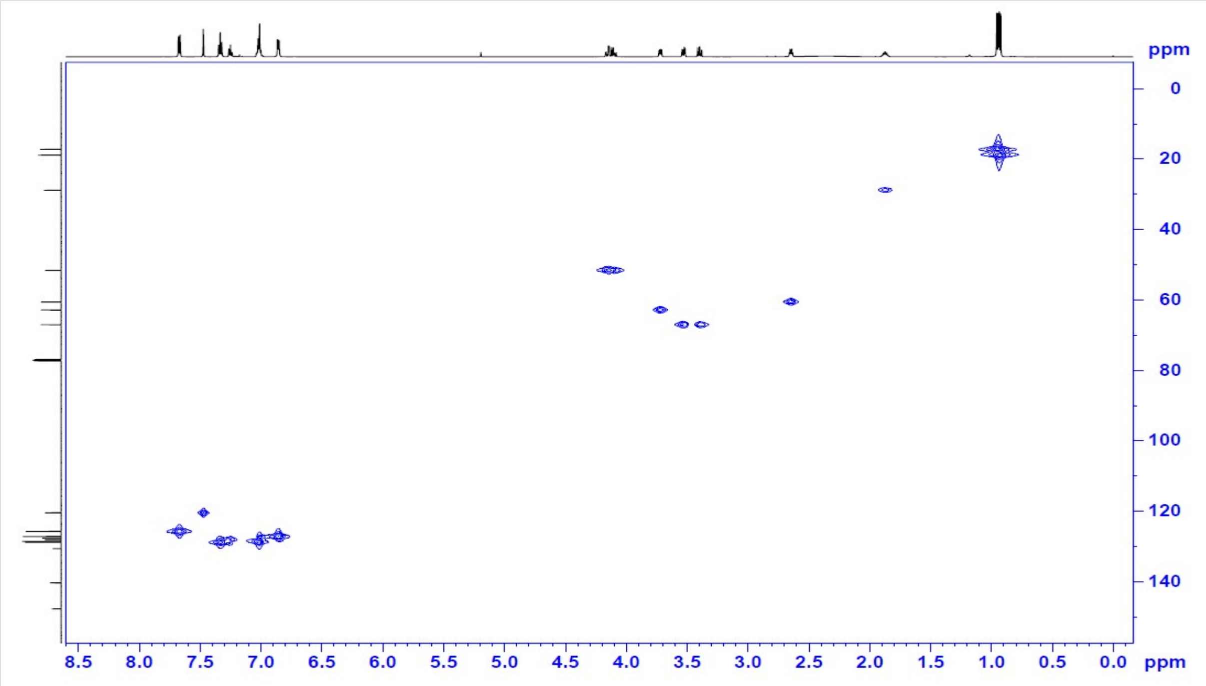

147.9
142.0
137.4
130.4
129.2
128.9
128.8
128.4
128.2
127.6
127.0
125.8
125.7
119.9
71.9
65.5
56.9
53.3
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


ppm
50 60 70 80 90 100 110 120 130 140 150
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 ppm

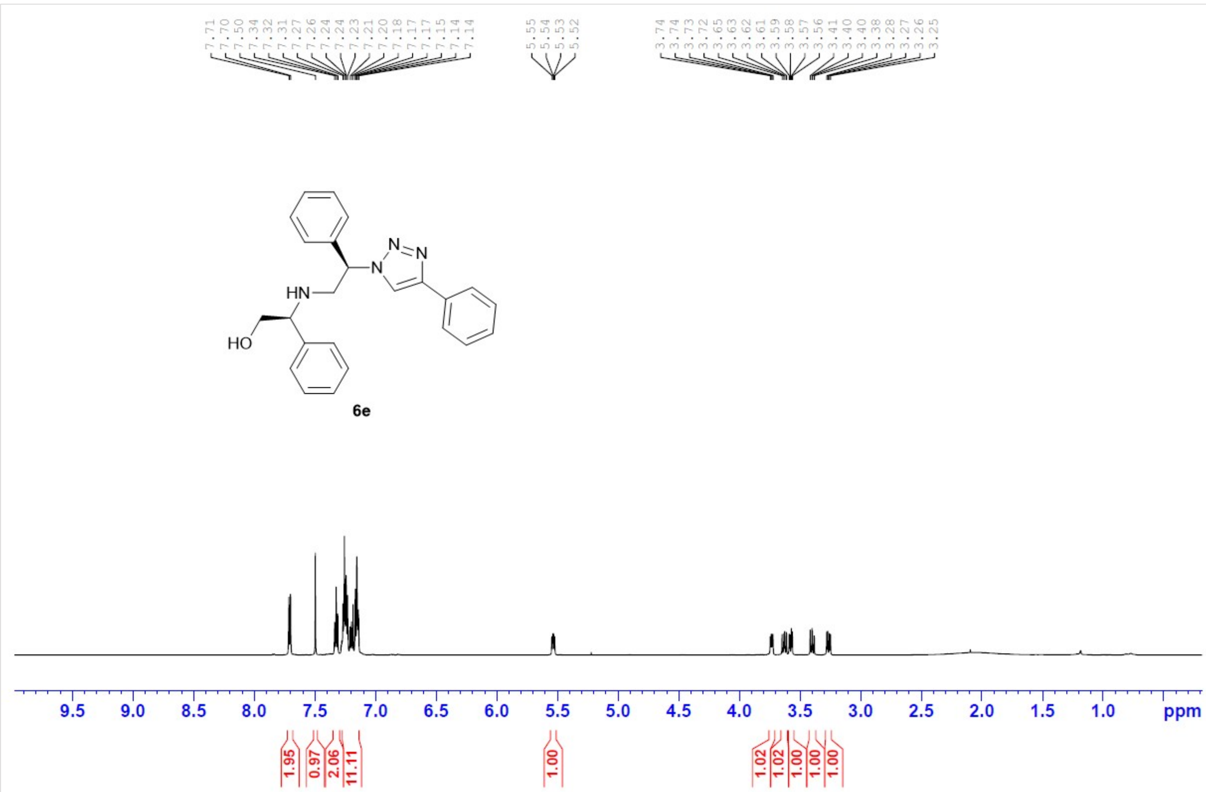
^{1}H NMR (600 MHz, $CDCl_3$), $^{13}C\{1H\}$ NMR (151 MHz, $CDCl_3$) and HMQC ($CDCl_3$) spectra for compound **6c**.

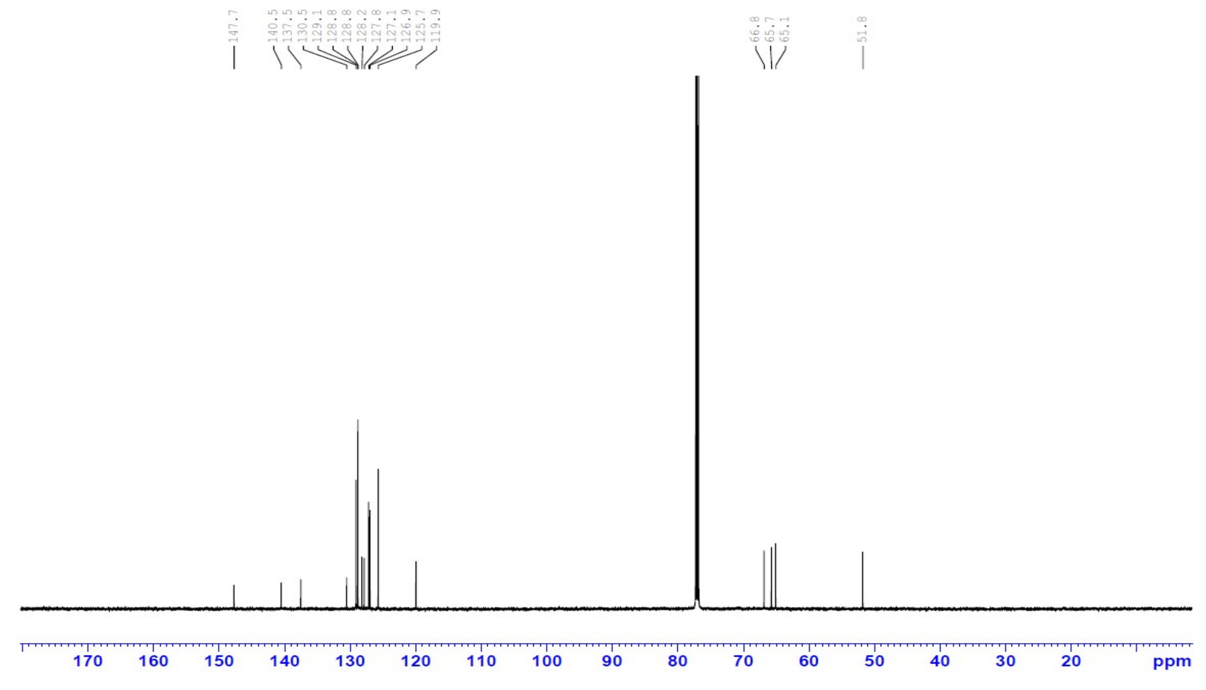


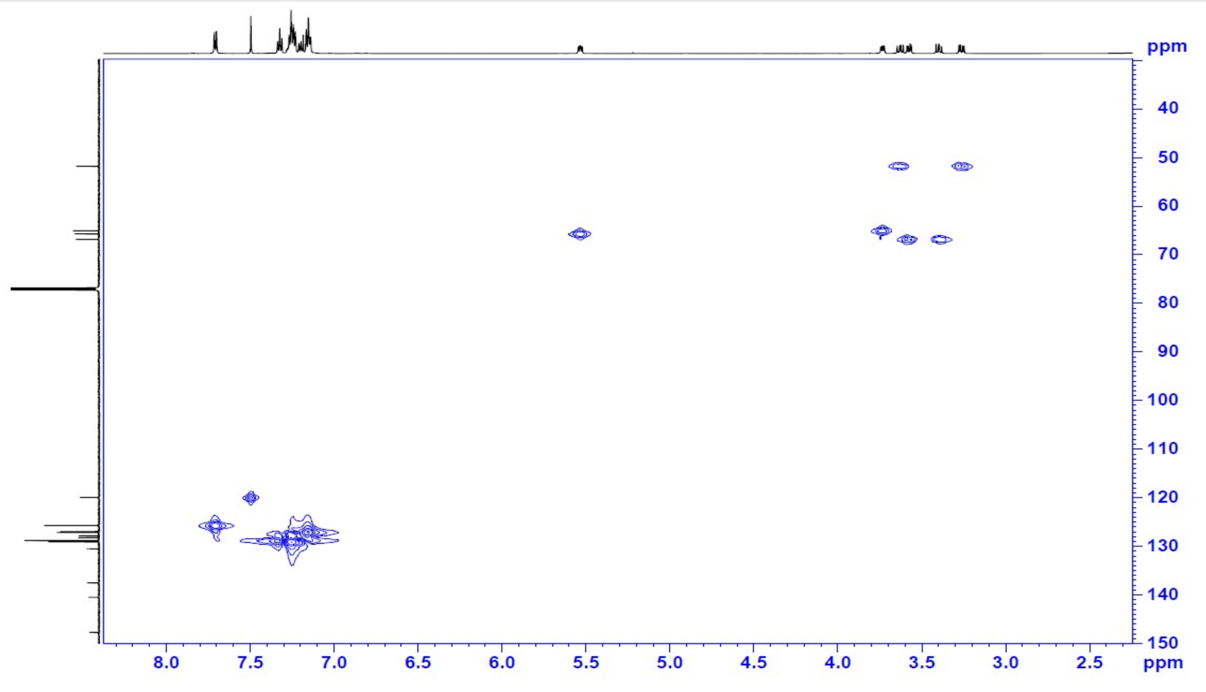




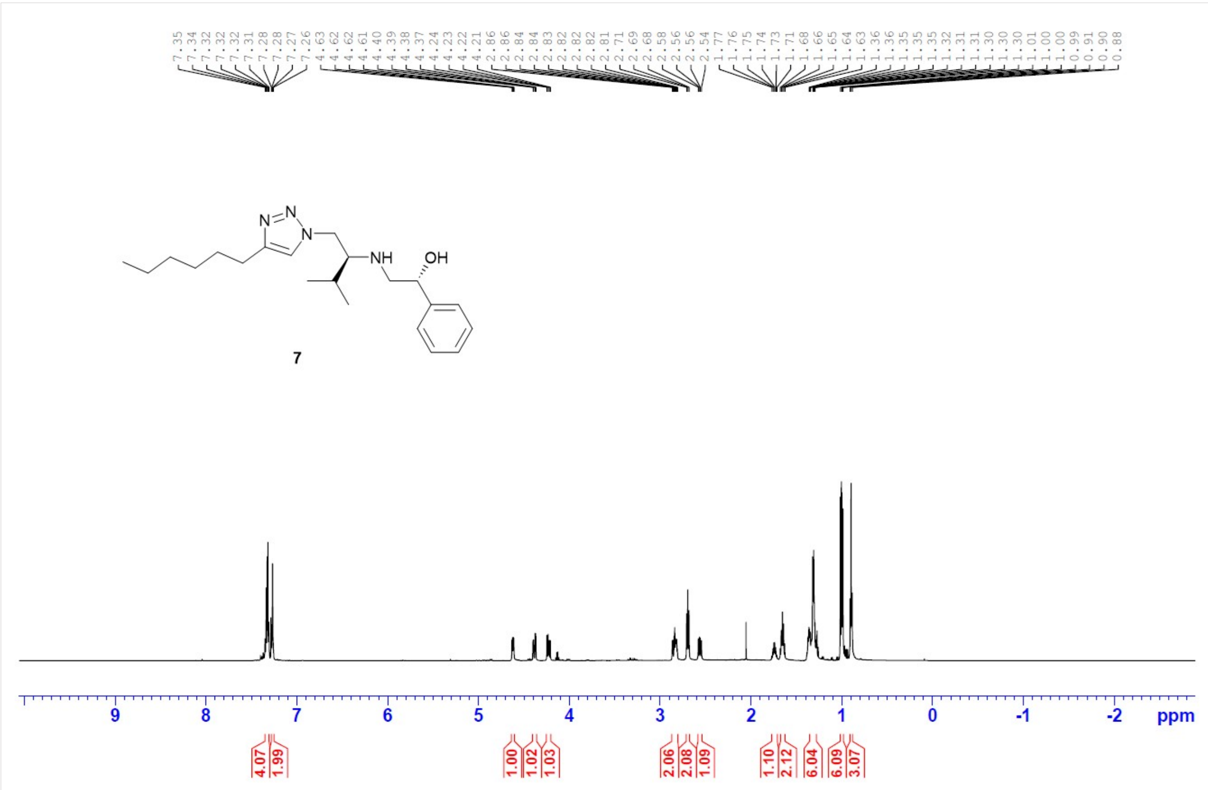
[1]H NMR (600 MHz, $CDCl_3$), [13]C{1H} NMR (151 MHz, $CDCl_3$) and HMQC ($CDCl_3$) spectra for compound **6e**.

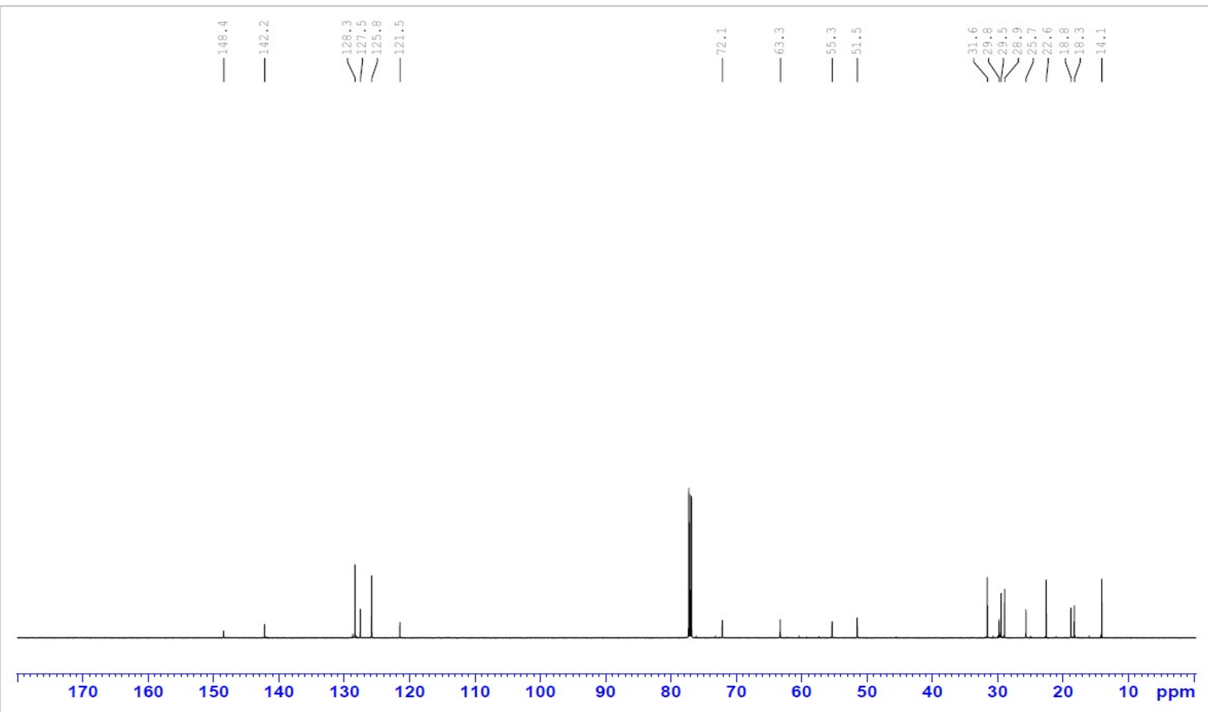


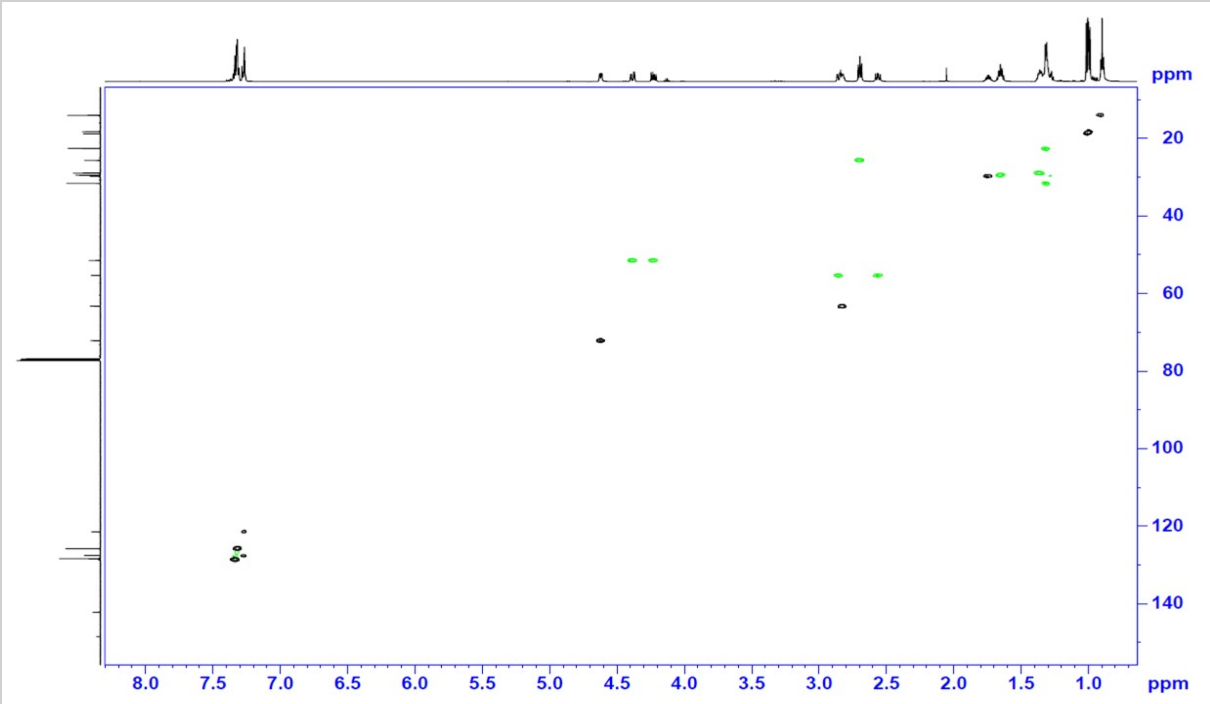

147.7
140.5
137.5
130.5
129.1
128.8
128.8
128.2
127.8
127.1
126.9
125.7
119.9
66.8
65.7
65.1
51.8
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


ppm
40
50
60
70
80
90
100
110
120
130
140
150
ppm
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
ppm

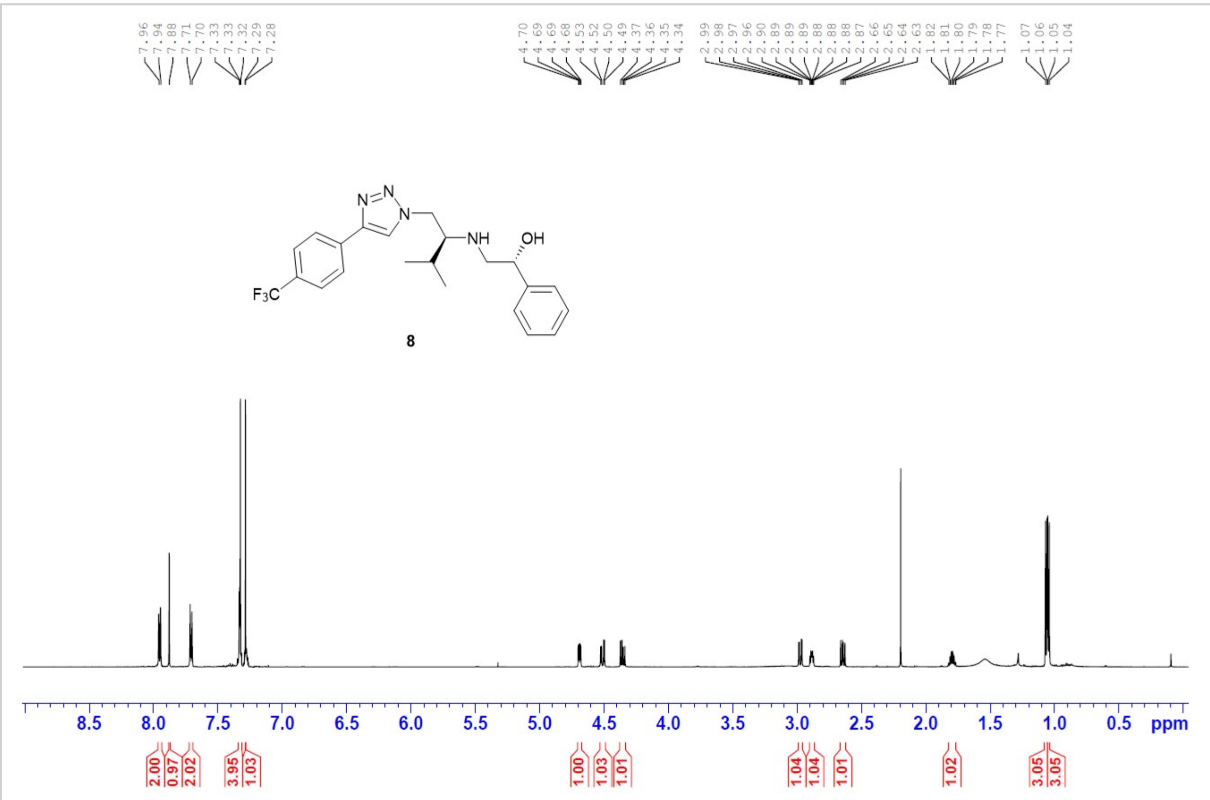
^{1}H NMR (600 MHz, $CDCl_3$), ^{13}C{1H} NMR (151 MHz, $CDCl_3$) and HSQC ($CDCl_3$) spectra for compound **7**.

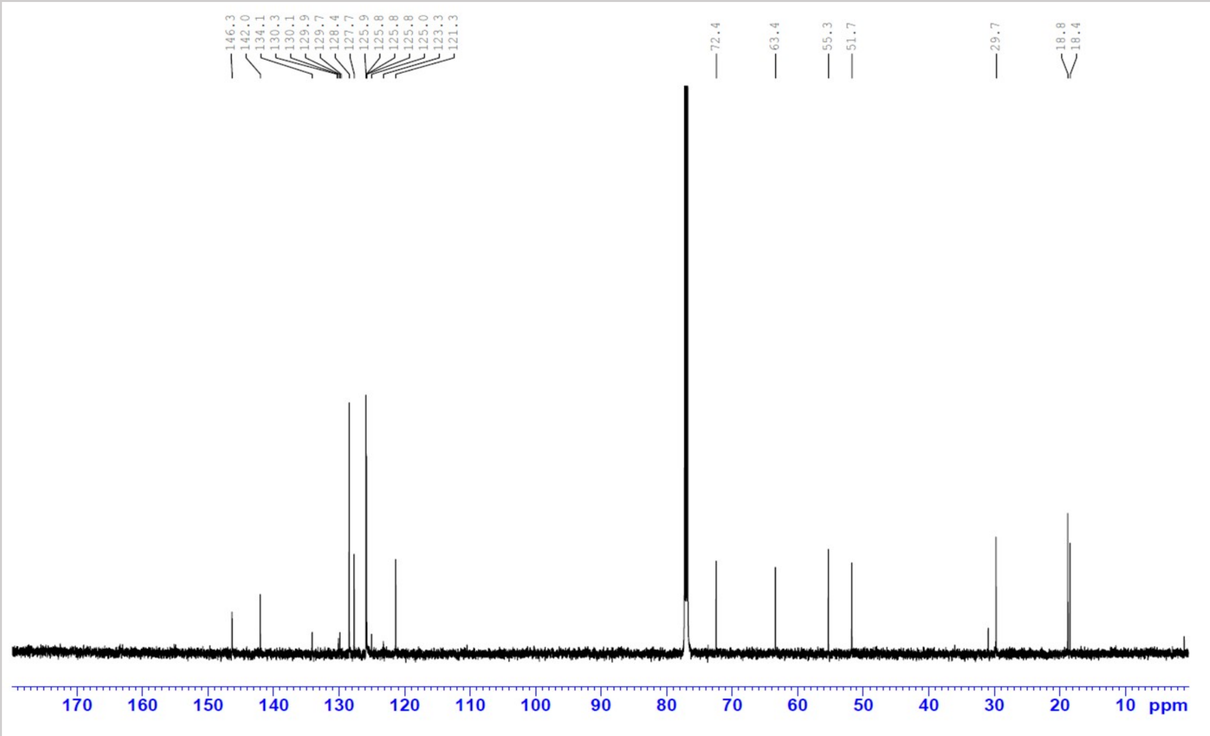


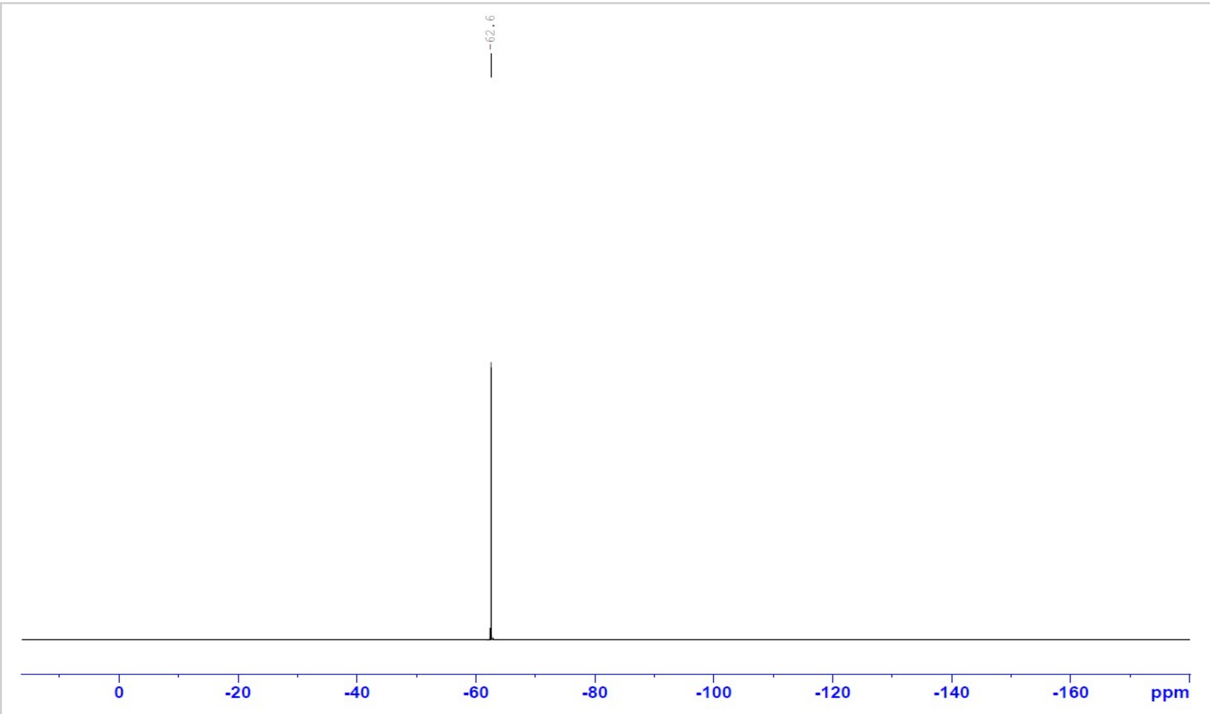


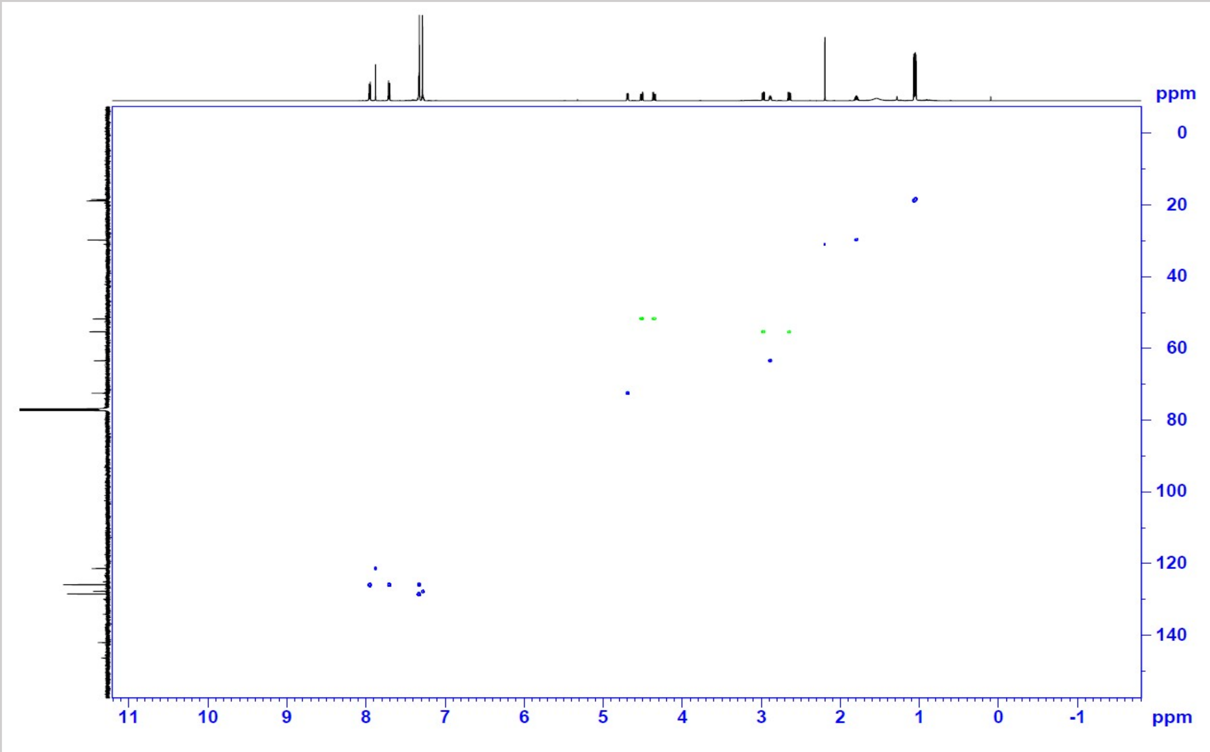


^{1}H NMR (600 MHz, $CDCl_3$), $^{13}C\{1H\}$ NMR (151 MHz, $CDCl_3$), ^{19}F NMR (565 MHz, $CDCl_3$) and HSQC ($CDCl_3$) spectra for compound **8**.

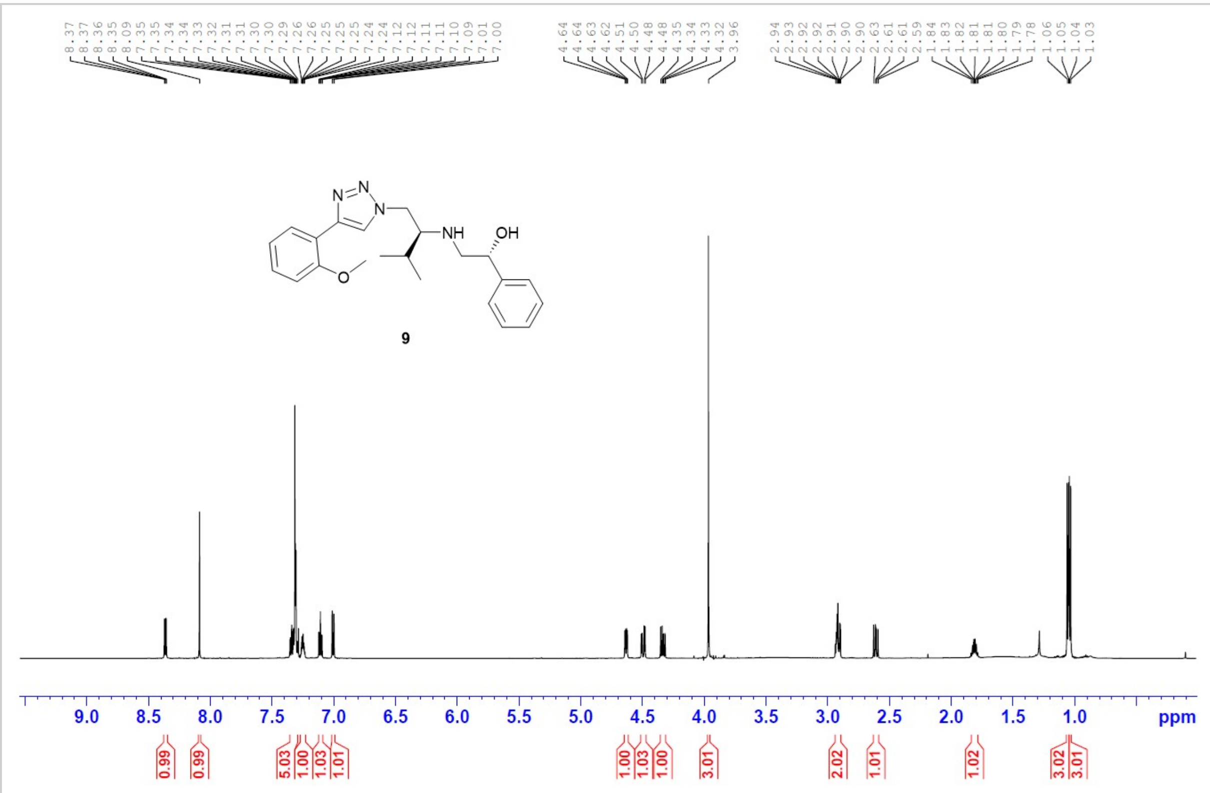


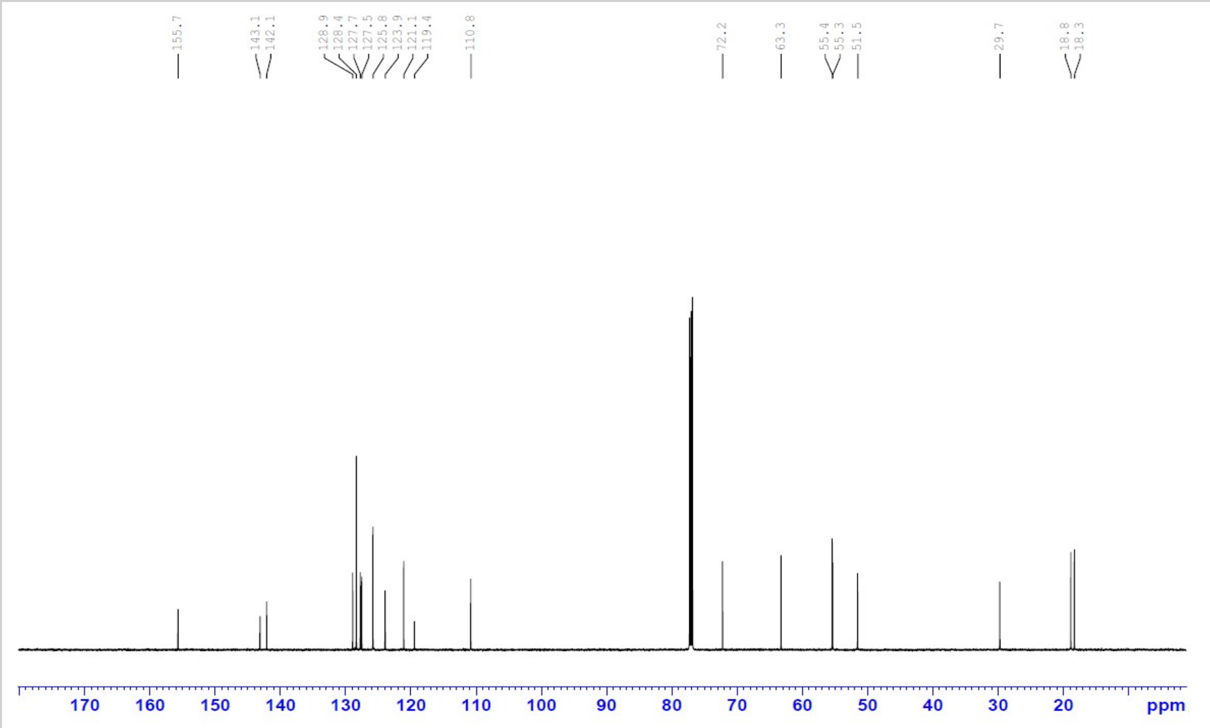

146.3
142.0
134.1
130.3
130.1
129.9
129.7
128.4
127.7
125.9
125.8
125.8
125.8
125.0
123.3
121.3
72.4
63.4
55.3
51.7
29.7
18.8
18.4
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


-62.6
0
-20
-40
-60
-80
-100
-120
-140
-160
ppm

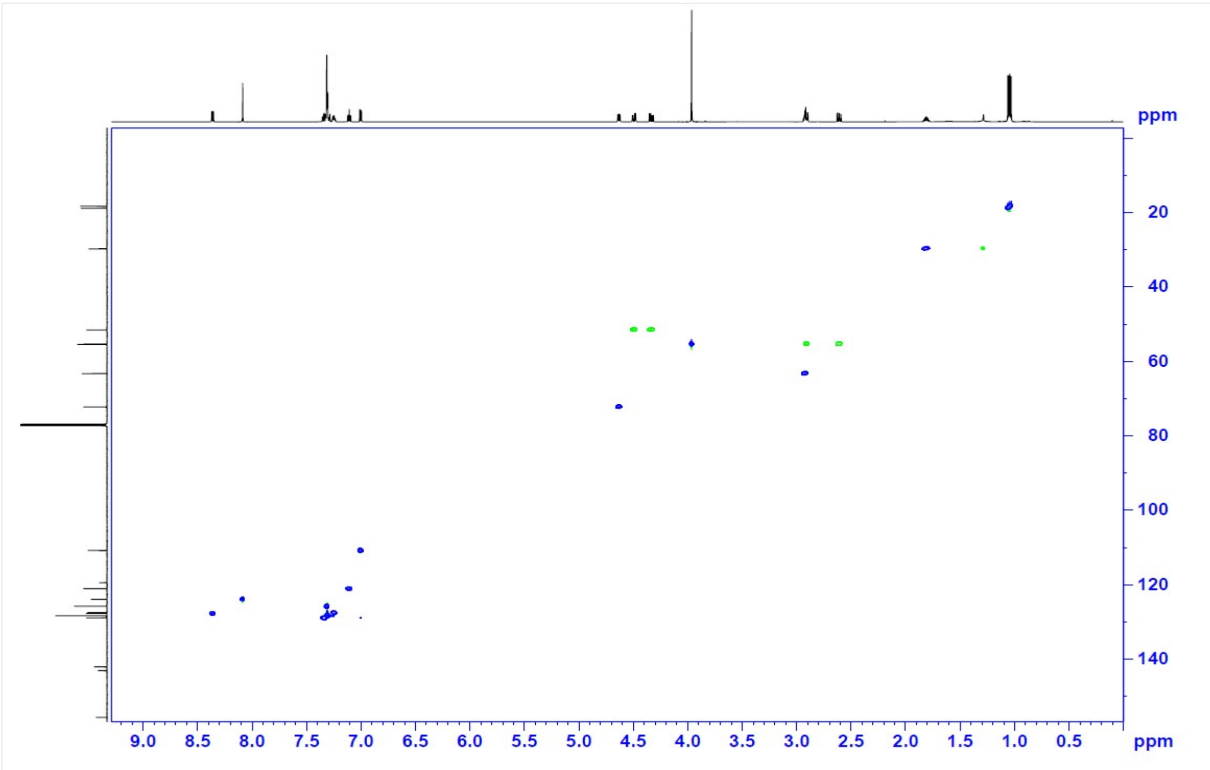


^{1}H NMR (600 MHz, $CDCl_3$), $^{13}C\{1H\}$ NMR (151 MHz, $CDCl_3$) and HSQC ($CDCl_3$) spectra for compound **9**.



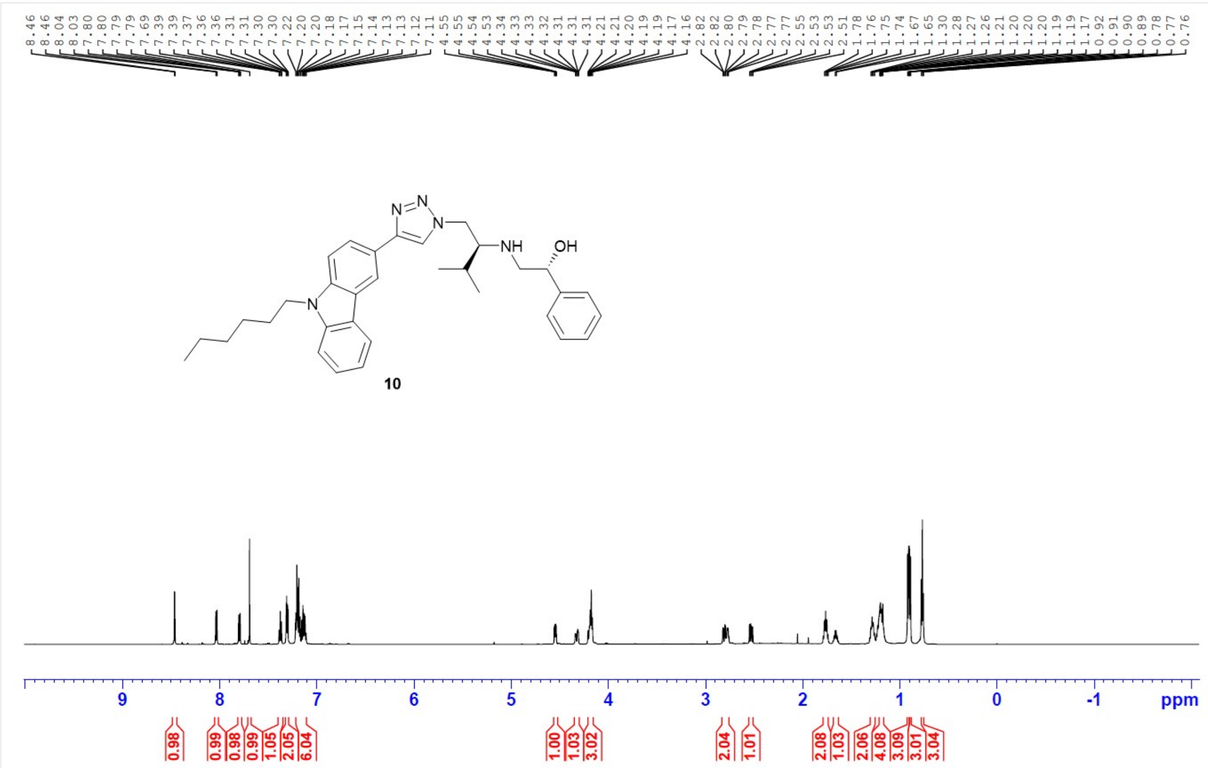


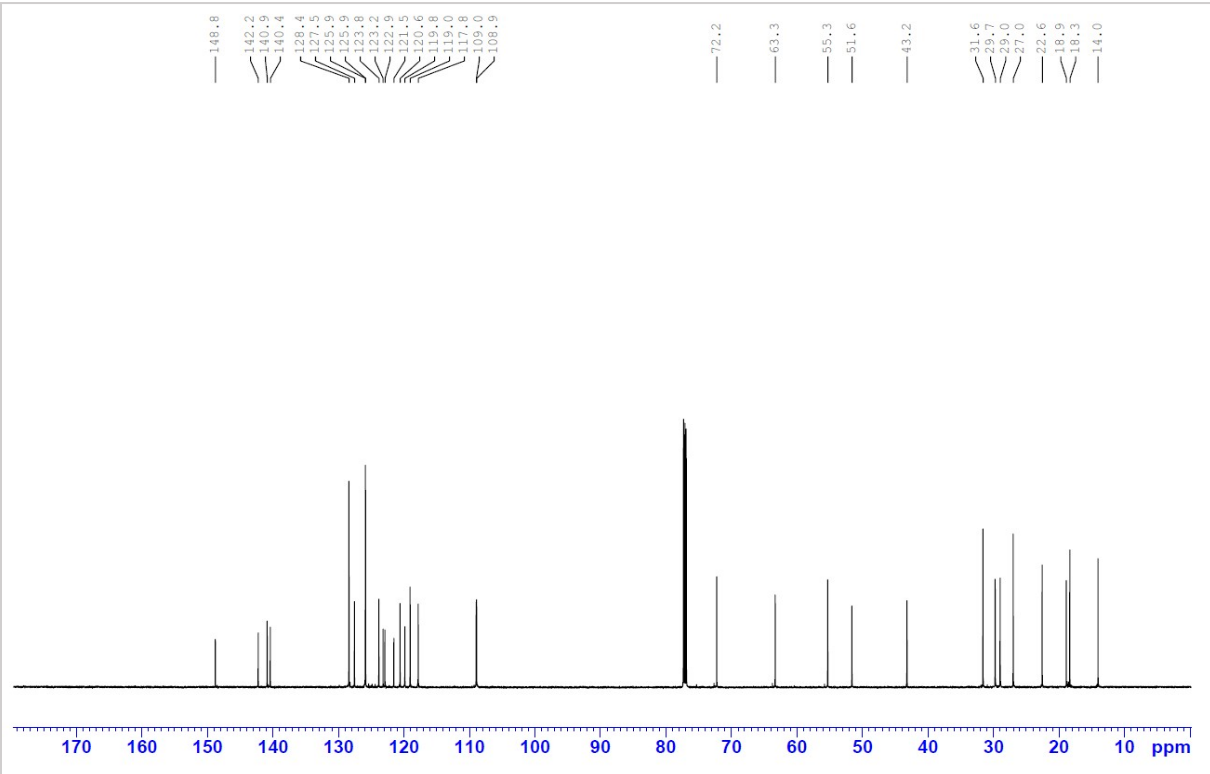
155.7
143.1
142.1
128.9
128.4
127.7
127.5
125.8
123.9
121.1
119.4
110.8
72.2
63.3
55.4
55.3
51.5
29.7
18.8
18.3
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

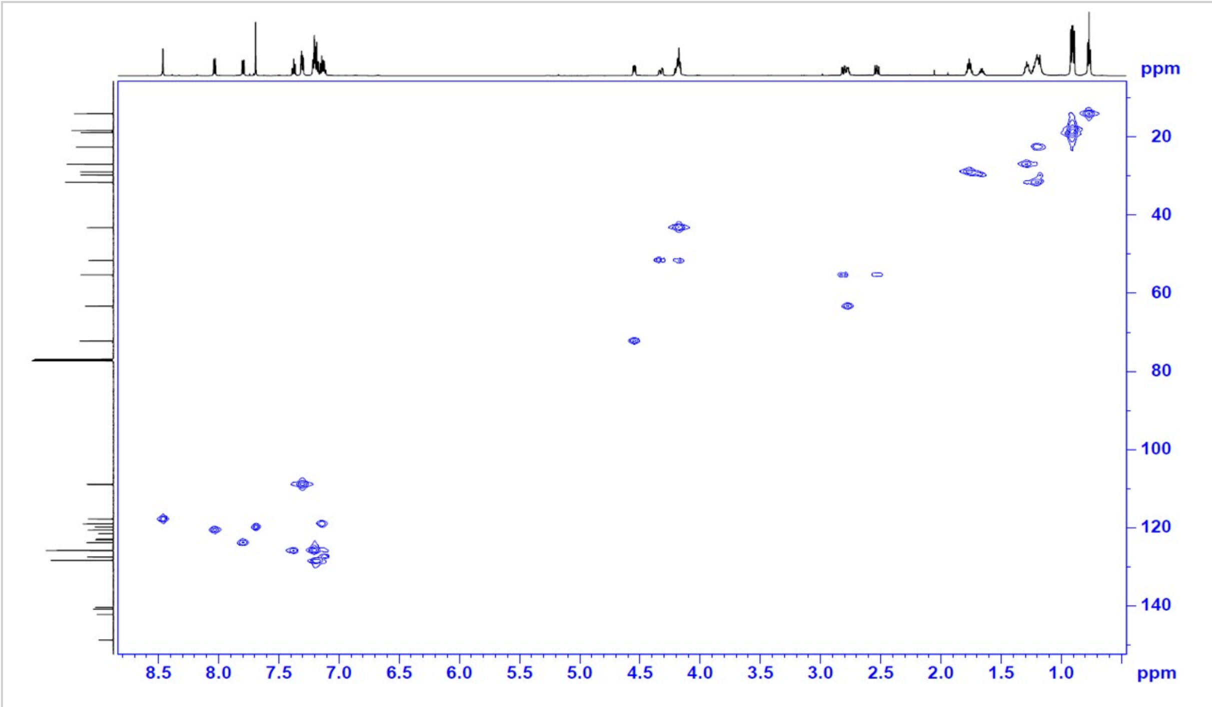


ppm
20
40
60
80
100
120
140
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

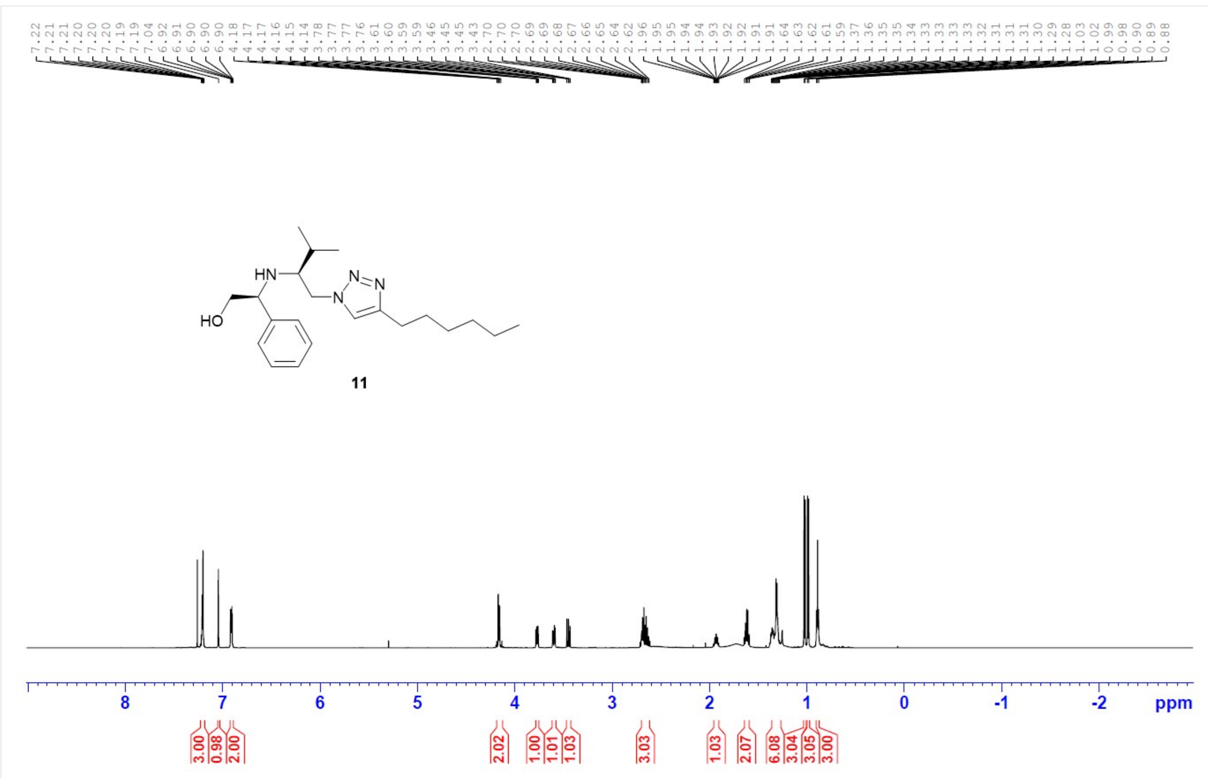
^{1}H NMR (600 MHz, $CDCl_3$), $^{13}C\{1H\}$ NMR (151 MHz, $CDCl_3$) and HMQC ($CDCl_3$) spectra for compound **10**.

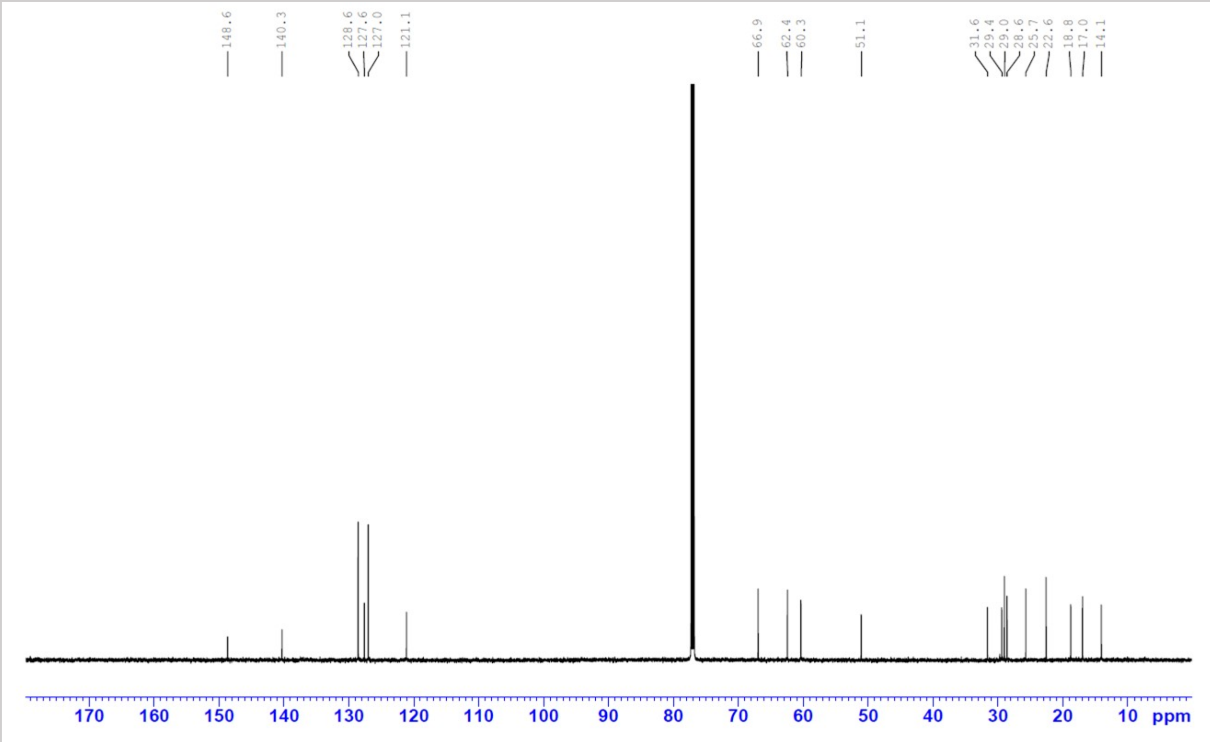


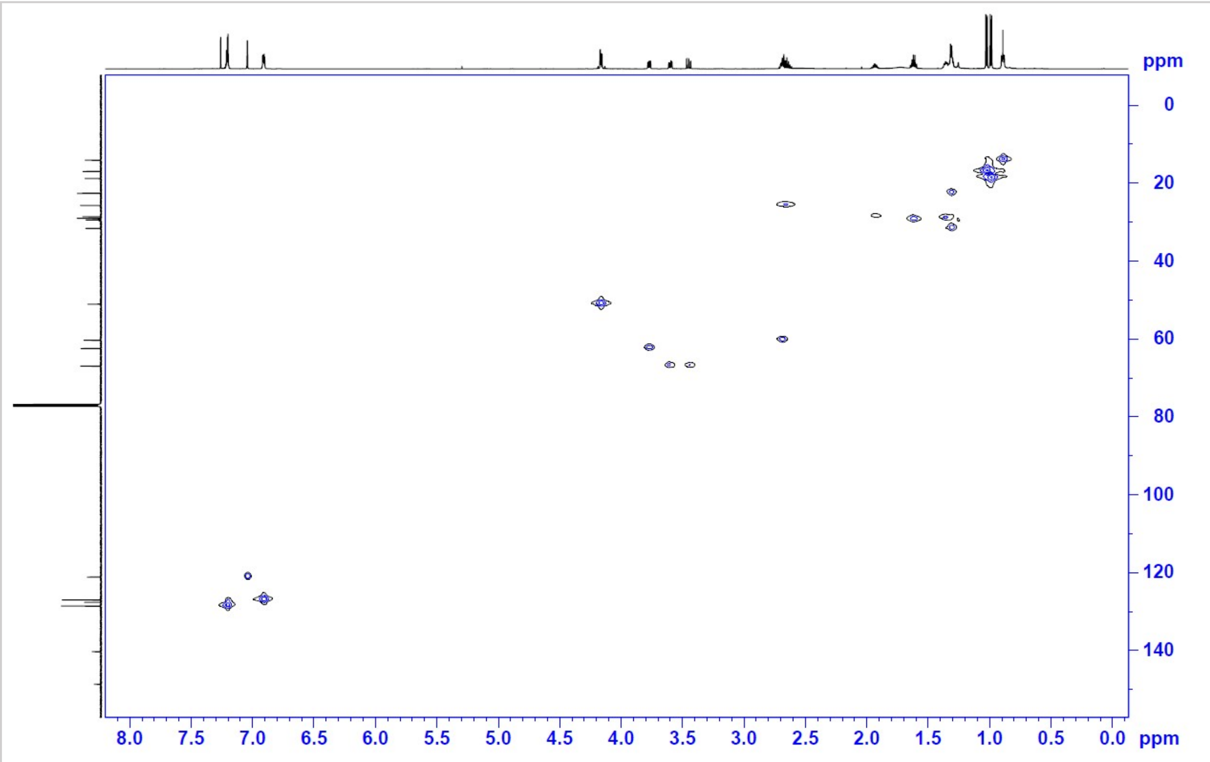




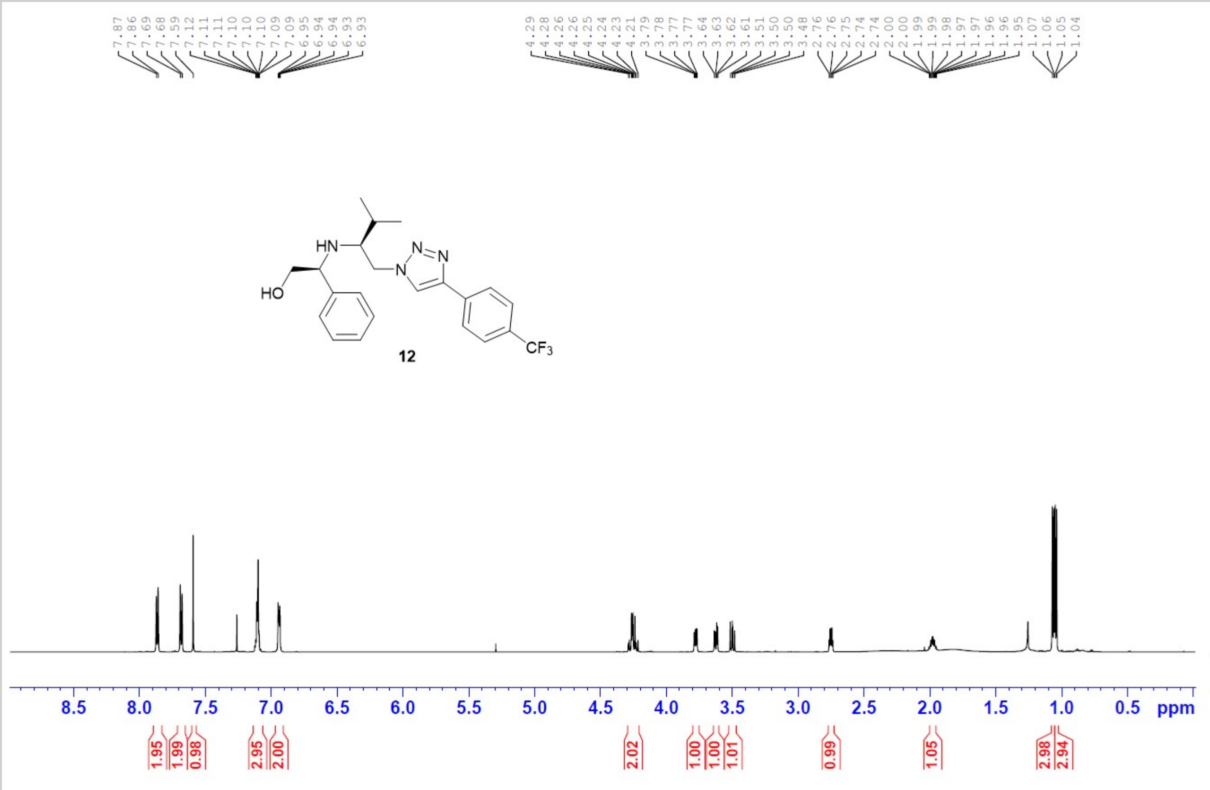
^{1}H NMR (600 MHz, $CDCl_3$), ^{13}C{1H} NMR (151 MHz, $CDCl_3$) and HMQC ($CDCl_3$) spectra for compound **11**.

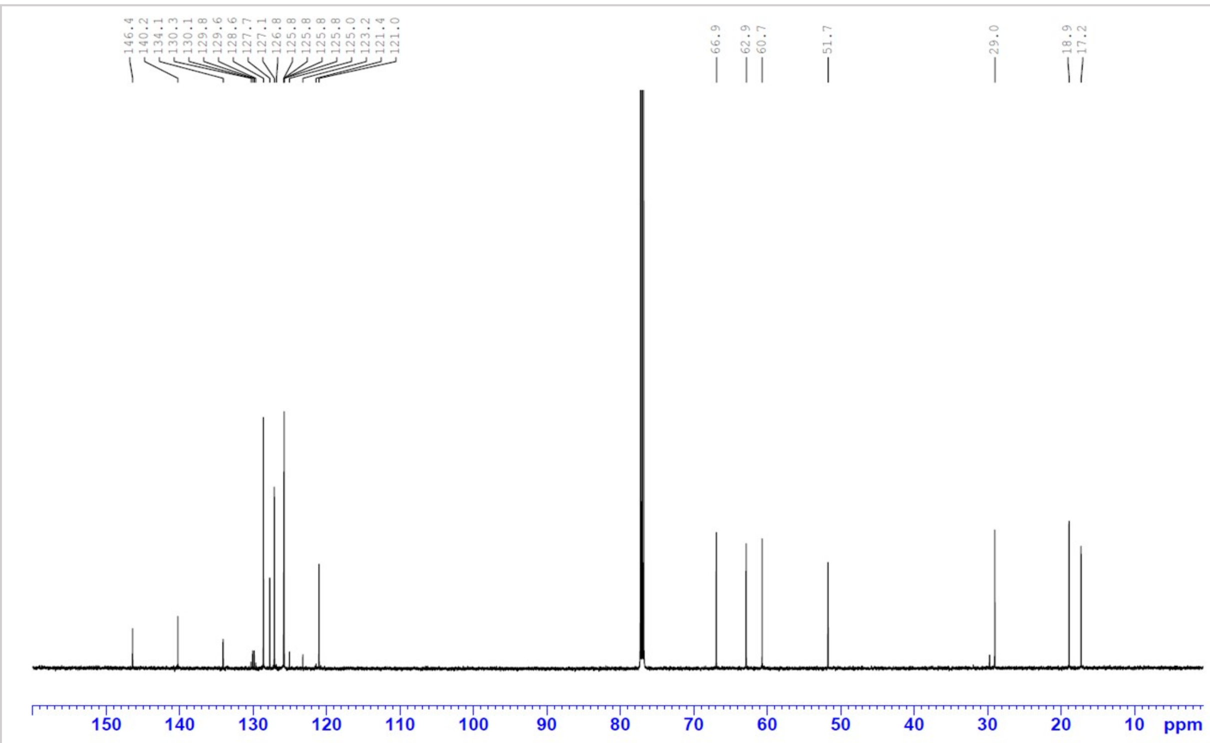


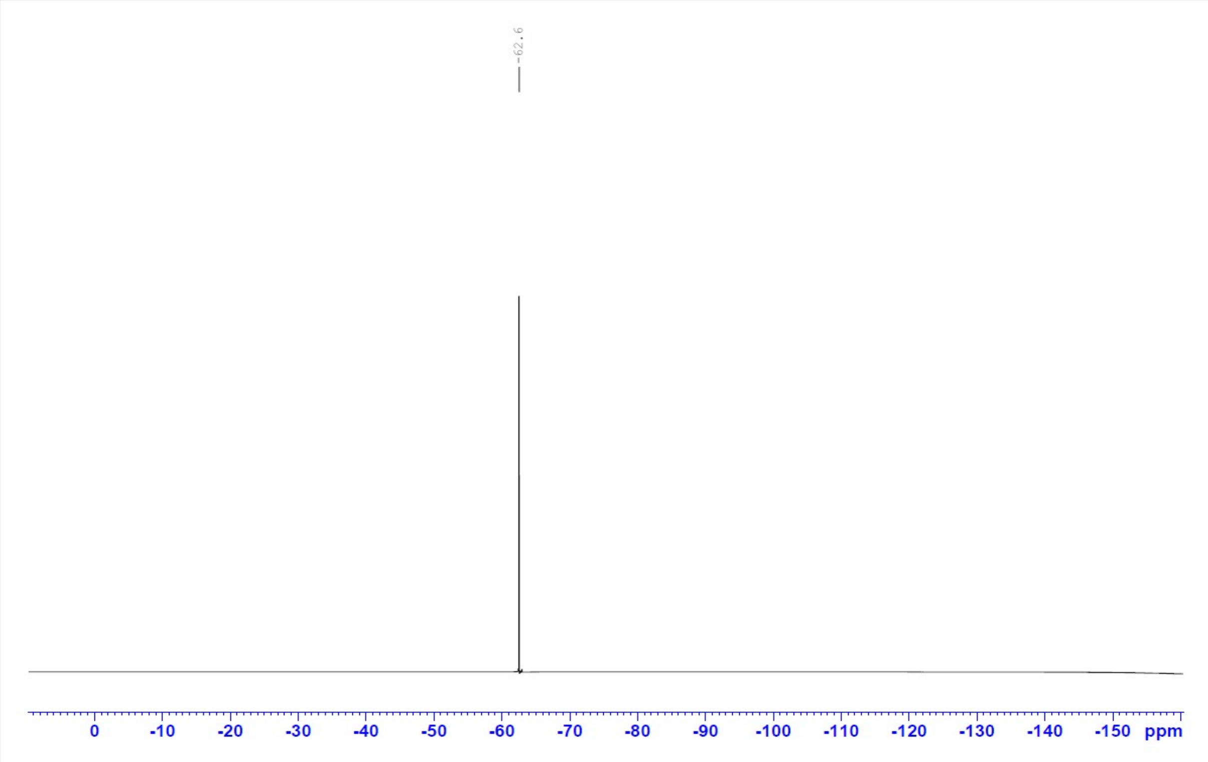

148.6
140.3
128.6
127.6
127.0
121.1
66.9
62.4
60.3
51.1
31.6
29.4
29.0
28.6
25.7
22.6
18.8
17.0
14.1
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


ppm
0
20
40
60
80
100
120
140
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm

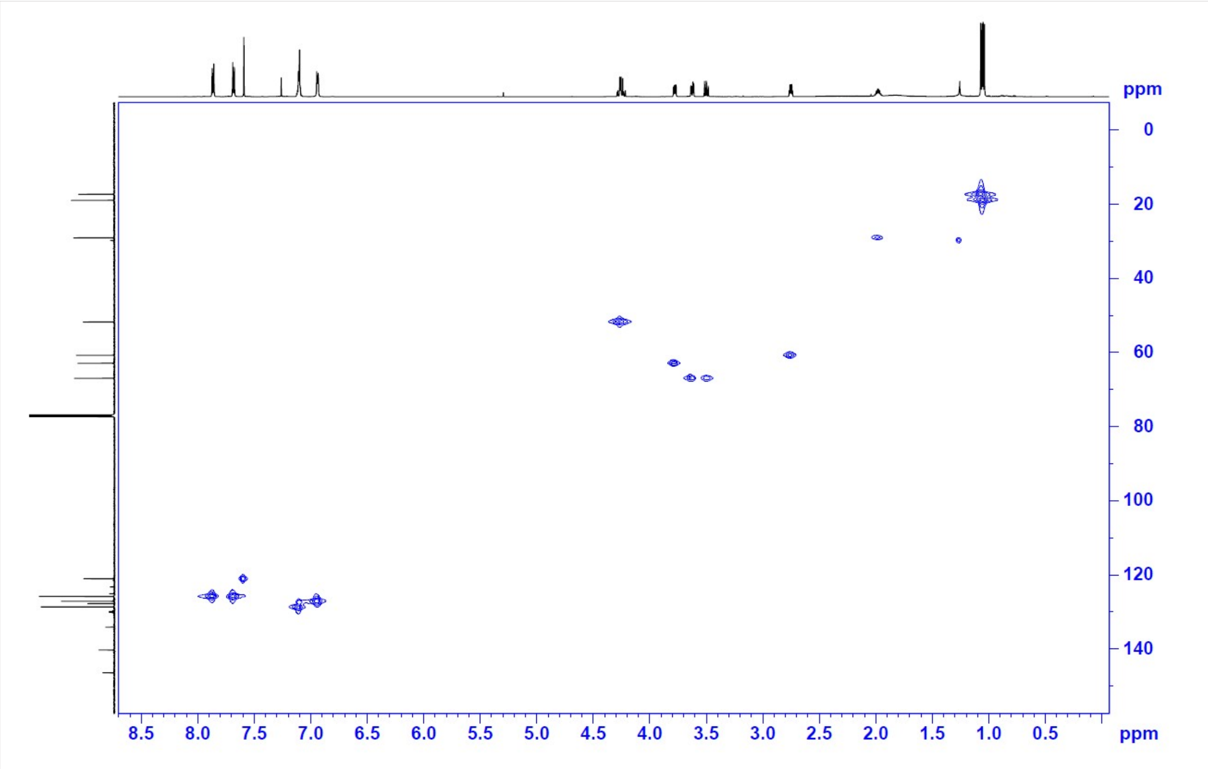
^{1}H NMR (600 MHz, $CDCl_3$), $^{13}C\{1H\}$ NMR (151 MHz, $CDCl_3$), ^{19}F NMR (565 MHz, $CDCl_3$) and HMQC ($CDCl_3$) spectra for compound **12**.





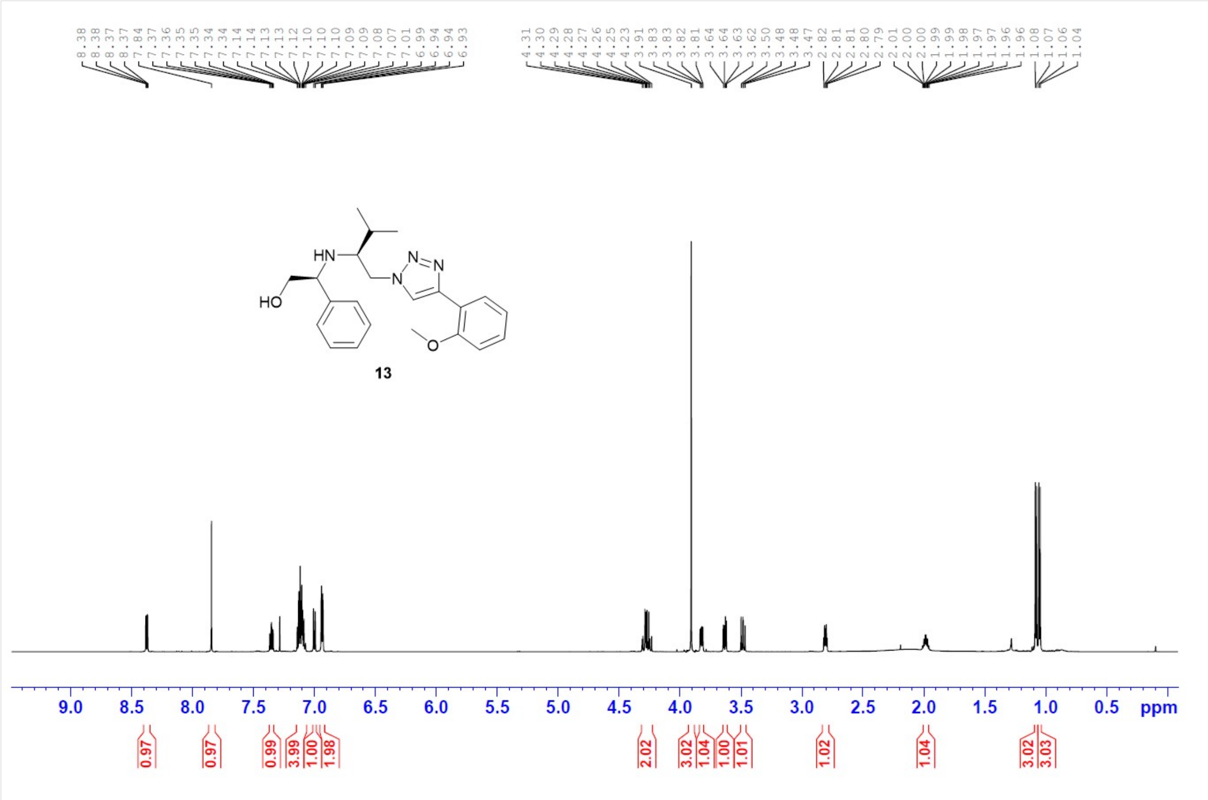


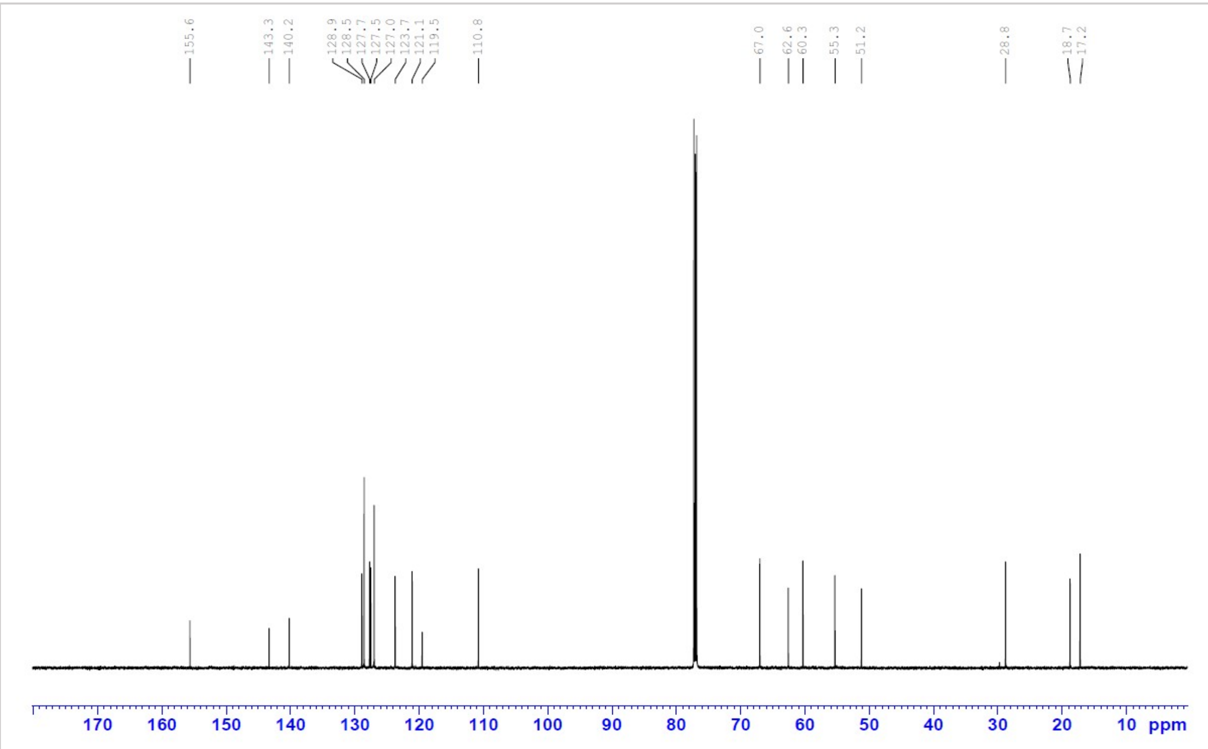
-62.6
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
ppm

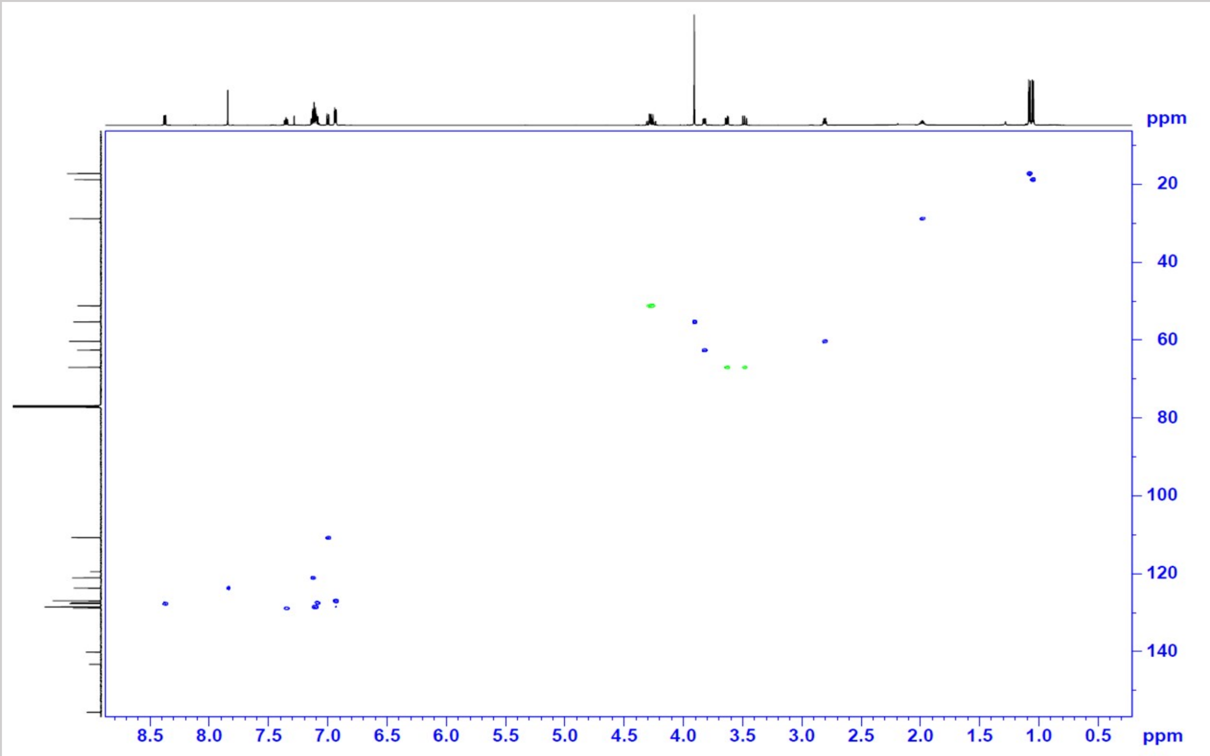


ppm
0
20
40
60
80
100
120
140
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm

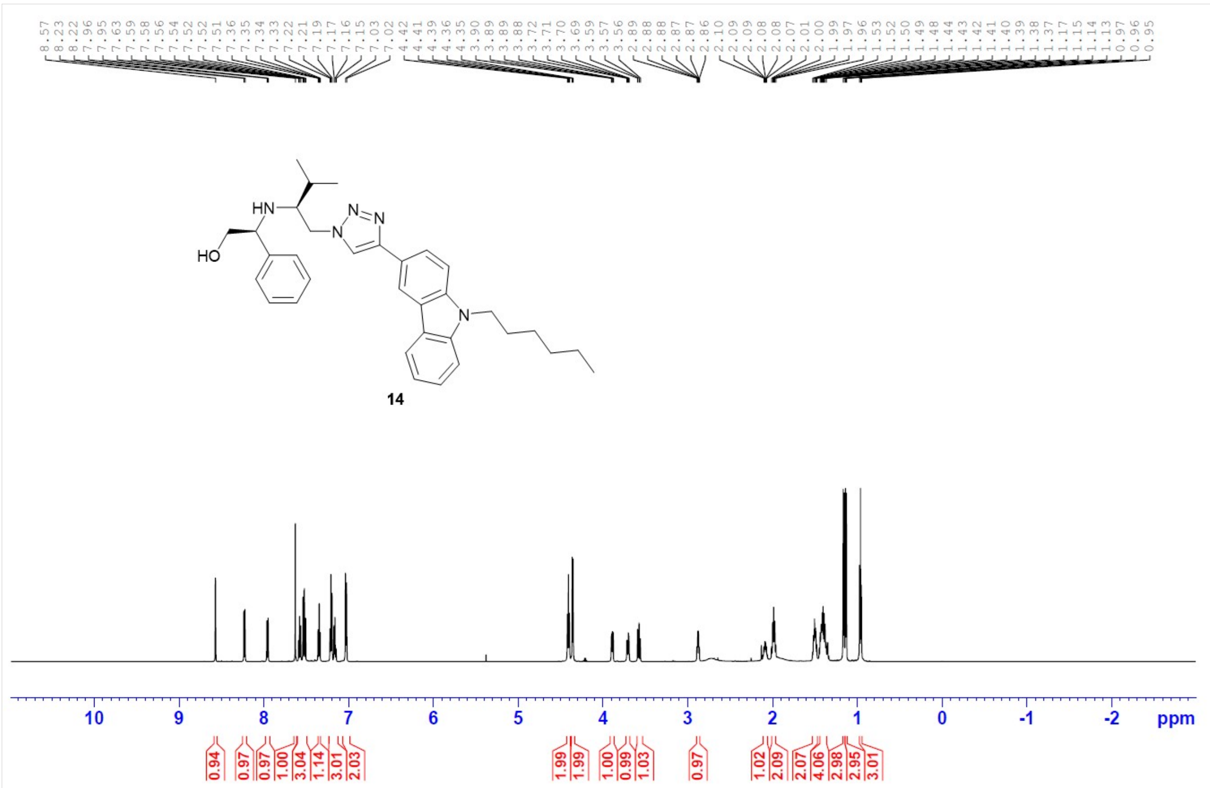
^{1}H NMR (600 MHz, $CDCl_3$), $^{13}C\{1H\}$ NMR (151 MHz, $CDCl_3$) and HSQC ($CDCl_3$) spectra for compound **13**.

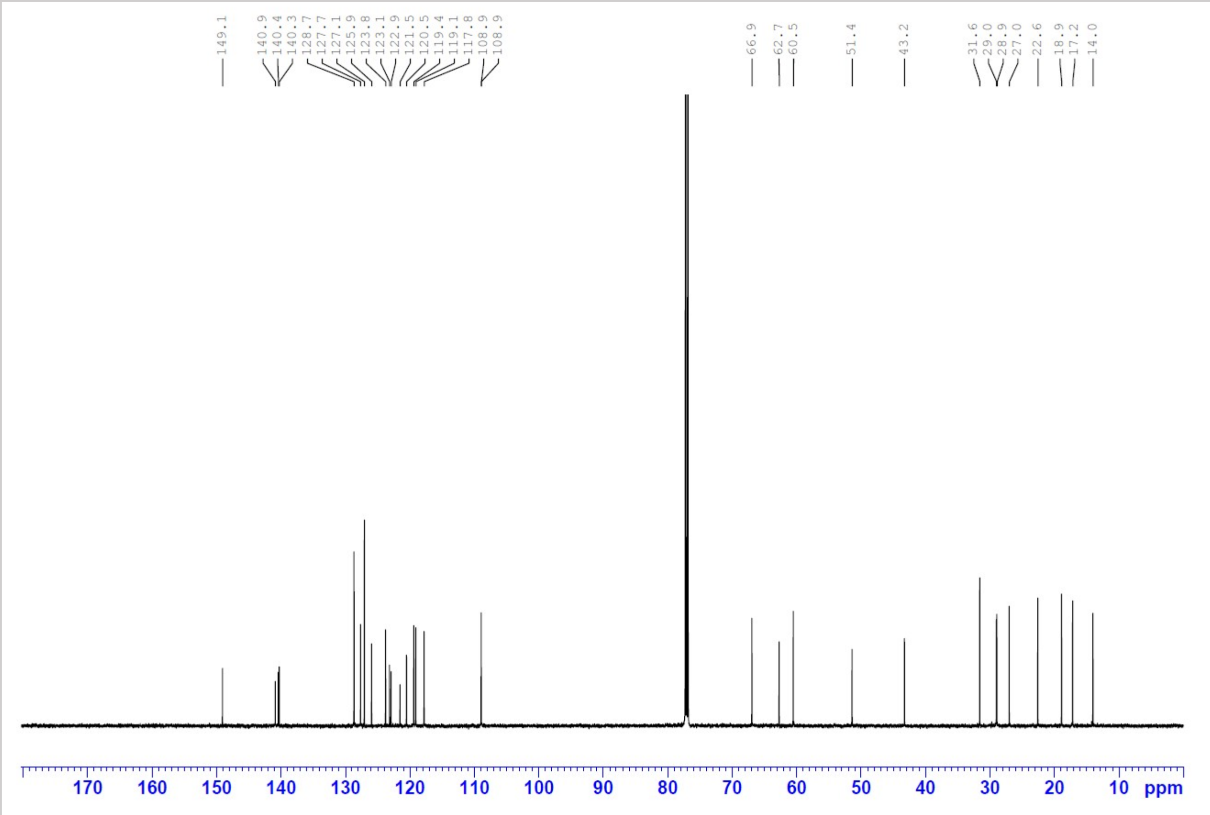


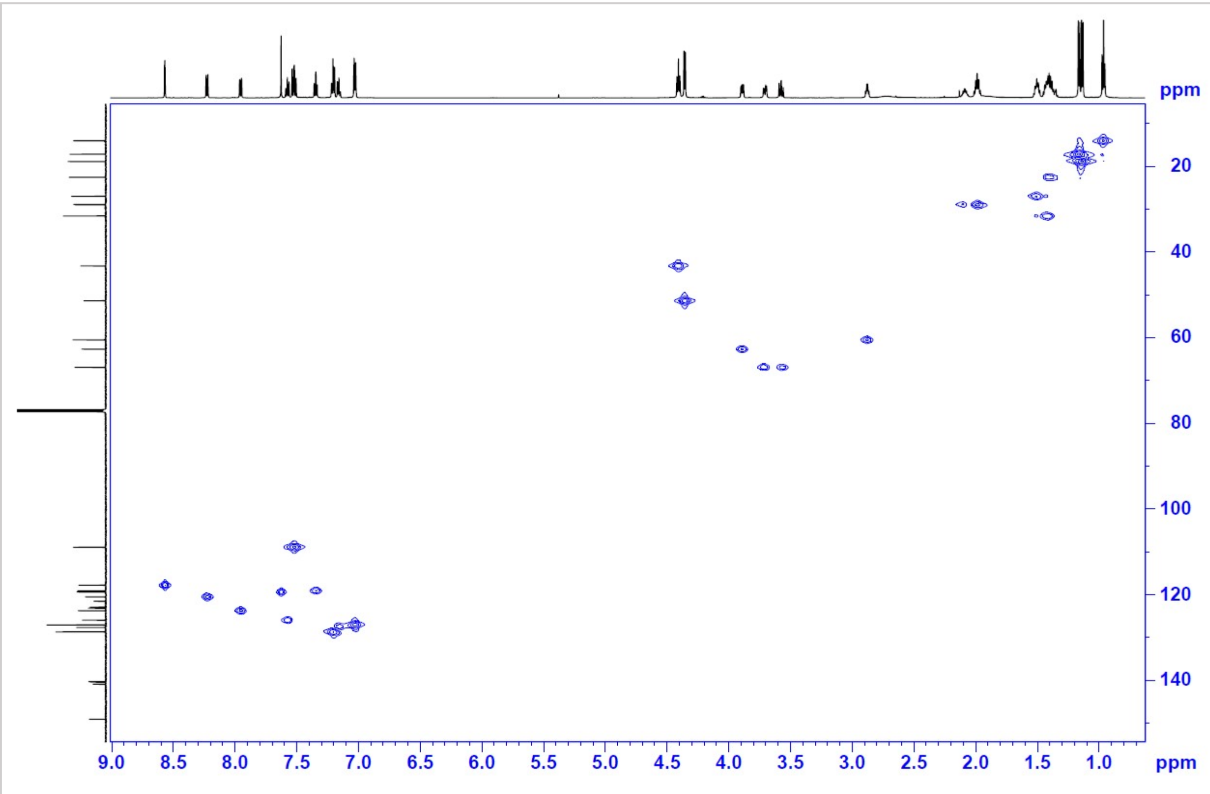




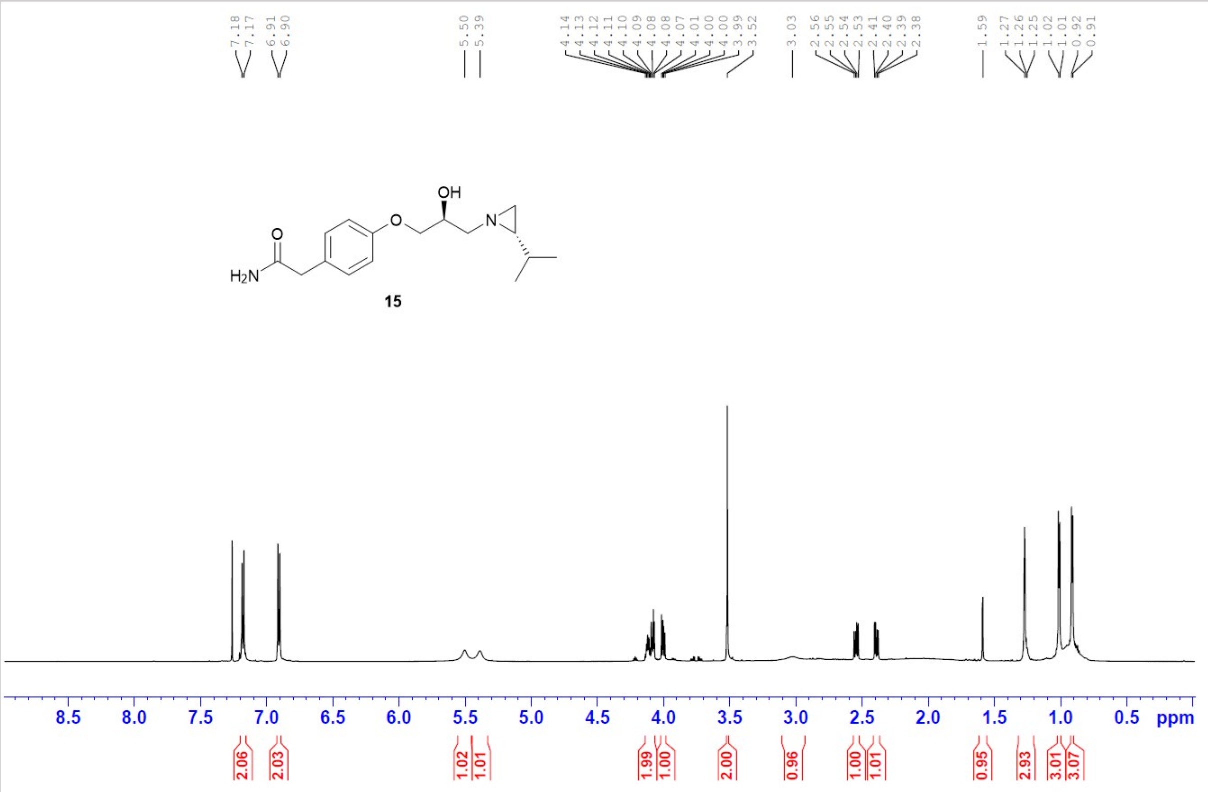
^{1}H NMR (600 MHz, $CDCl_3$), $^{13}C\{1H\}$ NMR (151 MHz, $CDCl_3$) and HMQC ($CDCl_3$) spectra for compound **14**.

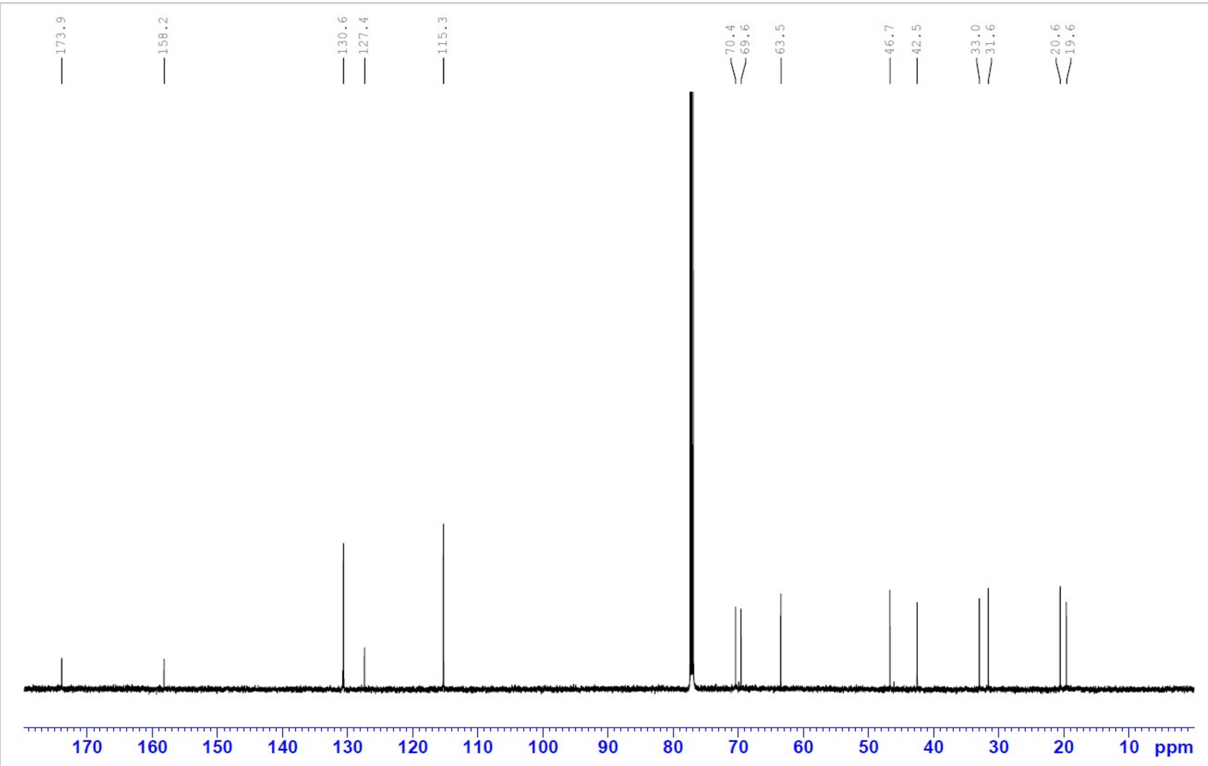


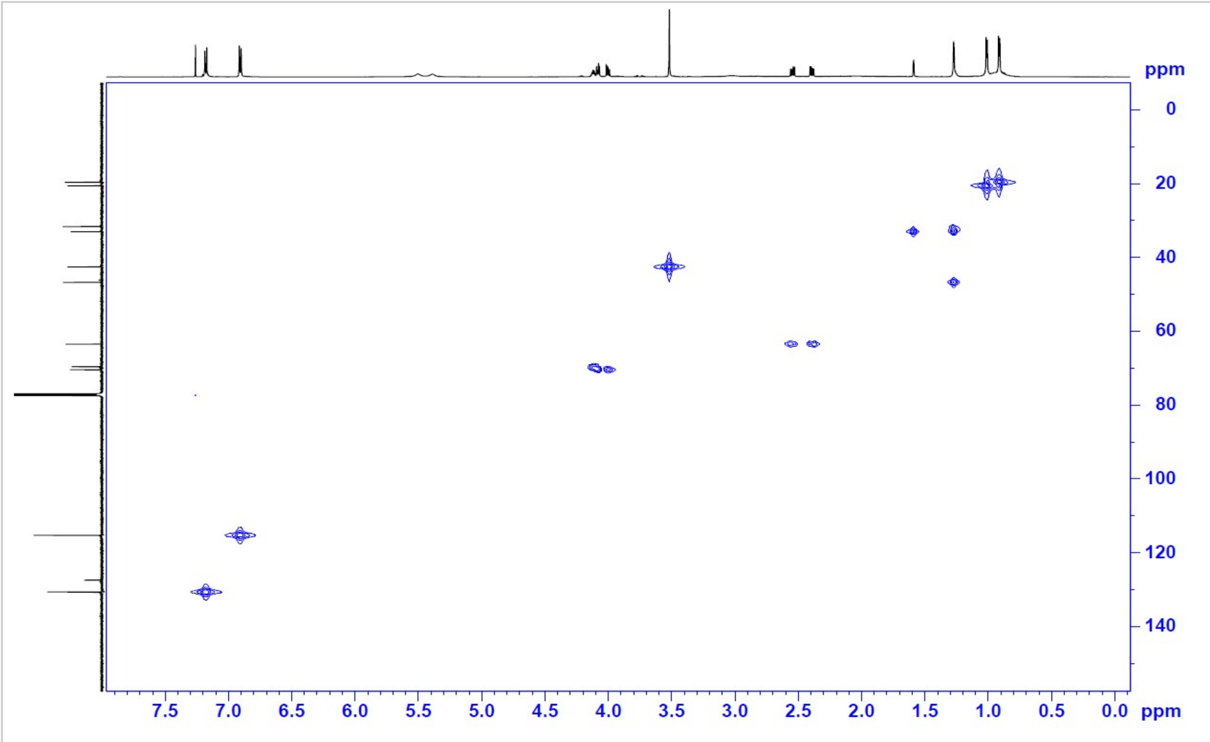

149.1
140.9
140.4
140.3
128.7
127.7
127.1
125.9
123.8
123.1
122.9
121.5
120.5
119.4
119.1
117.8
108.9
108.9
66.9
62.7
60.5
51.4
43.2
31.6
29.0
28.9
27.0
22.6
18.9
17.2
14.0
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


ppm
20
40
60
80
100
120
140
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm

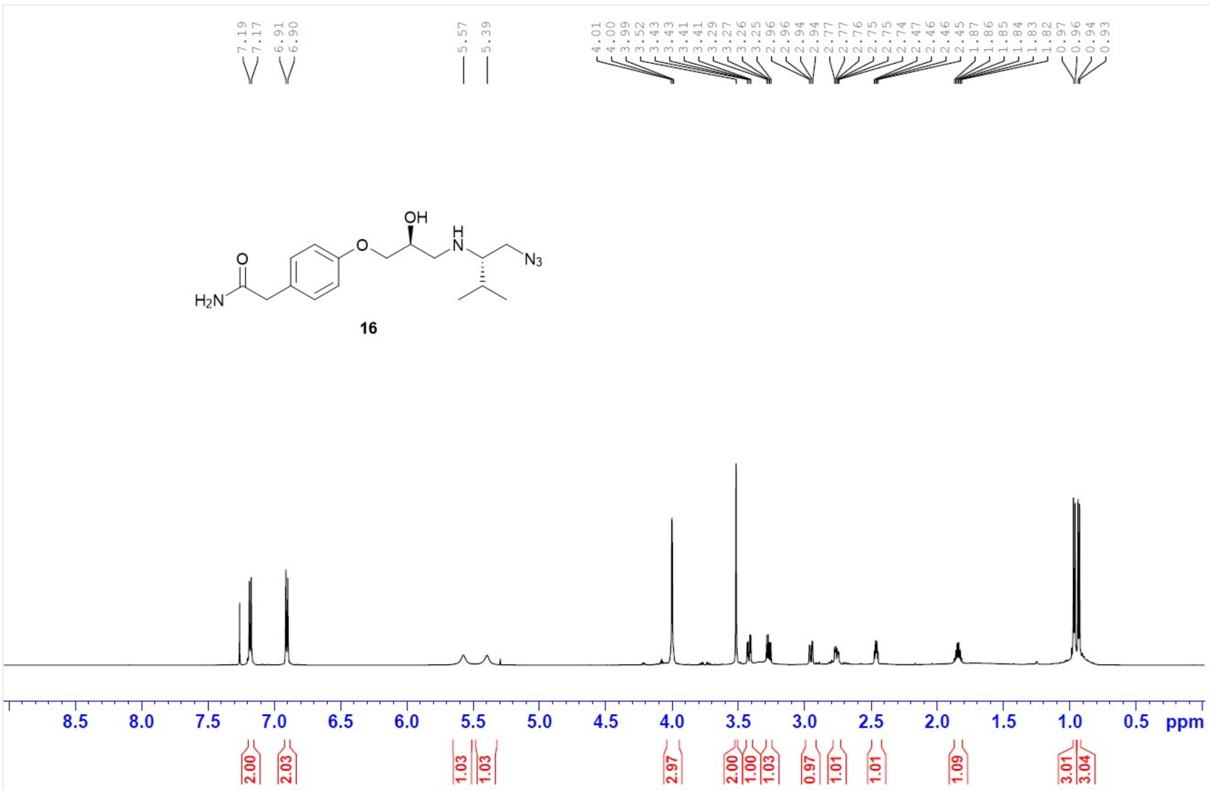
^{1}H NMR (600 MHz, $CDCl_3$), ^{13}C{1H} NMR (151 MHz, $CDCl_3$) and HMQC ($CDCl_3$) spectra for compound **15**.

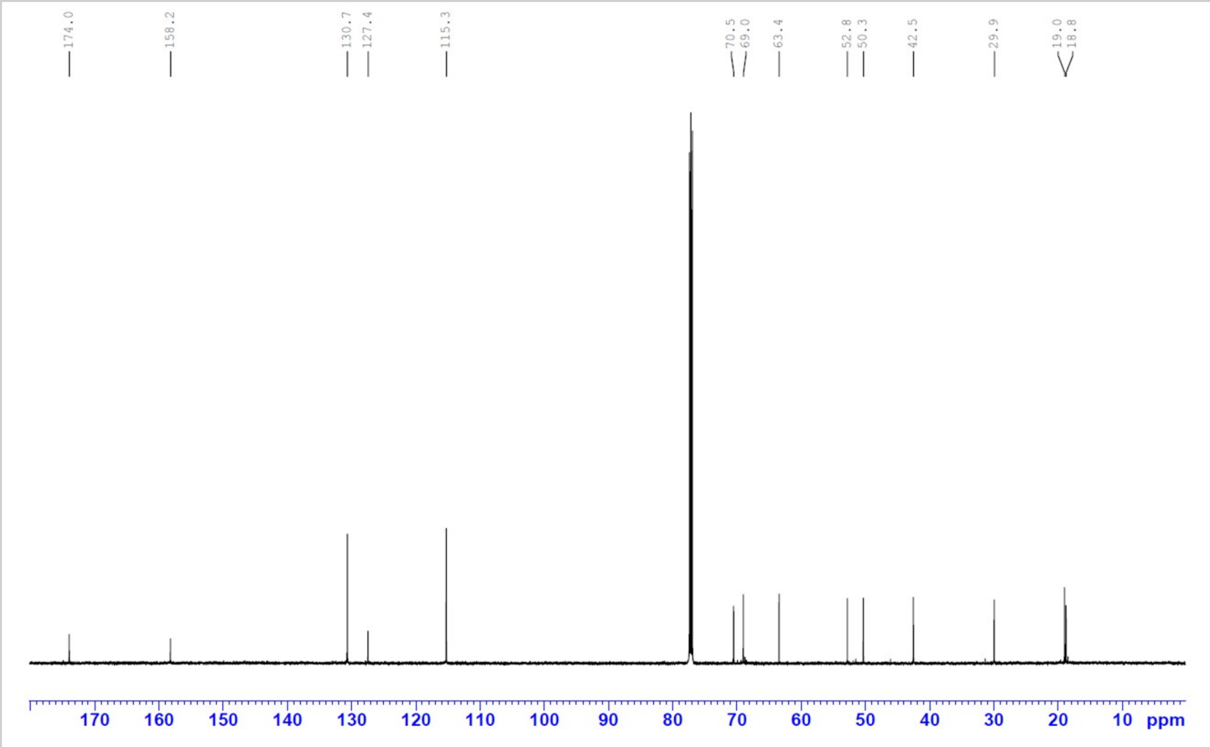


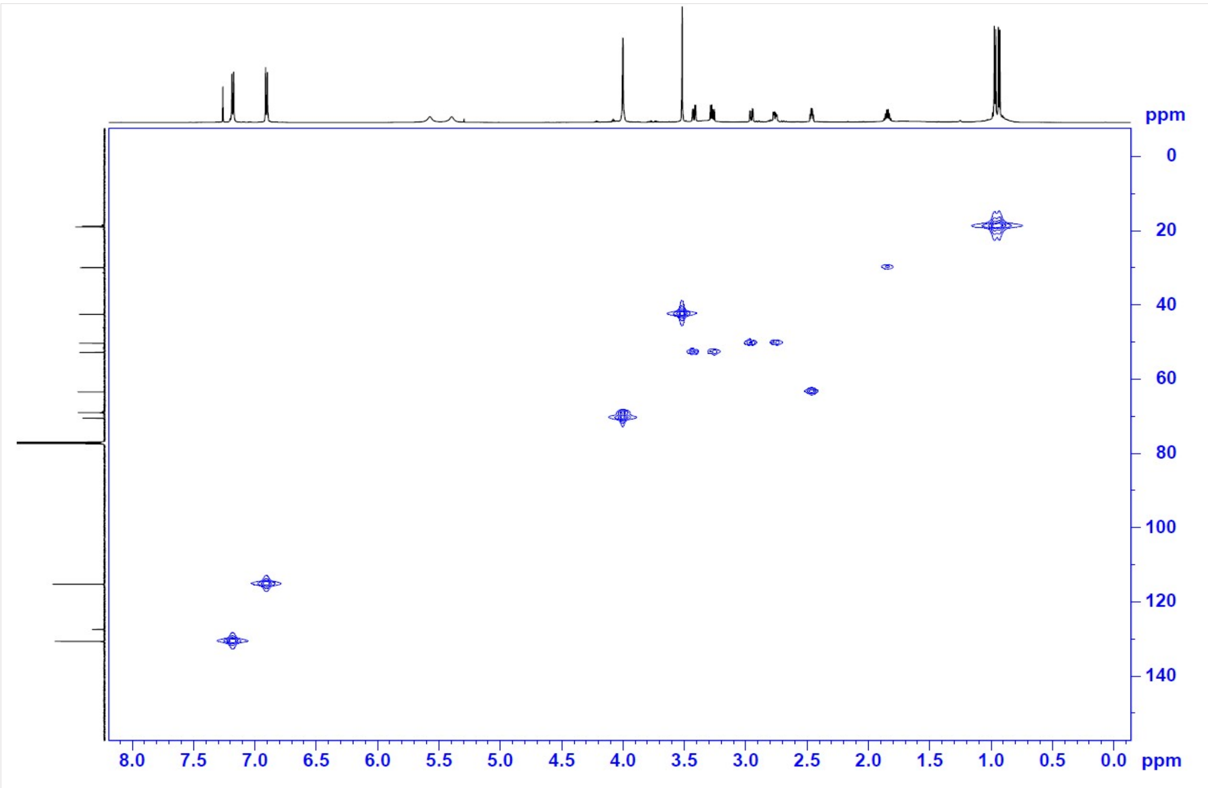




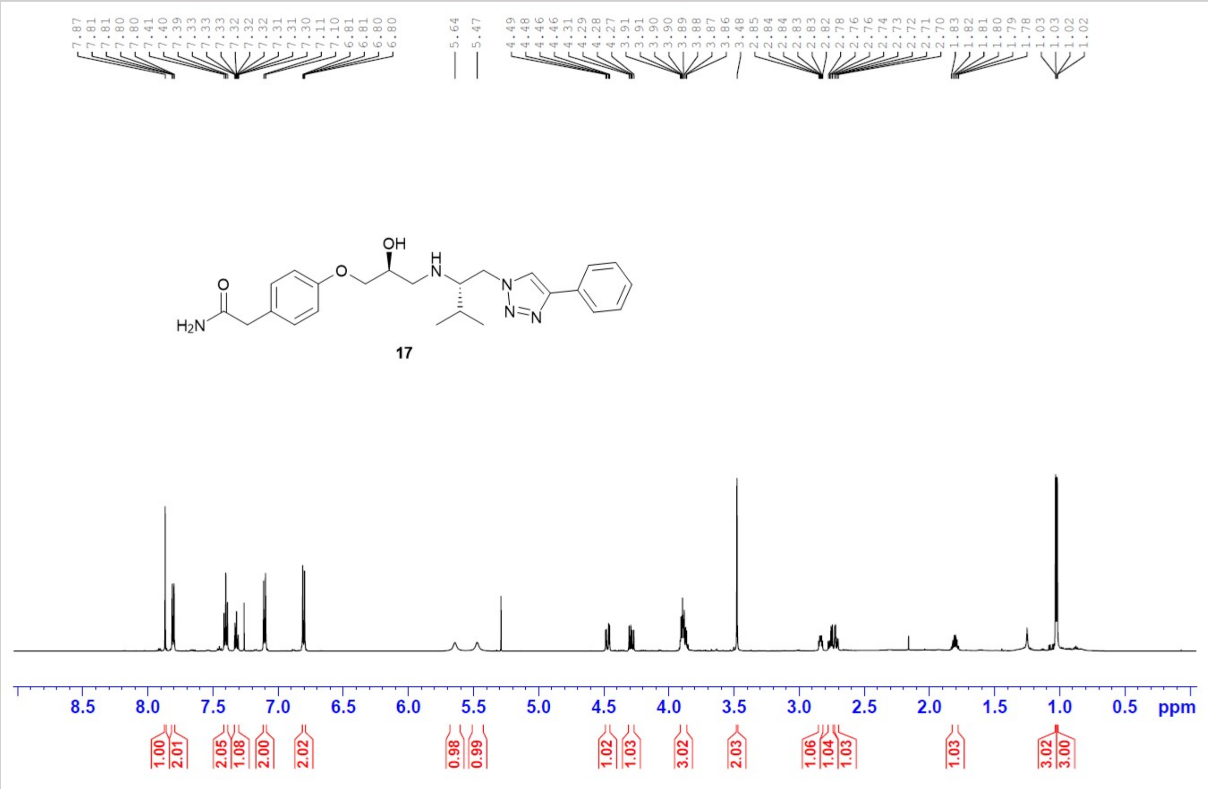
^{1}H NMR (600 MHz, $CDCl_3$), $^{13}C\{1H\}$ NMR (151 MHz, $CDCl_3$) and HMQC ($CDCl_3$) spectra for compound **16**.

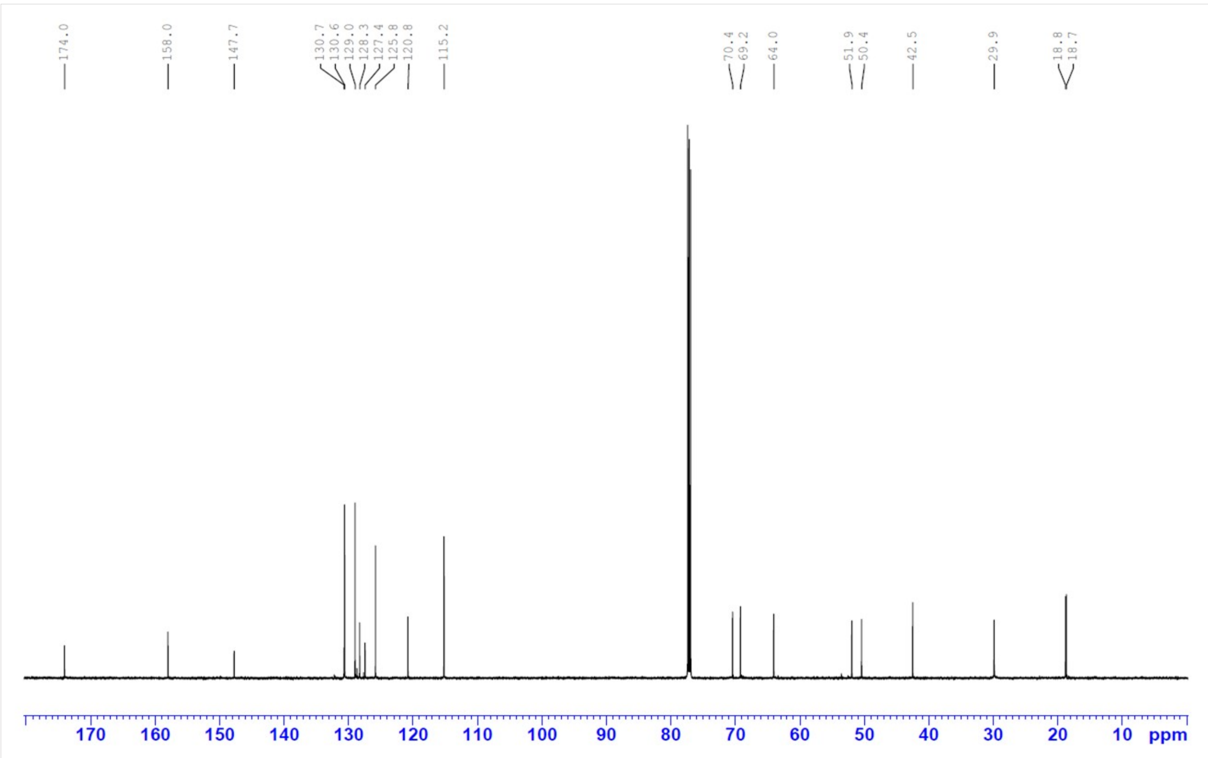


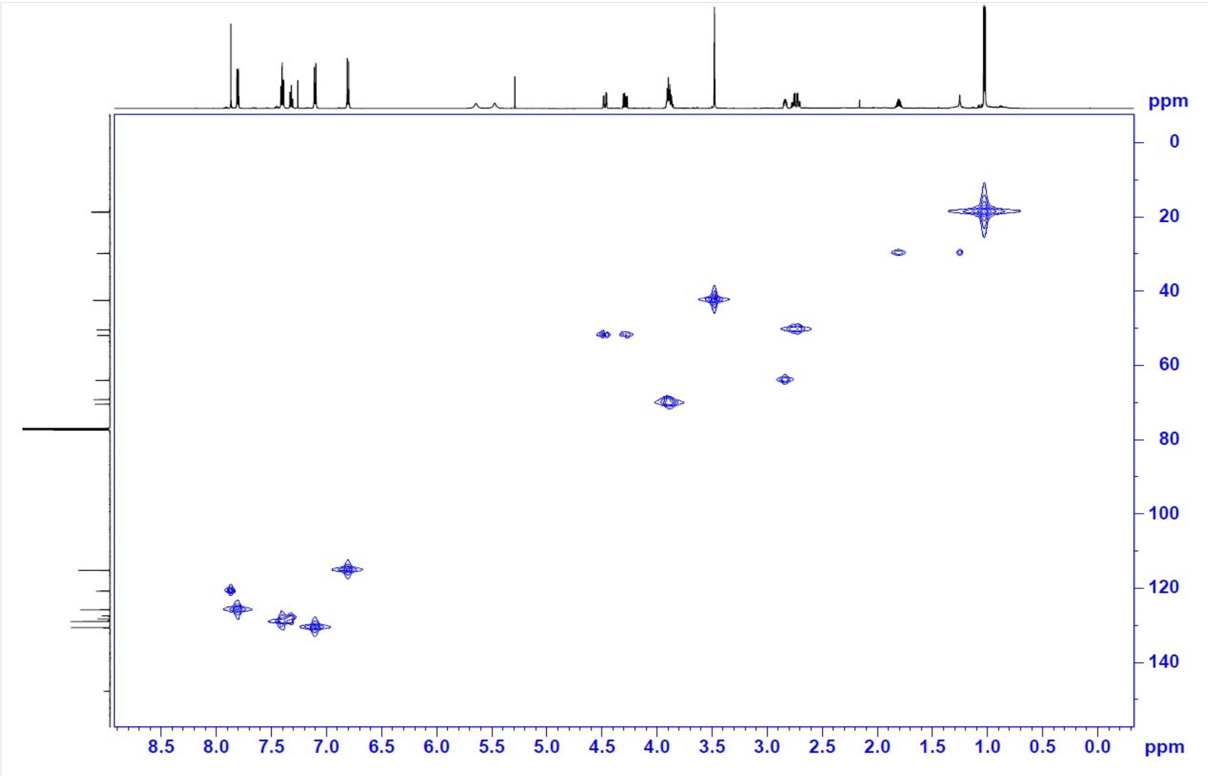

174.0
158.2
130.7
127.4
115.3
70.5
69.0
63.4
52.8
50.3
42.5
29.9
19.0
18.8
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


ppm
0
20
40
60
80
100
120
140
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm

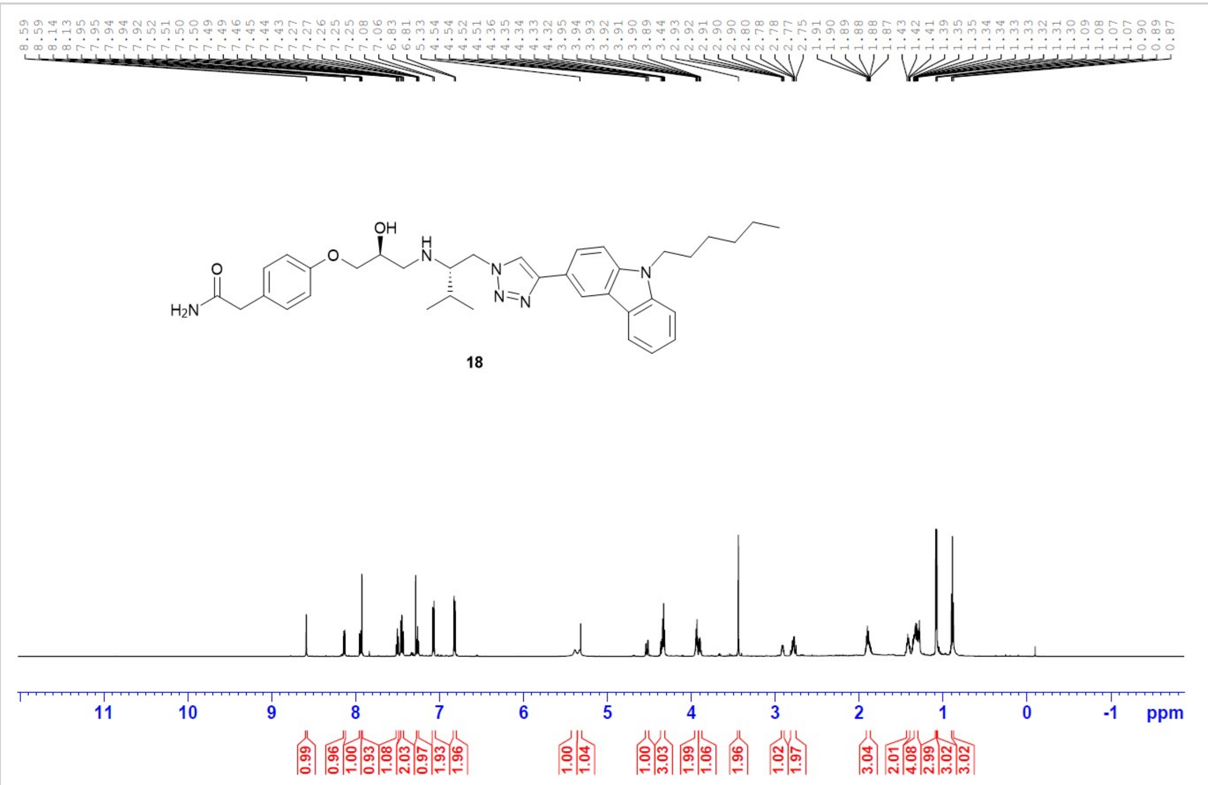
^{1}H NMR (600 MHz, $CDCl_3$), ^{13}C{1H} NMR (151 MHz, $CDCl_3$) and HMQC ($CDCl_3$) spectra for compound **17**.

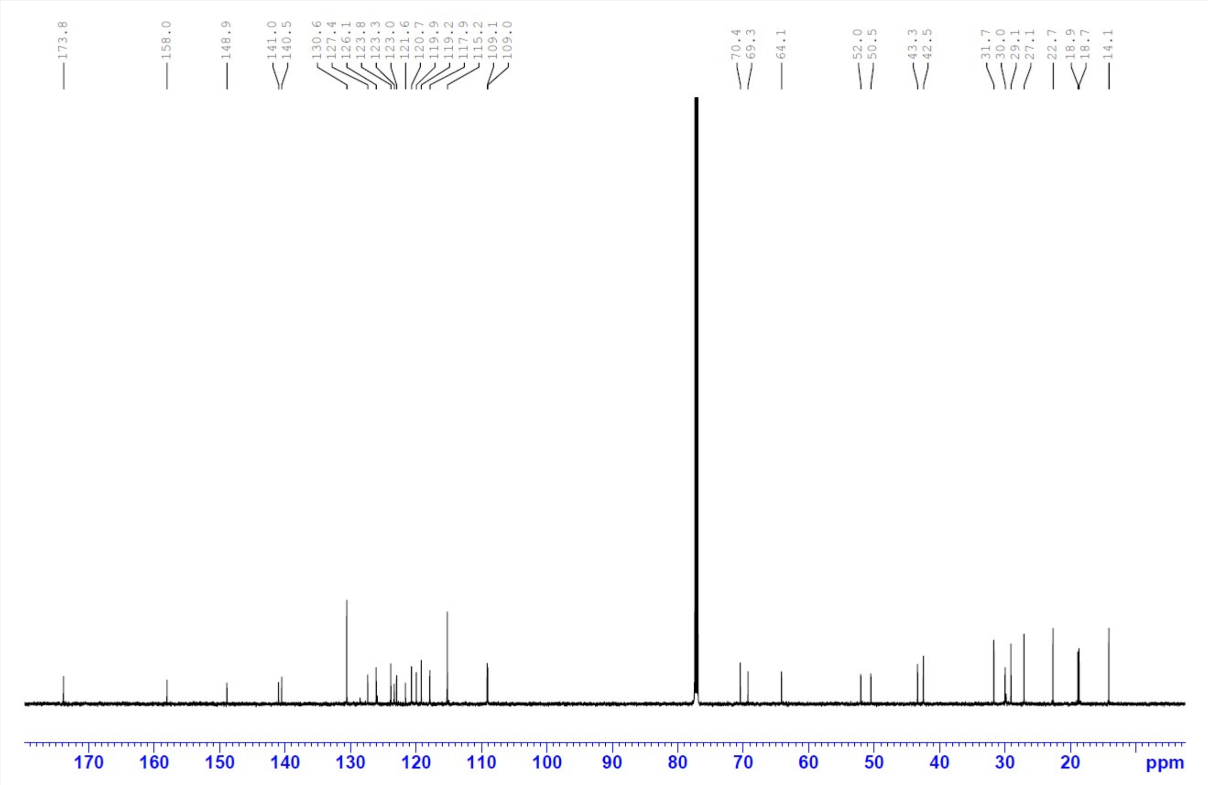


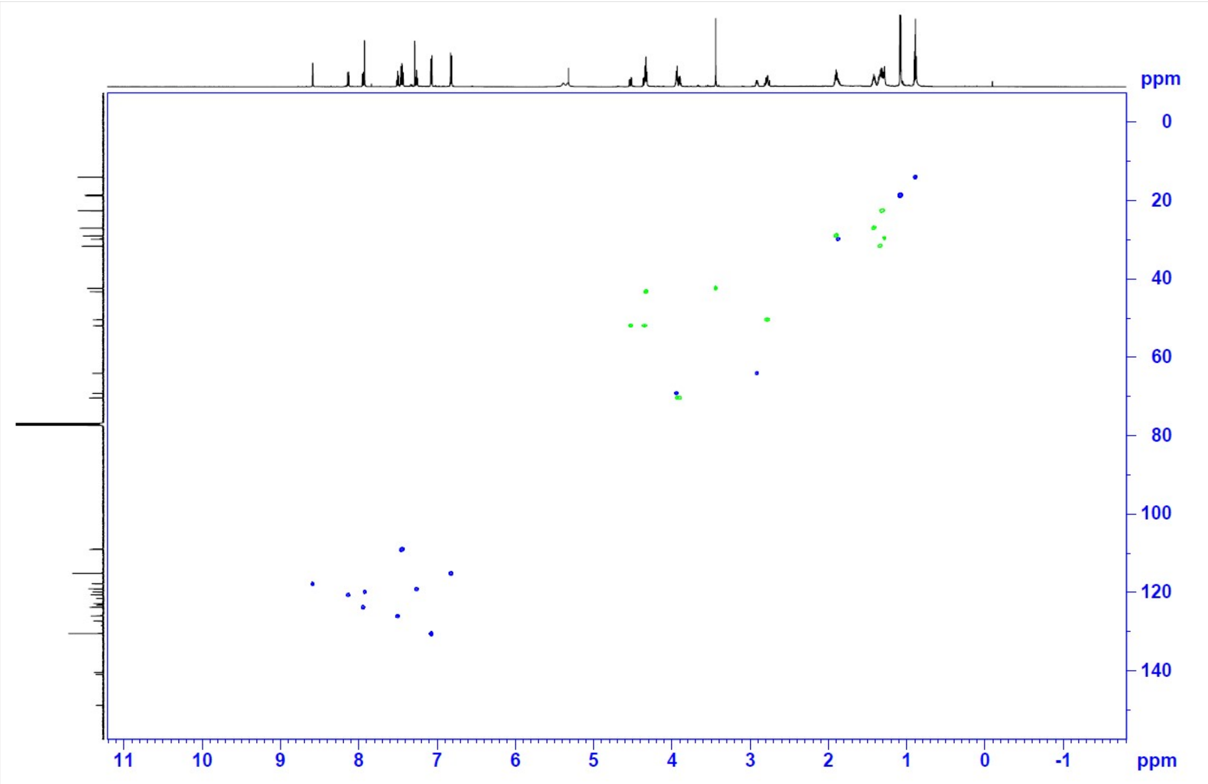




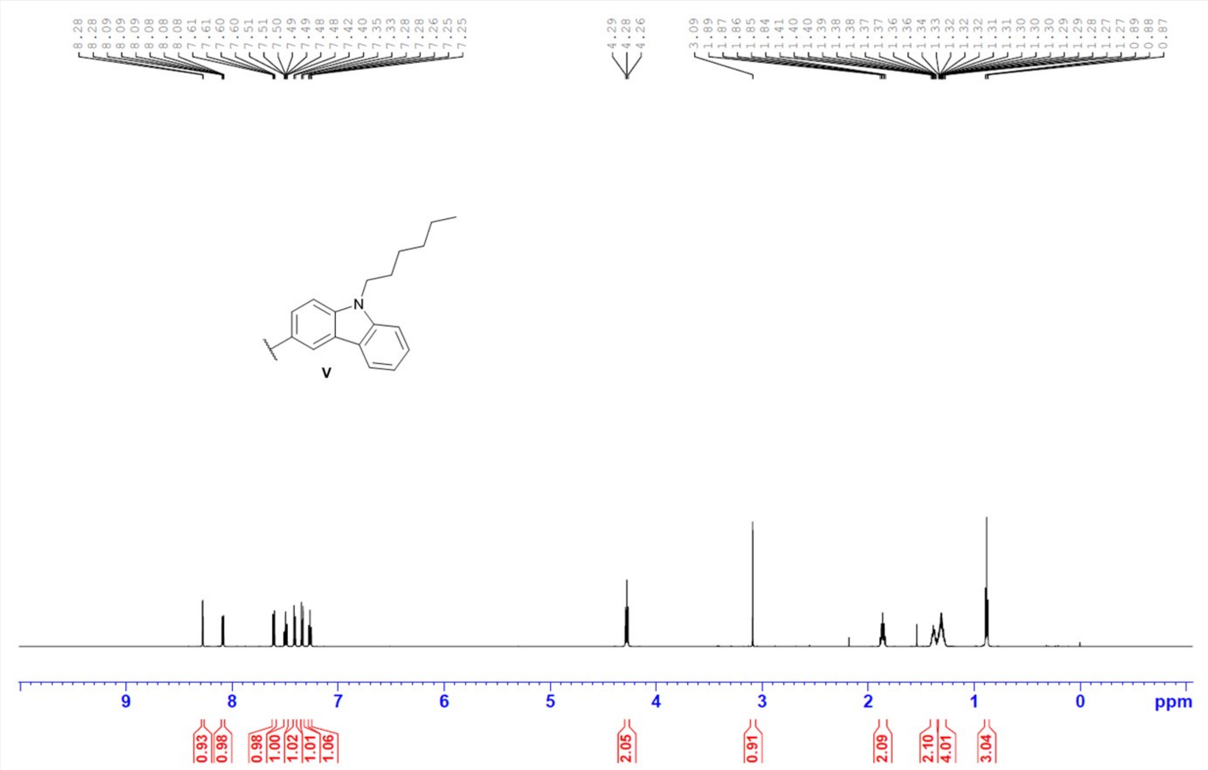
^1H NMR (600 MHz, $CDCl_3$), $^{13}C\{1H\}$ NMR (151 MHz, $CDCl_3$) and HSQC ($CDCl_3$) spectra for compound **18**.

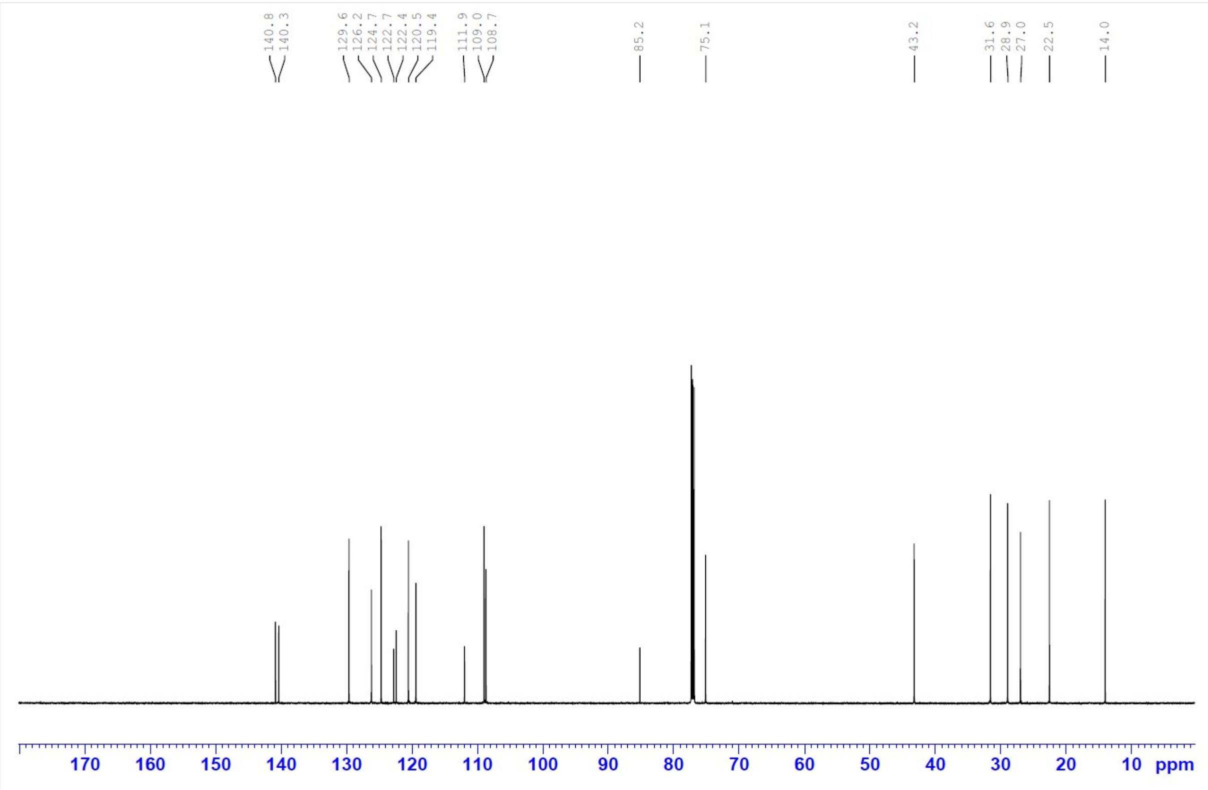



173.8
158.0
148.9
141.0
140.5
130.6
127.4
126.1
123.8
123.3
123.0
121.6
120.7
119.9
119.2
117.9
115.2
109.1
109.0
70.4
69.3
64.1
52.0
50.5
43.3
42.5
31.7
30.0
29.1
27.1
22.7
18.9
18.7
14.1
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


ppm
0 20 40 60 80 100 120 140
11 10 9 8 7 6 5 4 3 2 1 0 -1 ppm

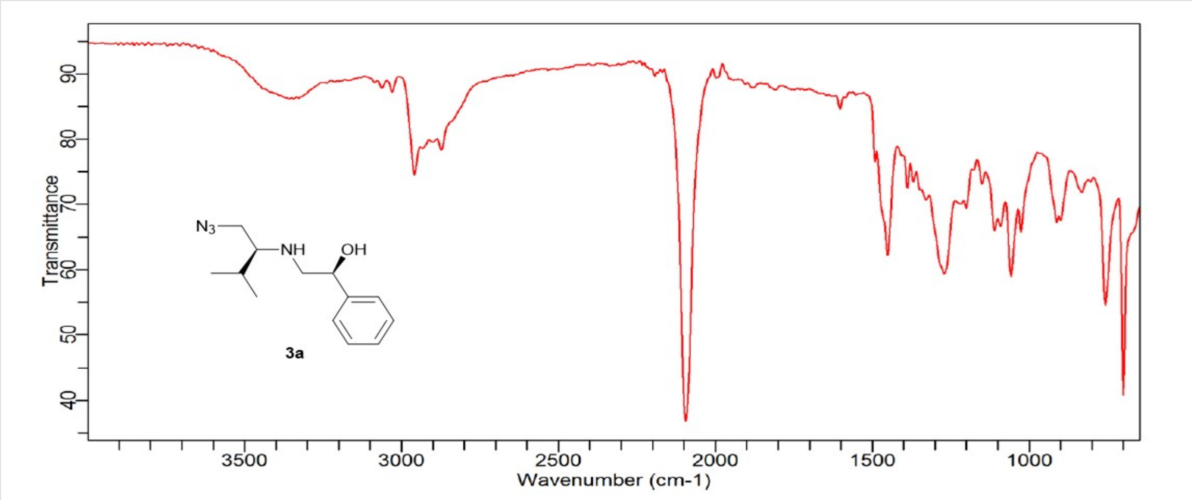
[1]H NMR (600 MHz, $CDCl_3$) and [13]C{1H} NMR (151 MHz, $CDCl_3$) spectra of compound **V** – 3-Ethynyl-9-hexyl-9*H*-carbazole.



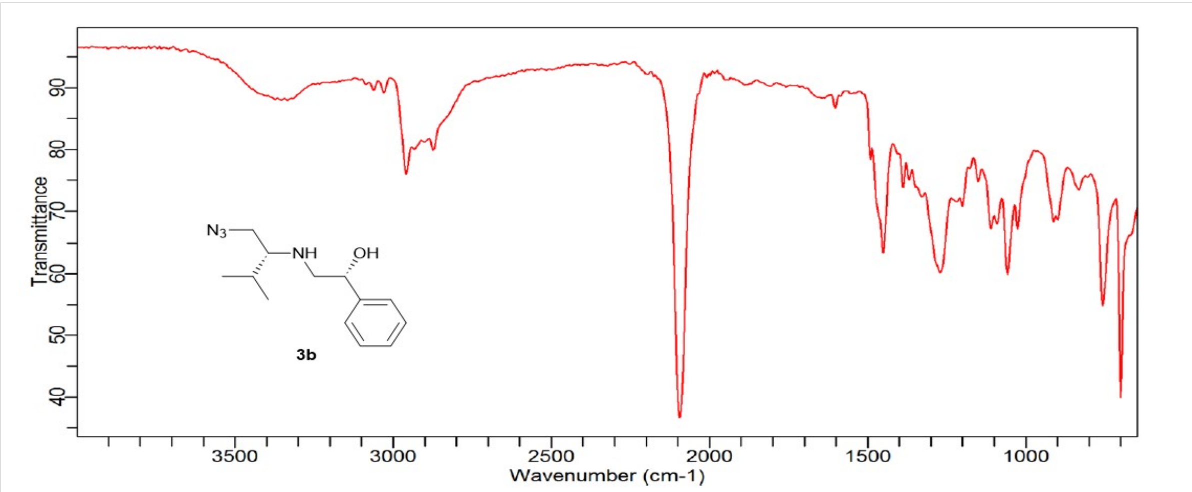


5. Copies of IR spectra

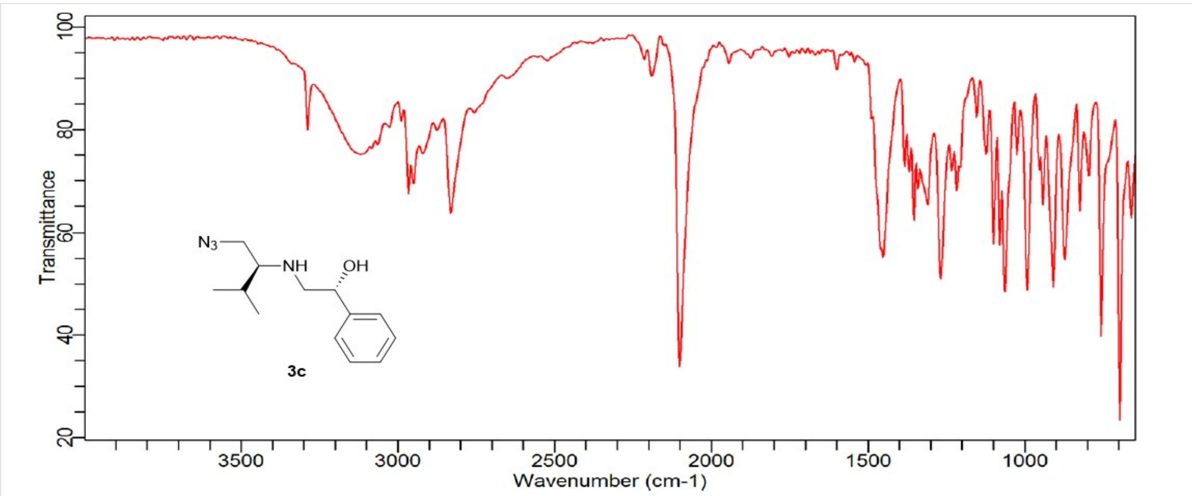
IR spectra for compound **3a**.



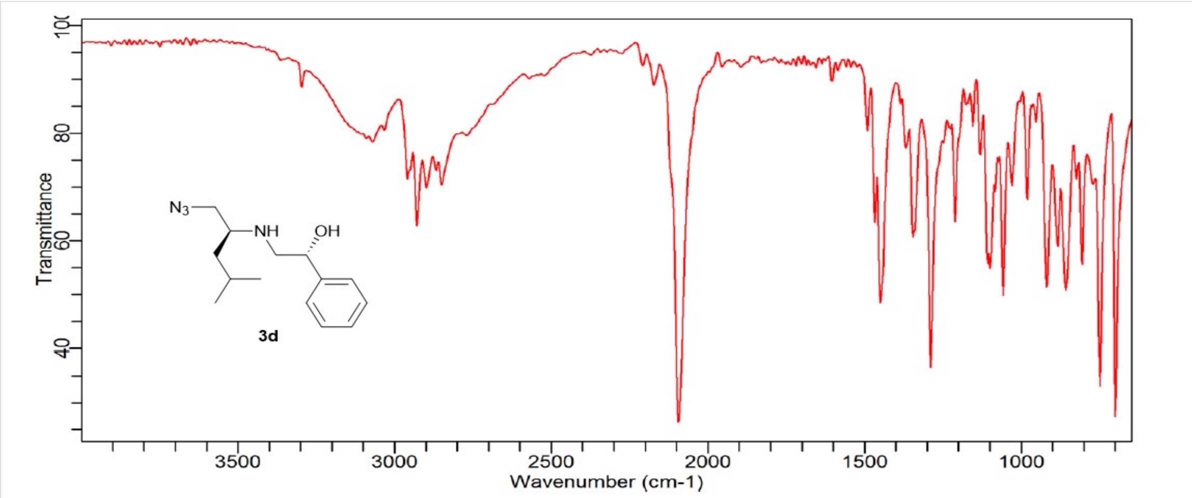
IR spectra for compound **3b**.



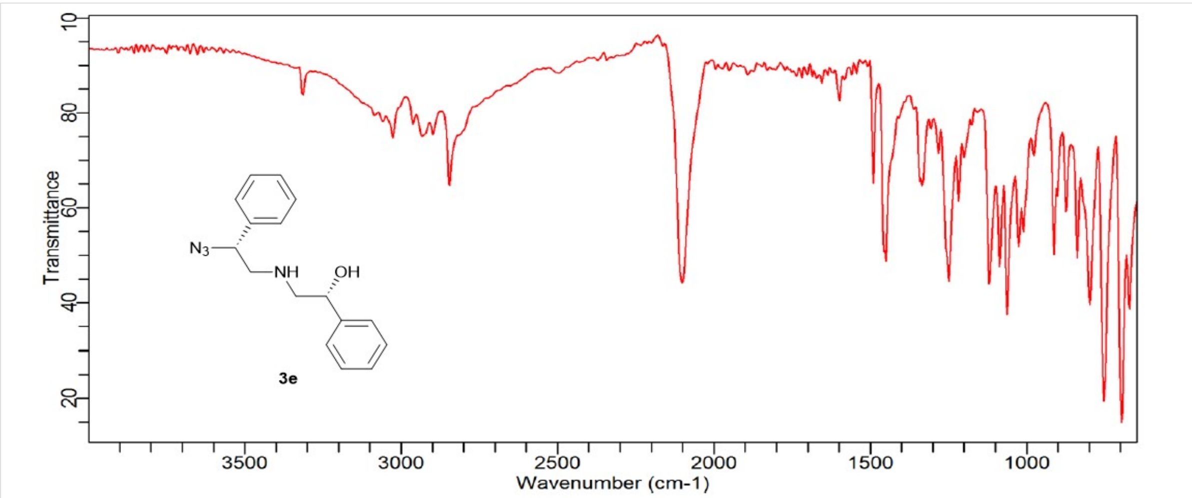
IR spectra for compound **3c**.



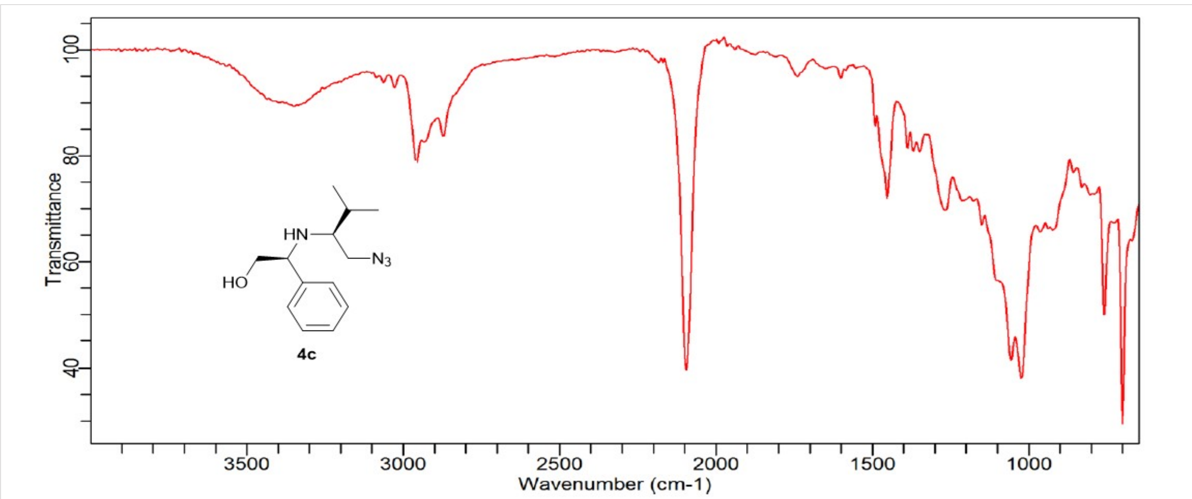
IR spectra for compound **3d**.



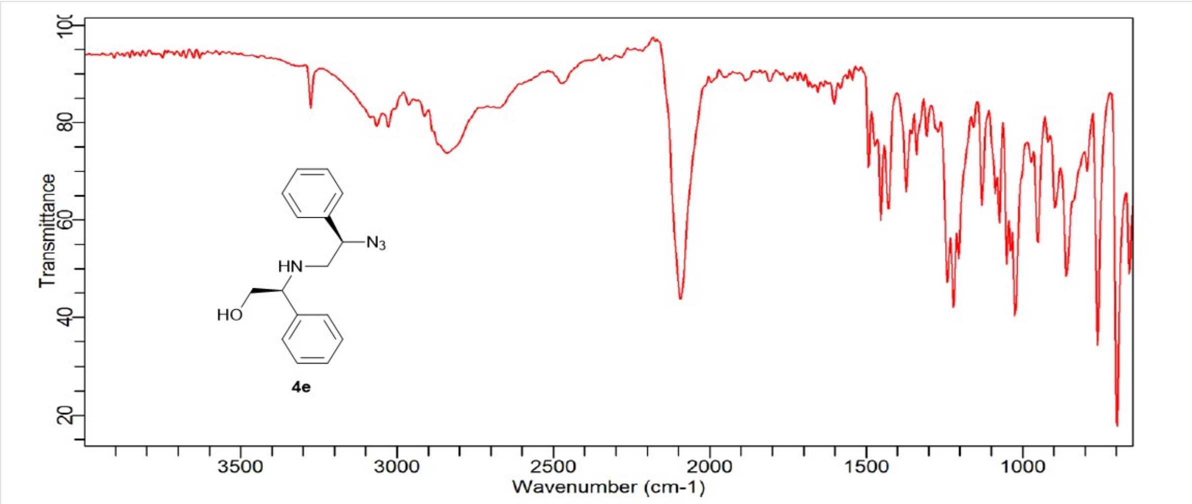
IR spectra for compound **3e**.



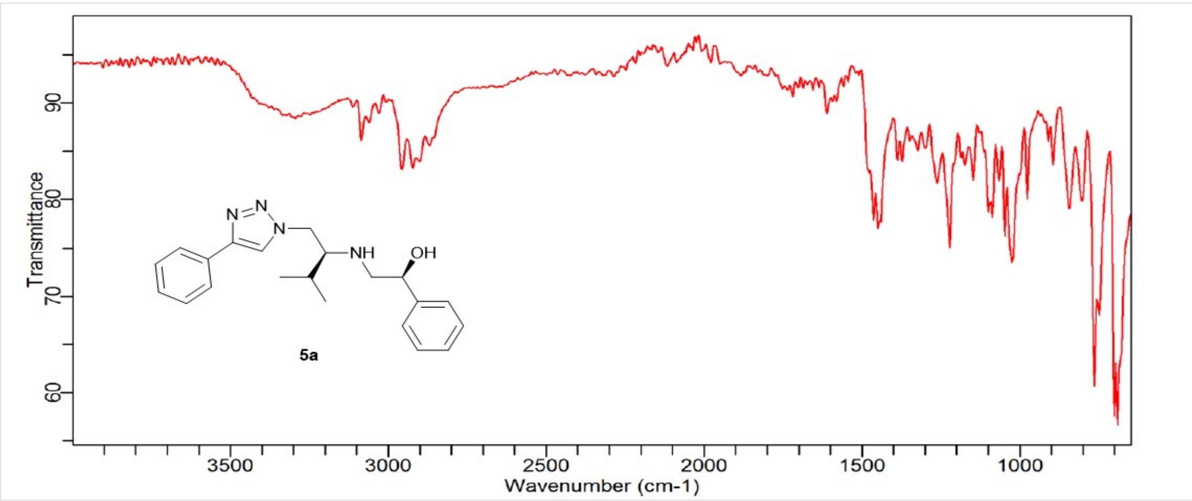
IR spectra for compound **4c**.



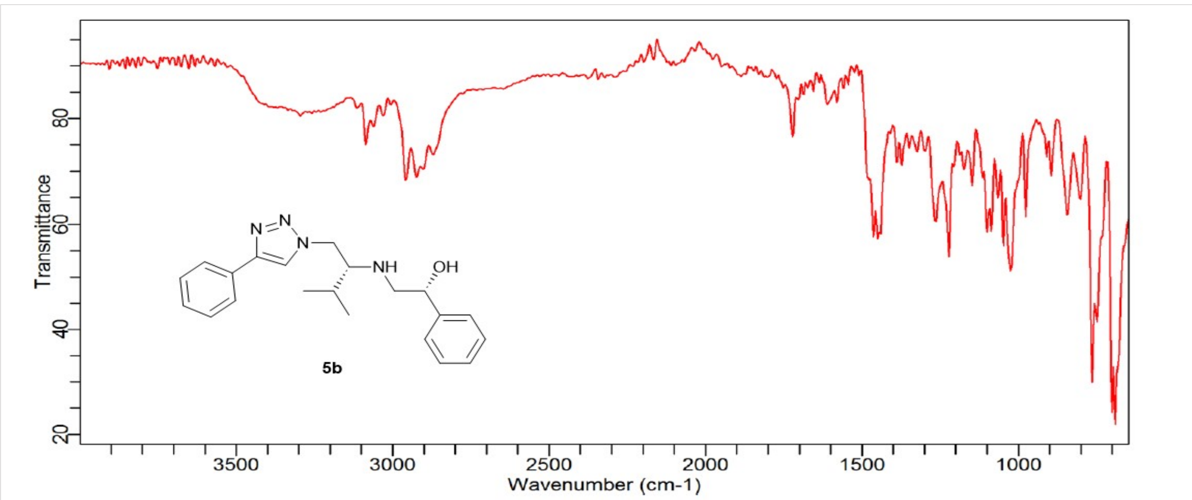
IR spectra for compound **4e**.



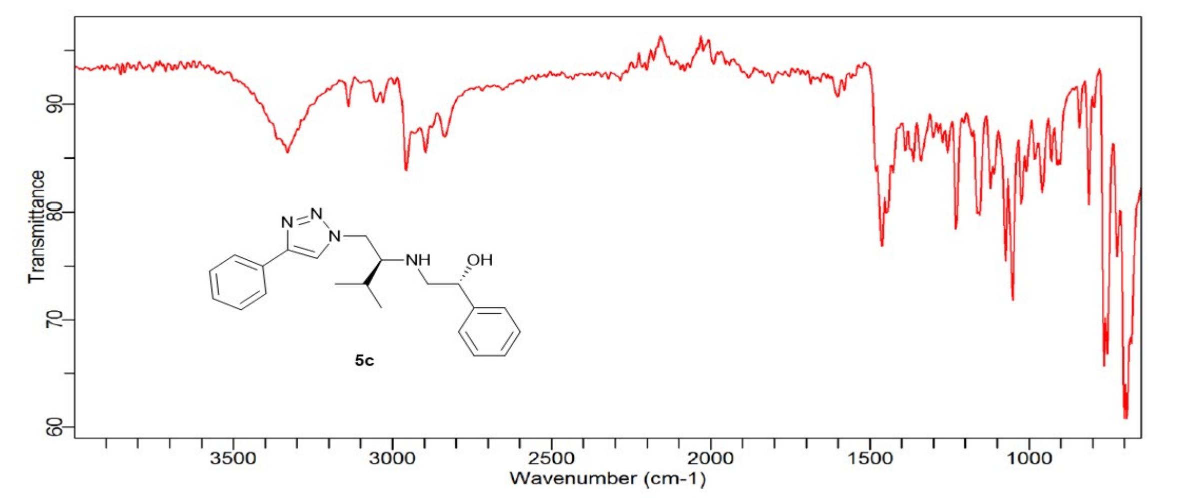
IR spectra for compound **5a**.



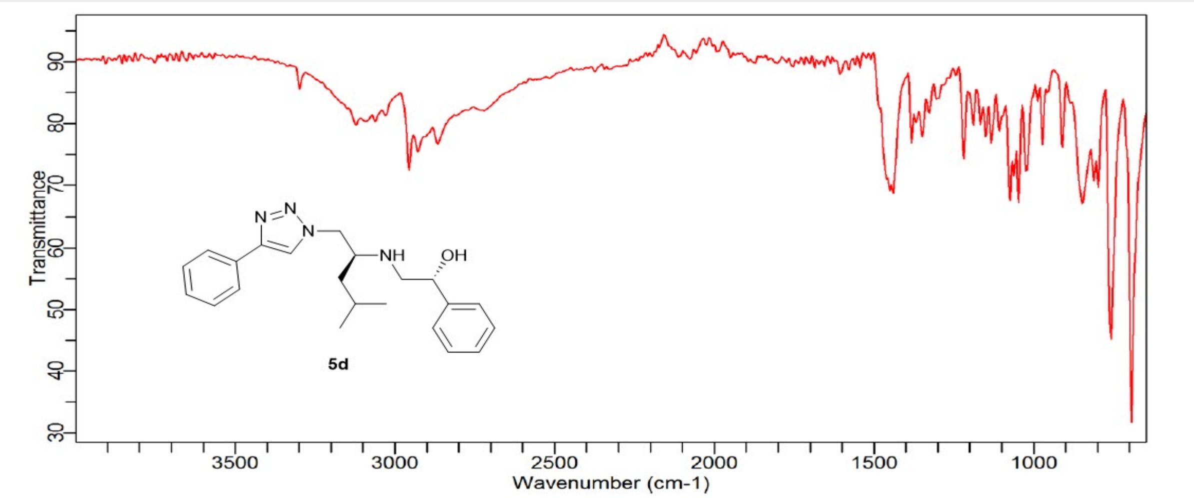
IR spectra for compound **5b**.



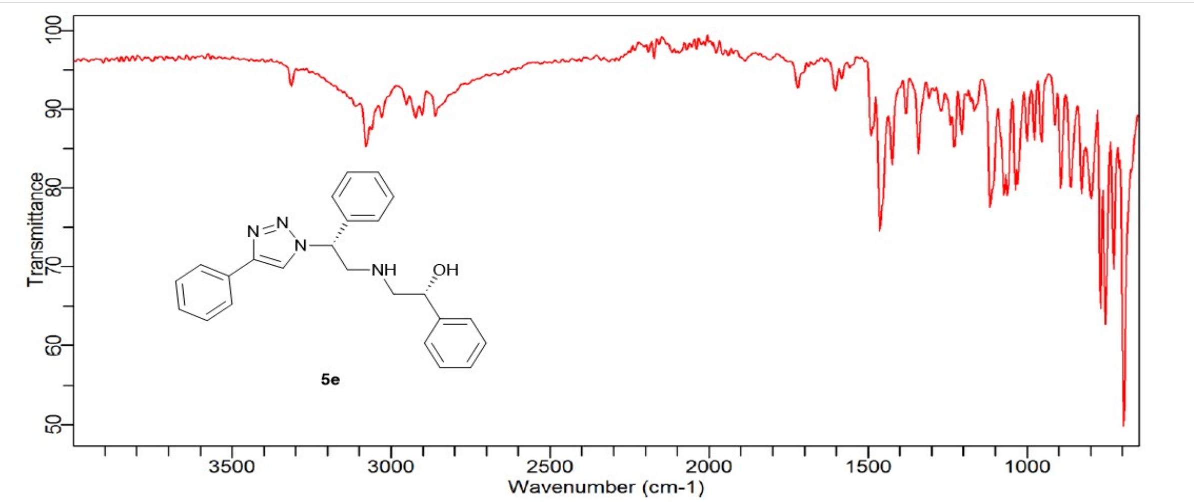
IR spectra for compound **5c**.



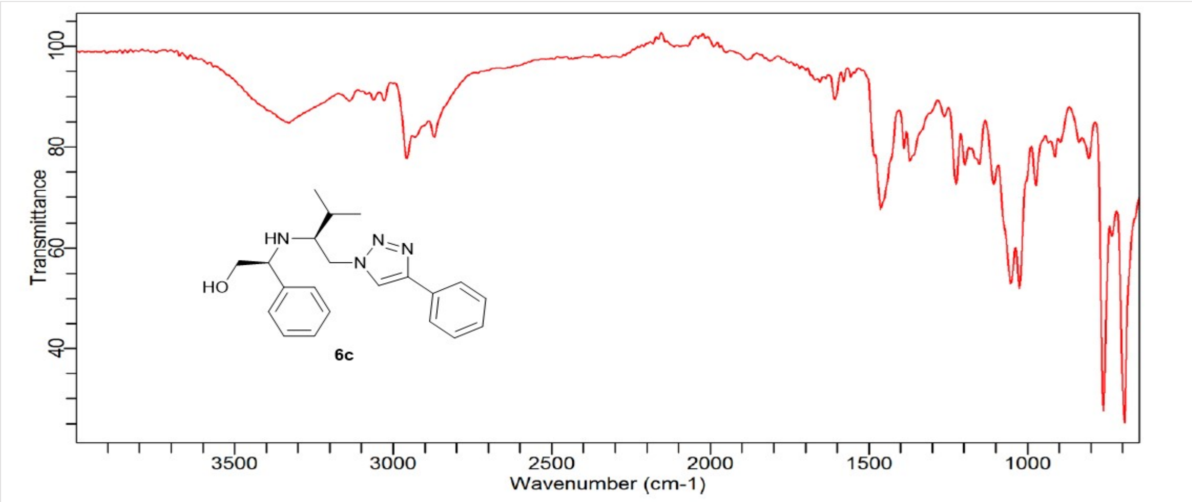
IR spectra for compound **5d**.



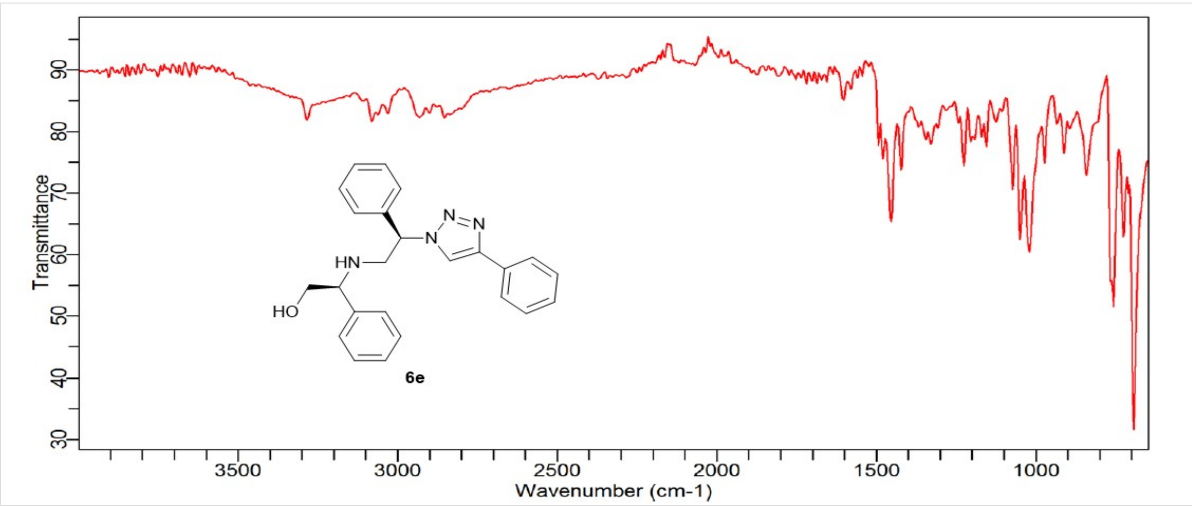
IR spectra for compound **5e**.



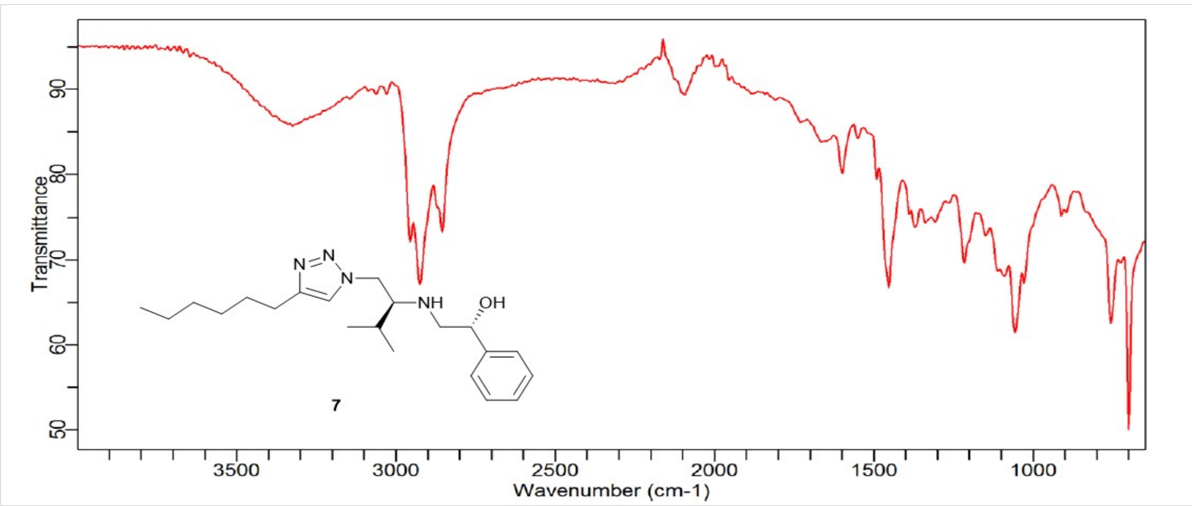
IR spectra for compound **6c**.



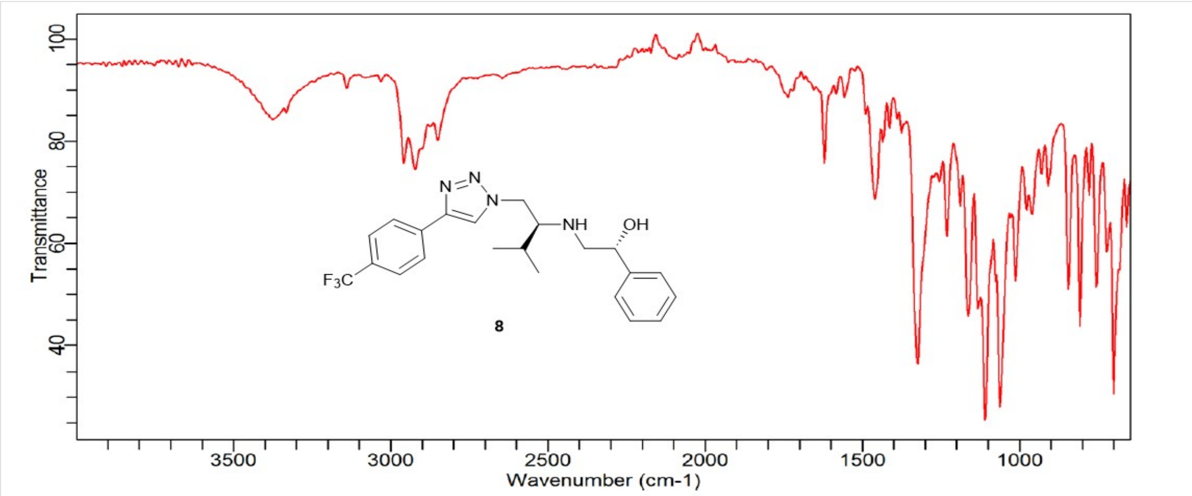
IR spectra for compound **6e**.



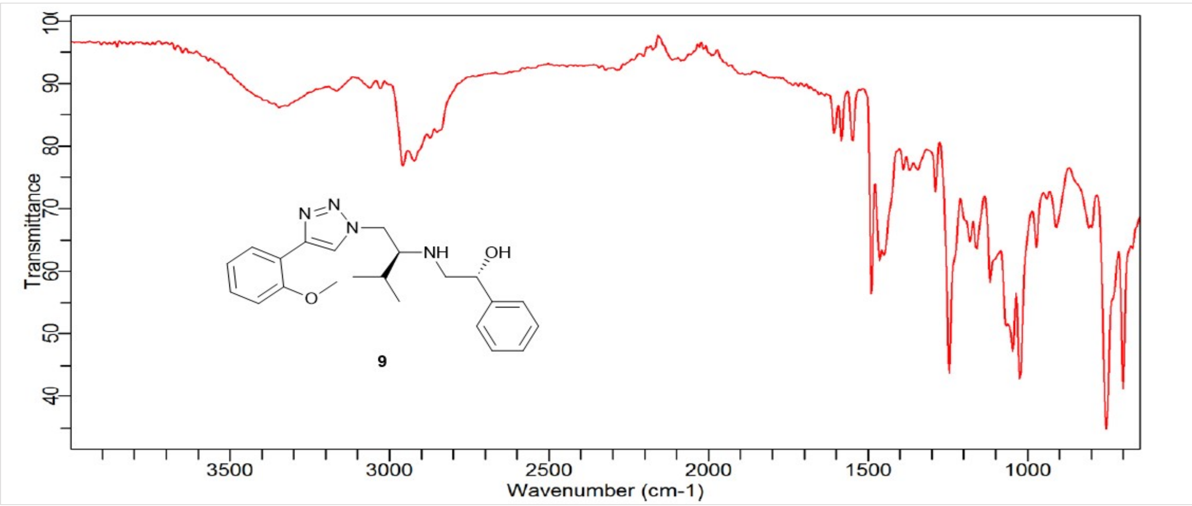
IR spectra for compound **7**.



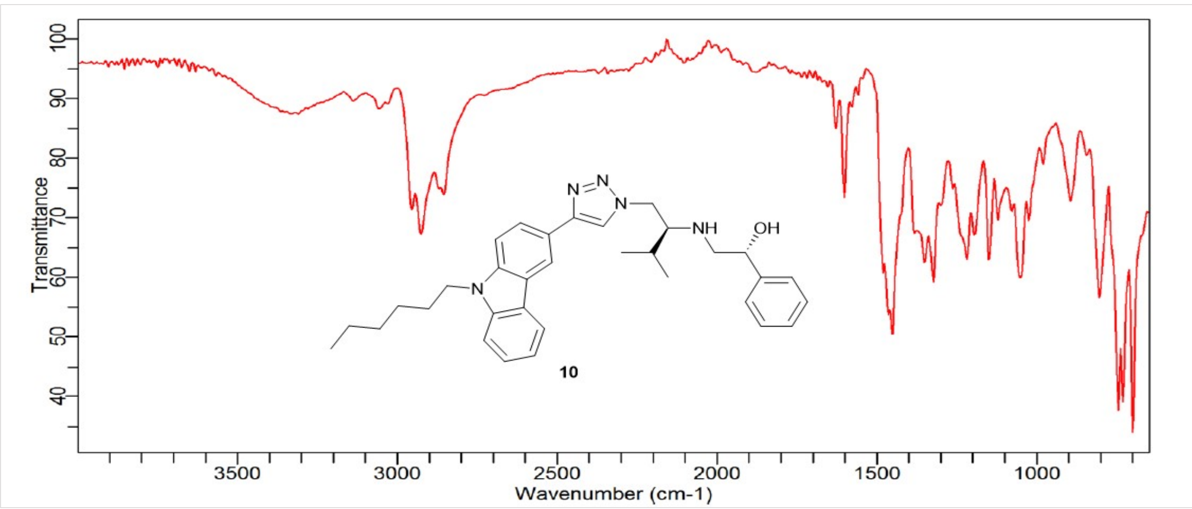
IR spectra for compound **8**.



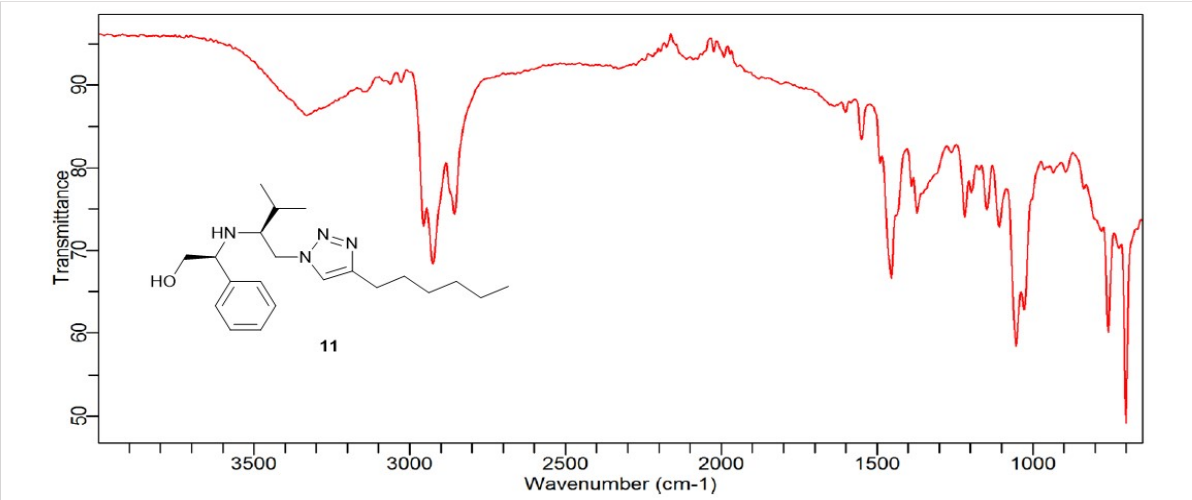
IR spectra for compound **9**.



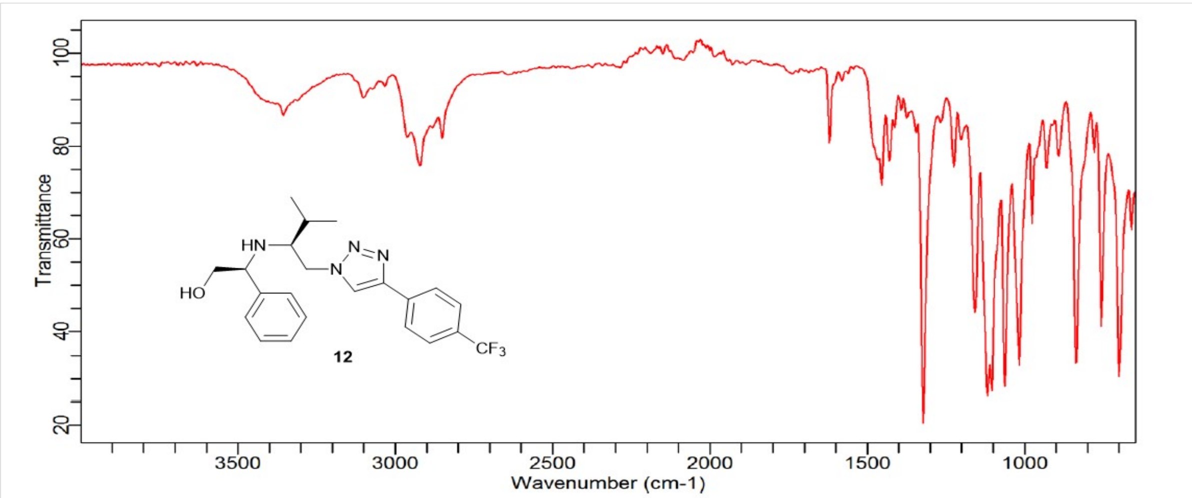
IR spectra for compound **10**.



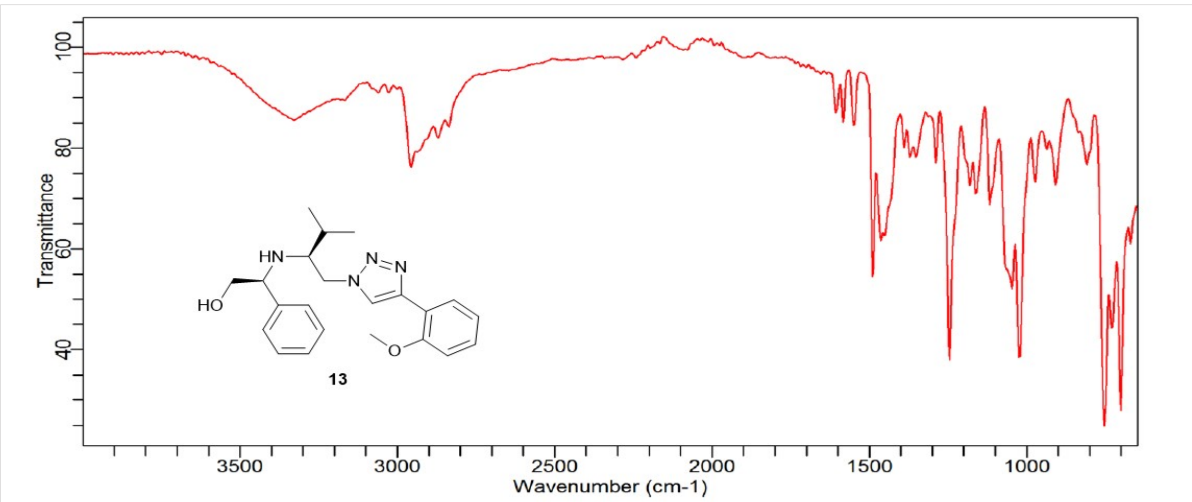
IR spectra for compound **11**.



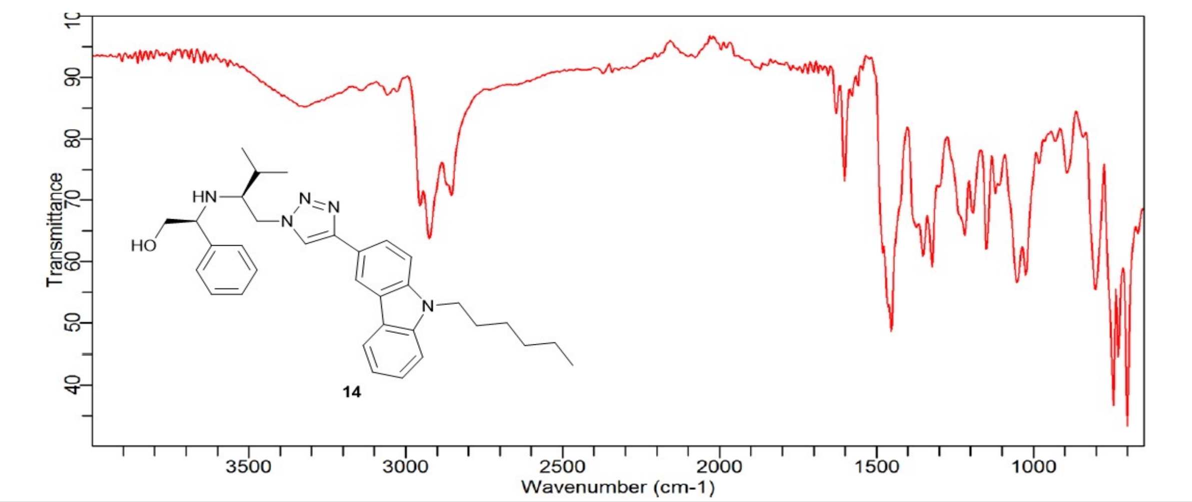
IR spectra for compound **12**.



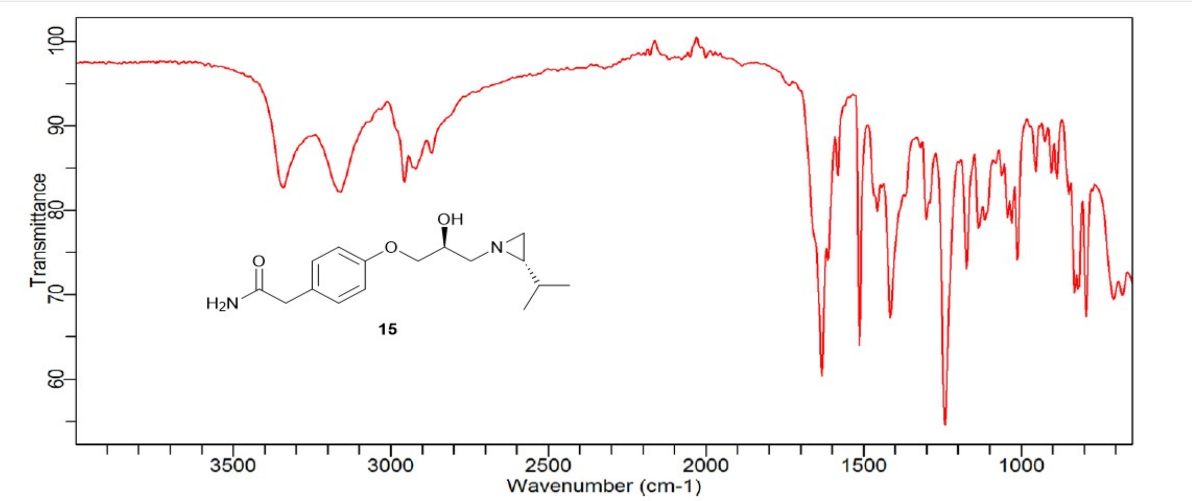
IR spectra for compound **13**.



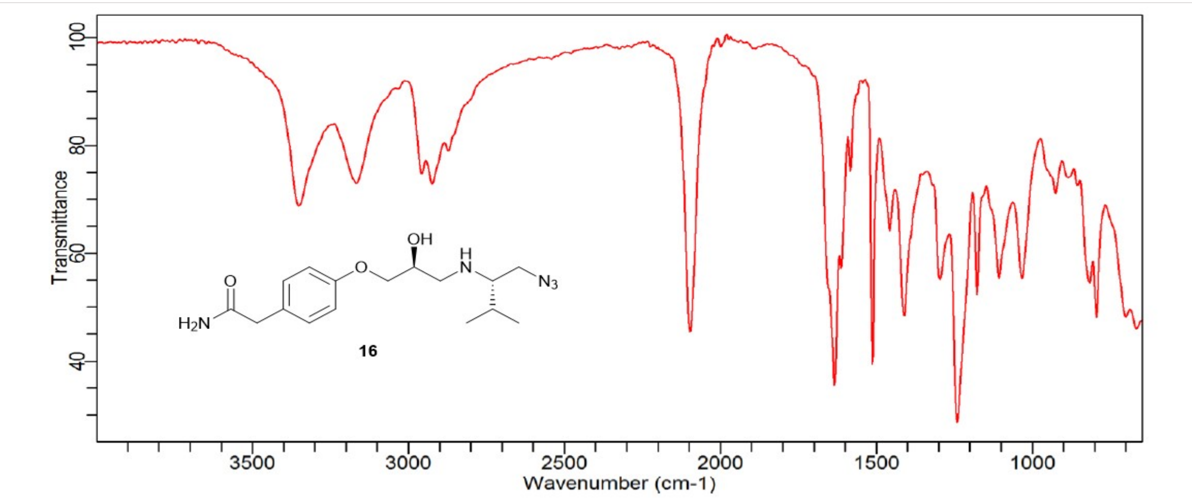
IR spectra for compound **14**.



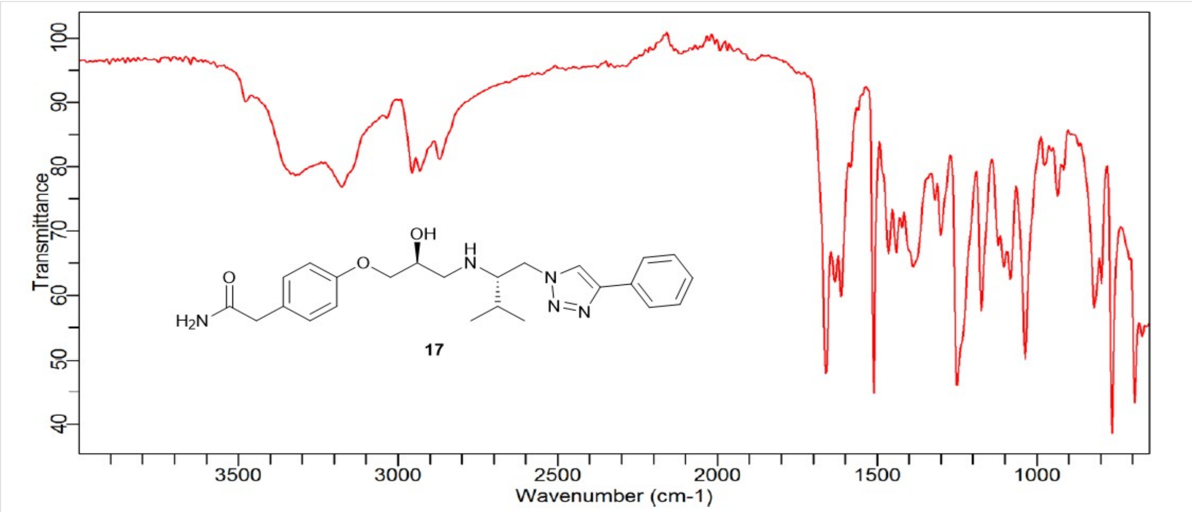
IR spectra for compound **15**.



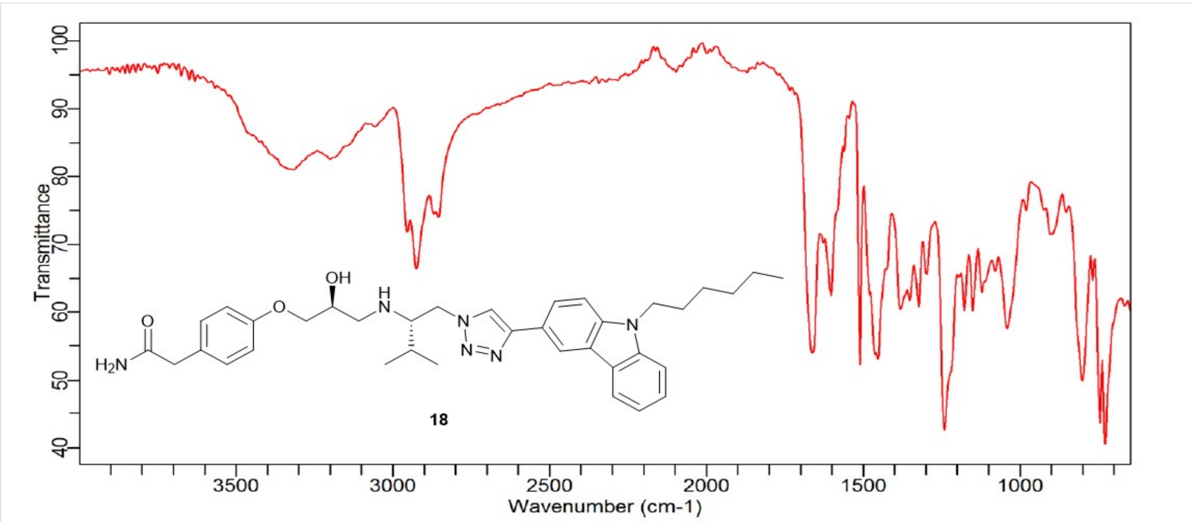
IR spectra for compound **16**.



IR spectra for compound **17**.

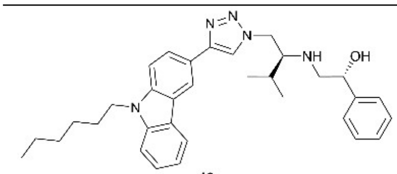
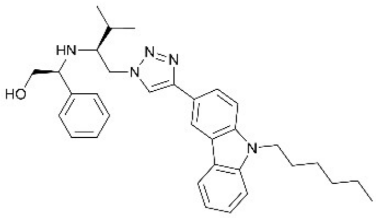
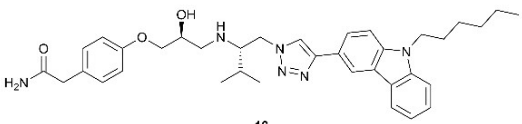


IR spectra for compound **18**.



6. Photophysical research

Table S1. Data of absorption maxima and emission maxima for compounds **10**, **14**, **18**.

Compounds	Solvent	Absorption maxima [nm]	Emission maxima [nm]	Photoluminscence Quantum Yield [%]
 **10**	DCM	342, 357	366, 382	19.47 (**10**)
 **14**	DCM	342, 357	368, 385	19.88 (**14**)
 **18**	DCM	342, 357	368, 385	17.42 (**18**)

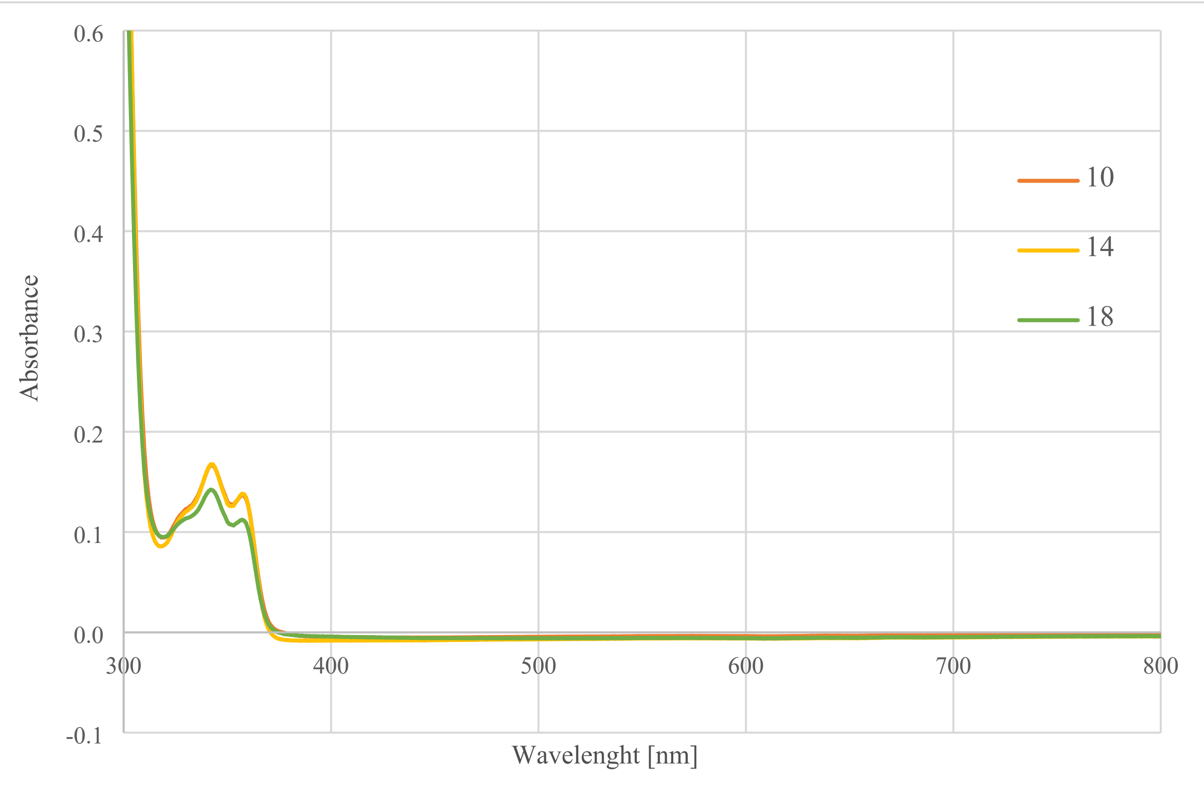


Fig. S1. Absorption spectra of compounds **10**, **14**, **18** in DCM.

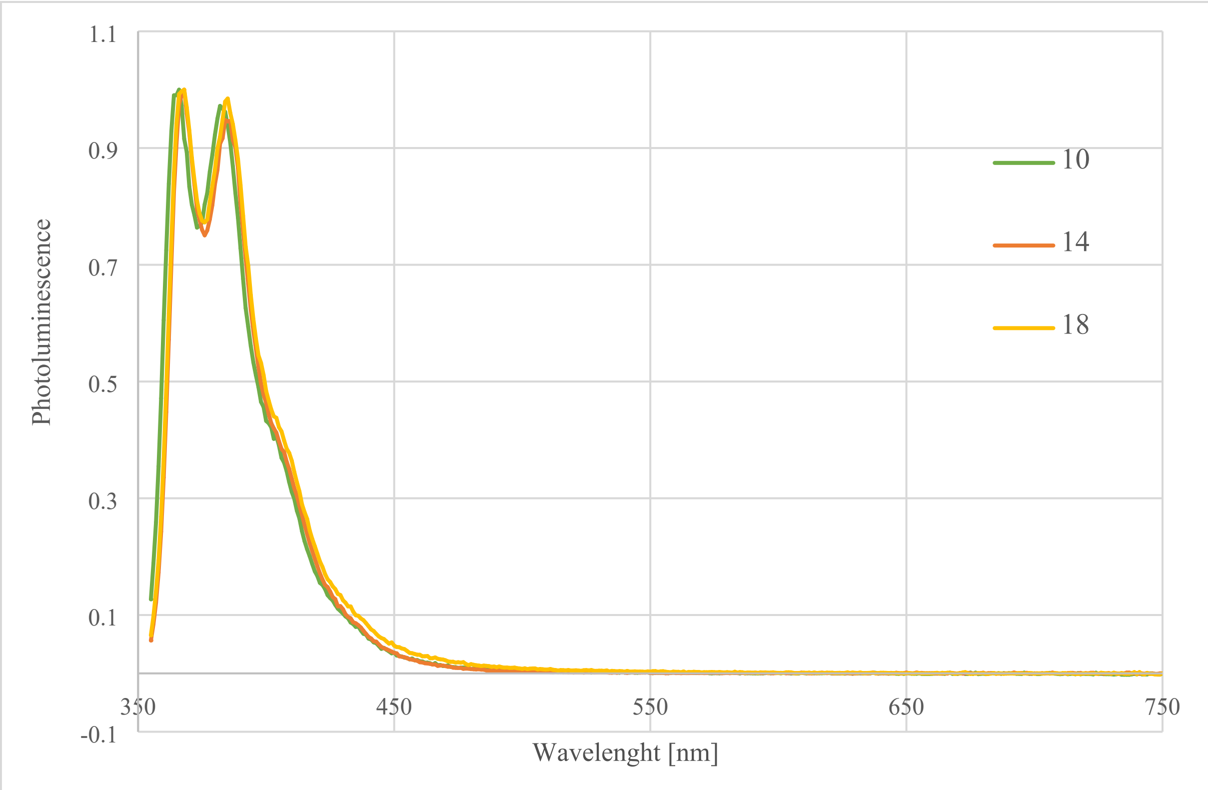


Fig. S2. Emission spectra of compounds **10**, **14**, **18** in DCM.

7. Crystallographic analysis

X-ray structure determination details

X-ray diffraction data for the investigated compound were measured on a four-circle Oxford Diffraction Supernova Dual diffractometer using a two-dimensional area CCD detector and a low-temperature device Oxford Cryosystem cooler. Integration of the intensities, corrections for Lorentz effects, polarization effects, and analytical absorption were performed with CrysAlis PRO [3].

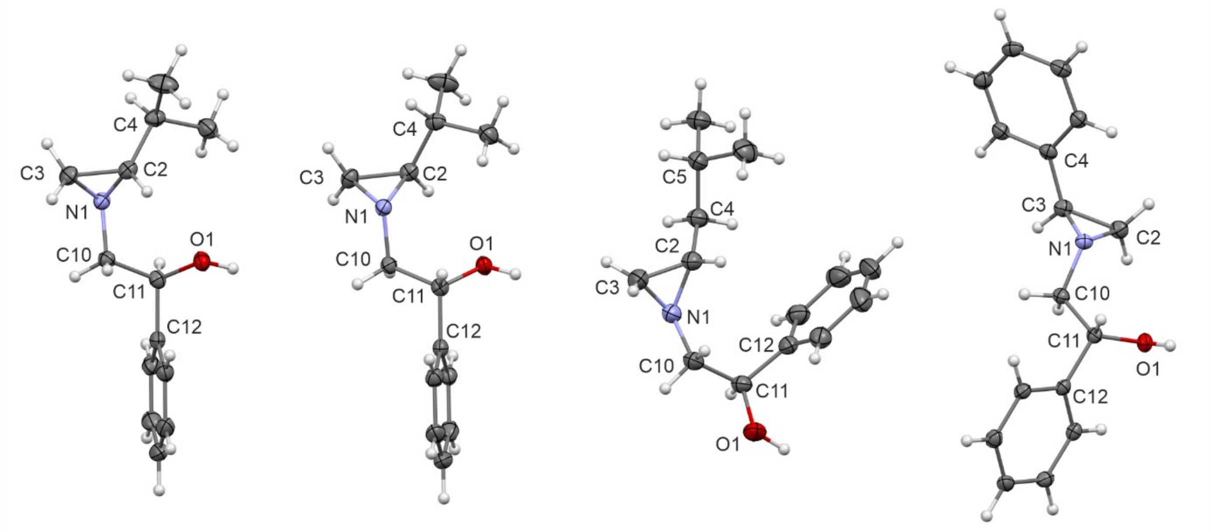
The crystal structure was solved by direct methods and refined on F^2 using a full-matrix least-squares procedure (SHELXL-2014) [4]. All the analyzed crystals belong to non-centrosymmetric space groups (monoclinic $P2_1$ or orthorhombic $P2_12_12_1$). During refinement procedure some structures show evidence of atoms positional disorder. Hence, finally **5a** was refined with isopropyl group disordered over two positions (ratio of disorder components 0.7 : 0.3). Also **6e** shows disorder involving hydroxymethylene group (component ratio 0.65 : 0.35). For **12**, there are two symmetrically independent molecules in the asymmetric unit. Both however, show disorder of trifluoromethyl groups with two independent position of fluorine atoms sets (0.7 : 0.3 for one molecule (A) and 0.5 : 0.5 for the other (B)).

In the process of crystal structure refinement the positions of the hydrogen were introduced in the calculated positions with an idealized geometry and constrained using a rigid body model with isotropic displacement parameters equal to 1.2 of equivalent displacement parameters of their parent C atoms Ueq(C) for aromatic rings, or 1.5 Ueq(C) for methyl and isopropyl groups. Hydrogen atoms bonded to heteroatoms (nitrogen and oxygen) as involved in hydrogen bonds were located in difference Fourier maps and refined freely.

Final results of crystal structure determination were evaluated by CheckCif service [5] in order to check the consistency of crystal structure data and to confirm that the obtained results fulfill the International Union of Crystallography (IUCr) standards. The most important crystallographic data are given as a Supplementary material in **XRD_data.cif** file.

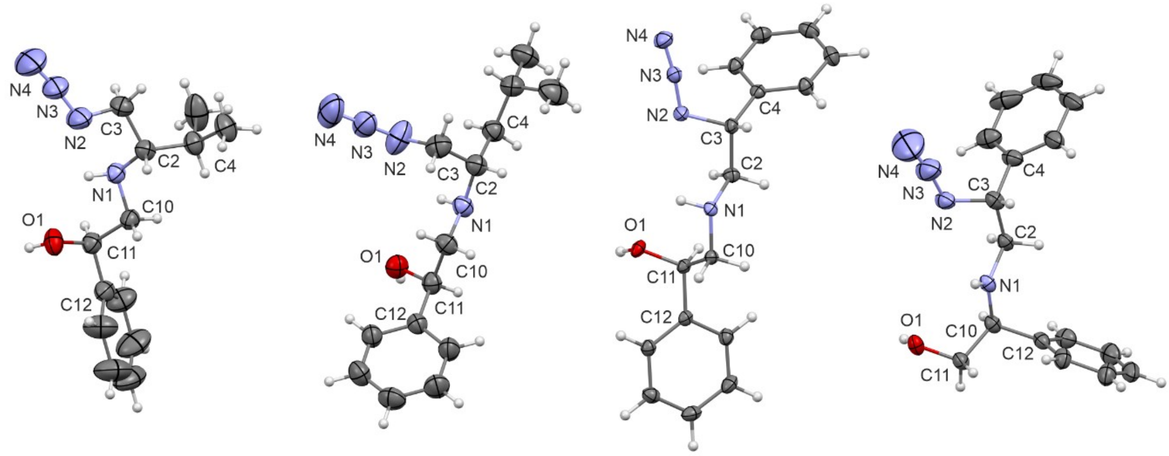
The full set of relevant crystallographic data, atomic coordinates, displacement parameters, and structure factors of the all crystal structures are deposited with Cambridge Crystallographic Data Centre CCDC (**reference deposit numbers: 2501469-2501480**). These data can be obtained free of charge from The Cambridge Crystallographic Data Centre [6].

Graphical presentation of X-ray diffraction results was prepared with the use of Mercury program [7]. In the **Fig. S5** only major disorder components of **5a**, **6e**, and **12** are shown for clarity. As the conformations of two crystallographic symmetry independent molecules of **12** is almost the same, only one of them (molecule A) is presented.



1a 1b 1d 1e

Fig. S3. The molecular structures of aziridine alcohol derivatives **1a**, **1b**, **1d** and **1e**. The labelling scheme is presented for selected non-hydrogen atoms, displacement ellipsoids are drawn in 50% probability level.



3c 3d 3e 4e

Fig. S4. The molecular structures of azide derivatives **3c**, **3d**, **3e** and **4e**. The labelling scheme is presented for selected non-hydrogen atoms, displacement ellipsoids are drawn in 50% probability level.

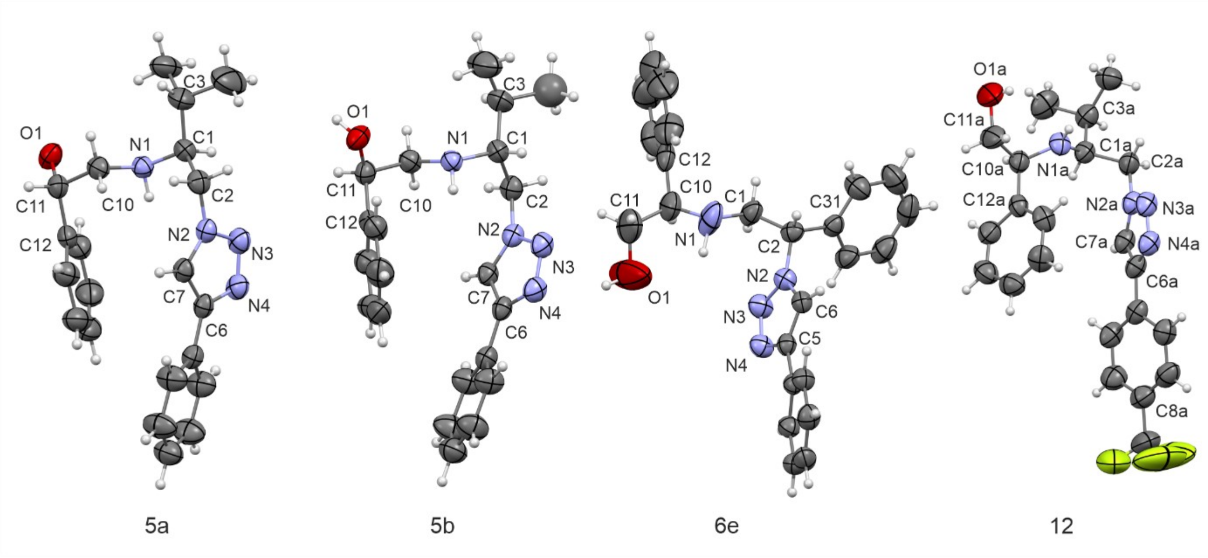


Fig. S5. The molecular structures of 1,2,3-triazole derivatives **5a**, **5b**, **6e** and **12**. For clarity only major disorder components of **5a**, **6e** and **12** are shown. The labelling scheme is presented for selected non-hydrogen atoms, displacement ellipsoids are drawn in 50% probability level.

8. References

1. J. Xu, A new and expeditious asymmetric synthesis of (*R*)- and (*S*)-2-aminoalkanesulfonic acids from chiral amino alcohols, *Tetrahedron: Asymmetry*, 2002, **13**, 1129–1134.

2. M. Rachwalski, S. Jarzyński, S. Leśniak, Highly efficient conjugate addition of diethylzinc to enones catalyzed by chiral ligands derived from (*S*)-mandelic acid, *Tetrahedron: Asymmetry*, 2013, **24**, 1117–1119.

3. CrysAlisPRO software system, Rigaku Oxford Diffraction 2020.

4. G. M. Sheldrick, Crystal structure refinement with SHELXL. Acta Crystallographica. 2015, C71, 3–8.

5. Spek, A. L., Structure validation in chemical crystallography. Acta Crystallographica 2009, D65, 148–155.

6. The Cambridge Crystallographic Data Centre, 12, Union Road, Cambridge CB2 1EZ, UK, https://www.ccdc.cam.ac.uk/conts/retrieving.html.

7. C. F. Macrae, I. Sovago, S. J. Cottrell, P. T. A. Galek, P. McCabe, E. Pidcock, M. Platings, G. P. Shields, J. S. Stevens, M. Towler and P. A. Wood, Mercury 4.0: from visualization to analysis, design and prediction J. Appl. Cryst., 2020, 53, 226–235.