SUPPORTING INFORMATION

Microwave-Assisted One-Pot Synthesis and Anti-Biofilm Activity of 2-Amino-1*H*-imidazole/Triazole Conjugates

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Materials and Methods

General Information

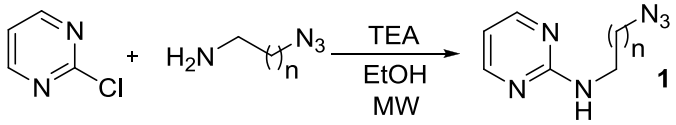
Reactions were carried out under ambient temperature unless otherwise specified. All chemicals were used without purification. Yields refer to purified and spectroscopic pure compounds. Solvents for column chromatography and TLC were laboratory grade and distilled before use. For thin-layer chromatography (TLC), analytical TLC plates (Alugram SIL G/UV_{254} (E. M. Merk) were used. Column chromatography was performed with flash silica gel (100-200 mesh). ^{1}H and ^{13}C NMR spectra were recorded on a Bruker Avance 300 (300 MHz) or a Bruker AMX-400 (400 MHz) spectrometers. NMR samples were run in the indicated solvents and were referenced internally. Chemical shift values were quoted in ppm and coupling constants were quoted in Hz. Chemical shift multiplicities were reported as s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet and br = broad. High-resolution mass spectra (EI) were recorded on a KRATOS MS50TC instrument.

Microwave Irradiation Experiments

Microwave irradiation experiments were carried out in a dedicated CEM-Discover mono-mode microwave apparatus or Milestone MicroSYNTH multi-mode microwave reactor (Laboratory Microwave Systems). Microwave apparatuses were used in the standard configuration as delivered, operating at a frequency 2.45 GHz with continuous irradiation power from 0 to 400 W. The reactions were carried out in 10, 20, 30 and 50 mL glass tubes. The temperature was measured with an IR sensor on the outer surface of the process vial or fibre optic sensor inside the process vial. After the irradiation period, the reaction vessel was cooled rapidly (2-5 min) to ambient temperature by air jet cooling.

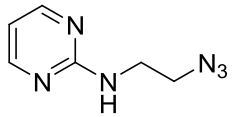
Experimental procedures and compound characterization

General Procedure for the Preparation of *N*-(3-azidopropyl)pyrimidin-2-amines 1.



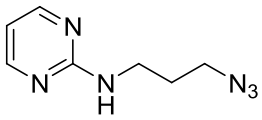
In a 50 mL microwave vial were successively dissolved in EtOH (20 mL) 2-chloropyrimidine (3.43 g, 30 mmol), azidoamine (48 mmol, 1.6 equiv) and triethylamine (6.2 mL, 45 mmol, 1.5 equiv). The reaction tube was sealed, and irradiated in the cavity of a Milestone MicroSYNTH microwave reactor at a ceiling temperature of 120 °C at 100 W maximum power for 30 min. After the reaction mixture was cooled with an air flow for 15 min, it was diluted with water (100 mL), extracted with DCM (2×150 mL) and dried over Na_2SO_4. The solvent was evaporated *in vaccuo*, and the crude mixture was purified by silica gel flash chromatography using 0-5% MeOH−DCM as the eluent.

N-(2-Azidoethyl)pyrimidin-2-amine (1a)



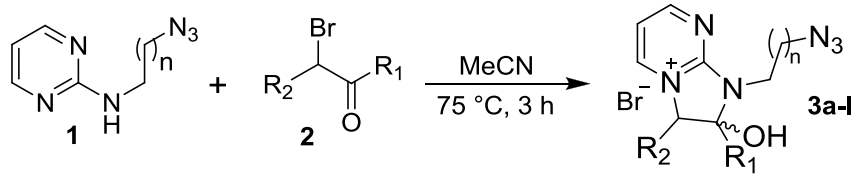
Yield: 67 %. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.30 (d, *J* = 4.74 Hz, 2H), 6.58 (t, *J* = 4.74 Hz, 1H), 5.44 (brs, 1H), 3.64 (m, 2H), 3.54 (t, *J* = 5.58 Hz, 2H). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 162.0, 158.1, 111.1, 50.8, 40.7. HRMS (EI) $C_6H_8N_6$, calcd 164.0810, found: 164.0825.

N-(3-Azidopropyl)pyrimidin-2-amine (1b)



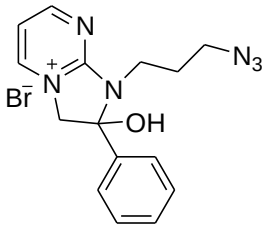
Yield: 69 %. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.28 (d, *J* = 4.80 Hz, 2H), 6.54 (t, *J* = 4.80 Hz, 1H), 5.30 (brs, 1H), 3.52 (m, 2H), 3.42 (t, *J* = 6.57 Hz, 2H), 1.90 (m, 2H). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 162.5, 158.0 (×2), 110.6, 49.2, 38.6, 28.8. HRMS (EI) $C_7H_{10}N_6$, calcd 178.0967, found: 178.0974.

General Procedure for the Preparation of Hydroxy Salts 3a-l.



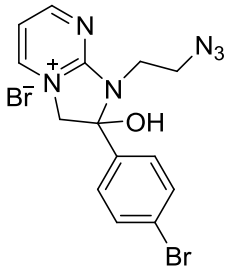
To a solution of *N*-(azidoalkyl)pyrimidin-2-amine **1** (6 mmol) and α-bromoacetophenone **2** (7.2 mmol, 1.2 equiv) in acetonitrile (12 mL) was added 4-dimethylaminopyridine (6 mg, 0.05 mmol). After being stirred at 75 °C for 3 h, the reaction mixture was diluted with ether (20 mL) and the precipitate was filtered off and washed with acetone (2×20 mL), ether (2×20 mL) and dried over P_2O_5 to give salt **3** as a white solid.

1-(3-Azidopropyl)-2-hydroxy-2-phenyl-2,3-dihydro-1*H*-imidazo[1,2-*a*]pyrimidin-4-ium bromide (3a)



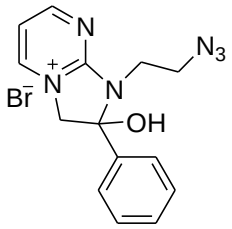
Yield: 86 %. ^{1}H NMR (300 MHz, DMSO-d_6): δ = 9.05 (m, 2H), 7.93 (s, 1H), 7.80 (m, 2H), 7.48 (m, 3H), 7.37 (t, *J* = 4.86 Hz, 1H), 4.95 (m, 2H), 3.41 (m, 4H), 1.64 (m, 2H). ^{13}C NMR (75.5 MHz, DMSO-d_6): δ = 167.4, 154.6, 148.2, 138.1, 129.3, 128.4 (×2), 126.9 (×2), 111.4, 90.6, 62.7, 47.9, 38.2, 27.0. MS (*m/z*) 297 $[(M - Br)]^+$.

1-(2-Azidoethyl)-2-(4-bromophenyl)-2-hydroxy-2,3-dihydro-1*H*-imidazo[1,2-*a*]pyrimidin-4-ium bromide (3b)



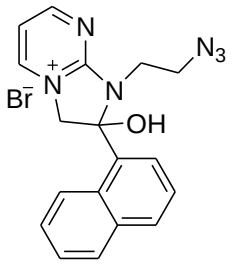
Yield: 90 %. ^{1}H NMR (300 MHz, DMSO-d_6): δ = 9.11 (m, 1H), 8.07 (s, 1H), 7.74 (d, *J* = 9.1 Hz, 2H), 7.72 (d, *J* = 9.1 Hz, 2H), 7.42 (m, 1H), 4.92 (dd, *J* = 14.3/26.4 Hz, 2H), 3.56-3.30 (m, 4H). ^{13}C NMR (75.5 MHz, DMSO-d_6): δ = 167.6, 154.8, 148.4, 137.4, 131.4, 129.4, 123.0, 112.0, 90.4, 62.6, 48.1. MS (*m/z*) 362 $[(M - Br)]^+$.

1-(2-Azidoethyl)-2-hydroxy-2-phenyl-2,3-dihydro-1*H*-imidazo[1,2-*a*]pyrimidin-4-ium bromide (3c)



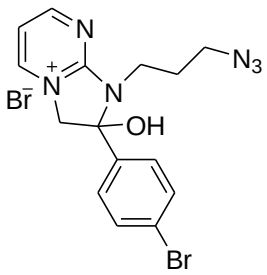
Yield: 89 %. ^{1}H NMR (300 MHz, DMSO-d_6): δ = 9.02 (m, 2H), 7.99 (s, 1H), 7.80 (m, 2H), 7.49 (m, 3H), 7.41 (t, *J* = 4.92 Hz, 1H), 4.95 (m, 2H), 3.38 (m, 4H). ^{13}C NMR (75.5 MHz, DMSO-d_6): δ = 167.5, 154.7, 148.4, 137.8, 129.4, 128.4 (×2), 126.9 (×2), 111.8, 90.6, 62.8, 48.1 (×2). MS (*m/z*) 283 $[(M - Br)]^{+}$.

1-(2-Azidoethyl)-2-hydroxy-2-(naphthalen-1-yl)-2,3-dihydro-1*H*-imidazo[1,2-*a*]pyrimidin-4-ium bromide (3d)



Yield: 69 %. ^{1}H NMR (300 MHz, DMSO-d_6): δ = 9.10 (m, 2H), 8.38 (s, 1H), 8.16 (s, 1H), 8.02 (m, 3H), 7.88 (m, 1H), 7.59 (m, 2H), 7.44 (m, 1H), 5.05 (s, 2H), 3.42 (m, 4H). ^{13}C NMR (75.5 MHz, DMSO-d_6): δ = 167.5, 154.9, 148.5, 135.0, 132.9, 132.1, 128.4, 128.2, 127.5, 127.1, 126.7 (×2), 124.1, 111.9, 90.8, 62.6, 48.2 (×2). MS (*m/z*) 333 $[(M - Br)]^{+}$.

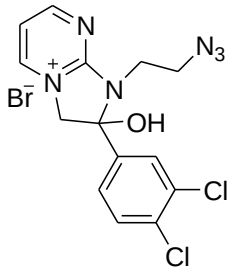
1-(3-Azidopropyl)-2-(4-bromophenyl)-2-hydroxy-2,3-dihydro-1*H*-imidazo[1,2-*a*]pyrimidin-4-ium bromide (3e)



Yield: 83 %. ^{1}H NMR (300 MHz, DMSO-d_6): δ = 9.06 (dd, *J* = 1.62, 4.60 Hz, 1H), 8.98 (dd, *J* = 1.62, 6.24 Hz,1H) 8.00 (s, 1H), 7.72 (m, 4H), 7.37 (m, 1H), 4.85 (m, 2H), 3.37 (m, 4H),

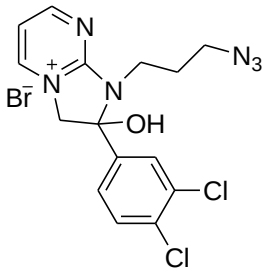
1.66 (m, 2H). ^{13}C NMR (75.5 MHz, DMSO-d_6): δ = 167.5, 154.7, 148.2, 137.6, 131.4(×2), 129.3 (×2), 122.9, 111.5, 90.3, 62.5, 47.9, 38.2, 27.0. MS (*m/z*) 375 $[(M - Br)]^+$.

1-(2-Azidoethyl)-2-(3,4-dichlorophenyl)-2-hydroxy-2,3-dihydro-1*H*-imidazo[1,2-*a*]pyrimidin-4-ium bromide (3f)



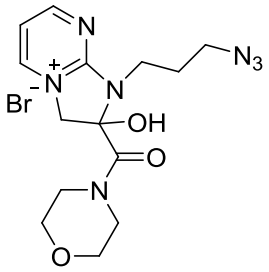
Yield: 75 %. ^{1}H NMR (300 MHz, DMSO-d_6): δ = 9.12 (m, 2H), 8.20 (s, 1H), 8.09 (s, 1H), 7.79 (m, 2H), 7.43 (m, 1H), 4.93 (m, 2H), 3.42 (m, 4H). ^{13}C NMR (75.5 MHz, DMSO-d_6): δ = 167.5, 154.9, 148.3, 139.0, 132.2, 131.3, 130.5, 129.5, 127.4, 112.1, 89.8, 62.5, 48.0 (×2). MS (*m/z*) 351 $[(M - Br)]^+$.

1-(3-Azidopropyl)-2-(3,4-dichlorophenyl)-2-hydroxy-2,3-dihydro-1*H*-imidazo[1,2-*a*]pyrimidin-4-ium bromide (3g)



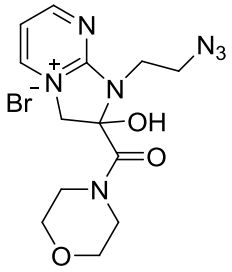
Yield: 77 %. ^{1}H NMR (300 MHz, DMSO-d_6): δ = 9.07 (m, 1H), 8.97 (m,1H), 8.12 (s, 1H), 8.08 (brs, 1H), 7.97 (m, 2H), 7.38 (t, *J* = 4.92 Hz, 1H), 4.86 (m, 2H), 3.37 (m, 4H), 1.68 (m, 2H). ^{13}C NMR (75.5 MHz, DMSO-d_6): δ = 167.5, 154.7, 148.1, 139.2, 132.2, 131.3, 130.6, 129.3, 127.4, 111.6, 89.8, 62.4, 47.8, 38.3, 26.9. MS (*m/z*) 365 $[(M - Br)]^+$.

1-(3-Azidopropyl)-2-hydroxy-2-(morpholine-4-carbonyl)-2,3-dihydro-1*H*-imidazo[1,2-*a*]pyrimidin-4-ium bromide (3h)



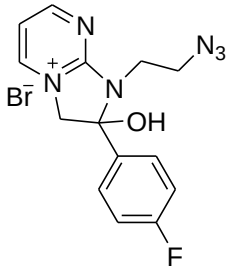
Yield: 65 %. ^{1}H NMR (300 MHz, DMSO-d_6): δ = 9.01 (m, 1H), 8.82 (m,1H), 7.28 (t, *J* = 6.0 Hz, 1H), 5.05 (dd, *J* = 14.3/45.6 Hz, 2H), 3.66 (m, 12H), 2.07 (m, 2H). ^{13}C NMR (75.5 MHz, DMSO-d_6): δ = 167.9, 164.7, 154.4, 148.3, 111.2, 91.5, 65.7, 57.4, 48.4, 46.5, 43.0, 27.0. MS (*m/z*) 334 $[(M - Br)]^{+}$.

1-(2-Azidoethyl)-2-hydroxy-2-(morpholine-4-carbonyl)-2,3-dihydro-1*H*-imidazo[1,2-*a*]pyrimidin-4-ium bromide (3i)



Yield: 76 %. ^{1}H NMR (300 MHz, DMSO-d_6): δ = 9.06 (m, 1H), 8.90 (m, 1H), 8.50 (brs, 1H), 7.35 (t, *J* = 6.0 Hz, 1H), 5.07 (dd, 14.3/48.2 Hz, 2H), 3.70 (m, 12 H). ^{13}C NMR (75.5 MHz, DMSO-d_6): δ = 168.0, 164.7, 154.5, 148.4, 111.7, 91.4, 65.7, 48.4, 46.4, 43.0, 41.5, 30.7. MS (*m/z*) 320 $[(M - Br)]^{+}$.

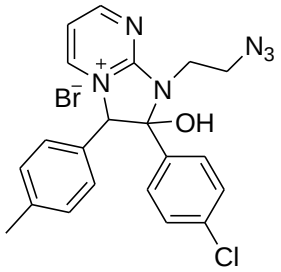
1-(2-Azidoethyl)-2-(4-fluorophenyl)-2-hydroxy-2,3-dihydro-1*H*-imidazo[1,2-*a*]pyrimidin-4-ium bromide (3j)



Yield: 69 %. ^{1}H NMR (300 MHz, DMSO-d_6): δ = 9.09 (d, *J* = 4.53 Hz, 1H), 9.01 (d, *J* = 6.00 Hz, 1H), 8.04 (s, 1H), 7.85 (m, 2H), 7.37 (m, 3H), 4.92 (m, 2H), 3.38 (m, 4H). ^{13}C NMR

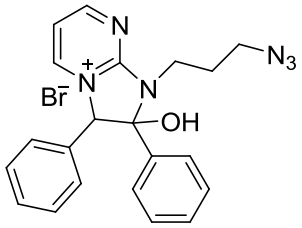
(75.5 MHz, DMSO-d_6): δ = 167.5, 164.1, 160.9, 154.7, 148.4, 134.0 (d), 129.4 (d), 115.4, 115.1, 111.9, 90.3, 62.7, 48.1 (×2). MS (*m/z*) 301 $[(M - Br)]^+$.

1-(2-Azidoethyl)-2-(4-chlorophenyl)-2-hydroxy-3-*p*-tolyl-2,3-dihydro-1*H*-imidazo[1,2-*a*]pyrimidin-4-ium bromide (3k)



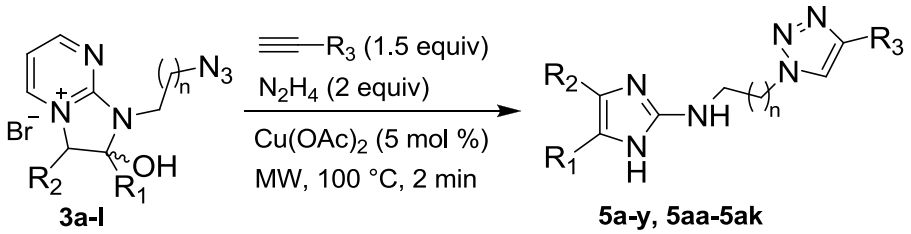
Yield: 72 %. ^{1}H NMR (300 MHz, DMSO-d_6): δ = 9.19 (d, *J* = 3.06 Hz, 1H), 8.55 (d, *J* = 5.43 Hz, 1H), 7.71 (d, *J* = 8.52 Hz, 2H), 7.70 (s, 1H), 7.55 (d, *J* = 8.49 Hz, 2H), 7.38 (m, 1H), 7.42 (d, *J* = 7.80 Hz, 2H), 7.08 (d, *J* = 7.80 Hz, 2H), 6.10 (s, 1H), 3.36 (m, 4H), 2.33 (s, 3H). ^{13}C NMR (75.5 MHz, DMSO-d_6): δ = 168.2, 156.1, 146.9, 139.5, 135.9, 134.4, 129.4 (×6), 128.4 (×2), 124.4, 112.8, 93.5, 74.9, 47.9, 41.0, 20.7. MS (*m/z*) 407 $[(M - Br)]^+$.

1-(3-Azidopropyl)-2-hydroxy-2,3-diphenyl-2,3-dihydro-1*H*-imidazo[1,2-*a*]pyrimidin-4-ium bromide (3l)



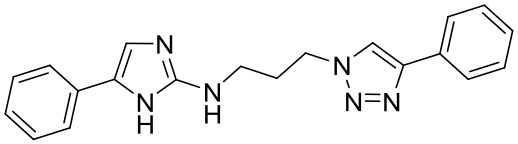
Yield: 75 %. ^{1}H NMR (300 MHz, DMSO-d_6): δ = 9.17 (d, *J* = 3.0 Hz, 1H), 8.57 (d, *J* = 6.0 Hz, 1H), 7.71 (m, 2H), 7.49 (m, 6H), 7.34 (m, 1H), 7.14 (m, 3H), 6.09 (s, 1H), 3.47 (m, 2H), 3.36 (m, 1H), 1.73 (m, 2H). ^{13}C NMR (75.5 MHz, DMSO-d_6): δ = 168.3, 157.0, 147.0, 137.0, 129.8, 129.5, 128.8, 128.5, 127.8, 127.4, 112.3, 96.6, 93.8, 75.2, 48.1, 39.4, 27.0. MS (*m/z*) 373 $[(M - Br)]^+$.

General Procedure for the Preparation of 2-AIT 5a-y, 5aa-5aj.



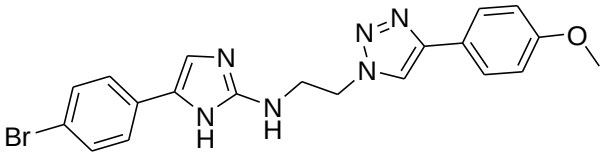
To the cooled solution of hydrazine hydride (2 equiv) in ethanol (0.8 mL) were added $Cu(OAc)_2$ (5 mol %) in water (0.2 mL) and stirred for 2 min at 0 °C. To suspension were added acetylene (1.5 equiv) and hydroxyl salt **3** (1 equiv). The reaction mixture was irradiated at 100 °C at the maximum power 35 W for 2 min. After completion of the reaction, the solvent was removed under reduce pressure. The crude product was purified by column chromatography over silica gel using DCM/methanol/7N methanolic NH_3 (96:3:1) as the eluent.

5-phenyl-*N*-(3-(4-phenyl-1*H*-1,2,3-triazol-1-yl)propyl)-1*H*-imidazol-2-amine (5a)



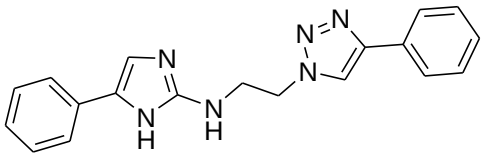
Yield: 90 %. ^{1}H NMR (300 MHz, DMSO-d_6): δ = 11.09 (brs, 1H), 8.63 (s, 1H), 7.85 (d, *J* = 7.2 Hz, 2H), 7.62 (d, *J* = 7.5, 2H), 7.45 (t, *J* = 7.9 Hz, 2H), 7.33 (m, 3H), 7.12 (t, *J* = 6.9 Hz, 2H), 6.30 (brs, 1H), 4.51 (t, *J* = 7.2 Hz, 2H), 3.23 (m, 2H), 2.17 (m, 2H). ^{13}C NMR (75.5 MHz, DMSO-d_6): δ = 150.3, 146.3, 133.0, 130.8, 128.9, 128.4, 127.8, 125.7, 125.1, 123.7, 121.4, 104.2, 47.4, 29.9. HRMS (EI) $C_{20}H_{20}N_6$, calcd 344.1749, found: 344.1754.

5-(4-Bromophenyl)-*N*-(2-(4-(4-methoxyphenyl)-1*H*-1,2,3-triazol-1-yl)ethyl)-1*H*-imidazol-2-amine (5b)



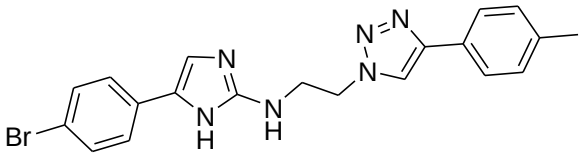
Yield: 66 %. ^{1}H NMR (300 MHz, DMSO-d_6): δ = 10.62 (brs, 1H), 8.45 (s, 1H), 7.43 (d, *J* = 8.8 Hz, 2H), 7.57 (d, *J* = 7.9 Hz, 2H), 7.43 (d, *J* = 8.8 Hz, 2H), 7.10 (s, 1H), 6.98 (d, *J* = 8.8 Hz, 2H), 6.02 (m, 1H), 4.60 (t, *J* = 5.90 Hz, 2H), 3.78 (s, 3H), 3.68 (m, 2H). ^{13}C NMR (75.5 MHz, DMSO-d_6): δ = 158.8, 150.0, 146.0, 131.0, 126.4 (×4), 125.5 (×2), 123.4, 120.7, 117.5, 114.2 (×4), 55.0, 49.2. 42.8. HRMS (EI) $C_{20}H_{19}BrN_6O$, calcd 438.0804, found: 438.0811.

5-Phenyl-*N*-(2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)ethyl)-1*H*-imidazol-2-amine (5c)



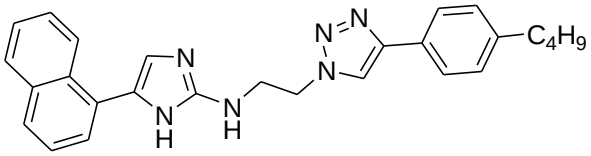
Yield: 84 %. ^{1}H NMR (300 MHz, DMSO-d_6): δ = 10.68 (brs, 1H), 8.57 (s, 1H), 7.82 (d, *J* = 7.3 Hz, 2H), 7.61 (m, 2H), 7.43 (t, *J* = 7.6 Hz, 2H), 7.28 (m, 3H), 7.06 (m, 2H), 6.01 (brs, 1H), 4.63 (t, *J* = 6.1 Hz, 2H), 3.70 (m, 2H). ^{13}C NMR (75.5 MHz, DMSO-d_6): δ = 150.3, 146.1, 130.4, 128.8 (×4), 128.2, 127.7, 125.1, 125.0 (×4), 123.4, 121.7, 104.1, 49.3. 42.9. HRMS (EI) $C_{19}H_{18}N_6$, calcd 330.1593, found: 330.1582.

5-(4-Bromophenyl)-*N*-(2-(4-p-tolyl-1*H*-1,2,3-triazol-1-yl)ethyl)-1*H*-imidazol-2-amine (5d)



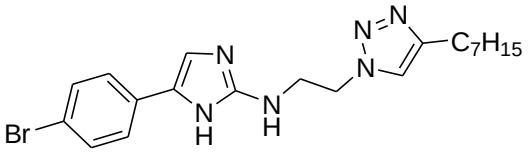
Yield: 73 %. ^{1}H NMR (300 MHz, DMSO-d_6): δ = 10.66 (brs, 1H), 8.50 (s, 1H), 7.70 (d, *J* = 8.07 Hz, 2H), 7.57 (d, *J* = 8.31 Hz, 2H), 7.43 (d, *J* = 8.56 Hz, 2H), 7.22 (d, *J* = 8.07 Hz, 2H), 7.13 (s, 1H), 6.03 (br s, 1H), 4.61 (t, *J* = 5.80 Hz, 2H), 3.68 (m, 2H), 2.32 (s, 3H). ^{13}C NMR (75.5 MHz, DMSO-d_6): δ = 150.4, 146.1, 136.9 (×2), 130.9 (×2), 129.3 (×4), 128.0, 125.3, 124.9 (×3), 121.2, 117.4, 49.2, 42,8, 20.7. HRMS (EI) $C_{20}H_{19}BrN_6$, calcd 422.0855, found: 422.0863.

***N*-(2-(4-(4-Butylphenyl)-1*H*-1,2,3-triazol-1-yl)ethyl)-5-(naphthalen-1-yl)-1*H*-imidazol-2-amine (5e)**



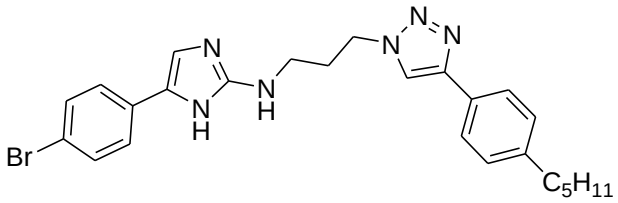
Yield: 64 %. ^{1}H NMR (300 MHz, DMSO-d_6): δ = 10.9 (brs, 1H), 8.54 (s, 1H), 8.14 (s, 1H), 7.73 (m, 6H), 7.37 (m, 2H), 7.23 (m, 3H), 6.01 (m, 1H), 4.68 (m, 2H), 3.74 (m, 2H), 2.58 (t, *J* = 7.4 Hz, 2H), 1.56 (m, 2H), 1.32 (m, 2H), 0.89 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (75.5 MHz, DMSO-d_6): δ = 150.7, 146.2, 141.8, 133.5, 131.3, 128.7 (×3), 128.3, 127.5, 127.3 (×3), 126.0, 125.0 (×3), 124.6, 123.2, 121.3, 120.2, 49.3, 42.9, 34.5, 32.9, 21.7, 13.7. HRMS (EI) $C_{27}H_{28}N_6$, calcd 436.2375, found: 436. 2349.

5-(4-Bromophenyl)-*N*-(2-(4-heptyl-1*H*-1,2,3-triazol-1-yl)ethyl)-1*H*-imidazol-2-amine (5f)



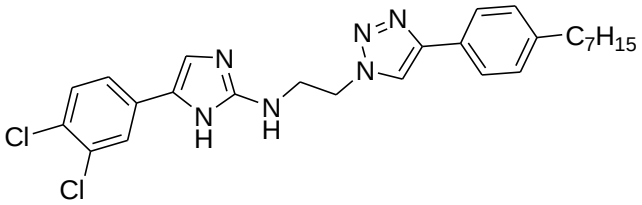
Yield: 73 %. ^{1}H NMR (300 MHz, DMSO-d_6): δ = 10.56 (brs, 1H), 7.82 (s, 1H), 7.59 (d, *J* = 8.2 Hz, 2H), 7.42 (d, *J* = 7.9 Hz, 2H), 7.13 (s, 1H), 5.93 (brs, 1H), 4.51 (t, *J* = 5.90 Hz, 2H), 3.60 (m, 2H), 2.57 (d, *J* = 7.7 Hz, 2H), 1.57 (m, 2H), 1.25 (m, 8H), 0.85 (t, *J* = 6.9 Hz, 3H). ^{13}C NMR (75.5 MHz, DMSO-d_6): δ = 150.5, 146.7 (×2), 131.0 (×3), 125.3, 121.9 (×2), 117.4, 104.1, 48.9, 42.9, 31.1, 28.9, 28.5, 28.4, 25.0, 22.0, 13.9. HRMS (EI) $C_{20}H_{27}BrN_6$, calcd 430.1481, found: 430.1488.

5-(4-Bromophenyl)-*N*-(3-(4-(4-pentylphenyl)-1*H*-1,2,3-triazol-1-yl)propyl)-1*H*-imidazol-2-amine (5g)



Yield: 80 %. ^{1}H NMR (300 MHz, DMSO-d_6): δ = 10.58 (brs, 1H), 8.55 (s, 1H), 7.72 (d, *J* = 8.06 Hz, 2H), 7.53 (d, *J* = 8.06 Hz, 2H), 7.38 (d, *J* = 8.27 Hz, 2H), 7.23 (d, *J* = 8.06 Hz, 2H), 7.11 (s, 1H), 5.96 (m, 1H), 4.47 (t, *J* = 6.57 Hz, 2H), 3.19 (m, 2H), 2.59 (t, *J* = 7.63 Hz, 2H), 2.14 (m, 2H), 1.59 (m, 2H), 1.30 (m, 4H), 0.86 (t, *J* = 6.78 Hz, 3H). ^{13}C NMR (75.5 MHz, DMSO-d_6): δ = 146.3, 142.9, 131.0 (×2), 128.7 (×4), 128.3, 125.4, 124.0 (×4), 121.0, 117.3 (×2), 47.3, 39.9, 34.8, 30.8, 30.5, 30.6, 21.9, 13.8. HRMS (EI) $C_{25}H_{29}BrN_{6.}$ calcd.492.1637, found: 492. 1621.

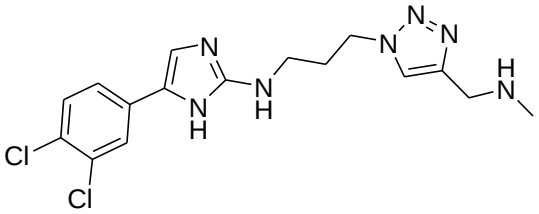
5-(3,4-Dichlorophenyl)-*N*-(2-(4-(4-heptylphenyl)-1*H*-1,2,3-triazol-1-yl)ethyl)-1*H*-imidazol-2-amine (5h)



Yield: 84 %. ^{1}H NMR (300 MHz, DMSO-d_6): δ = 10.66 (brs, 1H), 8.50 (s, 1H), 7.86 (s, 1H), 7.71 (d, *J* = 8.3 Hz, 2H), 7.62 (m, 1H), 7.48 (d, *J* = 8.3 Hz, 1H), 7.22 (d, *J* = 8.3 Hz, 3H), 6.06

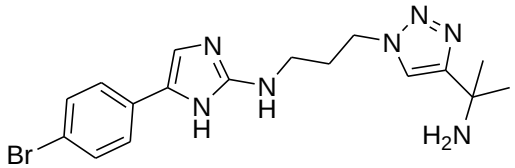
(m, 1H), 4.61 (t, *J* = 5.77 Hz, 2H), 3.69 (m, 2H), 2.58 (t, *J* = 7.58Hz, 2H), 1.57 (m, 2H), 1.28 (m, 8H), 0.86 (m, 3H). ^{13}C NMR (75.5 MHz, DMSO-d_6): δ = 146.1, 141.8, 130.9 (×2), 130.3, 128.6 (×3), 128.2 (×2), 126.5,124.9 (×3), 124.8, 124.7, 121.2, 49.2, 42.8, 34.8, 31.1, 30.7, 28.5, 28.4, 22.0, 13.8. HRMS (EI) $C_{26}H_{30}Cl_2N_6$, calcd 496.1909, found: 496.1919.

5-(3,4-Dichlorophenyl)-*N*-(3-(4-((methylamino)methyl)-1*H*-1,2,3-triazol-1-yl)propyl)-1*H*-imidazol-2-amine (5i)



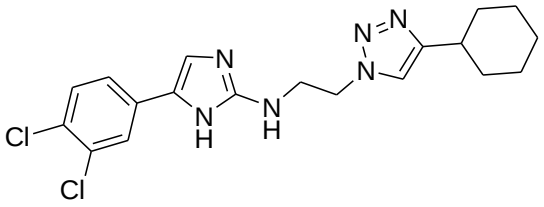
Yield: 81 %. ^{1}H NMR (300 MHz, DMSO-d_6): δ = 10.70 (brs, 1H), 7.99 (s, 1H), 7.82 (s, 1H), 7.58 (d, *J* = 8.7 Hz, 1H), 7.48 (d, *J* = 8.2 Hz, 1H), 7.23 (s, 1H), 6.01 (m, 1H), 4.41 (t, *J* = 6.95 Hz, 2H), 3.67 (m, 2H), 3.14 (m, 2H), 2.26 (s, 3H), 2.07 (t, *J* = 6.5 Hz, 2H), 1.86 (s,1H) ^{13}C NMR (75.5 MHz, DMSO-d_6): δ = 151.4, 145.9, 135.9, 130.9 (×2), 130.3, 126.4 (×2), 124.6, 123.4, 122.6, 47.0 (×2), 41.0, 35.4, 30.3. HRMS (EI) $C_{16}H_{19}Cl_2N_7$, calcd 389.1079, found: 389.1064.

***N*-(3-(4-(2-aminopropan-2-yl)-1*H*-1,2,3-triazol-1-yl)propyl)-5-(4-bromophenyl)-1*H*-imidazol-2-amine (5j)**



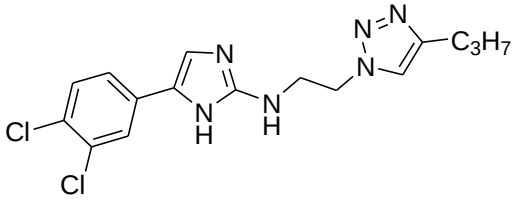
Yield: 75 %. ^{1}H NMR (300 MHz, DMSO-d_6): δ = 10.57 (brs, 1H), 7.92 (s, 1H), 7.55 (d, *J* = 8.3 Hz, 2H), 7.42 (d, *J* = 8.3 Hz, 2H), 7.11 (s, 1H), 5.94 (t, *J* = 5.6 Hz, 1H), 4.38 (t, *J* = 7.0 Hz, 2H), 4.10 (m, 2H), 3.16 (m, 2H), 2.07 (m, 2H), 1.37 (s, 6H). ^{13}C NMR (75.5 MHz, DMSO-d_6): δ = 156.0, 151.3, 134.0, 131.0 (×3), 125.3 (×2), 120.1 (×2), 117.3, 54.8, 48.5, 47.1, 30.8 (×2), 30.1. HRMS (EI) $C_{17}H_{22}BrN_7$, calcd 403.1120, found: 403.1131.

5-(3,4-Dichlorophenyl)-*N*-(2-(4-cyclohexyl-1*H*-1,2,3-triazol-1-yl)ethyl)-1*H*-imidazol-2-amine (5k)



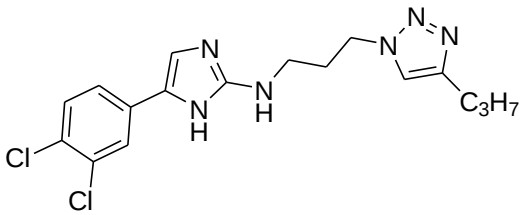
Yield: 89 %. ^{1}H NMR (300 MHz, DMSO-d_6): δ = 10.64 (brs, 1H), 7.58 (s, 1H), 7.80 (s, 1H), 7.60 (m, 1H), 7.48 (d, *J* = 8.3 Hz, 1H), 7.24 (s, 1H), 6.00 (m, 1H), 4.50 (t, *J* = 5.76 Hz, 2H), 3.61 (m, 2H), 2.61 (m, 1H), 1.91 (m, 2H), 1.69 (m, 3H), 1.32 (m,5H). ^{13}C NMR (75.5 MHz, DMSO-d_6): δ = 151.9, 150.6, 131.0 (×2), 130.3, 126.6 (×2), 124.7, 123.4, 120.7, 104.1, 54.8, 49.0, 42.8, 34.5, 32.4 (×2), 25.5 (×2). HRMS (EI) $C_{19}H_{22}Cl_2N_6$, calcd 404.1283, found: 404.1278.

5-(3,4-Dichlorophenyl)-*N*-(2-(4-propyl-1*H*-1,2,3-triazol-1-yl)ethyl)-1*H*-imidazol-2-amine (5l)



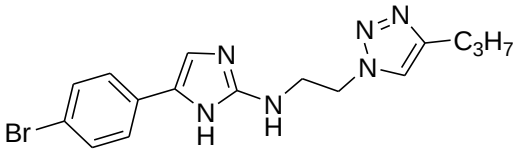
Yield: 85 %. ^{1}H NMR (300 MHz, DMSO-d_6): δ = 10.80 (brs, 1H), 7.84 (d, *J* = 1.7 Hz, 1H), 7.82 (s, 1H), 7.59 (dd, *J* = 8.4, 1.7 Hz, 1H), 7.53 (d, *J* = 8.4 Hz, 1H), 7.26 (s, 1H), 6.14 (br s, 1H), 4.51 (t, *J* = 6.04 Hz, 2H), 3.62(m, 2H), 2.56 (t, *J* = 7.49 Hz, 2H), 1.57 (m, 2H), 0.89 (t, *J* = 7.25 Hz, 3H). ^{13}C NMR (75.5 MHz, DMSO-d_6): δ = 150.4, 146.5, 135.0, 131.0 (×2), 130.4 126.8 (×2), 124.8, 123.5, 122.0, 48.8, 42.8, 27.0, 22.0, 13.6. HRMS (EI) $C_{16}H_{18}Cl_2N_6$, calcd 364.0970, found: 364.0980.

5-(3,4-Dichlorophenyl)-*N*-(3-(4-propyl-1*H*-1,2,3-triazol-1-yl)propyl)-1*H*-imidazol-2-amine (5m)



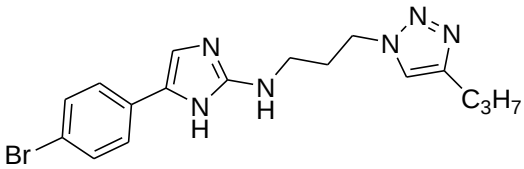
Yield: 91 %. ^{1}H NMR (300 MHz, DMSO-d_6): δ = 10.80 (brs, 1H), 7.88 (s, 1H), 7.83 (d, *J* = 1.7 Hz 1H), 7.58 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.52 (s, 1H), 7.49 (s, 1H), 6.13 (br s, 1H), 4.38 (t, *J* = 6.98 Hz, 2H), 3.15 (m, 2H), 2.57 (t, *J* = 7.51 Hz, 2H), 2.06 (m, 2H), 1.58 (m, 2H), 0.89 (t, *J* = 7.51 Hz, 3H). ^{13}C NMR (75.5 MHz, DMSO-d_6): δ = 150.0, 146.6, 135.1, 131.0 (×2), 130.3 126.8 (×2), 124.8, 123.5, 121.7, 54.8, 46.9, 30.0, 27.0, 22.2, 13.5. HRMS (EI) $C_{17}H_{20}Cl_2N_6$, calcd 378.1127, found: 378.1114.

5-(4-Bromophenyl)-*N*-(2-(4-propyl-1*H*-1,2,3-triazol-1-yl)ethyl)-1*H*-imidazol-2-amine (5n)



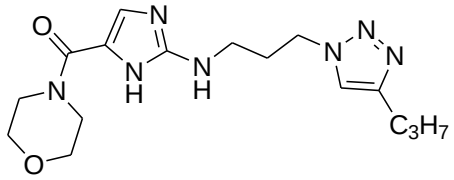
Yield: 94 %. ^{1}H NMR (300 MHz, DMSO-d_6): δ = 10.63 (brs, 1H), 7.87(s, 1H), 7.62 (m, 2H), 7.48 (d, *J* = 8.6 Hz, 2H), 7.17 (s, 1H), 5.98 (t, *J* = 5.3 Hz, 1H), 4.59 (t, *J* = 6.04 Hz, 2H), 3.66 (m, 2H), 2.61 (t, *J* = 7.44 Hz, 2H), 1.62 (m, 2H), 0.94 (t, *J* = 7.21 Hz, 3H). ^{13}C NMR (75.5 MHz, DMSO-d_6): δ = 150.5, 146.5, 134.6, 131.0 (×3), 125.4 (×2), 122.0 (×2), 117.4, 48.9, 42.9, 27.0, 22.2, 13.6. HRMS (EI) $C_{16}H_{19}BrN_6$, calcd 374.0855, found: 374.0844.

5-(4-Bromophenyl)-*N*-(3-(4-propyl-1*H*-1,2,3-triazol-1-yl)propyl)-1*H*-imidazol-2-amine (5o)



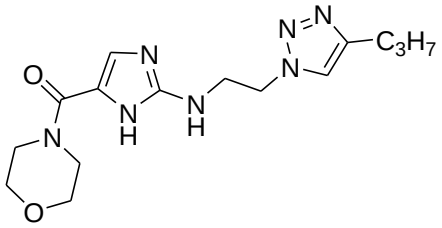
Yield: 75 %. ^{1}H NMR (300 MHz, DMSO-d_6): δ = 10.59 (brs, 1H), 7.89 (s, 1H), 7.55 (d , *J* = 8.1 Hz, 2H), 7.42 (d, *J* = 8.4 Hz, 2H), 7.11 (s, 1H), 5.93 (t, *J* = 5.25 Hz, 1H), 4.38 (t, *J* = 6.83 Hz, 2H), 3.14 (m, 2H), 2.48 (t, *J* = 7.62 Hz, 2H), 2.06 (m, 2H), 1.58 (m, 2H), 0.90 (t, *J* = 7.35 Hz, 3H). ^{13}C NMR (75.5 MHz, DMSO-d_6): δ = 151.1, 146.6, 134.6, 131.0 (×3), 125.4 (×2), 121.7 (×2), 117.4, 47.9, 30.0, 27.0 (×2), 22.2, 13.5. HRMS (EI) $C_{17}H_{21}BrN_6$, calcd 388.1011, found: 388.1023.

(2-(3-(4-Propyl-1*H*-1,2,3-triazol-1-yl)propylamino)-1*H*-imidazol-5-yl)(morpholino)methanone (5p)



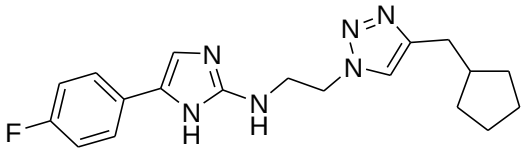
Yield: 45 %. ^{1}H NMR (300 MHz, DMSO-d_6): δ = 10.02 (brs, 1H), 7.85 (s, 1H), 7.10 (s, 1H), 6.05 (m, 1H), 4.35 (t, *J* = 6.8 Hz, 2H), 3.75 (m, 4H), 3.57 (t, *J* = 4.31 Hz, 4H), 3.10 (m, 2H), 2.57 (t, *J* = 7.42 Hz, 2H), 2.05 (m, 2H), 1.60 (m, 2H), 0.90 (t, *J* = 7.42 Hz, 3H). ^{13}C NMR (75.5 MHz, DMSO-d_6): δ = 161.2, 150.1, 146.6, 122.8, 121.7 (×2), 66.3 (×2), 54.8 (×2), 46.9, 44.4, 29.9, 27.0, 22.2, 13.5. HRMS (EI) $C_{16}H_{25}N_7O_2$, calcd 347.2070, found: 347.2085.

(2-(2-(4-Propyl-1*H*-1,2,3-triazol-1-yl)ethylamino)-1*H*-imidazol-5-yl)(morpholino)methanone (5q)



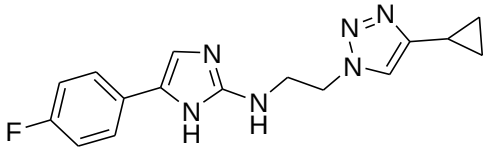
Yield: 39 %. ^{1}H NMR (300 MHz, DMSO-d_6): δ = 10.89 (brs, 1H), 7.78 (s, 1H), 7.08 (s, 1H), 5.98 (m, 1H), 4.45 (m, 2H), 3.74 (m, 3H), 3.58 (m, 6H), 3.16 (m, 1H), 2.56 (m, 2H), 1.57 (m, 2H), 0.89 (t, *J* = 7.25 Hz, 3H). ^{13}C NMR (75.5 MHz, DMSO-d_6): δ = 161.4, 149.7, 146.5 (×2), 121.9 (×2), 66.3 (×2), 48.7 (×2), 44.4, 44.7, 27.0, 22.2, 13.6. HRMS (EI) $C_{15}H_{23}N_7O_2$, calcd 333.1913, found: 333.1920.

***N*-(2-(4-(Cyclopentylmethyl)-1*H*-1,2,3-triazol-1-yl)ethyl)-5-(4-fluorophenyl)-1*H*-imidazol-2-amine (5r)**



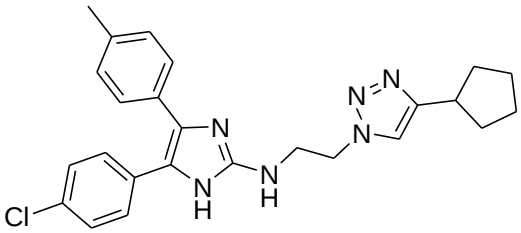
Yield: 68 %. ^{1}H NMR (300 MHz, DMSO-d_6): δ = 10.63 (brs, 1H), 7.82 (s, 1H), 7.63 (q, *J* = 2.9, 5.7 Hz, 2H), 7.11 (t, *J* = 8.7 Hz, 2H), 7.03 (s, 1H), 5.96 (t, *J* = 5.4 Hz, 1H), 4.51 (t, *J* = 5.99 Hz, 2H), 3.61 (m, 2H), 2.59 (d, *J* = 7.08 Hz, 2H), 2.07 (m, 1H), 1.66 (m, 6H), 1.70 (m, 2H). ^{13}C NMR (75.5 MHz, DMSO-d_6): δ = 161.8, 158.6, 150.3, 146.2, 146.1, 130.9, 125.2, 125.1, 122.2, 115.1, 114.8, 48.9, 42.9, 31.8 (×3), 31.0, 24.5 (×2). HRMS (EI) $C_{19}H_{23}FN_6$, calcd 354.1968, found: 354.1974.

_N_-(2-(4-Cyclopropyl-1_H_-1,2,3-triazol-1-yl)ethyl)-5-(4-fluorophenyl)-1_H_-imidazol-2-amine (5s)



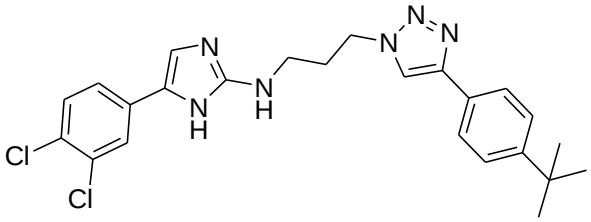
Yield: 80 %. ^{1}H NMR (300 MHz, DMSO-d_6): δ = 10.55 (brs, 1H), 7.79 (s, 1H), 7.64 (m, 2H), 7.10 (t , J = 8.7 Hz, 2H), 7.02 (s, 1H), 5.90 (m, 1H), 4.99 (t, J = 5.85 Hz, 2H), 3.61 (m, 2H), 1.91 (m, 1H), 0.85 (m, 2H), 0.69 (m, 2H). ^{13}C NMR (75.5 MHz, DMSO-d_6): δ = 161.8, 158.6, 150.4, 148.6 (×2), 131.1, 125.1, 125.0, 120.9, 115.1, 114.8, 48.9, 42.9, 7.6(×2), 6.5. HRMS (EI) $C_{16}H_{17}FN_6$, calcd 312.1499, found: 312.1487.

5-(4-Chlorophenyl)-_N_-(2-(4-cyclopentyl-1_H_-1,2,3-triazol-1-yl)ethyl)-4-_p_-tolyl-1_H_-imidazol-2-amine (5t)



Yield: 56 %. ^{1}H NMR (300 MHz, DMSO-d_6): δ = 10.89 (brs, 1H), 7.84 (s, 1H), 7.40 (m, 2H), 7.29 (m, 4H), 7.14 (m, 2H), 5.87 (m, 1H), 4.52 (t, J = 5.87 Hz, 2H), 3.64 (m, 2H), 3.06 (m, 1H), 2.29 (s, 3H), 1.95 (m, 2H), 1.60 (m, 6H). ^{13}C NMR (75.5 MHz, DMSO-d_6): δ = 150.9, 150.1, 135.7, 130.0, 128.9 (×3), 128.1 (×3), 128.0 (×2), 127.2 (×3), 121.1, 104.1, 49.0, 42.7, 36.1, 32.7 (×2), 24.6 (×2), 20.7. HRMS (EI) $C_{25}H_{27}ClN_6$ calcd.446.1986, found: 446.1990.

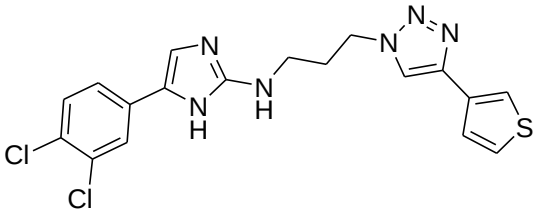
_N_-(3-(4-(4-_tert_-Butylphenyl)-1_H_-1,2,3-triazol-1-yl)propyl)-5-(3,4-dichlorophenyl)-1_H_-imidazol-2-amine (5u)



Yield: 85 %. ^{1}H NMR (300 MHz, DMSO-d_6): δ = 10.68 (brs, 1H), 8.53 (s, 1H), 7.82 (s, 1H), 7.73 (d, J = 7.9 Hz, 2H), 7.57 (m, 1H), 7.43 (m, 3H), 7.25 (s, 1H) 6.02 (m, 1H), 4.48 (t, J =

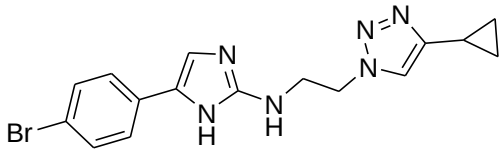
6.73 Hz, 2H), 3.20 (m, 2H), 2.14 (m, 2H), 1.30 (s, 9H). ^{13}C NMR (75.5 MHz, DMSO-d_6): δ = 150.2, 146.2, 131.0, 130.3, 128.0, 126.6, 125.5 (×3), 124.8 (×3), 124.7, 123.4, 121.0 (×2), 104.1, 47.3, 39.6, 34.2, 31.0 (×3), 29.9. HRMS (EI) $C_{24}H_{26}Cl_2N_6$, calcd 468.1596, found: 468.1602.

5-(3,4-Dichlorophenyl)-*N*-(3-(4-(thiophen-3-yl)-1*H*-1,2,3-triazol-1-yl)propyl)-1*H*-imidazol-2-amine (5v)



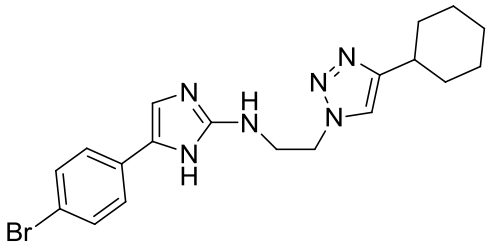
Yield: 91 %. ^{1}H NMR (300 MHz, DMSO-d_6): δ = 10.67 (brs, 1H), 8.46 (s, 1H), 7.82 (m, 2H), 7.63 (m, 1H), 7.58 (m, 1H), 7.51 (m, 2H), 7.26 (s, 1H) 6.02 (m, 1H), 4.47 (t, *J* = 6.8 Hz, 2H), 3.19 (m, 2H), 2.14 (m, 2H). ^{13}C NMR (75.5 MHz, DMSO-d_6): δ = 151.3, 142.8, 132.1 (×2), 131.0, 130.0, 127.0, 126.5, 125.7, 124.7, 123.4, 121.1, 120.6 (×2), 104.1, 47.3, 39.5, 29.9. HRMS (EI) $C_{18}H_{16}Cl_2N_6S$, calcd 418.0534, found: 418.0522.

5-(4-Bromophenyl)-*N*-(2-(4-cyclopropyl-1*H*-1,2,3-triazol-1-yl)ethyl)-1*H*-imidazol-2-amine (5w)



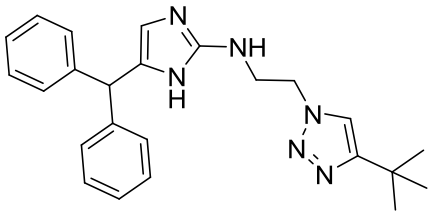
Yield: 80 %. ^{1}H NMR (300 MHz, DMSO-d_6): δ = 10.56 (brs, 1H), 7.80 (s, 1H), 7.60 (d, *J* = 7.3 Hz, 2H), 7.43 (d, *J* = 7.3 Hz, 2H), 7.14 (s, 1H), 5.93 (m, 1H), 4.49 (t, *J* = 5.48 Hz, 2H), 3.59 (m, 2H), 3.16 (dd, *J* = 5.2, 1.4 Hz, 1H), 0.87 (m, 2H), 0.69 (m, 2H). ^{13}C NMR (75.5 MHz, DMSO-d_6): δ = 150.4, 148.7 (×3), 131.0, 130.9, 125.3, 120.9 (×3), 117.4, 48.9, 42.8, 7.5 (×2), 6.5. HRMS (EI) $C_{16}H_{17}BrN_6$, calcd 372.0698, found: 372.0689.

5-(4-Bromophenyl)-*N*-(2-(4-cyclohexyl-1*H*-1,2,3-triazol-1-yl)ethyl)-1*H*-imidazol-2-amine (5x)



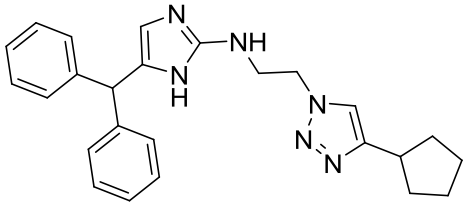
Yield: 71 %. ^{1}H NMR (300 MHz, DMSO-d_6): δ = 10.61 (brs, 1H), 7.81 (s, 1H), 7.57 (m, 2H), 7.45 (d, J = 8.3 Hz), 7.13 (s, 1H), 5.96 (brs, 1H), 4.49 (m, 2H), 3.62 (m, 2H), 2.62 (m, 1H), 1.91 (m, 2H), 1.71 (m, 3H), 1.37-1.17 (m, 5H). ^{13}C NMR (75.5 MHz, DMSO-d_6): δ = 152.0, 131.1 (×2), 125.5, 120.8, 117.5, 49.0, 43.0, 34.6, 32.5 (×2), 25.6 (×2). HRMS (EI) $C_{19}H_{23}BrN_6$, calcd 414.1168, found: 414.1175.

5-benzhydryl-*N*-(2-(4-tert-butyl-1*H*-1,2,3-triazol-1-yl)ethyl)-1*H*-imidazol-2-amine (5y)



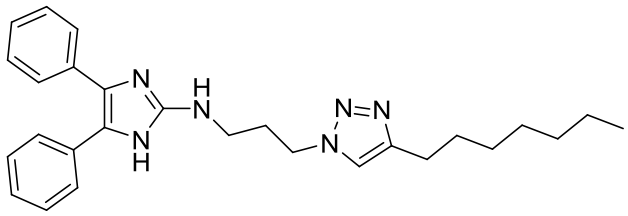
^{1}H NMR (300 MHz, DMSO-d_6): δ = 7.77 (s, 1H), 7.28-7.21 (m, 10H), 6.25 (s, 1H), 5.98 (brs, 1H), 5.17 (s, 1H), 4.43 (m, 2H), 3.53 (m, 2H), 1.25 (s, 9H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 144.4 (x2), 129.1 (x4), 128.5(x4), 126.4 , 120.4 , 117.2, 113.2, 110.9, 109.0, 104.6, 50.2, 49.4, 47.4, 43.4, 30.8 (x3). HRMS (EI) $C_{24}H_{28}N_6$, calcd 400.2375, found: 400.2369.

5-benzhydryl-*N*-(2-(4-cyclopentyl-1*H*-1,2,3-triazol-1-yl)ethyl)-1*H*-imidazol-2-amine (5z):



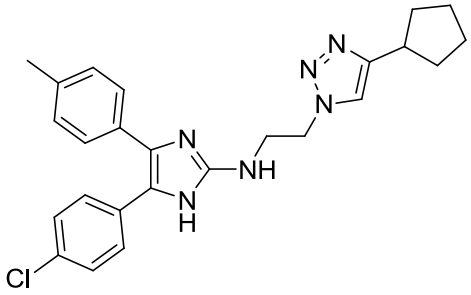
^{1}H NMR (300 MHz, DMSO-d_6): δ = 7.78 (s, 1H), 7.29-7.14 (m, 10H), 5.98 (s,1H), 5.17 (s, 1H), 4.43 (m, 2H), 3.52 (m, 2H), 3.09 (m, 1H), 1.66 (m, 2H), 1.63 (m, 6H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 151.5, 150.5, 144.5 (x2), 129.1 (x4), 128.5(x4) , 126.4 (x2), 1221.5, 50.3, 49.5, 43.5, 38.7, 33.3 (x2), 25.2 (x2). HRMS (EI) $C_{25}H_{28}N_6$, calcd 412.2375, found: 412.2380.

***N*-(3-(4-Heptyl-1*H*-1,2,3-triazol-1-yl)propyl)-4,5-diphenyl-1*H*-imidazol-2-amine (5aa)**



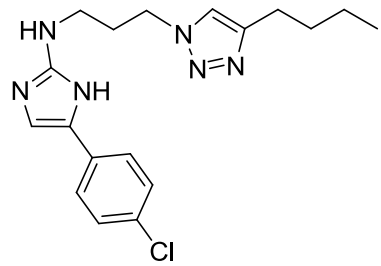
Yield: 84 %. ^{1}H NMR (300 MHz, DMSO-d_6): δ = 9.54 (brs, 1H), 8.13-6.97 (m, 11H), 6.26 (brs, 1H), 4.45 (m, 2H), 3.65 (m, 2H), 2.57 (m,2H), 2.24 (m, 2H), 1.53 (m, 4H), 1.24 (m, 6H), 0.85 (m, 3H). ^{13}C NMR (75.5 MHz, DMSO-d_6): δ = 177.2, 166.8, 156.3, 137.3, 135.5, 133.7, 132.0, 129.6, 129.1, 128.1, 127.4, 126.7, 121.8, 47.1, 31.2, 29.4, 28.9, 28.6, 28.4, 25.1, 22.1, 13.9. HRMS (EI) $C_{27}H_{34}N_6$, calcd 442.2845, found: 442.2833.

5-(4-chlorophenyl)-*N*-(2-(4-cyclopentyl-1*H*-1,2,3-triazol-1-yl)ethyl)-4-*p*-tolyl-1*H*-imidazol-2-amine (5ab)



^{1}H NMR (300 MHz, DMSO-d_6): δ = 10.92 (brs, 1H), 7.85 (s, 1H), 7.40 (m, 2H), 7.30 (m, 4H), 7.13 (m, 2H), 6.25 (s, 1H), 4.52 (m, 2H), 3.67 (m, 2H), 3.07 (m, 1H), 1.93 (m, 2H), 1.62 (m, 6H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 151.5, 150.6, 136.3, 130.6, 129.5 (x2), 128.7 (x5), 127.7 (x4), 121.6, 104.6, 49.6, 43.3, 36.7, 33.3 (x2), 25.2 (x2), 21.3. HRMS (EI) $C_{25}H_{27}N_6Cl$, calcd 446.1986, found: 446.1974.

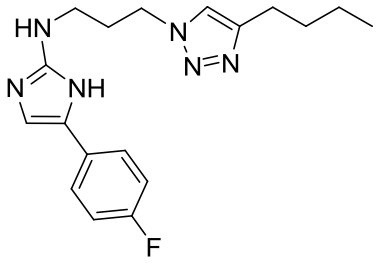
***N*-(3-(4-butyl-1*H*-1,2,3-triazol-1-yl)propyl)-5-(4-chlorophenyl)-1*H*-imidazol-2-amine (5ac):**



^{1}H NMR (300 MHz, DMSO-*d*6) δ= 7.89 (s, 1H), 7.63 (d, *J* = 8.7 Hz, 2H) , 7.34 (d, *J* = 8.7 Hz, 2H), 7.16 (s, 1H), 6.17 (br s, 1H), 4.38 (t, 2H), 3.17 (m, 2H), 2.60 (t, 2H), 2.08 (m, 2H), 1.57 (m, 2H), 1.32 (m, 2H), 0.89 (t, 3H). ^{13}C NMR (75,5 MHz, DMSO-*d*6) δ= 159.0, 149.5,

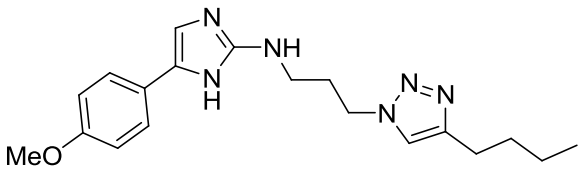
146.9 (x2), 130.6, 128.5(x2), 125.6 (x2), 121.7, 110.6, 46.8, 31.1, 29.7, 24.7, 21.7, 17.6, 13.7. HRMS (EI) $C_{18}H_{23}N_6Cl$, calcd 358.1673, found: 358.1647.

_N_-(3-(4-butyl-1_H_-1,2,3-triazol-1-yl)propyl)-5-(4-fluorophenyl)-1_H_-imidazol-2-amine (5ad):



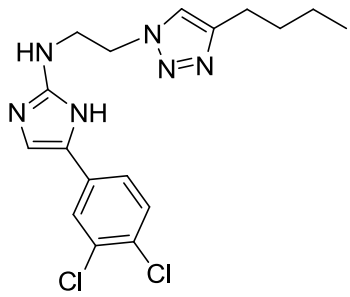
^{1}H NMR (300 MHz, DMSO *d*6) δ7.89 (s,1H), 7.64 (m, 2H), 7.12 (m, 3H), 6.25 (br s, 1H), 4.39 (m, 2H), 3.17 (m, 2H), 2.60 (t, 2H), 2.09 (m, 2H), 1.57 (m, 2H), 1.32 (m, 2H), 0.89 (t, 3H). ^{13}C NMR (75,5 MHz, DMSO-*d*6) δ 159.7, 148.4, 146.9, 128.1 (x2), 126.4 (x2), 121.8, 115.8, 115.5, 109.7, 46.7, 31.1 (x2) , 29.5, 24.7, 21.7, 13.7. HRMS (EI) $C_{18}H_{23}N_6F$, calcd 342.1968, found: 342.1966.

_N_-(3-(4-butyl-1_H_-1,2,3-triazol-1-yl)propyl)-5-(4-methoxyphenyl)-1_H_-imidazol-2-amine (5ae):



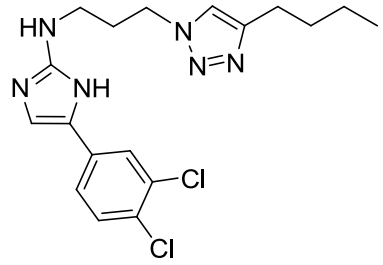
^{1}H NMR (300 MHz, DMSO *d*6) 7.63 (s, 1H), 7.15 (d, *J*=9.0, 1H), 6.90 (d, *J*=9.0, 1H), 6.43 (s, 1H), 4.20 (m, 2H), 3.77 (s, 3H), 3.74 (m, 2H), 2.58 (m, 2H), 2.06 (m, 2H), 1.53 (m, 2H), 1.31 (m, 2H), 0.88 (m, 3H), ^{13}C NMR (75,5 MHz, DMSO-*d*6) δ 158.1 (x2), 150.2, 146.9, 128.8 (x2), 126.9, 123.2, 121.5, 114.1 (x2), 55.0, 46.5, 31.0 (x2), 29.5, 24.7, 21.7, 13.6. HRMS (EI) $C_{19}H_{26}N_6O$, calcd 354.2168, found: 354.2164.

_N_-(2-(4-butyl-1_H_-1,2,3-triazol-1-yl)ethyl)-5-(3,4-dichlorophenyl)-1_H_-imidazol-2-amine (5af):



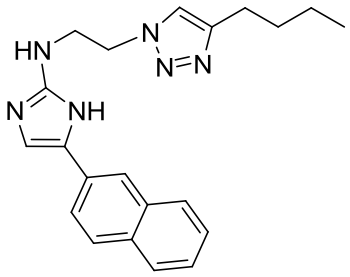
^{1}H NMR (75,5 MHz, DMSO-D6) δ 7.84 (m, 2H), 7.62 (m, 1H), 7.50 (m, 1H), 7.26 (s, 1H), 6.25 (m, 1H), 6.00 (m, 1H), 4.51(t, 2H), 3.62 (m, 2H), 2.59 (t, 2H), 1.53 (m, 2H), 1.30 (m, 2H), 0.87 (t, 3H); ^{13}C NMR (75,5 MHz, DMSO-*d*6) δ 150.7, 146.7 (x2), 131.1, 130.4, 126.6, 124.7, 122.2, 121.9(x2), 104.1, 49.0, 42.9, 31.1, 24.7, 21.7, 13.7. HRMS (EI) $C_{17}H_{20}N_6Cl_2$, calcd 378.1127, found: 378.1127.

_N_-(3-(4-butyl-1_H_-1,2,3-triazol-1-yl)propyl)-5-(3,4-dichlorophenyl)-1_H_-imidazol-2-amine (5ag):



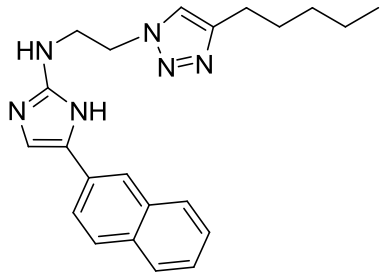
^{1}H NMR (300 MHz, DMSO-*d*6) δ 10.69 (br s, 1H), 7.88 (s, 1H), 7.83 (d, *J*=1.7, 1H), 7.60 (dd, *J*=8.3, 1.7, 1H), 7.50 (d, *J*=8.3, 1H), 7.25 (s, 1H), 6.01 (brs, 1H), 4.38 (m, 2H), 3.12 (m, 2H), 2.61 (m, 2H), 2.07 (m, 2H), 1.56 (m, 2H), 1.31 (m, 2H), 0.88 (m, 3H). ^{13}C NMR (75,5 MHz, DMSO-*d*6) δ 156.9, 146.8 (x2), 139.7, 130.9, 130.6, 130.1 (x2), 129.2, 121.7 (x2), 46.8, 31.1, 30.1, 29.2, 24.7, 21.7, 13.7. HRMS (EI) $C_{18}H_{22}N_6Cl_2$, calcd 392.1283, found: 392.1281.

_N_-(2-(4-butyl-1_H_-1,2,3-triazol-1-yl)ethyl)-5-(naphthalen-2-yl)-1_H_-imidazol-2-amine (5ah):



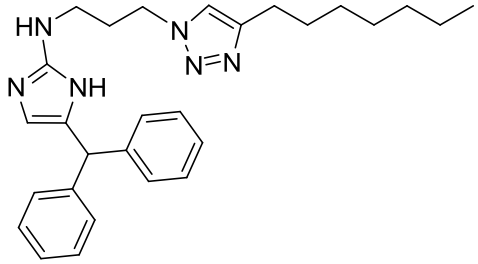
^{1}H NMR (75,5 MHz, DMSO-*d*6) δ 8.11 (s, 1H), 7.87-7.80 (m, 5H), 7.52-7.40 (m, 2H), 7.3 (s, 1H), 6.38 (br s, 1H), 4.58 (m, 2H), 3.70 (m, 2H), 2.61 (m, 2H), 1.57 (m, 2H), 1.30 (m, 2H), 0.88 (m, 3H). ^{13}C NMR (75,5 MHz, DMSO-*d*6) δ 149.9, 146.8, 133.3, 131.9, 131.7, 127.9, 127.6, 127.5, 127.0, 126.3, 125.2, 123.2, 122.1, 120.9, 104.2, 48.9, 49.2, 31.1, 24.7, 21.7, 13.7. HRMS (EI) $C_{21}H_{24}N_6$, calcd 360.2062, found: 360.2038.

5-(naphthalen-2-yl)-*N*-(2-(4-pentyl-1*H*-1,2,3-triazol-1-yl)ethyl)-1*H*-imidazol-2-amine (5ai):



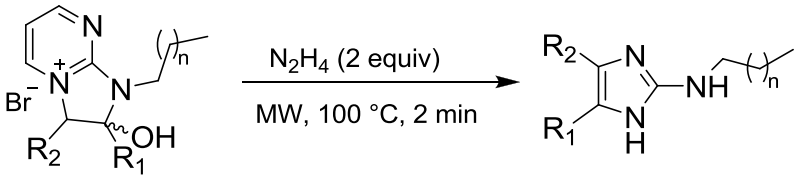
^{1}H NMR (75,5 MHz, DMSO-D6) δ 8.10 (m, 1H), 7.87-7.83 (m, 5H), 7.50-7.39 (m, 2H), 7.26 (s, 1H), 6.20 (brs, 1H), 4.57 (m, 2H), 3.72 (m, 2H), 2.60 (m, 2H), 1.59 (m, 2H), 1.30 (m, 4H), 0.86 (m, 3H); ^{13}C NMR (75,5 MHz, DMSO-*d*6) δ 150.8, 146.8 (x2), 133.5 (x2), 131.4 (x3), 127.5, 126.1, 124.7, 123.3, 122.0, 120.3, 104.2, 49.0, 43.0, 28.7, 25.0, 21.9, 18.5, 13.9. HRMS (EI) $C_{22}H_{26}N_6$, calcd 374.2219, found: 374.2220.

5-benzhydryl-*N*-(3-(4-heptyl-1*H*-1,2,3-triazol-1-yl)propyl)-1*H*-imidazol-2-amine (5aj):



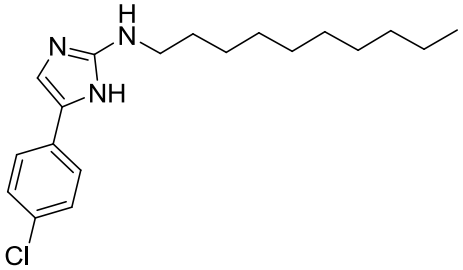
^{1}H NMR (300 MHz, DMSO-*d*6) δ 7.77 (s, 1H), 7.27 (m, 10H), 6.06 (s, 1H), 5.22 (m, 1H), 4.46 (m, 2H), 3.56 (m, 2H), 3.44 (m, 2H), 2.58 (m, 2H), 1.27 (m, 6H), 0.87 (m, 3H). ^{13}C NMR (75,5 MHz, DMSO-*d*6) δ 150.5, 147.2(x2), 129.1(x4), 128.5(x4), 126.4, 122.4, 104.6 (x2), 49.4, 43.5, 31.7, 29.5, 29.1, 28.9, 25.5, 22.5, 14.4. HRMS (EI) $C_{27}H_{34}N_6$, calcd 442.2845, found: 442.2829.

General Procedure for the Preparation of 2-AIT 6a-h.



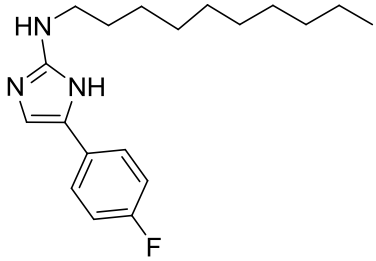
To the suspension of hydroxyl salt (1 equiv) were added hydrazine hydride (5 equiv). The reaction mixture was irradiated at 100 °C at the maximum power 35 W for 2 min. After completion of the reaction, the solvent was removed under reduce pressure. The crude product was purified by column chromatography over silica gel using DCM/methanol/7N methanolic NH_3 (96:3:1) as the eluent.

5-(4-chlorophenyl)-*N*-decyl-1*H*-imidazol-2-amine (6a)



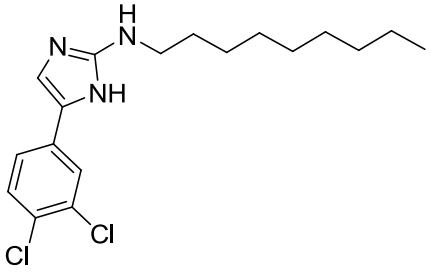
^{1}H NMR (300 MHz, DMSO-*d*6) δ 10.53 (br s, 1H), 7.62 (d, *J* = 8.67, 2H), 7.31 (d, *J* = 8.67, 2H), 7.07 (s, 1H), 5.72 (m, 1H), 3.11 (m, 2H), 1.50 (m, 2H), 1.25 (m, 14H), 0.85 (m, 3H). ^{13}C NMR (75,5 MHz, DMSO-*d*6) δ 140.1, 133.4, 131.0, 130.2, 128.1, 127.8, 104.1, 31.3, 29.5, 29.1, 29.0, 28.8, 28.7, 26.5, 26.1, 22.1, 13.9.

***N*-decyl-5-(4-fluorophenyl)-1*H*-imidazol-2-amine (6b)**



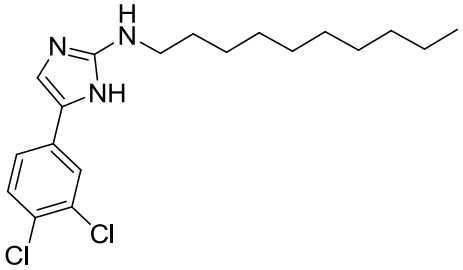
^{1}H NMR (300 MHz, DMSO-*d*6) δ 10.52 (br s, 1H), 7.62 (m, 2H), 7.09 (m, 2H), 7.00 (s, 1H), 5.73 (m, 1H), 3.11 (m, 2H), 1.50 (m, 2H), 1.25 (m, 14H), 0.85 (m, 3H). ^{13}C NMR (75,5 MHz, DMSO-*d*6) δ 174.0, 157.0, 131.5, 130.3, 129.3, 114.9, 104.2, 31.3, 29.5, 29.1, 29.0, 28.9, 28.7, 26.5, 26.1, 22.1, 13.9.

5-(3,4-dichlorophenyl)-*N*-nonyl-1*H*-imidazol-2-amine (6d)



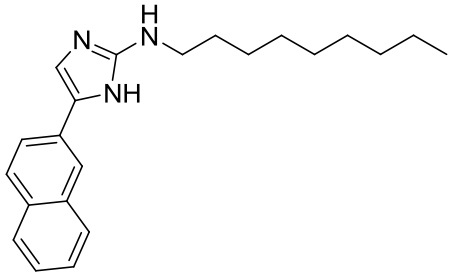
^{1}H NMR (300 MHz, DMSO-*d*6) δ 7.82 (s, 1H), 7.58 (d, *J*=8.67, 1H), 7.48 (d, *J*=8.67, 1H), 7.21 (s, 1H), 6.25 (brs, 1H), 5.80 (m, 1H), 3.13 (m, 2H), 1.51 (m, 2H), 1.25 (br, 12H), 0.85 (m, 3H).

***N*-decyl-5-(3,4-dichlorophenyl)-1*H*-imidazol-2-amine (6e)**



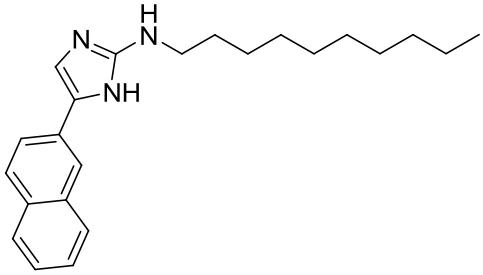
^{1}H NMR (300 MHz, DMSO-*d*6) δ 10.54 (br s, 1H), 7.82 (s, 1H), 7.57 (d, *J* = 8.67, 1H), 7.48 (d, *J* = 8.67, 1H), 7.21 (s, 1H), 5.80 (m, 1H), 3.14 (m, 2H), 1.52 (m, 2H), 1.25 (m, 14H), 0.85 (m, 3H). ^{13}C NMR (75,5 MHz, $CDCl_3$) δ 151.6, 133.7, 133.4, 132.6, 130.5, 129.5, 125.7, 123.3, 105.2, 44.2, 31.9, 29.9, 29.6 (×2), 29.4, 29.3, 26.9, 22.7, 14.1.

5-(naphthalen-2-yl)-*N*-nonyl-1*H*-imidazol-2-amine (6f)



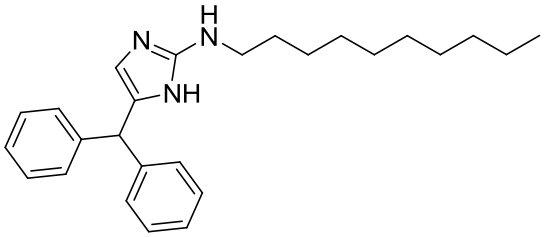
^{1}H NMR (300 MHz, DMSO-*d*6) δ 10.51(br s, 1H), 8.05 (s, 1H), 7.82 (m, 3H), 7.39 (m, 3H) 7.17 (s, 1H), 5.73 (t, 1H), 3.18 (q, 2H), 1.53 (m, 2H), 1.31-1.26 (br, 12H), 0.84 (m, 3H). ^{13}C NMR (75,5 MHz, $CDCl_3$) δ 146.5, 135.0, 132.8, 132.5, 130.2, 129.5, 129.4, 129.2, 128.4, 127.6, 126.5, 126.1, 105.0, 31.9, 29.6, 29.5, 29.4, 29.3 (×2), 29.2, 22.7, 14.1.

***N*-decyl-5-(naphthalen-2-yl)-1*H*-imidazol-2-amine (6g)**



^{1}H NMR (300 MHz, DMSO-*d*6) δ 8.06 (s, 1H), 7.82 (m, 4H), 7.42 (m, 2H), 7.19 (s, 1H), 5.80 (m, 1H), 3.18 (m, 2H), 1.55 (m, 2H), 1.25 (br, 14H), 0.85 (m, 3H).

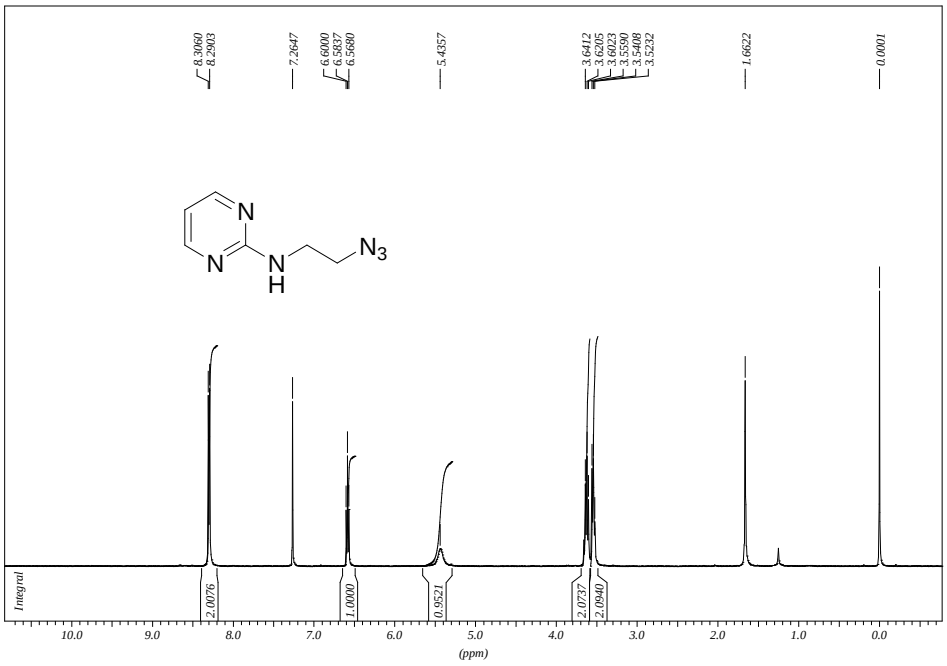
5-benzhydryl-*N*-decyl-1*H*-imidazol-2-amine (6h):

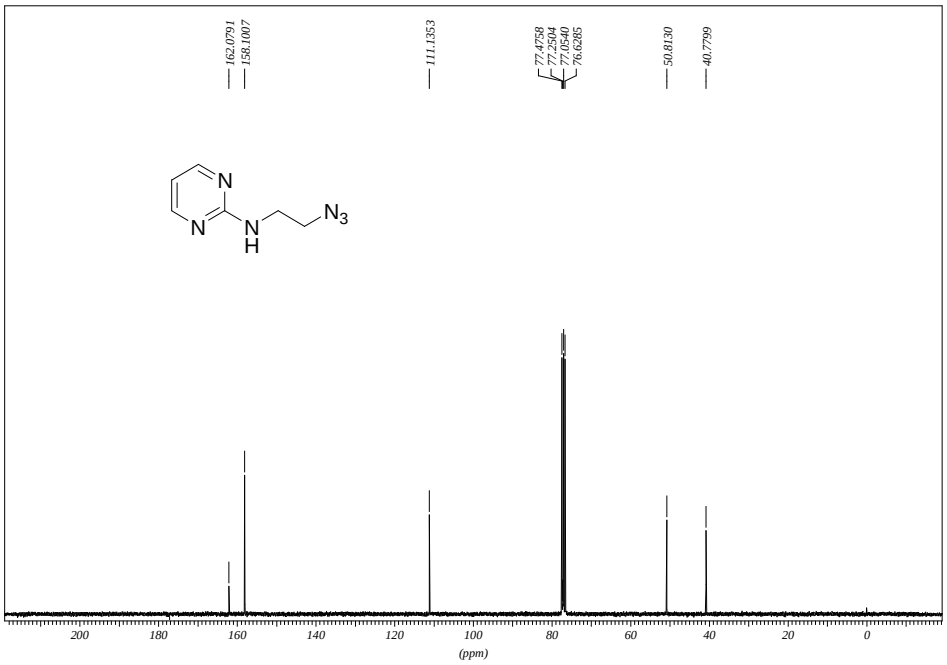


^{1}H NMR (300 MHz, DMSO-*d*6) δ 7.23 (m, 10H), 5.99 (s, 1H), 5.18 (s, 1H), 3.05 (m, 2H), 1.46 (m, 2H), 1.24 (br, 18H), 0.85 (m, 3H).

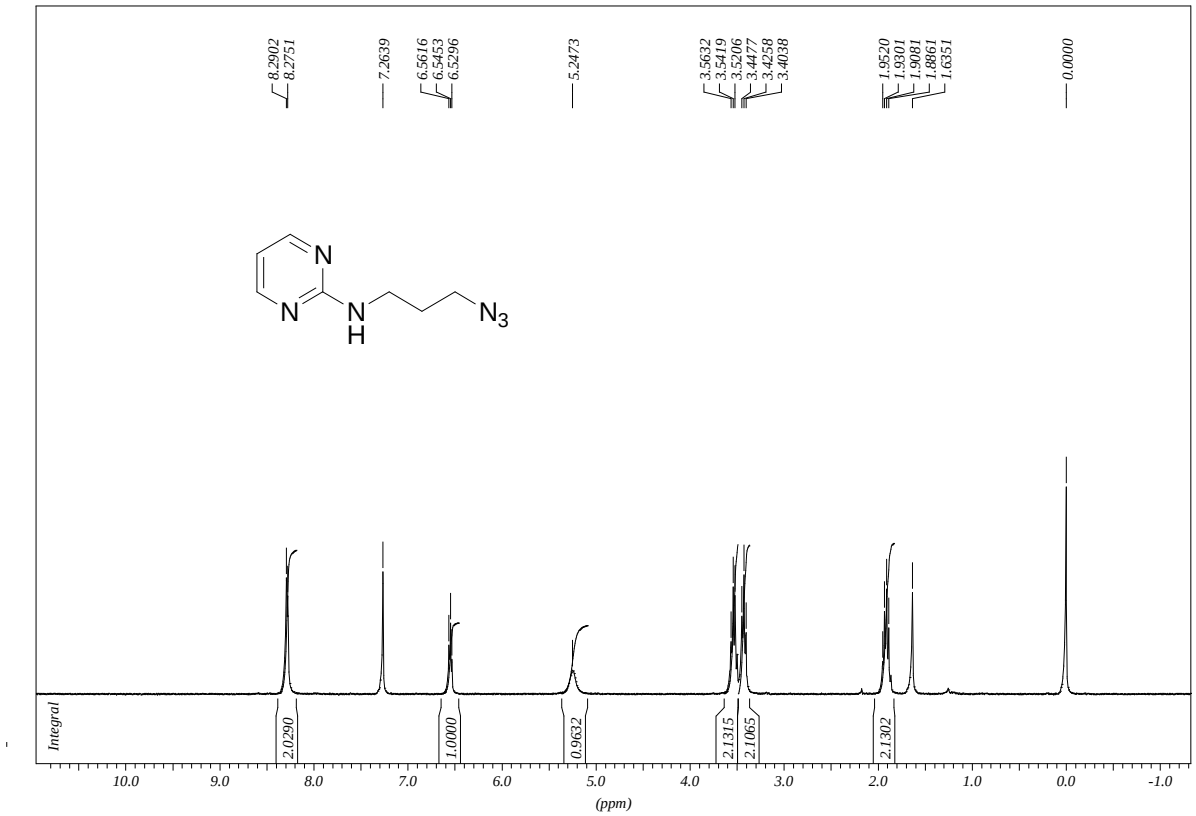
Copies of ^{1}H NMR and ^{13}C NMR spectra of new compounds

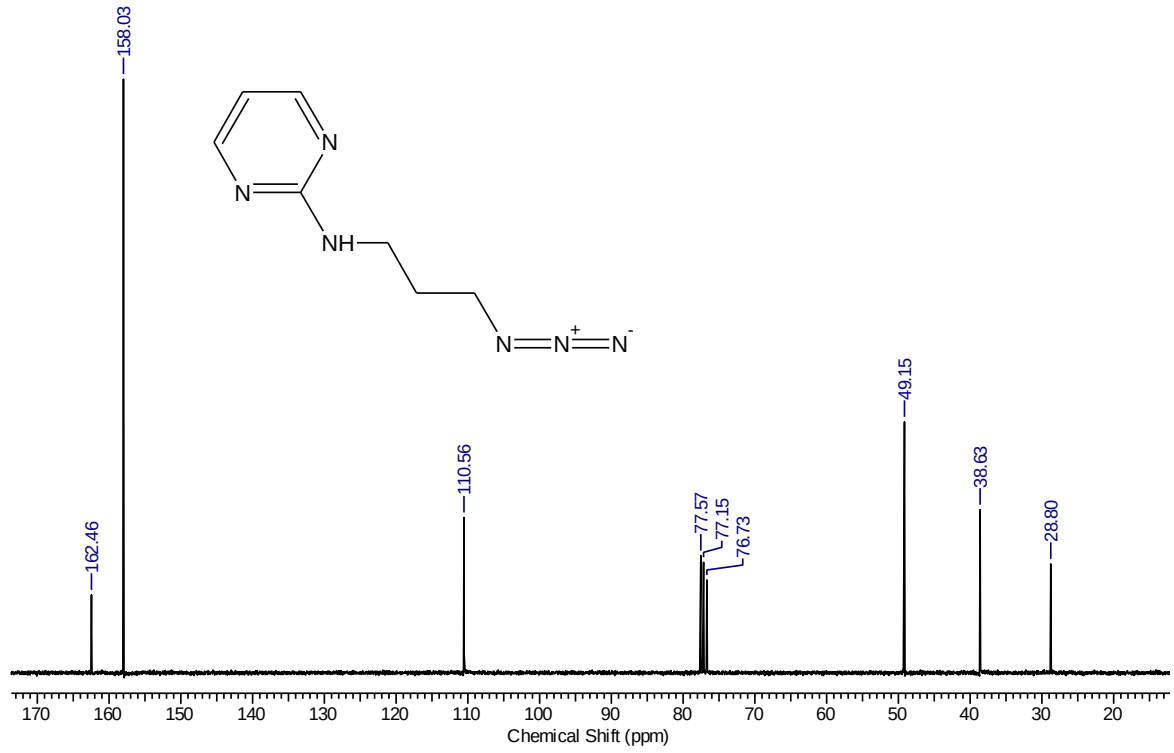
^{1}H NMR and ^{13}C NMR spectra of **1a** ($CDCl_3$)



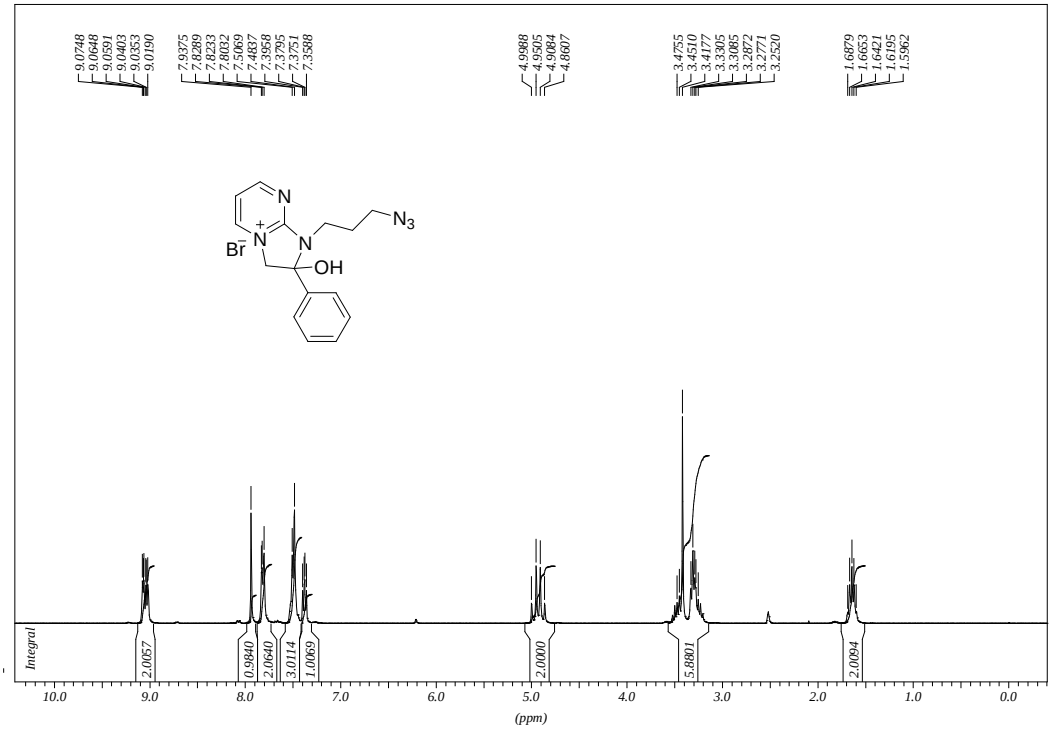


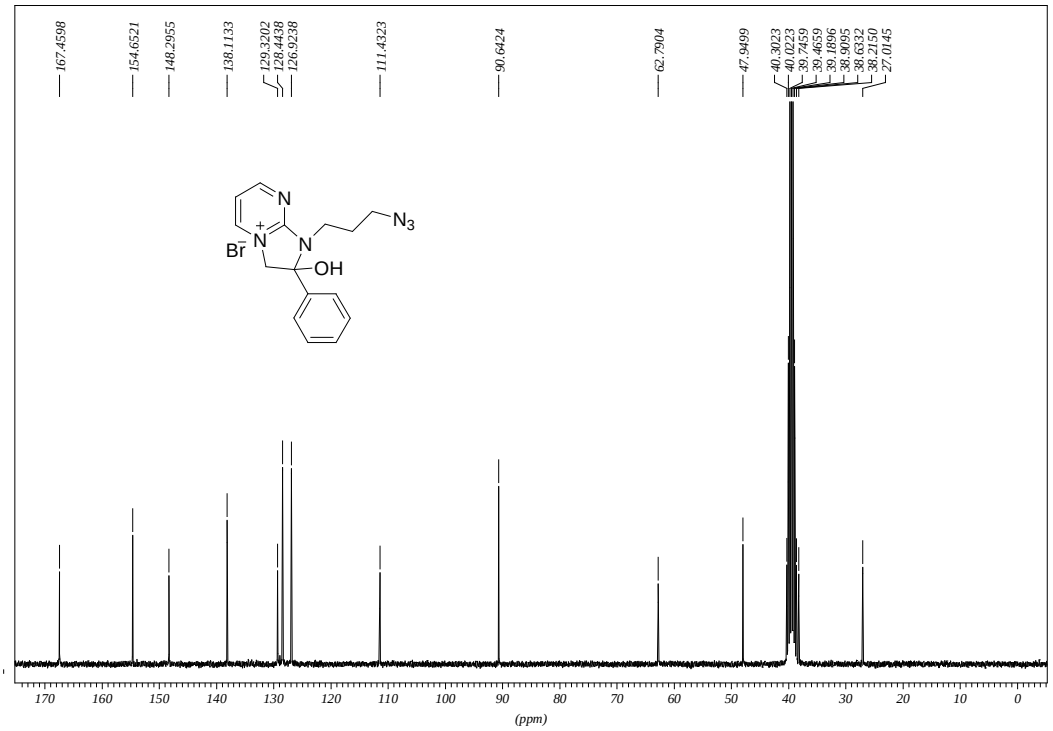
^{1}H NMR spectra of **1b** ($CDCl_3$)



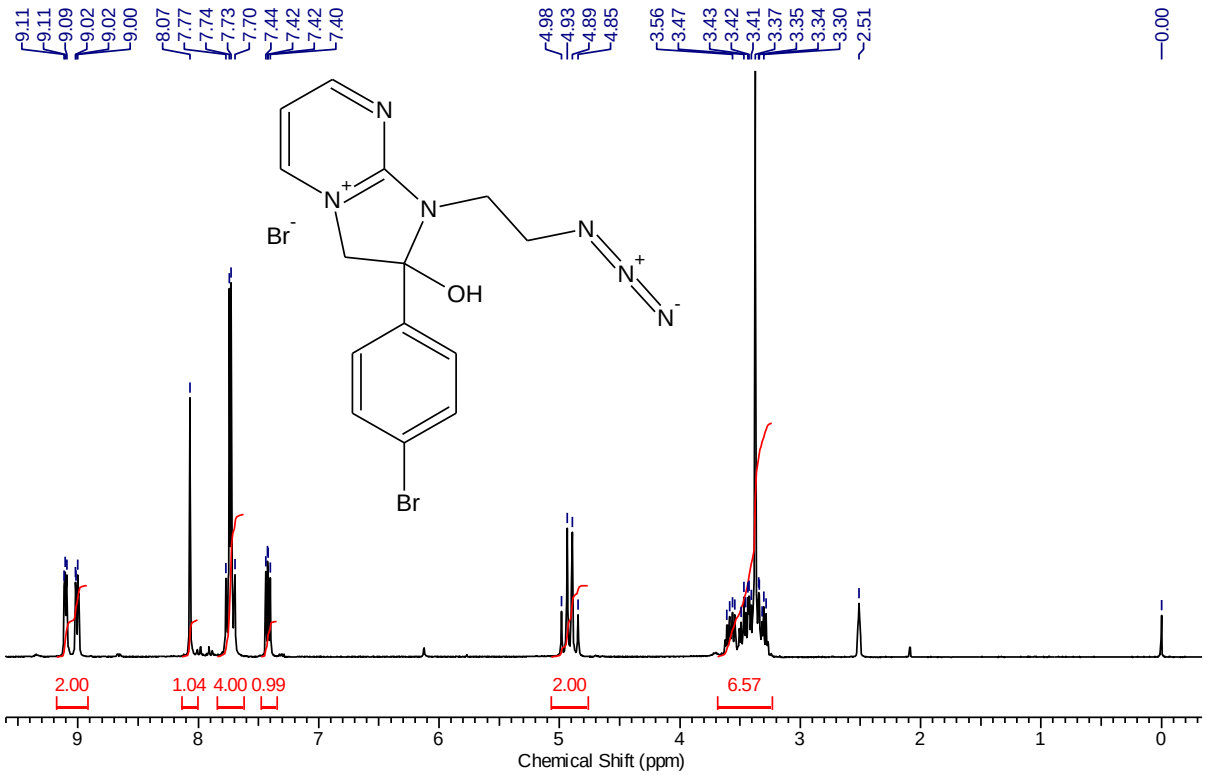


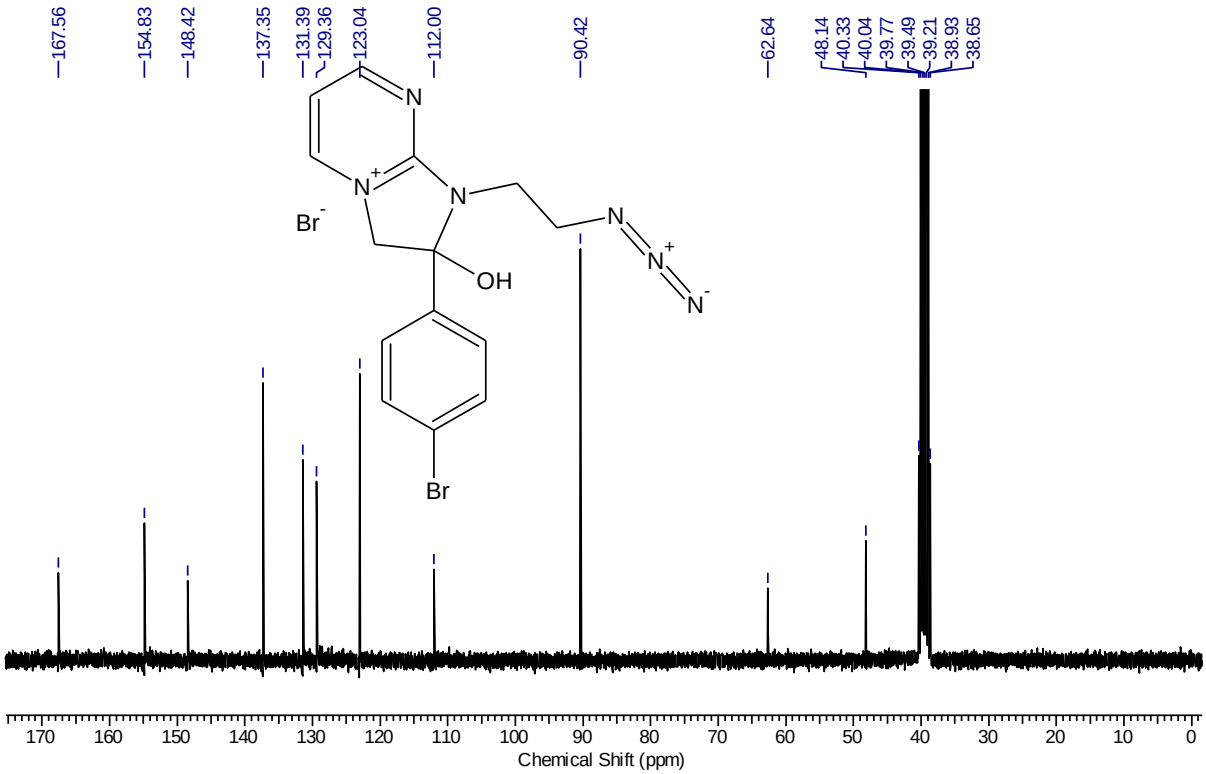
^{1}H NMR and ^{13}C NMR spectra of **3a** (DMSO-d_6)



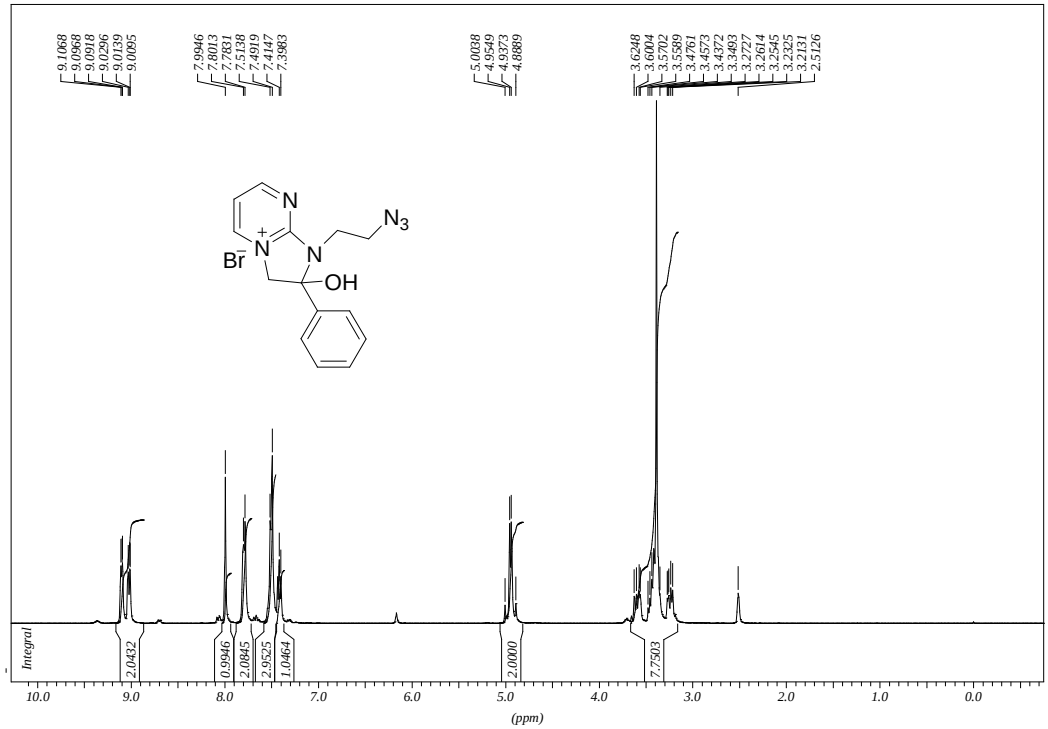


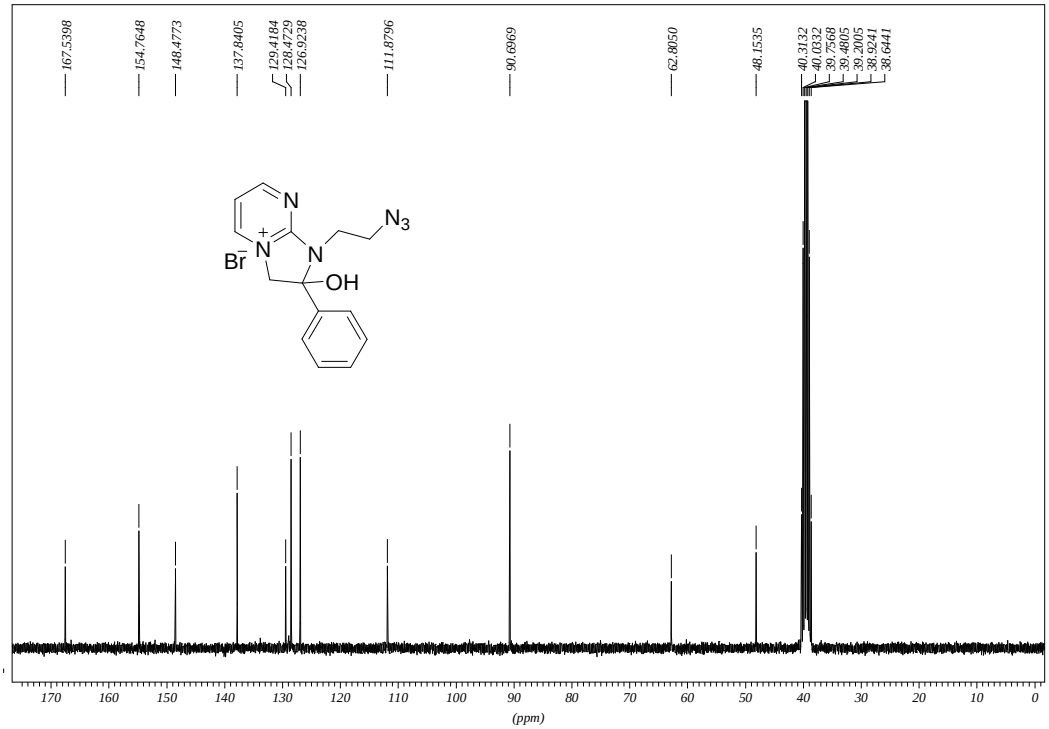
^{1}H NMR and ^{13}C NMR spectra of **3b** (DMSO-d_6)



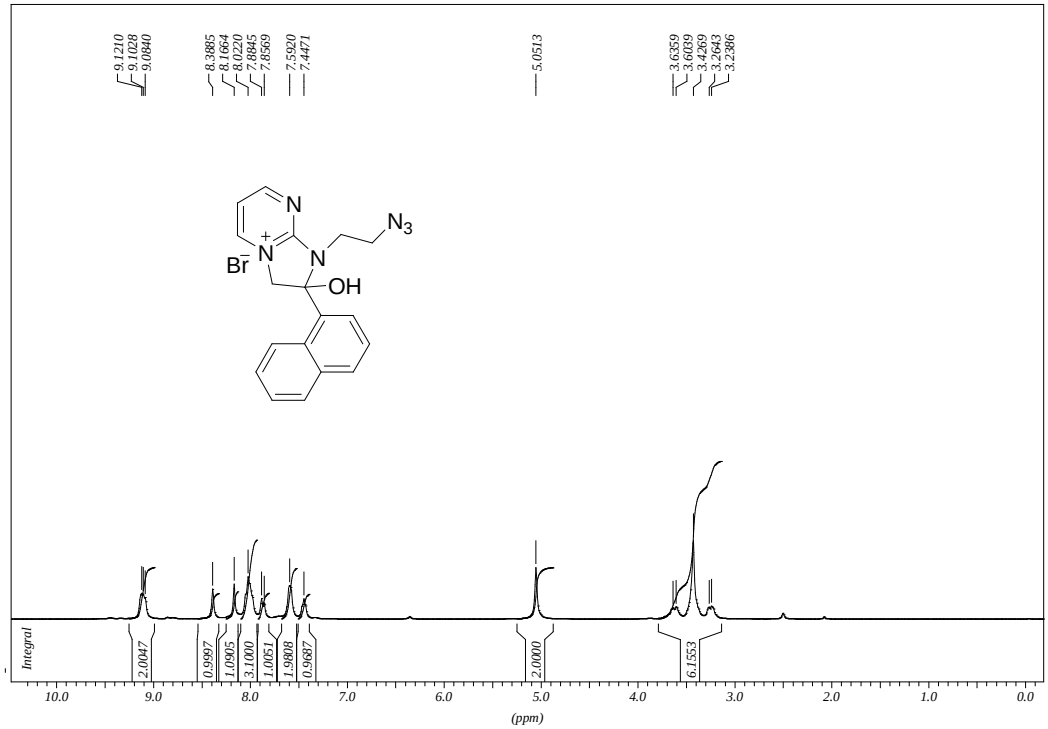


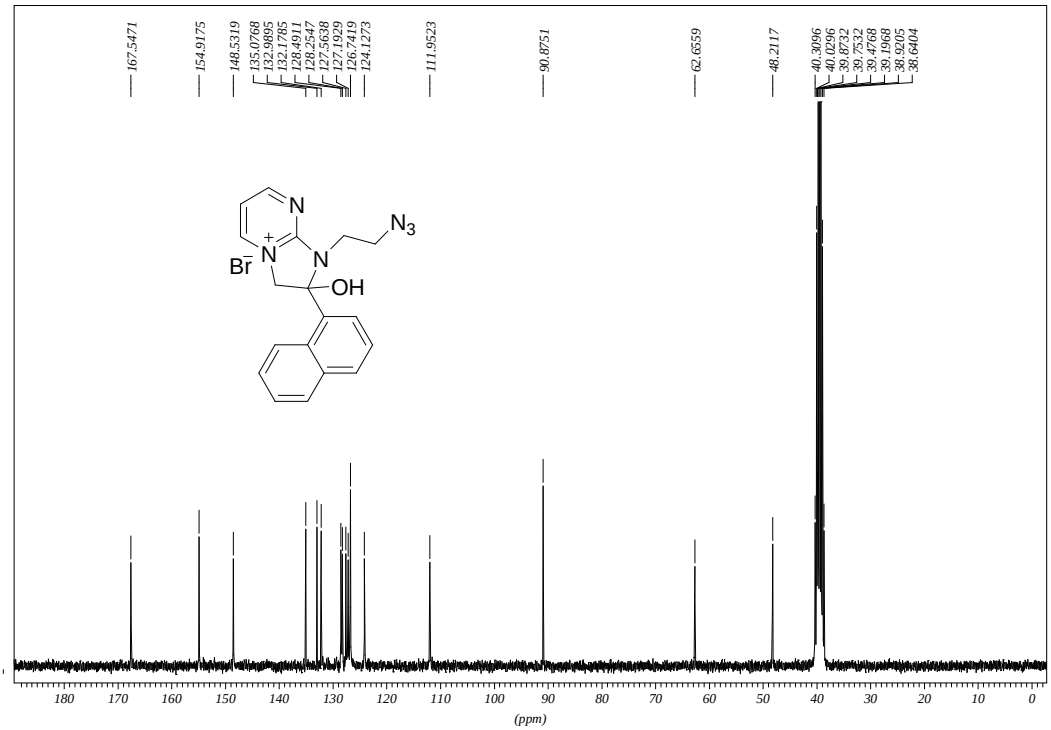
^{1}H NMR and ^{13}C NMR spectra of **3c** (DMSO-d_6)



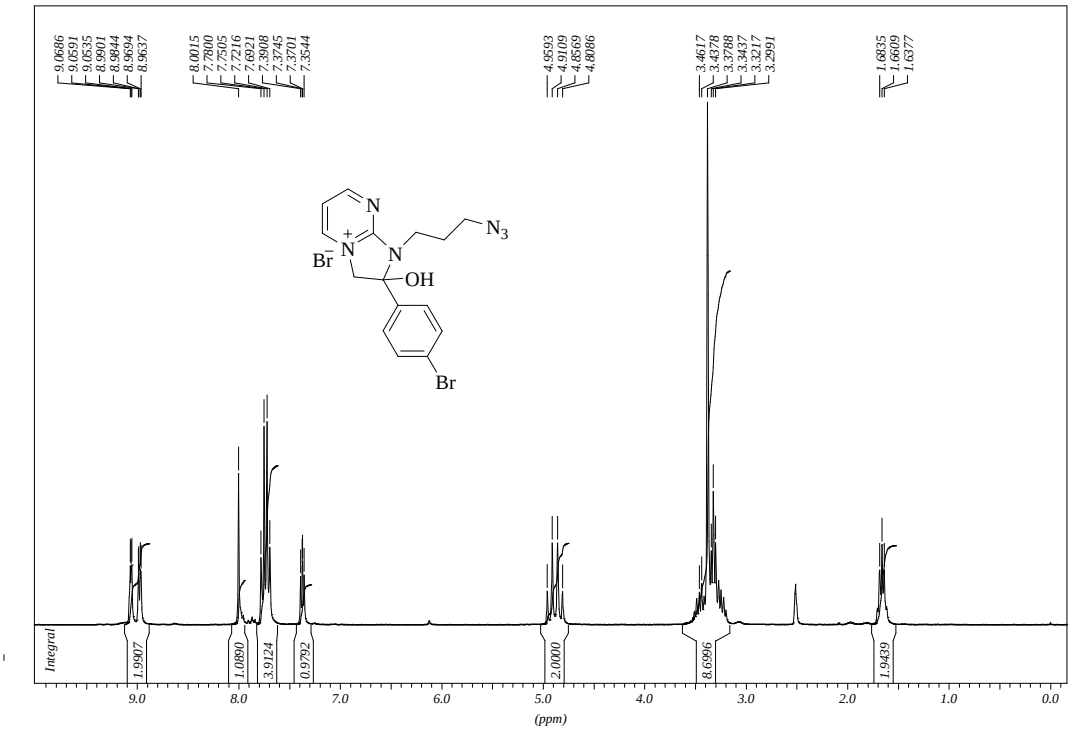


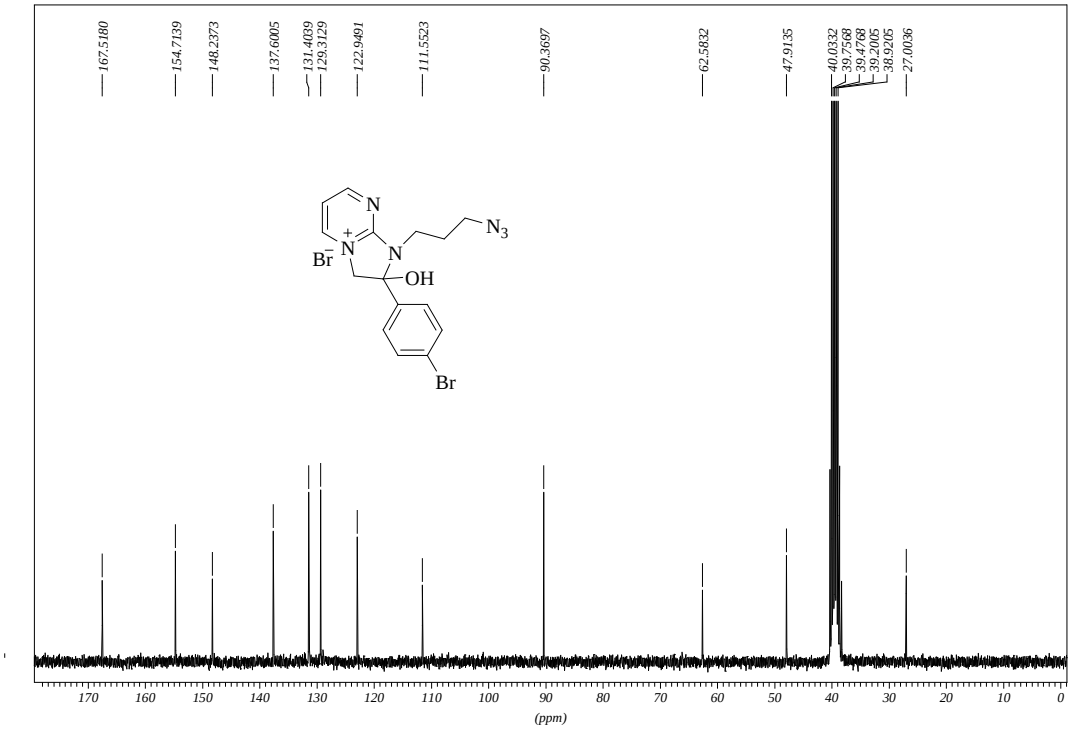
^{1}H NMR and ^{13}C-NMR spectra of **3d** (DMSO-d_6)



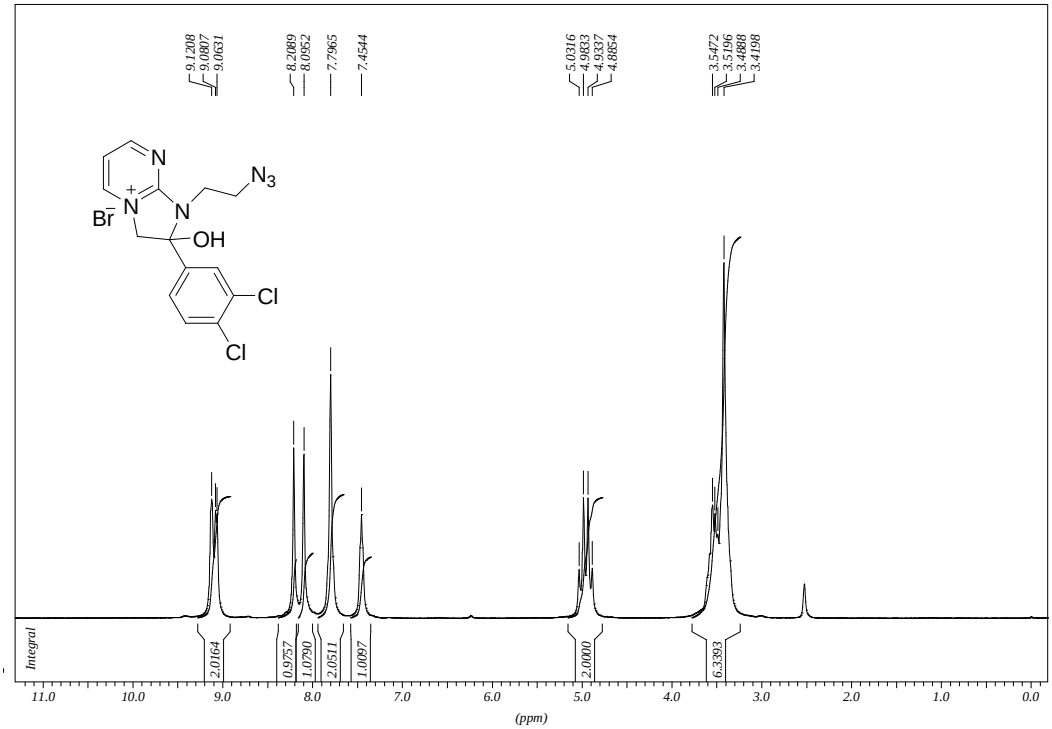


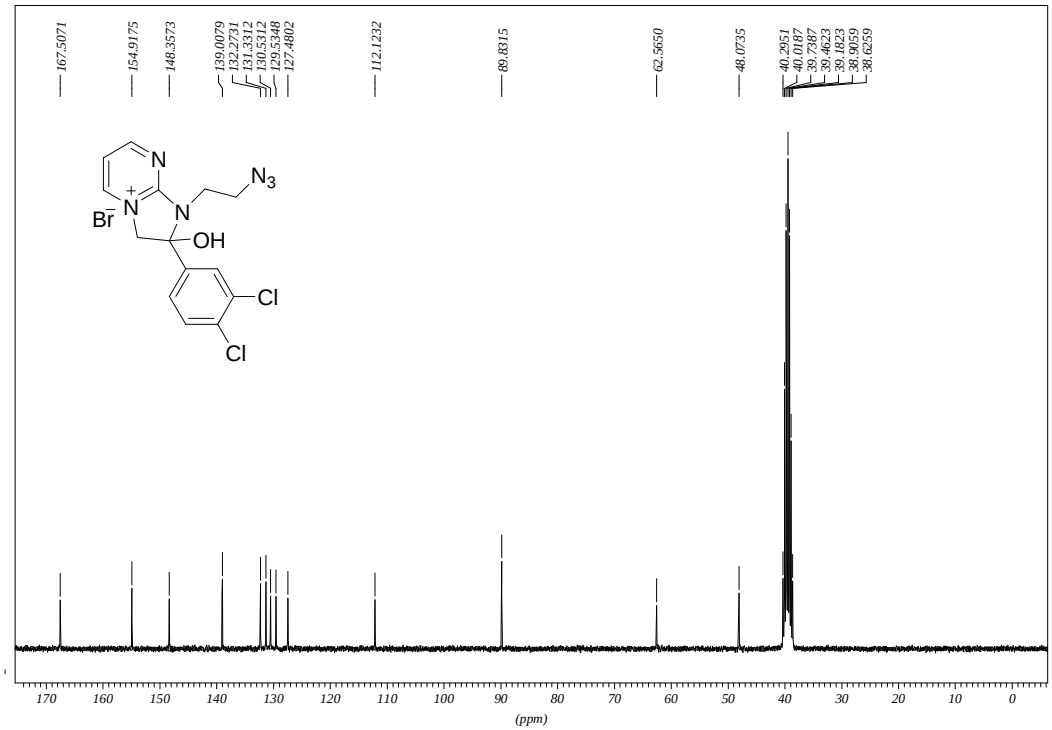
^{1}H NMR and ^{13}C NMR spectra of **3e** (DMSO-d_6)



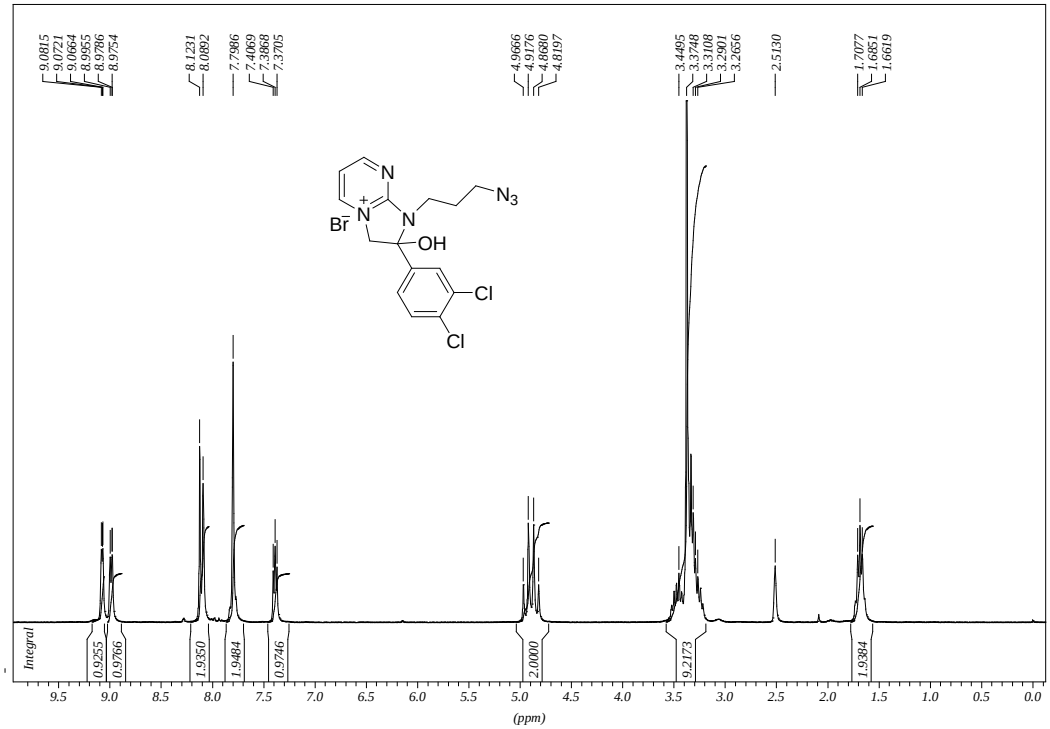


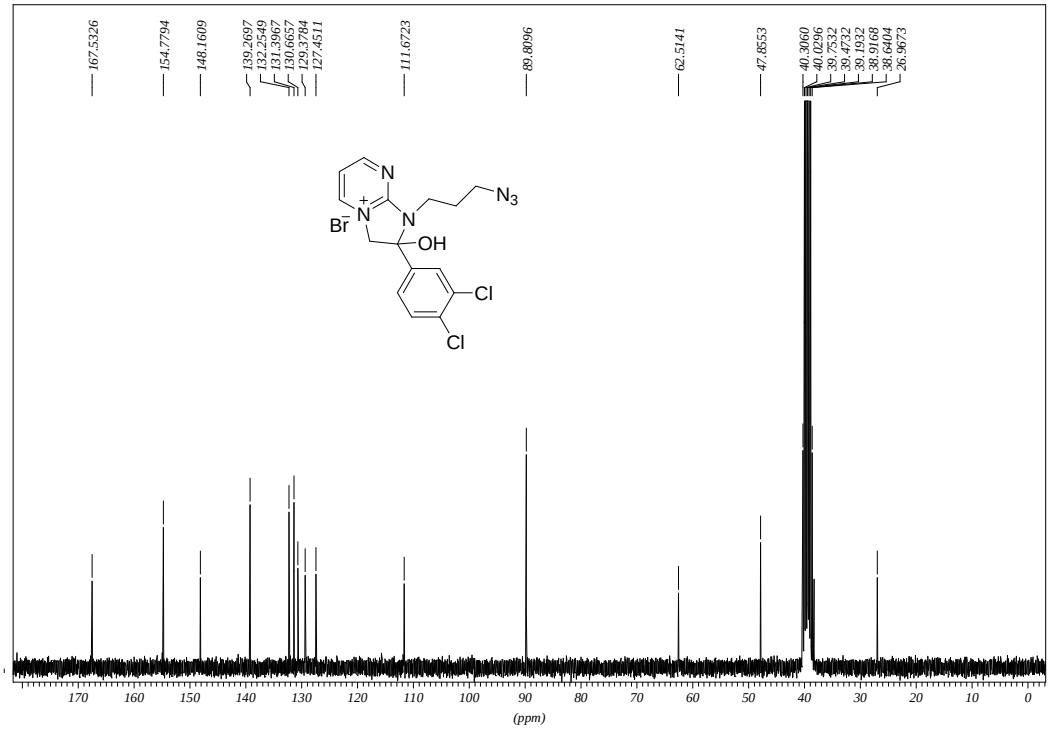
^{1}H NMR and ^{13}C NMR spectra of **3f** (DMSO-d_6)



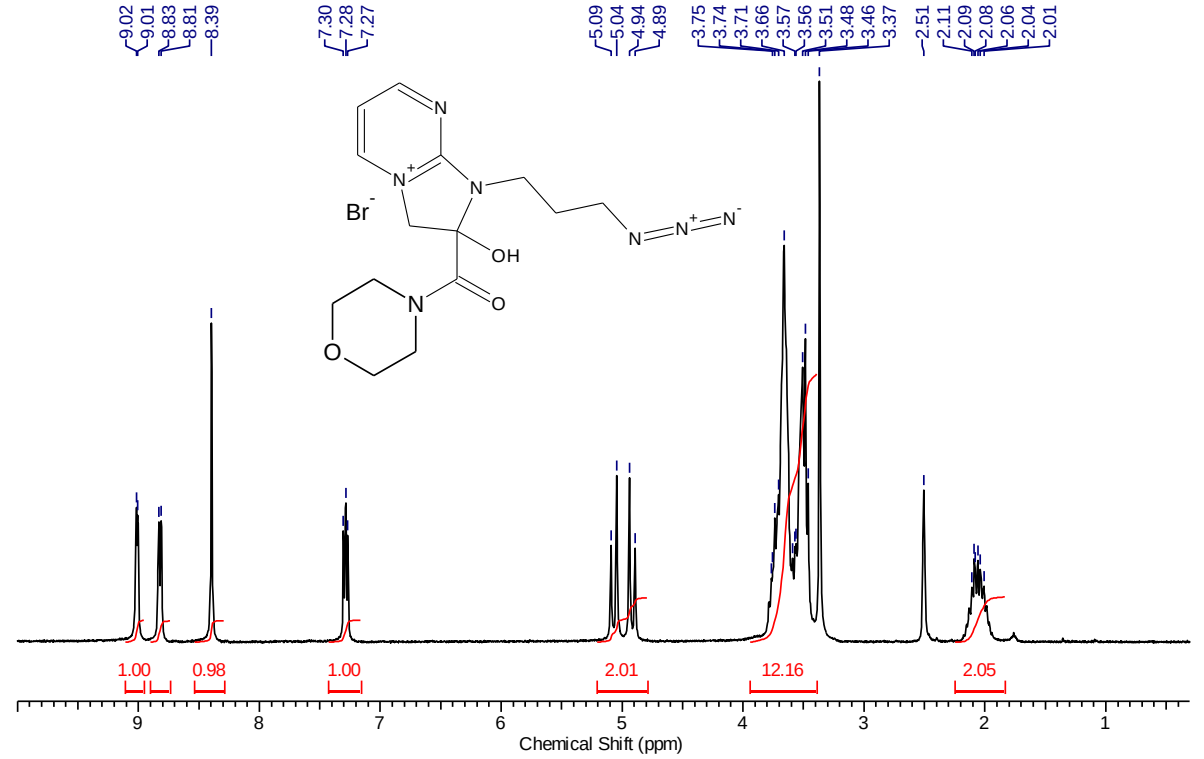


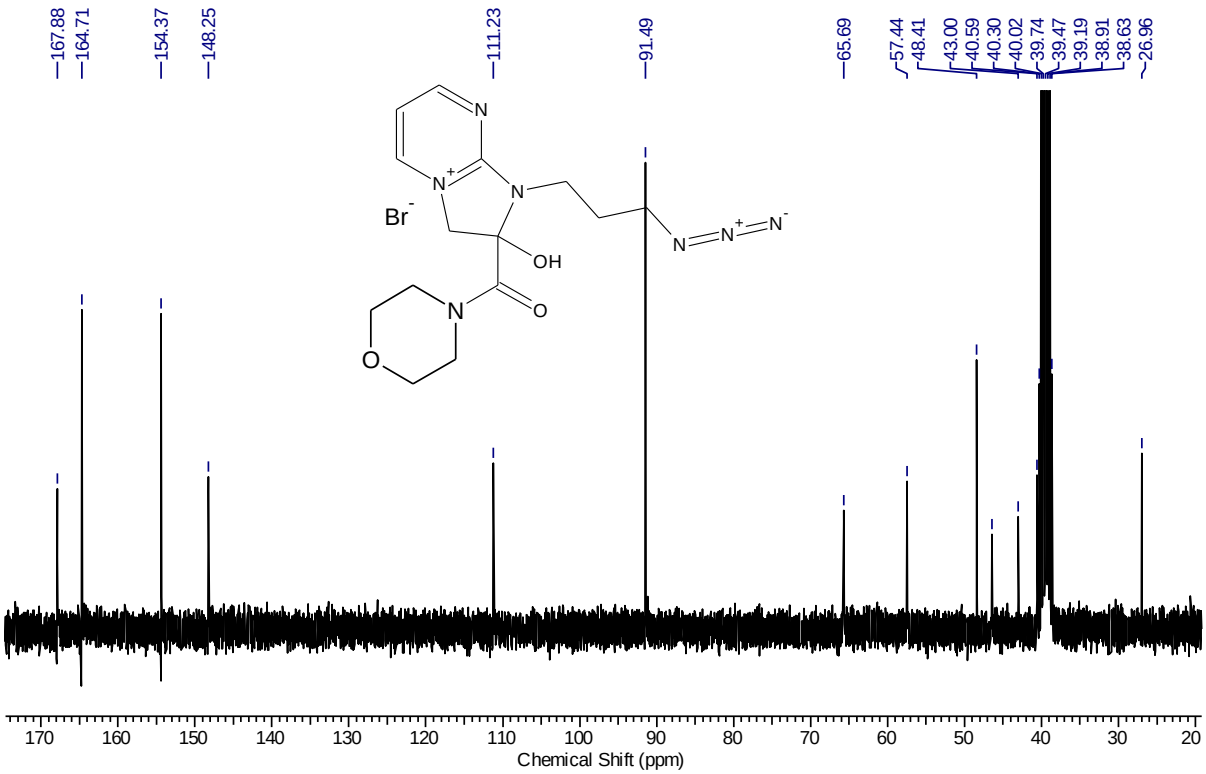
^{1}H NMR and ^{13}C NMR spectra of **3g** (DMSO-d_6)



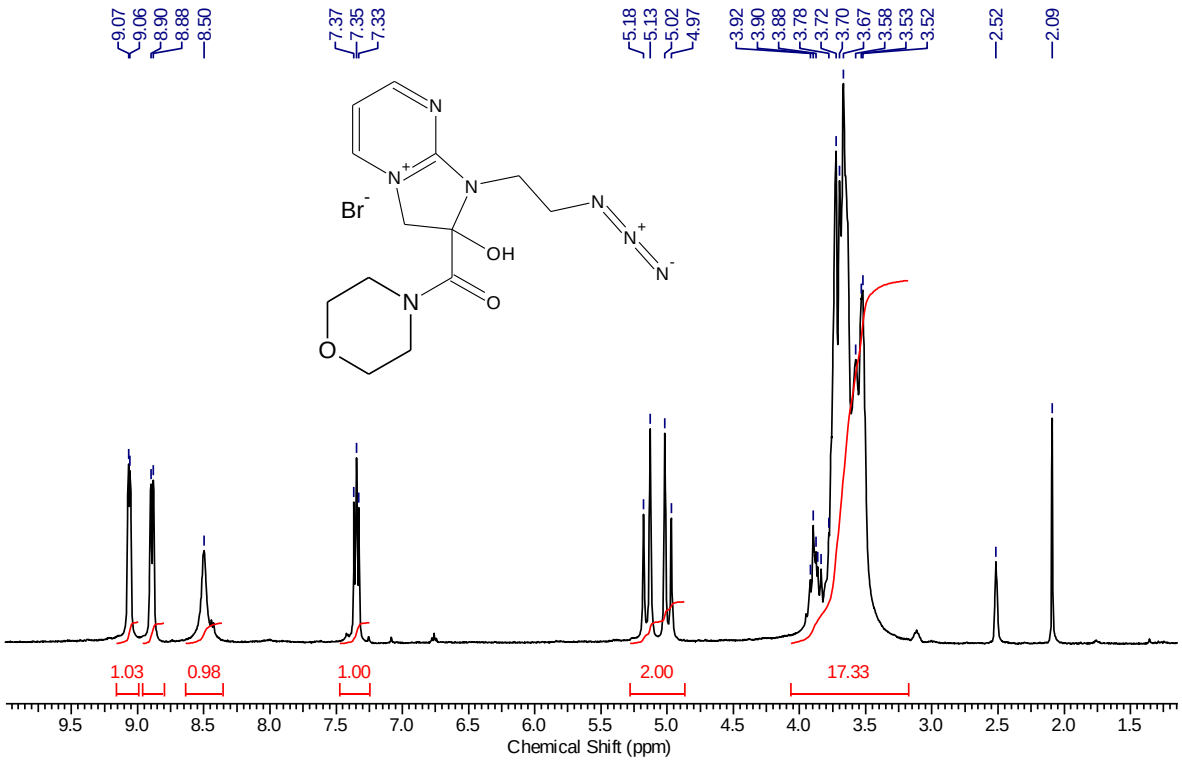


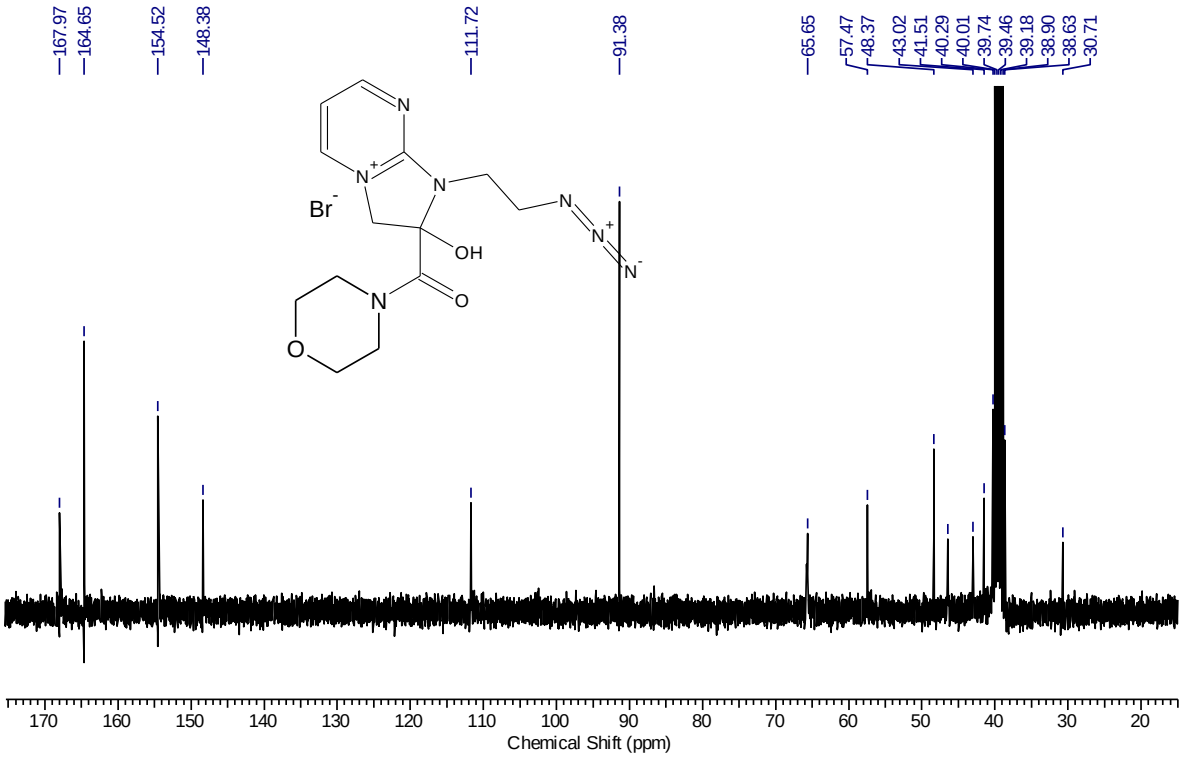
^{1}H NMR and ^{13}C NMR spectra of **3h** (DMSO-d_6)



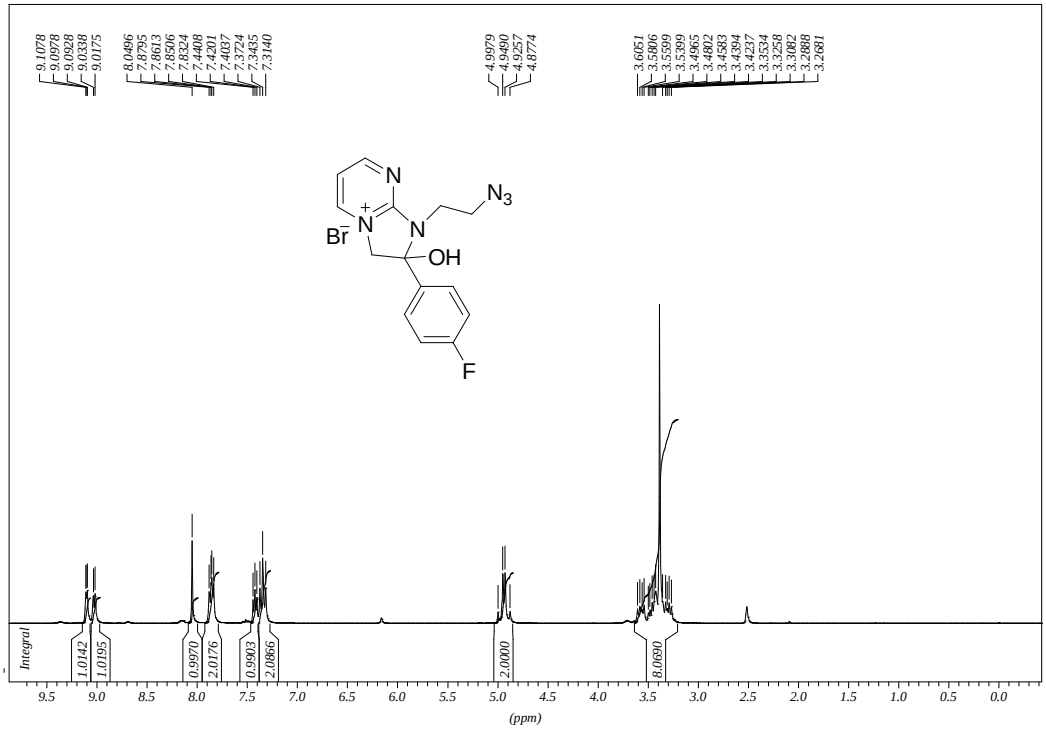


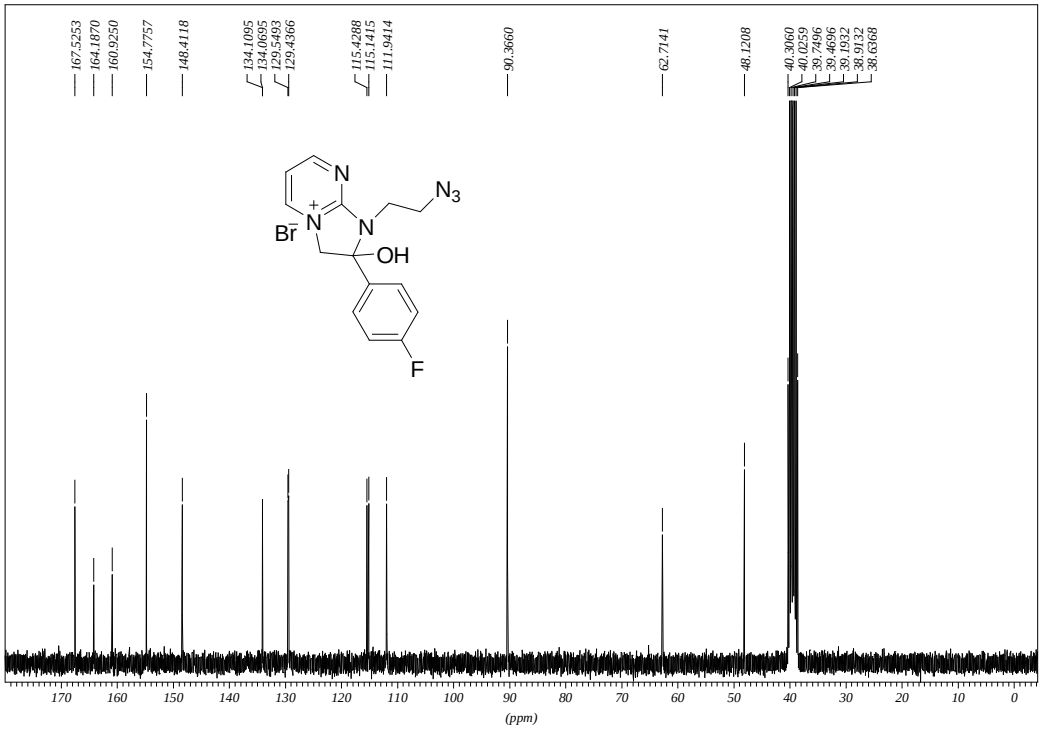
^{1}H NMR and ^{13}C NMR spectra of **3i** (DMSO-d_6)



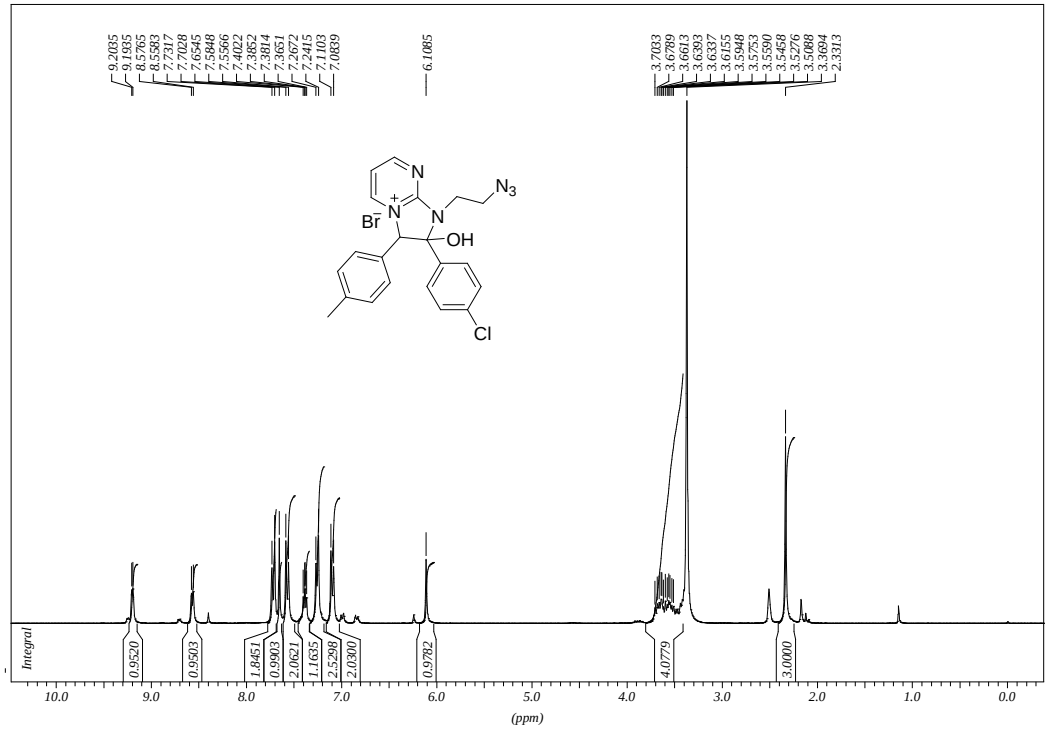


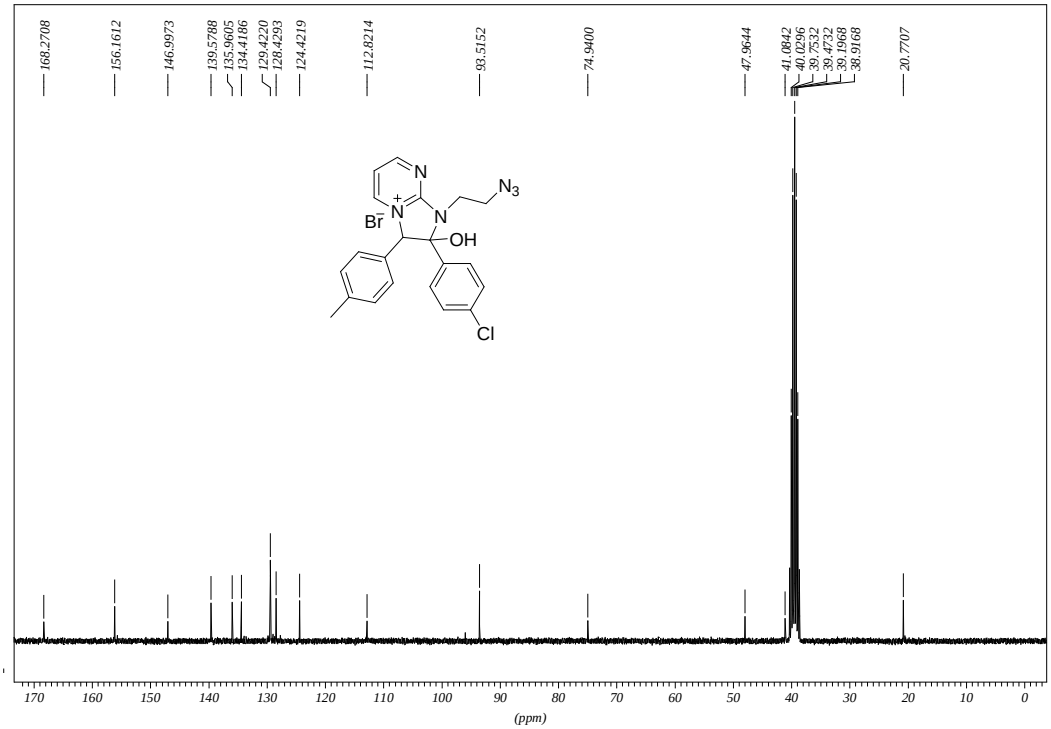
^{1}H NMR and ^{13}C NMR spectra of **3j** (DMSO-d_6)



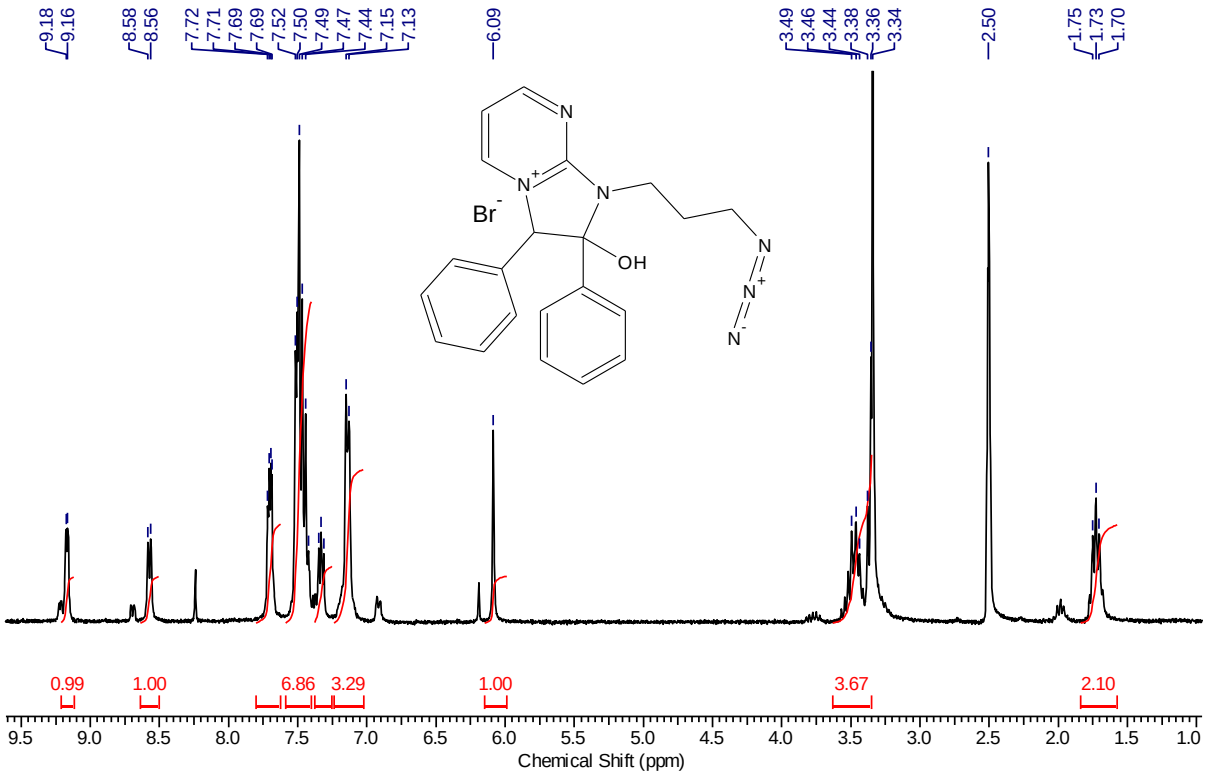


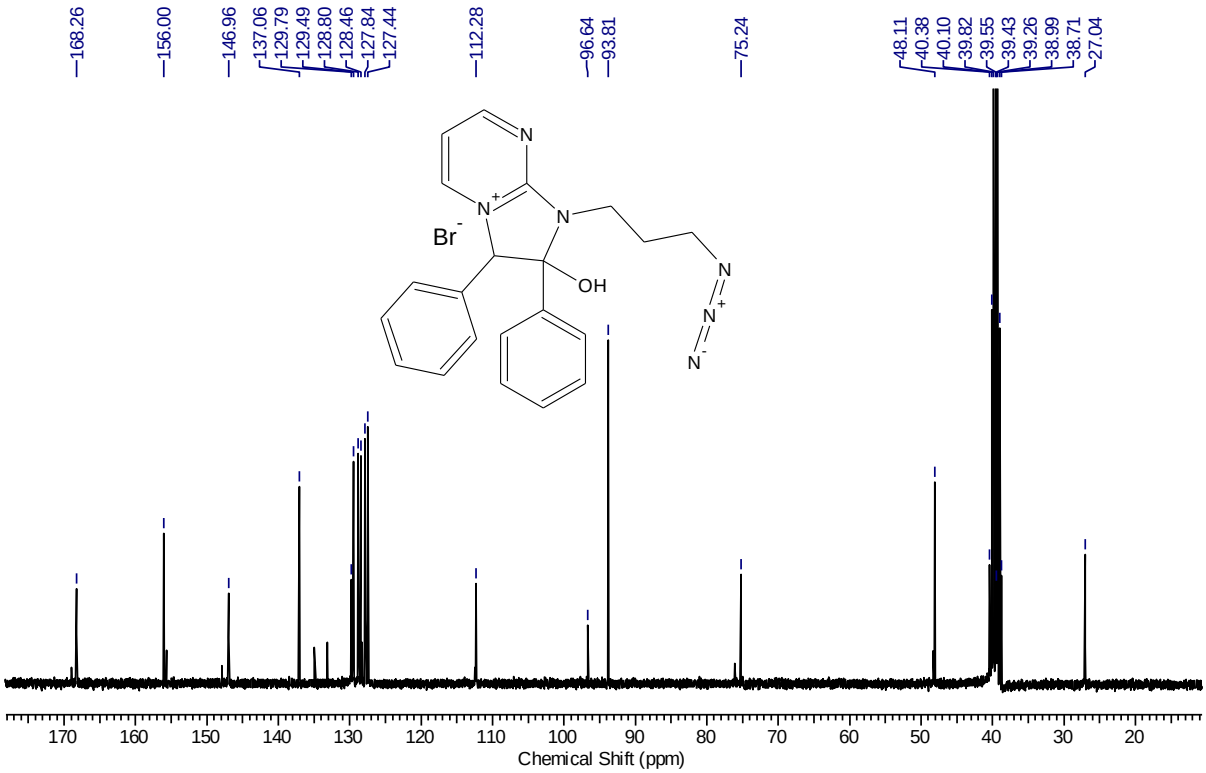
^{1}H NMR and ^{13}C NMR spectra of **3k** (DMSO-d_6)



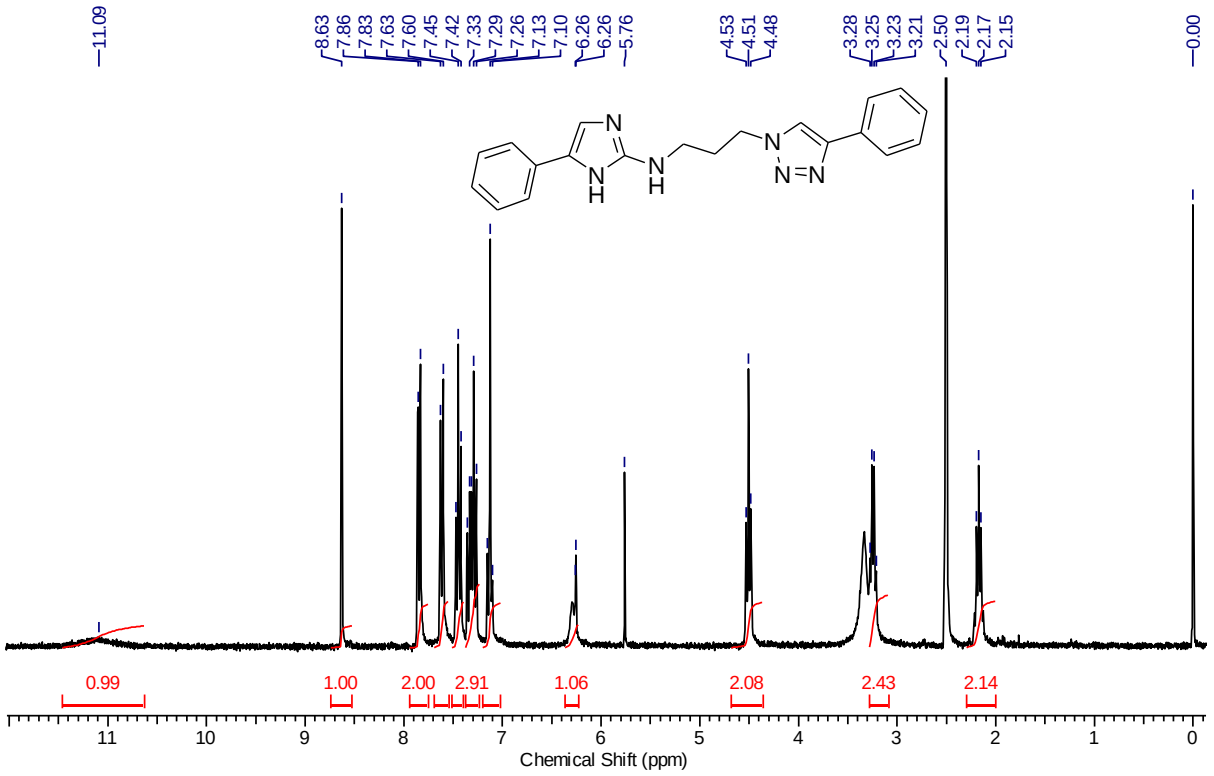


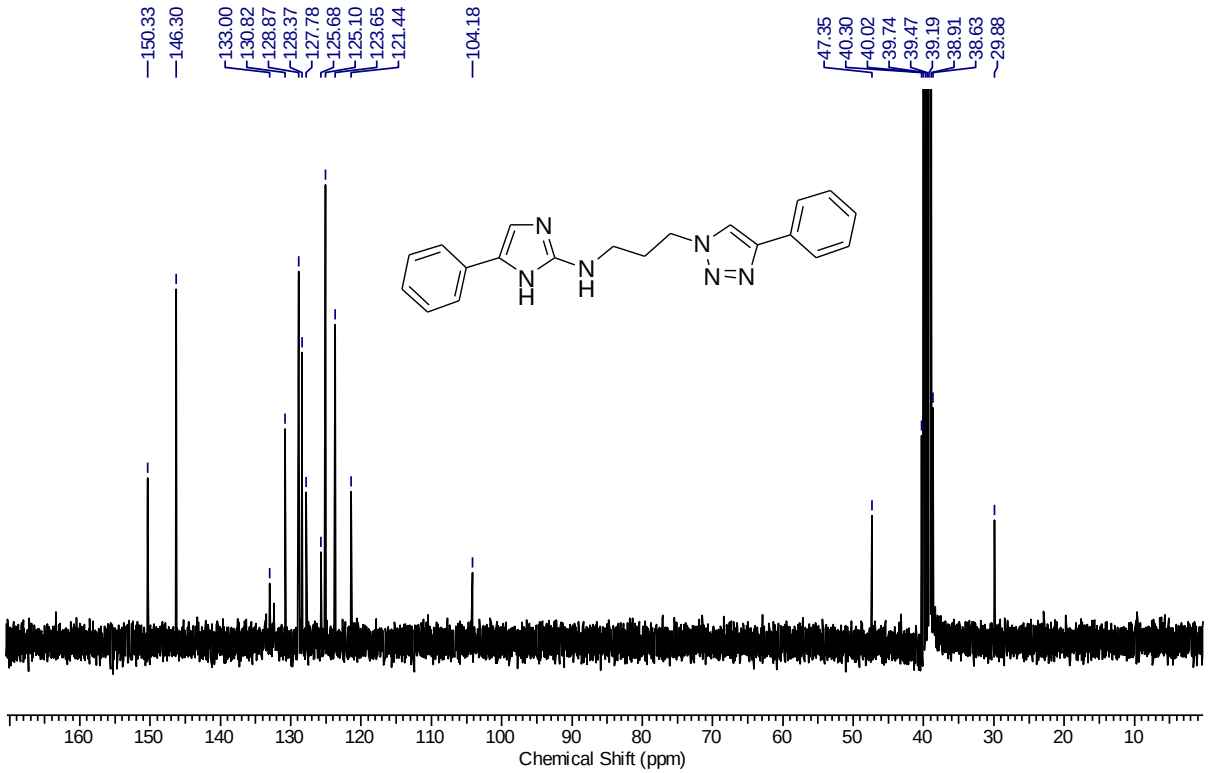
^{1}H NMR and ^{13}C NMR spectra of **3l** (DMSO-d_6)



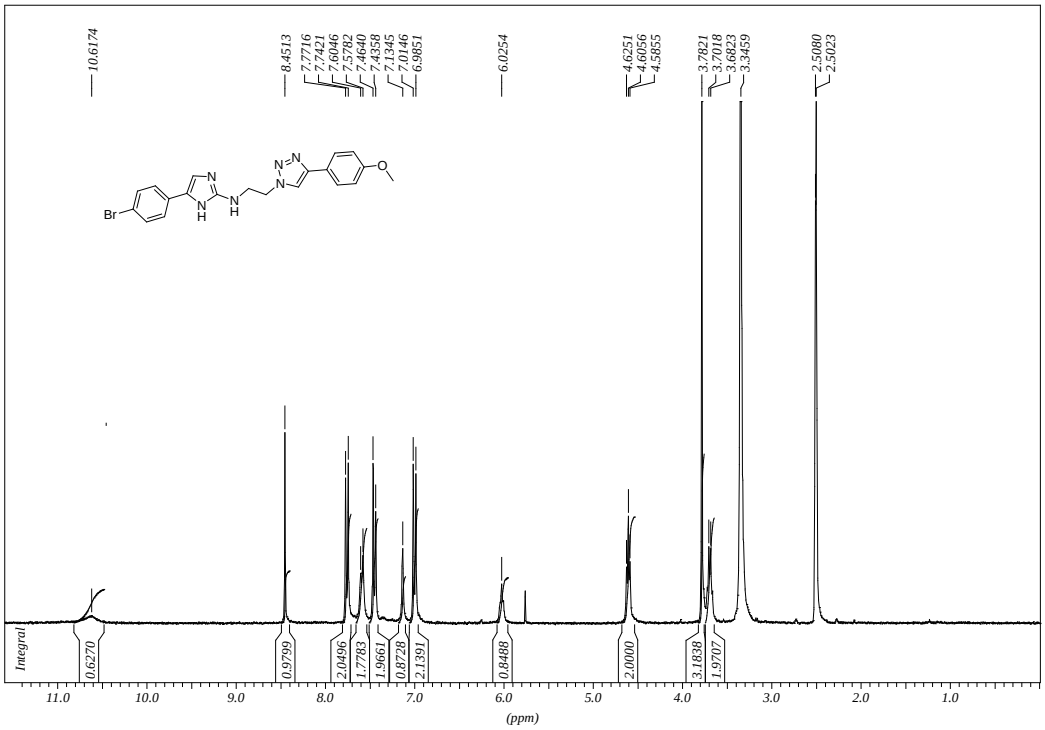


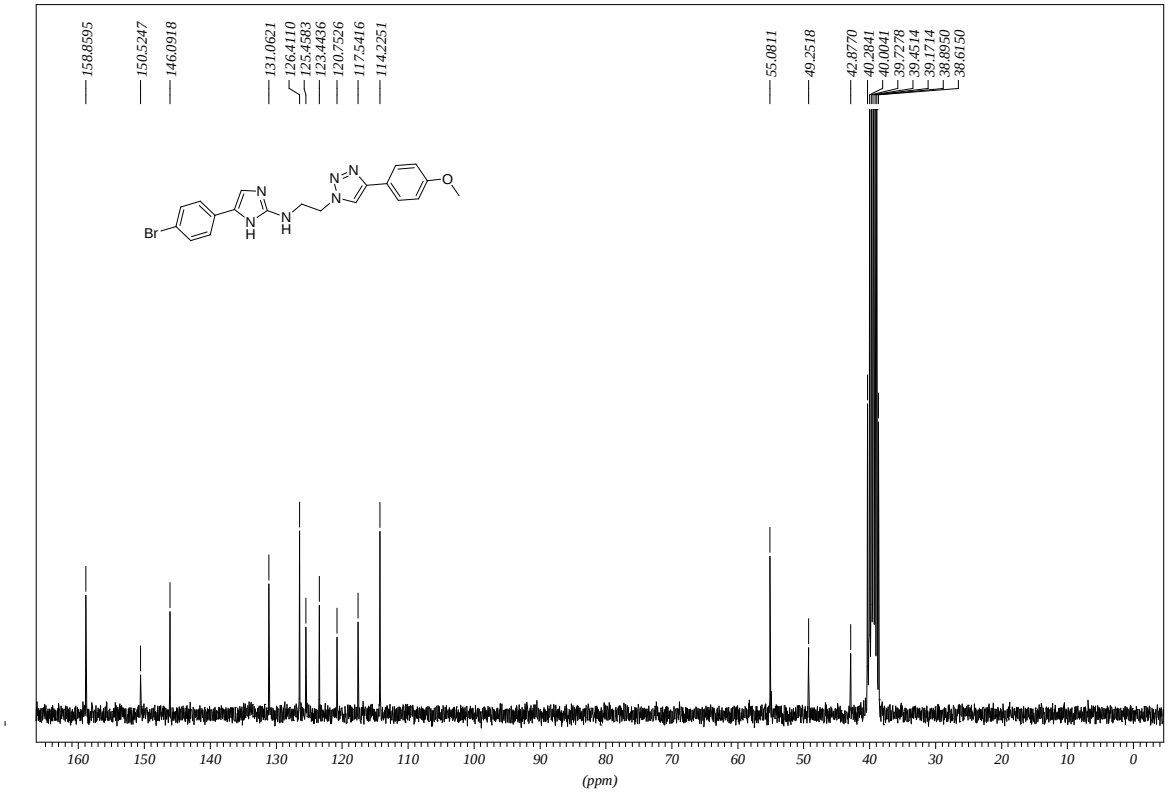
^{1}H NMR and ^{13}C NMR spectra of **5a** (DMSO-d_6)



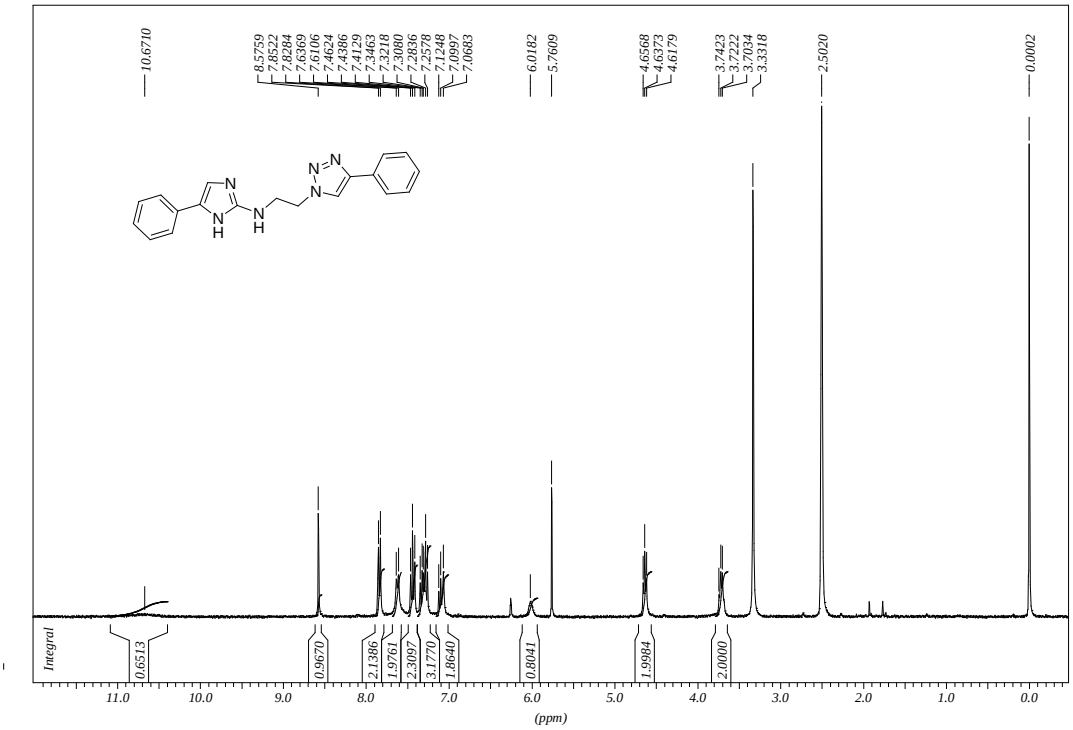


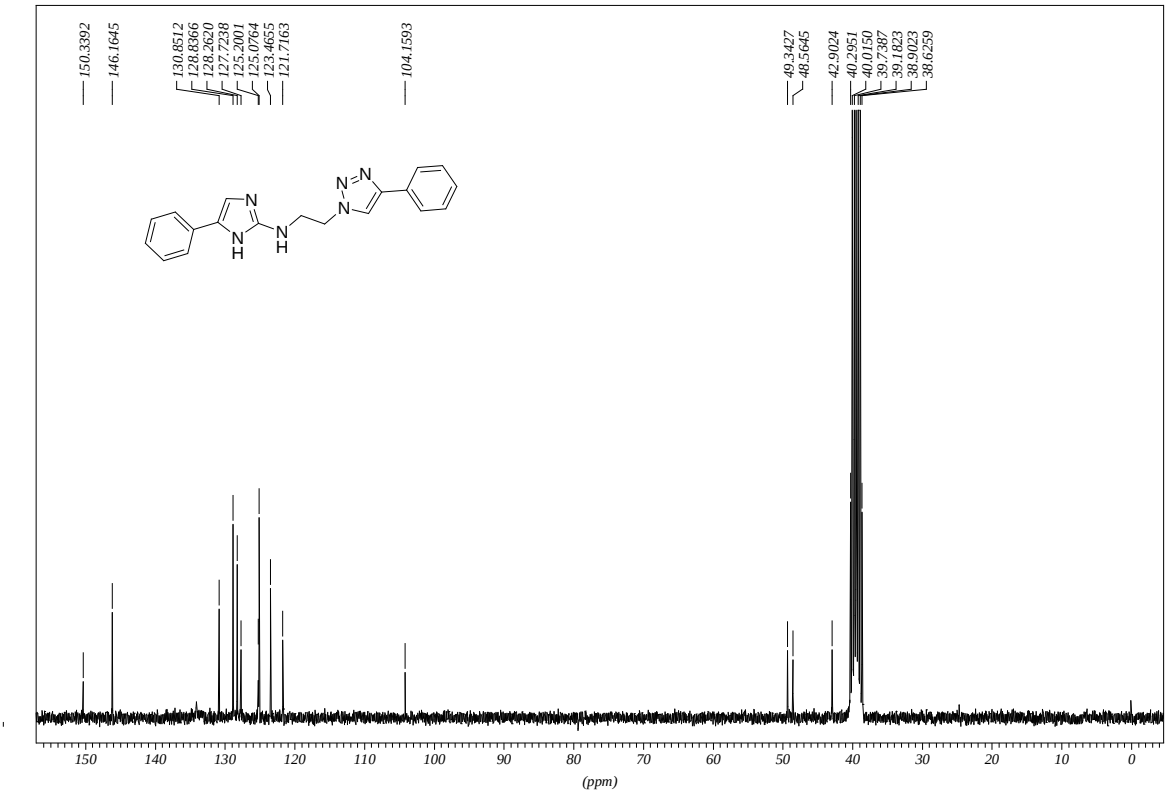
^{1}H NMR and ^{13}C NMR spectra of **5b** (DMSO-d_6)



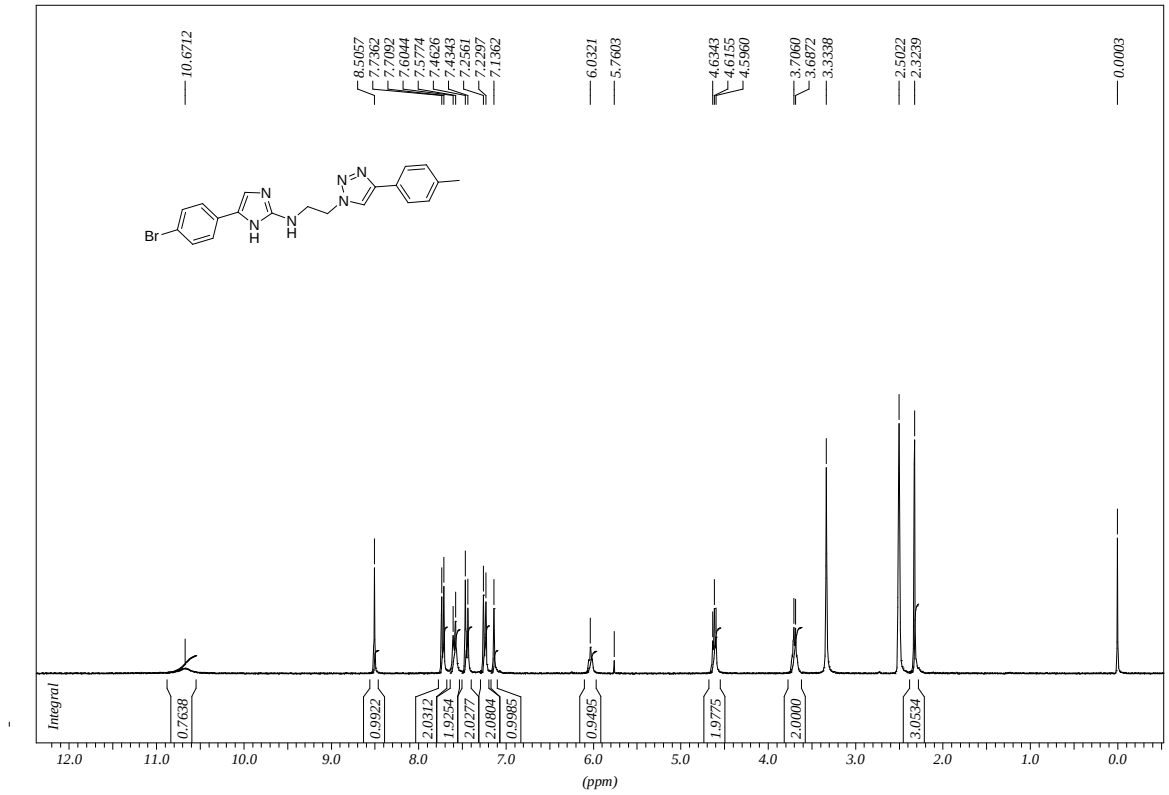


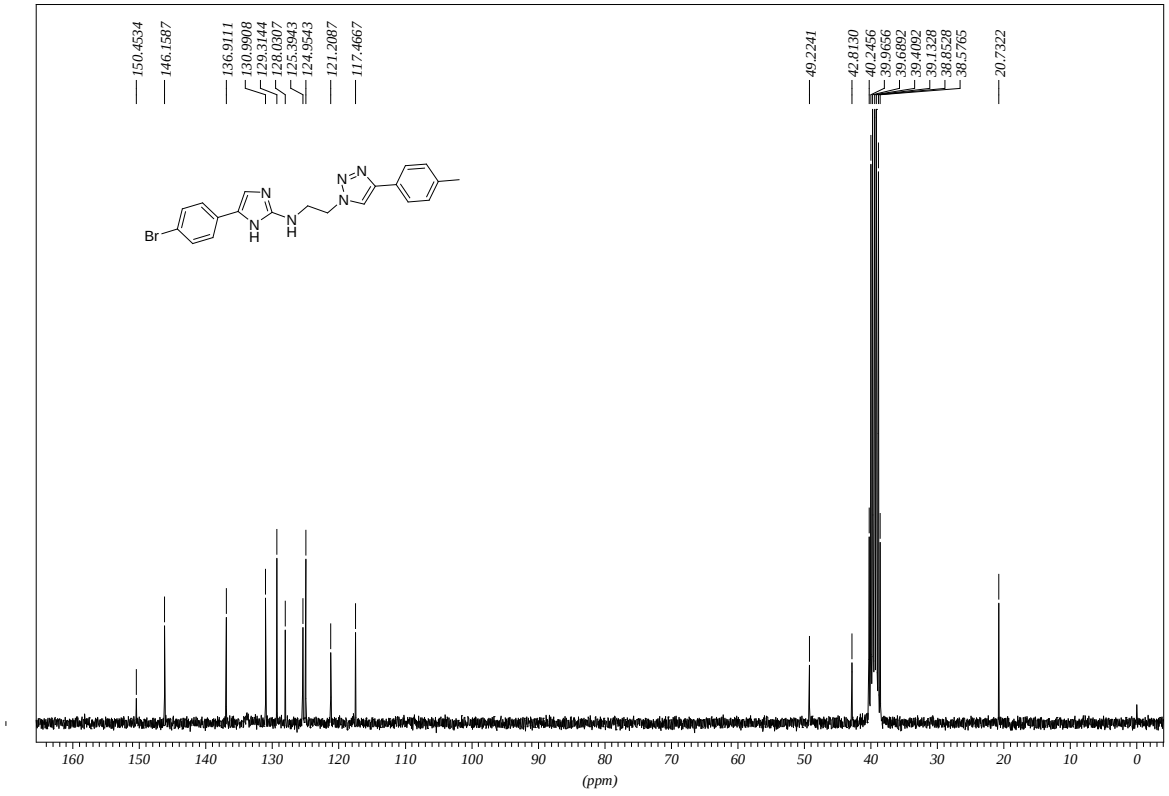
^{1}H NMR and ^{13}C NMR spectra of **5c** (DMSO-d_6)



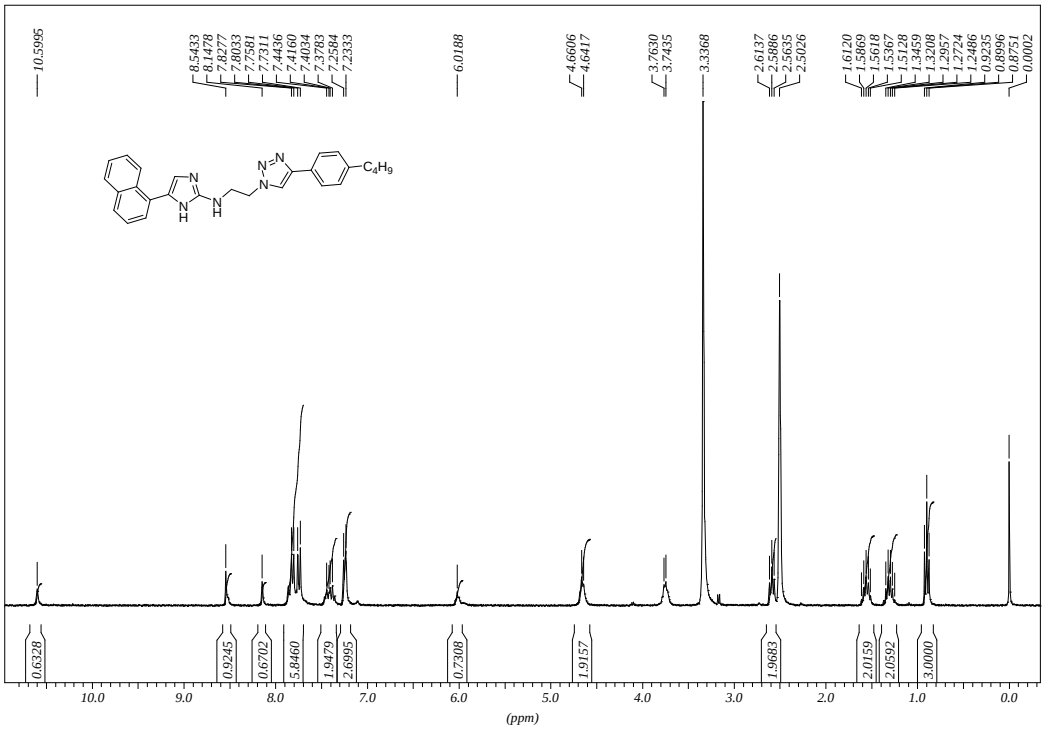


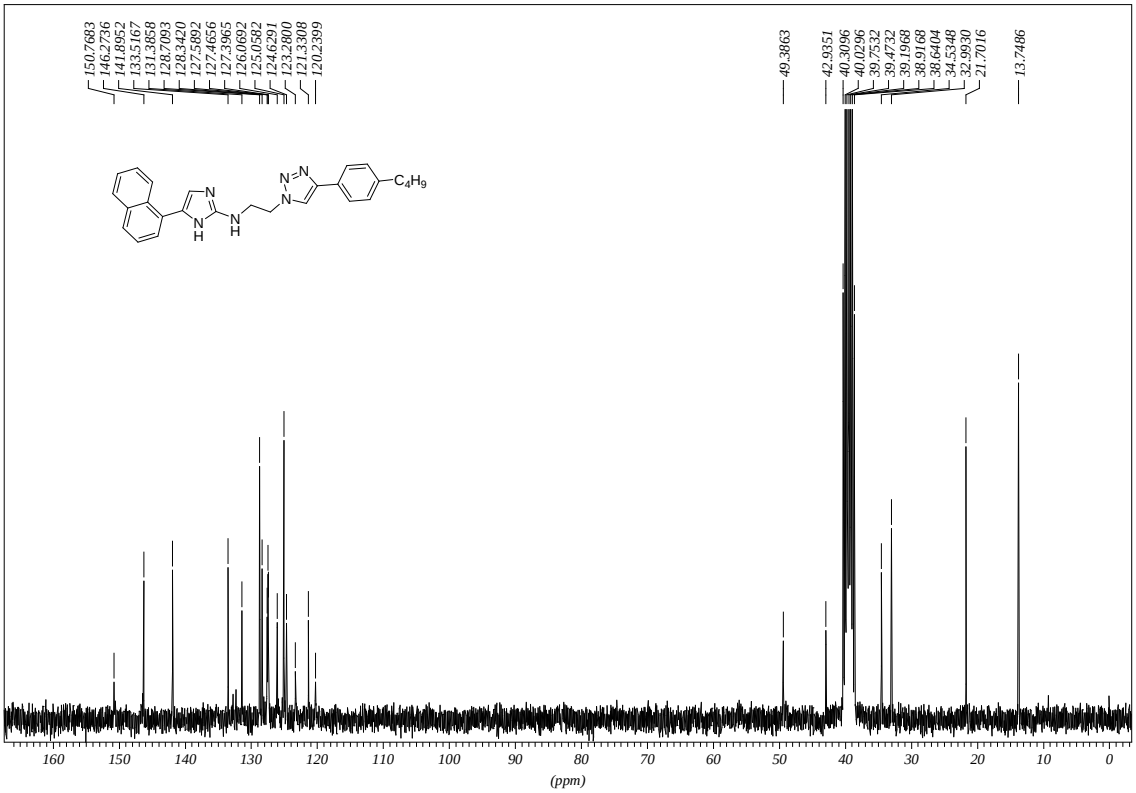
^{1}H NMR and ^{13}C NMR spectra of **5d** (DMSO-d_6)



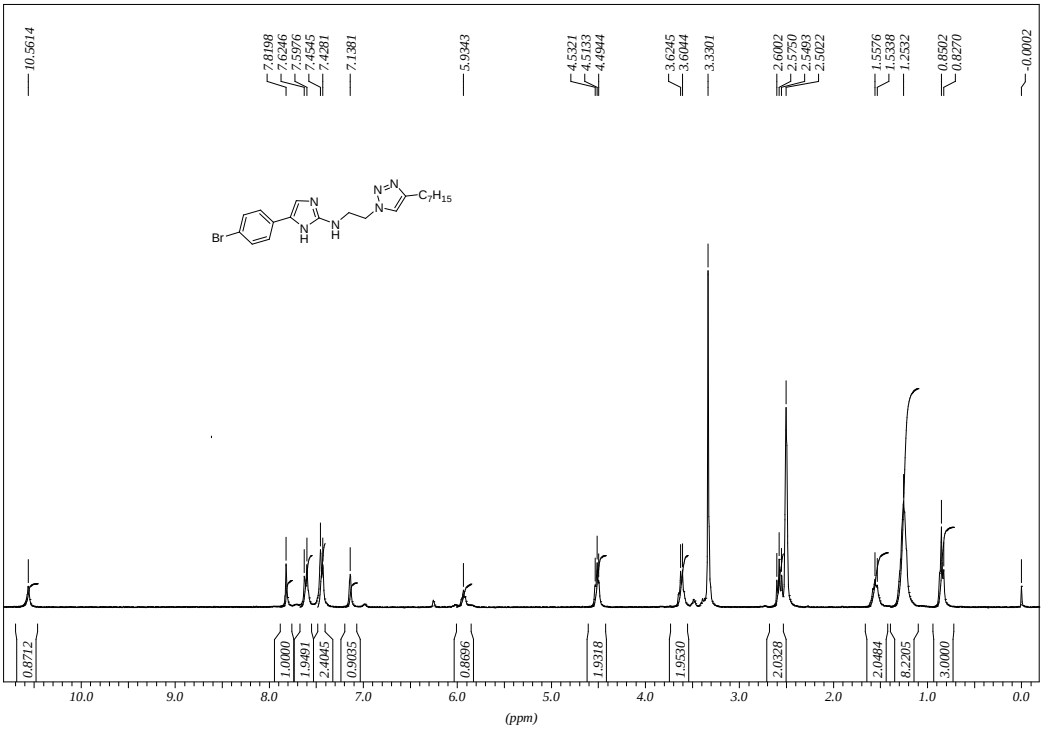


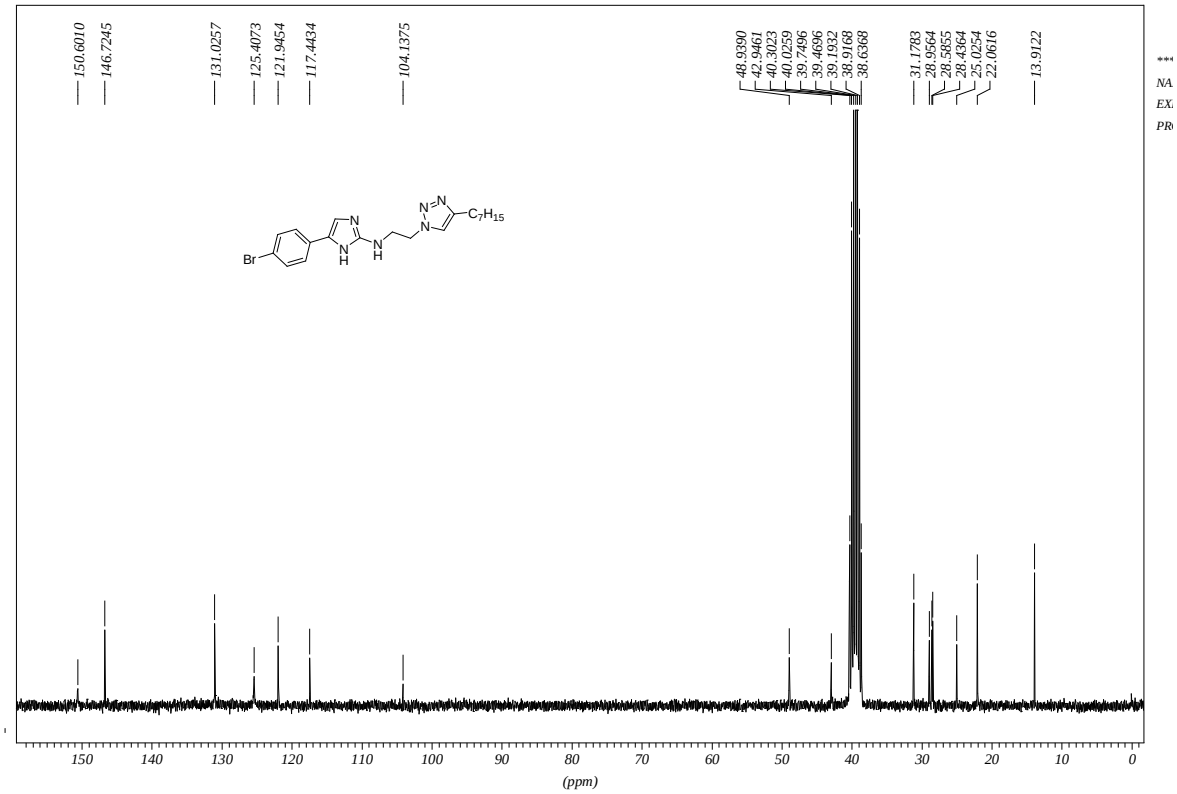
^{1}H NMR and ^{13}C NMR spectra of **5e** (DMSO-d_6)



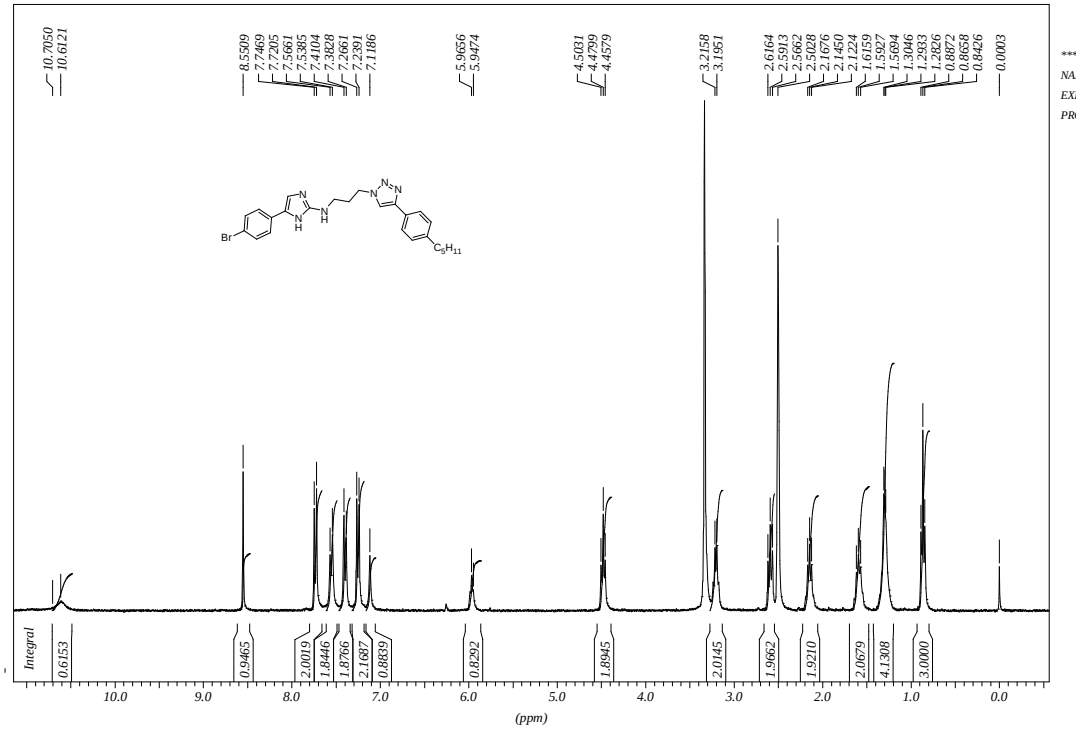


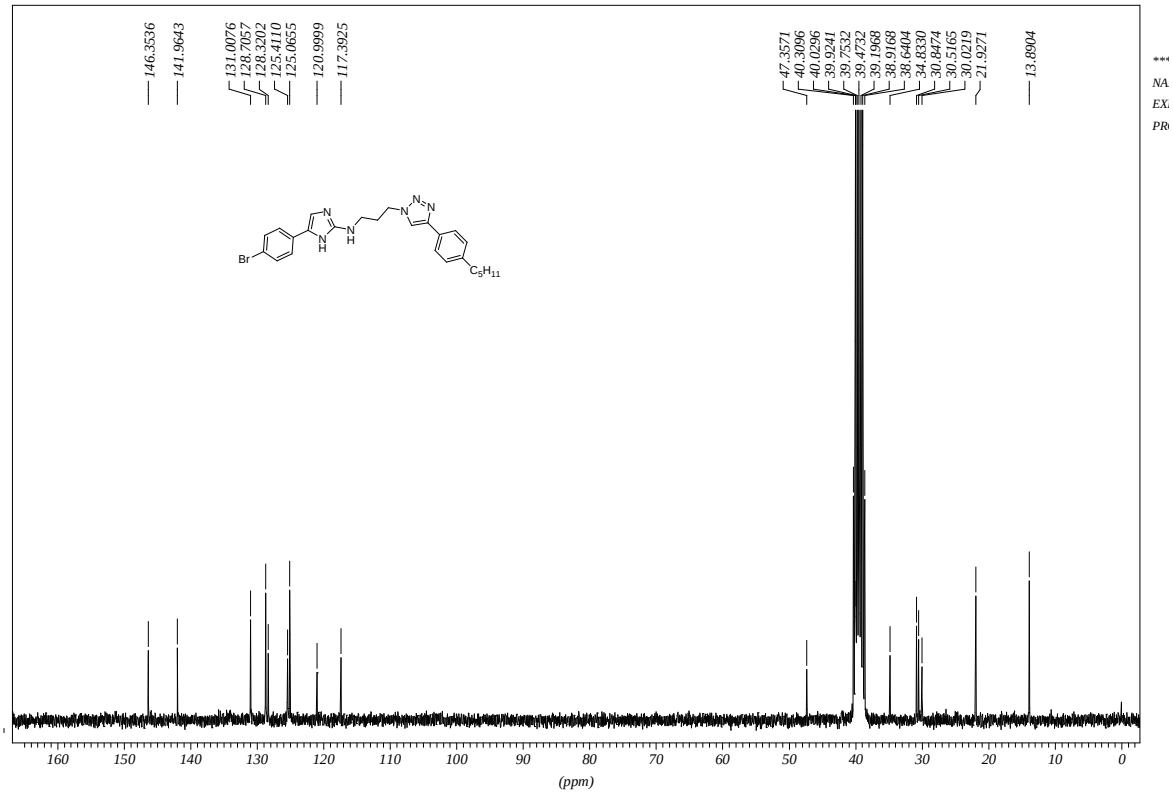
^{1}H NMR and ^{13}C NMR spectra of **5f** (DMSO-d_6)



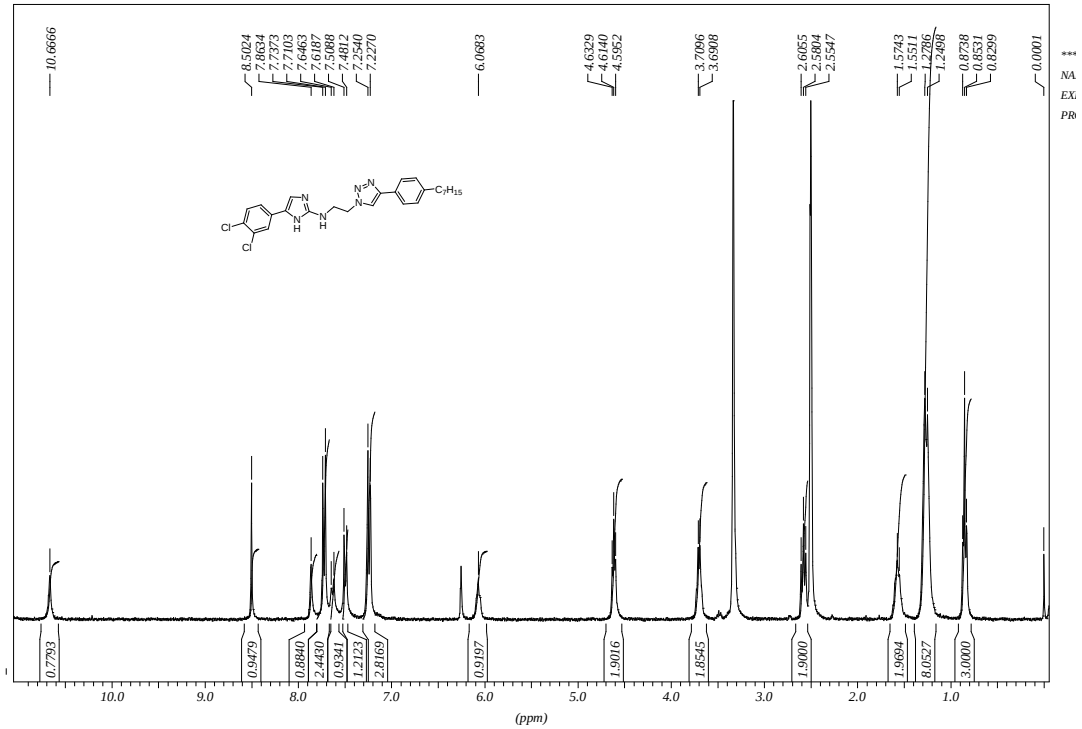


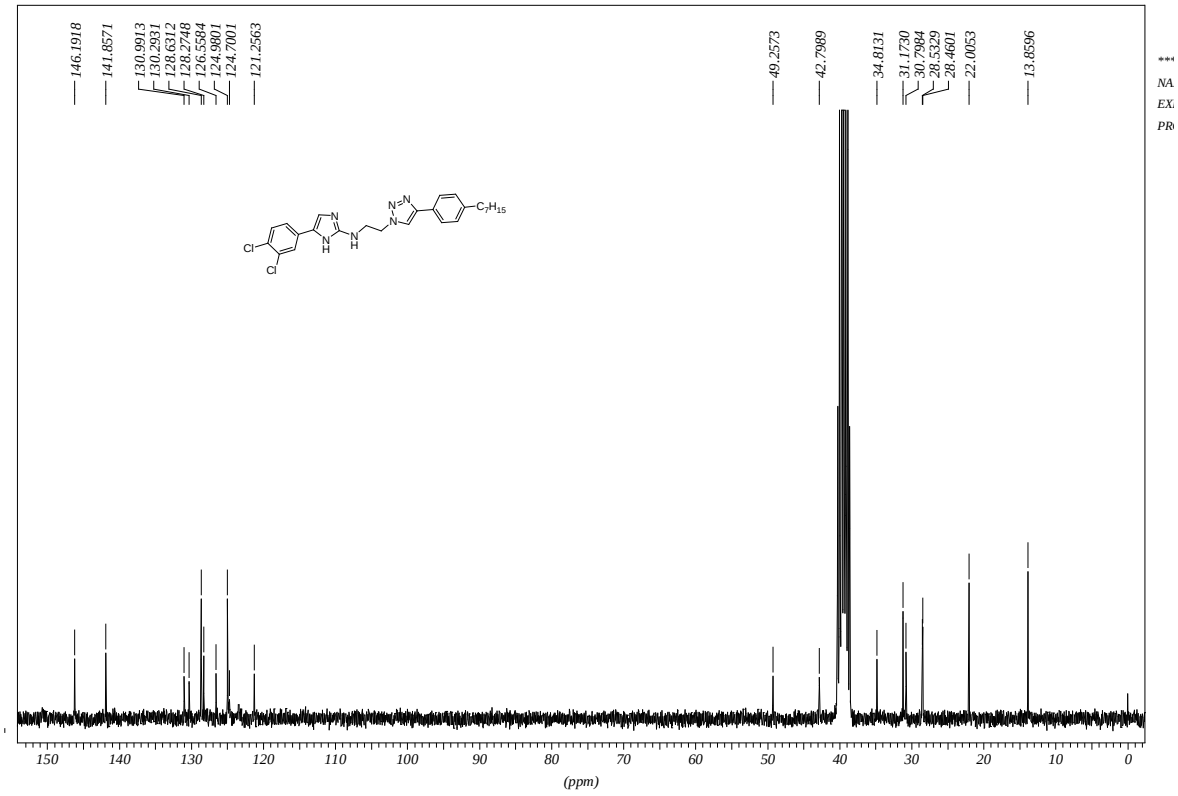
^{1}H NMR and ^{13}C NMR spectra of **5g** (DMSO-d_6)



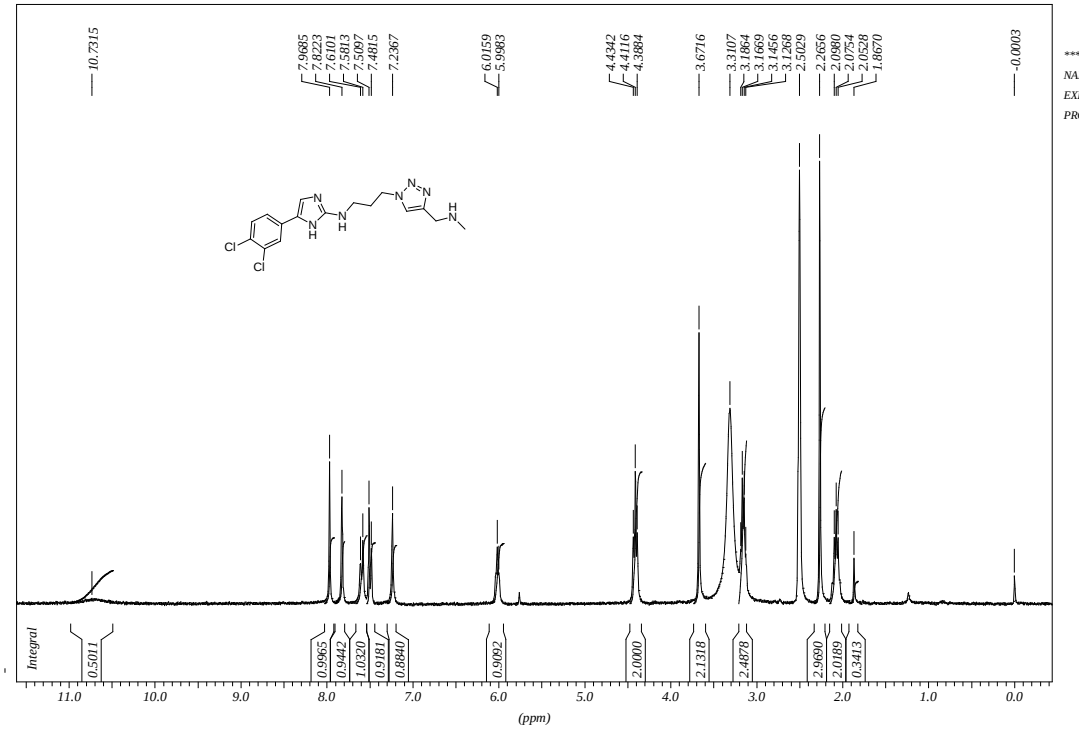


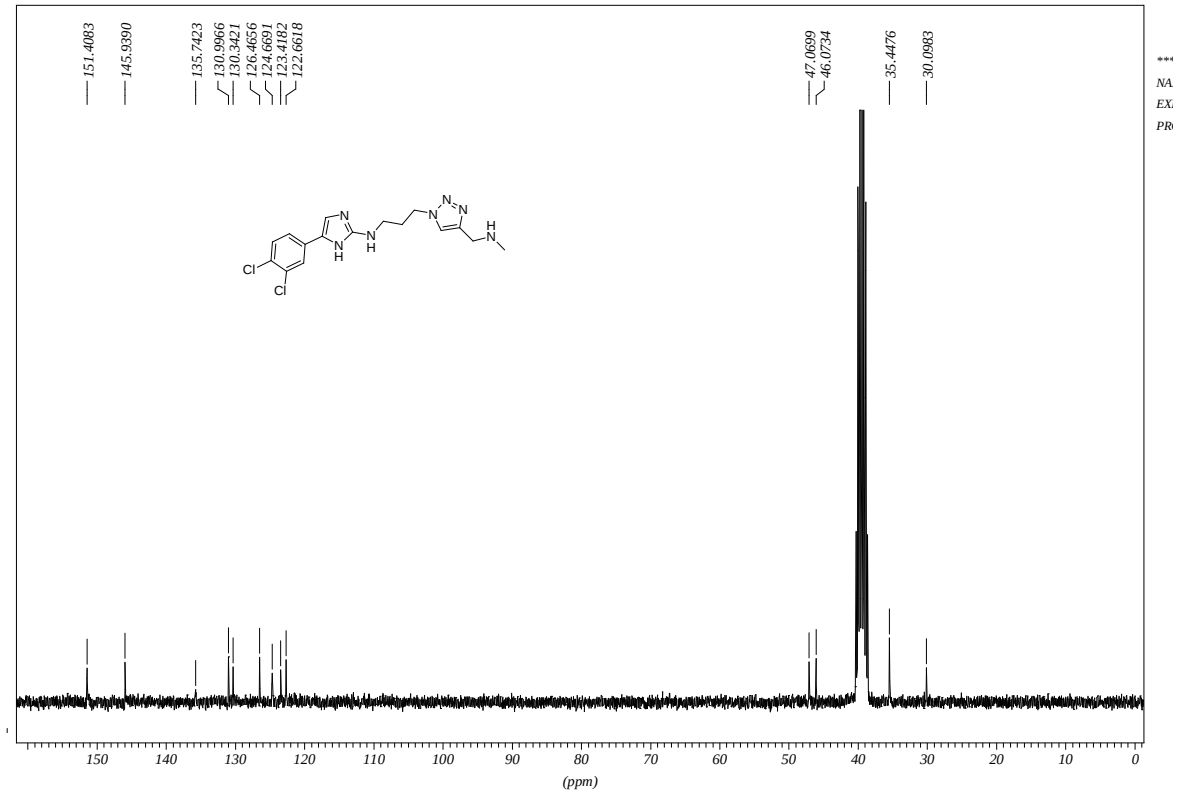
^{1}H NMR and ^{13}C NMR spectra of **5h** (DMSO-d_6)



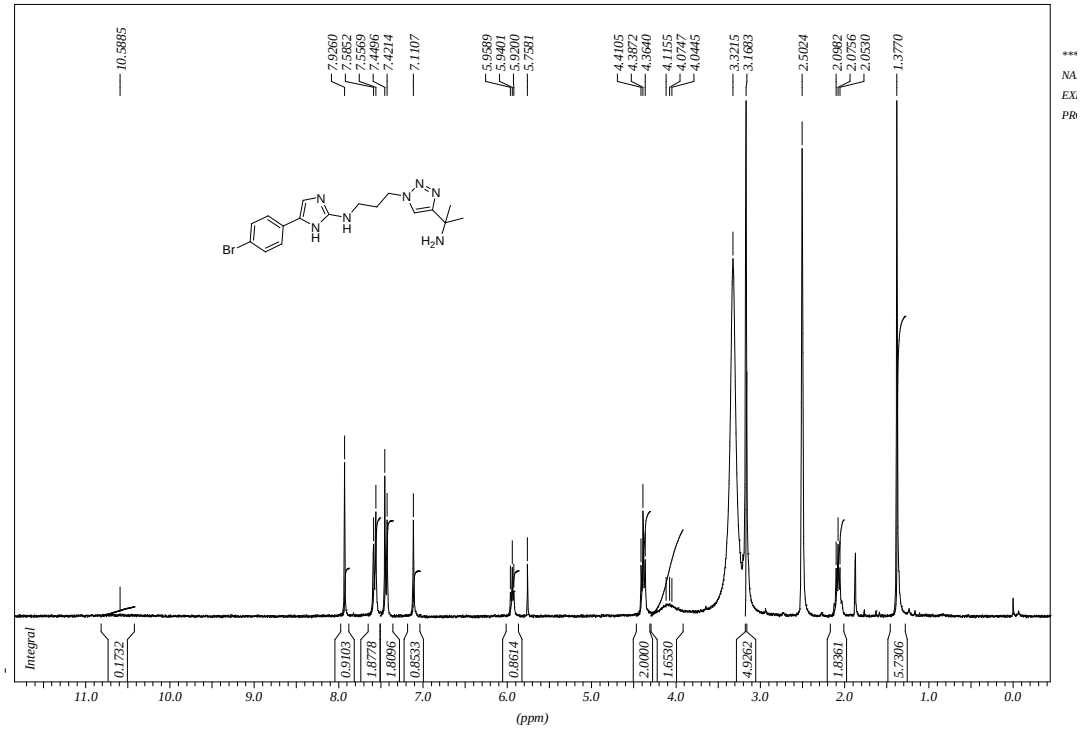


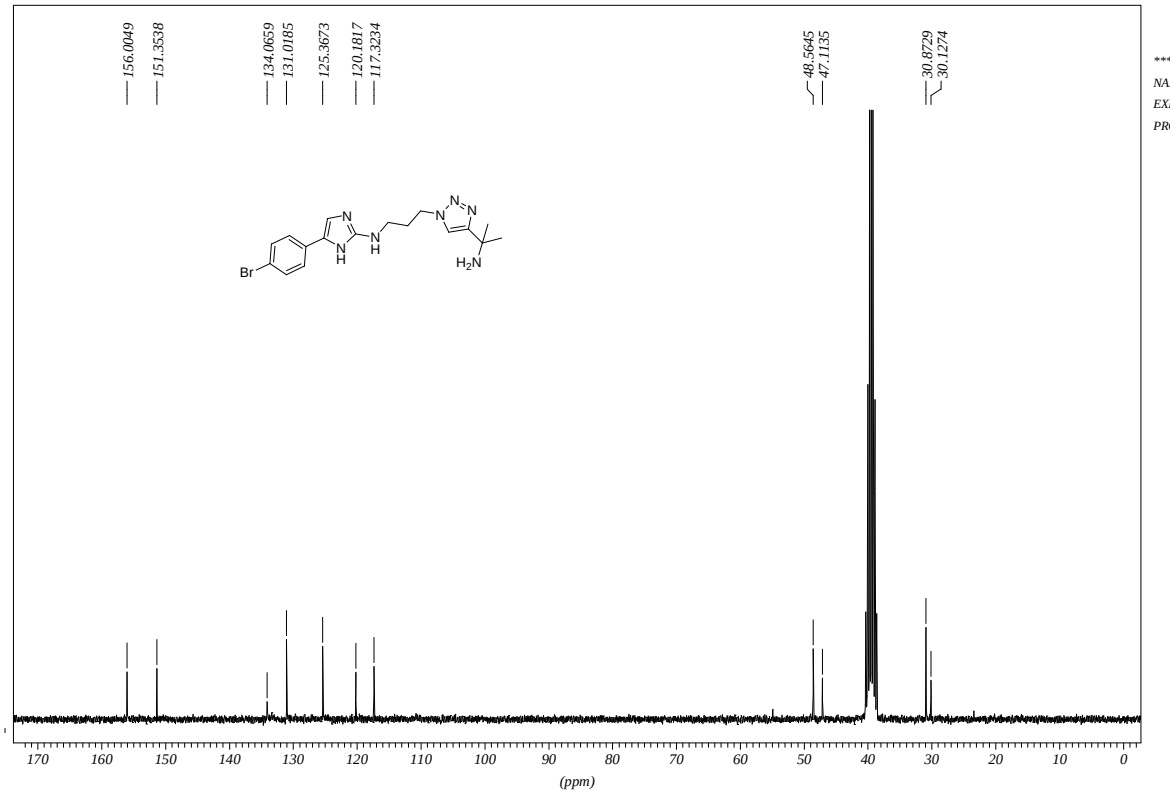
^{1}H NMR and ^{13}C NMR spectra of **5i** (DMSO-d_6)



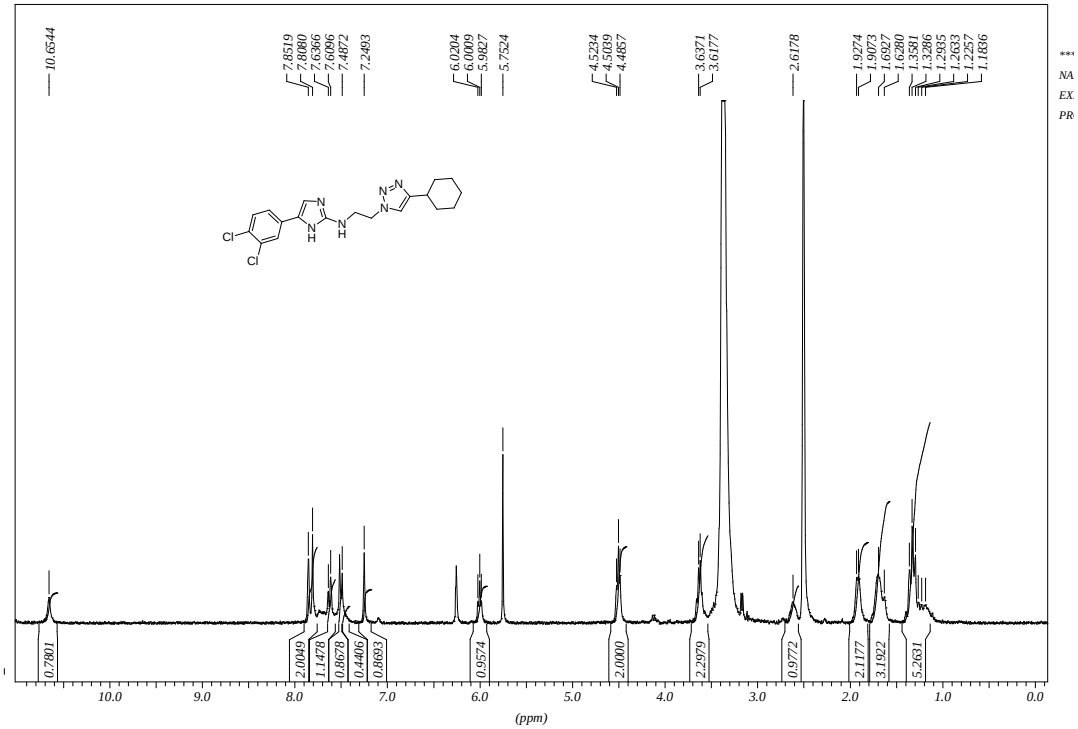


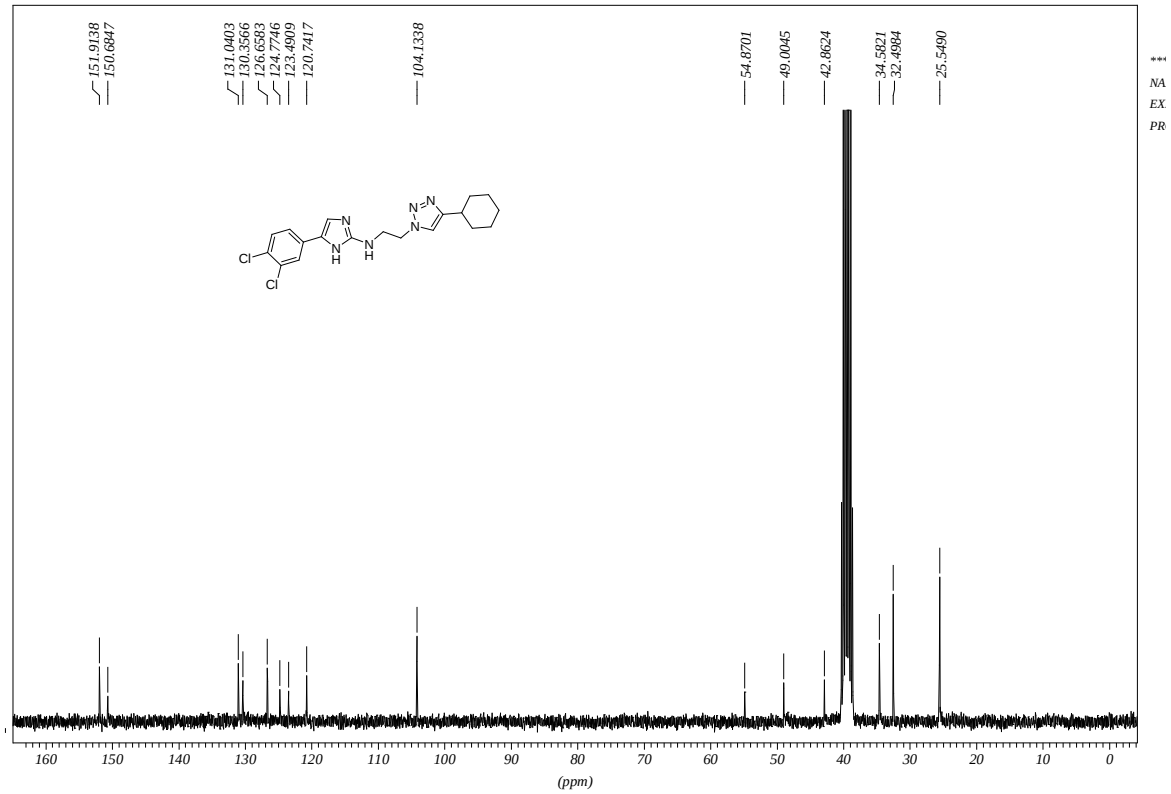
^{1}H NMR and ^{13}C NMR spectra of **5j** (DMSO-d_6)



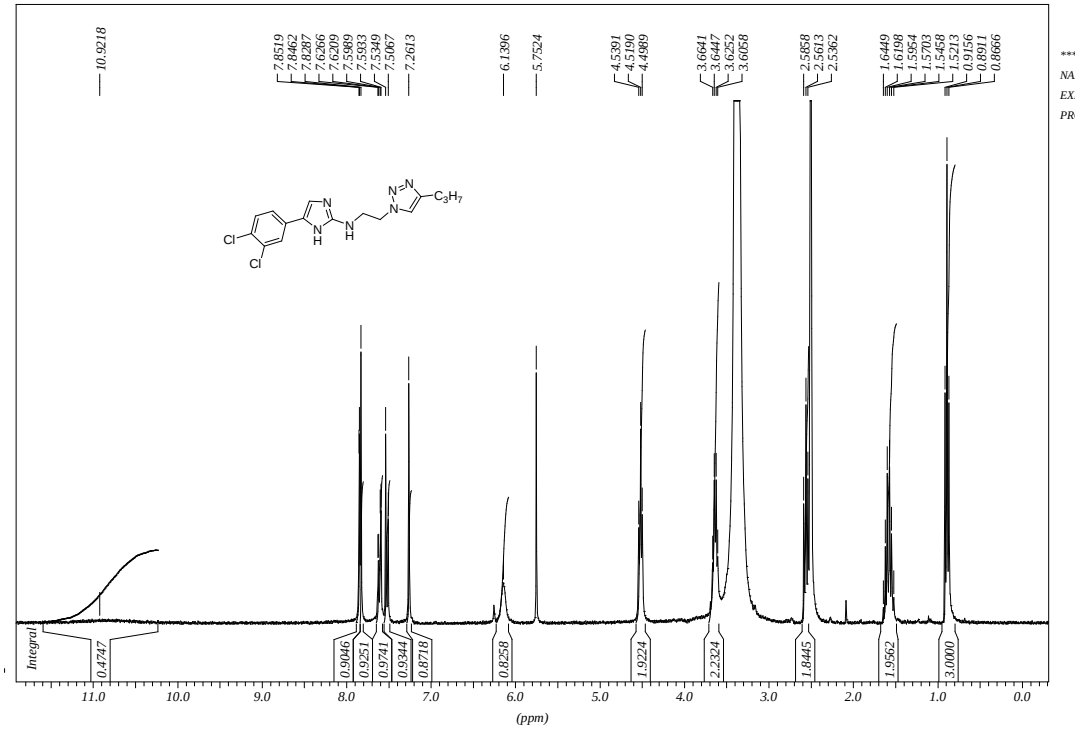


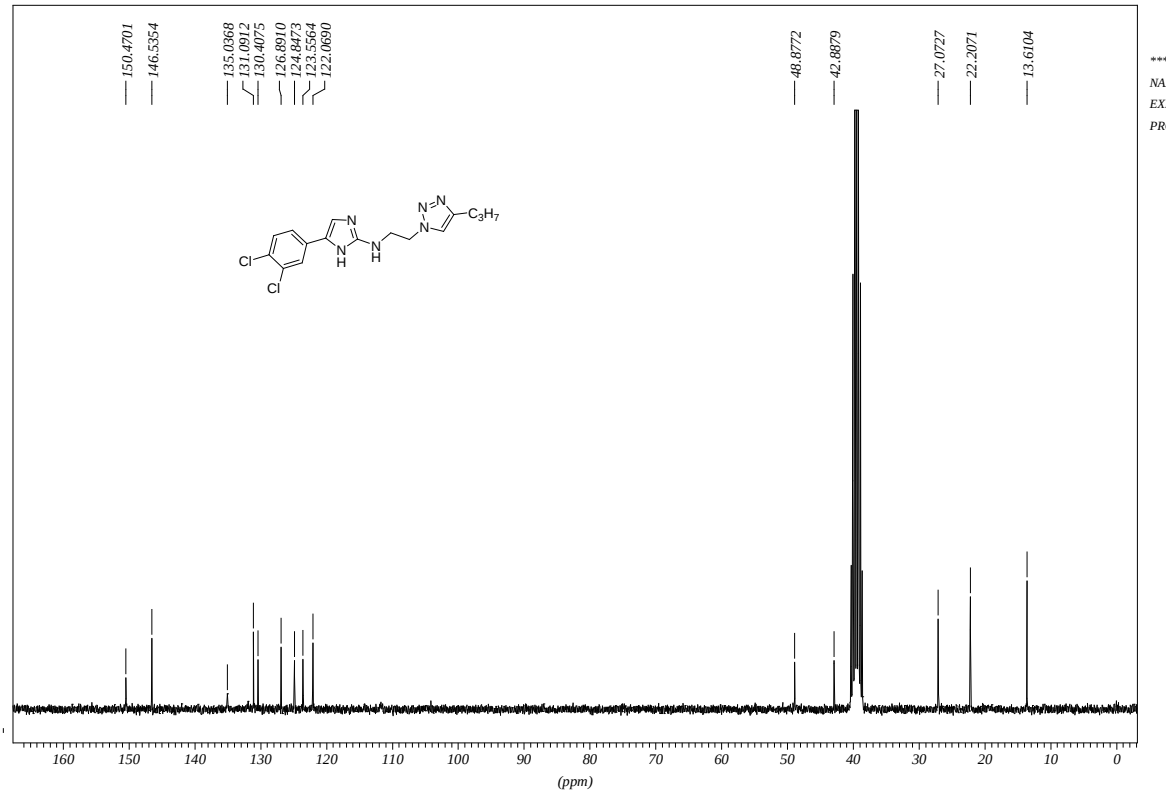
^{1}H NMR and ^{13}C NMR spectra of **5k** (DMSO-d_6)



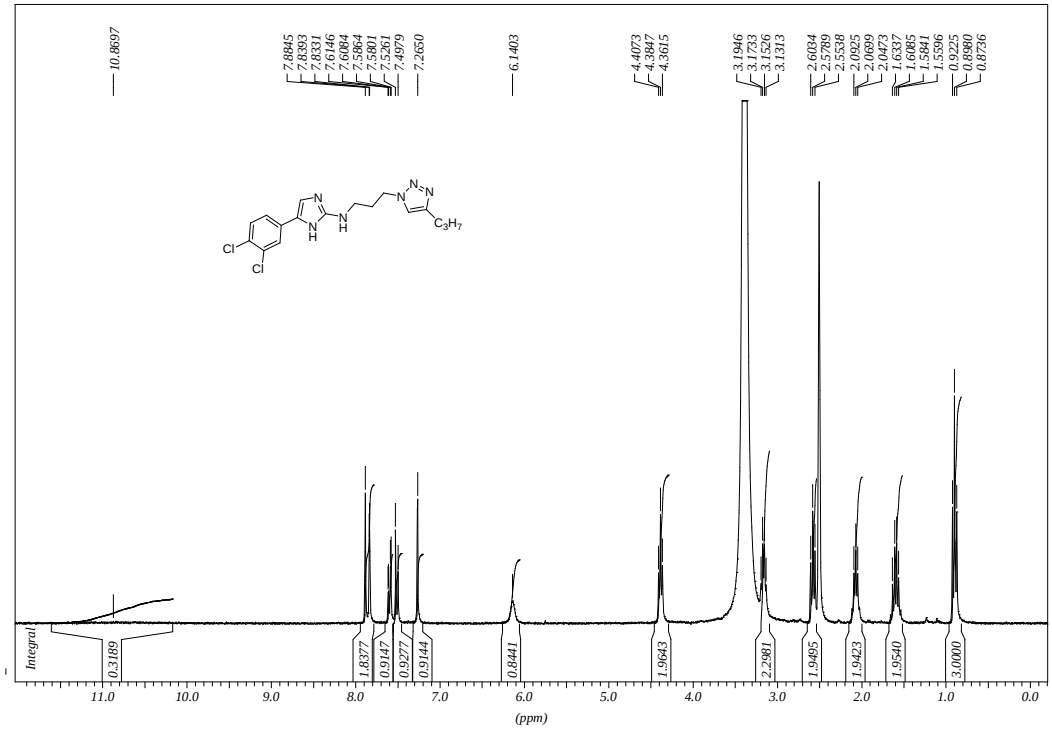


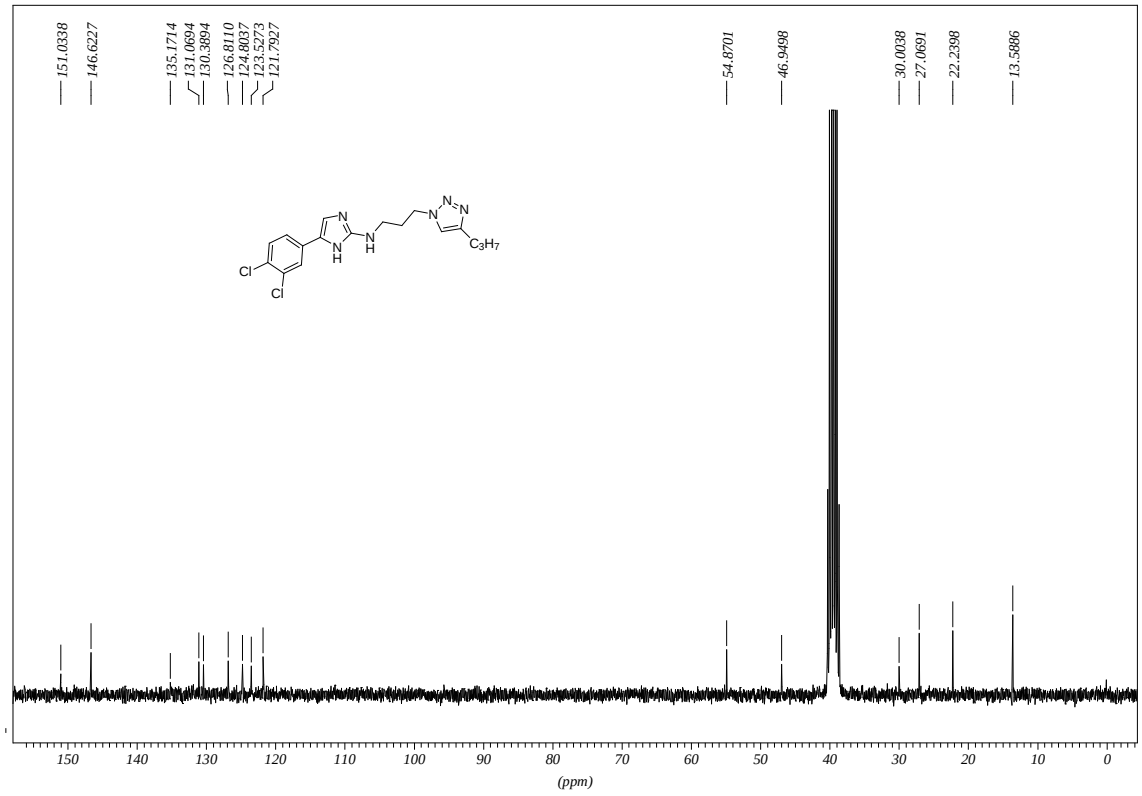
^{1}H NMR and ^{13}C NMR spectra of **5l** (DMSO-d_6)



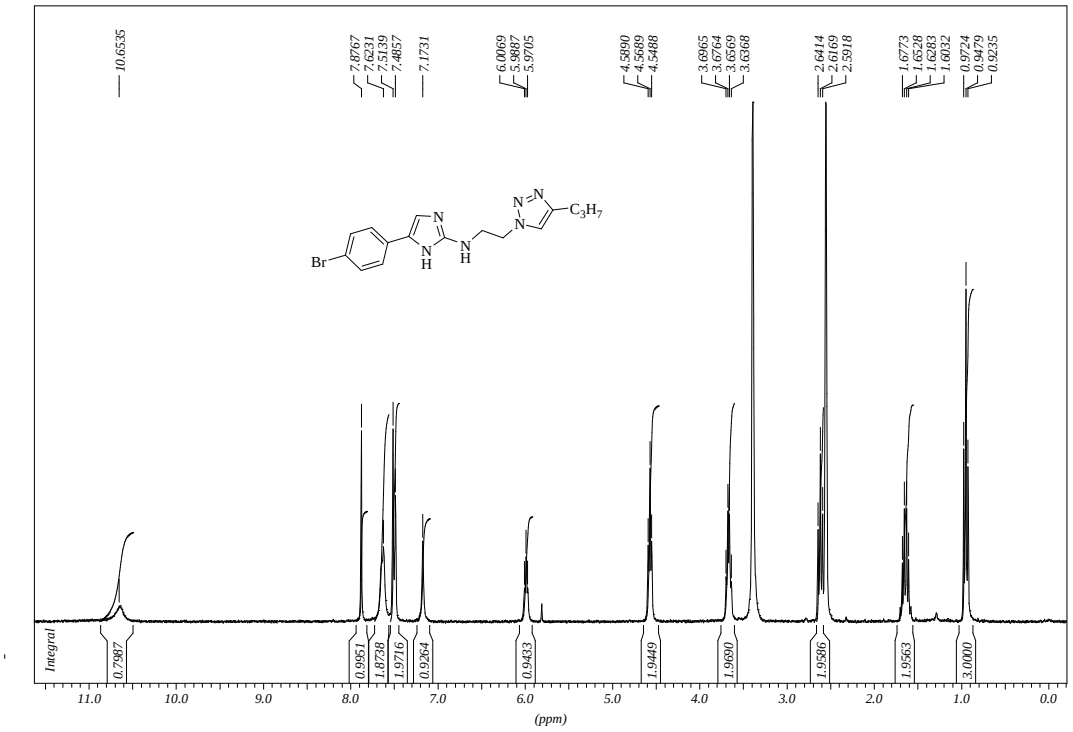


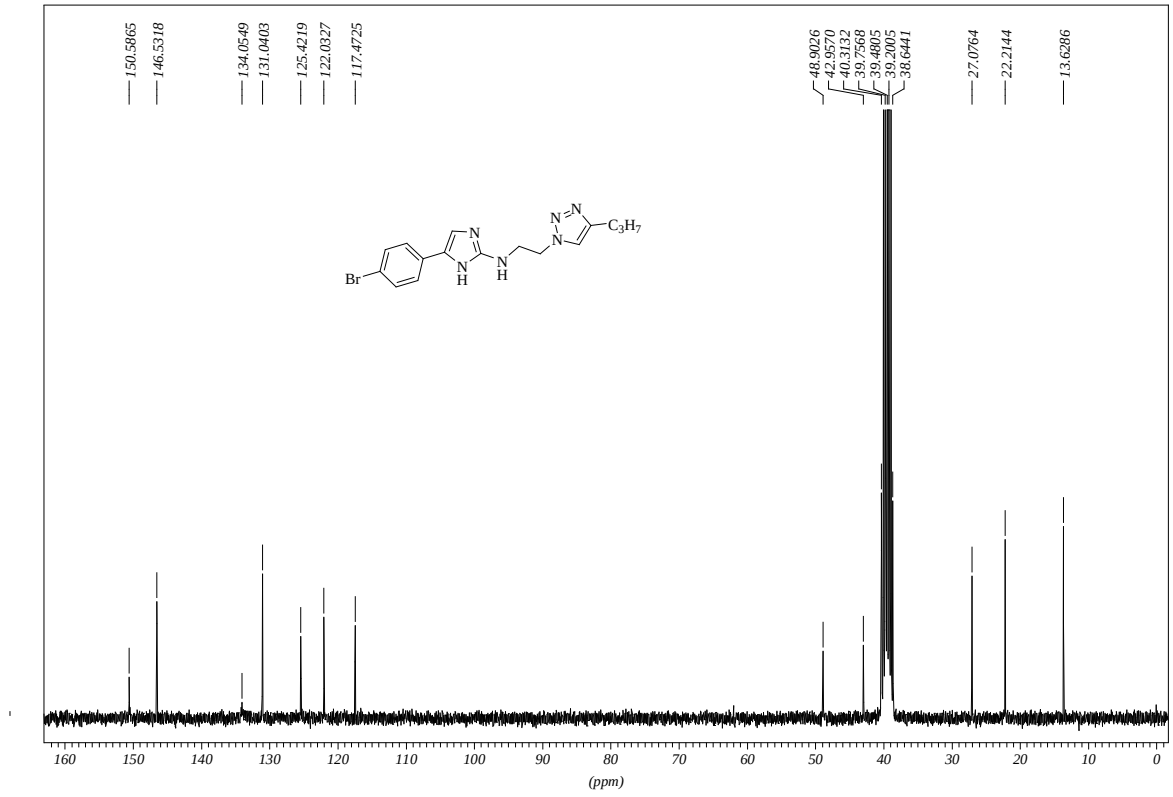
^{1}H NMR and ^{13}C NMR spectra of **5m** (DMSO-d_6)



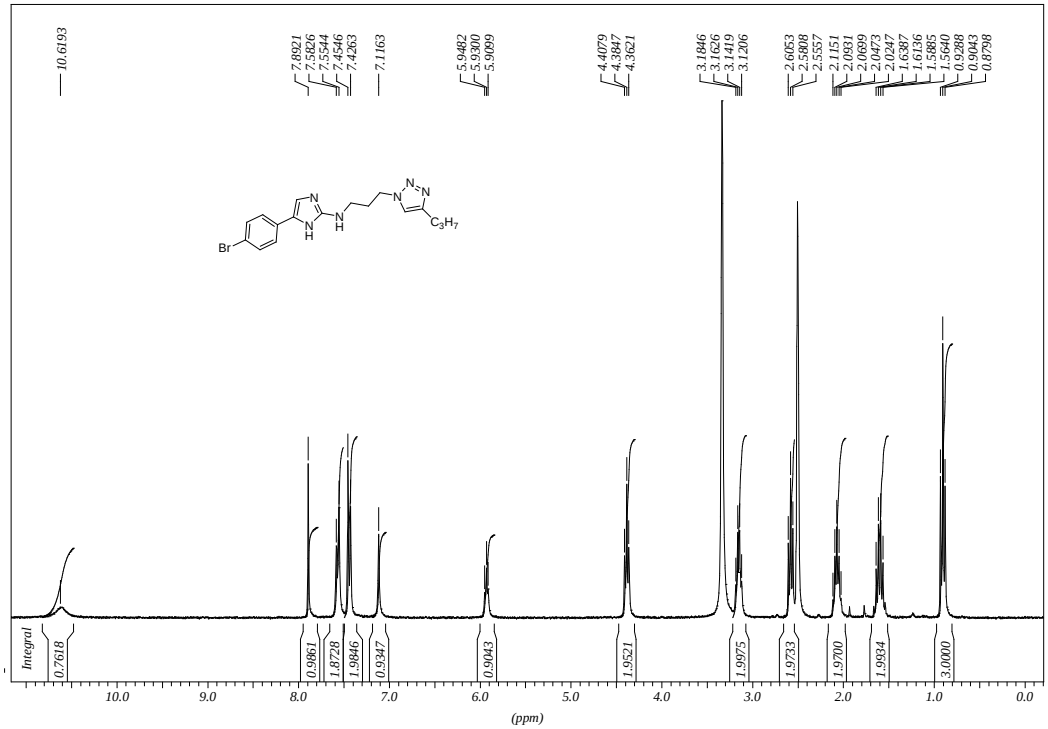


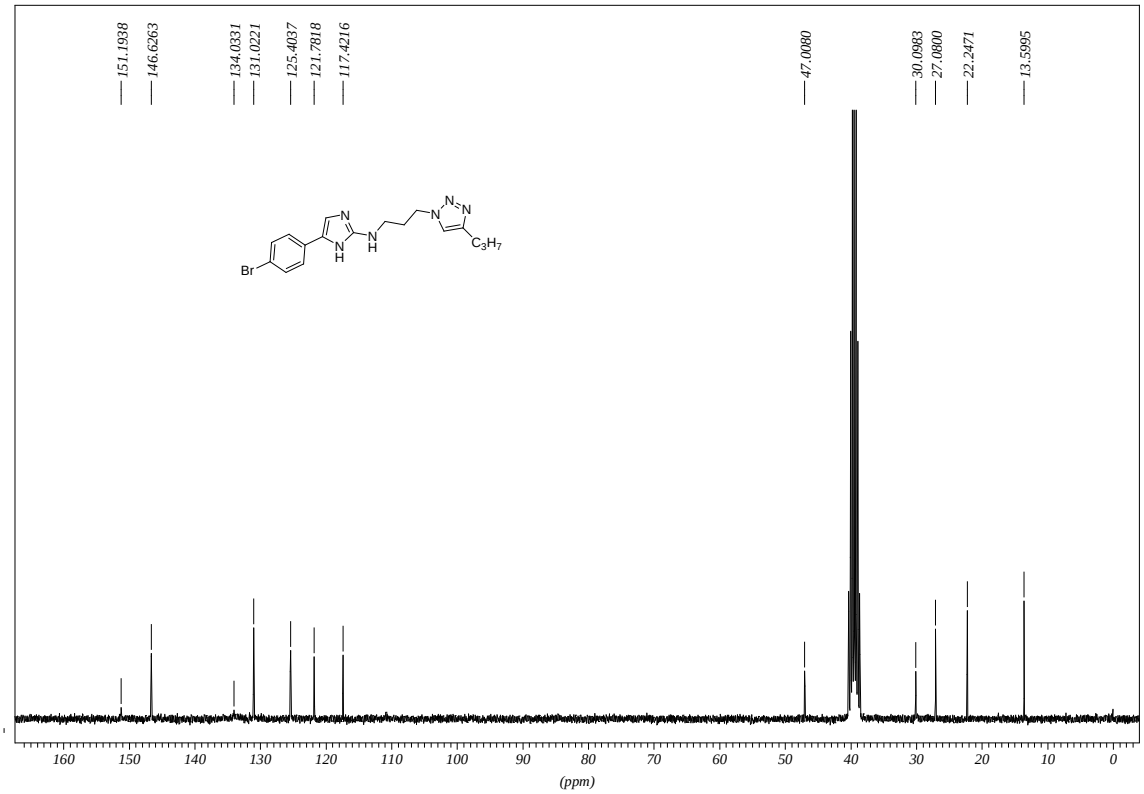
^{1}H NMR and ^{13}C NMR spectra of **5n** (DMSO-d_6)



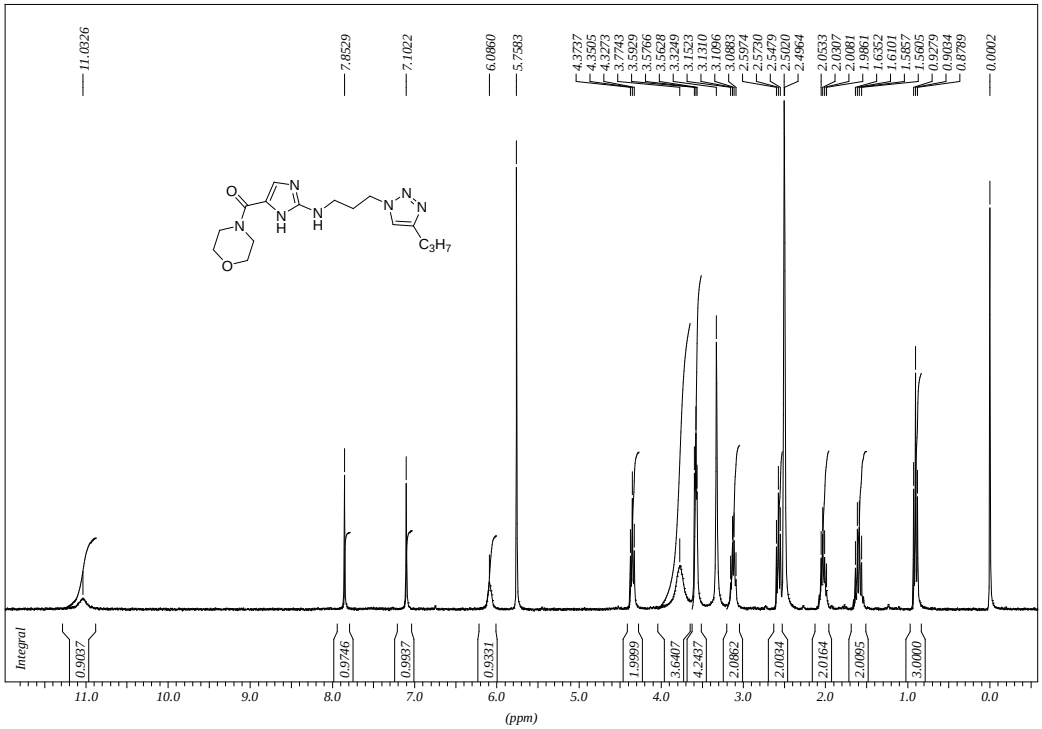


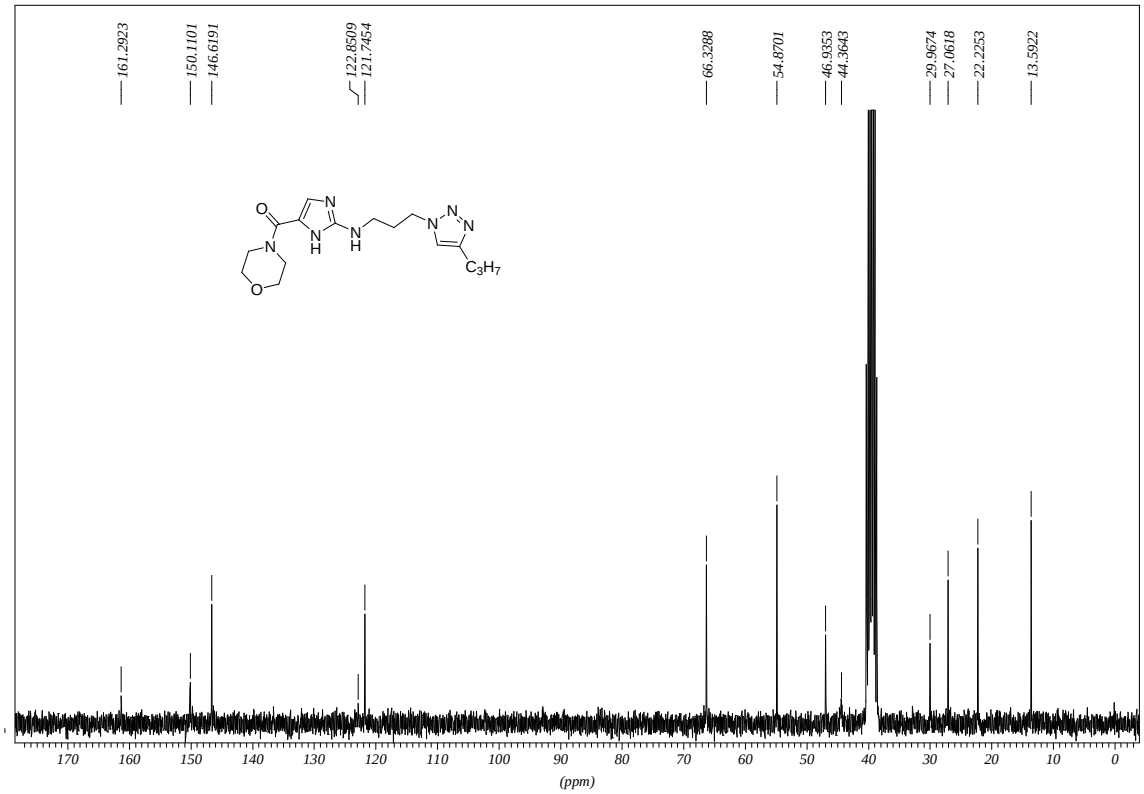
^{1}H NMR and ^{13}C NMR spectra of **5o** (DMSO-d_6)



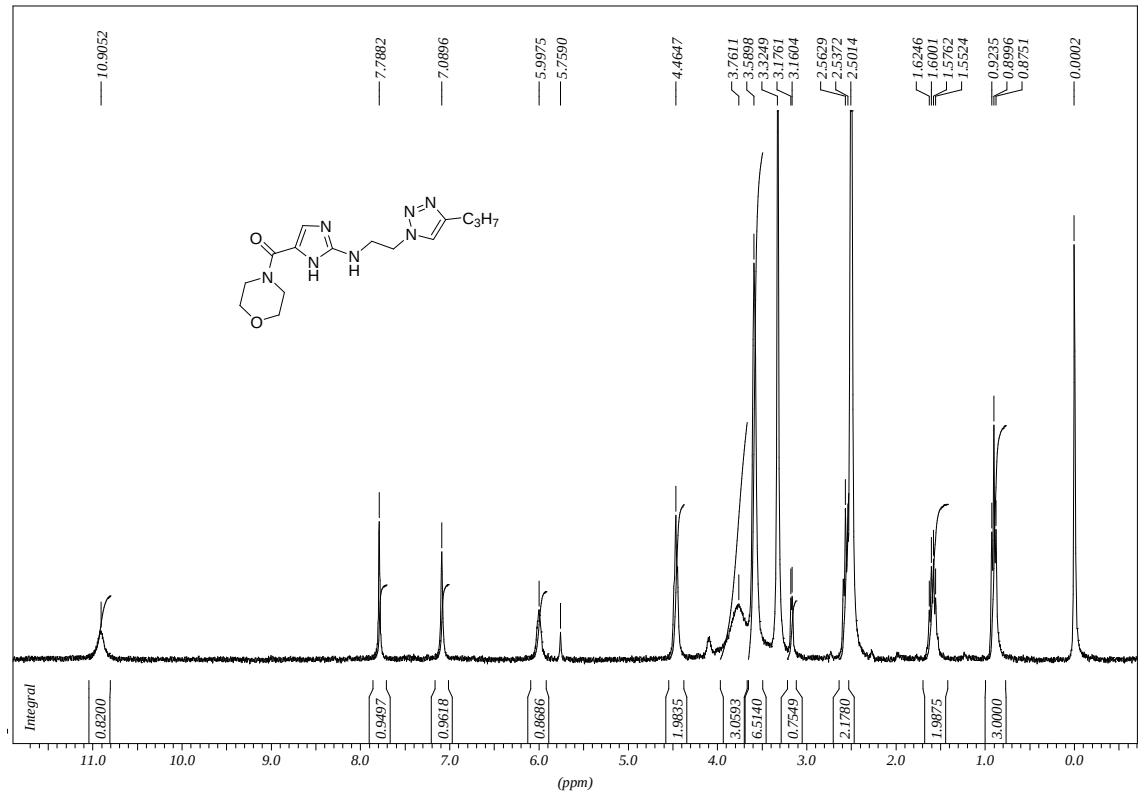


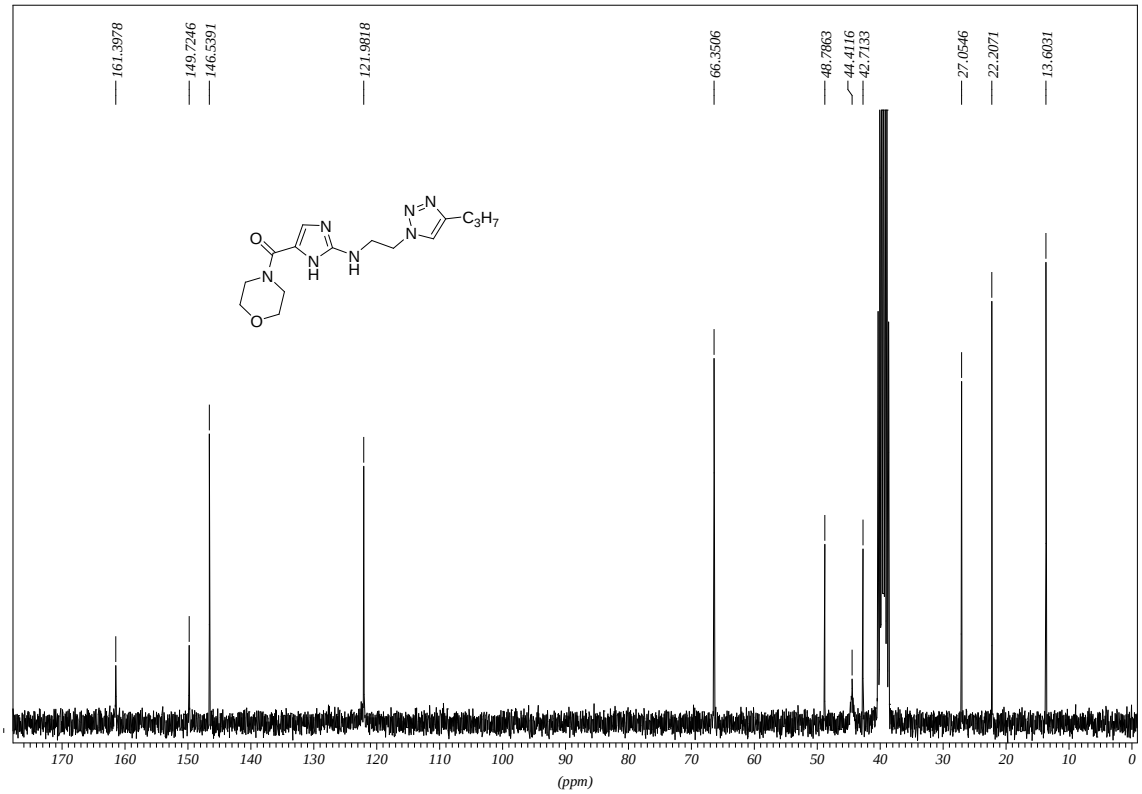
^{1}H NMR and ^{13}C NMR spectra of **5p** (DMSO-d_6)



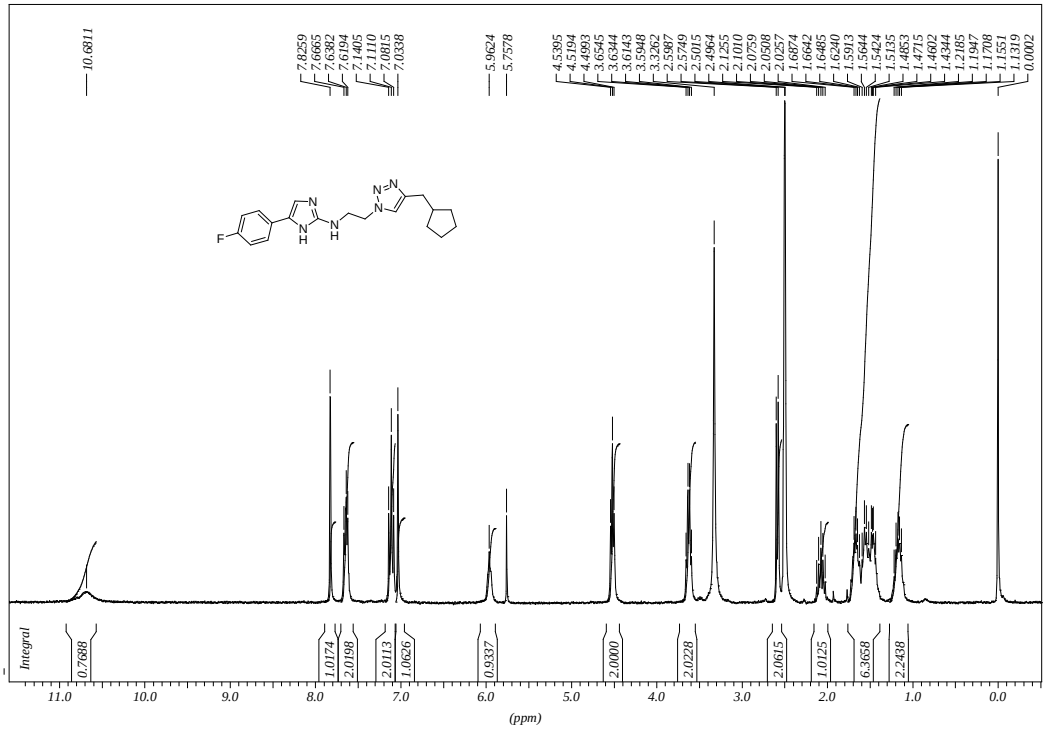


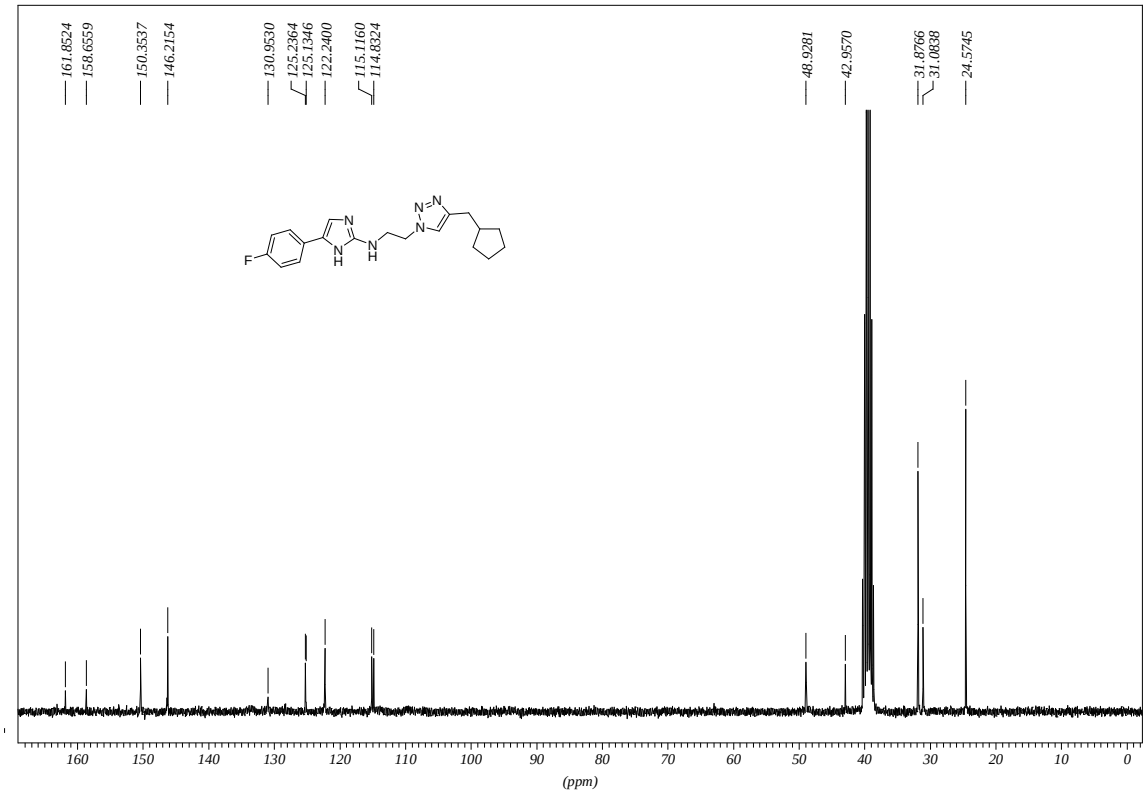
^{1}H NMR and ^{13}C NMR spectra of **5q** (DMSO-d_6)



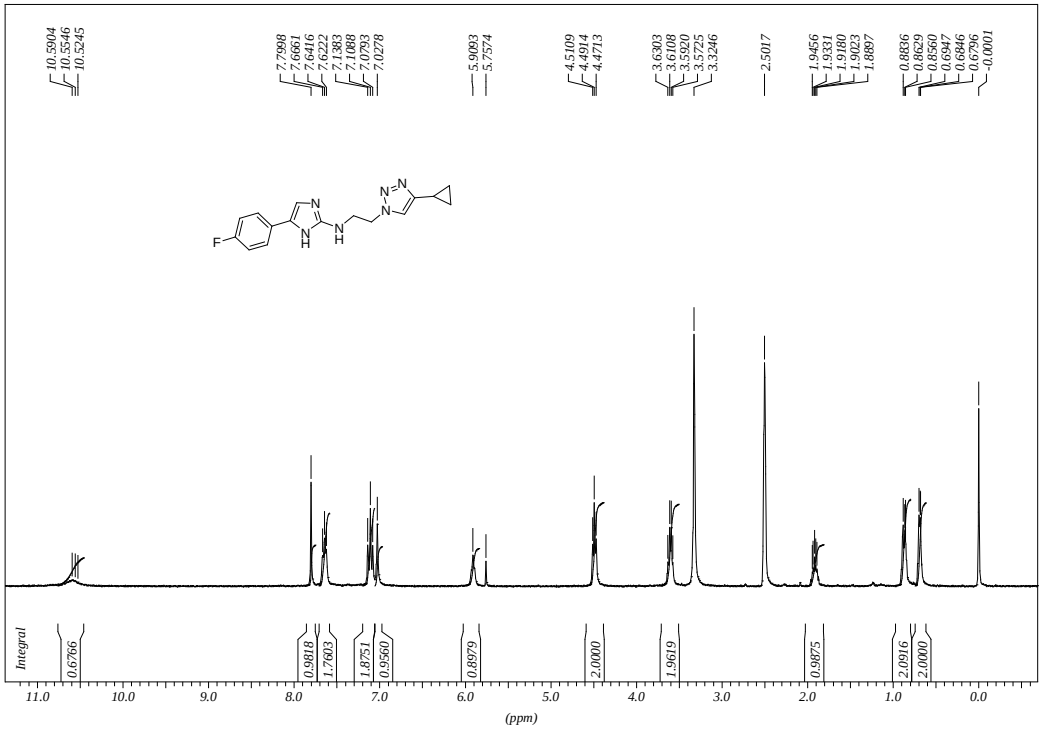


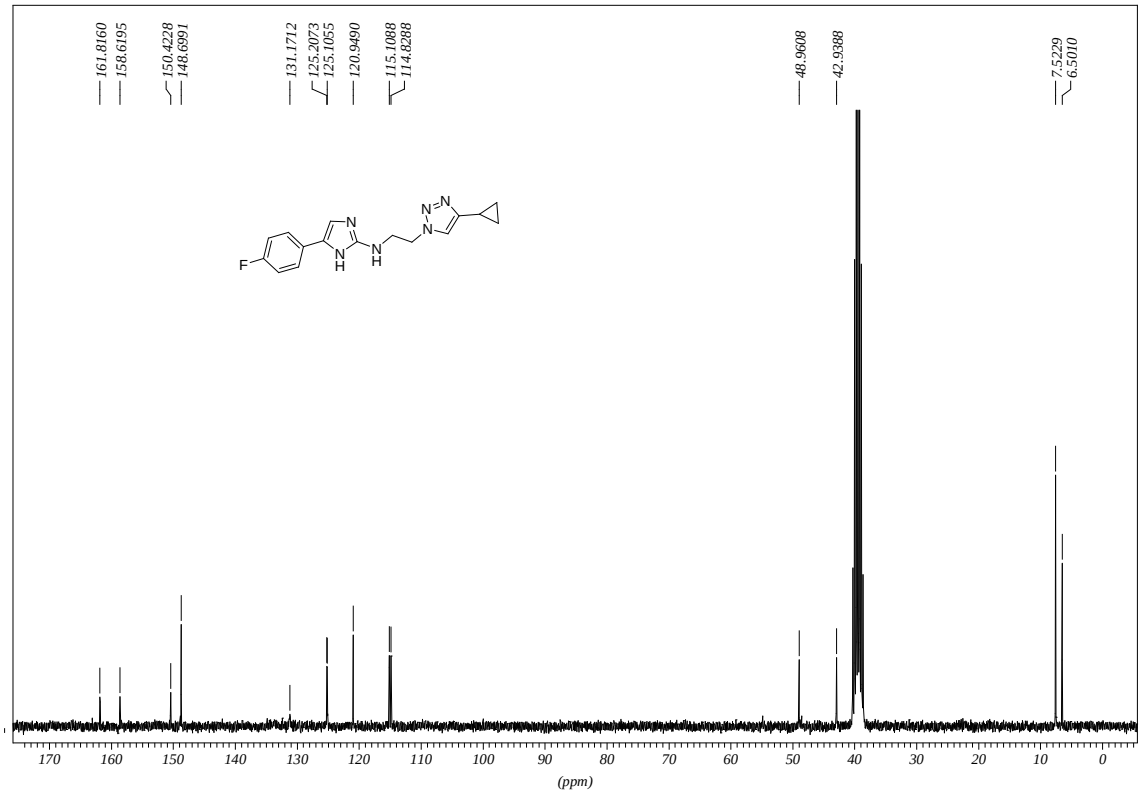
^{1}H NMR and ^{13}C NMR spectra of **5r** (DMSO-d_6)



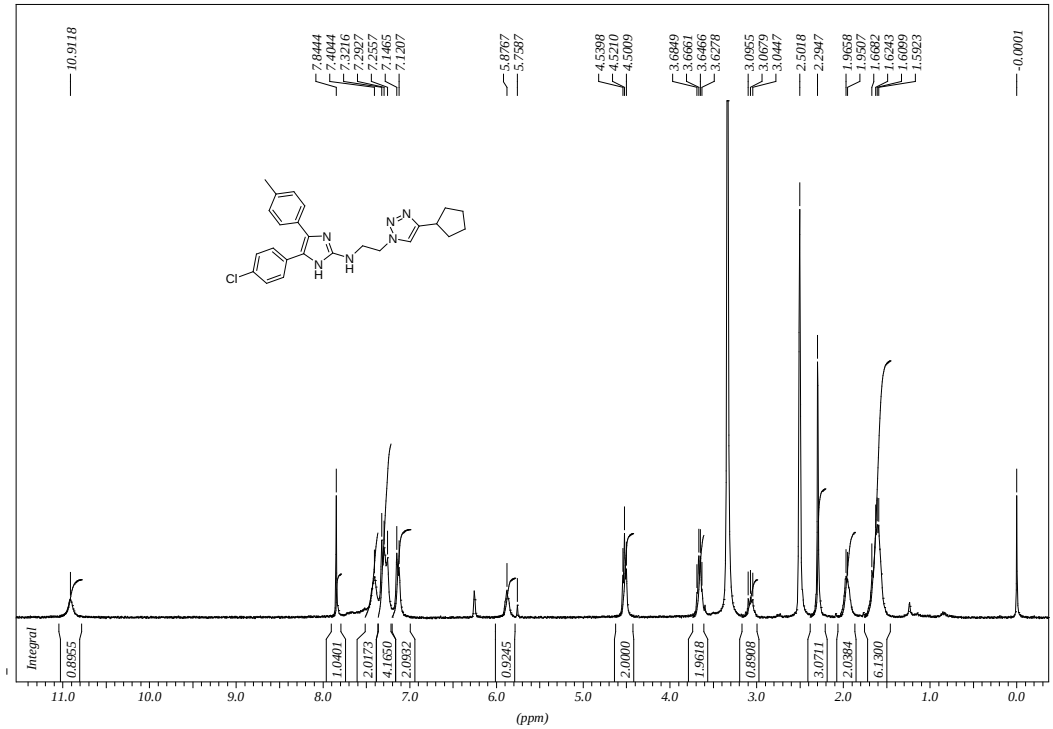


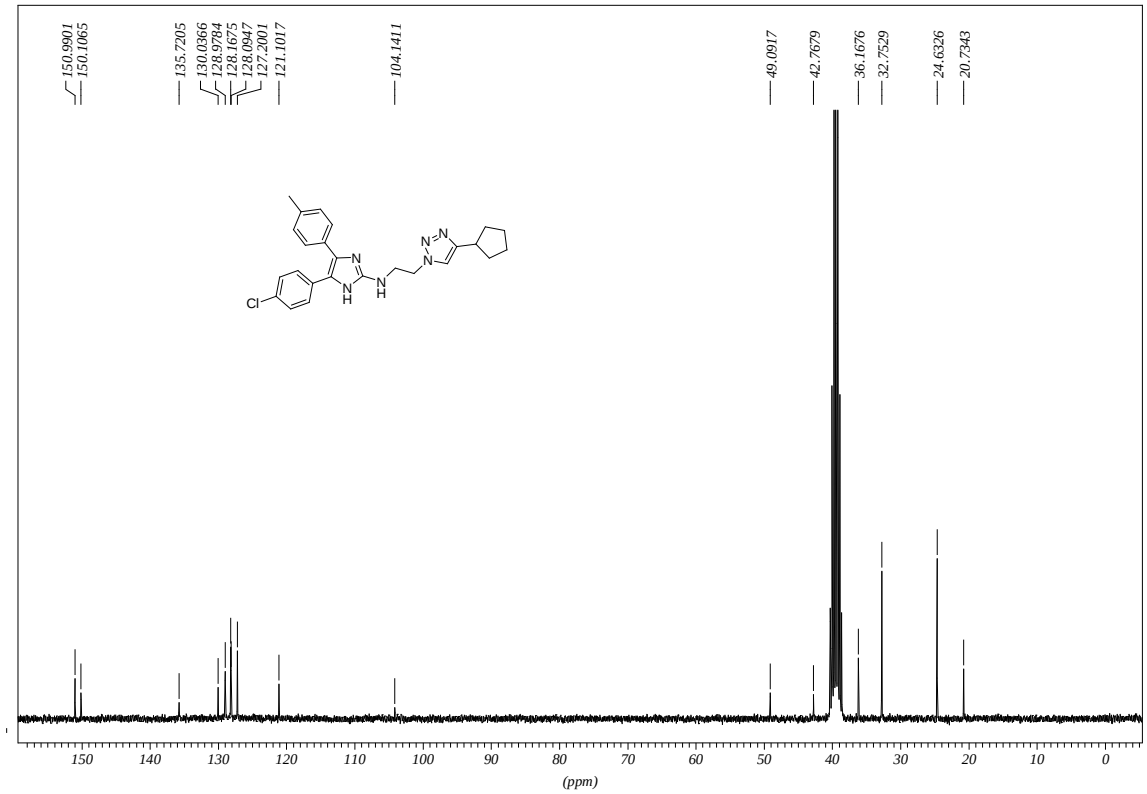
^{1}H NMR and ^{13}C NMR spectra of **5s** (DMSO-d_6)



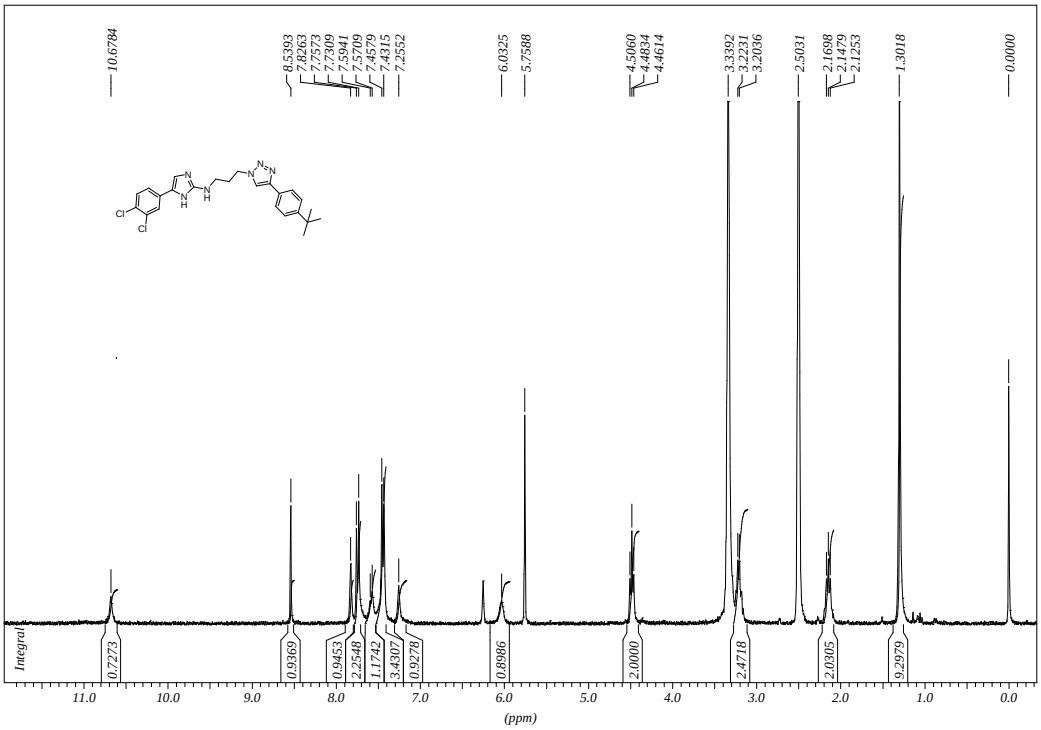


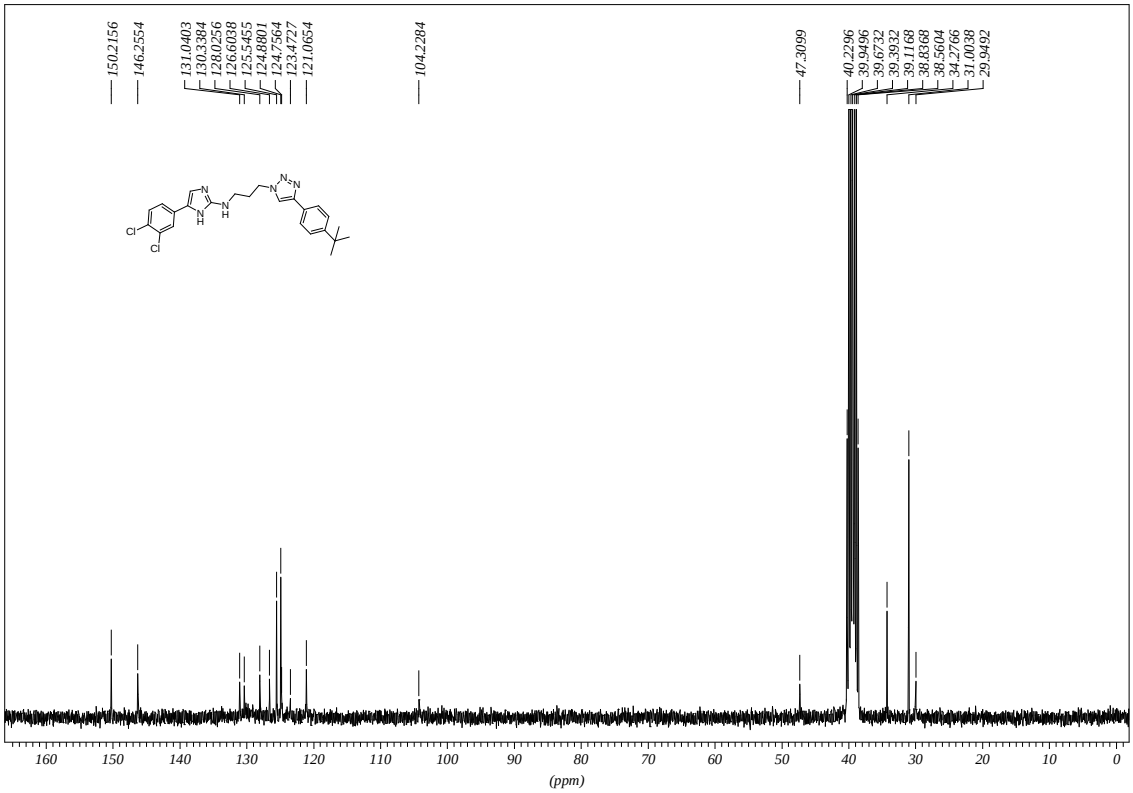
^{1}H NMR and ^{13}C NMR spectra of **5t** (DMSO-d_6)



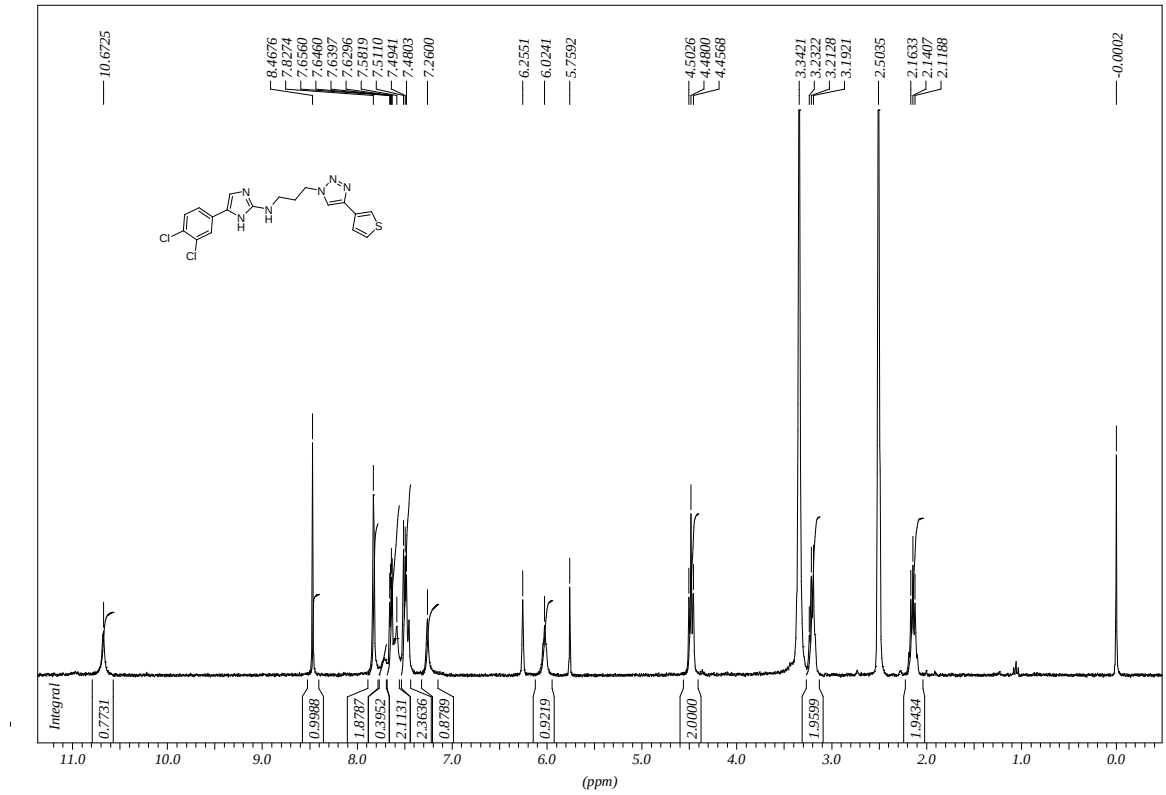


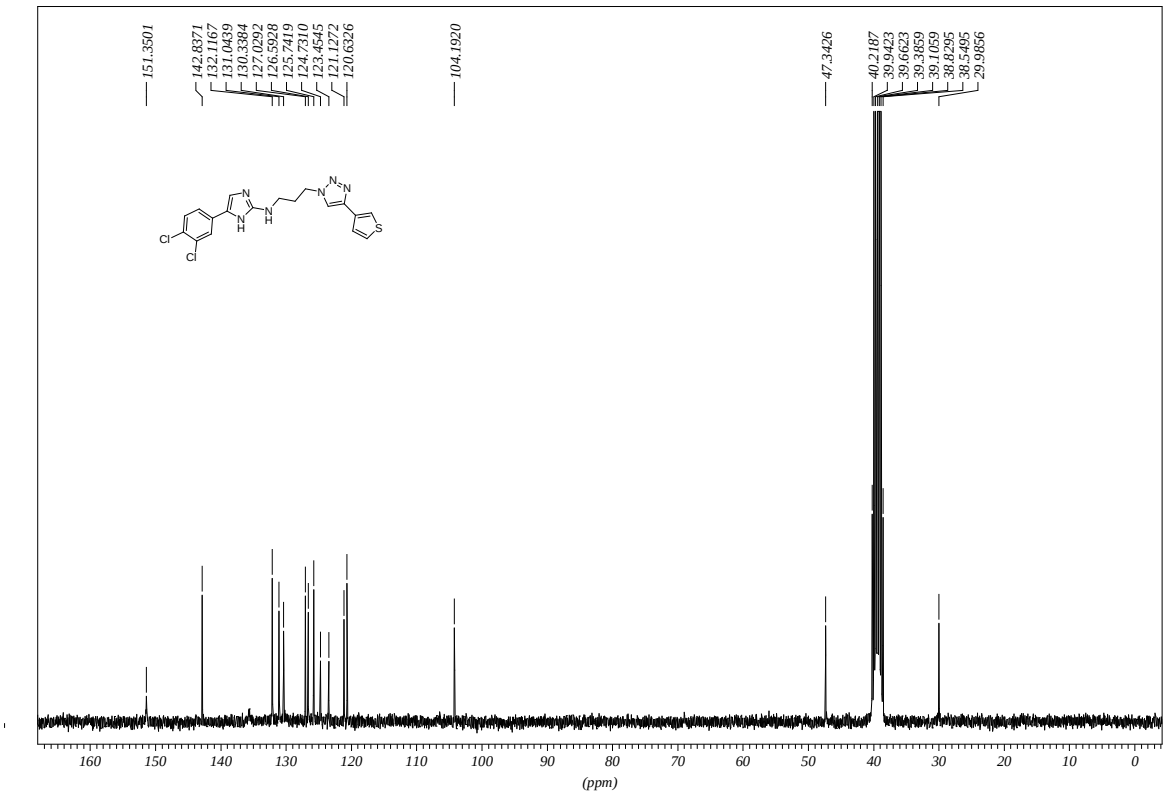
^{1}H NMR and ^{13}C NMR spectra of **5u** (DMSO-d_6)



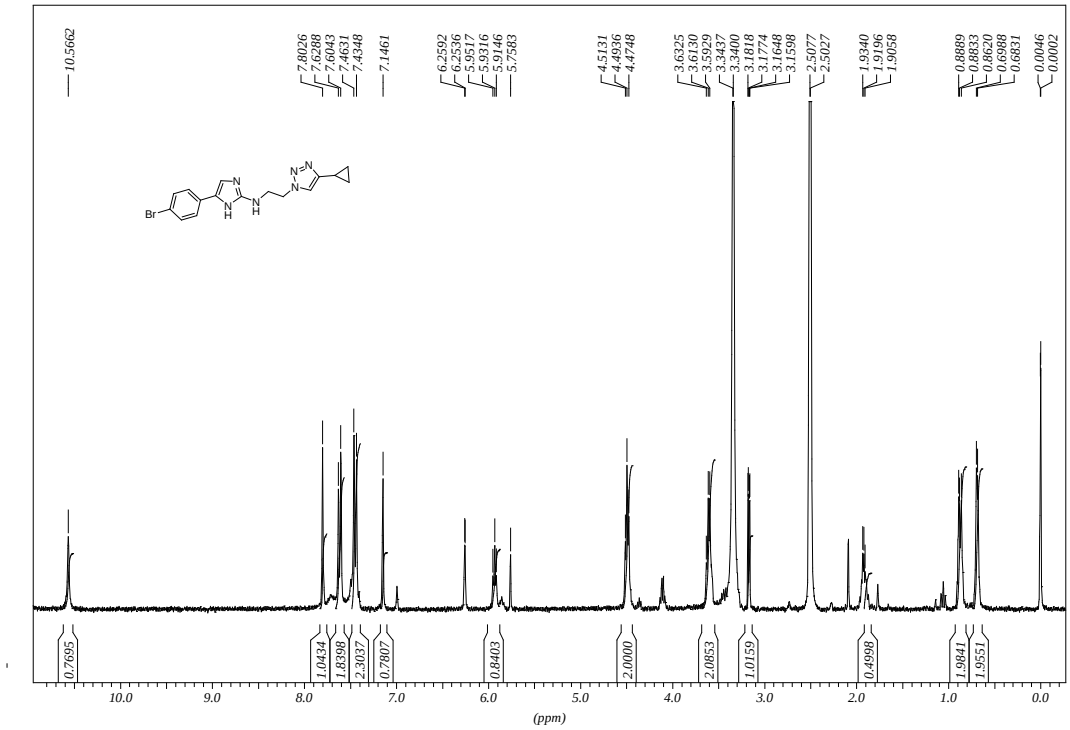


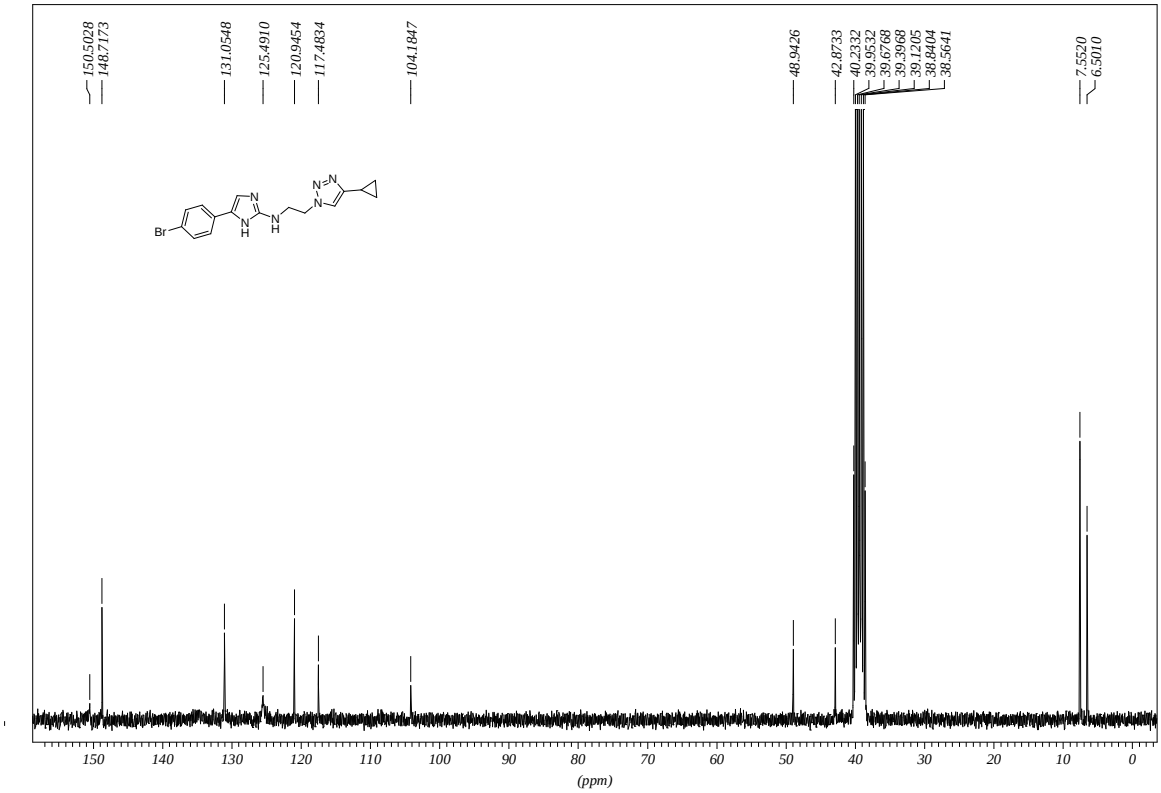
^{1}H NMR and ^{13}C NMR spectra of **5v** (DMSO-d_6)



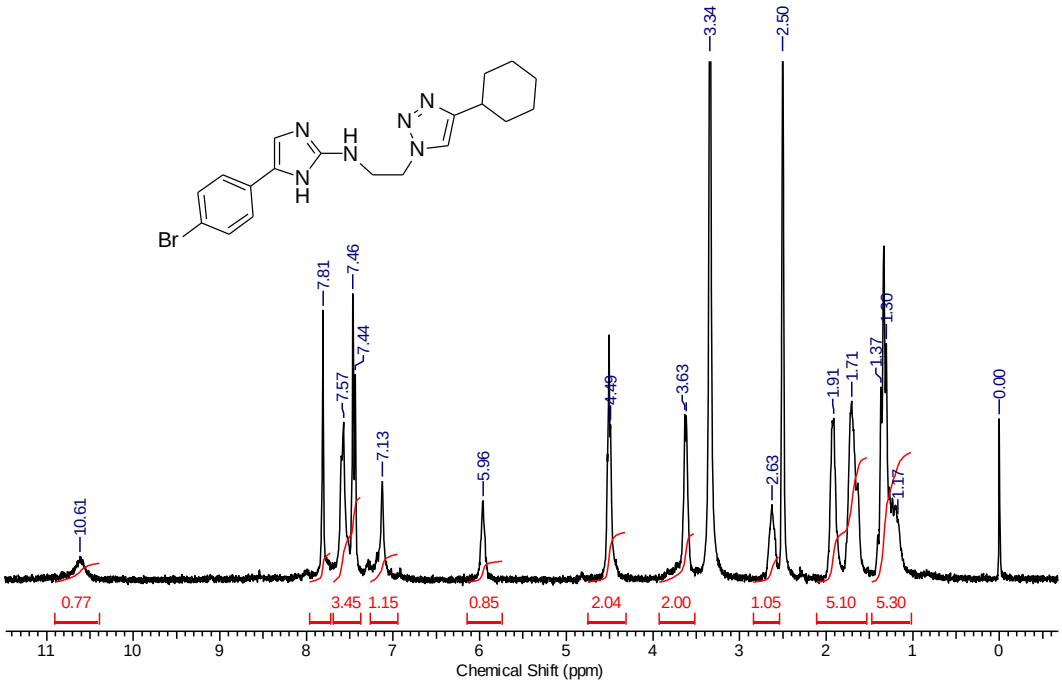


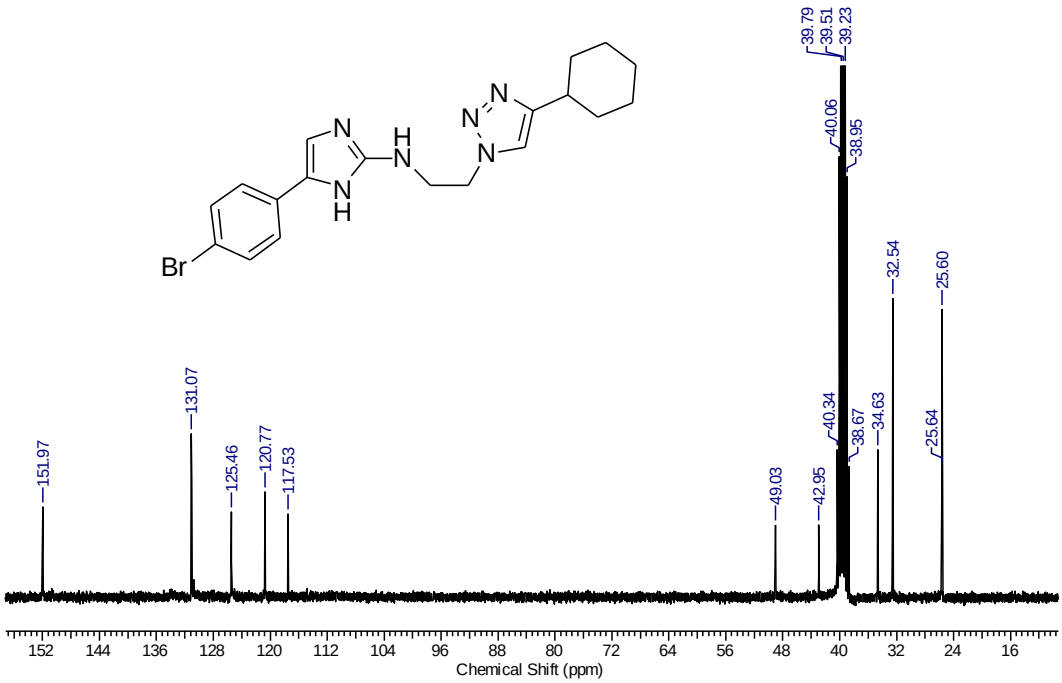
^{1}H NMR and ^{13}C NMR spectra of **5w** (DMSO-d_6)



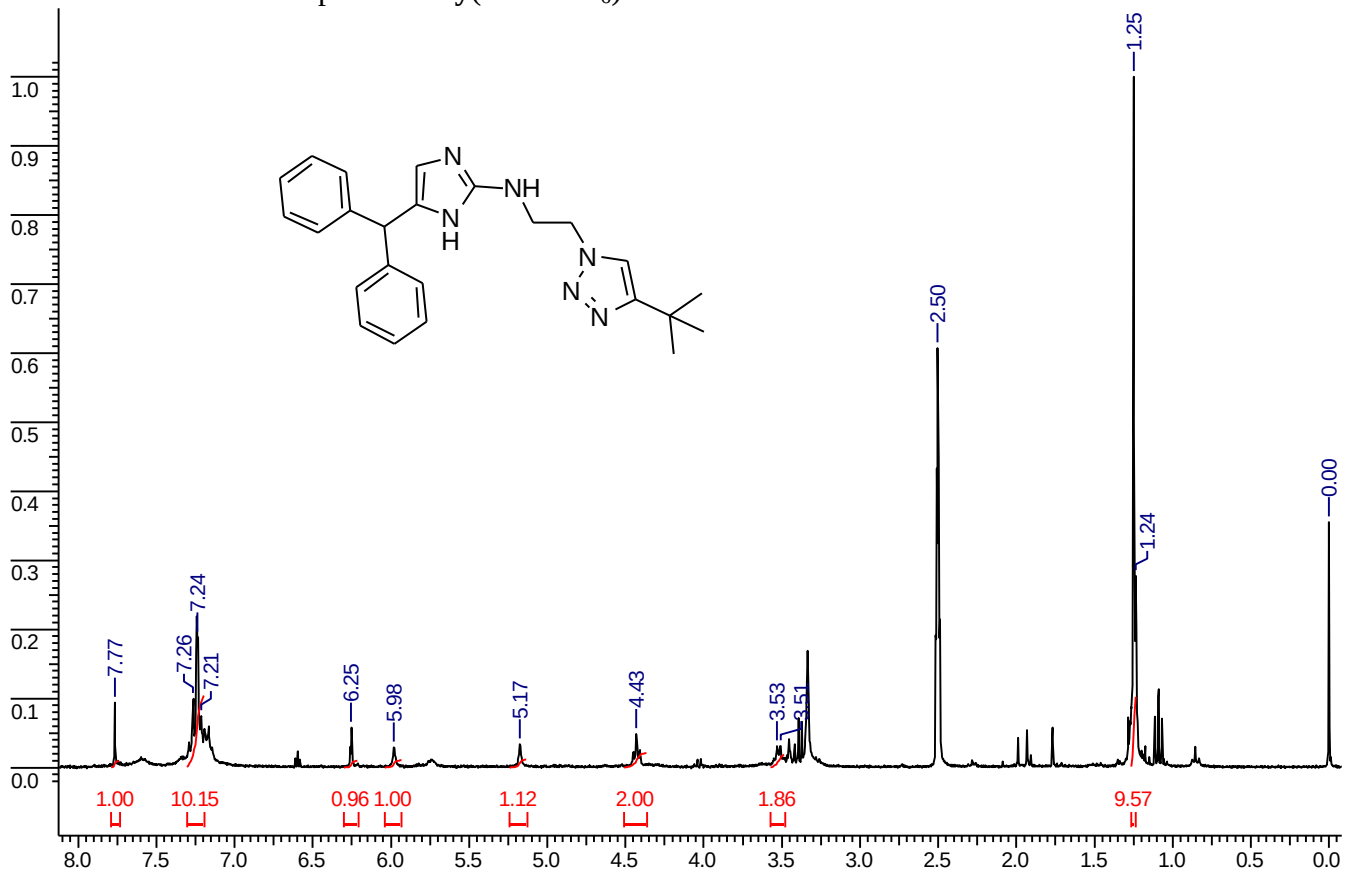


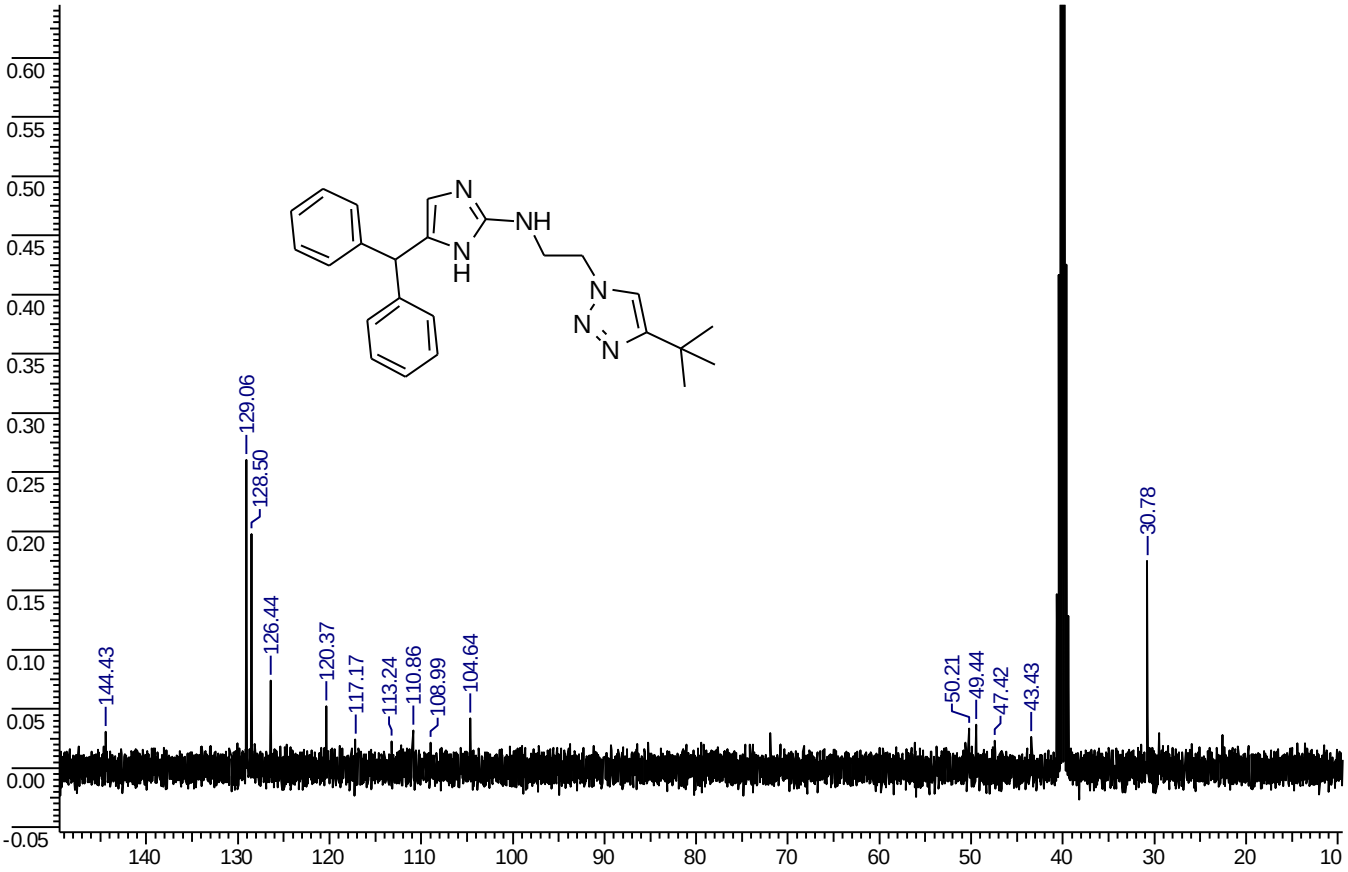
^{1}H NMR and ^{13}C NMR spectra of **5x** (DMSO-d_6)



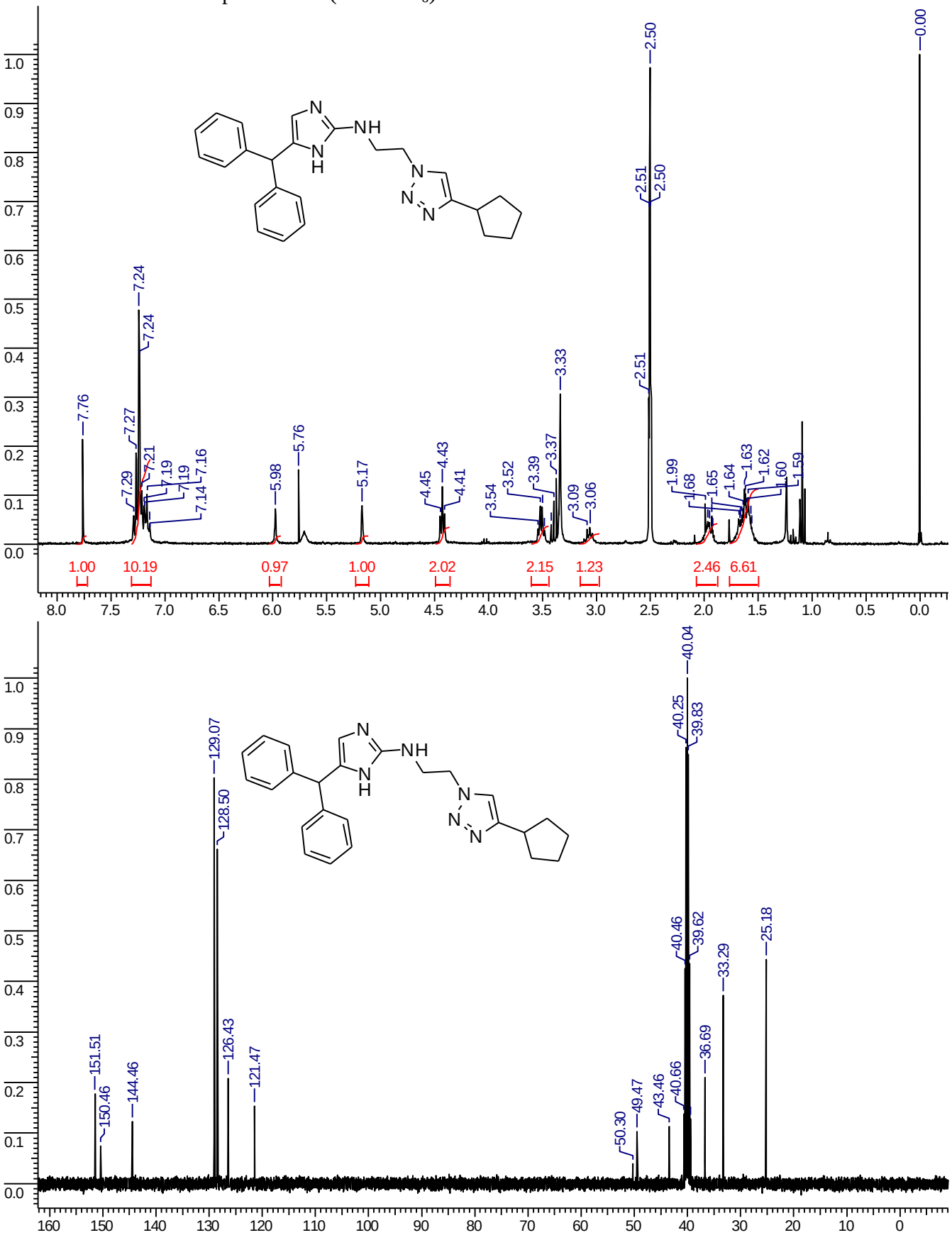


^{1}H NMR and ^{13}C NMR spectra of **5y**(DMSO-d_6)

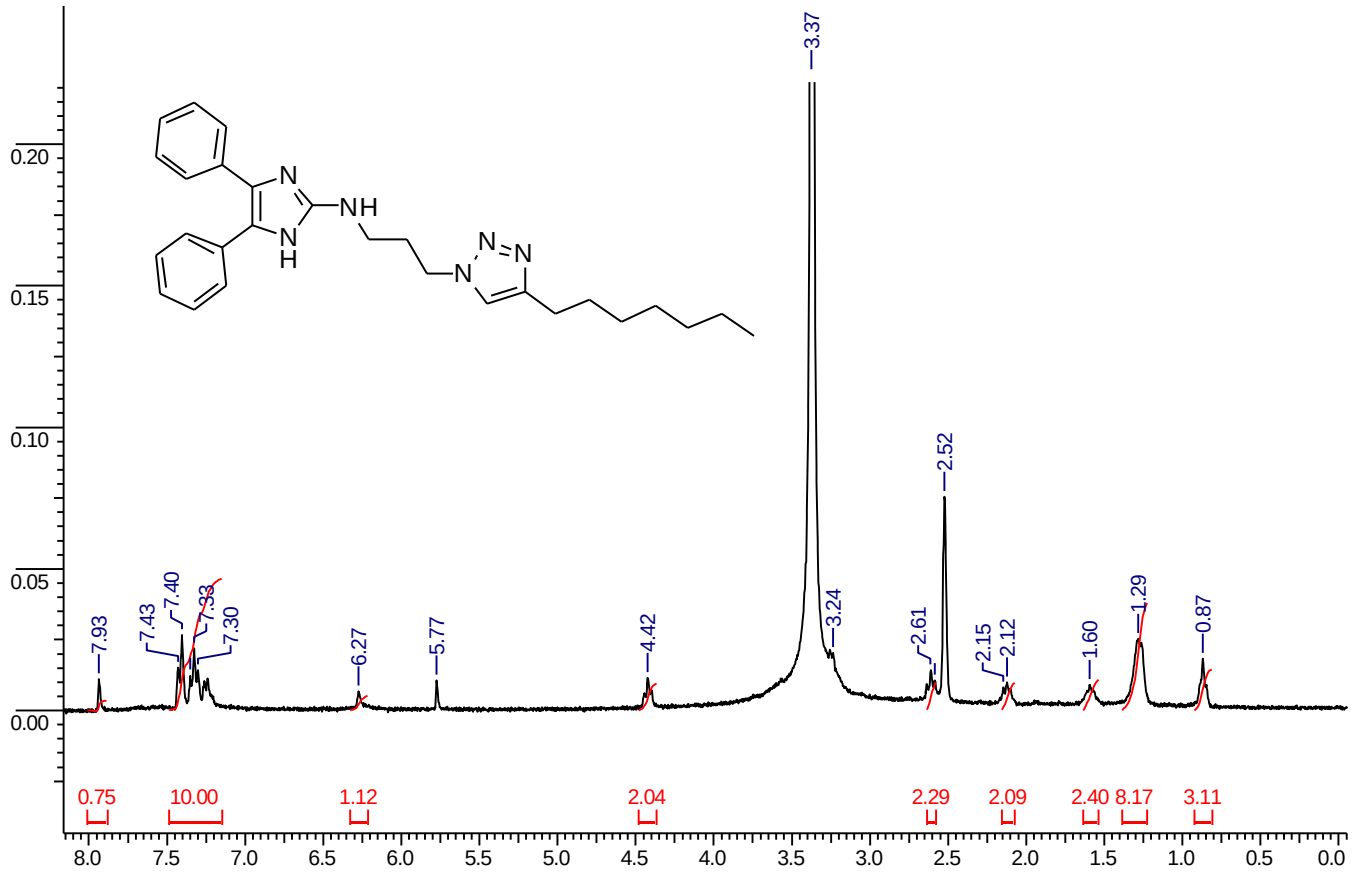


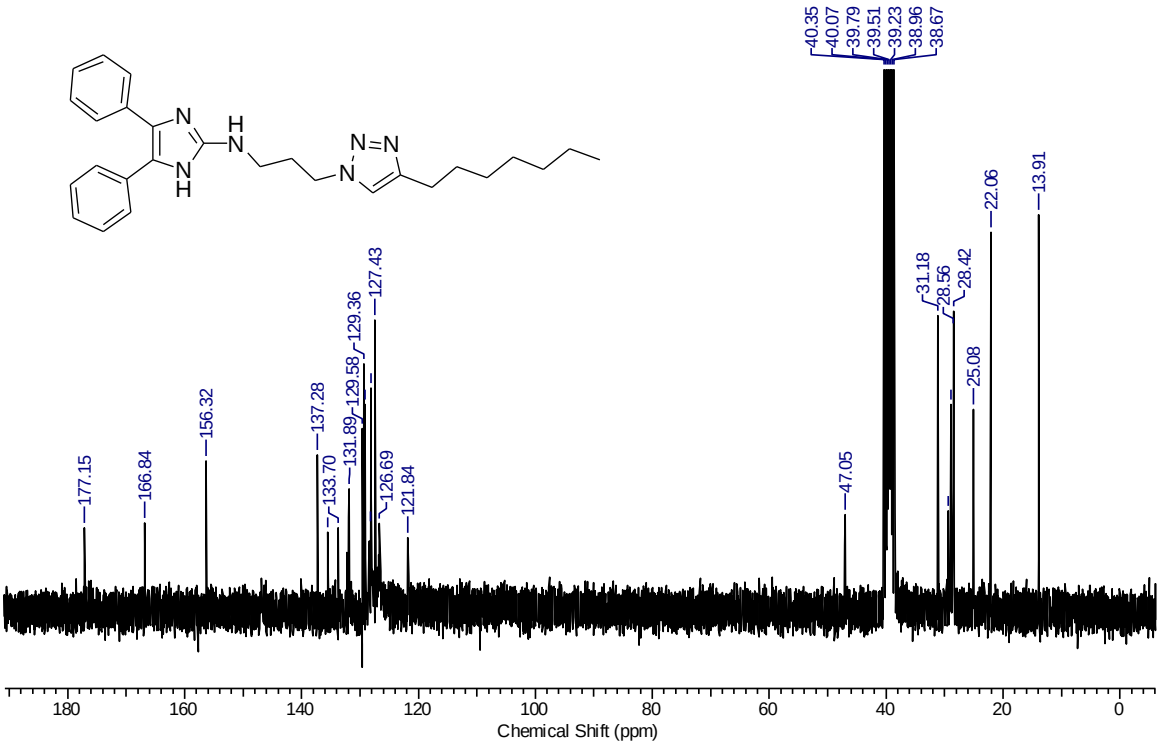


^{1}H NMR and ^{13}C NMR spectra of **5z**(DMSO-d_6)

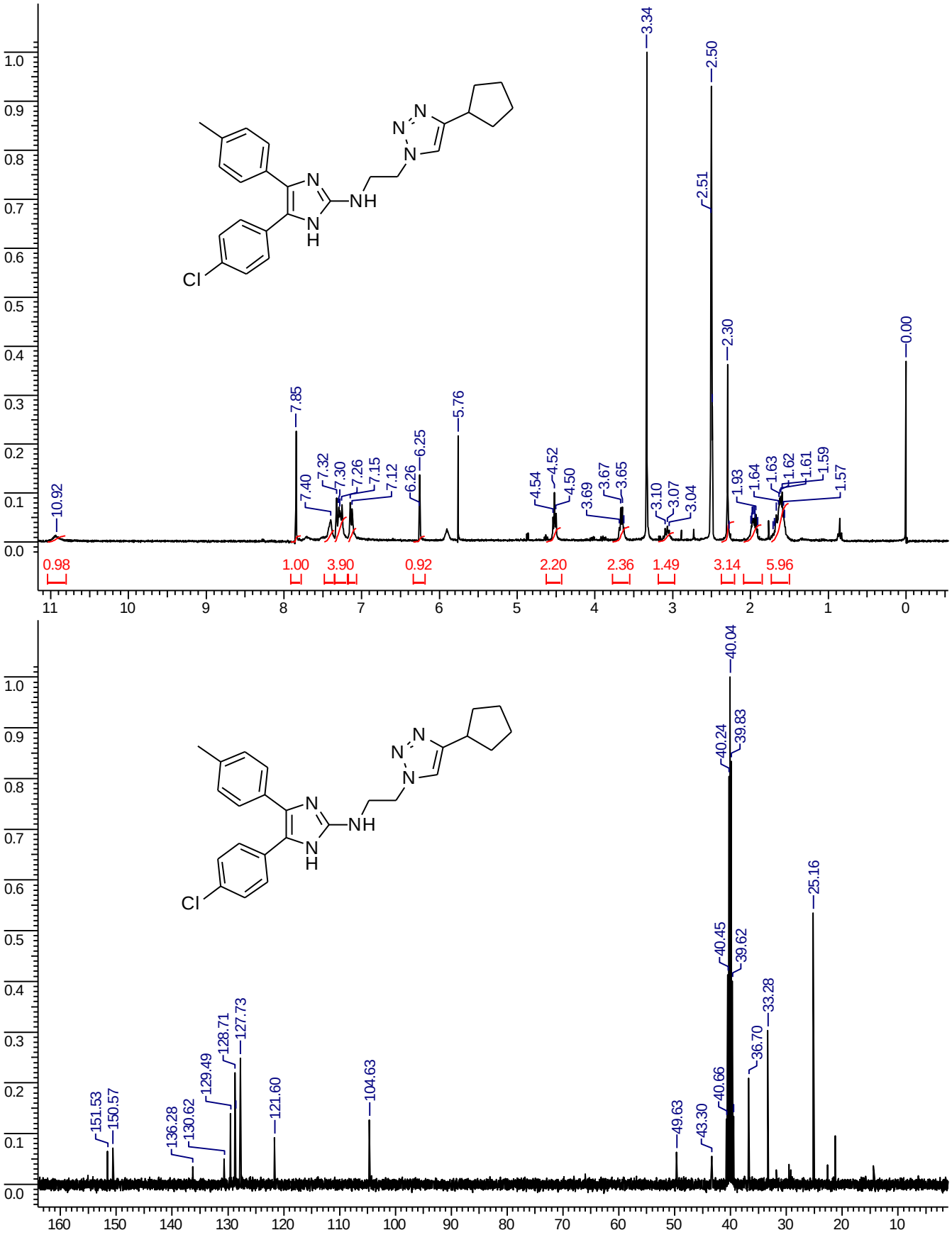


^{1}H NMR and ^{13}C NMR spectra of **5aa** (DMSO-d_6)

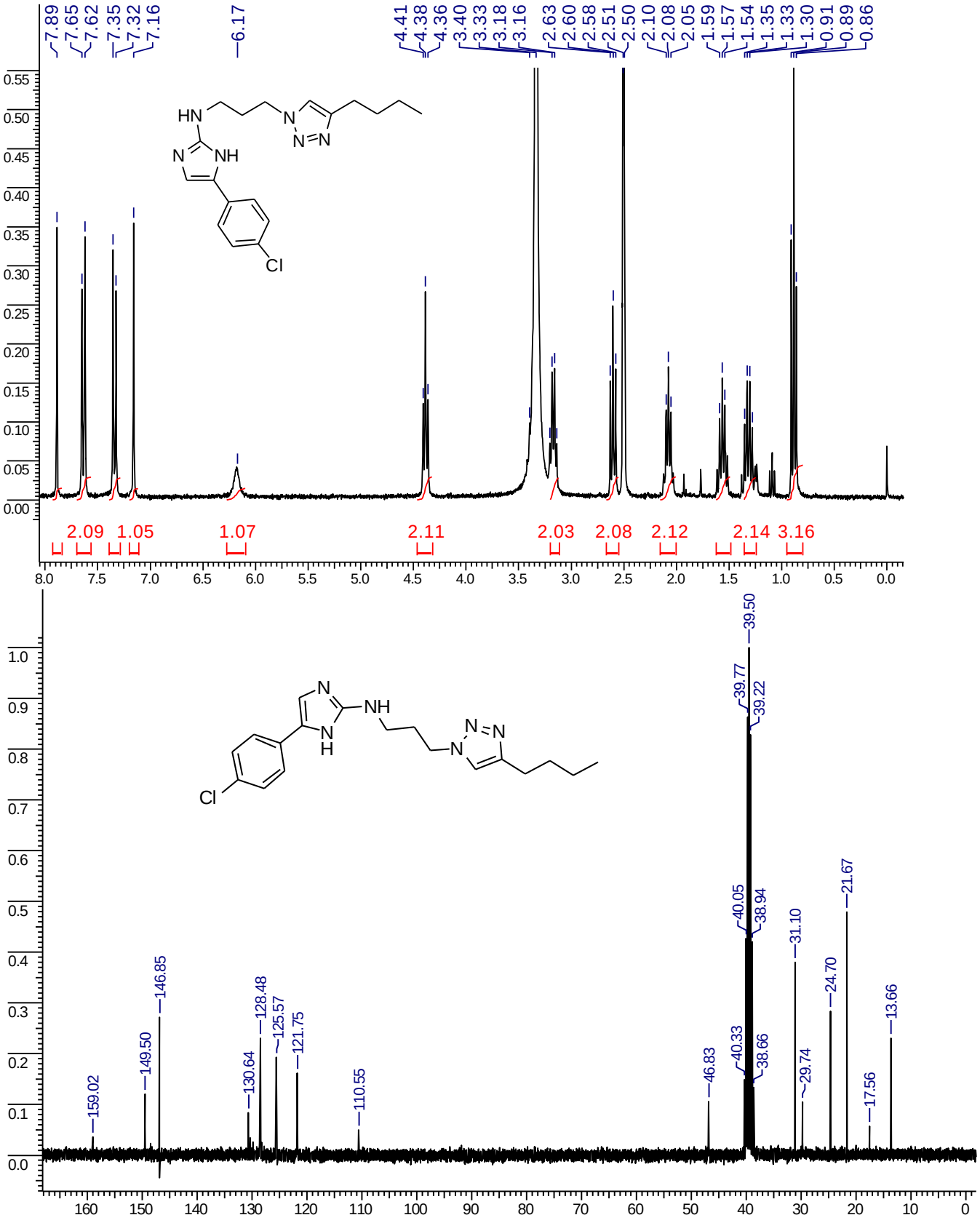




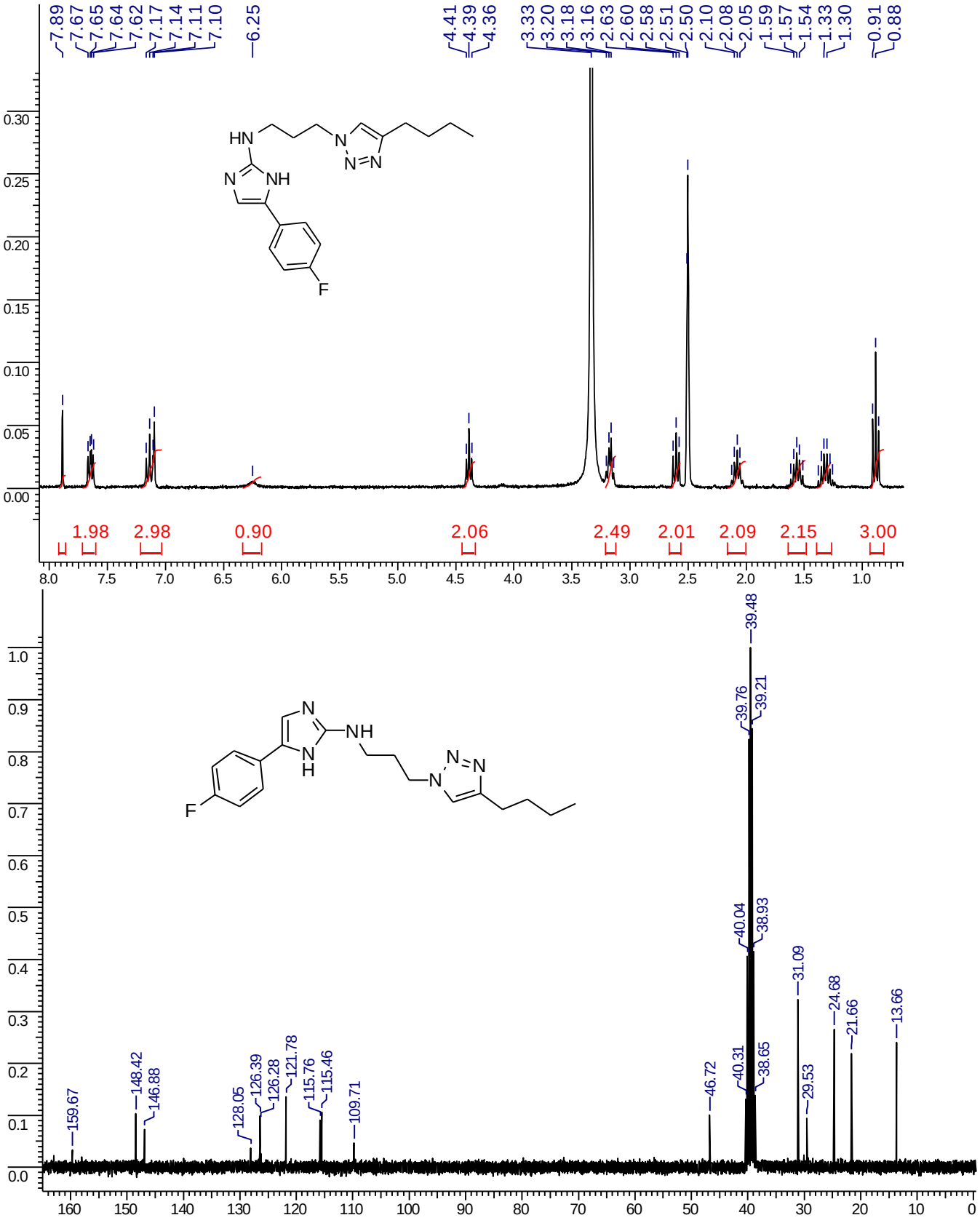
^{1}H NMR and ^{13}C NMR spectra of **5ab** (DMSO-d_6)



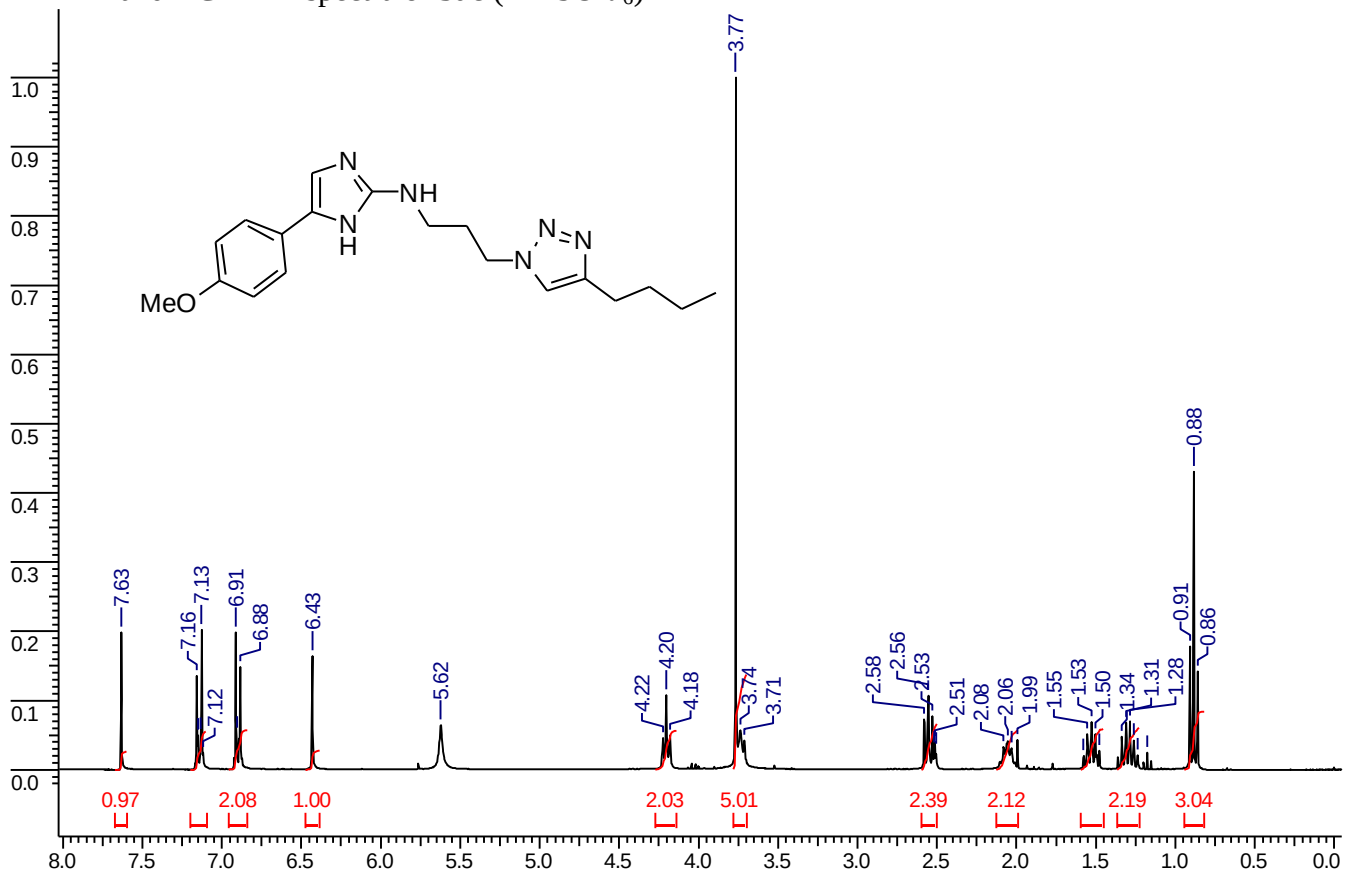
^{1}H NMR and ^{13}C NMR spectra of **5ac** (DMSO-d_6)

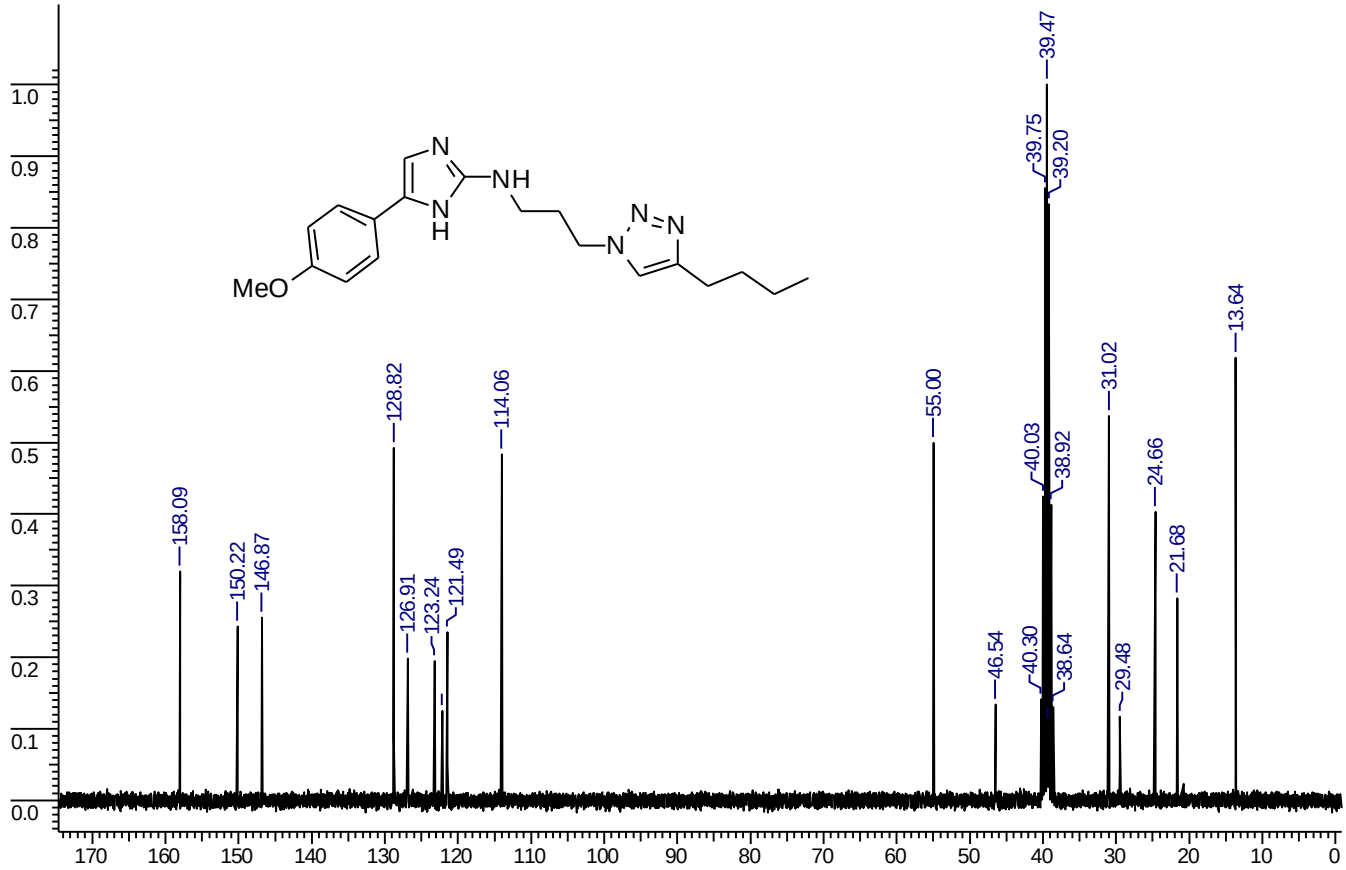


^{1}H NMR and ^{13}C NMR spectra of **5ad** (DMSO-d_6)

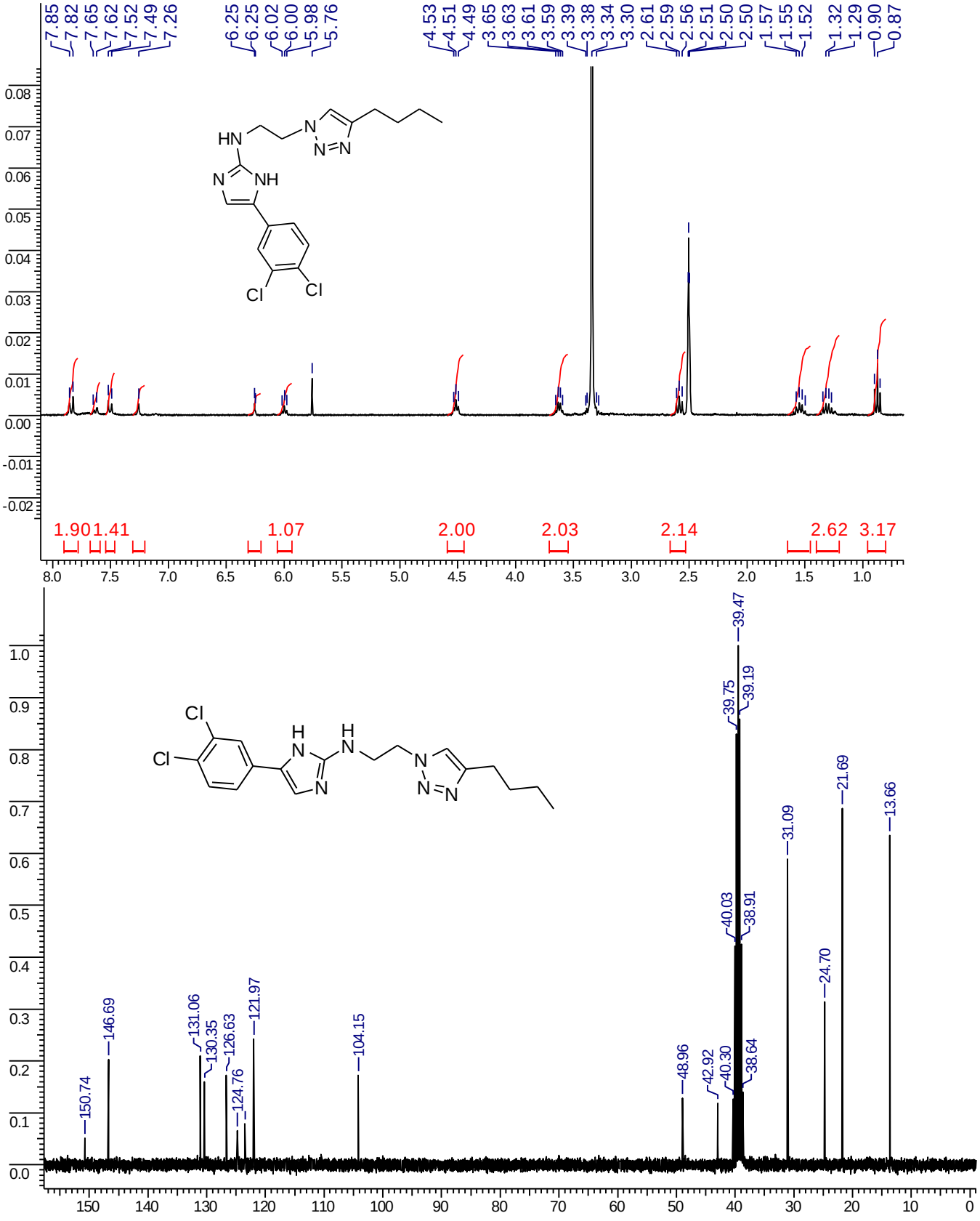


^{1}H NMR and ^{13}C NMR spectra of **5ae** (DMSO-d_6)

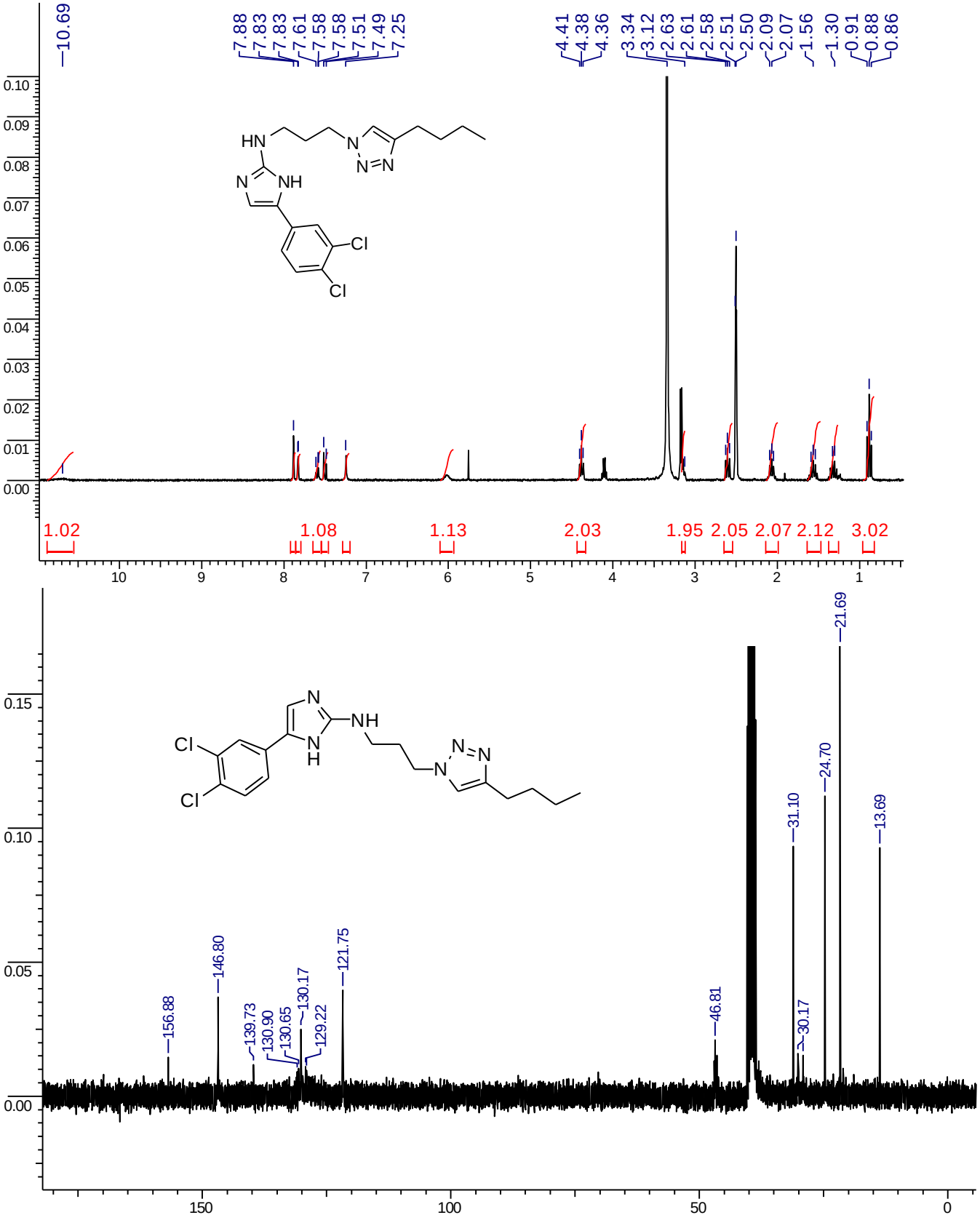




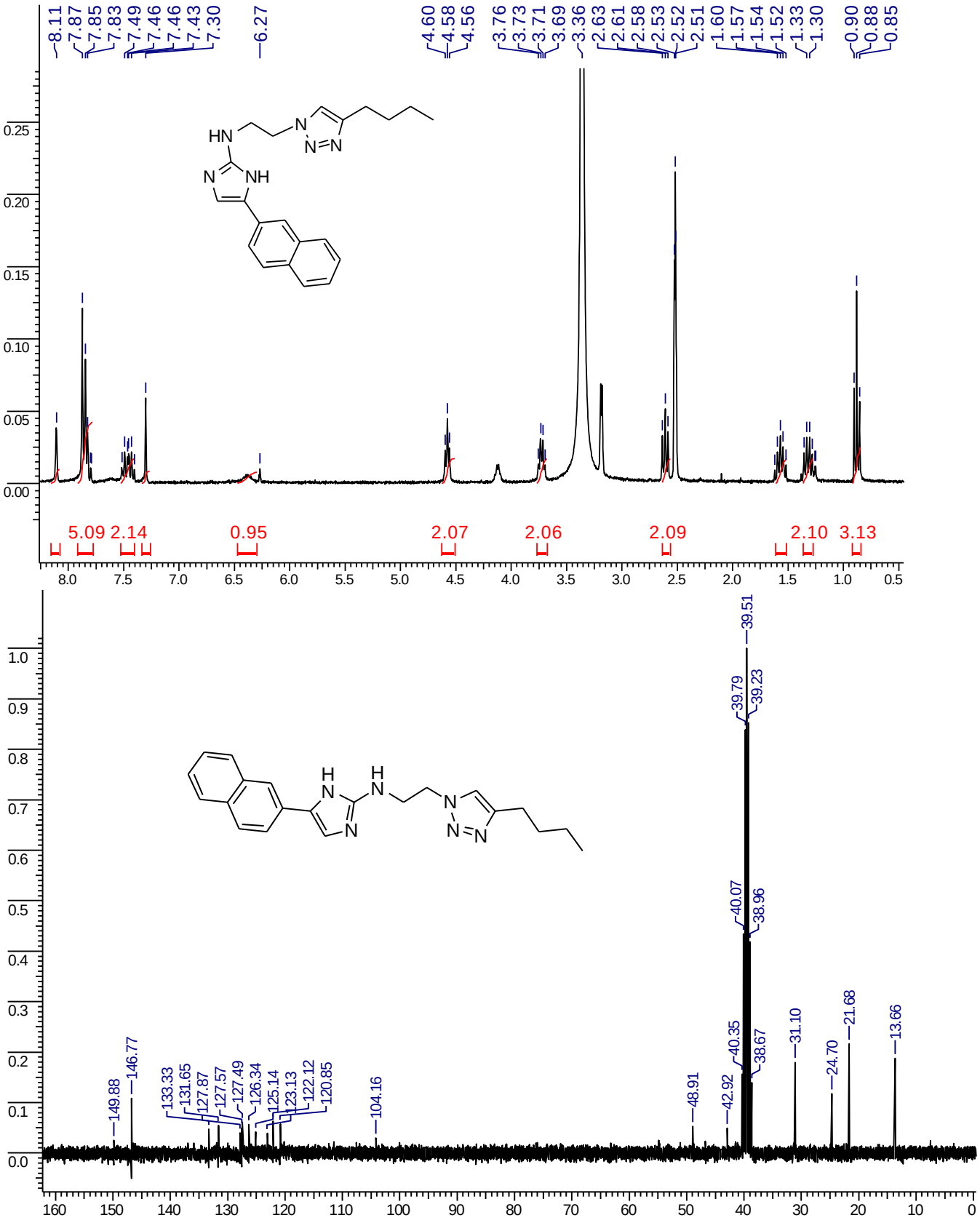
^{1}H NMR and ^{13}C NMR spectra of **5af** (DMSO-d_6)



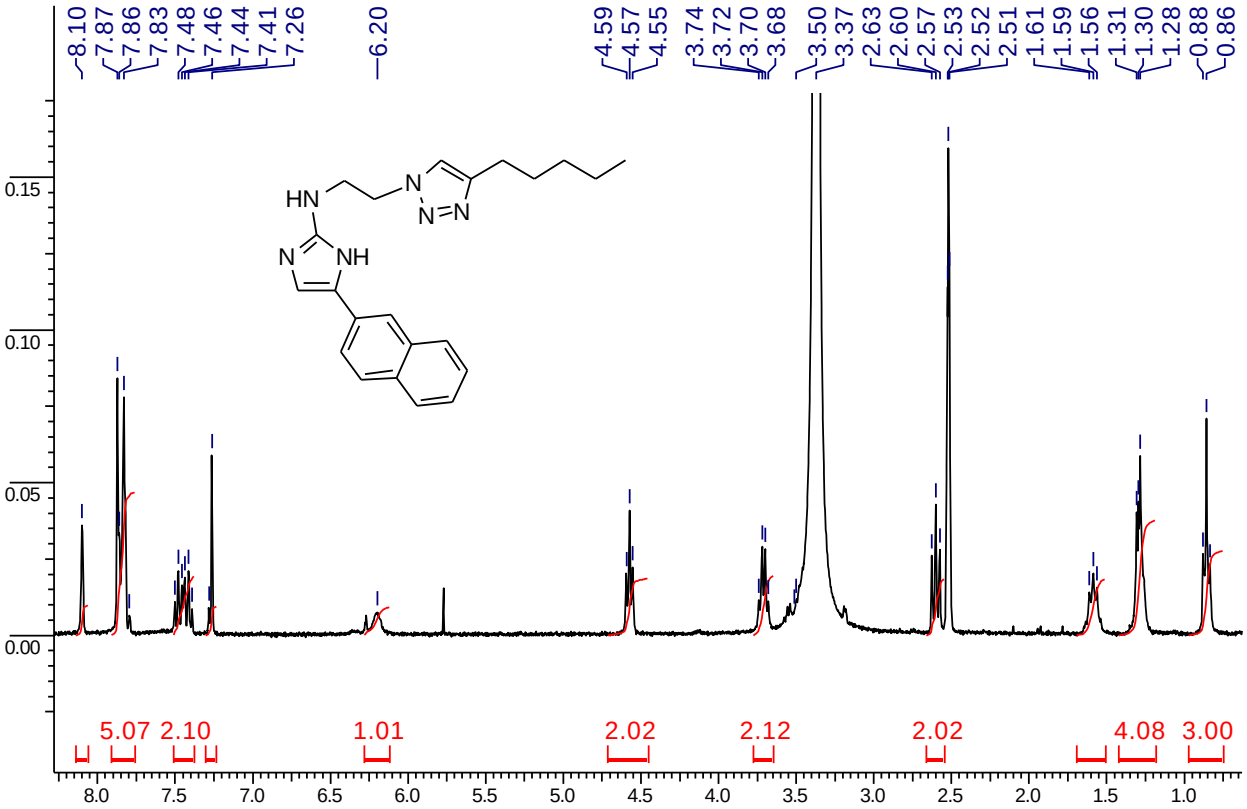
^{1}H NMR and ^{13}C NMR spectra of **5ag** (DMSO-d_6)

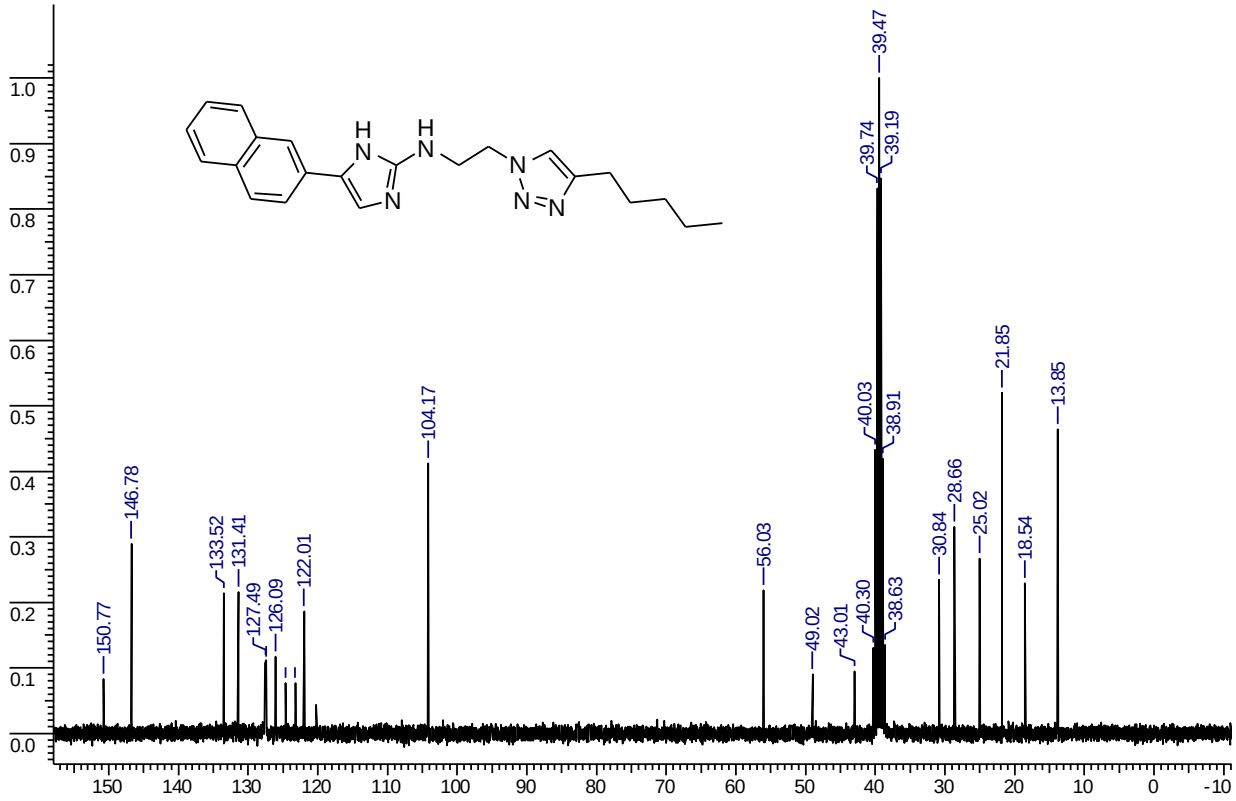


^{1}H NMR and ^{13}C NMR spectra of **5ah** (DMSO-d_6)

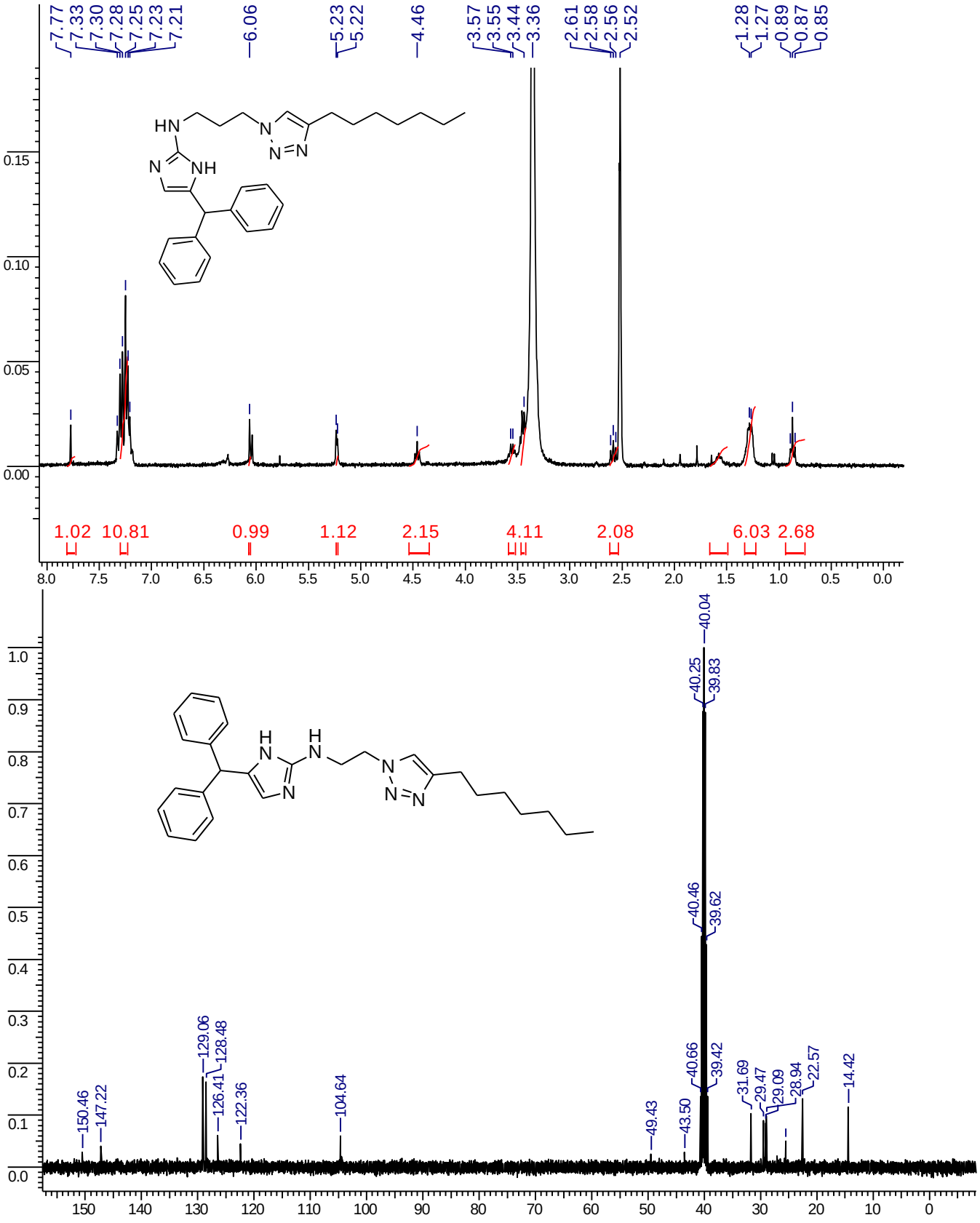


^{1}H NMR and ^{13}C NMR spectra of **5ai** (DMSO-d_6)

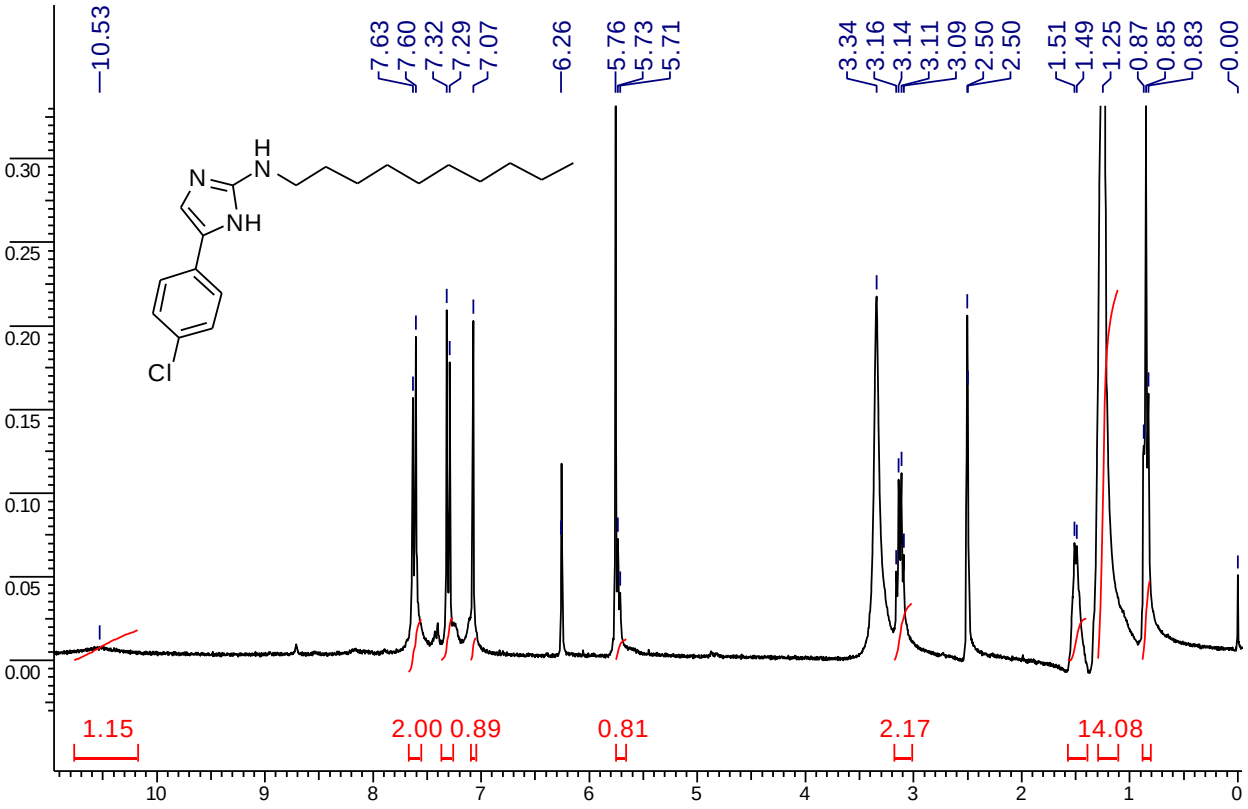




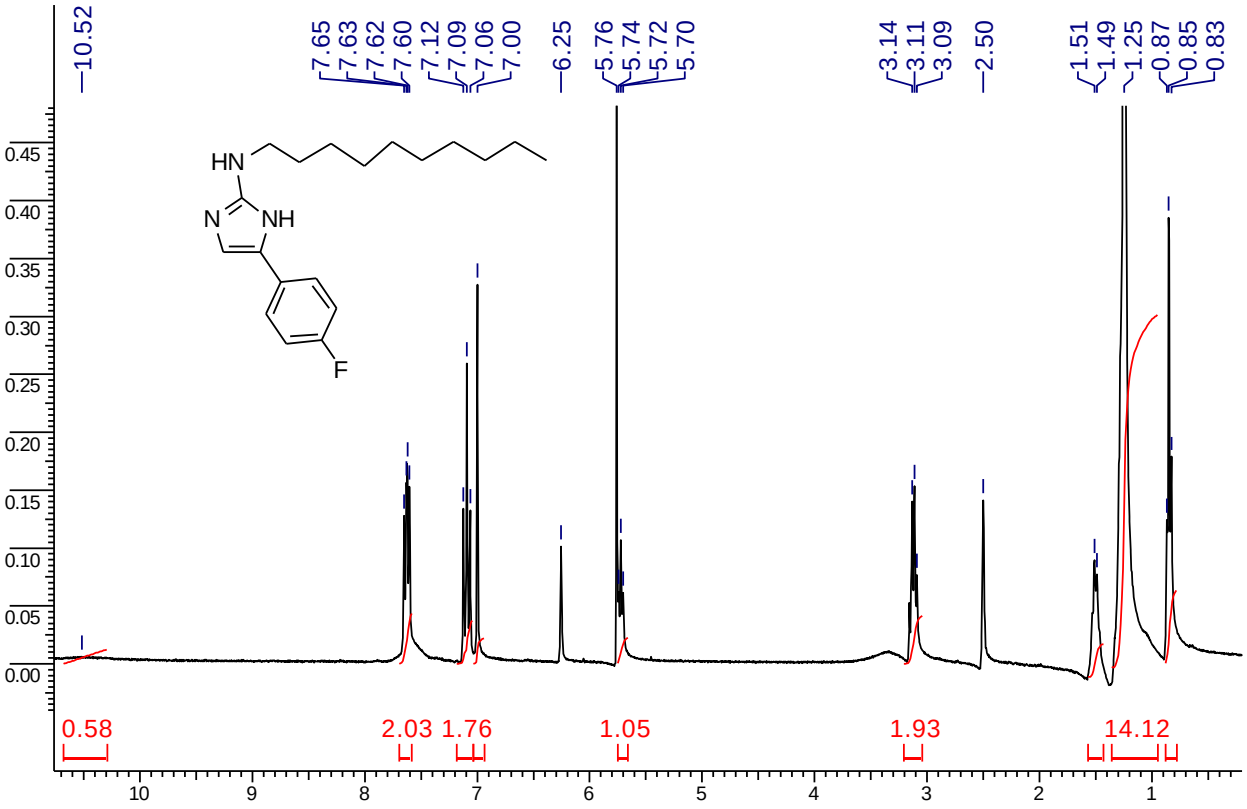
^{1}H NMR and ^{13}C NMR spectra of **5aj** (DMSO-d_6)



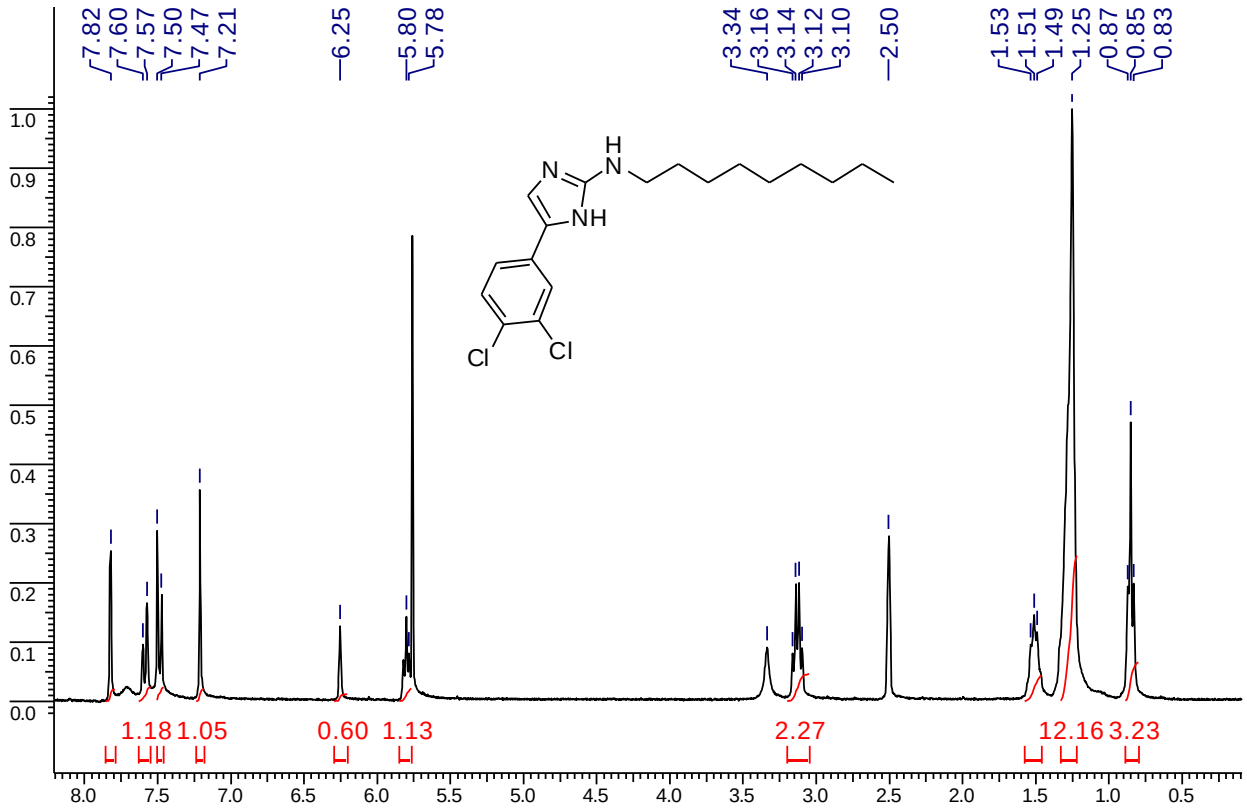
^{1}H NMR spectra of **6a** (DMSO-d_6)



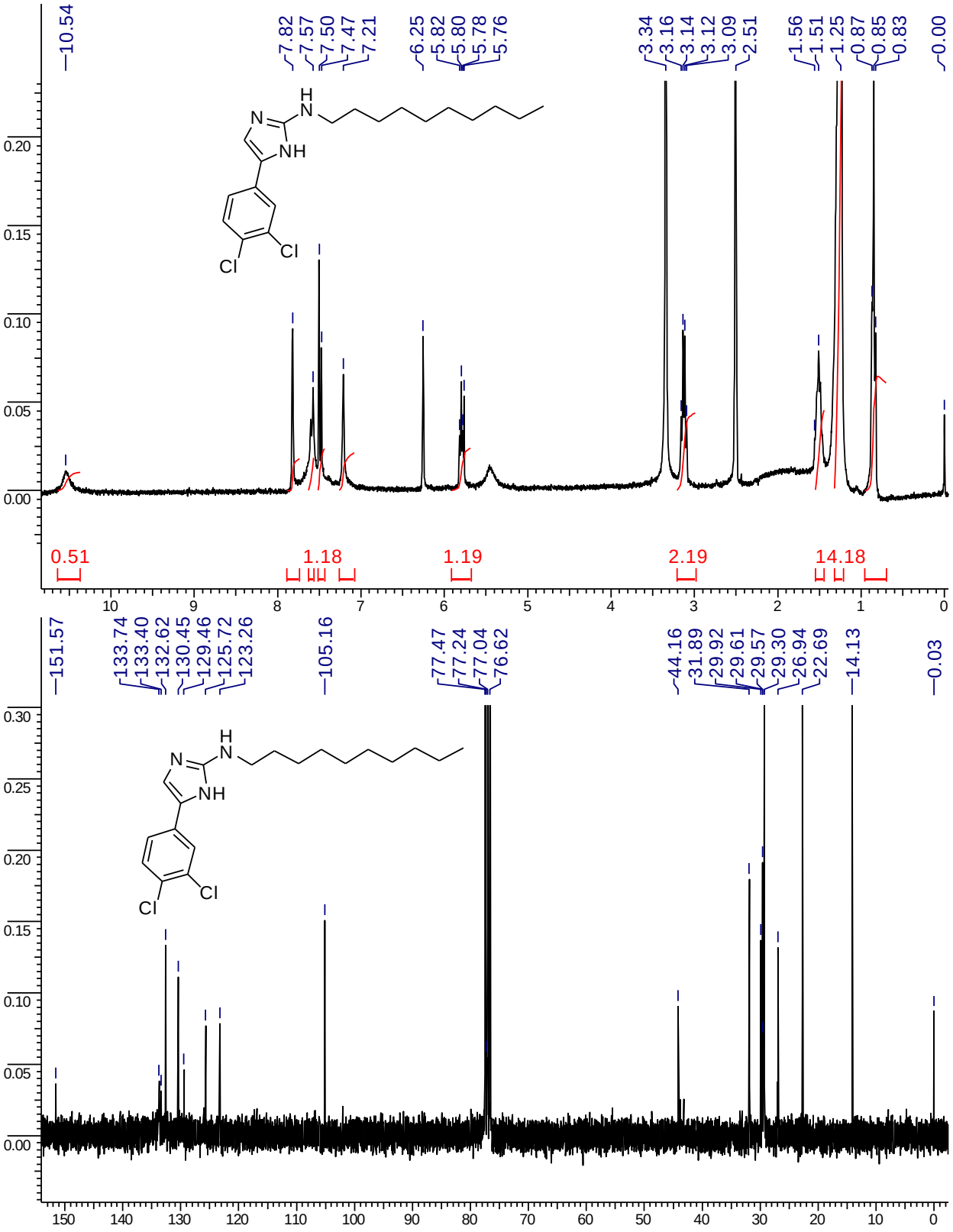
^{1}H NMR spectra of **6b** (DMSO-d_6)



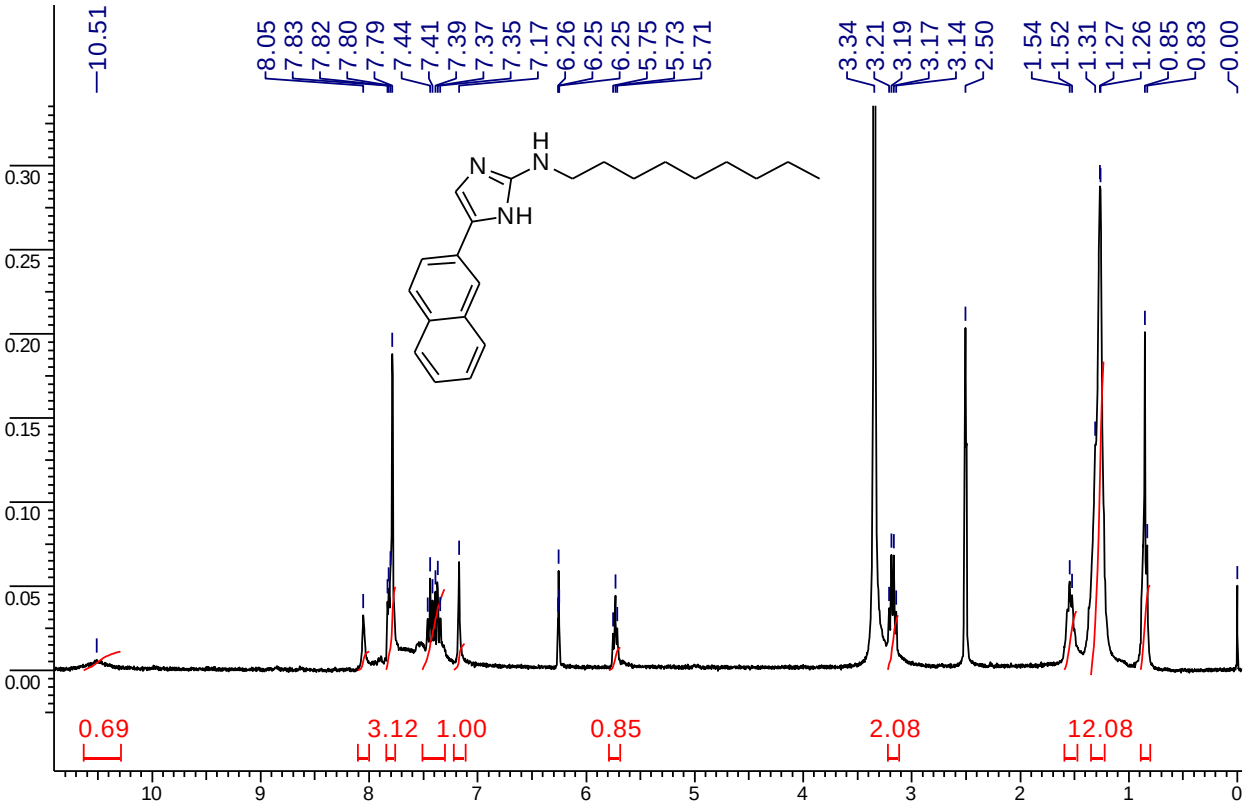
^{1}H NMR spectra of **6d** (DMSO-d_6)



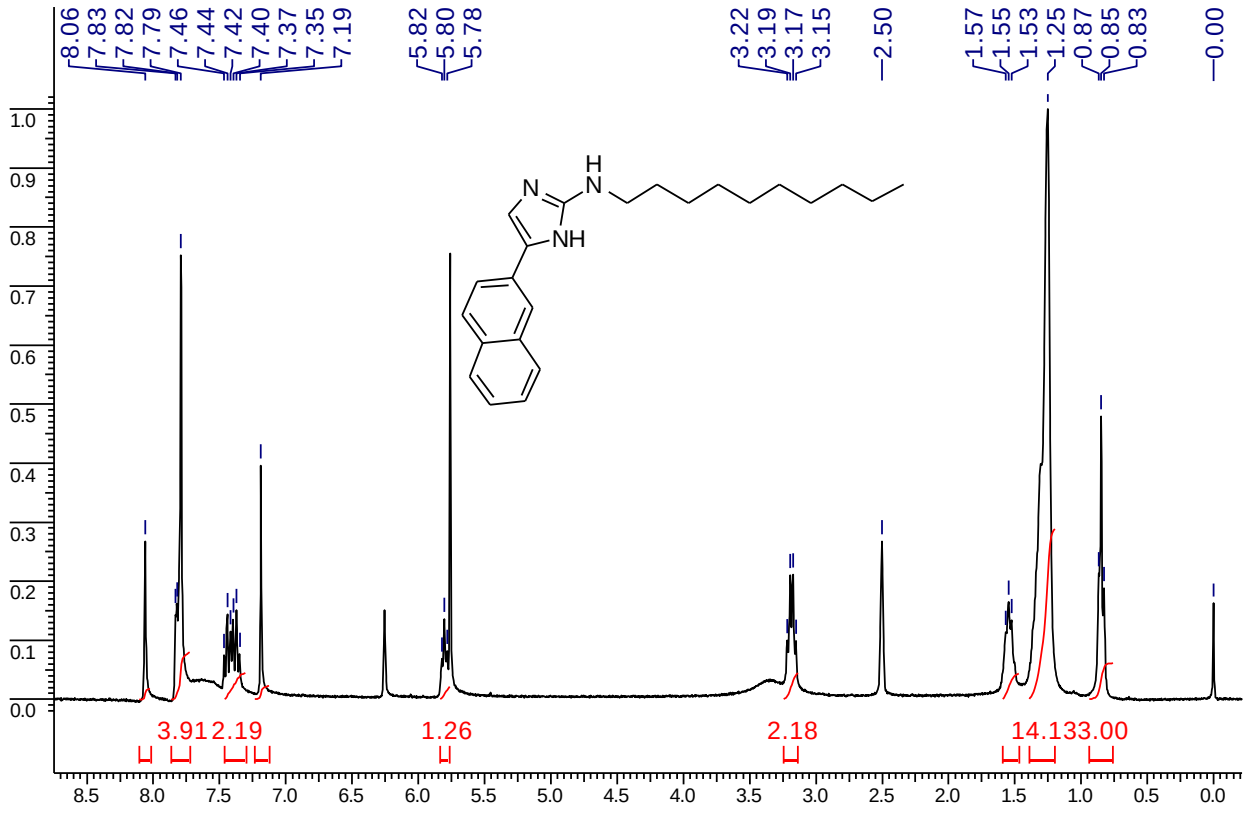
^{1}H NMR and ^{13}C NMR spectra of **6e** (DMSO-d_6)



^{1}H NMR and ^{13}C NMR spectra of **6f** (DMSO-d_6)



^{1}H NMR spectra of **6g** (DMSO-d_6)



^{1}H NMR spectra of **6h** (DMSO-d_6)