Electronic Supplementary Material (ESI) for Chemical Communications.

Supporting Information

N-Heterocyclic Imino Catalyzed 1,4-Regioselective Azide-Alkyne Cycloaddition (AAC): A Metal-free Approach

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1. General Experimental Details

The chemicals *o*–Phenylene diamine, 1,8-diamino naphthalene, $LiAlH_4$, cyanogen bromide, p-tolyl isocyanate, KOH, alkynes, amines, acetone, chloroform ($CDCl_3$), and other solvents pentane, hexane, PET ether, ethyl acetate were purchased from Sigma-Aldrich and Avra and used as received. Diethyl ether and toluene were distilled over sodium-benzophenone. Flash column chromatography was performed on silica gel (200–300 mesh) and thin-layer chromatography (TLC) analyses were performed on commercial silica gel plates (60 F254).

2. Instrumentation Methods

2.1 Infrared spectroscopy

FT-IR spectra were obtained using a SHIMADZU IR Affinity-1 instrument equipped with a high-sensitivity DLaTGS detector and the spectra were recorded in KBr discs. The scans were taken between 400 and 4000 cm^{-1} range.

2.2. Single crystal data collection and structure determination

The Photon II area detector 3-circle diffractometer was used to glue a suitable crystal to a nylon loop. The Bruker APEX4 Software was used to collect intensity data sets using Mo Kα radiation (λ = 0.71073). The crystal structure was solved in the monoclinic symmetry, space group P21/n using APEX4 software. The structures were solved with SHELXT[1] and refined with the full-matrix least-squares procedure on F2 by SHELXL.[2] All non-hydrogen atoms were refined anisotropically. The figures were drawn using the DIAMOND software.

2.3. NMR spectroscopy

^{1}H and ^{13}C NMR spectra were recorded on a BRUKER (400 MHz) spectrometer. The chemical shifts are reported in parts per million (ppm). Tetramethylsilane is used as an internal standard.

2.4. Melting point analysis

Melting points were determined in open-end capillary tubes on a Guna melting point apparatus with 130 watts, and 230 A/C volts, and were uncorrected.

3. Experimental Section

3.1. Synthesis of 1,3-dihydro-2H-benzo[d]imidazol-2-imine (C-A)

A 100 mL round bottom flask was charged with magnetic pellet, *o*–phenylene diamine (1g, 9.250 mmol), and dried toluene (30 mL). Then the round bottom flask was attached with a dropping funnel containing a dried toluene solution of cyanogen bromide (1.223g, 11.56

mmol). The whole setup was transferred to an oil bath at 110°C. After attending the 110°C temperature, dropwise addition of cyanogen bromide solution was started. Yellowish orange precipitate was formed instantaneously. This reaction was allowed to run overnight. The whole setup was allowed to cool at room temperature. The precipitate was filtered using a Buchner funnel followed by (3×10 mL) washings of diethyl ether to the precipitate and dried under vacuum. This precipitate was suspended in diethyl ether treated with an aqueous solution of potassium hydroxide (1.23 g, 21.98 mmol) at room temperature for 30 minutes. Finally, the product was extracted with diethyl ether (3 × 50 mL) and dried over anhydrous sodium sulphate, filtered and the solvent was evaporated under reduced pressure. The product 1,3-dihydro-2H-benzo[d]imidazol-2-imine was dried under vacuum. 1,3-dihydro-2H-benzo[d]imidazol-2-imine was isolated as a pale yellow solid (yield 88%). mp: 307-308°C ^{1}H NMR (400MHz, DMSO-d6): δ_H 10.70(s, 1H), 7.13-7.15(t, 2H), 6.85-9.93(s, 2H), 6.13(s, 2H) ^{13}C NMR (100MHz, DMSO-d6): δ_C 155.76, 135.40, 119.41, 117.76, 115.18.

3.2. Synthesis of 1H-perimidin-2(3H)-imine (C-B)

1H-perimidin-2(3H)-imine was synthesized using the same protocol as 1,3-dihydro-2H-benzo[d]imidazol-2-imine. 1H-perimidin-2(3H)-imine was isolated as reddish brown solid (yield 90%). mp: 244-245°C ^{1}H NMR (400MHz, DMSO-d_6): δ_H 9.67(s, 1H), 7.08-7.12(t, 2H), 6.90-6.92(d, 2H), 6.33-6.35(d, 2H), 5.92 (, 2H), ^{13}C NMR (100MHz, DMSO-d_6): δ_C 151.90, 143.09, 135.47, 128.62, 119.02, 116.45, 106.22.

3.3. Synthesis of N-(1,3-isopropyl perimidin-2-ylidene)-N′-p-tolyisoureate (C-D)

The 1,3-diisopropyl-1H-perimidin-2(3H)-imine (**C-C**) was synthesized using a methodology published in the literature. A solution of 5% excess para-tolyl isocyanate (0.133 g, 1 mmol) was dropwise added to a stirring suspension of **C-C**, (0.26 g, 1 mmol) in distilled toluene (20 ml). The resulting mixture was subsequently stirred for 24 hours at room temperature. The resultant solution was then evaporated under a vacuum to produce a pale yellow powder. The desired product was obtained with a 97% yield. The white block crystals were grown from slow diffusion pentane into a saturated solution of **1** in THF at –15 °C. mp: 253°C ^{1}H NMR (400MHz, $CDCl_3$): δ_H 7.25-7.35(d, 2H), 7.01-7.18(m, 4H), 6.90-6.94(m, 4H), 4.73-4.83(s, 2H), 2.23(s, 3H), 1.48-1.50(d, 12H), ^{13}C NMR (100MHz, $CDCl_3$): δ_C 157.55, 137.95, 135.67, 134.02, 131.43, 129.53, 129.28, 126.78, 120.52, 108.67, 54.17, 53.91, 20.81, 20.47, 20.13.

3.4. Synthesis of azide

In a 100-mL round, the bottom flask was charged magnetic pellet, aniline (1 g, 0.10 mol), and water (10 mL). Then 1.8 mL (0.21 mol) of concentrated HCl was added to the reaction mixture in an ice bath. Following 20–30 minutes of stirring and cooling to 0°C, a freshly prepared, ice-cold solution of $NaNO_2$ (0.7408 g, 0.10 mol) in water (10 mL) was added dropwise to the reaction mixture while maintaining the ice bath. After the addition of $NaNO_2$(aqueous), the reaction mixture was stirred for an additional 10 min. A freshly prepared solution of sodium azide (0.698 g, 0.10 mol) in water (10 mL) was added dropwise to the reaction mixture via an additional funnel while maintaining the internal temperature of the reaction mixture below 5°C. Upon complete addition of the sodium azide solution, the reaction mixture was stirred for an additional 20–30 min at 0°C, followed by stirring at room tempreature for another 3 h. The completion of the reaction was monitored by TLC. The reaction mixture was extracted with ethyl acetate (2 × 100 mL). The organic layer was removed under reduced pressure to get the crude product, which was further purified by silica gel chromatography (petroleum ether/ethyl acetate as eluent) to yield corresponding aromatic azide.

3.5. Optimization of catalyst, solvent, and base

A solution of phenylacetylene (1 equiv) and benzyl azide (1 equiv) in the selected solvent (5 mL) was added to the active catalyst suspension (0.10 equiv) and the reaction mixture was stirred at 90°C for 24 h. The reaction was quenched by pouring into ice-cold water (20 mL) in a 100-mL Erlenmeyer flask. The extraction was carried out with ethyl acetate and dried over anhydrous Na_2SO_4. The solvent was removed under reduced pressure, the crude was purified by flash column chromatography over silica gel, using 10% EA/PET ether as eluent, to give the target compound.

3.6. Formation of active catalyst (C-A'-C-D')

At ambient temperature, various N-heterocyclic imines (C-A/D) were suspended in dimethyl sulfoxide with sodium hydride (1:1) and stirred for 10 minutes resulting in an active imino catalysts (C-A'-C-D').

3.7. General procedures for imine-catalyzed triazoles synthesis from terminal alkynes and azides:

To a solution of phenylacetylene (1 equiv) and benzyl azide (1 equiv) in DMSO (5 mL) treated with active catalyst suspension (0.10 equiv) the reaction mixture was stirred at 90°C for 24h. The reaction was quenched by pouring into ice-cold water (20 mL) in a 100-mL Erlenmeyer flask. The extraction was carried out with ethyl acetate and dried over anhydrous

Na_2SO_4. The solid was washed twice with petroleum ether to remove any traces of side products, unreacted-alkynes, and catalysts. The solvent was removed under reduced pressure, the crude was purified by flash column chromatography over silica gel, using 10% EA/PET ether as eluent, to give the target compound.

4. Spectral data of the compounds

1-benzyl-4-phenyl-1H-1,2,3-triazole (1a): (table 1, entry 1) **1a** was isolated as a white crystalline solid (yield A'-71%, B'-84%, C'-91%, D'-87%). mp: 128-130ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 7.76−7.78(d, 2H), 7.64(s, 1H), 7.34−7.38(m, 5H), 7.23−7.28(m, 3H), 5.54(s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C 148.17, 134.63, 130.48, 129.08, 128.73, 128.70, 128.09, 127.98, 125.63, 119.46, 54.15.

1-benzyl-4-(4-fluorophenyl)-1*H*-1,2,3-triazole (1b): (table 1, entry 2). **1b** was isolated as a white solid (yield A'-74%, B'-79%, C'-86%, D'-84%). mp: 113-115ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 7.80-7.78(m, 2H), 7.71(s, 1H), 7.35-7.39(m, 3H), 7.30-7.32(m, 2H), 7.06-7.10(m, 2H), 5.55(s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C 163.84, 161.38, 147.27, 134.71, 129.14, 128.77, 128.04, 127.48, 127.40, 126.85, 119.53, 115.86, 115.64, 54.17.

1-benzyl-4-(p-tolyl)-1*H*-1,2,3-triazole (1c): (table 1, entry 3) **1c** was isolated as a white solid (yield A'-73%, B'-76%, C'-85%, D'-79%). mp: 113-115ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 7.64-7.70(m, 2H),7.63(s, 1H), 7.27-7.36(m, 5H), 7.18-7.20(m, 2H), 5.52(s, 2H), 2.35 (s, 3H). ^{13}C NMR (100MHz, $CDCl_3$): δ_C 148.11, 137.83, 134.67, 129.34, 128.96, 128.67, 128.55, 127.62, 125.46, 119.16, 53.98, 21.12.

1-benzyl-4-(4-methoxyphenyl)-1*H*-1,2,3-triazole (1d): (table 1, entry 4) **1d** was isolated as a white solid (yield A'-74%, B'-83%, C'-90%, D'-89%). mp: 113-115ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 7.72-7.75(m, 2H), 7.60(s, 1H), 7.36-7.39(m, 3H), 7.30-7.32(m, 2H), 6.90-6.95(m, 2H), 5.55(s, 2H) 3.83(s, 3H).^{13}C NMR (100 MHz, $CDCl_3$): δ_C 159.67, 148.14, 134.89, 129.18, 128.78, 128.10, 127.37, 123.37, 118.84, 114.28, 55.37, 54.22.

2-(1-benzyl-1*H*-1,2,3-triazol-4-yl)pyridine (1e): (table 1, entry 5) **1e** was isolated as a white solid (yield A'-75%, B'-78%, C'-88%, D'-81%). mp: 114-115ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 8.52(s,1H), 8.09-8.17(m, 2H), 7.73(s, 1H), 7.18-7.33(m, 6H), 5.56(s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C 150.02, 149.10, 148.47, 136.64, 134.20, 128.91, 128.68, 128.05, 122.63, 121.83, 119.99, 54.12.

1-benzyl-4-(cyclohexyl)-1*H*-1,2,3-triazole (1f): (table 1, entry 6) **1f** was isolated as a white solid (yield A'-73%, B'-77%, C'-83%, D'-81%). mp: 78-80ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 7.27-7.32(m, 3H), 7.15-7.24(m, 2H), 7.08(s, 1H), 5.39(s, 2H), 2.62-2.68(m, 1H), 1.93-

1.95(m, 2H), 1.68-1.69(m, 3H), 1.26-1.31(m, 4H), 1.12-1.14(m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C 154.17, 135.07, 129.01, 128.54, 127.97, 119.23, 53.94, 35.34, 32.99, 26.12, 26.03.

1-benzyl-4-butyl-1*H*-1,2,3-triazole (1g): (table 1, entry 7) **1g** was isolated as a white solid (yield A'-76%, B'-77%, C'-84%, D'-82%). mp: 82-84ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 7.34-7.38(m, 3H), 7.25-7.27(m, 2H), 7.16(s, 1H), 5.48(s, 2H), 2.67-2.71(t, 2H), 1.59-1.66(m, 2H), 1.31-1.41(m, 2H), 0.89-0.93(t, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C 147.73, 134.39, 128.08, 126.90, 119.76, 52.89, 30.48, 24.37, 20.28, 12.86.

1-benzyl-4-*tert*-butyl-1*H*-1,2,3-triazole (1h): (table 1, entry 8) **1h** was isolated as a white solid (yield A'-72%, B'-75%, C'-79%, D'-76%). mp: 84-85ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 7.34-7.38(m, 3H), 7.25-7.29(m, 2H), 7.16(s, 1H), 5.48(s, 2H), 1.32(s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C 158.07, 134.47, 128.94, 128.46, 127.92, 120.80, 118.29, 105.38, 53.83, 30.68.

2-(1-benzyl-1H-1,2,3-triazol-4-yl)ethan-1-ol (1i): (table 1, entry 9) **1i** was isolated as a white solid (yield A'-70%, B'-72%, C'-76%, D'-74%). mp: 78-80ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 7.29(s, 1H), 7.19-7.22(m, 3H), 7.14-7.20(m, 2H), 5.35(s, 2H), 3.76(s, 2H), 2.79(s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C 146.05, 134.78, 129.03, 128.63, 128.02, 121.93, 61.28, 53.99, 28.89,19.81.

2-(1-benzyl-1*H*-1,2,3-triazol-4-yl)propan-2-ol (1j): (table 1, entry 10) **1j** was isolated as a white solid (yield A'-71%, B'-73%, C'-78%, D'-75%). mp: 78-80ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 7.41(s, 1H), 7.31-7.35(m, 3H), 7.23-7.27(m, 2H), 5.45(s, 2H), 1.58(s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C 156.02, 134.46, 128.85, 128.46, 127.90, 119.16, 68.19, 53.86, 30.24.

1,4-diphenyl-1H-1,2,3-triazole (2a): (table 1, entry 11) **2a** was isolated as a white crystalline solid (yield A'-77%, B'-79%, C'-89%, D'-80%). mp: 183-184ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 8.12(s, 1H), 7.83-7.84(d, 2H), 7.70−7.72(d, 2H), 7.44−7.48(t, 2H), 7.27-7.39(m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C 147.40, 136.06, 129.24, 128.76, 127.90, 127.77, 127.41, 127.84, 119.51,116.68,116.59.

1-naphthyl-4-phenyl-1H-1,2,3-triazole (3a): (table 1, entry 12) **3a** was isolated as a white crystalline solid (yield A'-76%, B'-82%, C'-87%, D'-84%). mp: 183-184ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 7.97(s, 1H), 7.78-7.86(m, 4H), 7.53 −7.55 (d, 1H), 7.21−7.45(m, 8H). δ_C 147.75, 134.19, 133.70, 130.46, 130.36, 129.02, 128.60, 128.45, 128. 34. 127.93, 127.13, 125.92, 125.05, 123.56, 122.39.

1-(4-methoxyphenyl)-4-phenyl-1H-1,2,3-triazole (4a): (table 1, entry 13) **4a** was isolated as a white crystalline solid (yield A'-79%, B'-87%, C'-93%, D'-89%). mp: 183-184ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 8.11(s, 1H), 7.89-7.91(d, 2H), 7.66−7.69(d, 2H), 7.34−7.47(m, 3H), 7.02-7.04(d, 2H), 3.87(s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C 160.03, 148.42, 130.76,130.48,129.03, 128.45, 125.95, 122.31, 117.98, 114.86, 55.77.

1-(4-tolyl)-4-phenyl-1H-1,2,3-triazole (5a): (table 1, entry 14) **5a** was isolated as a white crystalline solid (yield A'-71%, B'-73%, C'-82%, D'-77%). mp: 183-184ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 8.15(s, 1H), 7.90-7.92(d, 2H), 7.66−7.68(d, 2H), 7.44−7.48(t, 2H), 7.33-7.39(m, 3H), 2.44 (s,3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C 148.53, 139.06, 135.00, 130.42, 120.33, 129.10, 128.51, 126.00, 120.69, 117.85, 21.20.

1-(3-tolyl)-4-phenyl-1H-1,2,3-triazole (6a): (table 1, entry 15) **6a** was isolated as a white crystalline solid (yield A'-80%, B'-83%, C'-86%, D'-86%). mp: 183-184ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 8.10(s, 1H), 7.83-7.85(d, 2H), 7.50(s, 1H), 7.34−7.40(d, 1H), 7.20-7.34(m, 4H),7.18-7.31(t, 1H),2.39(s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C 148.75, 140.38, 137.49, 130.62, 129.87, 129.86, 129.24, 128.72, 126.18, 121.54, 118.00, 117.93, 21.68.

1-(2-tolyl)-4-phenyl-1H-1,2,3-triazole (7a): (table 1, entry 16) **7a** was isolated as a white crystalline solid (yield A'-70%, B'-72%, C'-77%, D'-74%). mp: 183-184ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 7.96(s, 1H), 7.90-7.93(d, 2H), 7.33-7.48(m, 7H), 2.27 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C 147.46, 136.54, 136.46, 133.91, 133.81, 133.55, 131.55, 130.45, 129.93, 128.95, 128.35, 126.35, 126.00, 125.83, 121.16, 18.07.

1-(2,4,6-mesityl)-4-phenyl-1H-1,2,3-triazole (8a): (table 1, entry 17) **8a** was isolated as a white crystalline solid (yield A'-71%, B'-73%, C'-76%, D'-73%). mp: 183-184ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 7.90-7.94 (d, 2H), 7.83(s, 1H), 7.44-7.48(d, 2H), 7.35-7.42(m, 1H), 2.37 (s, 3H) 2.02 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C 147.59, 140.10, 135.14, 133.53, 130.53, 129.35, 129.13, 128.93, 128.28, 126.94, 125.77, 121.49.

1-(4-fluroophenyl)-4-phenyl-1H-1,2,3-triazole (9a): (table 1, entry 18) **9a** was isolated as a white crystalline solid (yield A'-73%, B'-77%, C'-84%, D'-79%). mp: 183-184ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 8.17(s, 1H), 7.89-7.92(d, 2H), 7.45−7.69(m, 4H), 7.36−7.40(m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C 133.14, 129.13, 128.74, 125.98, 122.56, 122.33, 117.49.

1-(4-chlorophenyl)-4-phenyl-1H-1,2,3-triazole (10a): (table 1, entry 19) **10a** was isolated as a white crystalline solid (yield A'-73%, B'-75%, C'-83%, D'-78%). mp: 183-184ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 8.17(s, 1H), 7.90-7.92(d, 2H), 7.75−7.77(d, 2H), 7.40−7.54(m, 4H), 7.26-7.40 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C 130.14, 129.13, 128.77, 126.04, 121.83, 117.57.

1-(4-bromophenyl)-4-phenyl-1H-1,2,3-triazole (11a): (table 1, entry 20) **11a** was isolated as a white crystalline solid (yield A'-70%, B'-71%, C'-75%, D'-75%). mp: 183-184ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 8.15(s, 1H), 7.90-7.92(d, 2H), 7.45−7.49(m, 2H), 7.36−7.40(m, 3H), 7.20-7.26 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C 161.41, 130.14, 129.11, 128.69, 125.96, 117.77, 117.11, 116.80.

1-(4-nitrophenyl)-4-phenyl-1H-1,2,3-triazole (12a): (table 1, entry 21) **12a** was isolated as a white crystalline solid (yield A'-71%, B'-74%, C'-80%, D'-76%). mp: 183-184ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 8.44-.8.47(d, 2H) 8.30(s, 1H), 8.04-8.06(d 2H) 7.92-7.93(d, 2H), 7.40−7.51(m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C 164.33, 161.68, 147.48, 137.02, 129.82, 128.86, 127.59, 127.49, 126.49, 120.56, 117.37, 116.06, 115.84.

1-(3-nitrophenyl)-4-phenyl-1H-1,2,3-triazole (13a): (table 1, entry 22) **13a** was isolated as a white crystalline solid (yield A'-72%, B'-73%, C'-78%, D'-75%). mp: 183-184ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 8.12(s, 1H), 7.70-7.84 (d, 2H), 7.44-7.48(d, 2H), 7.18-7.39(m, 5H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C 137.94, 131.19, 129.70, 129.21, 129.04, 126.09, 126.04, 123.35, 117.41, 115.26.

1-(2-nitrophenyl)-4-phenyl-1H-1,2,3-triazole (14a): (table 1, entry 23) **14a** was isolated as a white crystalline solid (yield A'-69%, B'-71%, C'-74%, D'-72%). mp: 183-184ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 8.00 (s, 1H), 7.95-7.97(d, 1H), 7.80-7.95(d, 2H), 7.78−7.80(m, 1H), 7.67-7.71 (m, 2H), 7.18-7.67 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C 148.41, 144.47, 134.00, 130.88, 130.26, 129.85, 129.04, 128.73, 127.91, 126.04, 125.66, 121.14.

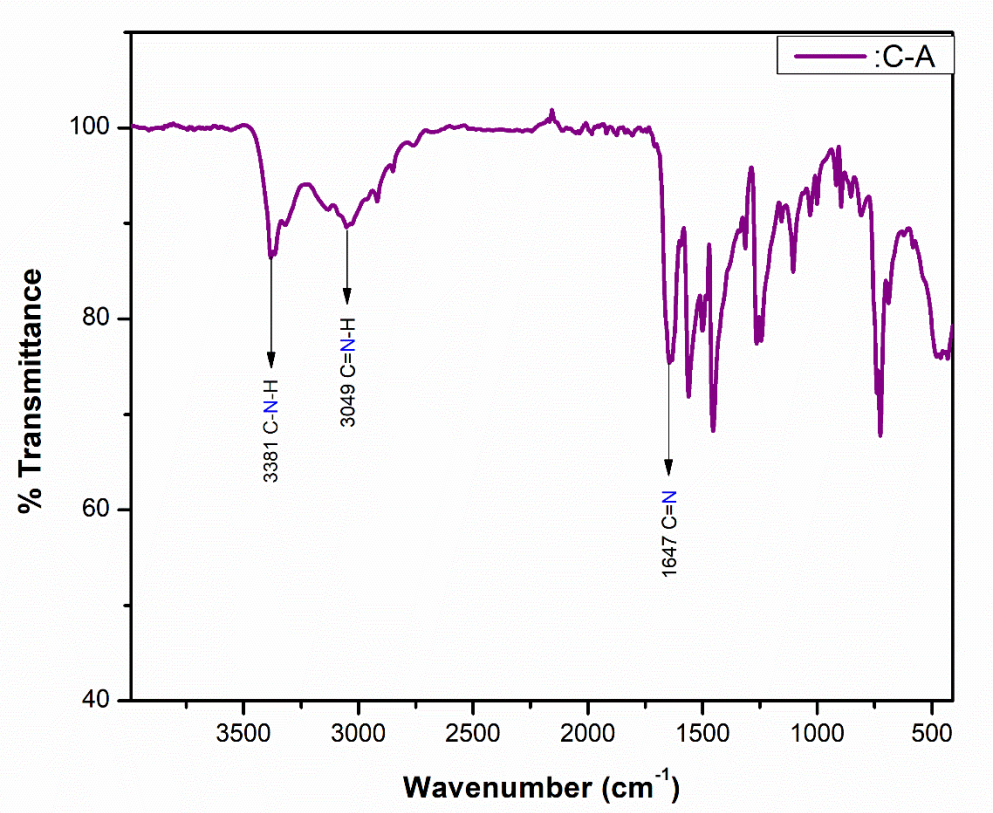


Figure S1: IR Spectrum of **C-A.**

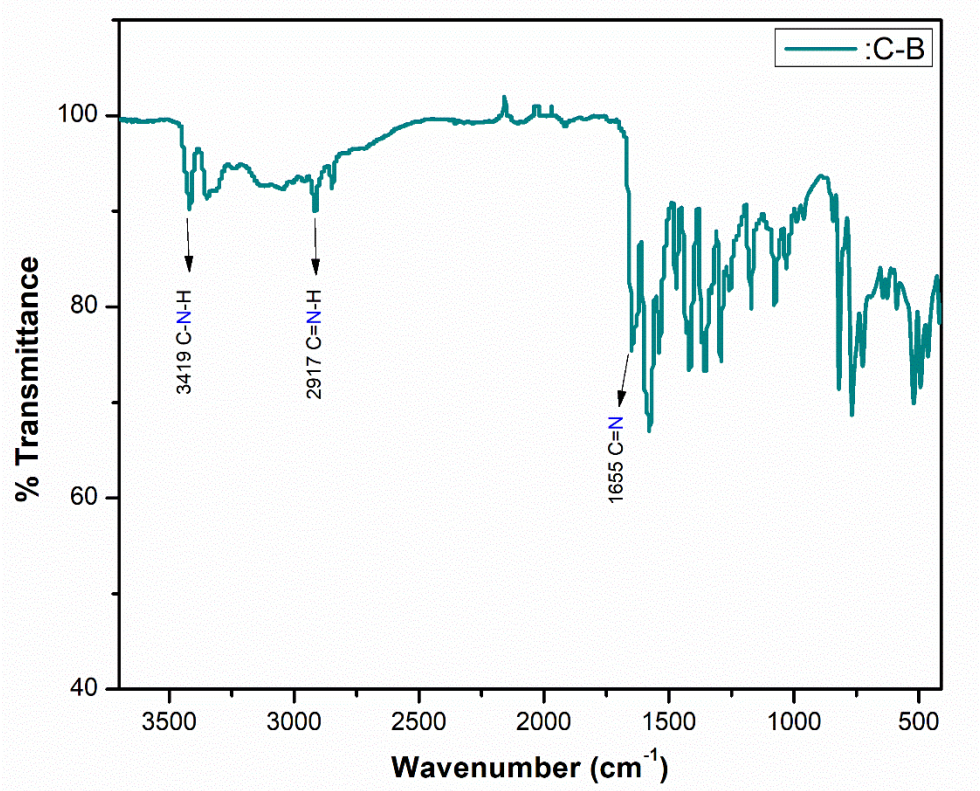


Figure S2: IR Spectrum of **C-B**

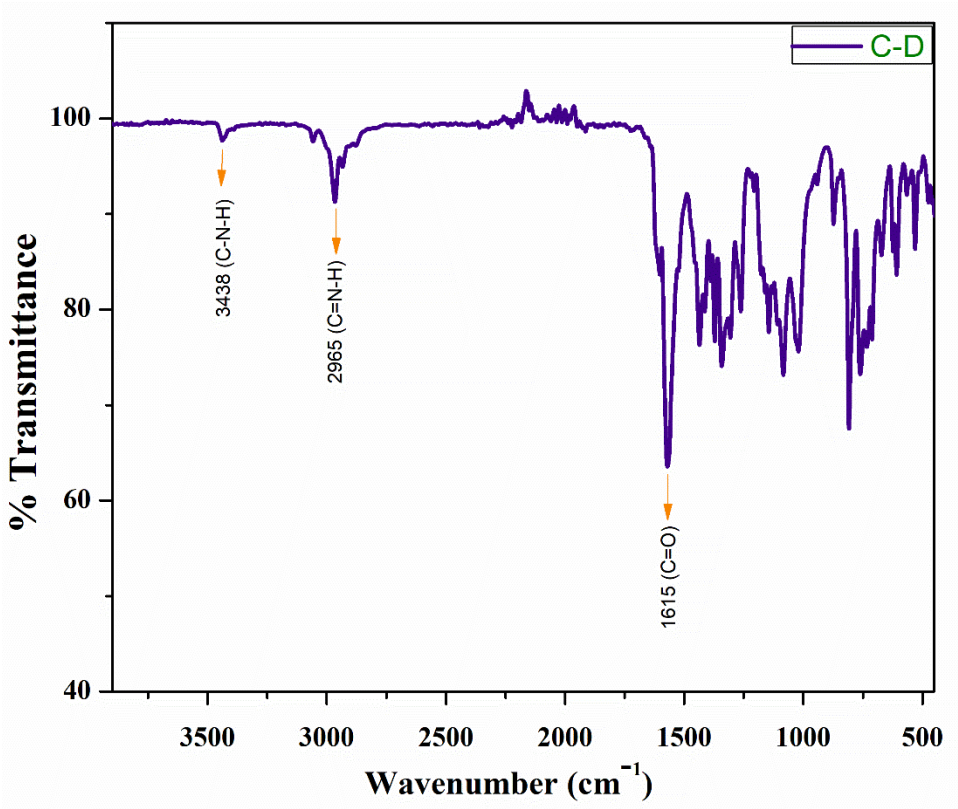


Figure S3: IR Spectrum of **C-D**

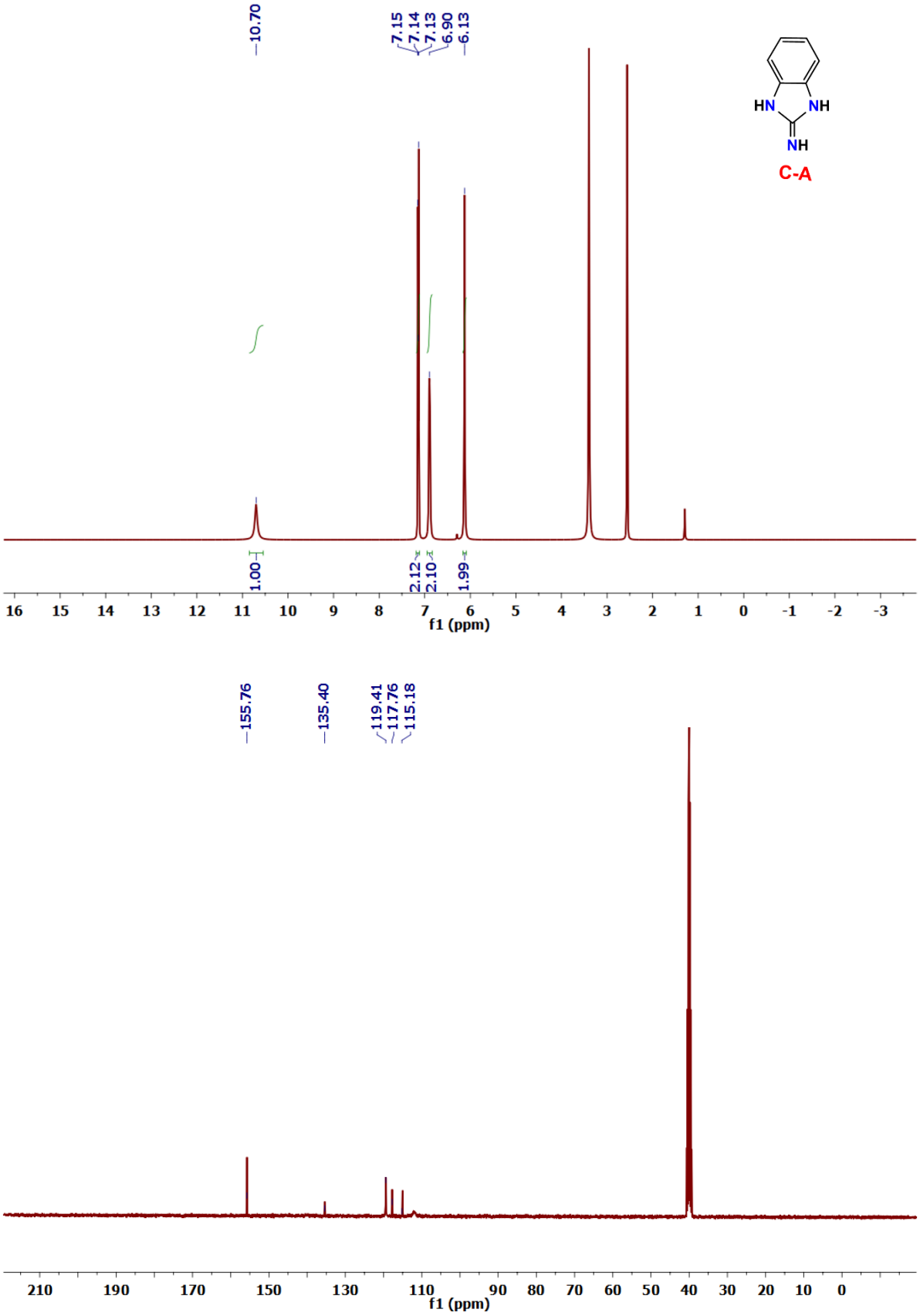


Figure S4: ^{1}H and ^{13}C NMR spectra of 1,3-dihydro-2H-benzo[d]imidazol-2-imine (**C-A**)

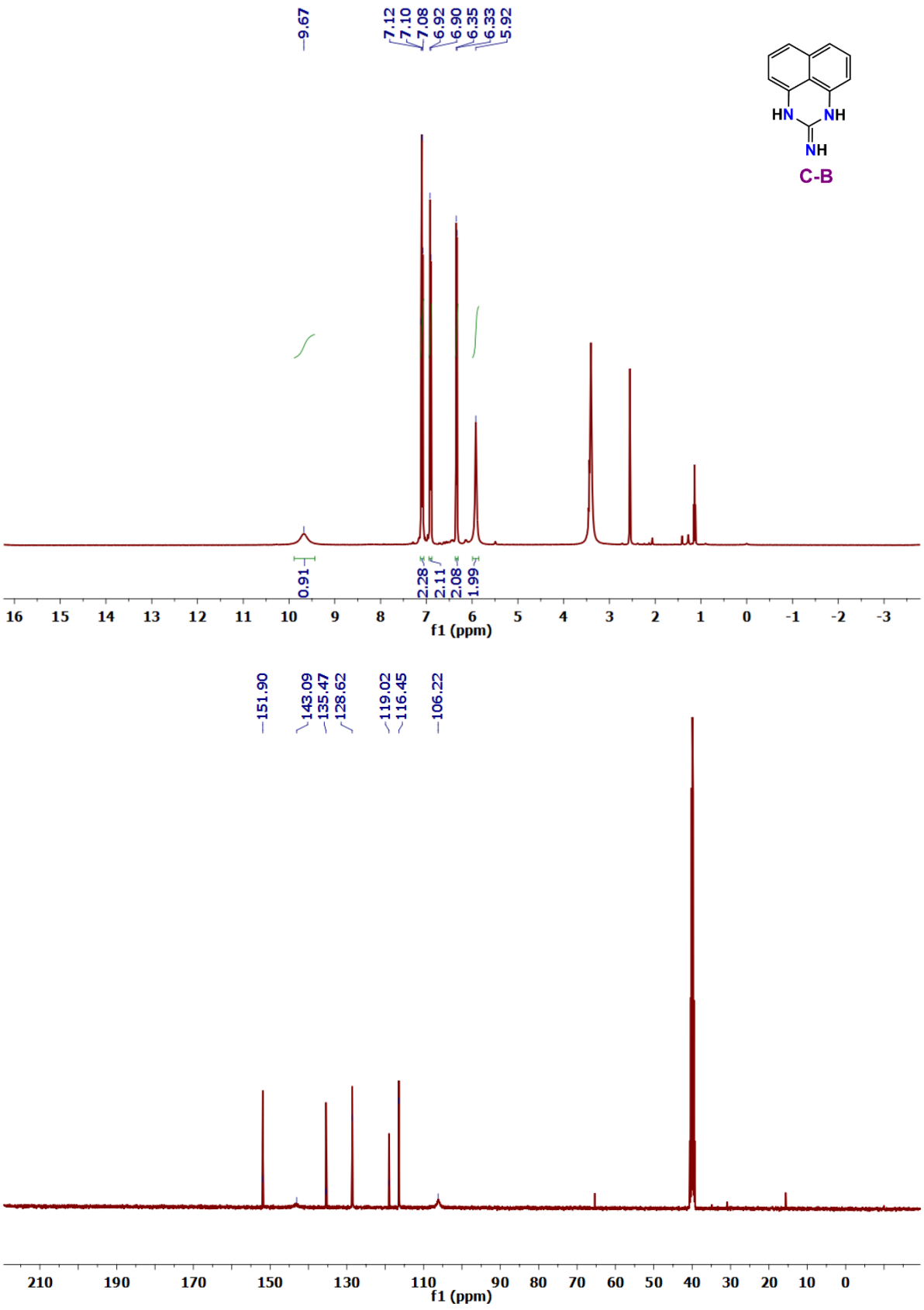


Figure S5: ^{1}H and ^{13}C NMR spectra of 1H-perimidin-2(3H)-imine (**C-B**)

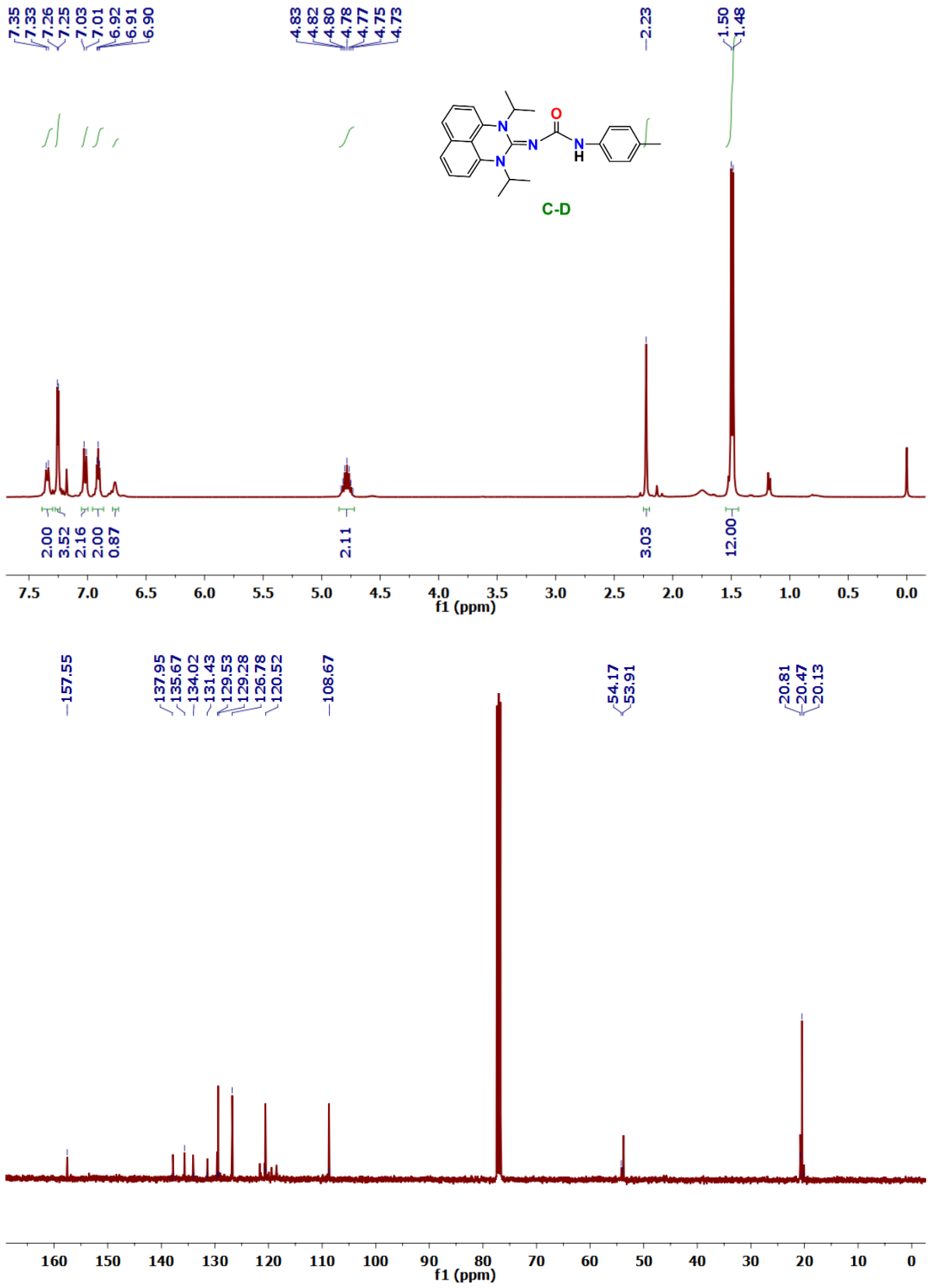


Figure S6: ^{1}H and ^{13}C NMR spectra of N,N-di-1,3-^{i}pr-perimidin-2-ylidene)-N′-*p*-tolyisoureate (**C-D**).

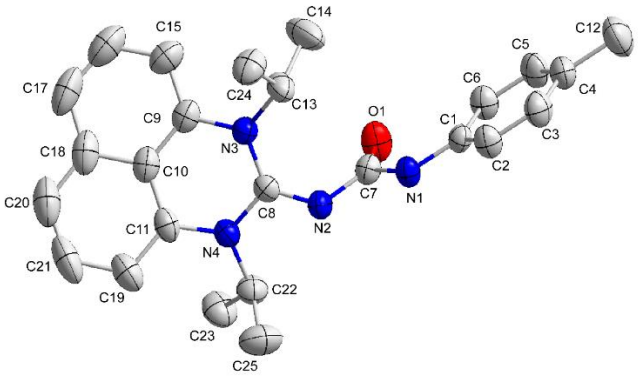
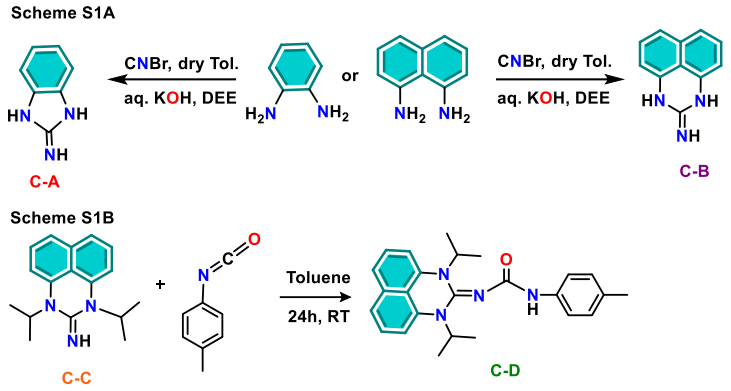


Figure S7: Molecular structure of compound **C-D** with thermal ellipsoid set at the 50% probability levels. All hydrogen atoms are omitted for clarity.

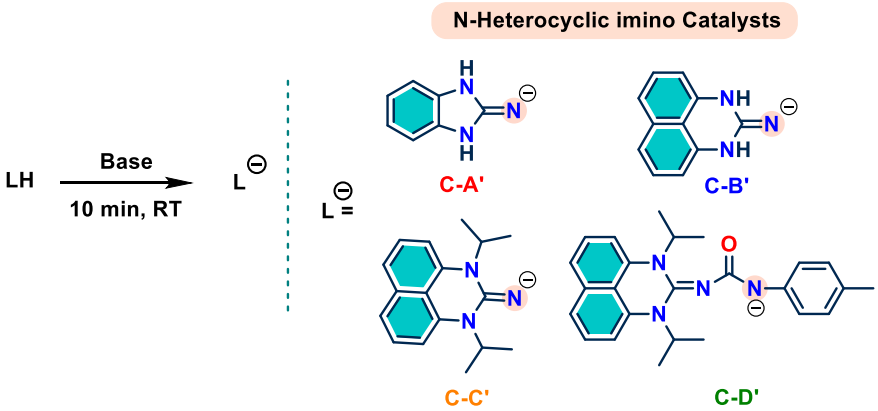
Table ST1: Crystal data and structure refinement parameters for **C-D**	
Empirical formula	$C_{25}H_{28}N_4O$
Formula weight ($gmol^{-1}$)	400.51 g/mol
Space group	P21/n
Temperature	301(2) K
λ (Å (Mo–Ka)	0.71073 Å
Crystal system	Monoclinic
a (Å)	8.0389(17) Å
b (Å)	31.902 (7) Å
c (Å)	9.109 (2) Å
α (°)	90°
β (°)	109.917 (6)°
γ (°)	90°
V ($Å^3$)	2196.3(8)$Å^3$
Z	4
qcalc (gcm^{-3})	1.211 g/cm^3
Crystal size (mm)	0.09 x 0.18 x 0.20 mm
F (000)	856
Theta range for data collection	2.699 to 25.019°
Index ranges	-9<=h<=9, -37<=k<=37, -10<=l<=10
GOF[a] on F^2	1.100
R1[b] [I[2r(I)]	R1 = 0.0699
R1 [all data]	R1 = 0.0457
wR2[c] [I[2r(I)]	wR2 = 0.1192
wR2 [all data]	wR2 = 0.1046
CCDC	**2278567**

Table ST2. Selected bond length (Å) for **C-D**			
Bond	**Bond length (Å)**	**Bond**	**Bond length (Å)**
O1 C7	1.227(2)	C1 C2	1.387(2)
N1 C7	1.366(2)	C1 C6	1.388(2)
N1 C1	1.408(2)	C2 C3	1.377(3)
N2 C8	1.295(2)	C3 C4	1.384(3)
N2 C7	1.372(2)	C4 C5	1.375(3)
N3 C8	1.385(2)	C4 C12	1.512(3)
N3 C9	1.419(2)	C5 C6	1.383(3)
N3 C13	1.498(2)	C9 C15	1.376(3)
N4 C8	1.383(2)	C9 C10	1.410(3)
N4 C11	1.412(2)	C10 C11	1.408(3)
N4 C22	1.496(2)	C10 C18	1.422(3)
C13 C24	1.520(3)	C11 C19	1.382(3)
C13 C14	1.534(3)	C17 C18	1.415(4)
C15 C16	1.350(4)	C18 C20	1.401(4)
C16 C17	1.399(3)	C19 C21	1.413(3)
C20 C21	1.352(4)	C22 C23	1.529(3)
C22 C25	1.521(3)		

Table ST3. Selected bond angles (˚) for **C-D**			
Bond	**Bond angle (º)**	**Bond**	**Bond angle (º)**
C7 N1 C1	128.24(15)	C15 C9 C10	119.67(18)
C8 N2 C7	126.23(15)	C15 C9 N3	122.61(18)
C8 N3 C9	120.79(14)	C10 C9 N3	117.62(17)
C8 N3 C13	118.68(14)	C11 C10 C9	120.03(16)
C9 N3 C13	119.45(15)	C11 C10 C18	119.99(19)
C8 N4 C11	121.48(15)	C9 C10 C18	120.0(2)
C8 N4 C22	116.36(14)	C19 C11 C10	119.82(18)
C11 N4 C22	122.11(14)	C19 C11 N4	123.18(19)
C2 C1 C6	118.27(16)	C10 C11 N4	116.95(16)
C2 C1 N1	117.08(15)	N3 C13 C24	111.87(16)
C6 C1 N1	124.64(16)	N3 C13 C14	113.84(19)
C3 C2 C1	120.87(17)	C24 C13 C14	112.94(18)
C2 C3 C4	121.57(18)	C9 C15 C16	119.8(2)
C5 C4 C3	116.90(17)	C17 C16 C15	121.7(2)
C5 C4 C12	121.34(19)	C16 C17 C18	120.6(2)
C3 C4 C12	121.8(2)	C20 C18 C17	123.6(2)
C4 C5 C6	122.84(18)	C20 C18 C10	118.5(2)
C5 C6 C1	119.54(17)	C17 C18 C10	118.0(2)
O1 C7 N1	123.18(16)	C11 C19 C21	119.0(2)
O1 C7 N2	124.19(16)	C21 C20 C18	120.6(2)
N1 C7 N2	112.46(15)	C20 C21 C19	121.8(2)
N2 C8 N4	117.04(15)	N4 C22 C25	112.35(17)
N2 C8 N3	125.10(15)	N4 C22 C23	112.27(16)
N4 C8 N3	117.80(15)	C25 C22 C23	114.37(18)

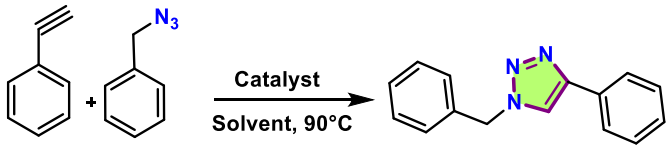


Scheme S1: Synthesis of various NHI precatalysts **C-A, C-B,** and **C-D.**



Scheme S2: Formation of active catalyst N-heterocyclic imino **(C-A'-C-D')** from N-heterocyclic imine **(C-A-C-D)**.

Table ST4. Optimization of the reaction conditions



Entry	Precatalyst	Base	Solvent	Yield (%)
1	C-C	—	DMSO	49
2	C-A	NaH	DMSO	71
3	C-B	NaH	DMSO	84
4	**C-C**	**NaH**	**DMSO**	**91**
5	C-D	NaH	DMSO	87
6	C-C	^{n}BuLi	DMSO	81
7	C-C	KO^{t}Bu	DMSO	0
8	C-C	KOH	DMSO	21
9	C-C	NaH	DMF	61
10	C-C	NaH	Toluene	>20

The reaction was carried out using a catalyst (C-A-C-D), phenylacetylene (1 mmol), and benzyl azide (1 mmol) in solvent (5 ml) at 90°C for 24h. Isolated yields after column chromatography.

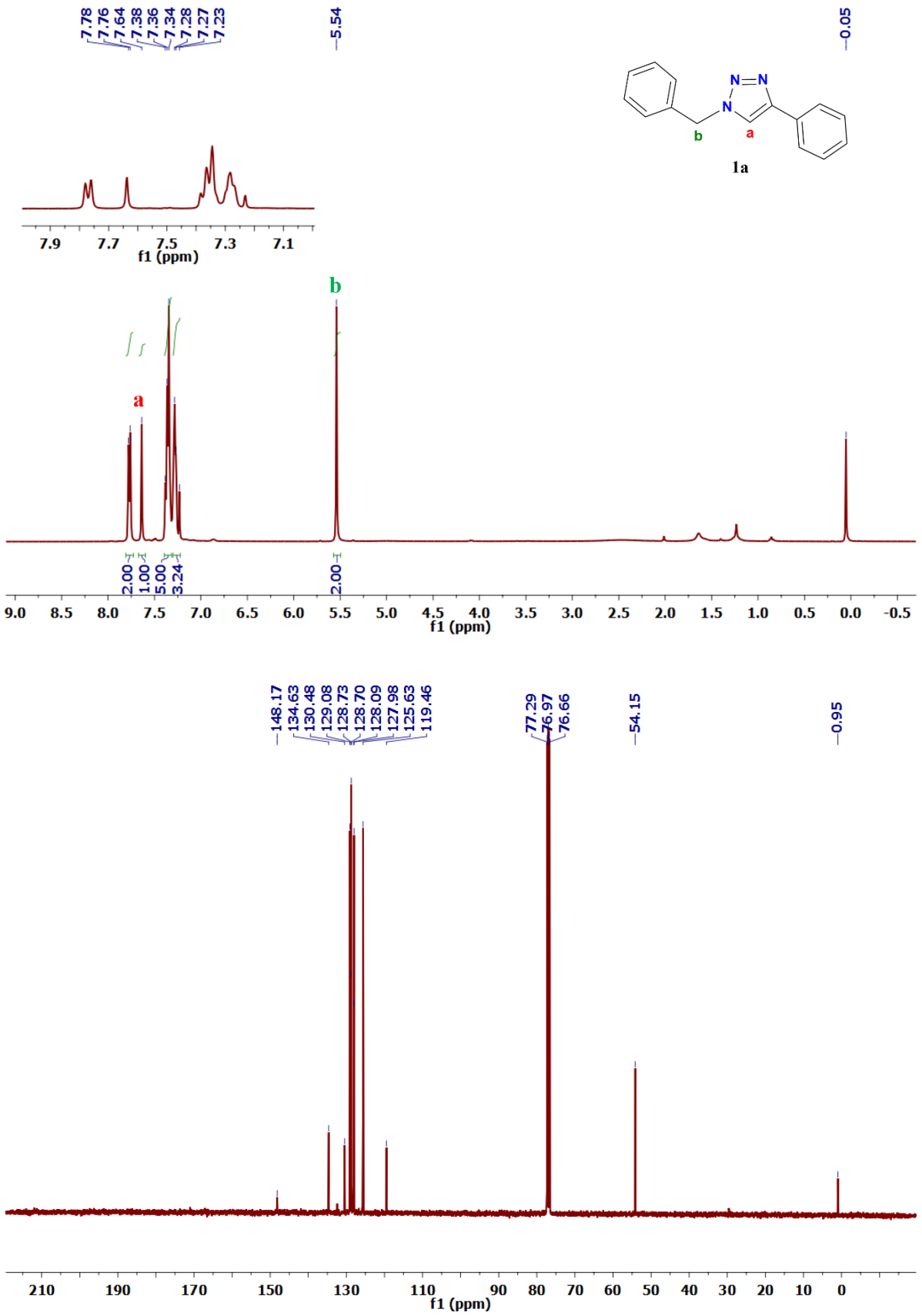


Figure S8: ^{1}H and ^{13}C NMR spectra of 1-benzyl-4-phenyl-1H-1,2,3-triazole (**1a**)

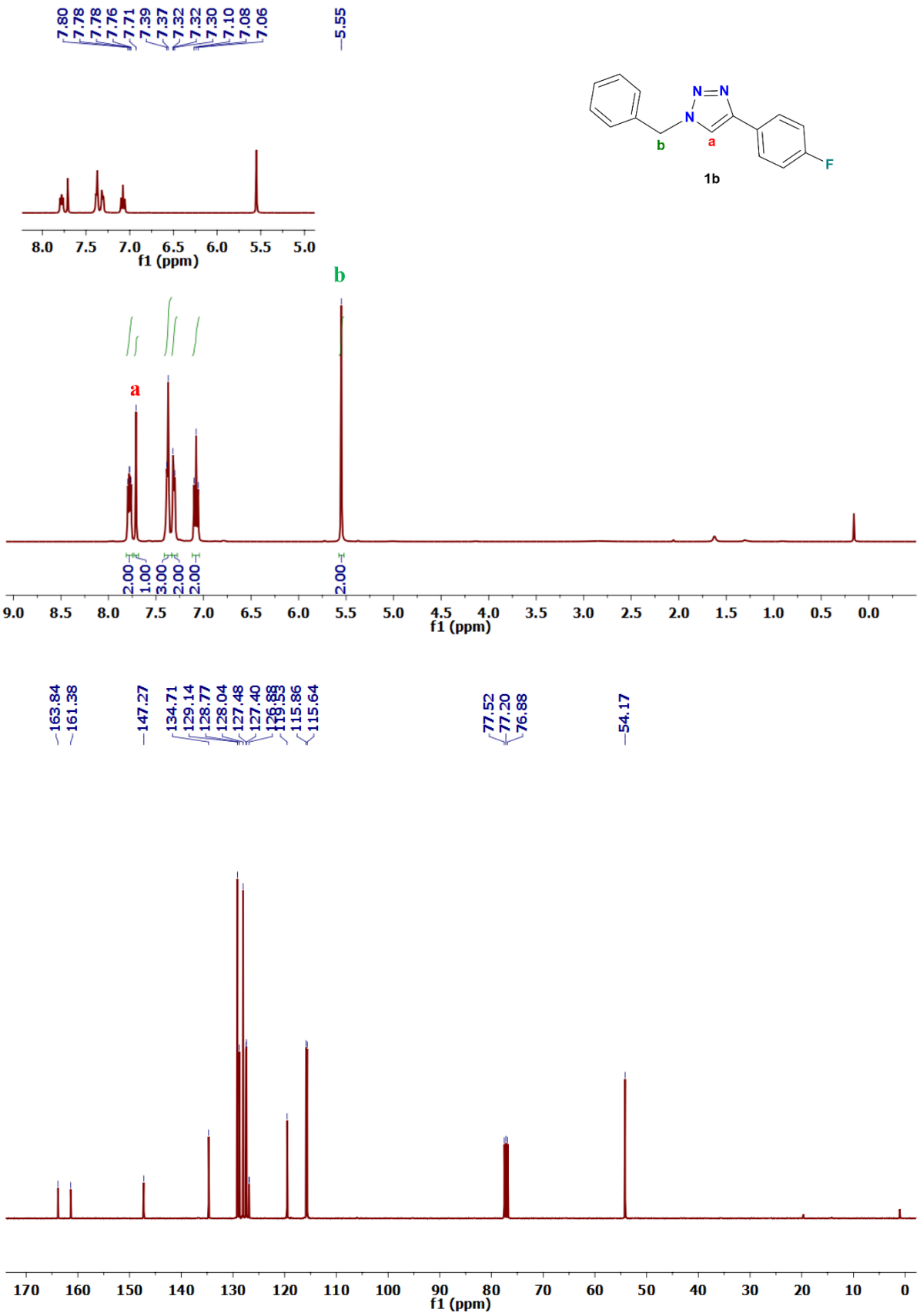


Figure S9: ^{1}H and ^{13}C NMR spectra of 1-benzyl-4-(4-fluorophenyl)-1H-1,2,3-triazole (**1b**)

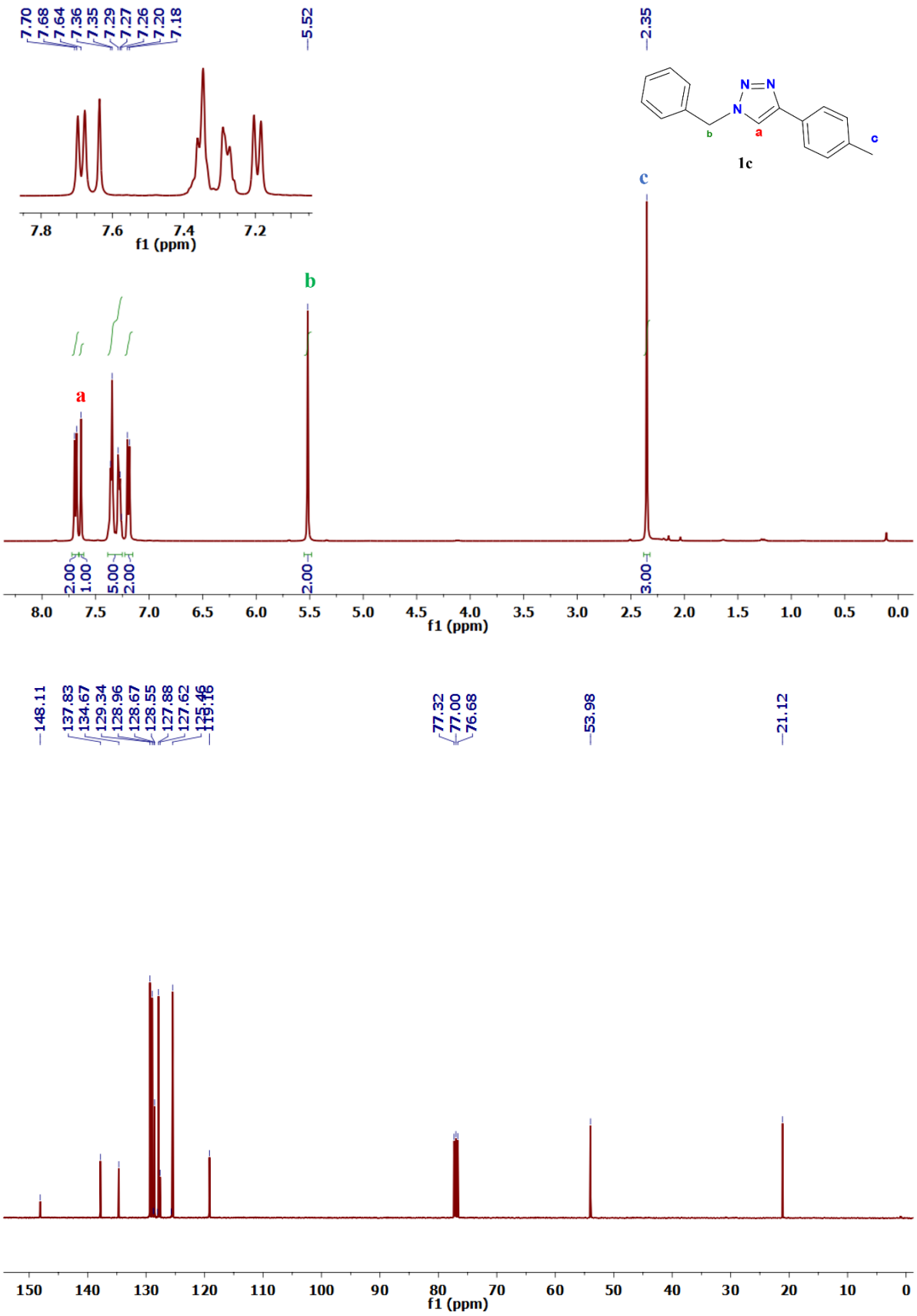


Figure S10: ^{1}H and ^{13}C NMR spectra of 1-Benzyl-4-(p-tolyl)-1H-1,2,3-triazole (**1c**)

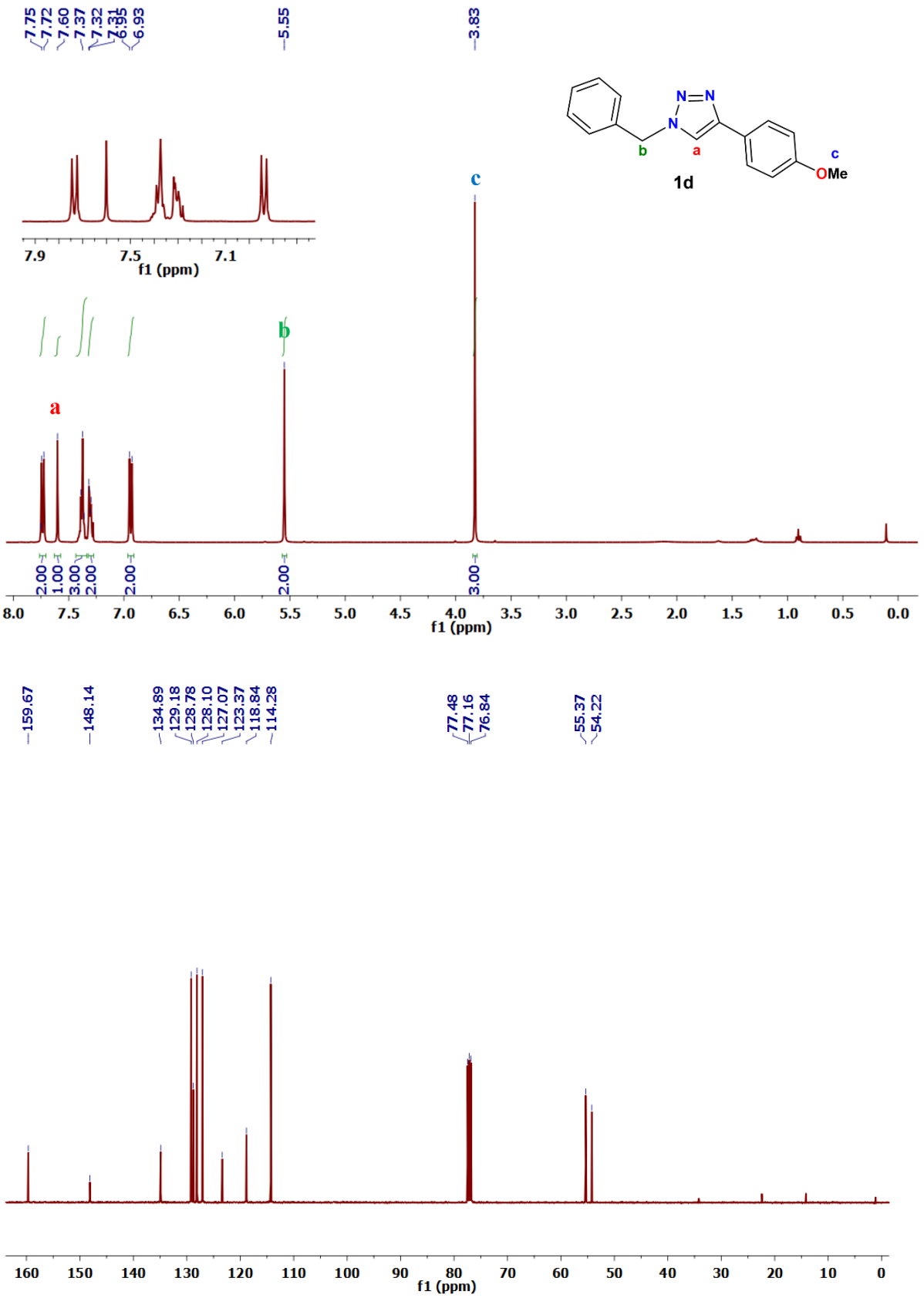


Figure S11: ^{1}H and ^{13}C NMR spectra of 1-benzyl-4-(4-methoxyphenyl)-1H-1,2,3-triazole (**1d**)

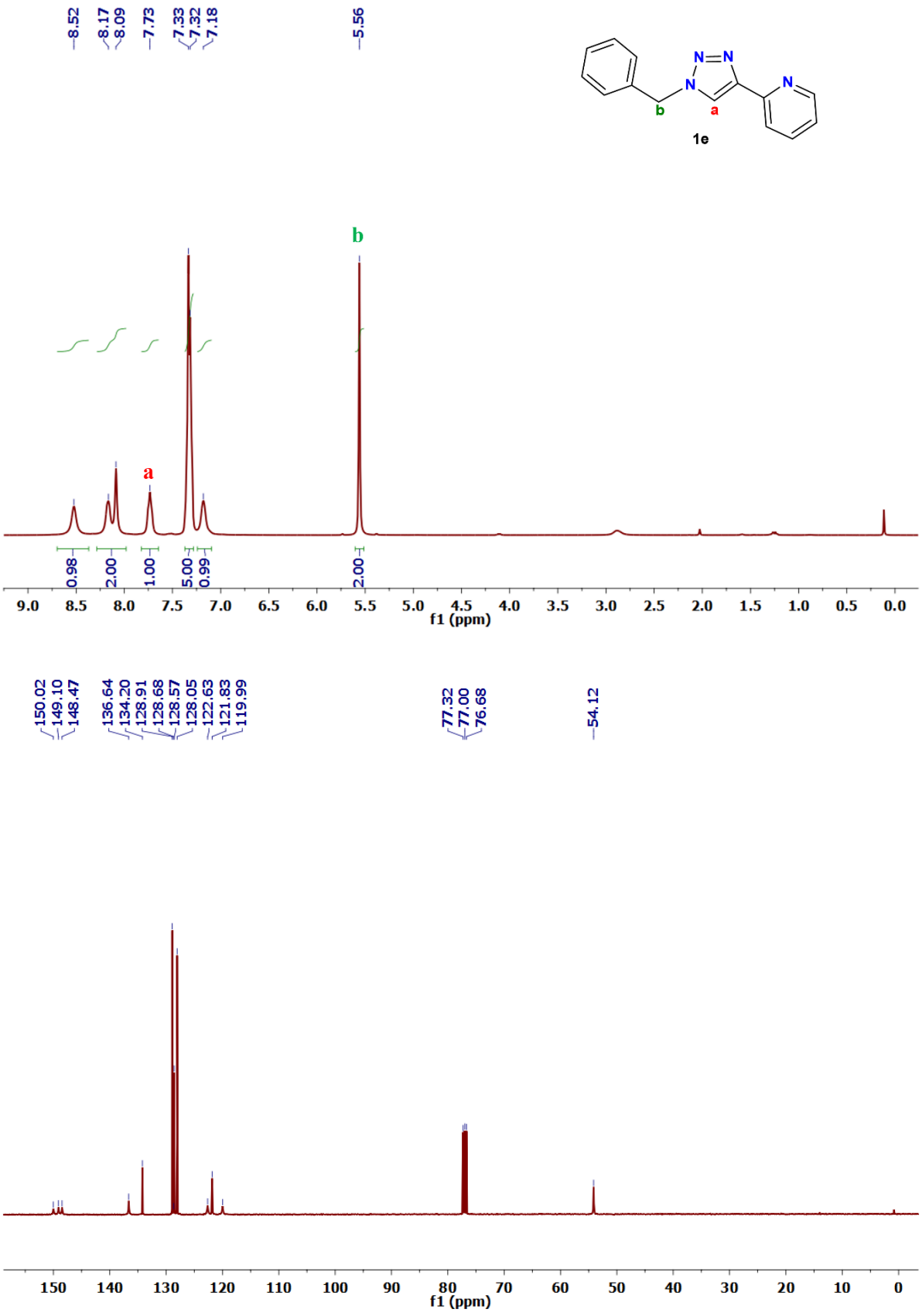


Figure S12: ^{1}H and ^{13}C NMR spectra of 2-(1-benzyl-1H-1,2,3-triazol-4-yl) pyridine (**1e**)

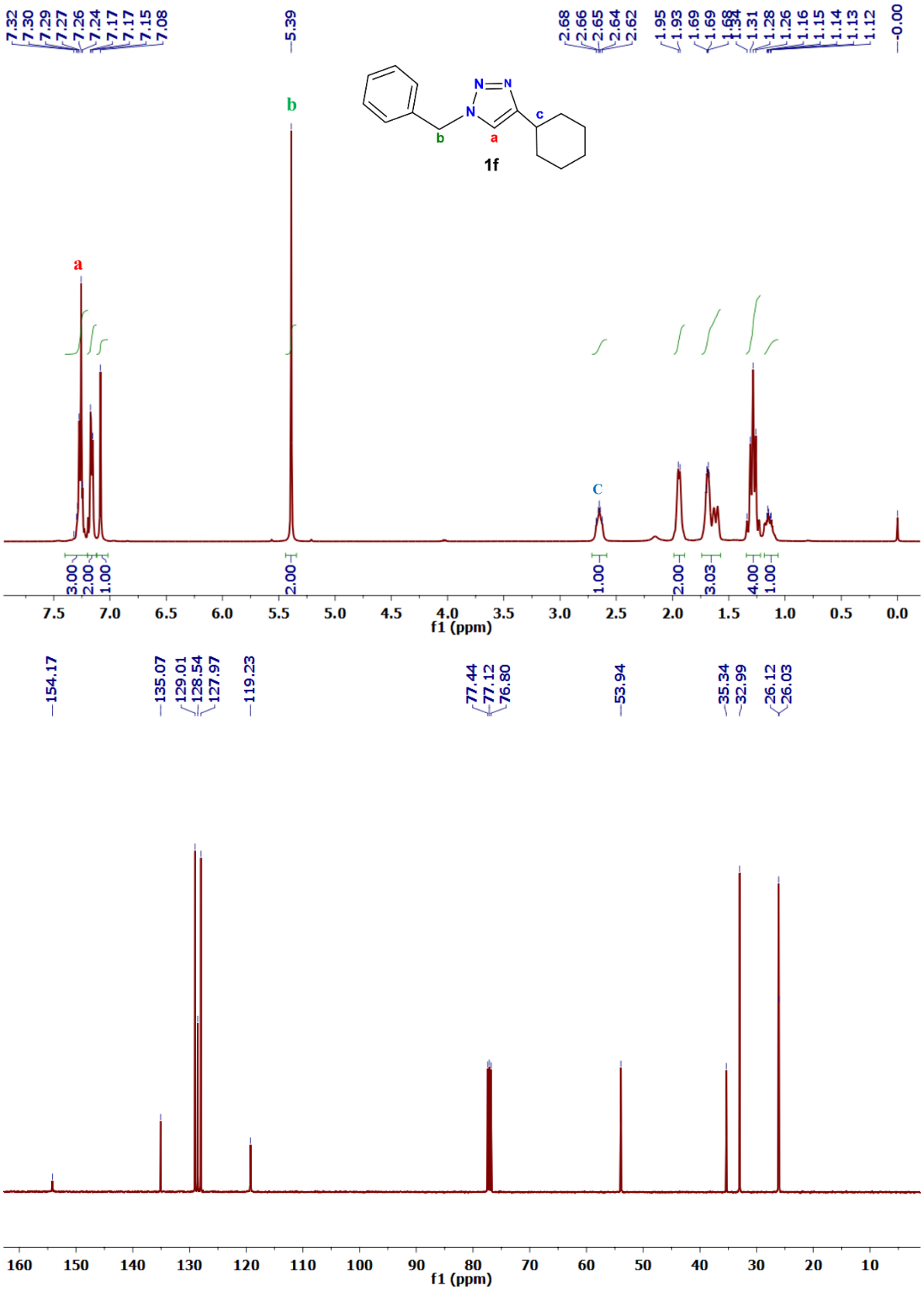


Figure S13: ^{1}H and ^{13}C NMR spectra of 1-benzyl-4-butyl-1H-1,2,3-triazole (**1f**)

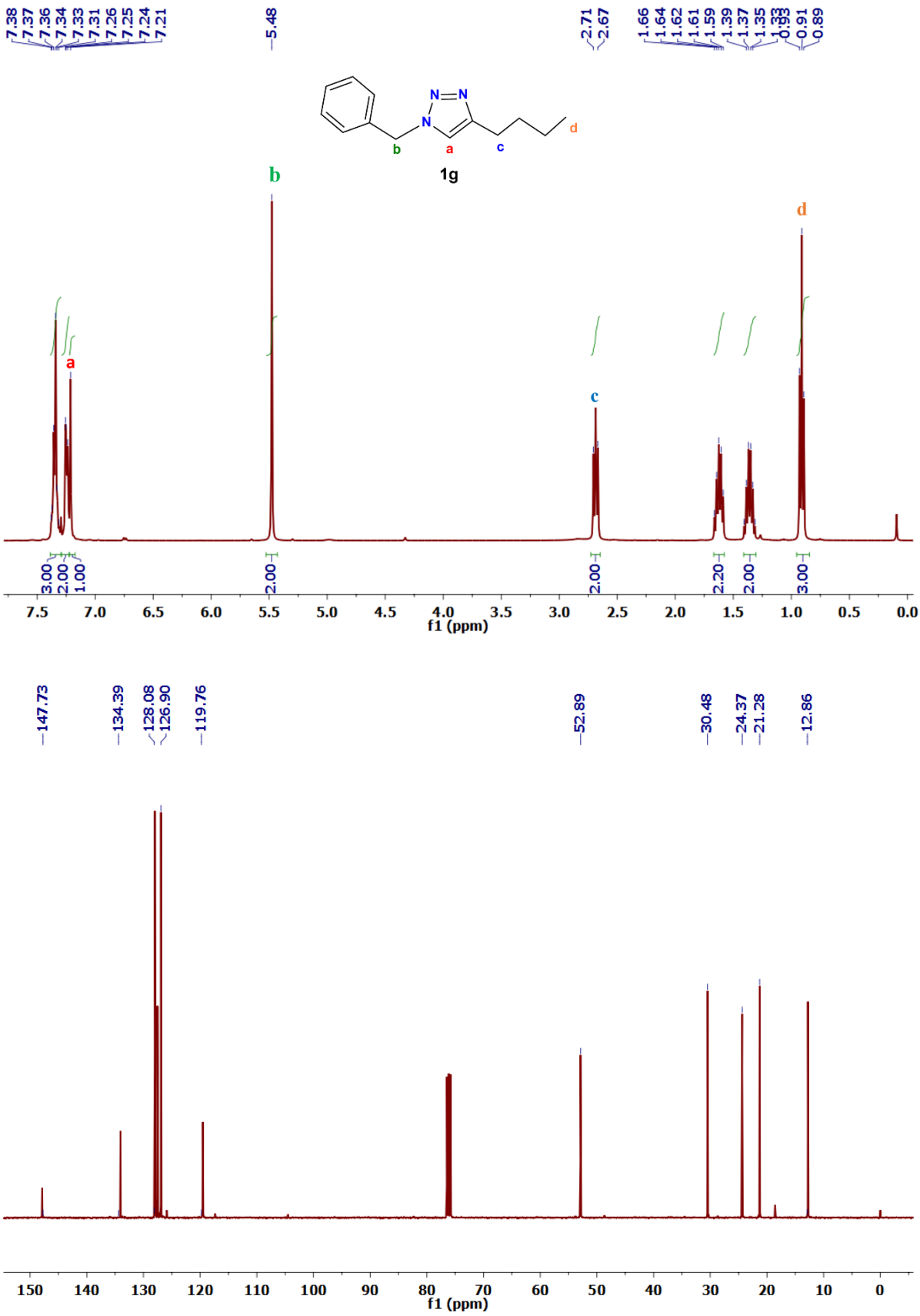


Figure S14: ^{1}H and ^{13}C NMR spectra of 1-benzyl-4-tert-butyl-1H-1,2,3-triazole (**1g**)

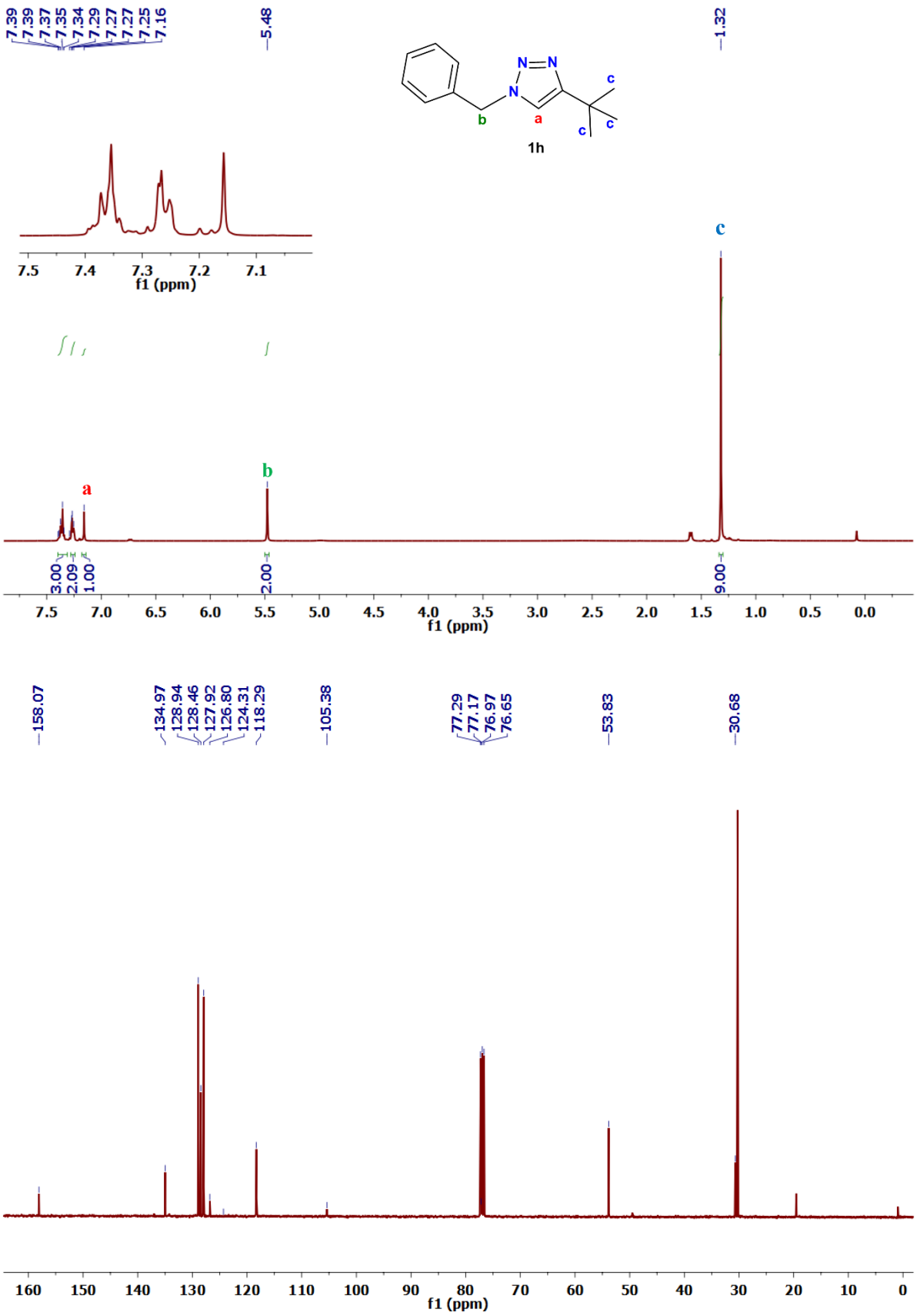


Figure S15: ^{1}H and ^{13}C NMR spectra of 1-benzyl-4-(cyclohexyl)-1H-1,2,3-triazole (**1h**)

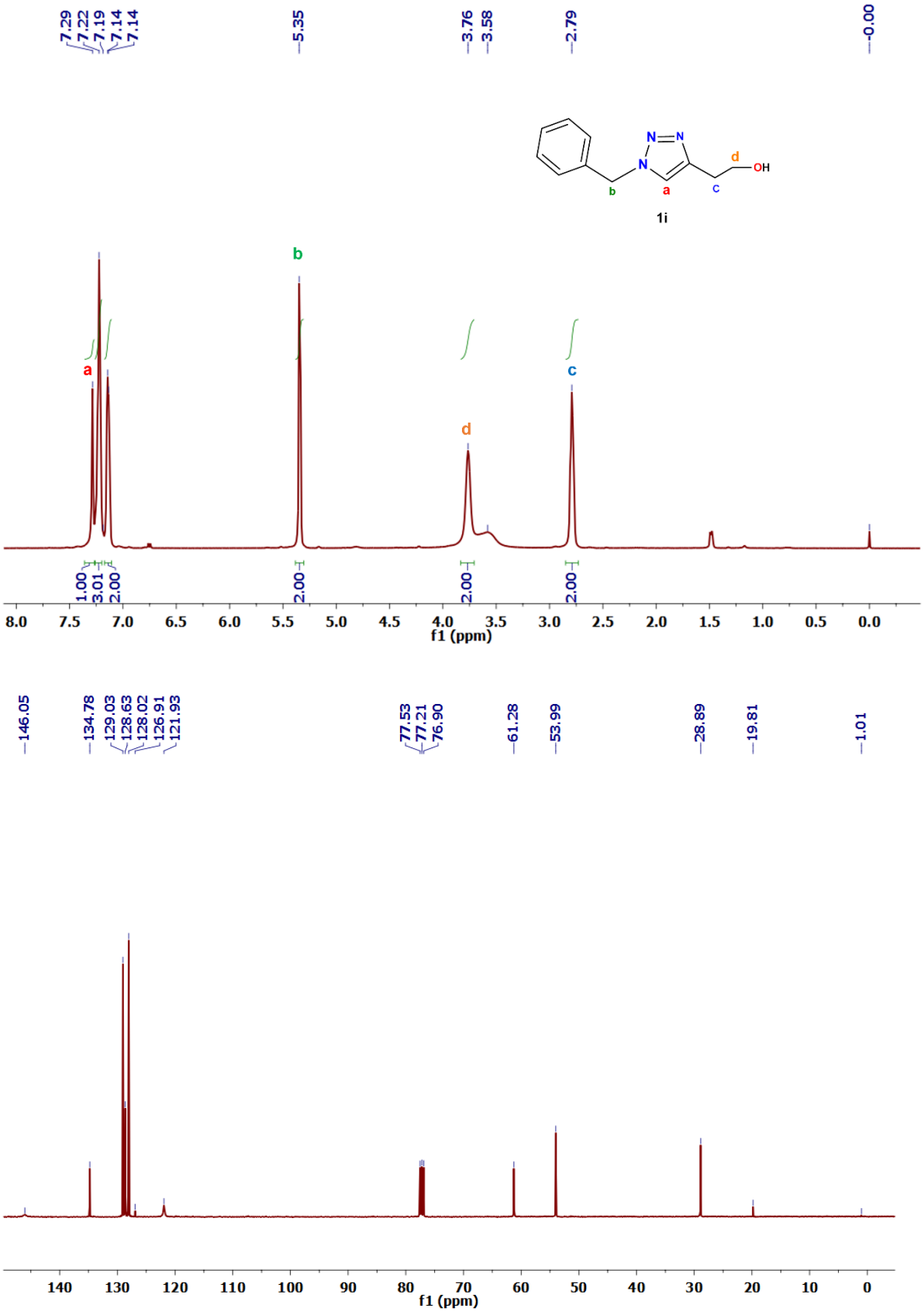


Figure S16: ^{1}H and ^{13}C NMR spectra of 2-(1-benzyl-1H-1,2,3-triazol-yl)ethan-1ol (**1i**)

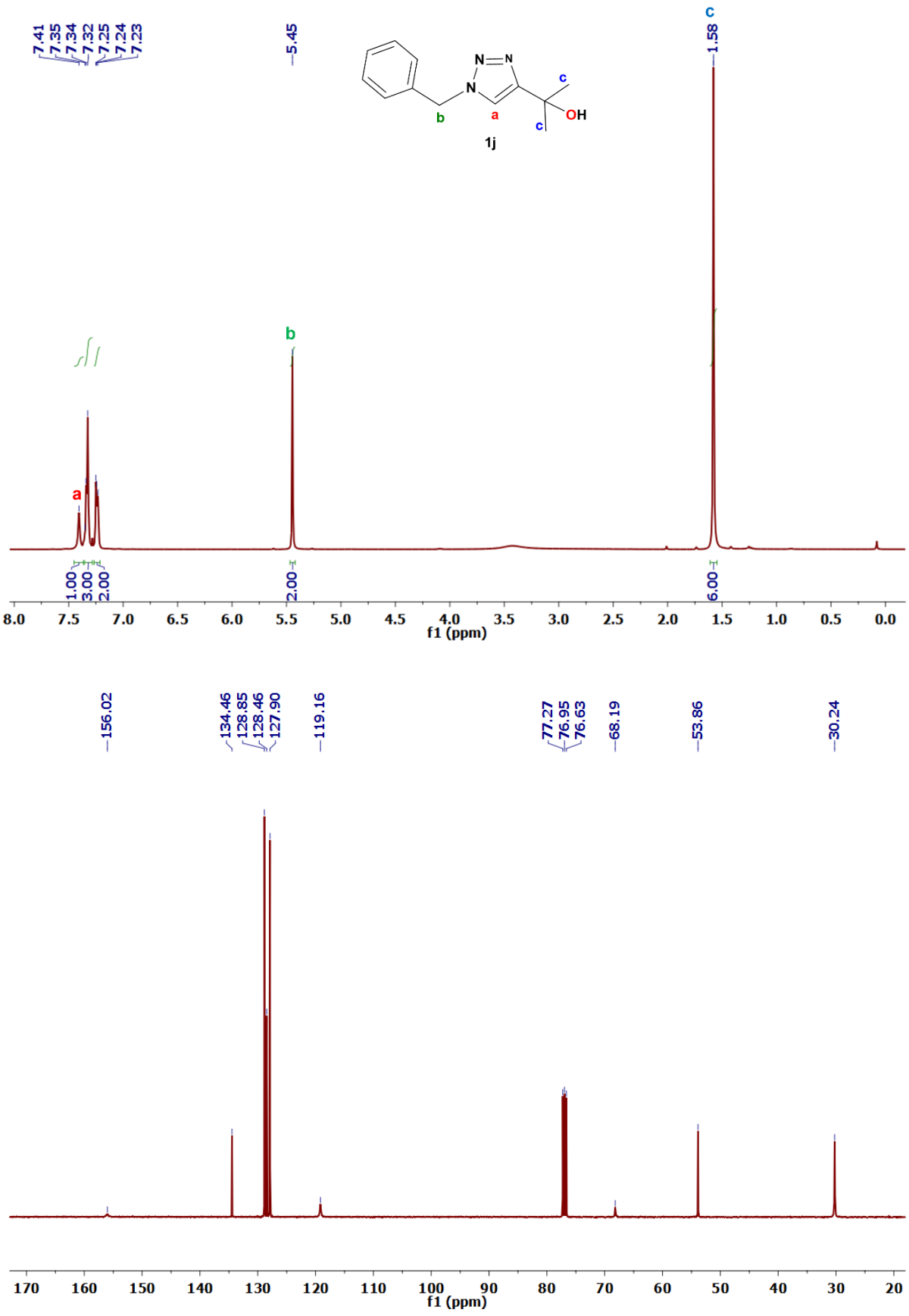


Figure S17: ^{1}H and ^{13}C NMR spectra of 2-(1-benzyl-1H-1,2,3-triazol-4-yl) propan-2-ol (**1j)**

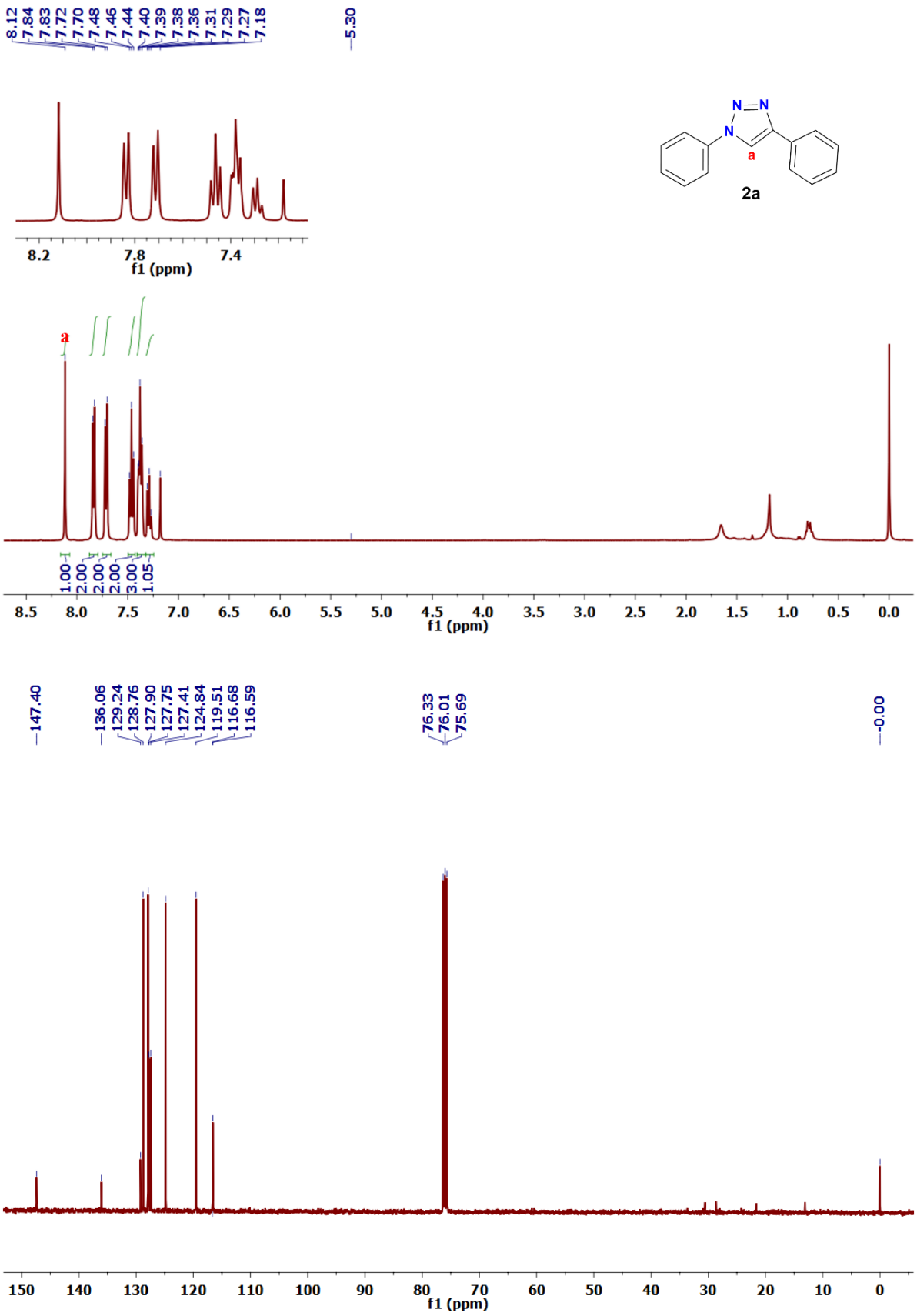


Figure S18: ^{1}H and ^{13}C NMR spectra of 1,4-diphenyl-1H-1,2,3-triazole (**2a**)

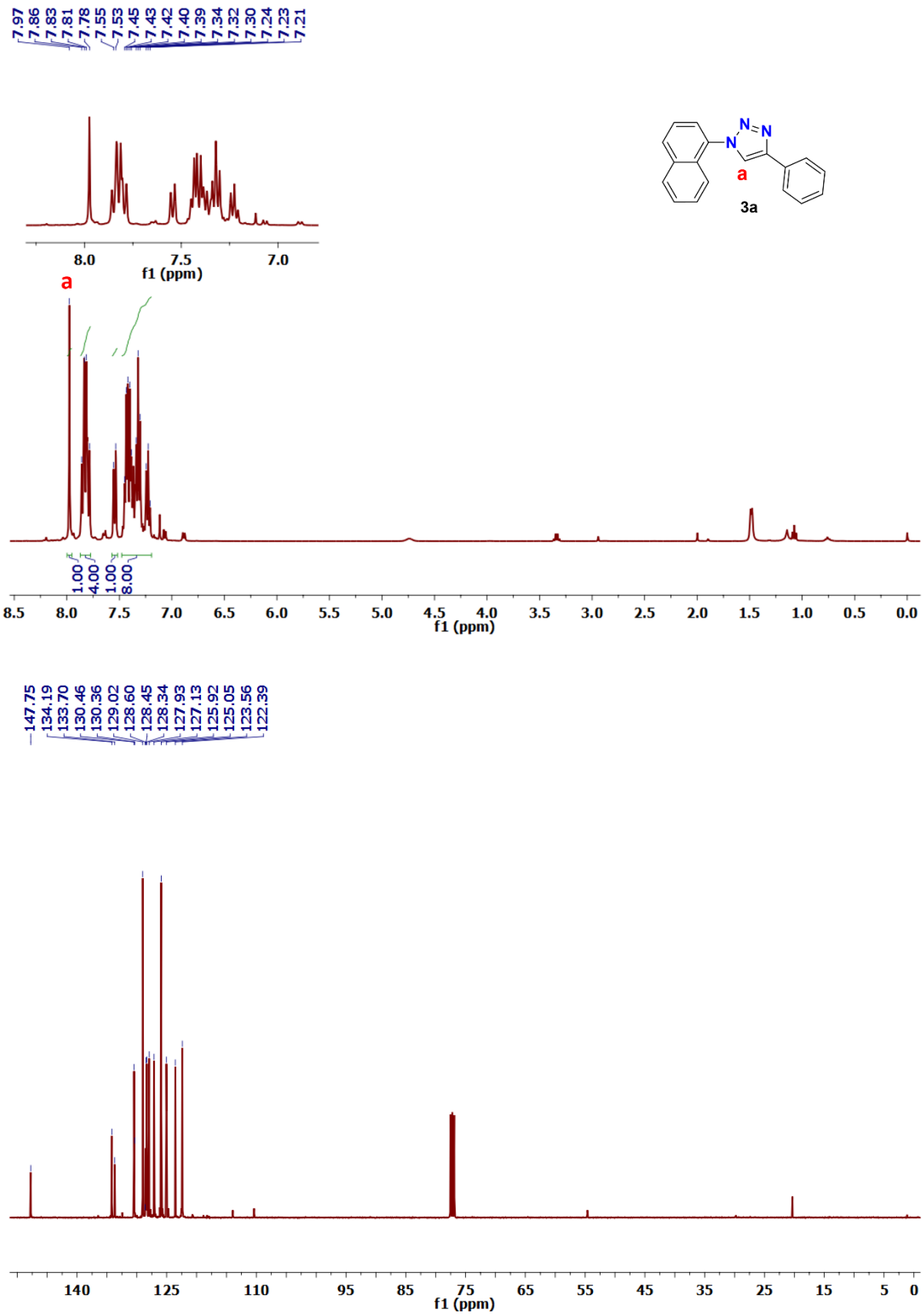


Figure S19: ^{1}H and ^{13}C NMR spectra of 1-naphthyl-4-phenyl-1H-1,2,3-triazole (**3a**)

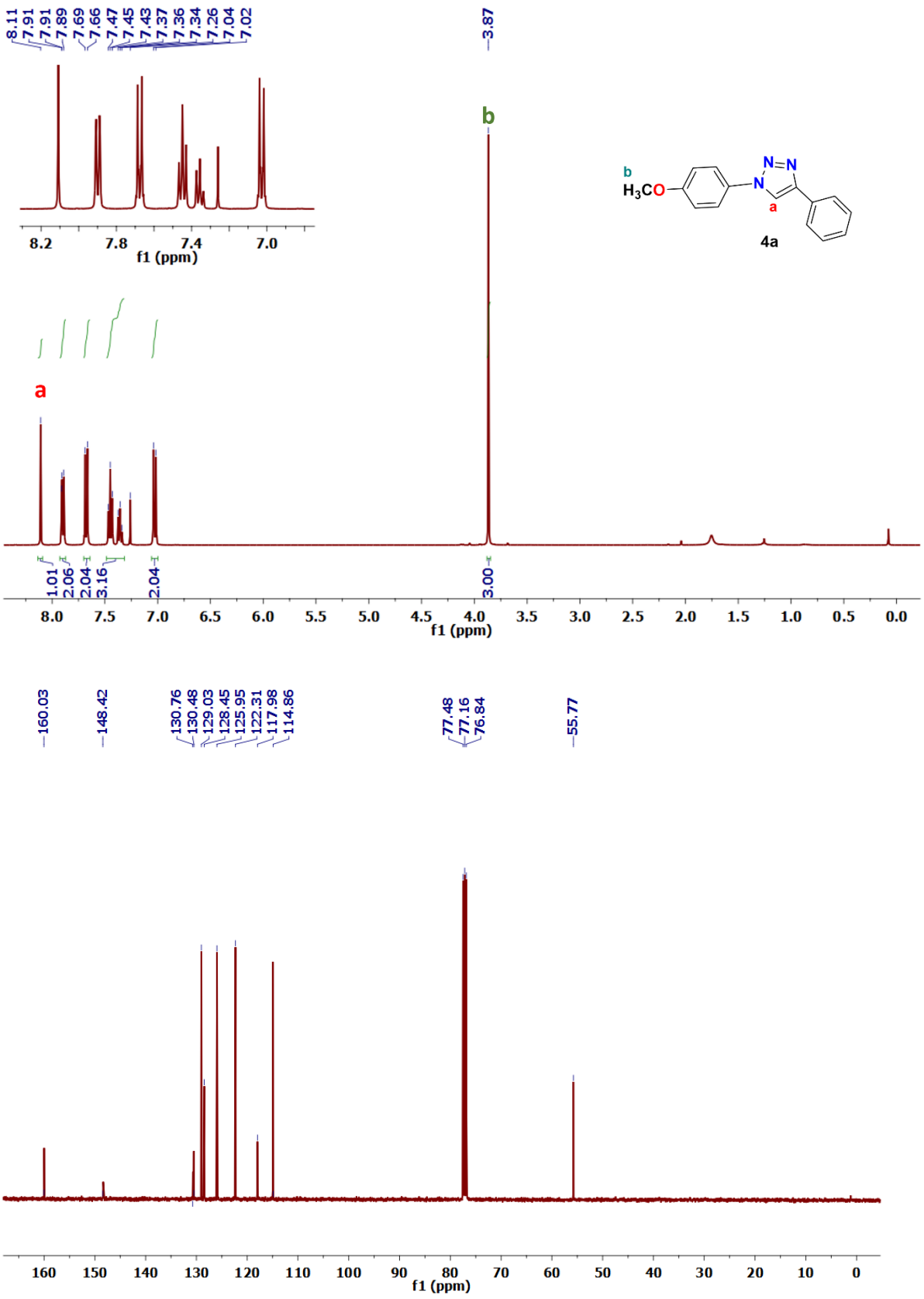


Figure S20: ^{1}H and ^{13}C NMR spectra of 1-(4-methoxyphenyl)-4-phenyl-1H-1,2,3-triazole (**4a**)

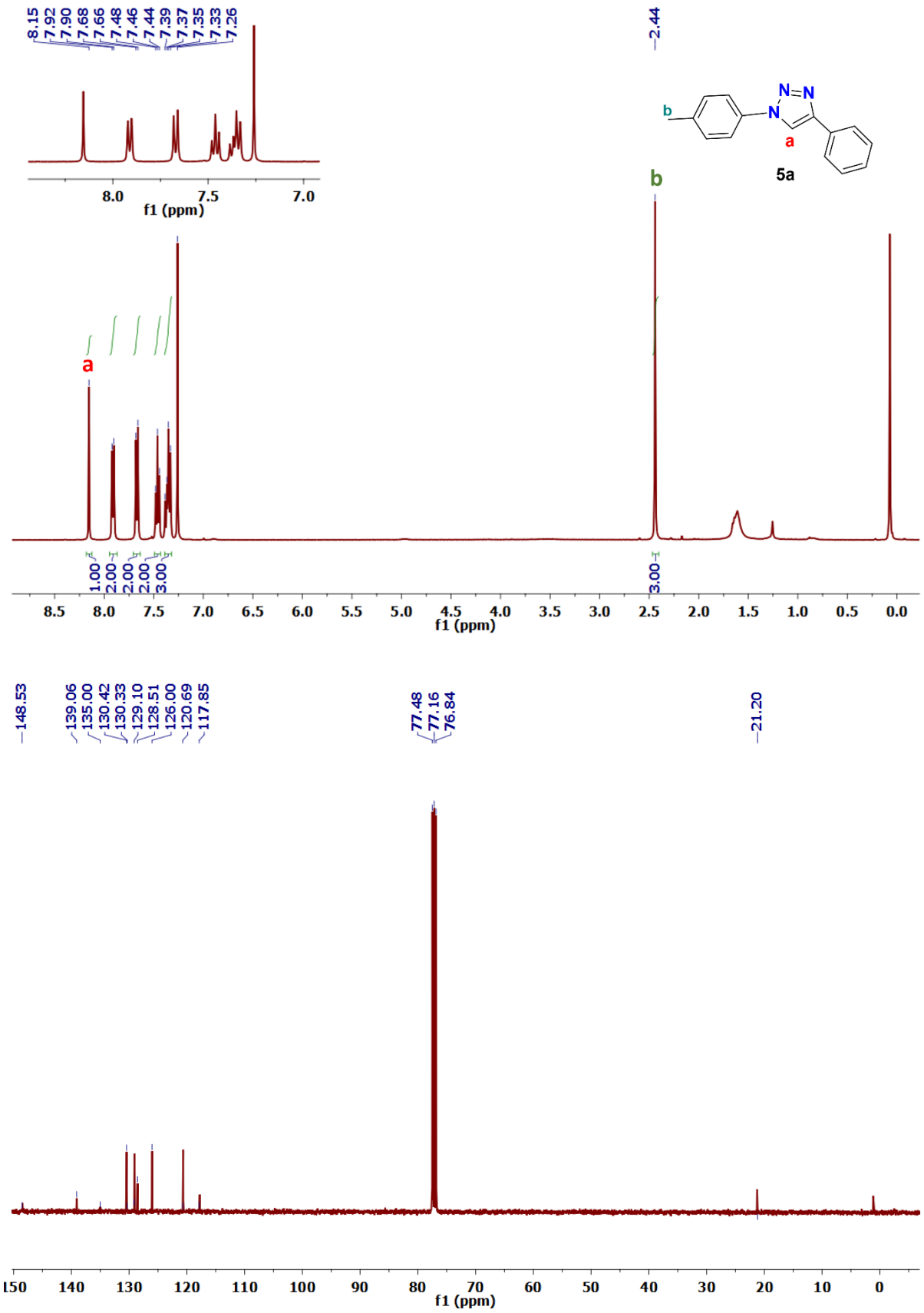


Figure S21: ^{1}H and ^{13}C NMR spectra of 1-(4-tolyl)-4-phenyl-1H-1,2,3-triazole (**5a**)

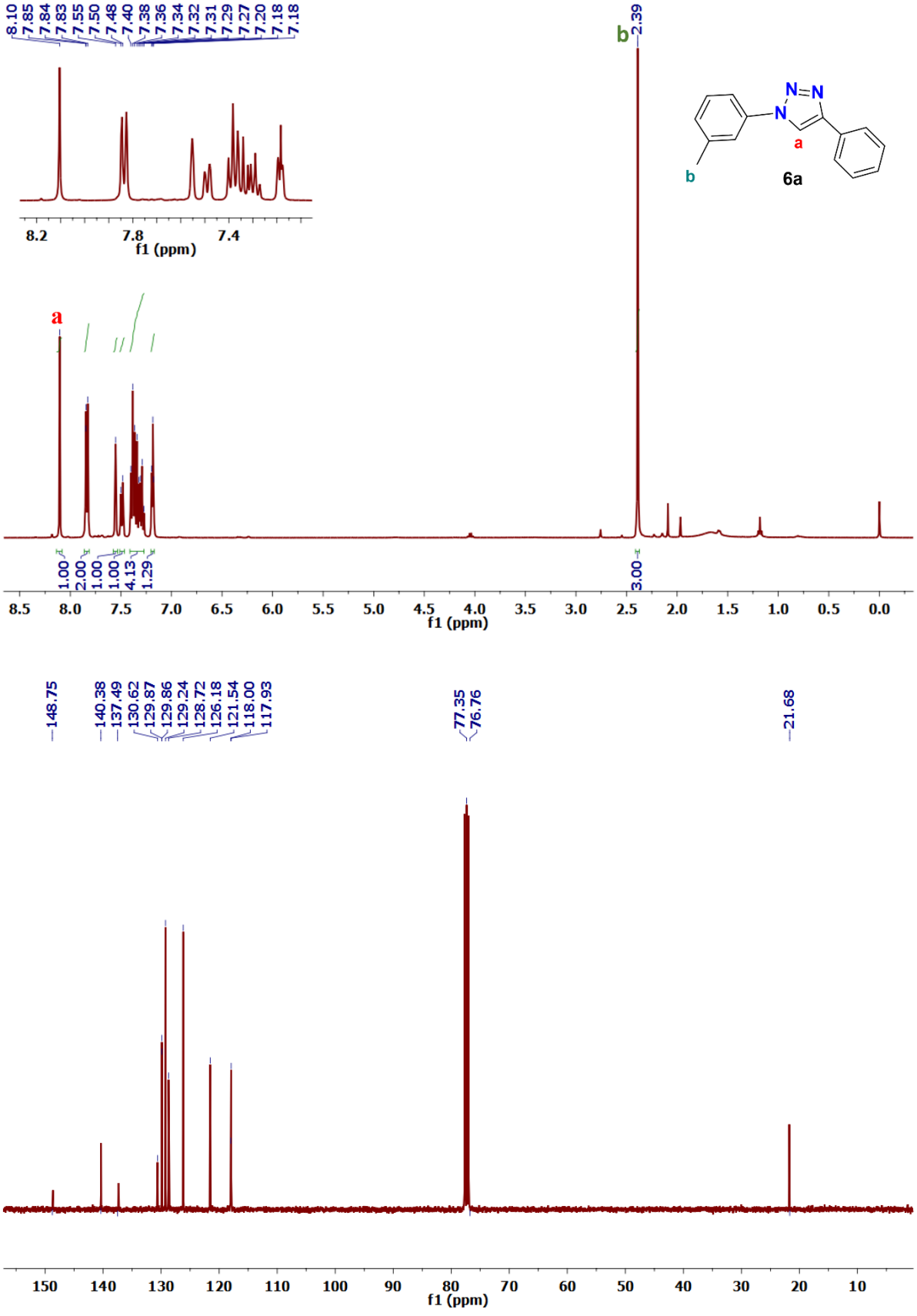


Figure S22: ^{1}H and ^{13}C NMR spectra of 1-(3-tolyl)-4-phenyl-1H-1,2,3-triazole (**6a**)

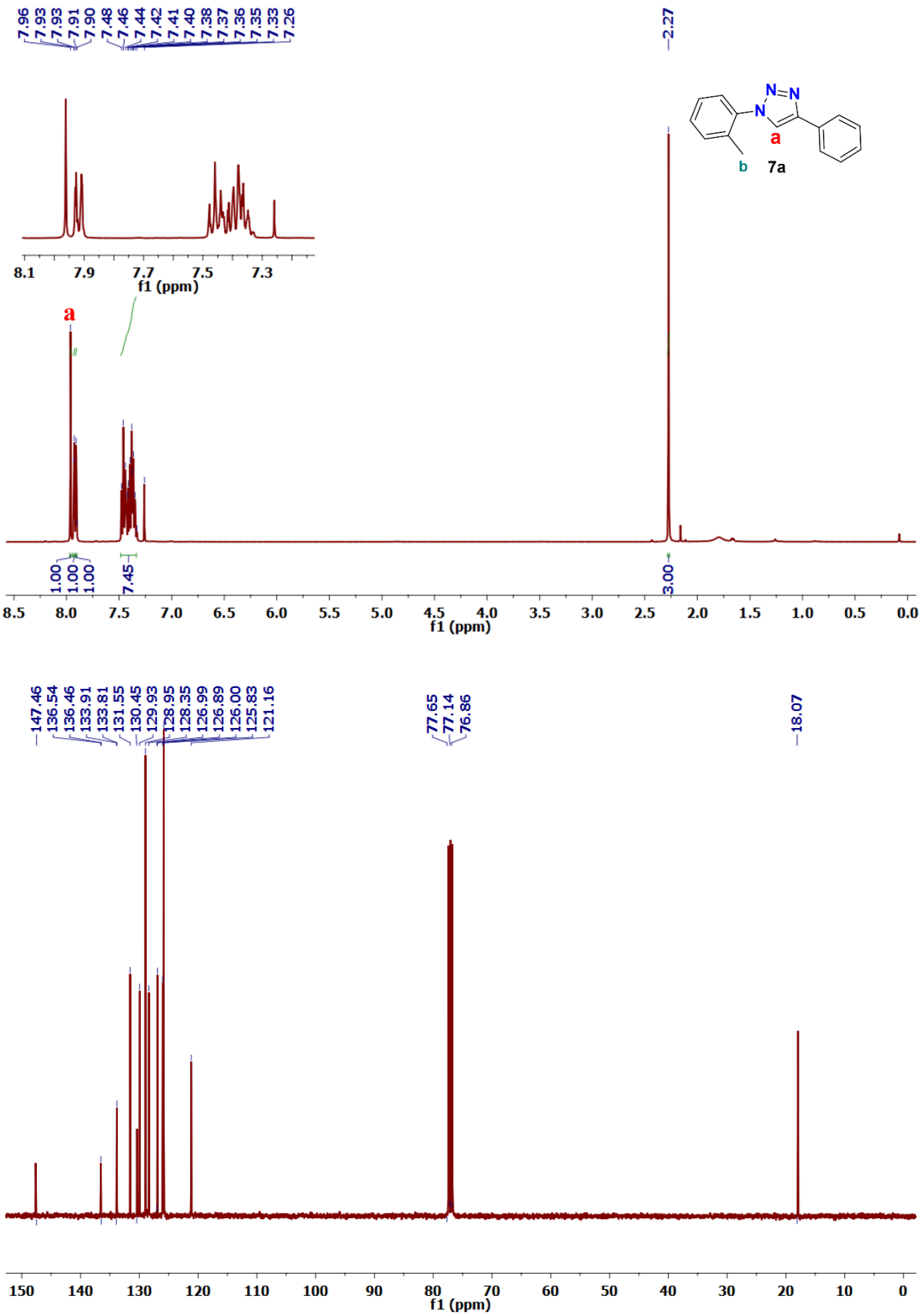


Figure S23: ^{1}H and ^{13}C NMR spectra of 1-(2-tolyl)-4-phenyl-1H-1,2,3-triazole (**7a**)

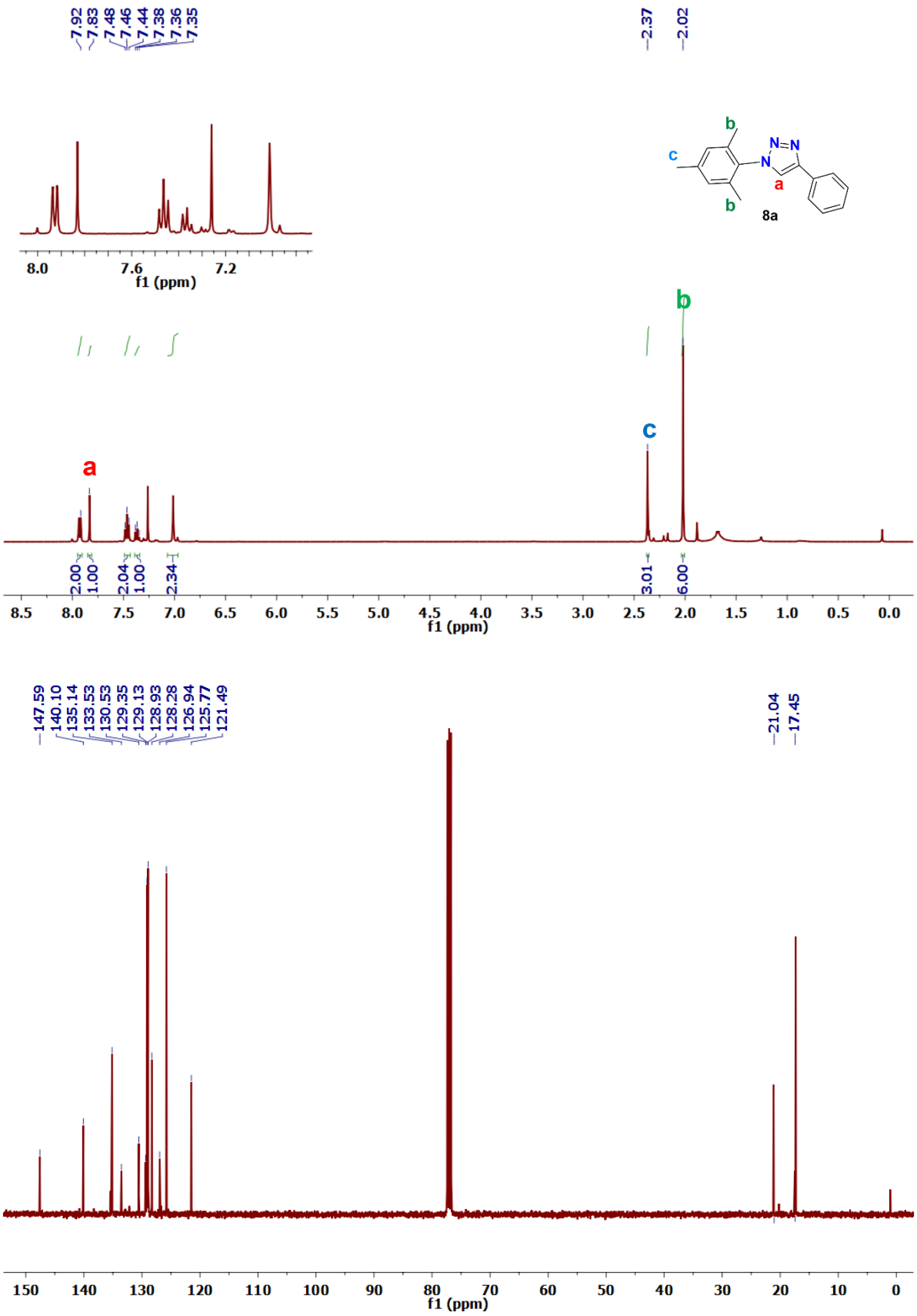


Figure S24: ^{1}H and ^{13}C NMR spectra of 1-(2,4,6-mesityl)-4-phenyl-1H-1,2,3-triazole (**8a**)

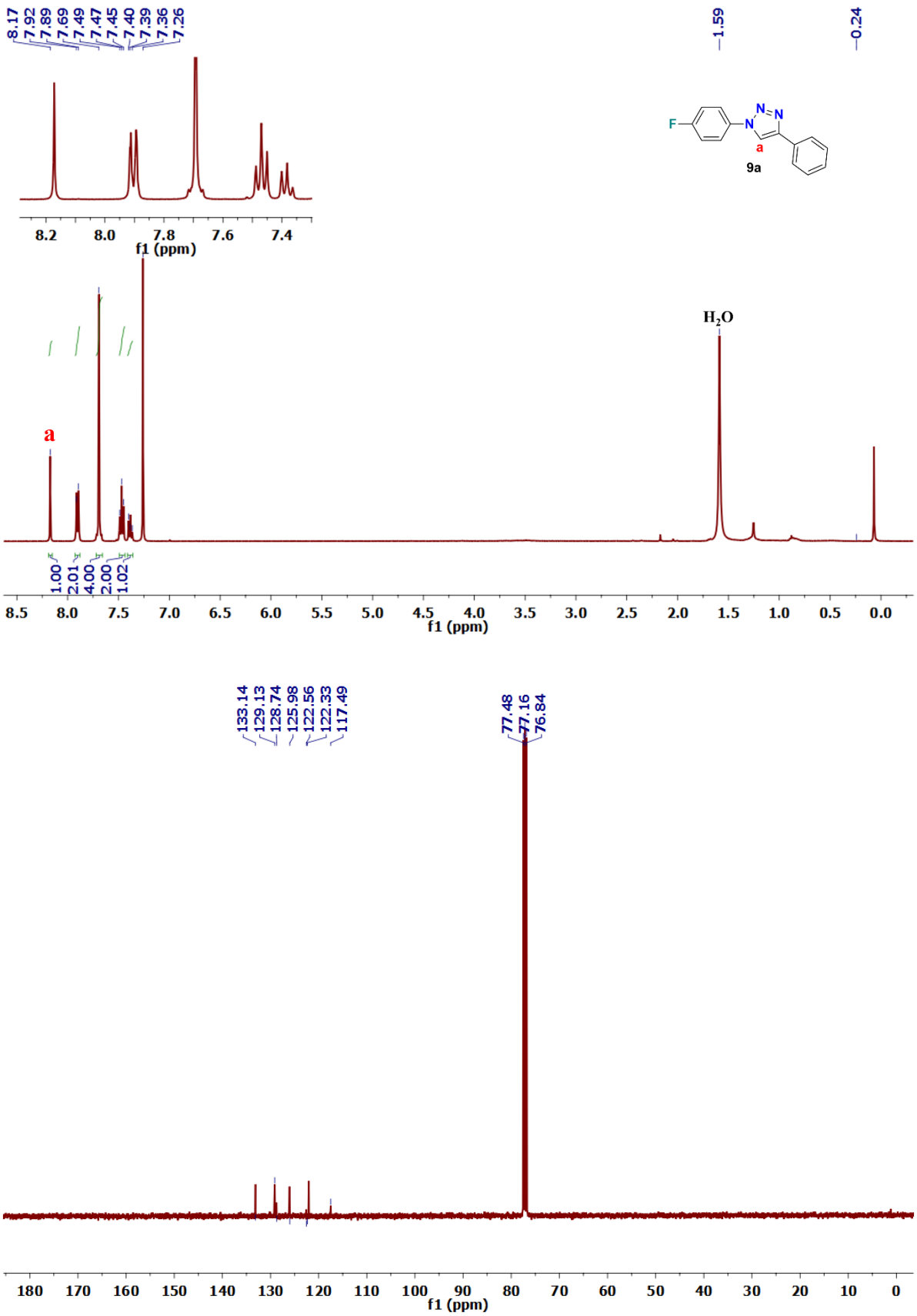


Figure S25: ^{1}H and ^{13}C NMR spectra of 1-(4-fluorophenyl)-4-phenyl-1H-1,2,3-triazole (**9a**)

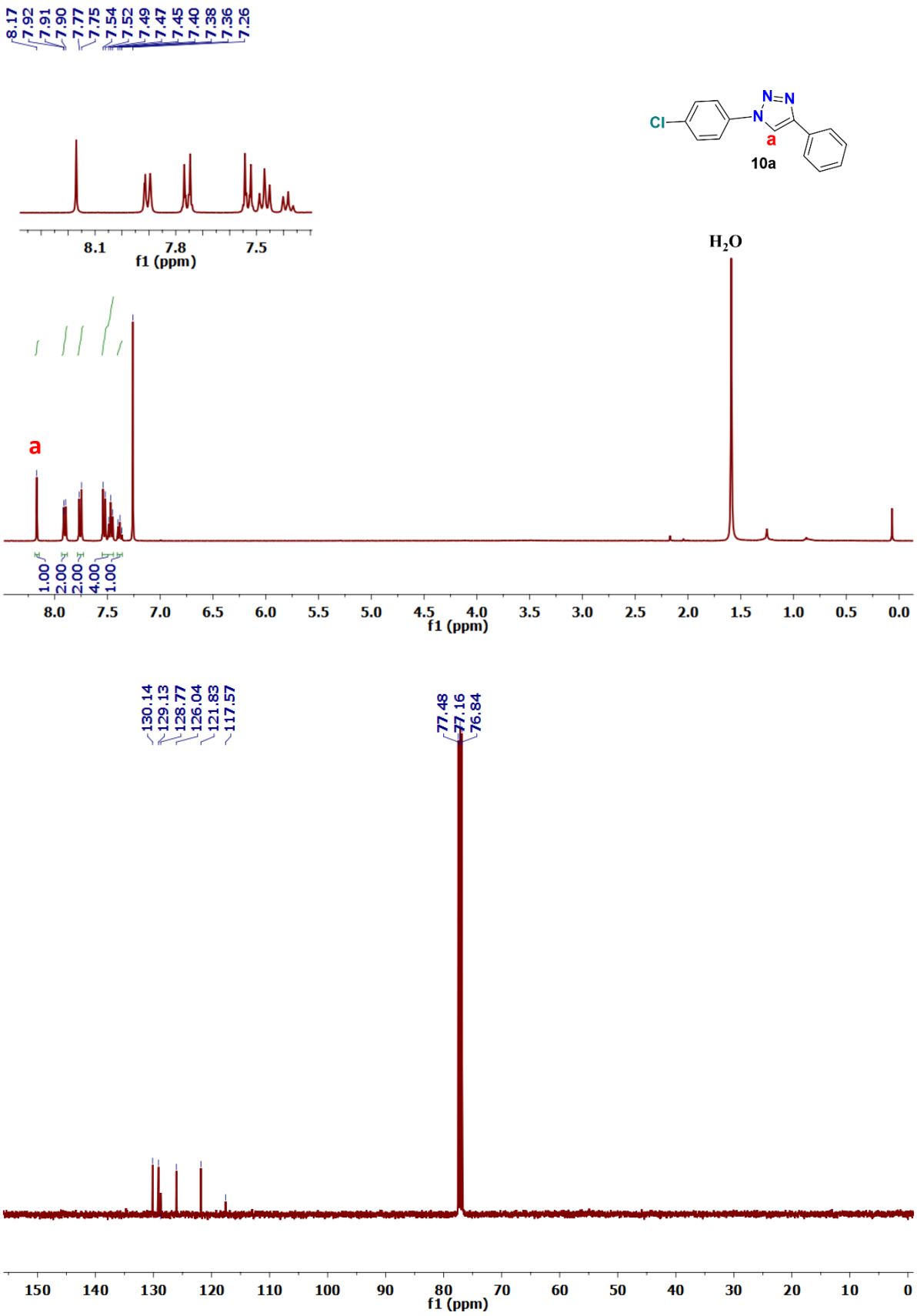


Figure S26: ^{1}H and ^{13}C NMR spectra of 1-(4-chlorophenyl)-4-phenyl-1H-1,2,3-triazole (**10a**)

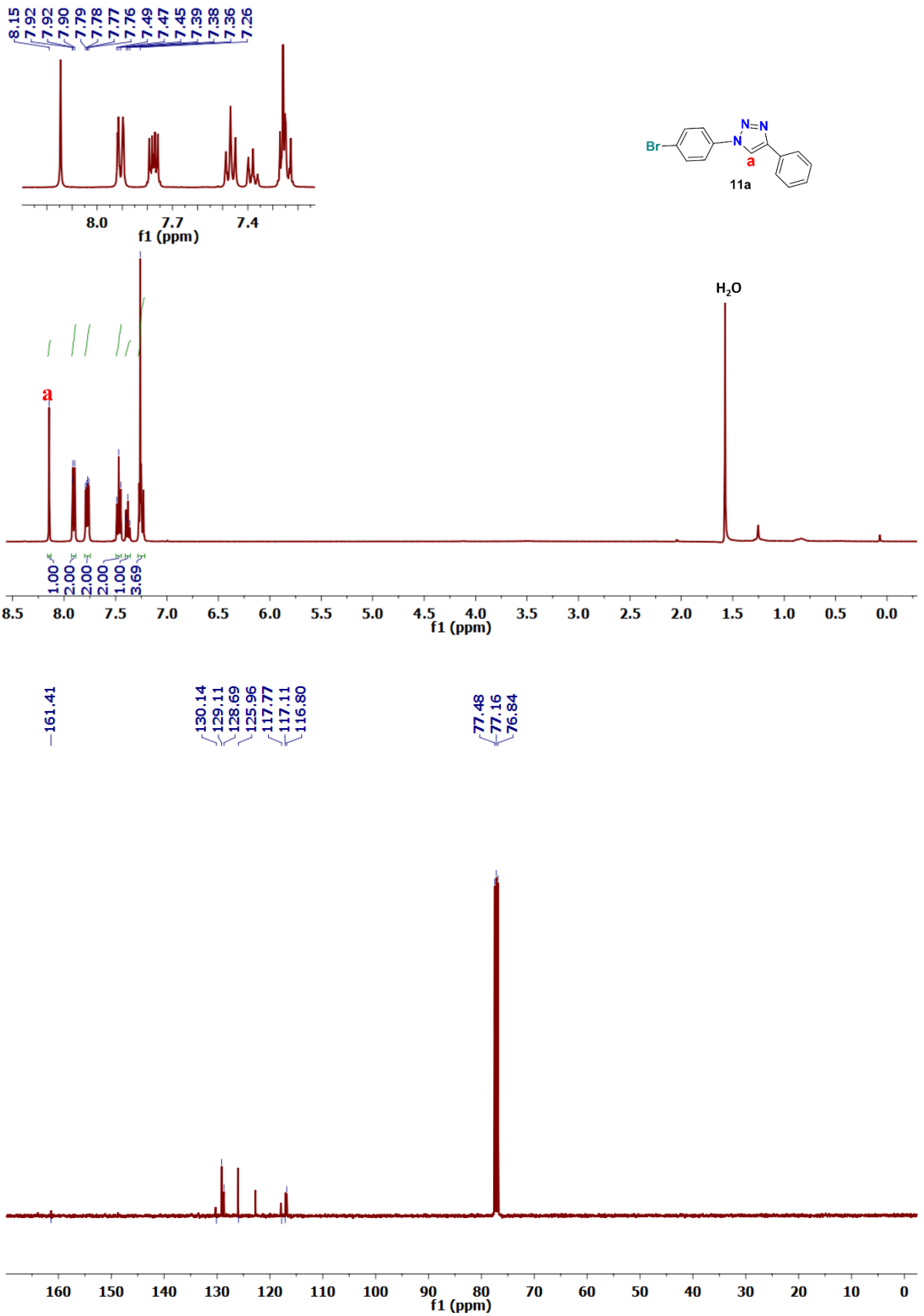


Figure S27: ^{1}H and ^{13}C NMR spectra of 1-(4-bromophenyl)-4-phenyl-1H-1,2,3-triazole (**11a**)

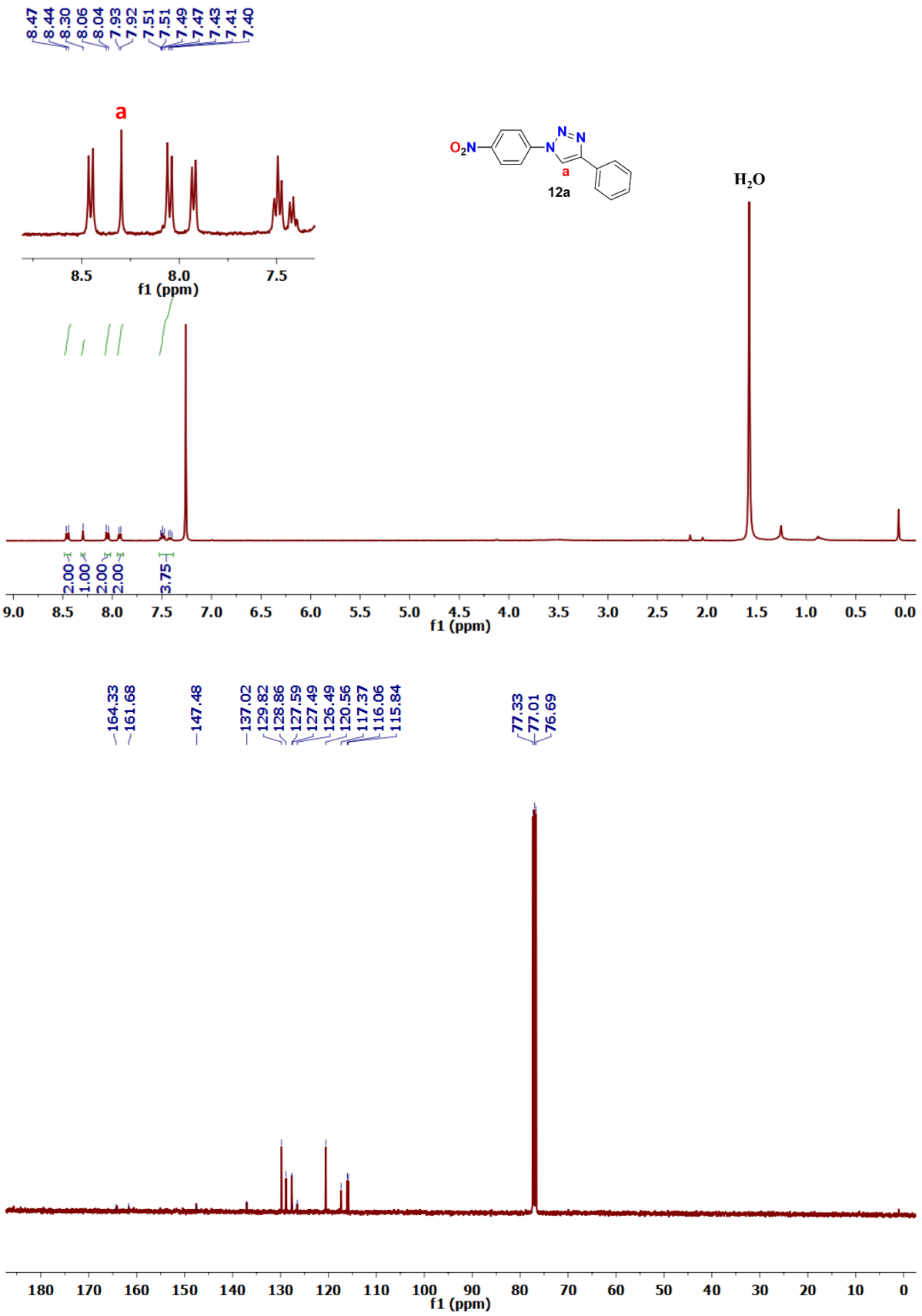


Figure S28: ^{1}H and ^{13}C NMR spectra of 1-(4-nitrophenyl)-4-phenyl-1H-1,2,3-triazole (**12a**)

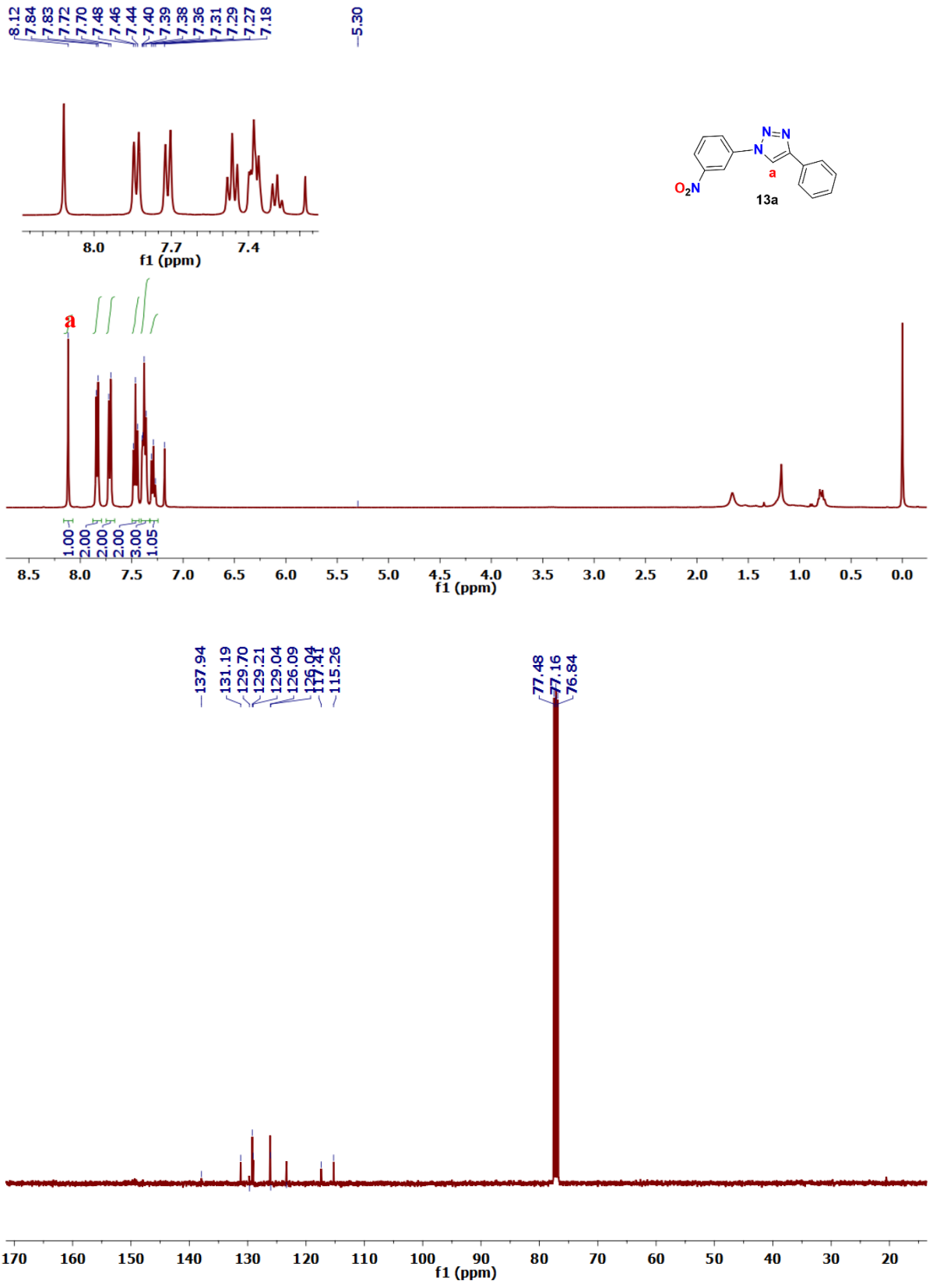


Figure S29: ^{1}H and ^{13}C NMR spectra of 1-(3-nitrophenyl)-4-phenyl-1H-1,2,3-triazole (**13a**)

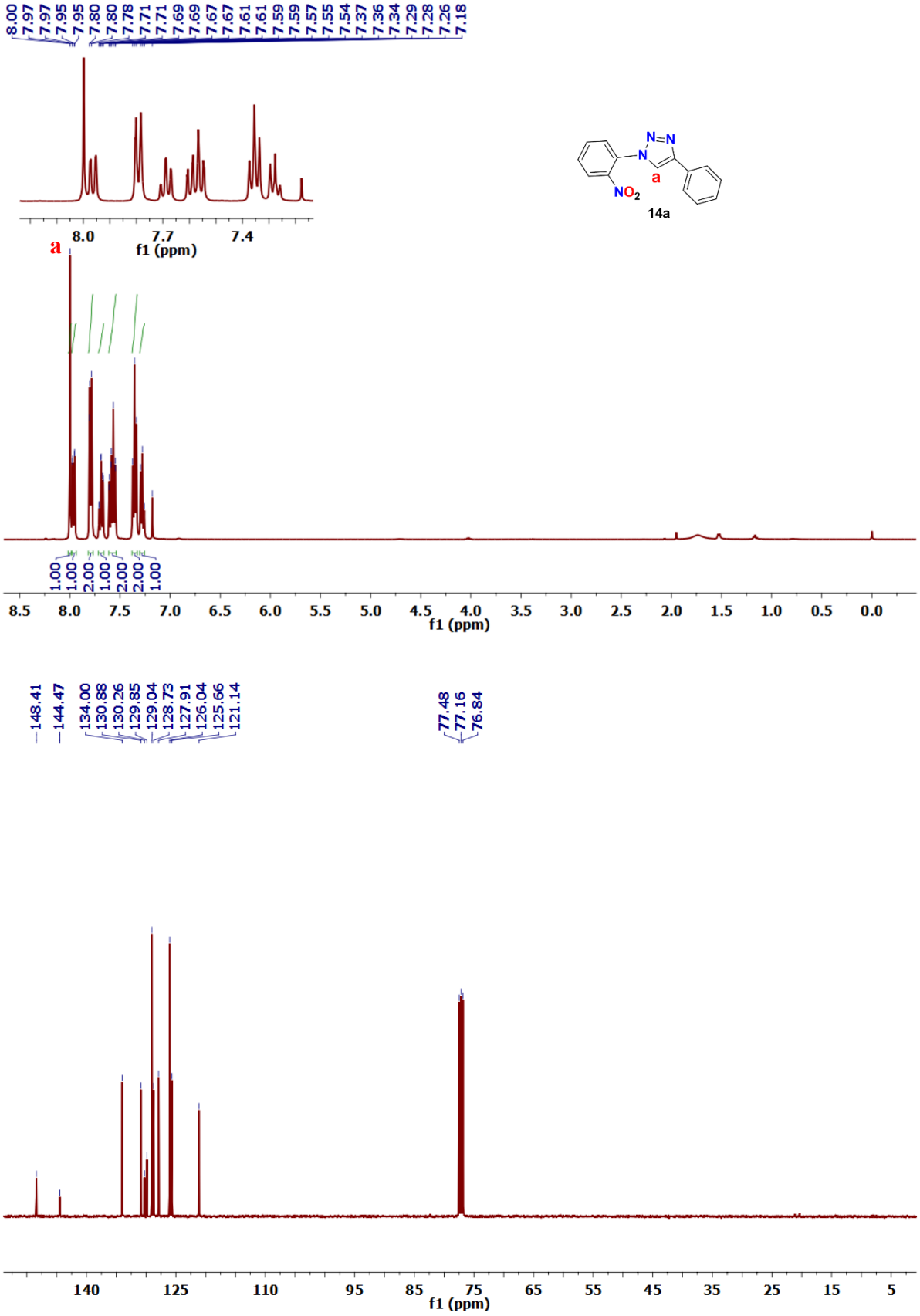


Figure S30: ^{1}H and ^{13}C NMR spectra of 1-(2-nitrophenyl)-4-phenyl-1H-1,2,3 triazole (**14a**)

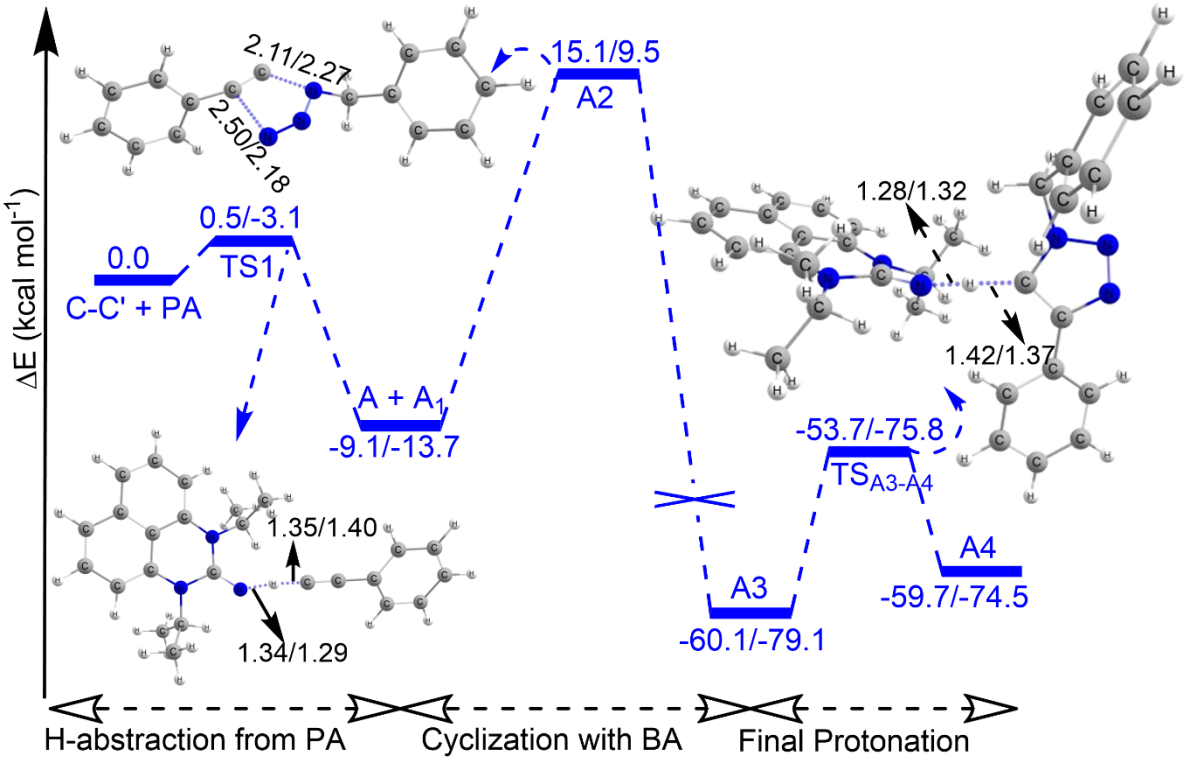


Figure S31: The potential energy profile and geometries of the transition states with important geometrical parameters

5. Computational Details

The Pka computed at the M062X/6-311++G** level of theory in the presence of water is considered as SMD solvation model.

Table ST5: Calculated p*K*a values	
Compound	**PKa**
Phenyl acetylene	20.1
C-C (Pre-catalyst)	30.4

The values from a benchmark study used to determine whether to use this method to calculate phenol's pka are as follows:

Method	**PKa**	**Expt**
S	12.6	9.95
B3LYP/6-31++G** SCRF (SMD)	10.6	
M062X/6-31++G** SCRF (SMD)	9.6	

The geometries have been optimized in two different density functional theory method (M062X and B3LYP) in combination with pople's split valance triple zeta basis set 6-311+G(d,p)[3]. M06-2X is a meta-GGA DFT functional with remarkable success in kinetic and thermodynamic calculations of the leading group elements.[4] B3LYP is the most popular DFT method consists of Becke's three-parameter hybrid exchange along with the Lee−Yang−Parr correlation.[5-7] Frequency calculations have also been performed to verify the stationary points as minima or transition states and to calculate free energy correction. Intrinsic reaction coordinate (IRC) analyses[8] were performed to confirm whether obtained transition states connect the exact minima. The self-consistent reaction field (SCRF), with solvation model density (SMD)[9], and polarizable continuum model (PCM)[10] were used to consider the influence of solvent dimethylsulphoxide on the reaction. All the computations were carried out using the Gaussian 16 program[11], and for the visualization and result analysis, Chemcraft software was used[12].

Thermochemistry and optimized coordinates of all the species computed at B3LYP/6-311+G** and M062X/6-311+G** level of theory.

B3LYP data:

C-C

Zero-point correction= 0.349425 (Hartree/Particle)
Thermal correction to Energy = 0.367838
Thermal correction to Enthalpy = 0.368783
Thermal correction to Gibbs Free Energy = 0.304098
Sum of electronic and zero-point Energies = -824.597336
Sum of electronic and thermal Energies = -824.578923
Sum of electronic and thermal Enthalpies = -824.577979
Sum of electronic and thermal Free Energies= -824.642664

C	-2.313318000	2.580296000	-0.605243000
C	-1.175972000	3.289766000	-0.301671000
C	0.020971000	2.597987000	0.018225000
C	0.010230000	1.170540000	0.019031000
C	-1.204722000	0.458013000	-0.192633000
C	-2.340652000	1.171449000	-0.550065000
H	1.244669000	4.355233000	0.339985000
H	-3.223580000	3.104103000	-0.875628000
H	-1.175314000	4.373778000	-0.309334000
C	1.230126000	3.271243000	0.334026000
C	1.216067000	0.447665000	0.228636000
H	-3.267945000	0.668024000	-0.766555000
C	2.364782000	1.138694000	0.582700000
C	2.359715000	2.548287000	0.634659000
H	3.282089000	0.616276000	0.801738000
H	3.277418000	3.060535000	0.901697000
C	-0.013282000	-1.662314000	0.094687000
N	-1.203307000	-0.925772000	0.045277000
N	1.184951000	-0.941348000	0.003137000
C	2.403656000	-1.692453000	-0.427673000
H	2.002488000	-2.592498000	-0.891833000
C	-2.462926000	-1.680653000	0.328048000
H	-2.091287000	-2.618834000	0.728597000
C	3.297541000	-2.140202000	0.738510000
H	4.045068000	-2.847233000	0.368983000
H	3.830255000	-1.309321000	1.203501000
H	2.714388000	-2.640651000	1.515158000
C	3.177818000	-0.985896000	-1.549170000
H	3.888022000	-1.701471000	-1.970899000
H	2.500552000	-0.673276000	-2.347261000
H	3.742384000	-0.116945000	-1.214673000
C	-3.243080000	-2.039767000	-0.943752000
H	-4.040637000	-2.742661000	-0.686961000
H	-3.706241000	-1.180137000	-1.430820000
H	-2.584760000	-2.527549000	-1.666081000

C	-3.316138000	-1.044003000	1.432967000
H	-2.701119000	-0.810269000	2.305730000
H	-3.839908000	-0.137743000	1.130892000
H	-4.069726000	-1.773596000	1.741258000
N	-0.084327000	-2.948623000	0.200178000
H	0.827069000	-3.367462000	0.334675000

C-C'

Zero-point correction= 0.334031 (Hartree/Particle)
Thermal correction to Energy = 0.352778
Thermal correction to Enthalpy = 0.353722
Thermal correction to Gibbs Free Energy = 0.287914
Sum of electronic and zero-point Energies = -824.087086
Sum of electronic and thermal Energies = -824.068339
Sum of electronic and thermal Enthalpies = -824.067395
Sum of electronic and thermal Free Energies = -824.133204

C	2.415685000	2.595805000	-0.027062000
C	1.234740000	3.300419000	-0.068140000
C	0.000001000	2.599613000	-0.064115000
C	0.000000000	1.166060000	-0.033795000
C	1.244070000	0.448489000	-0.002797000
C	2.433504000	1.192609000	0.007350000
H	-1.227303000	4.384568000	-0.092908000
H	3.363601000	3.125328000	-0.021921000
H	1.227308000	4.384566000	-0.092912000
C	-1.234736000	3.300420000	-0.068138000
C	-1.244070000	0.448491000	-0.002795000
H	3.388948000	0.698771000	0.037038000
C	-2.433503000	1.192613000	0.007353000
C	-2.415682000	2.595808000	-0.027058000
H	-3.388948000	0.698777000	0.037044000
H	-3.363598000	3.125333000	-0.021914000
C	-0.000001000	-1.720234000	-0.298660000
N	1.215538000	-0.931133000	0.019885000
N	-1.215540000	-0.931131000	0.019886000
C	-2.437293000	-1.758707000	0.118654000
H	-2.013671000	-2.762878000	0.102008000
C	2.437291000	-1.758708000	0.118657000
H	2.013669000	-2.762879000	0.102020000
C	-3.366491000	-1.698785000	-1.107427000
H	-4.086343000	-2.521390000	-1.048220000
H	-3.936055000	-0.772423000	-1.194616000
H	-2.787916000	-1.827911000	-2.025340000
C	-3.171136000	-1.595164000	1.458255000
H	-3.940134000	-2.369476000	1.540506000
H	-2.473736000	-1.727449000	2.290070000
H	-3.663363000	-0.629130000	1.582901000
C	3.171139000	-1.595157000	1.458254000
H	3.940136000	-2.369471000	1.540509000
H	3.663369000	-0.629125000	1.582893000

H	2.473741000	-1.727435000	2.290073000
C	3.366487000	-1.698795000	-1.107425000
H	2.787910000	-1.827918000	-2.025338000
H	3.936058000	-0.772436000	-1.194617000
H	4.086332000	-2.521405000	-1.048217000
N	-0.000004000	-2.892691000	-0.683447000

BA (benzyl azide)

Zero-point correction = 0.131665 (Hartree/Particle)
Thermal correction to Energy = 0.140118
Thermal correction to Enthalpy = 0.141062
Thermal correction to Gibbs Free Energy = 0.096436
Sum of electronic and zero-point Energies = -435.135950
Sum of electronic and thermal Energies = -435.127497
Sum of electronic and thermal Enthalpies = -435.126553
Sum of electronic and thermal Free Energies = -435.171179

C	-2.253531000	-0.796041000	-0.756280000
C	-1.016950000	-1.242356000	-0.296411000
C	-0.215763000	-0.418546000	0.504255000
C	-0.677747000	0.858734000	0.838134000
C	-1.917042000	1.307463000	0.378927000
C	-2.705959000	0.481648000	-0.419971000
H	-2.866486000	-1.444673000	-1.371889000
H	-0.670988000	-2.237290000	-0.556743000
H	-0.071701000	1.502903000	1.466696000
H	-2.264922000	2.298318000	0.648183000
H	-3.669792000	0.827955000	-0.775473000
C	1.135676000	-0.896450000	0.981099000
H	1.462321000	-0.330521000	1.857601000
H	1.105708000	-1.951319000	1.247292000
N	2.196036000	-0.815487000	-0.076191000
N	2.499316000	0.311274000	-0.454349000
N	2.859471000	1.299630000	-0.882915000

A3

Zero-point correction = 0.234901 (Hartree/Particle)
Thermal correction to Energy = 0.248853
Thermal correction to Enthalpy = 0.249798
Thermal correction to Gibbs Free Energy = 0.190622
Sum of electronic and zero-point Energies = -743.094268
Sum of electronic and thermal Energies = -743.080316
Sum of electronic and thermal Enthalpies = -743.079372
Sum of electronic and thermal Free Energies = -743.138547

C	4.753645000	1.419732000	-0.295521000
C	3.840309000	0.669516000	-1.039119000
C	2.976830000	-0.232498000	-0.411679000
C	3.041964000	-0.369617000	0.980240000
C	3.948899000	0.380719000	1.725879000

C	4.809749000	1.278016000	1.089847000
H	5.414501000	2.116918000	-0.798749000
H	3.797513000	0.790050000	-2.116877000
H	2.374861000	-1.064070000	1.479550000
H	3.986267000	0.264617000	2.803540000
H	5.515208000	1.861810000	1.670445000
C	2.013897000	-1.069536000	-1.234202000
H	2.029408000	-0.736407000	-2.272284000
H	2.320284000	-2.118745000	-1.213928000
N	0.633858000	-1.025698000	-0.761550000
N	0.178784000	-2.084949000	-0.011051000
N	-1.049910000	-1.796038000	0.305040000
C	-3.060801000	1.225540000	-0.649200000
C	-2.705423000	0.005195000	-0.044377000
C	-3.678098000	-0.635331000	0.746909000
C	-4.944138000	-0.080956000	0.924007000
C	-5.280054000	1.130806000	0.317246000
C	-4.326303000	1.778977000	-0.470970000
H	-2.327463000	1.733499000	-1.263871000
H	-3.429537000	-1.575088000	1.224776000
H	-5.672518000	-0.598064000	1.540286000
H	-6.265419000	1.561662000	0.455537000
H	-4.570336000	2.721161000	-0.951041000
C	-1.367096000	-0.572540000	-0.236263000
C	-0.275363000	-0.029782000	-0.950207000

A4

Zero-point correction = 0.248442 (Hartree/Particle)
Thermal correction to Energy = 0.262552
Thermal correction to Enthalpy = 0.263496
Thermal correction to Gibbs Free Energy = 0.202966
Sum of electronic and zero-point Energies = -743.603633
Sum of electronic and thermal Energies = -743.589523
Sum of electronic and thermal Enthalpies = -743.588579
Sum of electronic and thermal Free Energies = -743.649109

C	-4.406934000	1.652920000	0.401351000
C	-3.554249000	0.770323000	1.066685000
C	-2.977525000	-0.305544000	0.387506000
C	-3.267271000	-0.489926000	-0.969645000
C	-4.114552000	0.392087000	-1.635737000
C	-4.686781000	1.466342000	-0.950930000
H	-4.849295000	2.483329000	0.939788000
H	-3.339052000	0.919692000	2.119532000
H	-2.829141000	-1.325405000	-1.505419000
H	-4.332891000	0.239449000	-2.686594000
H	-5.348260000	2.151002000	-1.469455000
C	-2.059685000	-1.267405000	1.113865000
H	-2.065629000	-1.072168000	2.186594000
H	-2.363837000	-2.302018000	0.954241000
N	-0.667707000	-1.194966000	0.647799000

N	-0.141531000	-2.189985000	-0.089155000
N	1.086098000	-1.858879000	-0.382081000
C	2.877004000	1.345125000	0.397726000
C	2.682346000	0.009728000	0.012730000
C	3.768851000	-0.701309000	-0.519404000
C	5.013561000	-0.092907000	-0.660272000
C	5.198100000	1.234255000	-0.270909000
C	4.123796000	1.949715000	0.259266000
H	2.051464000	1.920376000	0.801090000
H	3.631493000	-1.732978000	-0.818129000
H	5.842124000	-0.657947000	-1.072402000
H	6.167800000	1.706220000	-0.379984000
H	4.254500000	2.982599000	0.561669000
C	1.371448000	-0.636976000	0.161761000
C	0.236667000	-0.207005000	0.828379000
H	0.014050000	0.678125000	1.398902000

PA (phenylacetylene)

Zero-point correction = 0.109099 (Hartree/Particle)
Thermal correction to Energy = 0.115526
Thermal correction to Enthalpy = 0.116470
Thermal correction to Gibbs Free Energy = 0.078666
Sum of electronic and zero-point Energies = -308.372595
Sum of electronic and thermal Energies = -308.366168
Sum of electronic and thermal Enthalpies = -308.365224
Sum of electronic and thermal Free Energies = -308.403028

C	-0.119161000	-1.212383000	0.000027000
C	0.593029000	-0.000014000	0.000055000
C	-0.119133000	1.212372000	0.000027000
C	-1.510610000	1.207654000	-0.000027000
C	-2.210103000	0.000018000	-0.000055000
C	-1.510638000	-1.207634000	-0.000026000
H	0.424323000	-2.149569000	0.000051000
H	0.424373000	2.149545000	0.000051000
H	-2.049452000	2.148114000	-0.000047000
H	-3.293961000	0.000031000	-0.000099000
H	-2.049501000	-2.148082000	-0.000047000
C	2.022730000	-0.000026000	0.000137000
C	3.229030000	-0.000024000	0.000070000
H	4.293358000	0.000186000	-0.001155000

A_1

Zero-point correction= 0.097215 (Hartree/Particle)
Thermal correction to Energy= 0.103458
Thermal correction to Enthalpy= 0.104402
Thermal correction to Gibbs Free Energy= 0.066858
Sum of electronic and zero-point Energies= -307.876782
Sum of electronic and thermal Energies= -307.870539
Sum of electronic and thermal Enthalpies= -307.869595

Sum of electronic and thermal Free Energies= -307.907139

C	-0.048411000	-1.206744000	-0.000002000
C	0.685112000	0.000000000	0.000017000
C	-0.048411000	1.206744000	-0.000002000
C	-1.440911000	1.204379000	-0.000041000
C	-2.147793000	0.000000000	-0.000060000
C	-1.440911000	-1.204379000	-0.000041000
H	0.490415000	-2.147421000	0.000013000
H	0.490415000	2.147421000	0.000013000
H	-1.977262000	2.147467000	-0.000055000
H	-3.231920000	0.000000000	-0.000090000
H	-1.977262000	-2.147467000	-0.000055000
C	2.116839000	0.000000000	0.000060000
C	3.358755000	0.000000000	0.000099000

TS1

Zero-point correction = 0.440632 (Hartree/Particle)
Thermal correction to Energy = 0.467395
Thermal correction to Enthalpy = 0.468339
Thermal correction to Gibbs Free Energy = 0.379365
Sum of electronic and zero-point Energies = -1132.458785
Sum of electronic and thermal Energies = -1132.432022
Sum of electronic and thermal Enthalpies = -1132.431078
Sum of electronic and thermal Free Energies = -1132.520052

C	-5.640659000	0.943951000	-0.636984000
C	-5.741910000	-0.426461000	-0.677313000
C	-4.592221000	-1.221964000	-0.434174000
C	-3.339084000	-0.584279000	-0.156852000
C	-3.254760000	0.845667000	-0.124043000
C	-4.418946000	1.582673000	-0.365370000
H	-5.616771000	-3.116621000	-0.657273000
H	-6.515828000	1.559094000	-0.820571000
H	-6.687218000	-0.914170000	-0.887515000
C	-4.666493000	-2.639002000	-0.446173000
C	-2.175930000	-1.376287000	0.110833000
H	-4.401497000	2.658127000	-0.356114000
C	-2.304500000	-2.768248000	0.089565000
C	-3.539033000	-3.380693000	-0.185916000
H	-1.457356000	-3.403509000	0.277400000
H	-3.587849000	-4.464899000	-0.192742000
C	-0.777397000	0.684202000	0.119974000
N	-2.027283000	1.432628000	0.140662000
N	-0.975478000	-0.728975000	0.376738000
C	0.252587000	-1.461438000	0.776471000
H	0.959317000	-0.659036000	0.964724000
C	-1.855142000	2.900193000	0.277847000
H	-0.796371000	2.974451000	0.517043000
C	0.880942000	-2.306394000	-0.344364000
H	1.879645000	-2.624386000	-0.033083000
H	0.312441000	-3.202602000	-0.595214000

H	0.991060000	-1.707040000	-1.250566000
C	0.099986000	-2.208101000	2.111738000
H	1.089265000	-2.536645000	2.442999000
H	-0.302775000	-1.537604000	2.875507000
H	-0.540258000	-3.089046000	2.063965000
C	-2.623009000	3.490397000	1.470374000
H	-2.273492000	4.513158000	1.639877000
H	-3.704619000	3.531813000	1.336632000
H	-2.416694000	2.913218000	2.375793000
C	-2.026680000	3.685004000	-1.033122000
H	-1.405645000	3.243019000	-1.815775000
H	-3.053569000	3.728187000	-1.398427000
H	-1.688265000	4.714245000	-0.878937000
N	0.327929000	1.246991000	-0.030606000
C	6.093339000	-0.928696000	-0.742716000
C	5.566606000	0.265269000	-0.210299000
C	6.471556000	1.229290000	0.277689000
C	7.845006000	1.005687000	0.234486000
C	8.351219000	-0.182313000	-0.295914000
C	7.467746000	-1.146884000	-0.783702000
H	5.412786000	-1.681626000	-1.123105000
H	6.084889000	2.153881000	0.690492000
H	8.522522000	1.761750000	0.616010000
H	9.421016000	-0.354275000	-0.328718000
H	7.850400000	-2.073265000	-1.198006000
C	4.154039000	0.492127000	-0.166885000
C	2.943847000	0.686453000	-0.131460000
H	1.622029000	0.878359000	-0.074088000

A2 (Cyclization transition state)

Zero-point correction = 0.228611 (Hartree/Particle)
Thermal correction to Energy = 0.244183
Thermal correction to Enthalpy = 0.245128
Thermal correction to Gibbs Free Energy = 0.181749
Sum of electronic and zero-point Energies = -742.974256
Sum of electronic and thermal Energies = -742.958683
Sum of electronic and thermal Enthalpies = -742.957739
Sum of electronic and thermal Free Energies = -743.021117

C	-5.047873000	-1.333538000	0.225688000
C	-3.837691000	-1.111231000	-0.427754000
C	-3.279638000	0.172308000	-0.482252000
C	-3.962934000	1.228291000	0.128082000
C	-5.177052000	1.009986000	0.782007000
C	-5.721974000	-0.272074000	0.833960000
H	-5.468348000	-2.332706000	0.257124000
H	-3.319304000	-1.939637000	-0.899627000
H	-3.544053000	2.228836000	0.090811000
H	-5.694766000	1.840625000	1.248944000
H	-6.664843000	-0.444172000	1.340843000
C	-1.958114000	0.409614000	-1.184184000

H	-1.947741000	-0.094843000	-2.151820000
H	-1.815091000	1.480295000	-1.365441000
N	-0.797545000	-0.159549000	-0.478128000
N	-0.389098000	0.435450000	0.566810000
N	0.607386000	0.624519000	1.147901000
C	3.864823000	-1.231926000	0.408585000
C	3.221426000	-0.190181000	-0.296610000
C	3.960864000	0.992862000	-0.520478000
C	5.271394000	1.121649000	-0.068951000
C	5.890892000	0.079326000	0.624667000
C	5.175419000	-1.097500000	0.858263000
H	3.320251000	-2.149888000	0.599603000
H	3.491275000	1.810913000	-1.055136000
H	5.812902000	2.042503000	-0.259686000
H	6.910948000	0.182351000	0.976912000
H	5.641473000	-1.917152000	1.395423000
C	1.878433000	-0.332362000	-0.775270000
C	0.944041000	-0.613568000	-1.578089000

$TS_{A3\text{-}A4}$

Zero-point correction = 0.579109 (Hartree/Particle)
Thermal correction to Energy = 0.613595
Thermal correction to Enthalpy = 0.614539
Thermal correction to Gibbs Free Energy = 0.505858
Sum of electronic and zero-point Energies = -1567.681181
Sum of electronic and thermal Energies = -1567.646695
Sum of electronic and thermal Enthalpies = -1567.645750
Sum of electronic and thermal Free Energies = -1567.754432

C	5.894671000	-1.514276000	1.134366000
C	6.268381000	-1.058394000	-0.107366000
C	5.332662000	-0.350172000	-0.904926000
C	4.007502000	-0.127742000	-0.406864000
C	3.636853000	-0.617844000	0.886769000
C	4.598808000	-1.302630000	1.635303000
H	6.695349000	-0.016137000	-2.554052000
H	6.605274000	-2.054658000	1.751533000
H	7.269283000	-1.225073000	-0.489463000
C	5.691801000	0.155480000	-2.181105000
C	3.061420000	0.605282000	-1.192092000
H	4.364178000	-1.691418000	2.610280000
C	3.466663000	1.084573000	-2.440156000
C	4.768643000	0.857016000	-2.918646000
H	2.788072000	1.634622000	-3.067352000
H	5.035967000	1.247782000	-3.895152000
C	1.283397000	0.083986000	0.466414000
N	2.342745000	-0.397459000	1.335691000
N	1.783380000	0.806655000	-0.680283000
C	0.791360000	1.690687000	-1.345347000
H	-0.042112000	1.682051000	-0.650279000
C	1.885078000	-0.809360000	2.687247000

H	0.857860000	-0.451857000	2.688254000
C	0.230286000	1.143514000	-2.668708000
H	-0.658016000	1.719495000	-2.941886000
H	0.928373000	1.201184000	-3.504324000
H	-0.072524000	0.101432000	-2.550246000
C	1.256341000	3.153564000	-1.426821000
H	0.410748000	3.772294000	-1.740063000
H	1.580567000	3.502758000	-0.443090000
H	2.069705000	3.324833000	-2.132048000
C	2.612092000	-0.072658000	3.822400000
H	2.076344000	-0.257636000	4.758139000
H	3.647835000	-0.379545000	3.971983000
H	2.602380000	1.005385000	3.640360000
C	1.782089000	-2.330516000	2.884191000
H	1.203154000	-2.773761000	2.070554000
H	2.743899000	-2.842501000	2.934045000
H	1.252399000	-2.532564000	3.820145000
N	0.075995000	-0.071606000	0.762125000
H	-1.039671000	0.186238000	0.174465000
C	-4.201278000	-5.185924000	-0.903187000
C	-3.615504000	-4.100123000	-1.556806000
C	-3.123528000	-3.011765000	-0.831656000
C	-3.230806000	-3.025348000	0.563912000
C	-3.819365000	-4.105335000	1.218509000
C	-4.305694000	-5.190759000	0.486612000
H	-4.579744000	-6.021931000	-1.480831000
H	-3.543733000	-4.099642000	-2.639655000
H	-2.855393000	-2.184821000	1.137558000
H	-3.896962000	-4.101835000	2.300145000
H	-4.763384000	-6.030916000	0.996634000
C	-2.452634000	-1.856148000	-1.551916000
H	-1.381606000	-1.849657000	-1.342886000
H	-2.584392000	-1.962842000	-2.629939000
N	-2.955127000	-0.542799000	-1.154516000
N	-4.181601000	-0.146923000	-1.596659000
N	-4.400494000	1.027187000	-1.073591000
C	-2.230399000	2.929308000	1.323478000
C	-3.278658000	2.651924000	0.427481000
C	-4.274115000	3.630019000	0.255172000
C	-4.222330000	4.836101000	0.950745000
C	-3.175340000	5.099178000	1.835807000
C	-2.179746000	4.136868000	2.015851000
H	-1.454063000	2.187765000	1.475851000
H	-5.089038000	3.437101000	-0.431850000
H	-5.002527000	5.574712000	0.799548000
H	-3.135817000	6.038231000	2.376332000
H	-1.360763000	4.326253000	2.701784000
C	-3.324138000	1.375953000	-0.299261000
C	-2.355500000	0.360421000	-0.336712000

M062X Data:

C-C

Zero-point correction = 0.353246 (Hartree/Particle)
Thermal correction to Energy = 0.371364
Thermal correction to Enthalpy = 0.372309
Thermal correction to Gibbs Free Energy = 0.308412
Sum of electronic and zero-point Energies = -824.256814
Sum of electronic and thermal Energies = -824.238696
Sum of electronic and thermal Enthalpies = -824.237751
Sum of electronic and thermal Free Energies = -824.301648

C	-2.316344000	2.554651000	-0.629067000
C	-1.188992000	3.269277000	-0.319128000
C	0.008308000	2.582863000	0.010358000
C	0.002857000	1.165064000	0.015286000
C	-1.205987000	0.445935000	-0.197165000
C	-2.339635000	1.144498000	-0.568340000
H	1.220499000	4.345904000	0.335370000
H	-3.226611000	3.072892000	-0.909616000
H	-1.189926000	4.353456000	-0.329155000
C	1.212060000	3.261653000	0.332923000
C	1.207351000	0.443464000	0.231049000
H	-3.261695000	0.633663000	-0.795459000
C	2.347914000	1.132031000	0.594561000
C	2.336313000	2.542837000	0.644741000
H	3.265055000	0.611378000	0.822537000
H	3.250492000	3.057419000	0.919018000
C	-0.007609000	-1.662618000	0.064434000
N	-1.193443000	-0.929917000	0.057389000
N	1.181667000	-0.938322000	-0.008638000
C	2.405886000	-1.667964000	-0.432481000
H	2.025939000	-2.541694000	-0.960009000
C	-2.441467000	-1.672895000	0.371617000
H	-2.079577000	-2.575028000	0.855856000
C	3.249922000	-2.160235000	0.742026000
H	4.045911000	-2.806665000	0.363881000
H	3.716272000	-1.336918000	1.285178000
H	2.649122000	-2.738078000	1.448317000
C	3.226728000	-0.907298000	-1.475025000
H	3.862789000	-1.633960000	-1.985567000
H	2.576038000	-0.445166000	-2.221034000
H	3.876210000	-0.142952000	-1.051716000
C	-3.190678000	-2.115298000	-0.882995000
H	-4.034335000	-2.746656000	-0.591830000
H	-3.583648000	-1.276024000	-1.459120000
H	-2.535391000	-2.701990000	-1.530371000
C	-3.328015000	-0.961569000	1.395058000
H	-2.725092000	-0.529094000	2.197353000
H	-3.959835000	-0.181225000	0.973480000
H	-3.986909000	-1.712022000	1.838241000

N	-0.076204000	-2.946904000	0.119908000
H	0.838891000	-3.367608000	0.226916000

C-C'

Zero-point correction = 0.338379 (Hartree/Particle)
Thermal correction to Energy = 0.356842
Thermal correction to Enthalpy = 0.357786
Thermal correction to Gibbs Free Energy= 0.292601
Sum of electronic and zero-point Energies= -823.747609
Sum of electronic and thermal Energies= -823.729147
Sum of electronic and thermal Enthalpies= -823.728202
Sum of electronic and thermal Free Energies= -823.793387

C	2.409407000	2.579470000	-0.052692000
C	1.233279000	3.283347000	-0.089217000
C	-0.000011000	2.581520000	-0.076664000
C	-0.000005000	1.157660000	-0.033655000
C	1.241768000	0.438662000	0.002939000
C	2.428845000	1.175470000	-0.006258000
H	-1.223027000	4.366987000	-0.123445000
H	3.357580000	3.107455000	-0.062008000
H	1.222986000	4.366999000	-0.123453000
C	-1.233309000	3.283335000	-0.089207000
C	-1.241770000	0.438651000	0.002948000
H	3.385683000	0.683270000	0.010284000
C	-2.428854000	1.175448000	-0.006240000
C	-2.409429000	2.579447000	-0.052674000
H	-3.385687000	0.683237000	0.010307000
H	-3.357608000	3.107423000	-0.061983000
C	0.000007000	-1.699982000	-0.322731000
N	1.203070000	-0.935771000	0.047602000
N	-1.203061000	-0.935782000	0.047601000
C	-2.420326000	-1.756472000	0.165081000
H	-2.014617000	-2.764274000	0.228080000
C	2.420339000	-1.756455000	0.165097000
H	2.014633000	-2.764254000	0.228146000
C	-3.311793000	-1.752062000	-1.080569000
H	-4.072919000	-2.530561000	-0.975252000
H	-3.828705000	-0.806785000	-1.248695000
H	-2.718557000	-1.980986000	-1.968885000
C	-3.191104000	-1.512334000	1.465078000
H	-3.882118000	-2.345718000	1.618253000
H	-2.503252000	-1.487153000	2.314190000
H	-3.780531000	-0.595582000	1.474804000
C	3.191139000	-1.512262000	1.465073000
H	3.882140000	-2.345649000	1.618281000
H	3.780582000	-0.595519000	1.474742000
H	2.503299000	-1.487025000	2.314193000
C	3.311791000	-1.752100000	-1.080564000
H	2.718543000	-1.981055000	-1.968864000
H	3.828707000	-0.806835000	-1.248733000

H	4.072912000	-2.530601000	-0.975226000
N	0.000009000	-2.842938000	-0.779376000

BA (benzyl azide)

Zero-point correction = 0.133127 (Hartree/Particle)
Thermal correction to Energy = 0.141483
Thermal correction to Enthalpy = 0.142427
Thermal correction to Gibbs Free Energy = 0.098305
Sum of electronic and zero-point Energies = -434.945350
Sum of electronic and thermal Energies = -434.936994
Sum of electronic and thermal Enthalpies = -434.936050
Sum of electronic and thermal Free Energies = -434.980171

C	-2.251752000	-0.749169000	-0.716567000
C	-1.027536000	-1.267807000	-0.309459000
C	-0.164684000	-0.504021000	0.479793000
C	-0.540847000	0.788133000	0.850361000
C	-1.766559000	1.309385000	0.441707000
C	-2.622736000	0.541270000	-0.341493000
H	-2.918433000	-1.350913000	-1.323812000
H	-0.736252000	-2.272299000	-0.600085000
H	0.125128000	1.382914000	1.468344000
H	-2.052352000	2.312258000	0.737919000
H	-3.578297000	0.944343000	-0.657200000
C	1.184970000	-1.042801000	0.873556000
H	1.530582000	-0.587314000	1.805128000
H	1.161181000	-2.123499000	0.992403000
N	2.207623000	-0.800357000	-0.190721000
N	2.350282000	0.385225000	-0.467620000
N	2.528281000	1.450071000	-0.783100000

A3

Zero-point correction = 0.238016 (Hartree/Particle)
Thermal correction to Energy = 0.251750
Thermal correction to Enthalpy = 0.252695
Thermal correction to Gibbs Free Energy = 0.194443
Sum of electronic and zero-point Energies = -742.797255
Sum of electronic and thermal Energies = -742.783520
Sum of electronic and thermal Enthalpies = -742.782576
Sum of electronic and thermal Free Energies = -742.840827

C	5.182049000	0.631454000	-0.341161000
C	4.276678000	-0.334961000	-0.763945000
C	2.958450000	-0.327213000	-0.300850000
C	2.560251000	0.665821000	0.591889000
C	3.467667000	1.636404000	1.015637000
C	4.778939000	1.622935000	0.552390000
H	6.201461000	0.613261000	-0.710132000
H	4.591788000	-1.104991000	-1.461825000
H	1.539695000	0.687960000	0.959578000
H	3.144723000	2.404439000	1.709585000

H	5.482484000	2.378734000	0.882397000
C	2.016624000	-1.413274000	-0.781245000
H	2.021239000	-1.452420000	-1.871021000
H	2.352939000	-2.383027000	-0.406829000
N	0.646504000	-1.219085000	-0.349282000
N	0.287640000	-1.736304000	0.847137000
N	-0.934270000	-1.364811000	1.054215000
C	-3.129471000	0.727910000	-1.135380000
C	-2.703946000	-0.052221000	-0.050715000
C	-3.615257000	-0.286768000	0.989305000
C	-4.902093000	0.239952000	0.945383000
C	-5.312305000	1.013807000	-0.137886000
C	-4.416188000	1.253694000	-1.177953000
H	-2.440946000	0.920374000	-1.950170000
H	-3.308203000	-0.887888000	1.837126000
H	-5.588071000	0.044024000	1.762454000
H	-6.315320000	1.423512000	-0.171612000
H	-4.720649000	1.854037000	-2.028486000
C	-1.340397000	-0.607030000	-0.009563000
C	-0.314376000	-0.479947000	-0.965166000

A4

Zero-point correction = 0.251217 (Hartree/Particle)
Thermal correction to Energy = 0.265153
Thermal correction to Enthalpy = 0.266097
Thermal correction to Gibbs Free Energy = 0.206719
Sum of electronic and zero-point Energies = -743.299928
Sum of electronic and thermal Energies = -743.285992
Sum of electronic and thermal Enthalpies = -743.285048
Sum of electronic and thermal Free Energies = -743.344426

C	-4.851026000	1.126589000	0.505865000
C	-4.004034000	0.161408000	1.044434000
C	-2.941122000	-0.339692000	0.294865000
C	-2.726161000	0.140444000	-0.997483000
C	-3.569366000	1.108870000	-1.533429000
C	-4.635052000	1.602566000	-0.784116000
H	-5.673914000	1.511186000	1.097644000
H	-4.166032000	-0.203451000	2.053619000
H	-1.897702000	-0.239790000	-1.587638000
H	-3.394131000	1.477948000	-2.537573000
H	-5.290350000	2.357815000	-1.202673000
C	-2.064616000	-1.423145000	0.882787000
H	-2.092870000	-1.392614000	1.972087000
H	-2.390796000	-2.411849000	0.555349000
N	-0.676062000	-1.297788000	0.456710000
N	-0.159441000	-2.134994000	-0.439709000
N	1.061767000	-1.764231000	-0.671954000
C	2.849618000	1.224604000	0.688173000
C	2.660795000	-0.004251000	0.047660000
C	3.737358000	-0.597526000	-0.618893000

C	4.978816000	0.028813000	-0.642687000
C	5.162013000	1.251171000	-0.000923000
C	4.092834000	1.846155000	0.664977000
H	2.020663000	1.698811000	1.202490000
H	3.599365000	-1.551445000	-1.114276000
H	5.806267000	-0.441532000	-1.161673000
H	6.130709000	1.737069000	-0.019681000
H	4.225664000	2.798661000	1.165213000
C	1.348500000	-0.664704000	0.077373000
C	0.219753000	-0.357291000	0.810456000
H	-0.010582000	0.414195000	1.527419000

PA (phenylacetylene)

Zero-point correction = 0.110185 (Hartree/Particle)
Thermal correction to Energy = 0.116554
Thermal correction to Enthalpy = 0.117498
Thermal correction to Gibbs Free Energy = 0.079785
Sum of electronic and zero-point Energies = -308.235104
Sum of electronic and thermal Energies = -308.228736
Sum of electronic and thermal Enthalpies = -308.227792
Sum of electronic and thermal Free Energies = -308.265505

C	-0.118344000	-1.211258000	0.000017000
C	0.584625000	0.000024000	0.000036000
C	-0.118394000	1.211277000	0.000017000
C	-1.507800000	1.206344000	-0.000018000
C	-2.204293000	-0.000034000	-0.000037000
C	-1.507751000	-1.206383000	-0.000019000
H	0.429490000	-2.146282000	0.000034000
H	0.429401000	2.146323000	0.000033000
H	-2.047552000	2.146106000	-0.000031000
H	-3.288207000	-0.000056000	-0.000066000
H	-2.047463000	-2.146167000	-0.000032000
C	2.020259000	0.000056000	0.000097000
C	3.223737000	0.000067000	0.000057000
H	4.292100000	-0.000479000	-0.000833000

A_1

Zero-point correction = 0.098327 (Hartree/Particle)
Thermal correction to Energy = 0.104561
Thermal correction to Enthalpy = 0.105505
Thermal correction to Gibbs Free Energy = 0.067920
Sum of electronic and zero-point Energies = -307.747691
Sum of electronic and thermal Energies = -307.741457
Sum of electronic and thermal Enthalpies = -307.740513
Sum of electronic and thermal Free Energies = -307.778098

C	-0.046888000	-1.205763000	-0.000005000
C	0.674219000	0.000000000	0.000013000
C	-0.046888000	1.205763000	-0.000005000
C	-1.437061000	1.203285000	-0.000041000

C	-2.139534000	0.000000000	-0.000059000
C	-1.437061000	-1.203284000	-0.000041000
H	0.495415000	-2.144665000	0.000010000
H	0.495415000	2.144665000	0.000010000
H	-1.973980000	2.145431000	-0.000054000
H	-3.223479000	0.000000000	-0.000085000
H	-1.973981000	-2.145431000	-0.000054000
C	2.113751000	0.000000000	0.000059000
C	3.349563000	0.000000000	0.000107000

TS1

Zero-point correction = 0.446074 (Hartree/Particle)
Thermal correction to Energy = 0.472241
Thermal correction to Enthalpy = 0.473185
Thermal correction to Gibbs Free Energy = 0.386703
Sum of electronic and zero-point Energies = -1131.987505
Sum of electronic and thermal Energies = -1131.961338
Sum of electronic and thermal Enthalpies = -1131.960394
Sum of electronic and thermal Free Energies = -1132.046876

C	-5.666959000	0.714108000	-0.557442000
C	-5.669059000	-0.651869000	-0.664874000
C	-4.459779000	-1.367961000	-0.473072000
C	-3.263646000	-0.658285000	-0.169121000
C	-3.282062000	0.769888000	-0.062690000
C	-4.492896000	1.430093000	-0.263414000
H	-5.343747000	-3.315031000	-0.803869000
H	-6.585560000	1.271877000	-0.707066000
H	-6.575357000	-1.200397000	-0.895485000
C	-4.427933000	-2.782781000	-0.572526000
C	-2.041197000	-1.372166000	0.044464000
H	-4.556501000	2.503033000	-0.214243000
C	-2.055092000	-2.759066000	-0.077806000
C	-3.244889000	-3.445991000	-0.379366000
H	-1.155172000	-3.336102000	0.042579000
H	-3.208185000	-4.527149000	-0.462893000
C	-0.808880000	0.771899000	0.131867000
N	-2.099875000	1.424431000	0.222758000
N	-0.904321000	-0.650372000	0.361203000
C	0.373567000	-1.307479000	0.705316000
H	0.992590000	-0.481245000	1.044033000
C	-2.038673000	2.885554000	0.427018000
H	-1.001756000	3.037726000	0.714859000
C	1.090111000	-1.922085000	-0.498670000
H	2.088307000	-2.249940000	-0.194719000
H	0.565671000	-2.785460000	-0.911141000
H	1.208538000	-1.178421000	-1.289906000
C	0.274040000	-2.258306000	1.903987000
H	1.269355000	-2.344282000	2.347502000
H	-0.396606000	-1.850368000	2.664373000
H	-0.055112000	-3.266759000	1.656329000

C	-2.888238000	3.370816000	1.605096000
H	-2.522201000	4.356277000	1.904955000
H	-3.951143000	3.472984000	1.389047000
H	-2.773365000	2.697862000	2.458692000
C	-2.235906000	3.699422000	-0.853604000
H	-1.534943000	3.364057000	-1.621640000
H	-3.245478000	3.638620000	-1.261446000
H	-2.025587000	4.751549000	-0.641972000
N	0.252095000	1.399996000	-0.042428000
C	5.962590000	-0.925927000	0.203250000
C	5.485402000	0.335479000	-0.182495000
C	6.404116000	1.311503000	-0.595204000
C	7.764968000	1.029691000	-0.621081000
C	8.230136000	-0.225799000	-0.236247000
C	7.324630000	-1.201149000	0.175775000
H	5.257049000	-1.684538000	0.523154000
H	6.041785000	2.288261000	-0.894820000
H	8.464141000	1.793150000	-0.942906000
H	9.291878000	-0.442929000	-0.257318000
H	7.679744000	-2.180192000	0.476908000
C	4.076193000	0.618346000	-0.156196000
C	2.877611000	0.843762000	-0.135832000
H	1.607434000	1.038836000	-0.096528000

A2 (transition state for cyclization)

Zero-point correction = 0.231734 (Hartree/Particle)
Thermal correction to Energy = 0.246922
Thermal correction to Enthalpy = 0.247866
Thermal correction to Gibbs Free Energy = 0.186028
Sum of electronic and zero-point Energies = -742.656001
Sum of electronic and thermal Energies = -742.640813
Sum of electronic and thermal Enthalpies = -742.639869
Sum of electronic and thermal Free Energies = -742.701707

C	-4.833807000	0.981610000	-0.308018000
C	-4.262672000	-0.288847000	-0.301886000
C	-2.959140000	-0.479167000	0.157241000
C	-2.227705000	0.625530000	0.601855000
C	-2.795786000	1.896099000	0.590591000
C	-4.100800000	2.077948000	0.137346000
H	-5.847963000	1.114672000	-0.667877000
H	-4.832888000	-1.140761000	-0.658932000
H	-1.211152000	0.484432000	0.956197000
H	-2.218247000	2.746193000	0.936523000
H	-4.541073000	3.068572000	0.127533000
C	-2.364137000	-1.869347000	0.183298000
H	-2.414921000	-2.284837000	1.193321000
H	-2.939284000	-2.533178000	-0.468457000
N	-0.942182000	-1.932040000	-0.155337000
N	-0.529363000	-1.244732000	-1.122620000
N	0.418086000	-0.664255000	-1.447700000

C	2.636784000	1.168658000	-0.076602000
C	2.660748000	-0.189721000	0.283462000
C	3.908919000	-0.830211000	0.359749000
C	5.084883000	-0.135848000	0.094443000
C	5.046771000	1.213002000	-0.251347000
C	3.814619000	1.860315000	-0.333260000
H	1.680211000	1.674486000	-0.153855000
H	3.947552000	-1.879779000	0.629709000
H	6.036194000	-0.652706000	0.160241000
H	5.964069000	1.752611000	-0.456892000
H	3.770120000	2.909832000	-0.603528000
C	1.438596000	-0.904576000	0.571492000
C	0.616325000	-1.520839000	1.305904000

$TS_{A3\text{-}A4}$

Zero-point correction = 0.586406 (Hartree/Particle)
Thermal correction to Energy = 0.620069
Thermal correction to Enthalpy = 0.621013
Thermal correction to Gibbs Free Energy = 0.517281
Sum of electronic and zero-point Energies = -1567.048910
Sum of electronic and thermal Energies = -1567.015246
Sum of electronic and thermal Enthalpies = -1567.014302
Sum of electronic and thermal Free Energies = -1567.118035

C	5.697840000	-2.126107000	0.198405000
C	6.092469000	-1.104594000	-0.624700000
C	5.164743000	-0.088533000	-0.969767000
C	3.840429000	-0.141237000	-0.450384000
C	3.452338000	-1.210345000	0.418179000
C	4.392479000	-2.192496000	0.718367000
H	6.551058000	1.015997000	-2.210176000
H	6.396675000	-2.913490000	0.460662000
H	7.099377000	-1.055963000	-1.023651000
C	5.539870000	0.982468000	-1.820563000
C	2.896386000	0.879609000	-0.787716000
H	4.140153000	-3.031152000	1.343247000
C	3.306215000	1.905560000	-1.634062000
C	4.619969000	1.947418000	-2.135364000
H	2.626119000	2.682181000	-1.936713000
H	4.894408000	2.766955000	-2.791201000
C	1.112654000	-0.401149000	0.354697000
N	2.161187000	-1.221148000	0.912587000
N	1.616257000	0.796558000	-0.264646000
C	0.608620000	1.853360000	-0.494079000
H	-0.216606000	1.546148000	0.137854000
C	1.701922000	-2.232423000	1.887583000
H	0.705876000	-1.879385000	2.140279000
C	0.062739000	1.889090000	-1.922757000
H	-0.793485000	2.569594000	-1.958414000
H	0.792334000	2.232055000	-2.657537000
H	-0.286710000	0.896801000	-2.220112000

C	1.018565000	3.228109000	0.043282000
H	0.109891000	3.830626000	0.143943000
H	1.465875000	3.130351000	1.036127000
H	1.706672000	3.782693000	-0.593508000
C	2.503833000	-2.230911000	3.192775000
H	1.883580000	-2.683642000	3.970688000
H	3.435355000	-2.794498000	3.155545000
H	2.731158000	-1.207184000	3.500782000
C	1.509555000	-3.625561000	1.285277000
H	0.854727000	-3.571321000	0.412338000
H	2.443036000	-4.102446000	0.983310000
H	1.030681000	-4.271335000	2.026898000
N	-0.093883000	-0.698404000	0.485019000
H	-1.203859000	-0.108702000	0.066186000
C	-5.314406000	-3.992846000	-0.551432000
C	-4.775257000	-3.002525000	-1.369507000
C	-3.484860000	-2.526153000	-1.140762000
C	-2.736572000	-3.049554000	-0.084450000
C	-3.274779000	-4.038620000	0.733529000
C	-4.564898000	-4.511706000	0.501156000
H	-6.317601000	-4.359797000	-0.737101000
H	-5.357348000	-2.597363000	-2.191418000
H	-1.734486000	-2.669672000	0.097356000
H	-2.687186000	-4.441914000	1.550983000
H	-4.983340000	-5.283816000	1.136927000
C	-2.909251000	-1.425118000	-1.999620000
H	-1.835053000	-1.563303000	-2.132972000
H	-3.390660000	-1.399534000	-2.977017000
N	-3.105574000	-0.112683000	-1.388750000
N	-4.104561000	0.675996000	-1.816037000
N	-4.065837000	1.755530000	-1.095497000
C	-1.956818000	2.445263000	1.888868000
C	-2.683493000	2.725462000	0.723894000
C	-3.011556000	4.056855000	0.441535000
C	-2.619629000	5.079794000	1.300029000
C	-1.888893000	4.792082000	2.450597000
C	-1.559310000	3.469150000	2.741105000
H	-1.702913000	1.415354000	2.121007000
H	-3.564080000	4.288001000	-0.462452000
H	-2.878156000	6.106290000	1.064327000
H	-1.579382000	5.590732000	3.115046000
H	-0.993733000	3.233977000	3.636051000
C	-3.045125000	1.640873000	-0.198848000
C	-2.395028000	0.417419000	-0.367939000

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