Supporting information

for

"Regioselective N^2-Arylation of Tetrazoles under CuO nanocatalysis: A route to potent anti-MRSA agents"

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Contents:

Section		Page No.
1	General information	S3-S4
2	Synthesis of tetrazoles	S4
3	Procedures	S5-S6
4	^{1}H and ^{13}C NMR spectral analysis of the 2,5-disubstituted tetrazole derivatives	S6-S10
5	Crystallographic data of 2,5-Diphenyl-2*H*-tetrazole (**3a**)	S10-S12
6	Powder XRD spectrum of Cu^{II}-tetrazole complex	S12
7	References	S13
8	Copies of ^{1}H and ^{13}C NMR spectra	S14-S42

1. General Information

All the reactions were performed using oven-dried glasswares such as round-bottom flasks and pressure tubes under an ambient atmosphere. The progress of the reaction was monitored through thin-layer chromatography (TLC) on Merck Kieselgel Silica gel 60 F_{254} plates and visualized using short wave UV light (λ=254 nm). The products were purified by column chromatography using silica gel (60-120 mesh) and freshly distilled ethyl acetate-hexane mixture as the solvent system. Concentration under reduced pressure was performed by rotary evaporation at 40-45 °C at an appropriate pressure.

1.1. *Reagents and starting materials*

Unless otherwise stated, all chemicals and solvents were purchased from commercial suppliers and used without purification. CuO NPs were purchased from Alfa Aesar having particle size of 30-50 nm and surface area of 13 m^2/g. Tetrazoles (**2a**-**2k**) were prepared using reported procedure.[1]

1.2. *Spectroscopy, spectrometry and instruments:*

The ^1H and ^{13}C NMR spectra were recorded on a 400 MHz JEOL NMR spectrometer (400 MHz for ^1H and 100 MHz for ^{13}C spectroscopy) at 298 K using $CDCl_3$ and DMSO-d_6 as solvents. Chemical shifts for both ^1H (δ_H) and 13C (δ_C) NMR are assigned in parts per million relative to the residual solvent peak [^1H NMR: $CDCl_3$ δ 7.26 and δ 1.56 ($CDCl_3$-water); DMSO-d_6 δ 2.50 and δ 3.3 (DMSO-water) and ^{13}C NMR: $CDCl_3$ δ 77.16; DMSO-d_6 δ 39.52] with multiplicities (br = broad, s = singlet, d = doublet, t = triplet, q = quartet, quin = quintet, sex = sextet, sep = septet, m = multiplet), coupling constants (in Hz), and integration. All the NMR spectra were plotted in the MestReNova software. High-resolution mass spectra were recorded on an ESI-Q-TOF mass spectrometer. Single-crystal X-ray diffraction data were recorded on a Bruker APEX-II CCD diffractometer using MoKα radiation (λ = 0.71073 Å).

1.3. *Melting Points and CHN content:*

Melting points were recorded on a Buchi M-560 melting point apparatus and are uncorrected. The organic content (wt % C, H, N) in the synthesized compounds was determined by combustion analysis using a PerkinElmer 2400 CHN analyzer.

1.4. *Materials and methods:*

The sterile discs (catalog no. SD067), and growth media for microbial culture: Mueller Hinton agar (catalog no. M173) and Mueller Hinton broth (catalog no. M391) were

purchased from HiMedia, Maharashtra, India. The antibiotic vancomycin (catalog no. 94747) was purchased from Sigma-Aldrich, Missouri, USA.

Preparation and storage of testing reagents:

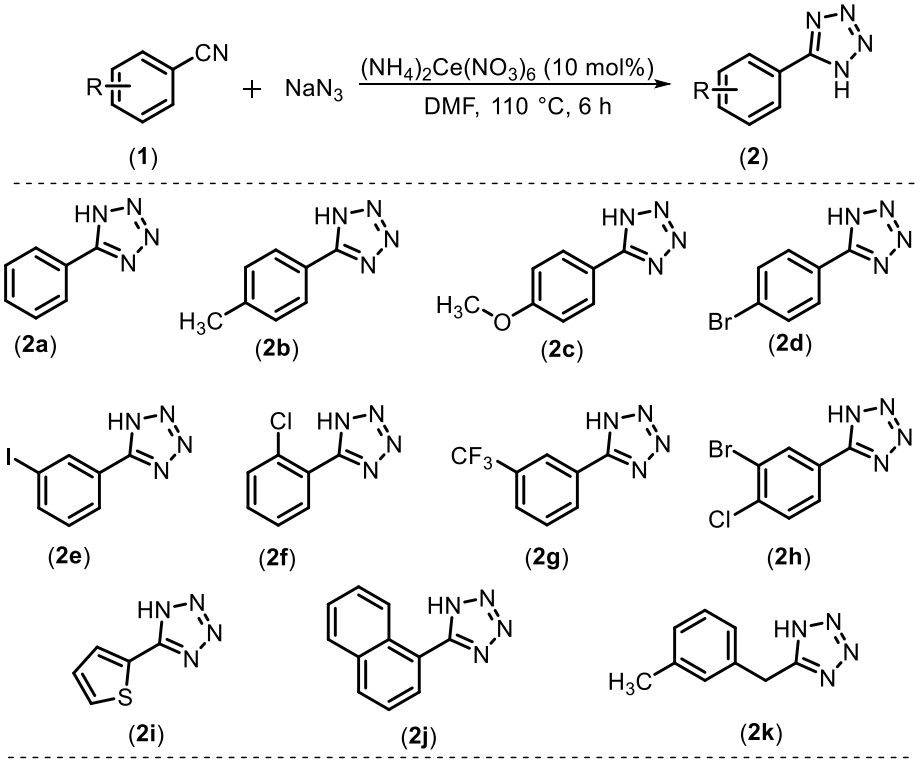
A concentration of 0.015 % resazurin was prepared by dissolving 0.015g in 100 mL sterile water, vortexed, and filter sterilised and stored at 4 ℃ for further experiments.

Test organism used:

Gram-positive MRSA was used for *in vitro* antibacterial activity. The bacterial strain was procured from American Type Culture Collection, Manassas, Virginia, USA (ATCC-BAA 43300).

2. Synthesis of Tetrazoles

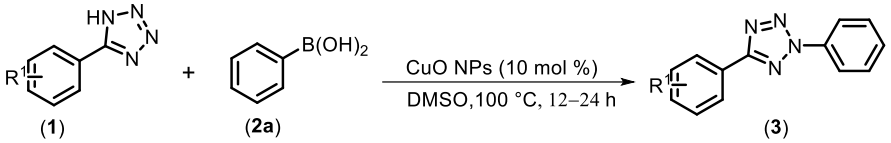
All the 5-substituted-1*H*-tetrazoles (**2a**-**2k**) were synthesized from previously known method without any alteration of the procedure. Analytical data were in agreement with previous literatures for all the compounds and confirmed by ^{1}H NMR spectroscopy.



Scheme S1: Synthesis of 5-substituted-1*H*-tetrazoles.

3. Procedures

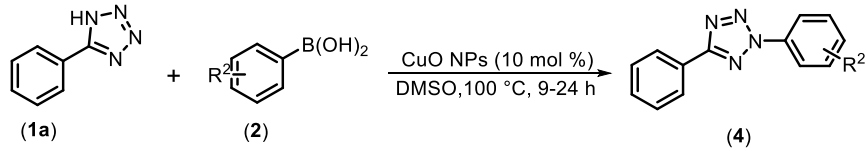
3.1 General experimental procedure for the Chan-Lam cross-coupling of 5-substituted-1*H*-tetrazoles (1a-1k) with phenylboronic acid (2a)



Scheme S2: Chan-Lam cross-coupling of 5-substituted-1*H*-tetrazoles with phenylboronic acid.

In an oven-dried round-bottomed flask with a magnetic stirring bead, 5-substituted-1*H*-tetrazole (**1a-1k**, 0.5 mmol) and phenylboronic acid (**2a**, 1 mmol, 2 equiv.) were taken. To it, 10 mol% of CuO NPs and 2 ml of DMSO were added. The reaction flask was then fitted to a condenser and stirred at 100-120 °C for 12-24 h in a pre-heated oil bath under reflux conditions. Progress of the reaction was monitored using TLC. The resulting reaction mixture was cooled to room temperature and work-up was performed with ethyl acetate and water. The organic layer was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The desired products (**3a-3k**) were obtained through purification by column chromatography using ethyl acetate-hexane as eluent.

3.2 General experimental procedure for the Chan-Lam cross-coupling of 5-phenyl-1*H*-tetrazole (1a) with arylboronic acids (2b-2q)



Scheme S3: Chan-Lam cross-coupling of 5-phenyl-1*H*-tetrazole with arylboronic acids.

In an oven-dried round-bottomed flask with a magnetic stirring bead, 5-phenyl-1*H*-tetrazole (**1a**, 0.5 mmol) and arylboronic acids (**2b-2q**, 1 mmol, 2 equiv.) were taken. To it, 10 mol% of CuO NPs and 2 ml of DMSO were added. The reaction flask was then fitted to a condenser and stirred at 100 °C for 9-24 h in a pre-heated oil bath under reflux conditions. Progress of the reaction was monitored using TLC. The resulting reaction mixture was cooled to room temperature and work-up was performed with ethyl acetate and water. The organic layer was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The desired products

(**4b**-**4q**) were obtained through purification by column chromatography using ethyl acetate-hexane as eluent.

4. ^{1}H and ^{13}C NMR spectral analysis of the 2,5-disubstituted tetrazole derivatives

2,5-Diphenyl-2*H*-tetrazole (**3a**)[2]. **3a** (106.4 mg, 96%) was prepared by the general experimental procedure A; white solid; mp 101-103 °C (lit. 102-104 °C); ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.29 (d, J = 7.4 Hz, 1H), 8.23 (d, J = 8.0 Hz, 1H), 7.60 (t, J = 7.7 Hz, 1H), 7.58-7.51 (m, 2H); $^{13}C\{^{1}H\}$ NMR (150 MHz, $CDCl_3$): δ 165.2, 136.9, 130.6, 129.7, 129.6, 129.0, 127.2, 127.1, 119.9.

2-Phenyl-5-(*p*-tolyl)-2*H*-tetrazole (**3b**)[2]. **3b** (87.4 mg, 74%) was prepared by the general experimental procedure A; white solid; mp 95-97 °C (lit. 94-96 °C); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.18 (d, J = 8.2 Hz, 2H), 8.14 (d, J = 8.2 Hz, 2H), 7.56 (t, J = 7.7 Hz, 2H), 7.48 (t, J = 7.4 Hz, 1H), 7.32 (d, J = 7.9 Hz, 2H), 2.42 (s, 3H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$): δ 165.3, 140.8, 137.0, 129.7, 129.6, 129.5, 127.0, 124.4, 119.8, 21.6.

5-(4-Methoxyphenyl)-2-phenyl-2*H*-tetrazole (**3c**)[3]. **3c** (111 mg, 88%) was prepared by the general experimental procedure A; white solid; mp 106-108 °C (lit. 104-106 °C); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.19 (d, J = 8.7 Hz, 4H), 7.56 (t, J = 7.8 Hz, 2H), 7.48 (t, J = 7.3 Hz, 1H), 7.03 (d, J = 8.7 Hz, 2H), 3.88 (s, 3H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$): δ 165.1, 161.5, 137.0, 129.6, 129.5, 128.6, 119.8, 119.7, 114.4, 55.4.

5-(4-Bromophenyl)-2-phenyl-2*H*-tetrazole (**3d**)[2]. **3d** (105.4 mg, 70%) was prepared by the general experimental procedure A; white solid; mp 108-110 °C (lit. 112-114 °C); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.17 (d, J = 7.9 Hz, 2H), 8.11 (d, J = 8.4 Hz, 2H), 7.65 (d, J = 8.4 Hz, 2H), 7.53 (dt, J = 27.7, 7.3 Hz, 3H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$): δ 164.4, 136.8, 132.2, 129.8, 129.7, 128.5, 126.1, 125.0, 119.8.

5-(3-Iodophenyl)-2-phenyl-2*H*-tetrazole (**3e**). **3e** (118.4 mg, 68%) was prepared by the general experimental procedure A; white solid; mp 86-88 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.61 (t, J = 1.6 Hz, 1H), 8.23-8.16 (m, 3H), 7.85-7.80 (m, 1H), 7.60-7.54 (m, 2H), 7.54-7.48 (m, 1H), 7.28-7.23 (m, 1H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$): δ 163.7, 139.5, 136.8, 135.8, 130.6, 129.8, 129.7, 129.1, 126.2, 119.9, 94.5. Anal. calcd. for $C_{13}H_9IN_4$: C, 44.85; H, 2.61; N, 16.09; found: C, 45.36; H, 2.46; N, 15.89.

5-(2-Chlorophenyl)-2-phenyl-2*H*-tetrazole (**3f**)[2]. **3f** (89.4 mg, 70%) was prepared by the general experimental procedure A; white solid; mp 74-76 °C (lit. 72-74 °C); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.22 (d, J = 8.0 Hz, 2H), 8.09-8.04 (m, 1H), 7.62-7.56 (m, 3H), 7.54-7.49 (m,

1H), 7.48-7.41 (m, 2H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$): δ 163.5, 136.9, 133.3, 131.4, 131.3, 131.0, 129.8, 129.7, 127.0, 126.3, 120.0.

2-Phenyl-5-(3-(trifluoromethyl)phenyl)-2*H*-tetrazole (**3g**)[3]. **3g** (93.2 mg, 64%) was prepared by the general experimental procedure A; white solid; mp 98-100 °C (lit. 96-98 °C); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.52 (s, 1H), 8.44 (d, J = 7.8 Hz, 1H), 8.20 (qd, J = 3.2, 0.9 Hz, 2H), 7.76 (dd, J = 7.8, 0.5 Hz, 1H), 7.66 (t, J = 7.8 Hz, 1H), 7.62-7.55 (m, 2H), 7.52 (t, J = 7.4 Hz, 1H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$): δ 164.1, 136.8, 131.6 (q, $^{2}J_{C-F}$ = 33 Hz), 130.3, 130.0, 129.8, 129.6, 128.1, 127.2 (q, $^{3}J_{C-F}$ = 4 Hz), 124.0 (q, $^{3}J_{C-F}$ = 4 Hz), 123.9 (q, $^{1}J_{C-F}$ = 271 Hz), 120.0; ^{19}F NMR (376 MHz, $CDCl_3$): δ -62.7.

5-(3-bromo-4-chlorophenyl)-2-phenyl-2H-tetrazole (**3h**). **3h** (93.9 mg, 56%) was prepared by the general experimental procedure A; white solid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.52 (d, J = 2.0 Hz, 1H), 8.20-8.16 (m, 2H), 8.13 (dd, J = 8.4, 2.0 Hz, 1H), 7.62-7.55 (m, 3H), 7.54-7.49 (m, 1H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$): δ 163.3, 136.84, 136.78 132.1, 131.0, 130.0, 129.8, 127.2, 126.9,123.3, 120.0.

2-Phenyl-5-(thiophen-2-yl)-2*H*-tetrazole (**3i**)[3]. **3i** (65.1 mg, 57%) was prepared by the general experimental procedure A; yellow solid; mp 94-96 °C (lit. 92-94 °C); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.17 (d, J = 8.4 Hz, 2H), 7.93-7.89 (m, 1H), 7.56 (t, J = 7.6 Hz, 2H), 7.53-7.46 (m, 2H), 7.19 (t, J = 4.3 Hz, 1H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$): δ 161.3, 136.7, 129.72, 129.68, 128.8, 128.3, 128.0, 119.9.

5-(Naphthalen-1-yl)-2-phenyl-2*H*-tetrazol (**3j**)[3]. **3j** (106.2 mg, 78%) was prepared by the general experimental procedure A; white solid; mp 124-126 °C (lit. 126-128 °C); ^{1}H NMR (600 MHz, $CDCl_3$): δ 9.06 (d, J = 8.6 Hz, 1H), 8.42 (dd, J = 7.2, 1.2 Hz, 1H), 8.31 (d, J = 7.5 Hz, 2H), 8.05 (d, J = 8.2 Hz, 1H), 7.98 (d, J = 8.1 Hz, 1H), 7.70-7.59 (m, 5H), 7.58-7.54 (m, 1H); $^{13}C\{^{1}H\}$ NMR (150 MHz, $CDCl_3$): δ 165.4, 136.9, 134.0, 131.3, 130.6, 129.8, 129.7, 128.7, 127.4, 126.3, 125.8, 125.3, 123.9, 119.9.

5-(3-Methylbenzyl)-2-phenyl-2*H*-tetrazole (**3k**). **3k** (40.0 mg, 32%) was prepared by the general experimental procedure A; colourless oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.11-8.07 (m, 2H), 7.55-7.43 (m, 3H), 7.24-7.15 (m, 3H), 7.06 (d, J = 7.1 Hz, 1H), 4.29 (s, 2H), 2.33 (s, 3H). $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$): δ 166.0, 138.5, 136.9, 136.5, 129.7, 129.6, 128.7, 127.8, 126.0, 119.9, 31.9, 21.5. HRMS (ESI/Q-TOF) m/z: $[M+H]^+$ calcd for $C_{19}H_{12}N_4O$, 251.1296; found, 251.1308.

5-Phenyl-2-(*p*-tolyl)-2*H*-tetrazole (**4b**)[4]. **4b** (111.2 mg, 94%) was prepared by the general experimental procedure A; white solid; mp 101-103 °C (lit. 104-105 °C); H^1 NMR (400 MHz,

$CDCl_3$): δ 8.24 (dd, J = 7.8, 1.8 Hz, 2H), 8.05 (d, J = 8.5 Hz, 2H), 7.54-7.46 (m, 3H), 7.34 (d, J = 8.3 Hz, 2H), 2.43 (s, 3H); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$): δ 165.1, 139.9, 134.7, 130.5, 130.2, 128.9, 127.3, 127.0, 119.7, 21.2.

2-(4-Methoxyphenyl)-5-phenyl-2*H*-tetrazole (**4c**)[2]. **4c** (123.8 mg, 98%) was prepared by the general experimental procedure B; white solid; mp 99-101 °C (lit. 100-102 °C); ^1H NMR (600 MHz, $CDCl_3$): δ 8.27 (d, J = 6.5 Hz, 2H), 8.13 (d, J = 9.1 Hz, 2H), 7.57-7.50 (m, 3H), 7.09 (d, J = 9.1 Hz, 2H), 3.92 (s, 3H); $^{13}C\{^1H\}$ NMR (150 MHz, $CDCl_3$): δ 165.0, 160.5, 130.5, 130.4, 128.9, 127.3, 127.0, 121.4, 114.7, 55.5.

2-(4-(*tert*-butyl)phenyl)-5-phenyl-2*H*-tetrazole (**4d**)[5]. **4d** (129 mg, 93%) was prepared by the general experimental procedure B; colourless oil; ^1H NMR (400 MHz, $CDCl_3$): δ 8.28-8.23 (m, 2H), 8.09 (d, J = 8.8 Hz, 2H), 7.56 (d, J = 8.8 Hz, 2H), 7.53-7.45 (m, 3H), 1.37 (s, 9H); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$): δ 165.1, 153.1, 134.6, 130.5, 128.9, 127.3, 127.1, 126.6, 119.6, 34.9, 31.3.

2-(4-Fluorophenyl)-5-phenyl-2*H*-tetrazole (**4e**)[6]. **4e** (113.1 mg, 94%) was prepared by the general experimental procedure B; white solid; mp 114-116 °C (lit. 119-120 °C); ^1H NMR (400 MHz, $CDCl_3$): δ 8.23 (dd, J = 7.2, 1.9 Hz, 2H), 8.18 (dd, J = 8.8, 4.5 Hz, 2H), 7.55-7.47 (m, 3H), 7.25 (t, J = 8.5 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.3, 163.0 (d, $^1J_{C–F}$ = 249 Hz), 133.2 (d, $^4J_{C–F}$ = 3 Hz), 130.6, 129.0, 127.05, 127.02, 121.8 (d, $^3J_{C–F}$ = 8 Hz), 116.7 (d, $^2J_{C–F}$ = 23 Hz); ^{19}F NMR (376 MHz, $CDCl_3$): δ -110.6.

2-(4-Chlorophenyl)-5-phenyl-2*H*-tetrazole (**4f**)[4]. **4f** (121 mg, 94%) was prepared by the general experimental procedure B; white solid; 118-120 °C (lit. 121-122 °C); ^1H NMR (400 MHz, $CDCl_3$): δ 8.25-8.20 (m, 2H), 8.13 (dd, J = 9.3, 2.4 Hz, 2H), 7.55-7.47 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.4, 135.5, 135.3, 130.7, 129.9, 129.0, 127.1, 126.9, 121.0.

2-(4-Bromophenyl)-5-phenyl-2*H*-tetrazole (**4g**)[4]. **4g** (134 mg, 89%) was prepared by the general experimental procedure B; white solid; mp 120-122 °C (lit. 123-124 °C); ^1H NMR (400 MHz, $CDCl_3$): δ 8.24-8.19 (m, 2H), 8.08-8.03 (m, 2H), 7.70-7.64 (m, 2H), 7.54-7.47 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.4, 135.8, 132.8, 130.7, 129.0, 127.1, 126.9, 123.5, 121.2.

2-(4-(trifluoromethyl)-5-phenyl-2*H*-tetrazole (**4h**). **4h** (123.1 mg, 85%) was prepared by the general experimental procedure B; white solid; mp 108-110°C; ^1H NMR (400 MHz, $CDCl_3$): δ 8.34 (d, J = 8.5 Hz, 2H), 8.28-8.22 (m, 2H), 7.84 (d, J = 8.6 Hz, 2H), 7.55-7.50 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.6, 139.1, 131.5 (q, $^2J_{C–F}$ = 33 Hz), 130.9, 129.0, 127.2, 127.0 (q, $^3J_{C–F}$ = 4 Hz), 126.7, 123.6 (q, $^1J_{C–F}$ = 270 Hz), 120.0; ^{19}F NMR (376 MHz, $CDCl_3$): δ -62.6. Anal. calcd. for $C_{14}H_9F_3N_4$: C, 57.93; H, 3.13; N, 19.30; found: C, 65.73; H, 5.20; N, 21.96.

1-(4-(5-phenyl-2*H*-tetrazol-2-yl)phenyl)ethan-1-one (**4i**)[6]. **4i** (94.6 mg, 72%) was prepared by the general experimental procedure B; off-white solid; mp 139-141 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.32 (d, J = 8.7 Hz, 2H), 8.28-8.23 (m, 2H), 8.16 (d, J = 8.8 Hz, 2H), 7.57-7.51 (m, 3H), 2.68 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 196.6, 165.6, 139.7, 137.6, 130.9, 130.0, 129.0, 127.2, 126.8, 119.7, 26.7.

4-(5-phenyl-2*H*-tetrazol-2-yl)benzaldehyde (**4j**). **4j** (99.6 mg, 80%) was prepared by the general experimental procedure B; pale green solid; mp 132-134 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.10 (s, 1H), 8.40 (d, J = 8.6 Hz, 2H), 8.25 (dd, J = 6.5, 3.1 Hz, 2H), 8.10 (d, J = 8.6 Hz, 2H), 7.53 (dd, J = 5.1, 1.9 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 190.7, 165.7, 140.5, 136.6, 131.2, 130.9, 129.1, 127.2, 126.7, 120.1. Anal. calcd. for $C_{14}H_{10}N_4O$: C, 67.19; H, 4.03; N, 22.39; found: C, 67.41; H, 5.31; N, 21.92.

2-(3,4-dichlorophenyl)-5-phenyl-2*H*-tetrazole (**4k**). **4k** (120.6 mg, 82%) was prepared by the general experimental procedure B; pale yellow solid; mp 122-124 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.31 (s, 1H), 8.21 (dd, J = 6.3, 2.7 Hz, 2H), 8.05 (dd, J = 8.7, 1.8 Hz, 1H), 7.63 (d, J = 8.7 Hz, 1H), 7.55-7.48 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.5, 135.7, 134.0, 133.8, 131.4, 130.9, 129.0, 127.1, 126.6, 121.6, 118.8. Anal. calcd. for $C_{13}H_8Cl_2N_4$: C, 53.63; H, 2.77; N, 19.24; found: C, 53.38; H, 2.28; N, 18.37.

5-phenyl-2-(3-(trifluoromethyl)phenyl)-2*H*-tetrazole (**4l**). **4l** (83.8 mg, 58%) was prepared by the general experimental procedure B; white solid; mp 99-101 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.52 (s, 1H), 8.46 (d, J = 8.0 Hz, 1H), 8.29 (dd, J = 7.7, 1.9 Hz, 2H), 7.77 (dt, J = 15.8, 7.8 Hz, 2H), 7.59-7.53 (m, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 165.6, 137.1, 132.4 (q, $^2J_{C-F}$ = 22 Hz), 130.9, 130.5, 129.0, 127.2, 126.7, 126.2 (q, $^3J_{C-F}$ = 2 Hz), 123.3 (q, $^1J_{C-F}$ = 180 Hz), 122.8, 116.9 (q, $^3J_{C-F}$ = 2 Hz); ^{19}F NMR (376 MHz, $CDCl_3$): δ -62.8. Anal. calcd. for $C_{14}H_9F_3N_4$: C, 57.93; H, 3.13; N, 19.30; found: C, 57.27; H, 2.31; N, 18.45.

5-phenyl-2-(*o*-tolyl)-2*H*-tetrazole (**4m**)[2]. **4m** (116 mg, 98%) was prepared by the general experimental procedure B; off-white solid; mp 53-55 °C (lit. 48-50 °C); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.25 (dd, J = 7.8, 1.8 Hz, 2H), 7.66 (d, J = 8.0 Hz, 1H), 7.55-7.48 (m, 3H), 7.48-7.35 (m, 3H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.0, 136.5, 133.1, 131.9, 130.5, 130.3, 129.0, 127.3, 127.0, 126.9, 125.3, 18.8.

2-mesityl-5-phenyl-2*H*-tetrazole (**4n**)[7]. **4n** (123.7 mg, 94%) was prepared by the general experimental procedure B; white solid; mp 99-101 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.28-

8.23 (m, 2H), 7.55-7.48 (m, 3H), 7.03 (s, 2H), 2.38 (s, 3H), 2.02 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.1, 140.9, 135.1, 133.9, 130.5, 129.2, 129.0, 127.4, 127.0, 21.2, 17.3.

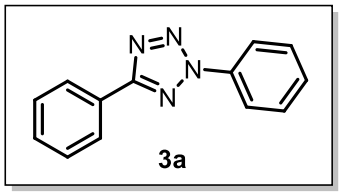
2-(naphthalen-2-yl)-5-phenyl-2*H*-tetrazole (**4o**)[8]. **4o** (117.9 mg, 87%) was prepared by the general experimental procedure B; white solid; mp 125-127 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.70 (s, 1H), 8.36 (dt, J = 8.8, 2.1 Hz, 1H), 8.33 (dd, J = 8.0, 1.3 Hz, 2H), 8.07 (dd, J = 8.8, 2.5 Hz, 1H), 8.03 (d, J = 7.4 Hz, 1H), 7.96 (d, J = 7.3 Hz, 1H), 7.65-7.53 (m, 5H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 165.3, 134.3, 133.4, 133.1, 130.6, 129.9, 129.0, 128.7, 128.0, 127.5, 127.4, 127.2, 127.1, 118.3, 117.9.

2-methoxy-5-(5-phenyl-2*H*-tetrazol-2-yl)pyridine (**4p**). **4p** (88.6 mg, 63%) was prepared by the general experimental procedure B; white solid; mp 134-136 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 9.01 (d, J = 2.6 Hz, 1H), 8.36 (dd, J = 8.9, 2.7 Hz, 1H), 8.27-8.24 (m, 2H), 7.54 (q, J = 6.2 Hz, 3H), 6.96 (d, J = 8.9 Hz, 1H), 4.05 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 165.4, 164.5, 138.8, 130.7, 129.0, 128.4, 127.1, 127.0, 111.7, 54.2. HRMS (ESI/Q-TOF) m/z: $[M+H]^+$ calcd for $C_{13}H_{11}N_5O$, 254.1042; found, 254.1021.

2-(dibenzo[b,d]furan-4-yl)-5-phenyl-2*H*-tetrazole (**4q**). **4q** (49.7 mg, 32%) was prepared by the general experimental procedure B; white solid; mp 141-143 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.36 (d, J = 6.9 Hz, 2H), 8.14 (dd, J = 16.4, 7.8 Hz, 2H), 8.05 (d, J = 7.7 Hz, 1H), 7.75 (d, J = 8.3 Hz, 1H), 7.61-7.53 (m, 5H), 7.45 (t, J = 7.5 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 165.2, 156.7, 146.9, 130.7, 129.0, 128.4, 127.5, 127.2, 127.1, 123.6, 123.2, 122.3, 122.1, 120.9, 120.5, 112.5. HRMS (ESI/Q-TOF) m/z: $[M+H]^+$ calcd for $C_{19}H_{12}N_4O$, 313.1089; found, 313.1074.

5. Crystallographic data of 2,5-Diphenyl-2*H*-tetrazole (3a)

Good-quality crystals of compound **3a** were obtained by slow evaporation of methanol from its solution.



3a

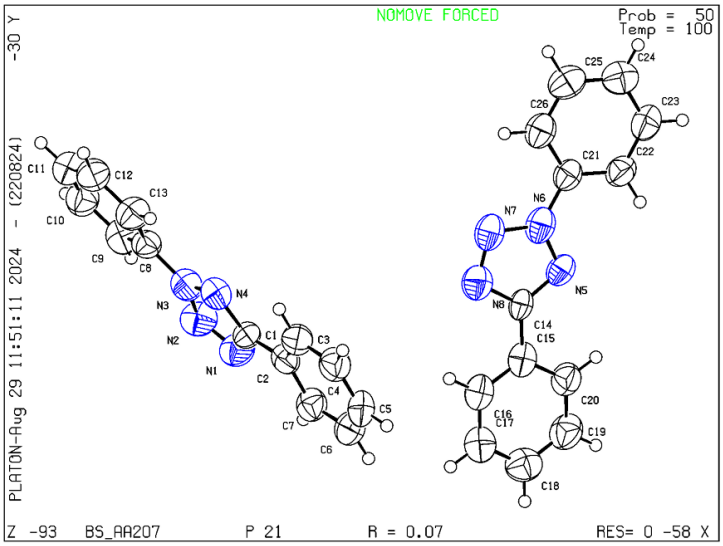


Figure S1: ORTEP of the compound **3a** with 50% probablity ellipsoid

Table S1. Crystal structure data of **3a**

Crystal Data	**3a**
CCDC No	2498997
Empirical Formula	$C_{13}H_{10}N_4$
Formula weight	222.25
Crystal system	monoclinic
Temperature [K]	100
a [Å]	5.08(2)
b [Å]	16.32(7)
c [Å]	13.82(6)
α [°]	90
β [°]	90.01(4)
γ [°]	90
Volume [Å^3]	1146(8)
Space group	P 21
Z	4

ρ_{calc} [g/cm^3]	1.288
μ [mm^{-1}]	0.082
F(000)	464
Reflections (R) collected	2055
Unique observed	4503
R1	0.0688
wR2	0.1576
Radiation	MoKα (λ = 0.71073 Å)
Instrument	Bruker APEX-II CCD

6. Powder XRD spectrum of Cu^{II}-tetrazole complex

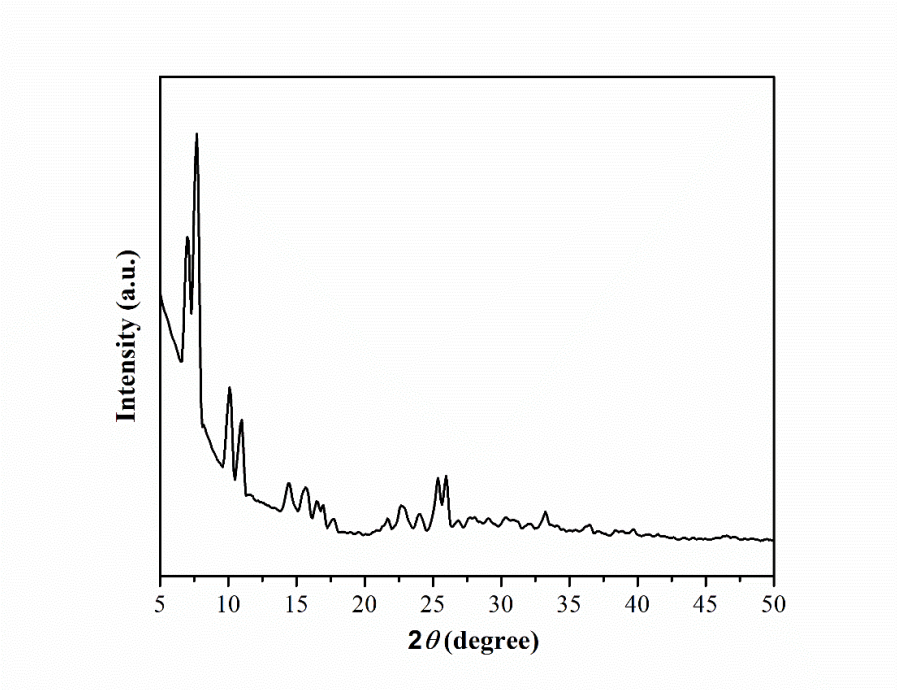


Figure S2: Powder X-ray diffraction pattern of the complex from CuO NPs and tetrazole, **1a**

7. References

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2. S. Rajamanickam, C. Sah, B. A. Mir, S. Ghosh, G. Sethi, V. Yadav, S. Venkataramani and B. K. Patel, *J. Org. Chem.*, 2020, **85**, 2118-2141.
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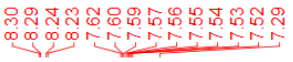
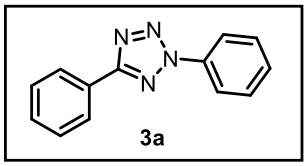
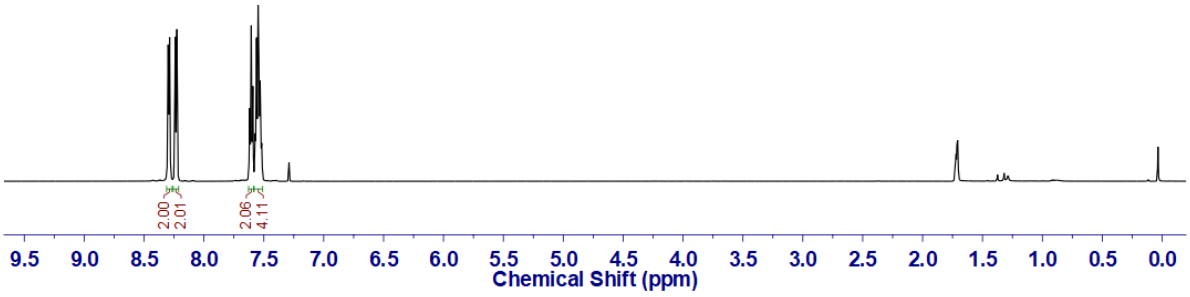
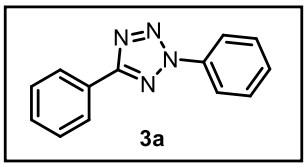
8. Copies of ^{1}H, ^{13}C and ^{19}F NMR spectra



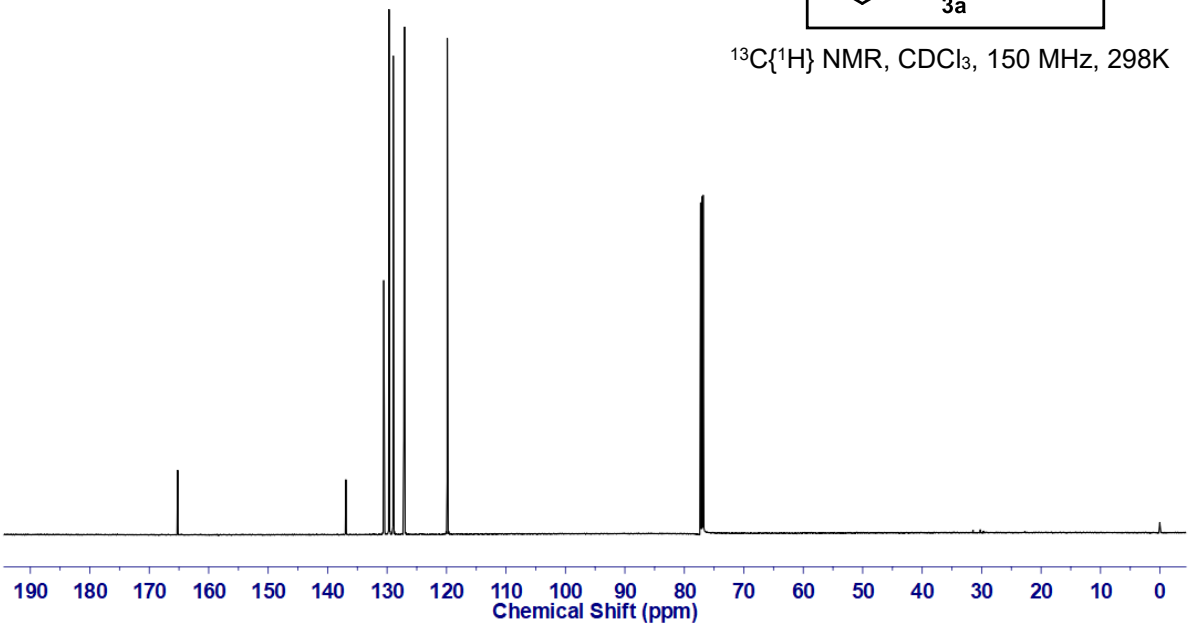


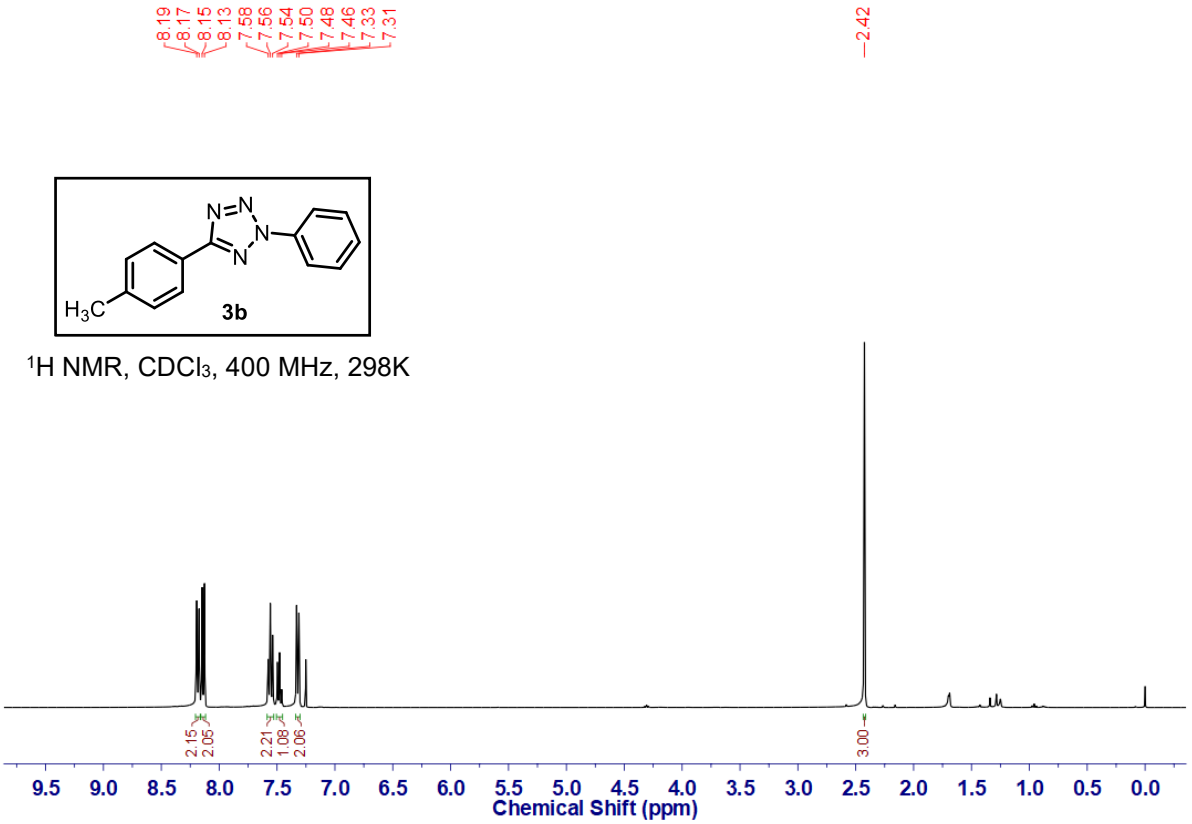
^{1}H NMR, $CDCl_3$, 600 MHz, 298K



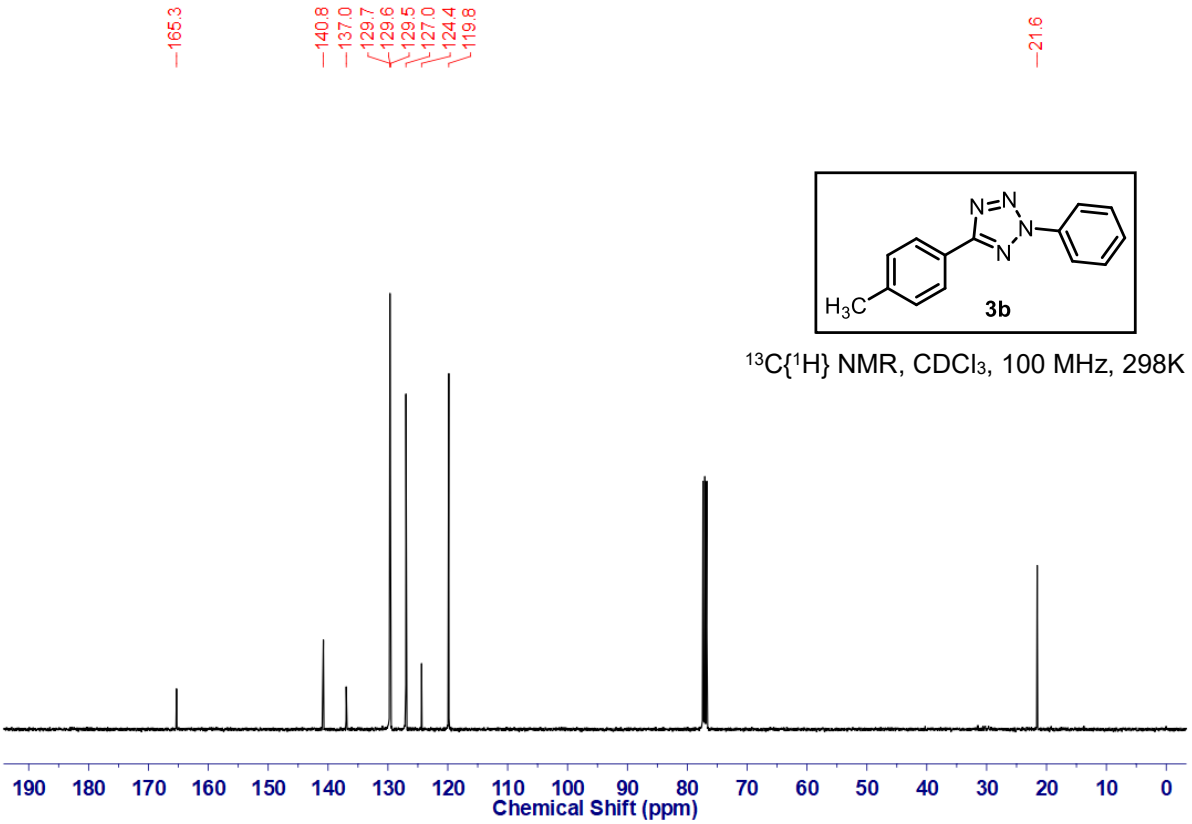


$^{13}C\{^{1}H\}$ NMR, $CDCl_3$, 150 MHz, 298K

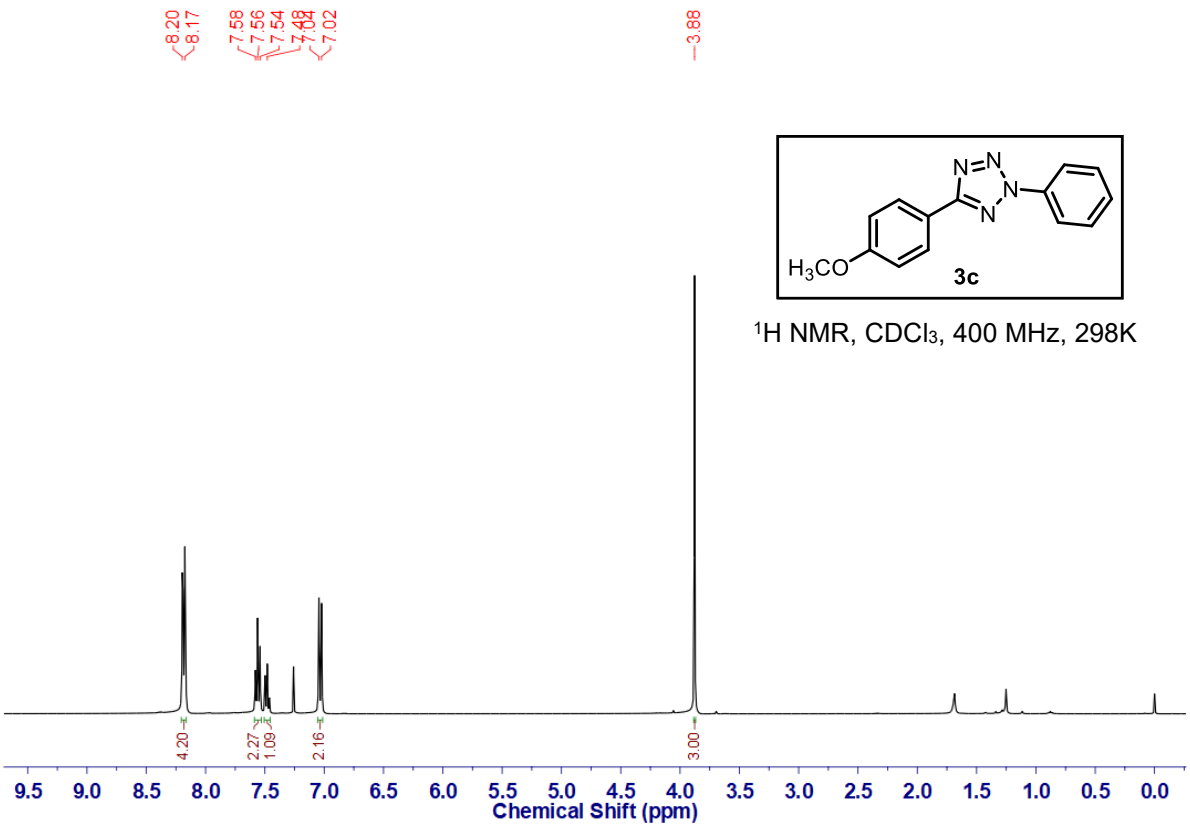




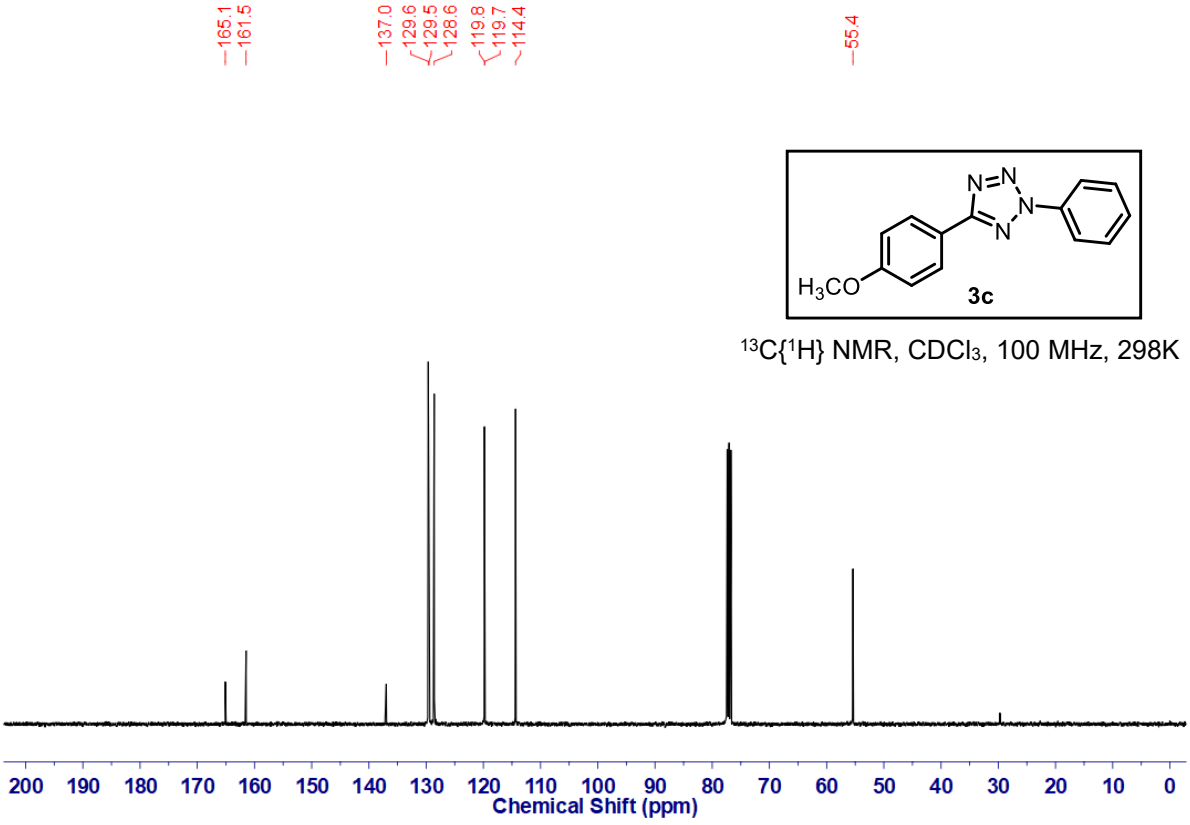
^{1}H NMR, $CDCl_3$, 400 MHz, 298K



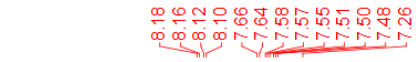
$^{13}C\{^{1}H\}$ NMR, $CDCl_3$, 100 MHz, 298K

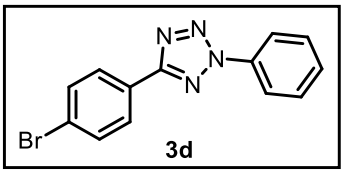


^{1}H NMR, $CDCl_3$, 400 MHz, 298K

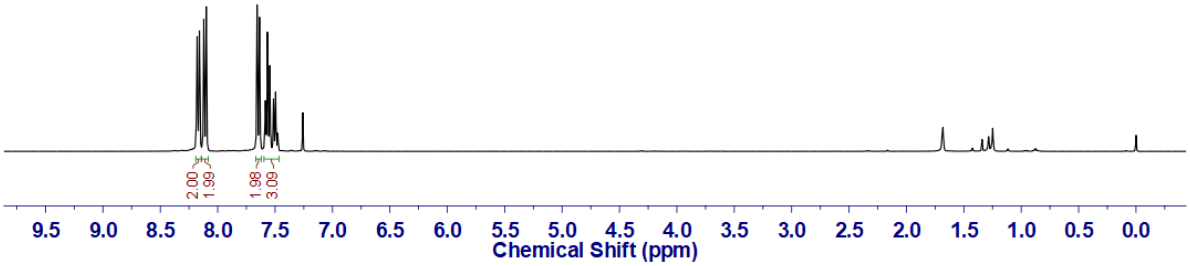


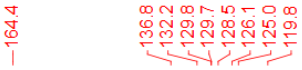
^{13}C{^{1}H} NMR, $CDCl_3$, 100 MHz, 298K

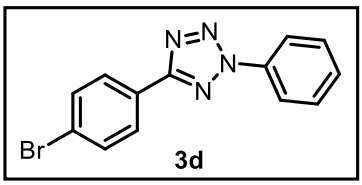




^{1}H NMR, $CDCl_3$, 400 MHz, 298K







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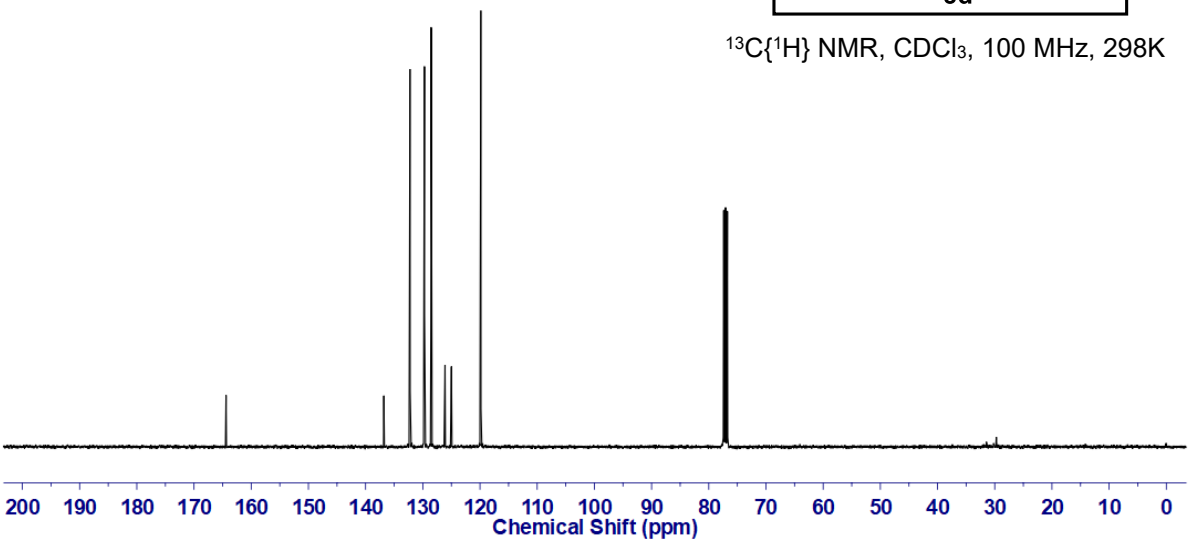

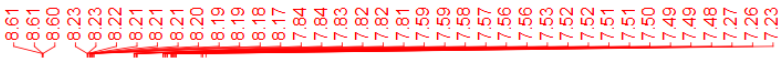

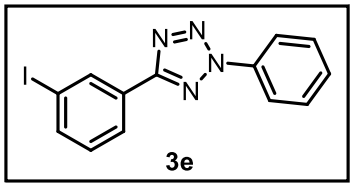

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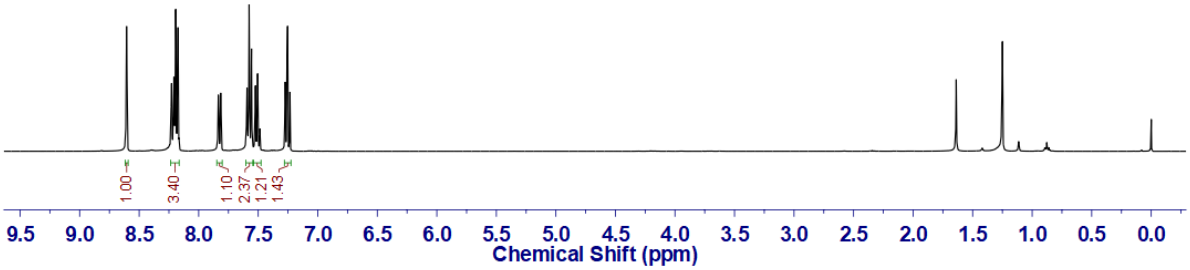

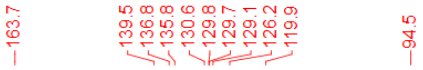

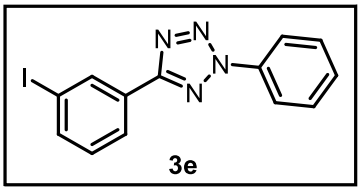

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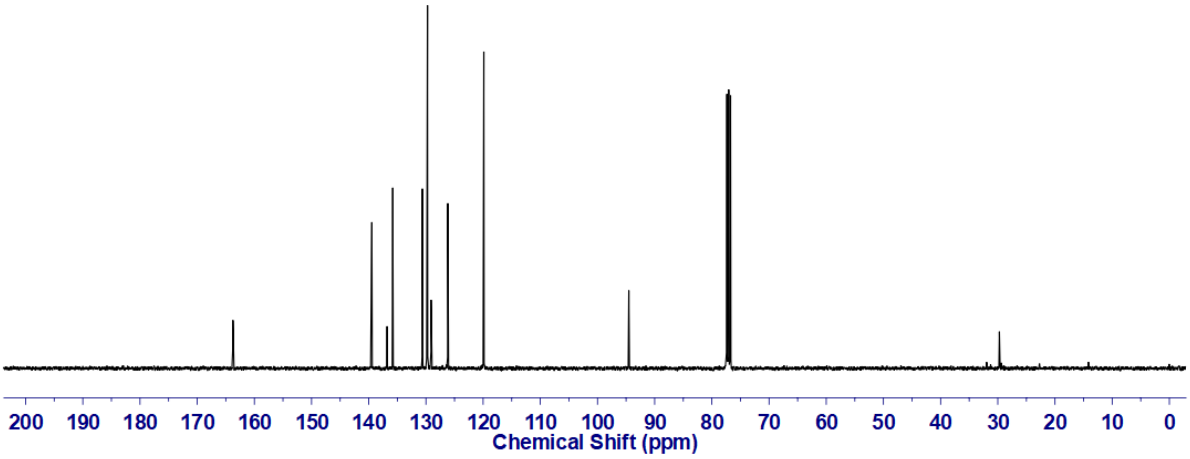

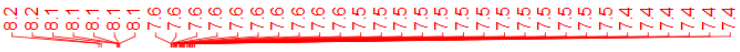

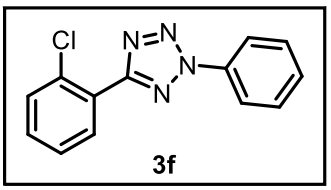

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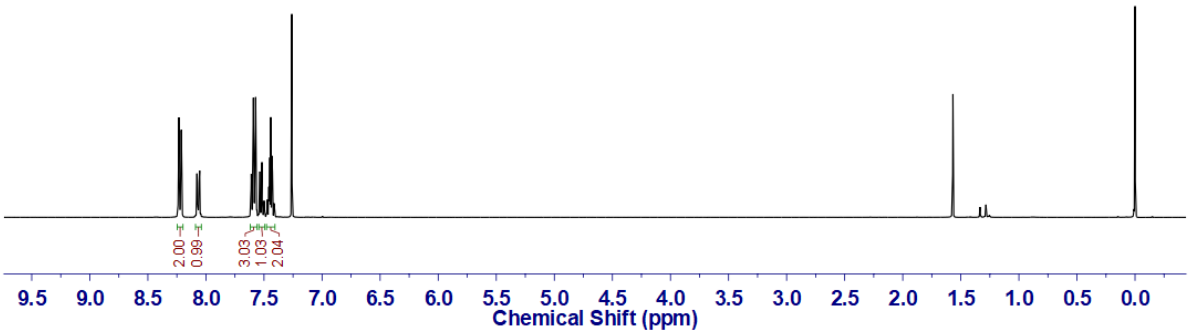
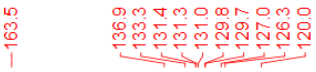
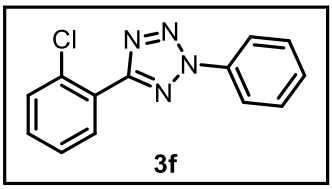
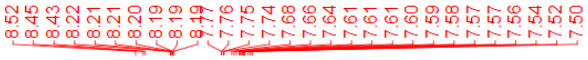
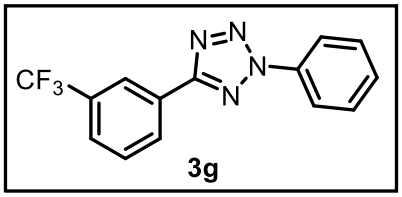






^{13}C{^{1}H} NMR, $CDCl_3$, 100 MHz, 298K





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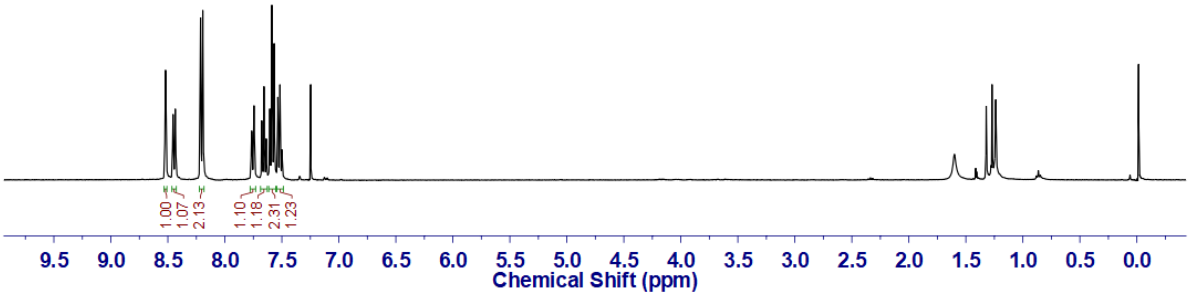
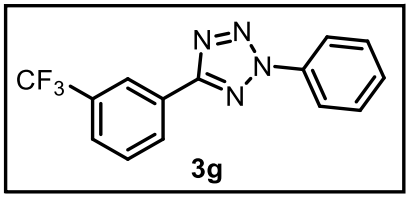
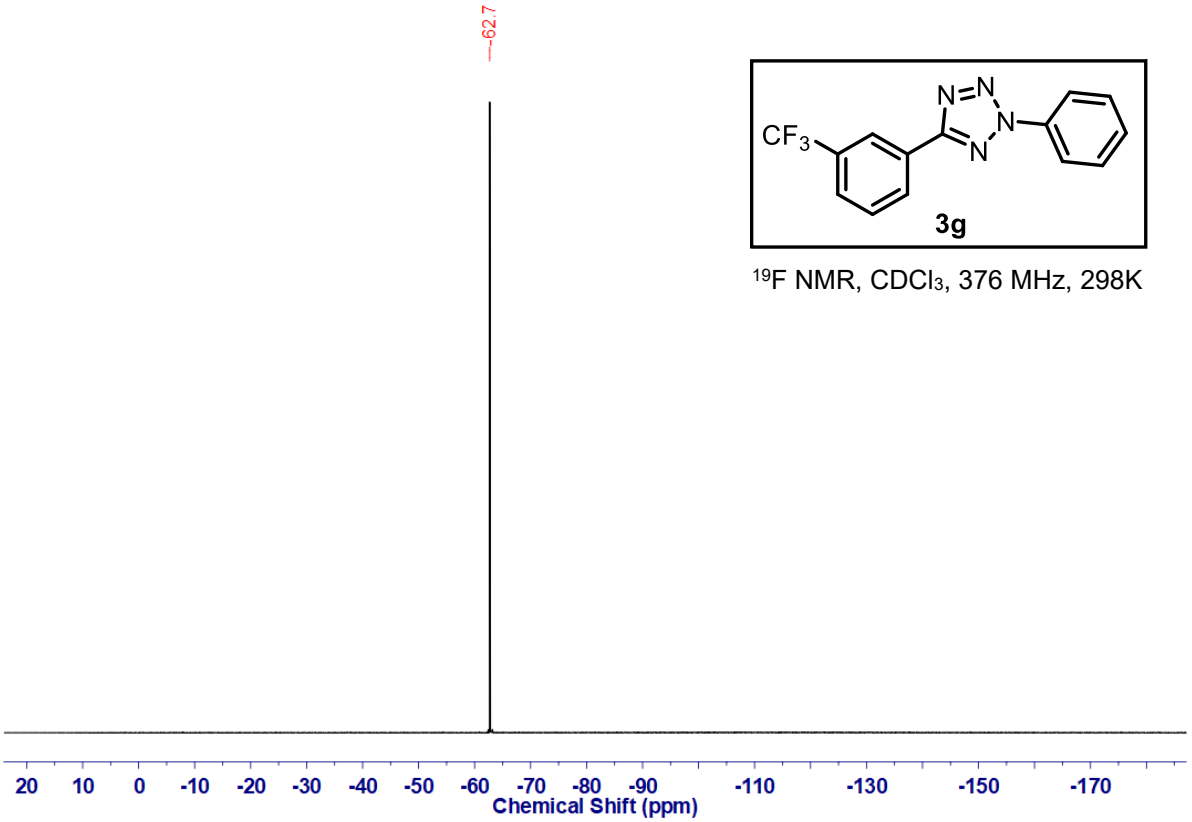




$^{13}C\{^{1}H\}$ NMR, $CDCl_3$, 100 MHz, 298K



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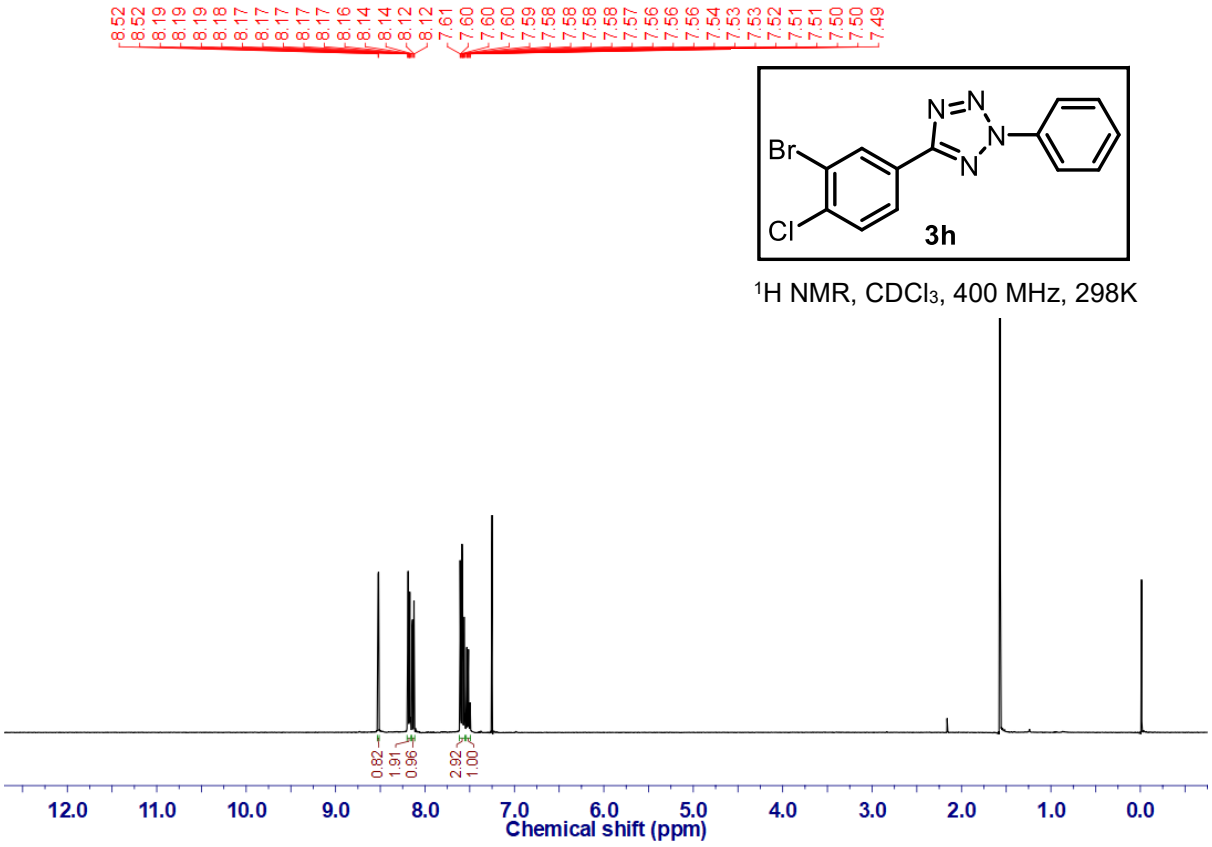

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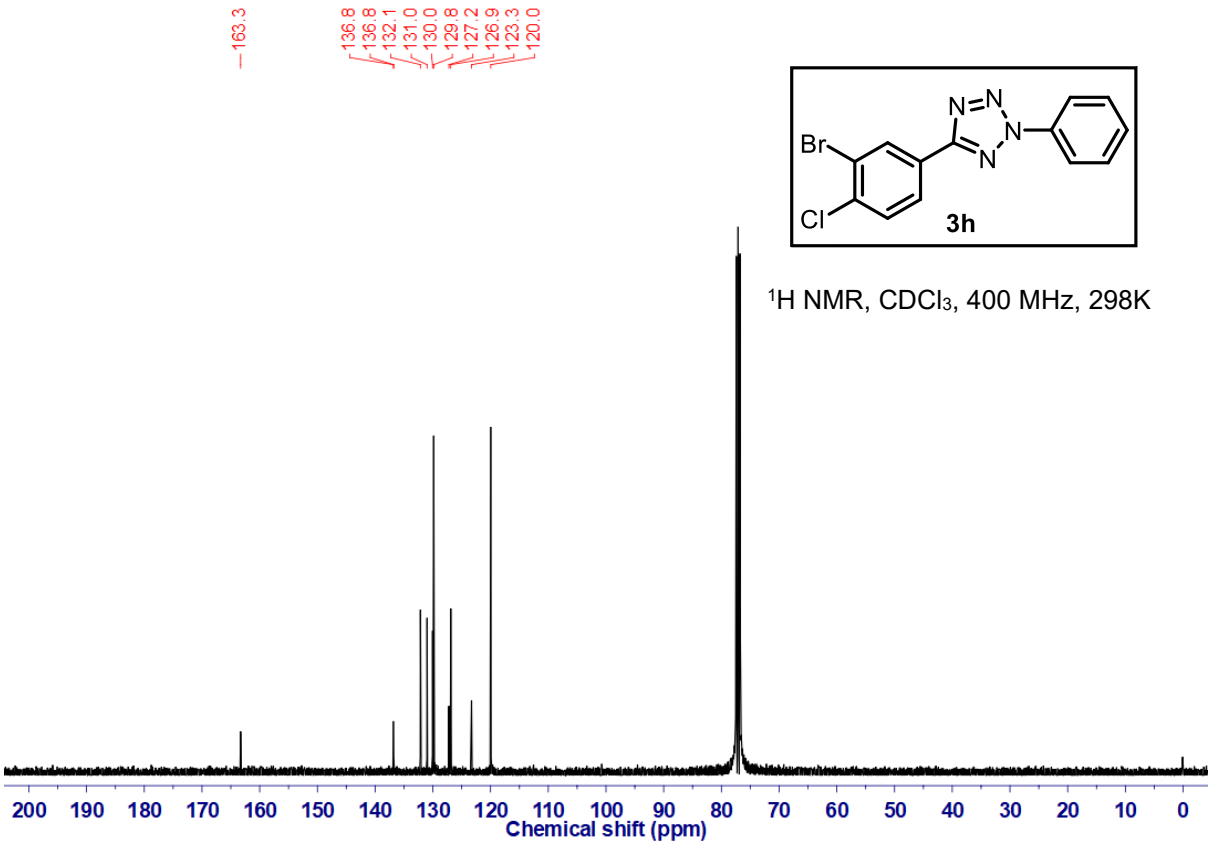
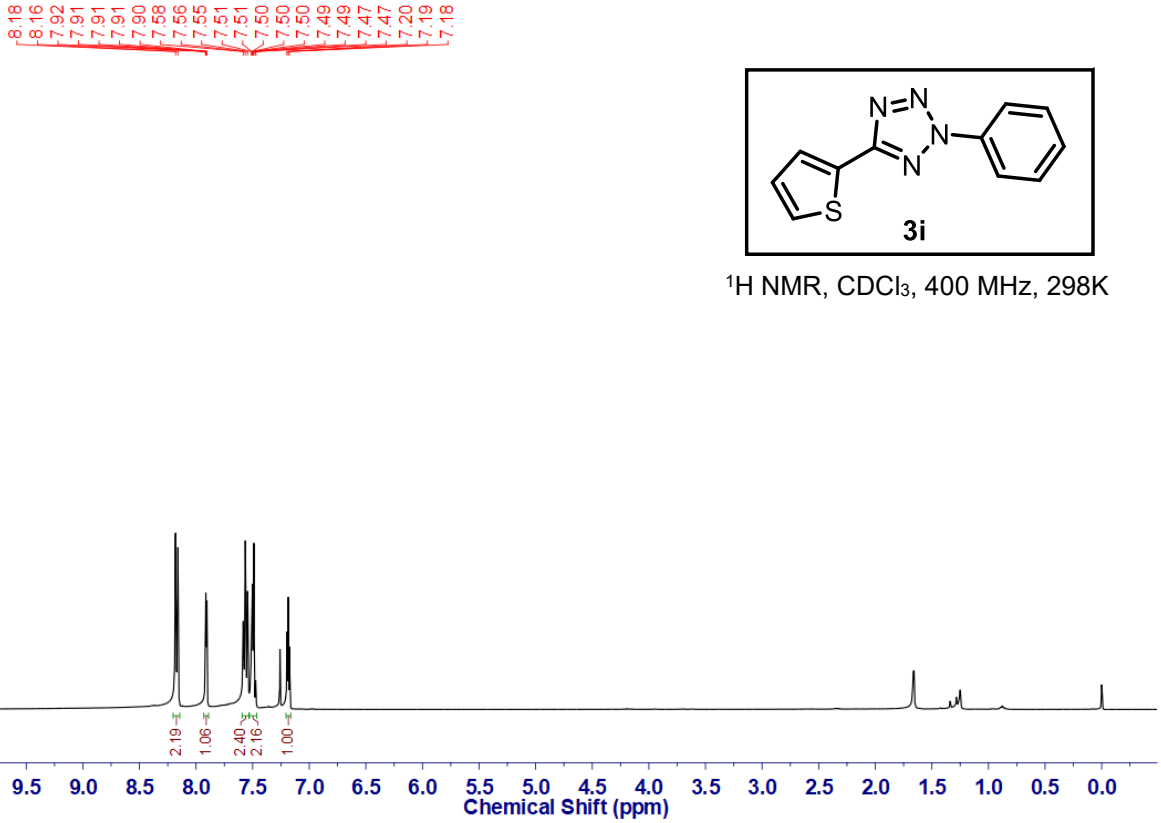


^{1}H NMR, $CDCl_3$, 400 MHz, 298K



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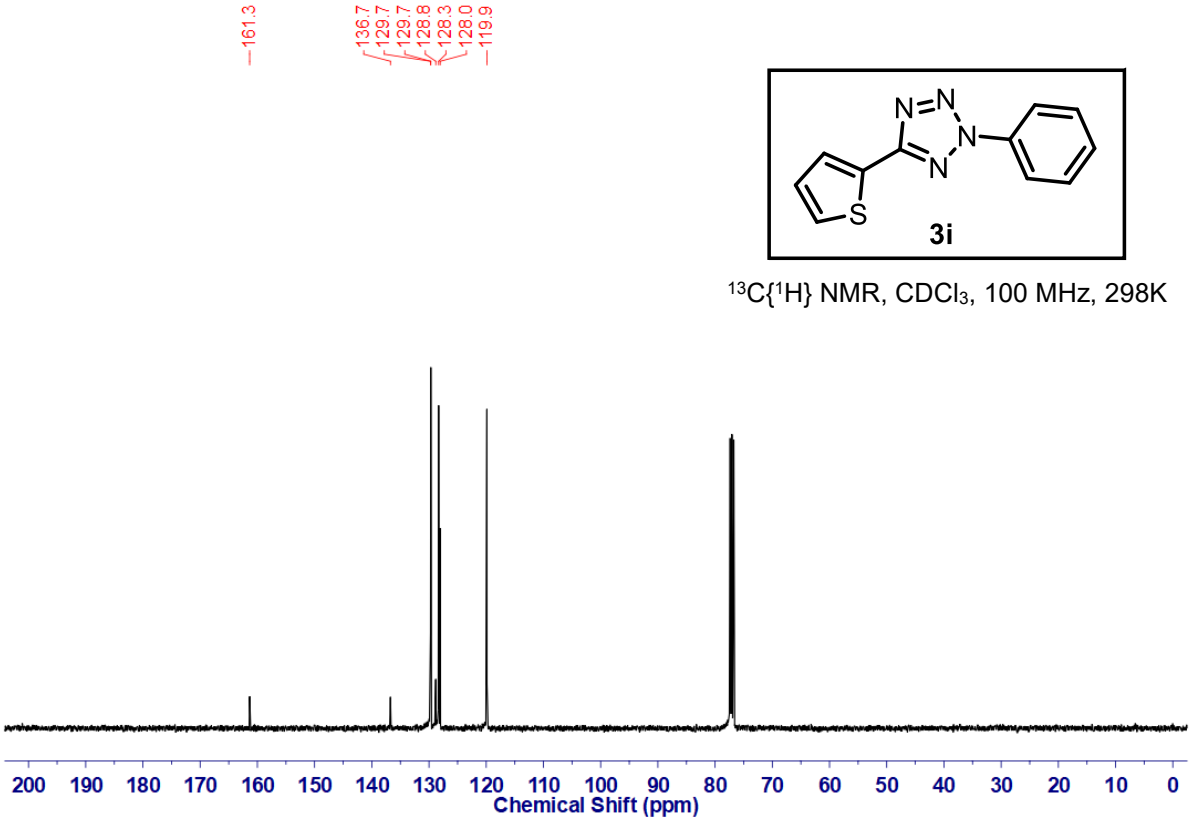

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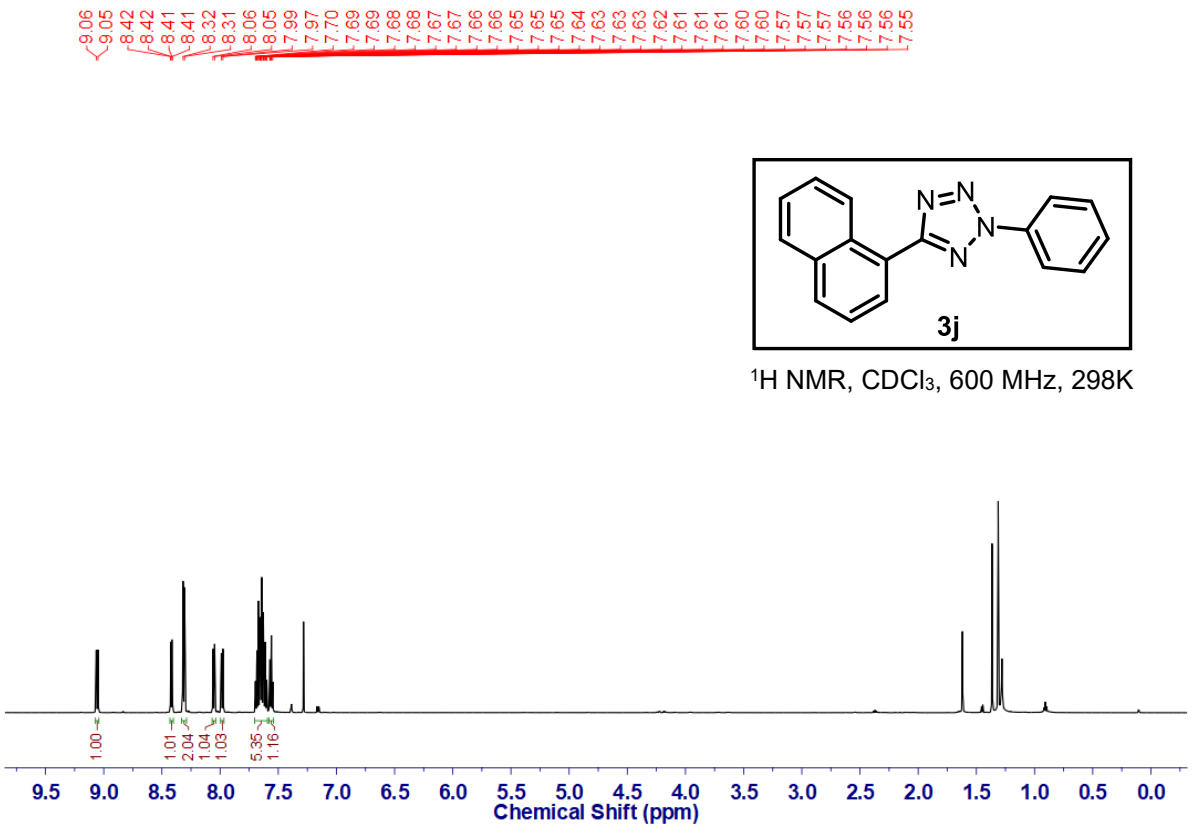

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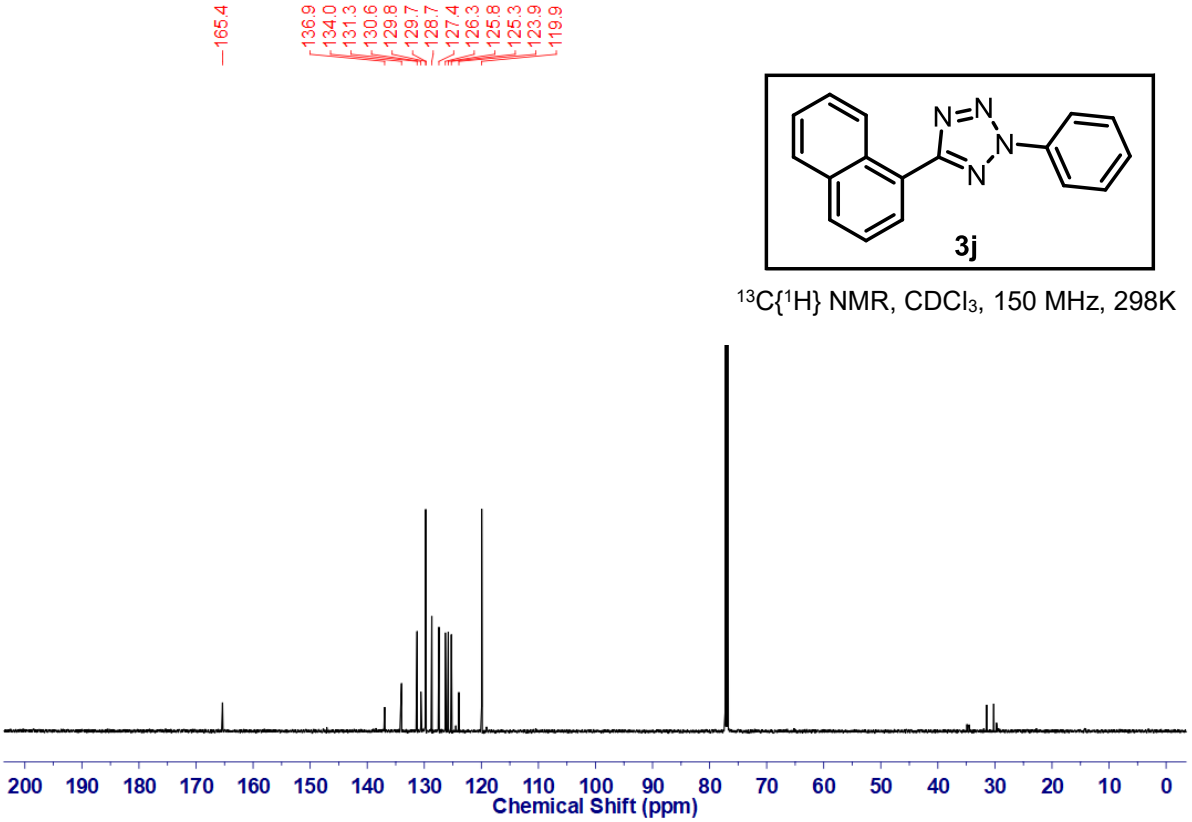

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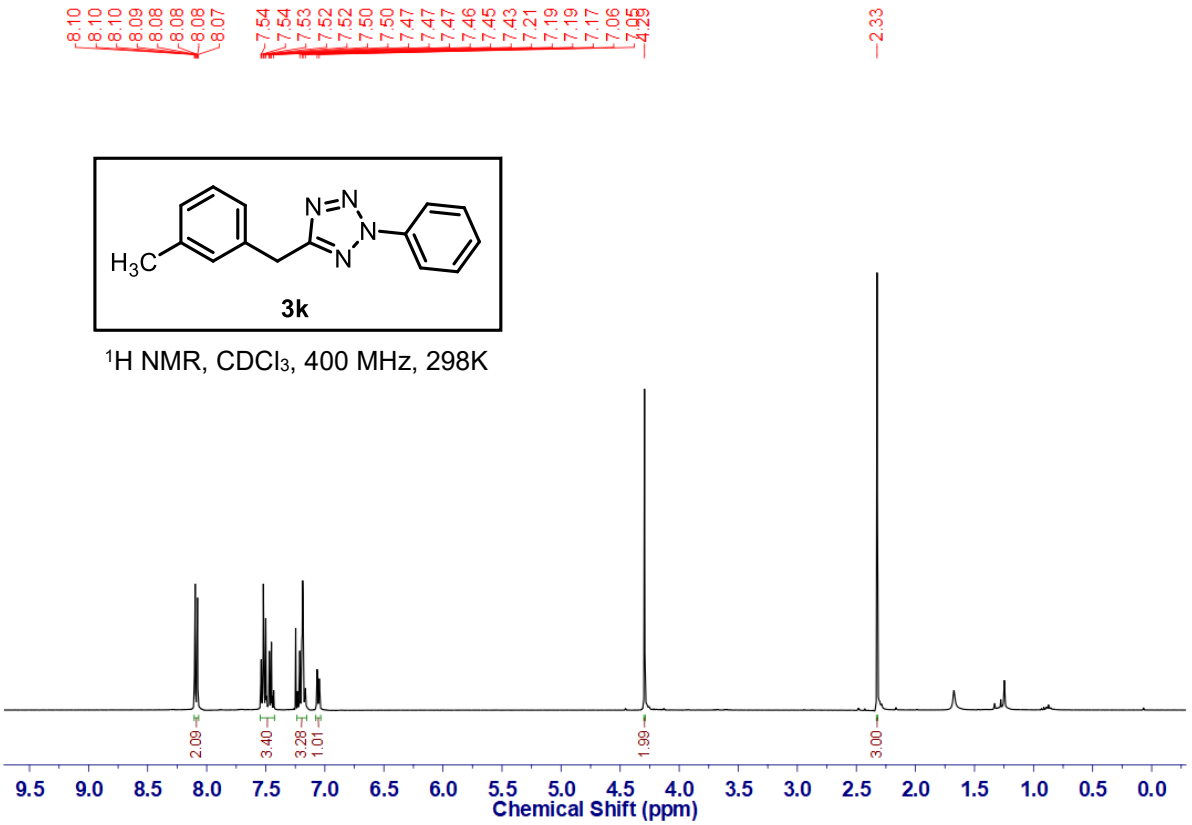

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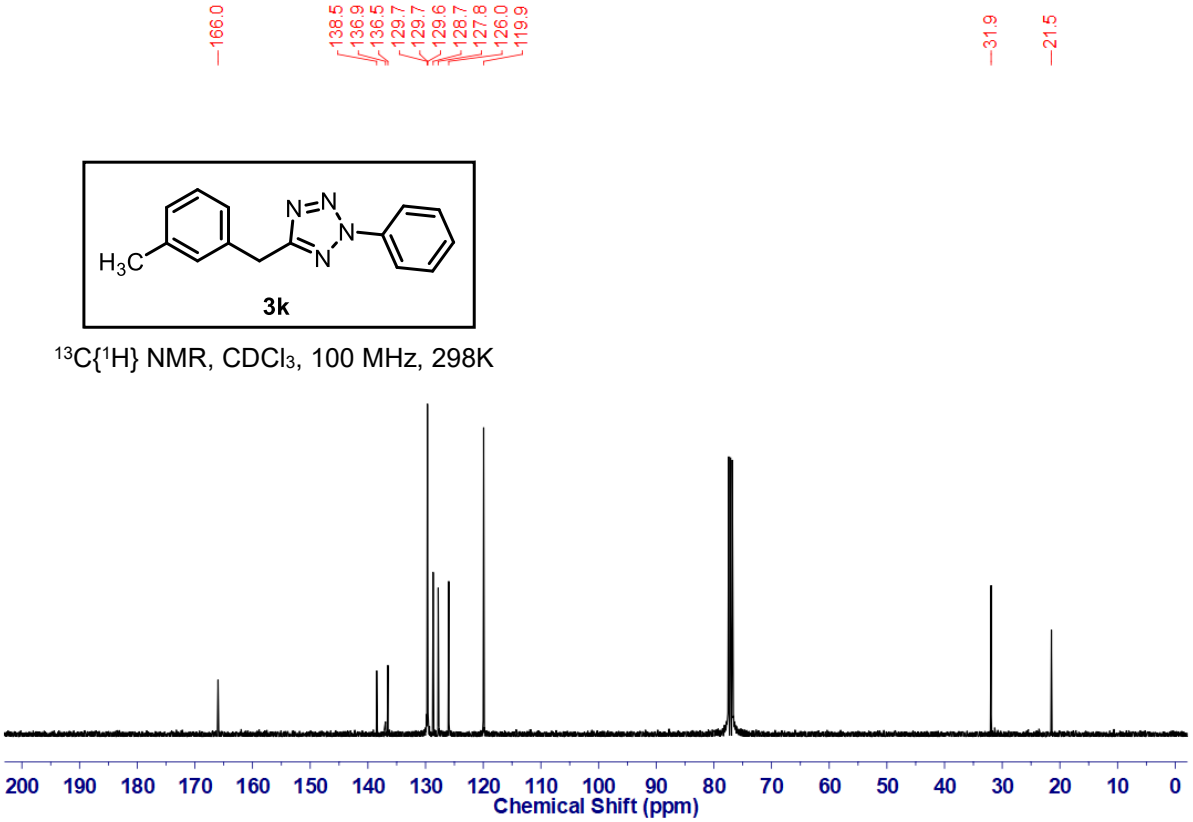

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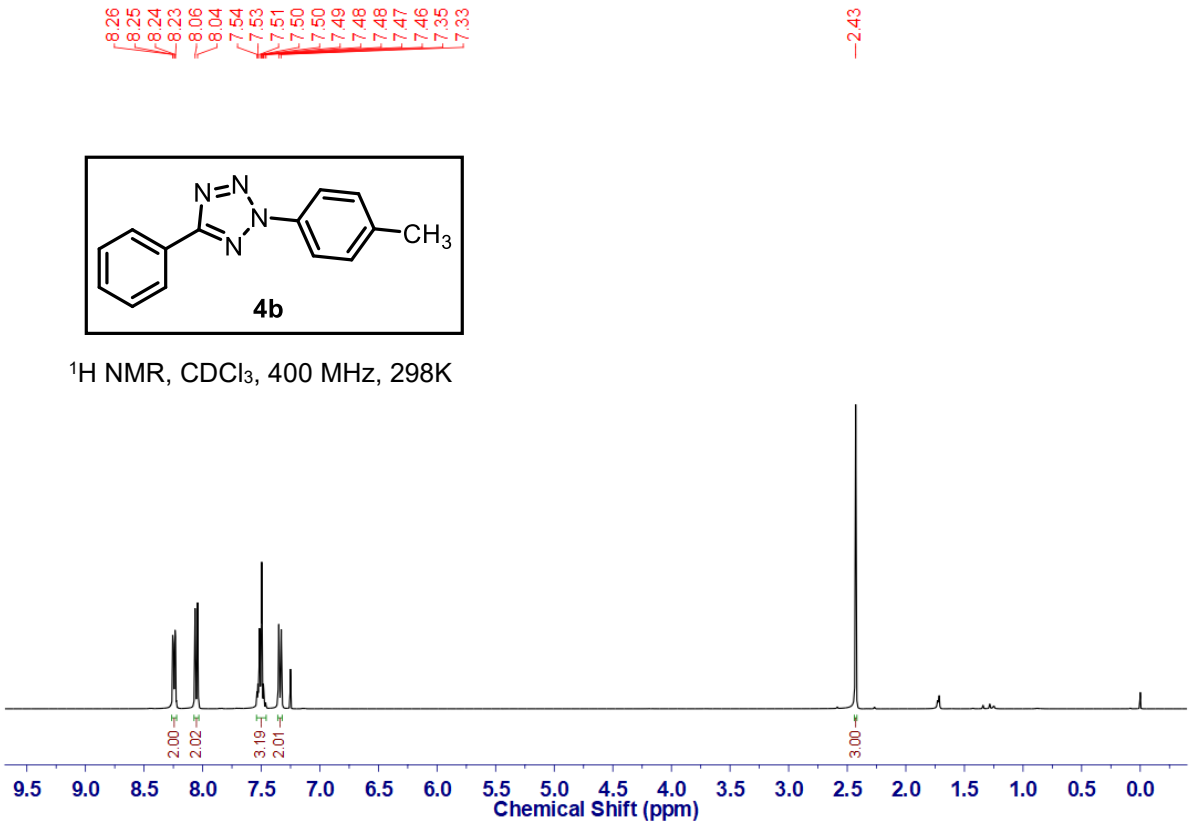
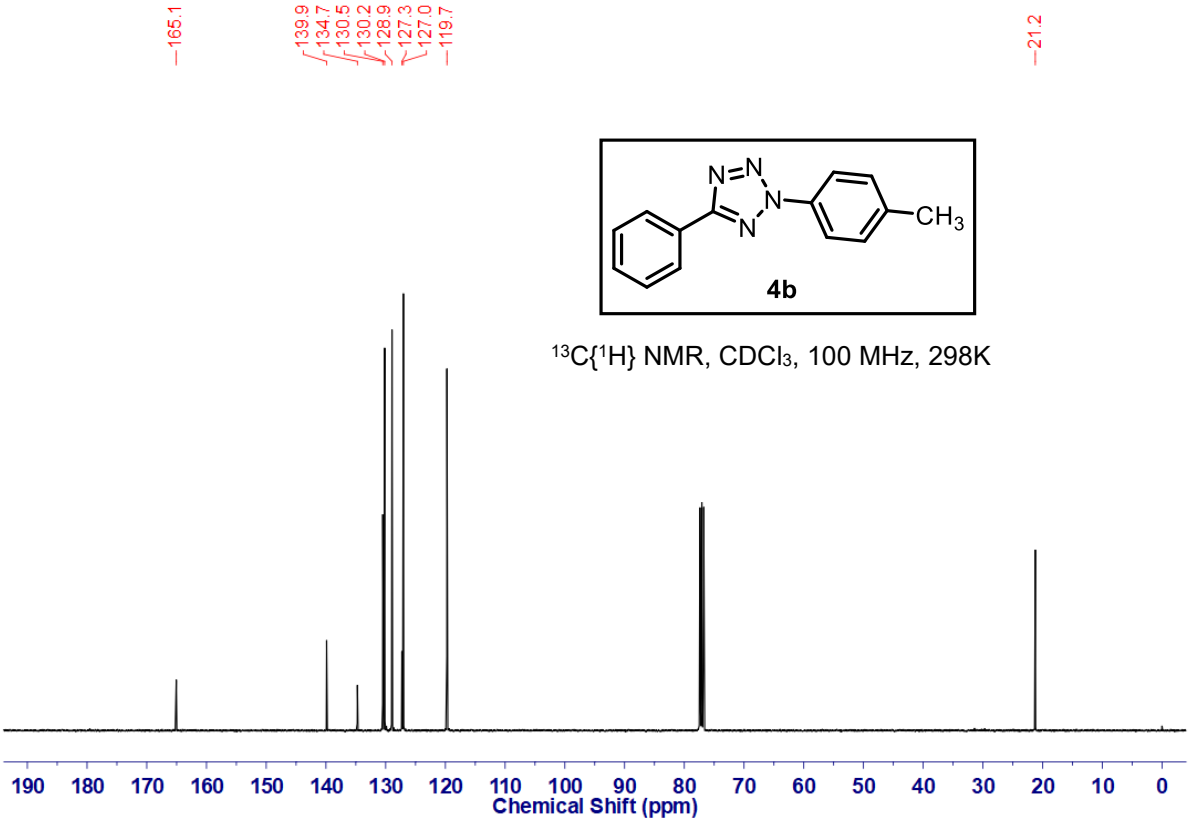
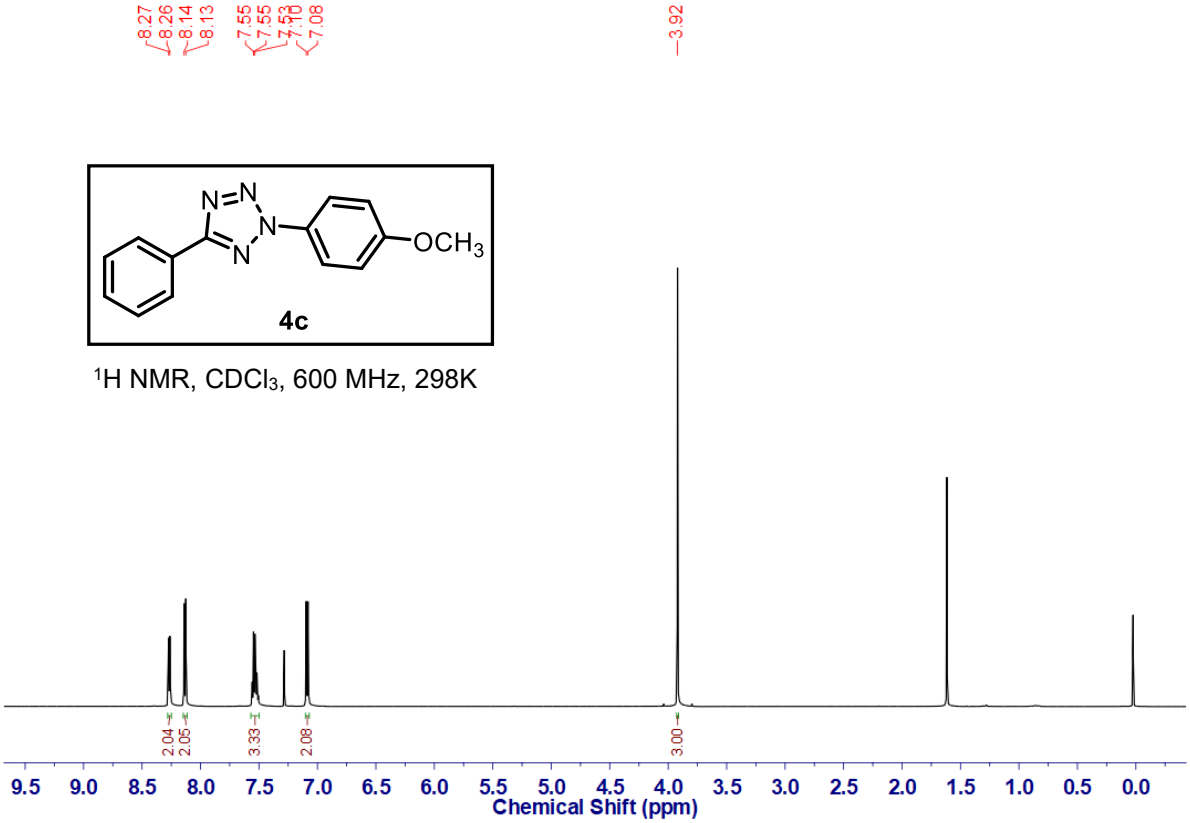


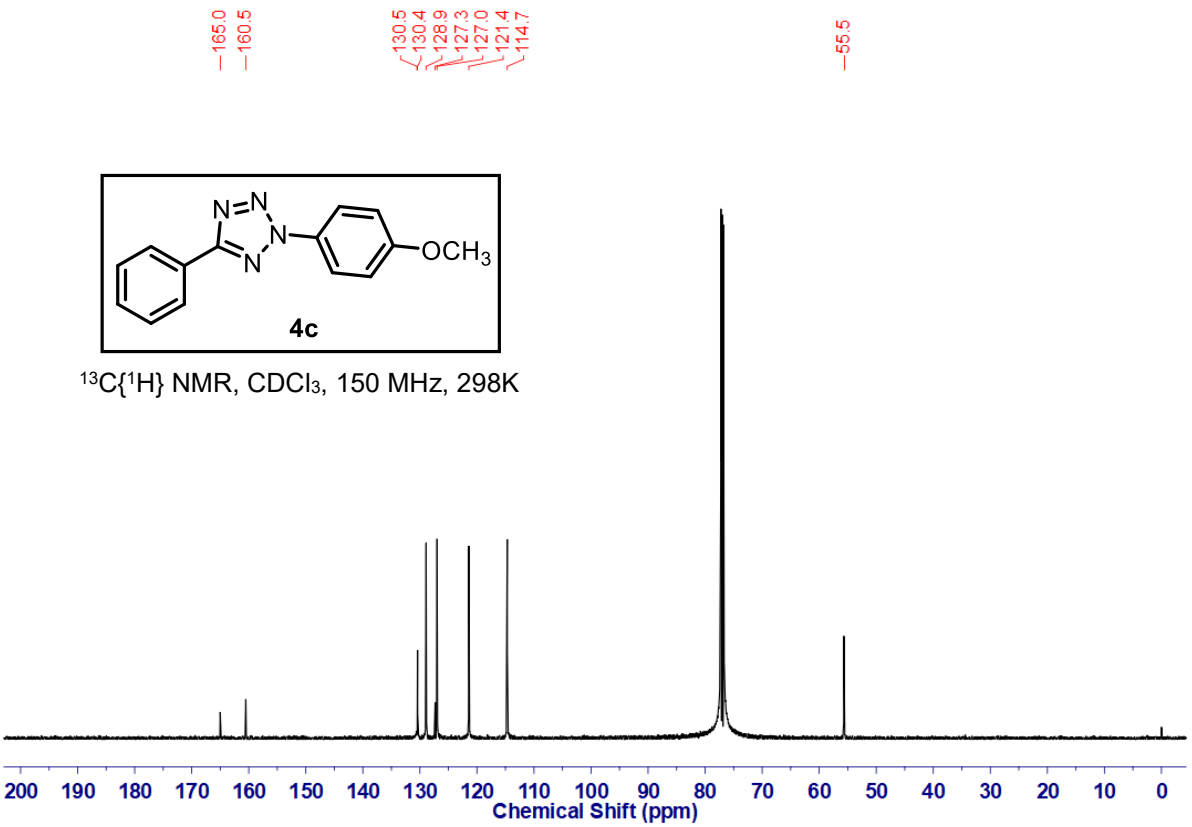
^{1}H NMR, $CDCl_3$, 400 MHz, 298K



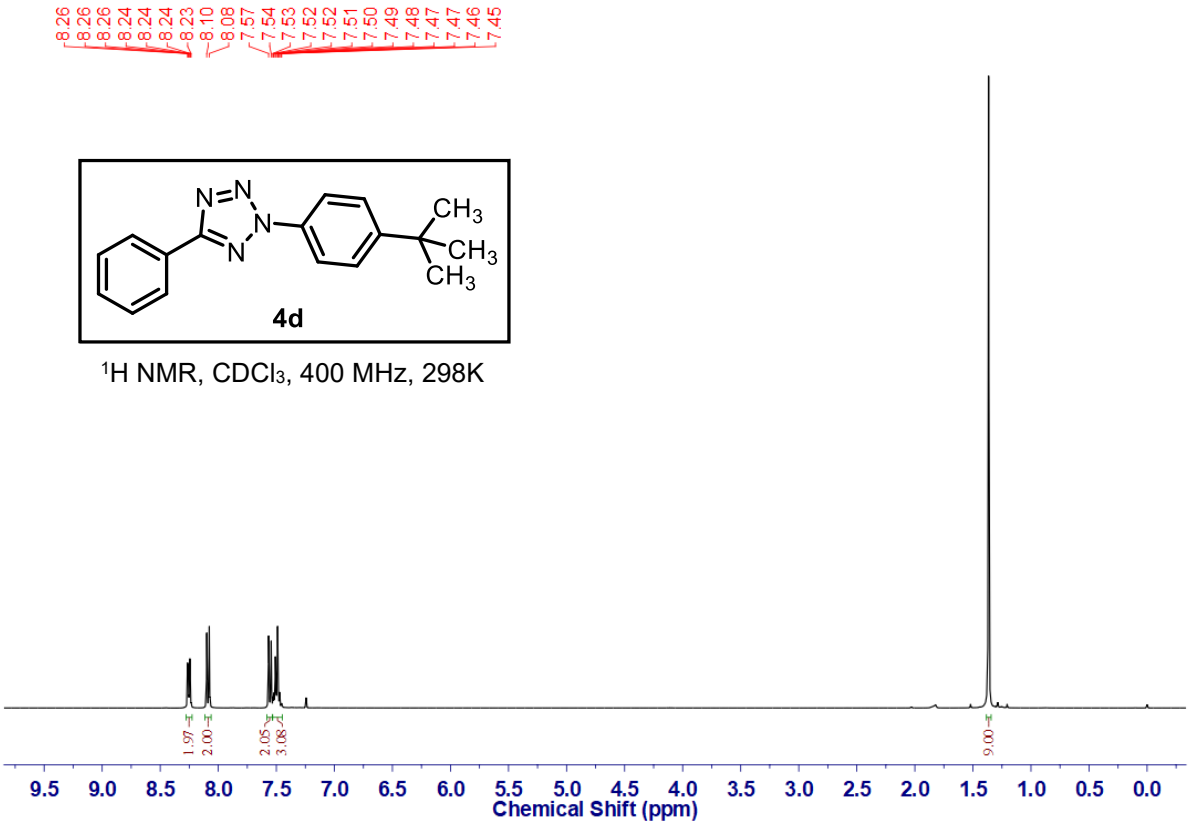
$^{13}C\{^{1}H\}$ NMR, $CDCl_3$, 100 MHz, 298K



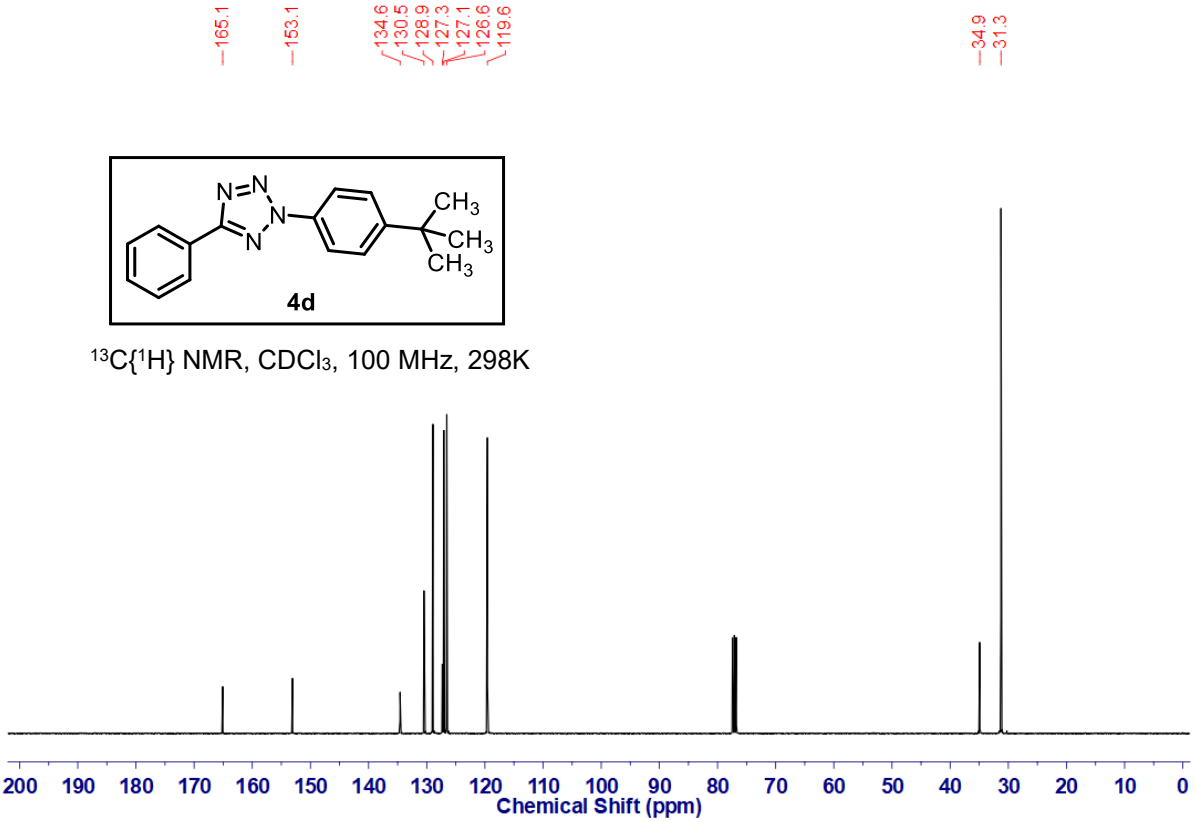
^{1}H NMR, $CDCl_3$, 600 MHz, 298K



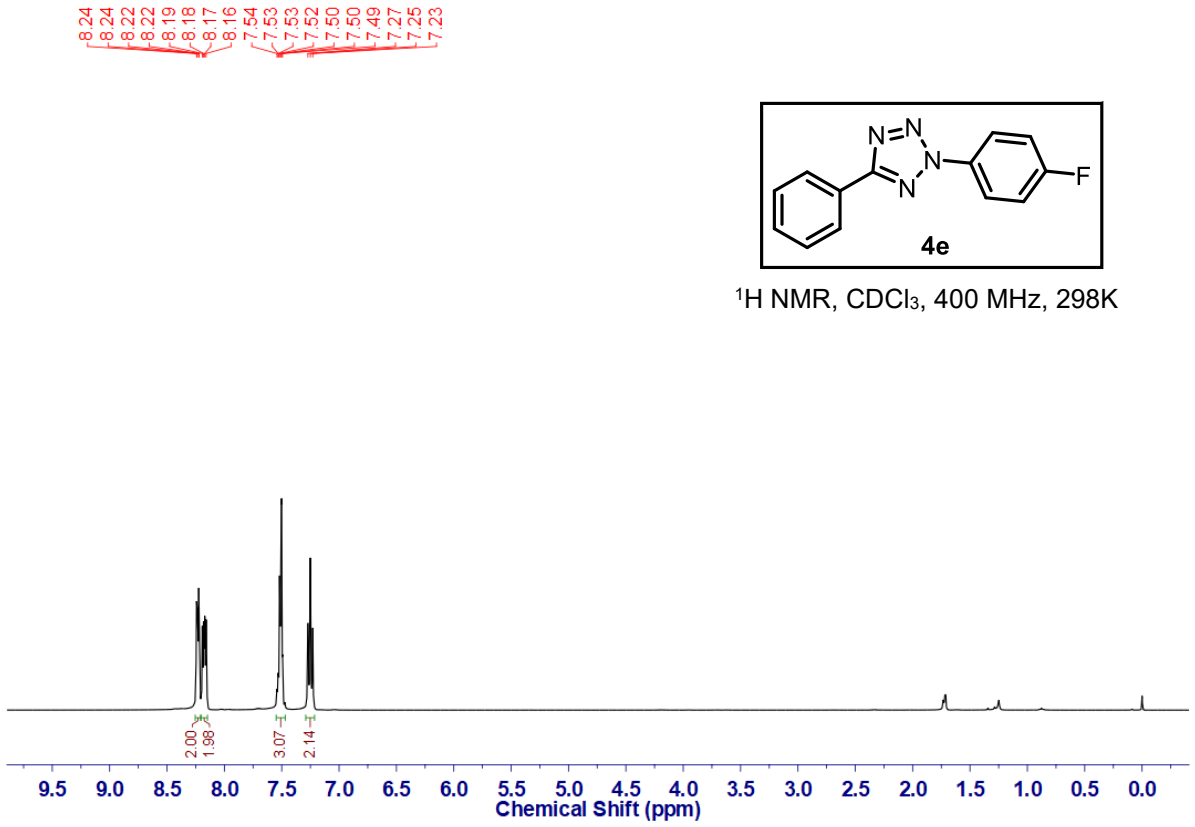
$^{13}C\{^{1}H\}$ NMR, $CDCl_3$, 150 MHz, 298K



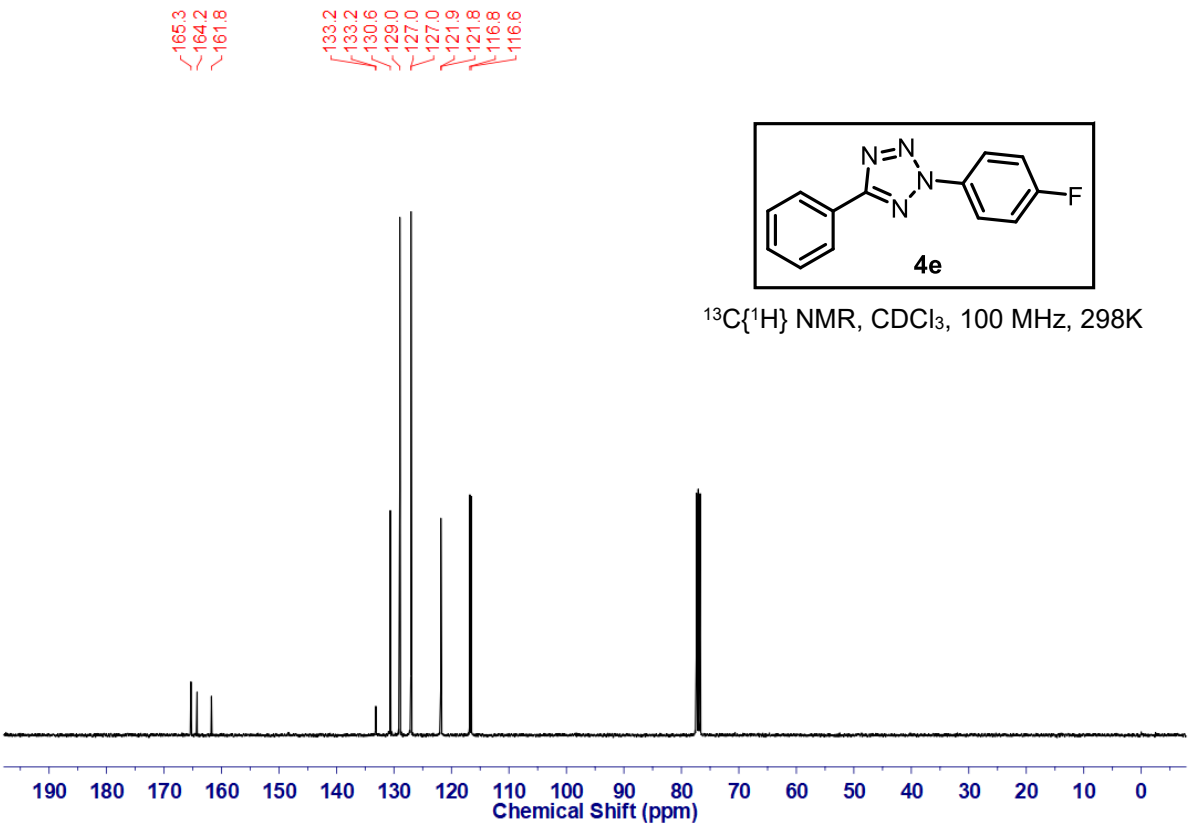
^{1}H NMR, $CDCl_3$, 400 MHz, 298K



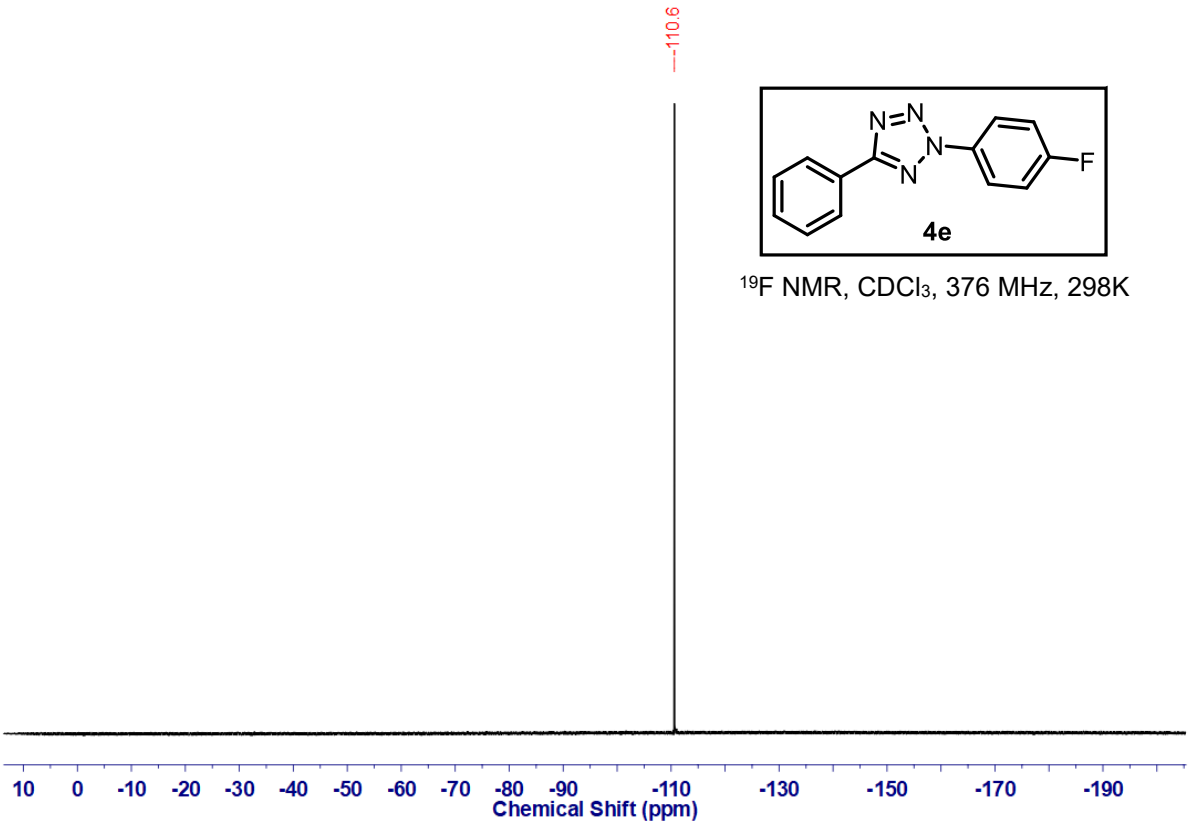
$^{13}C\{^{1}H\}$ NMR, $CDCl_3$, 100 MHz, 298K



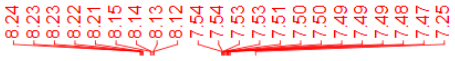
^{1}H NMR, $CDCl_3$, 400 MHz, 298K

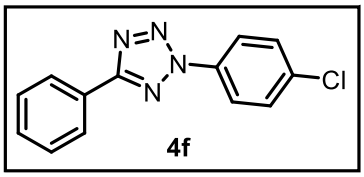


$^{13}C\{^{1}H\}$ NMR, $CDCl_3$, 100 MHz, 298K

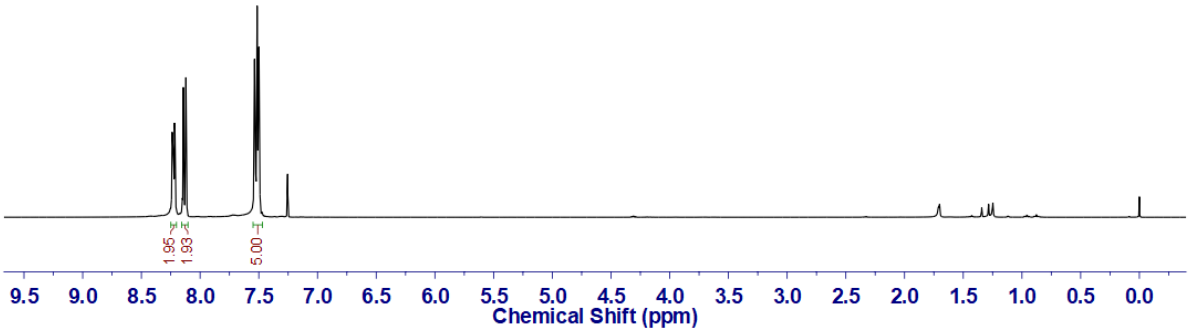


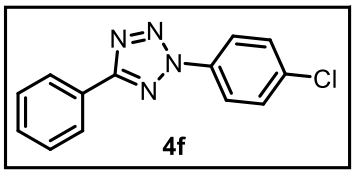
^{19}F NMR, $CDCl_3$, 376 MHz, 298K



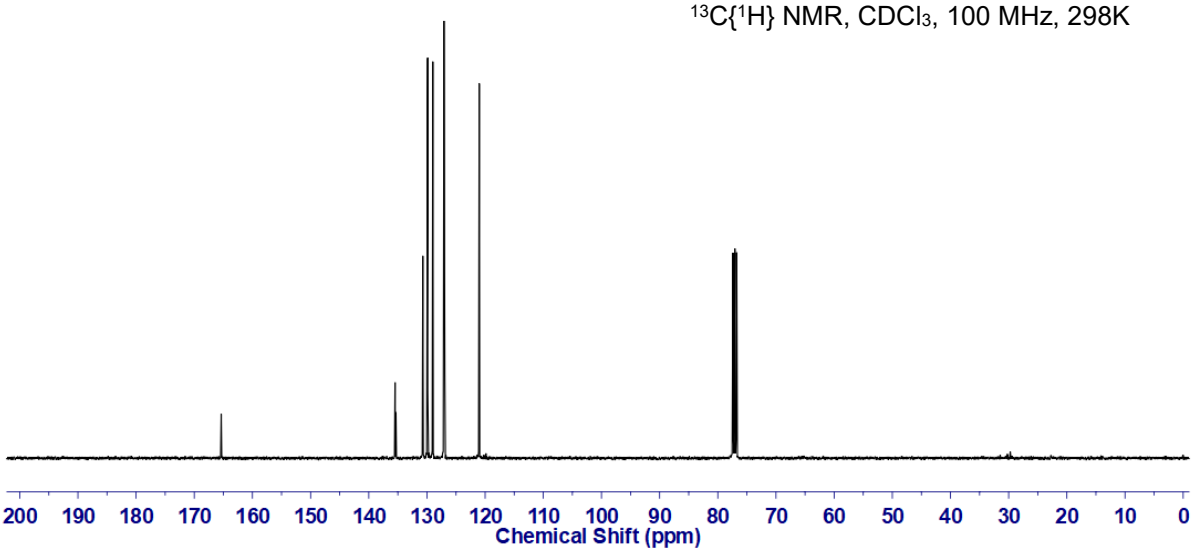


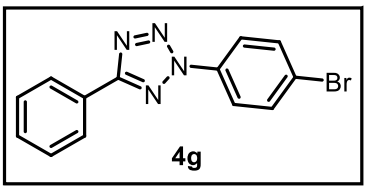
^{1}H NMR, $CDCl_3$, 400 MHz, 298K



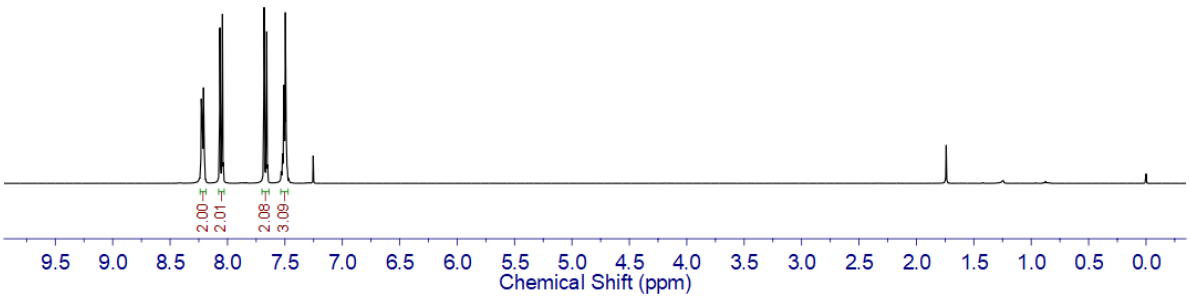


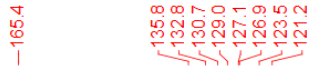
^{13}C{^{1}H} NMR, $CDCl_3$, 100 MHz, 298K

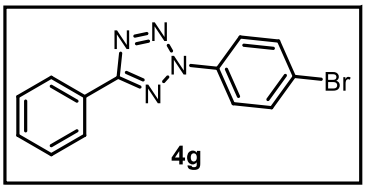




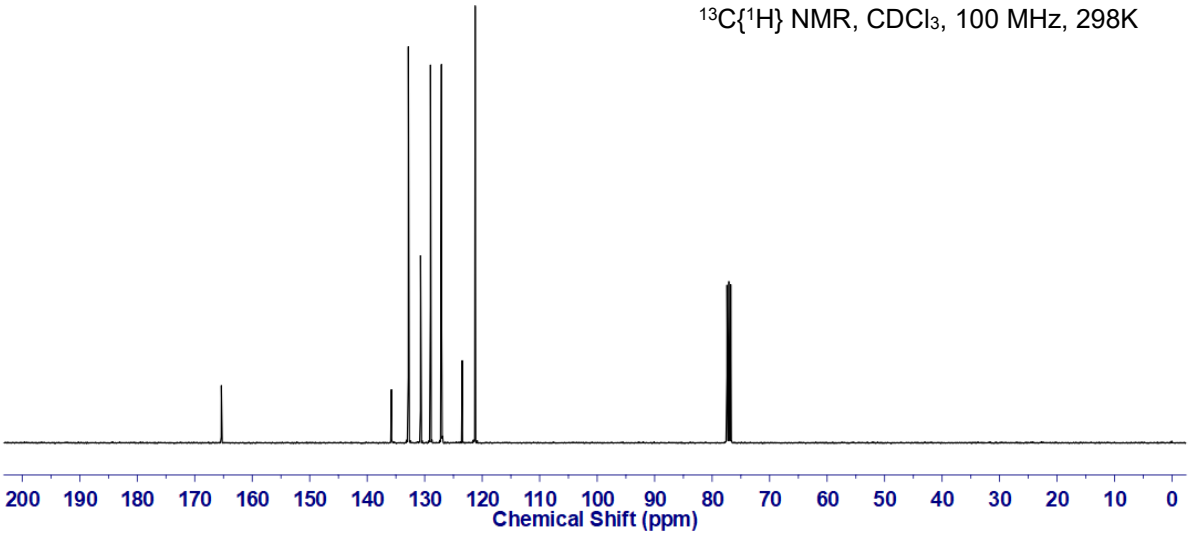
^{1}H NMR, $CDCl_3$, 400 MHz, 298K

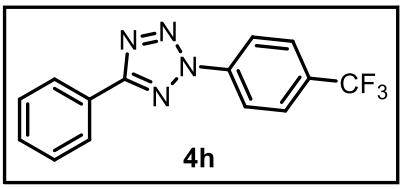




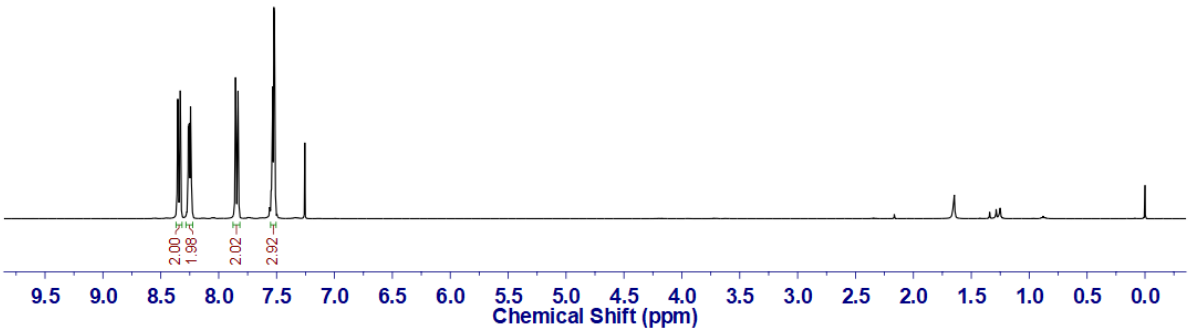


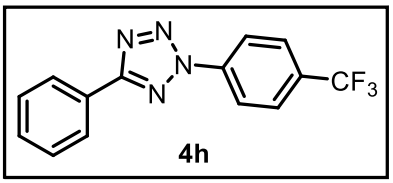
$^{13}C\{^{1}H\}$ NMR, $CDCl_3$, 100 MHz, 298K



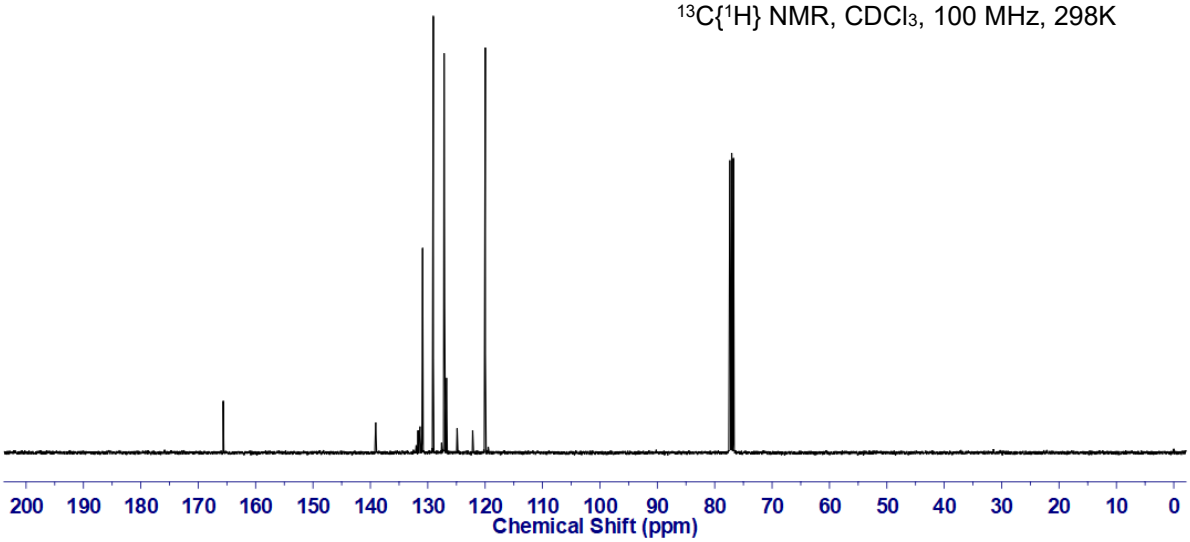


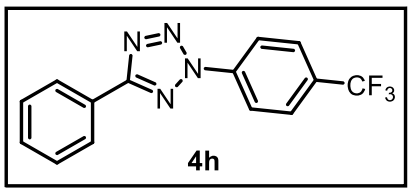
^{1}H NMR, $CDCl_3$, 400 MHz, 298K





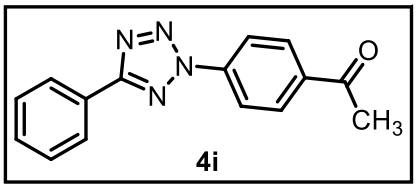
^{13}C{^{1}H} NMR, $CDCl_3$, 100 MHz, 298K





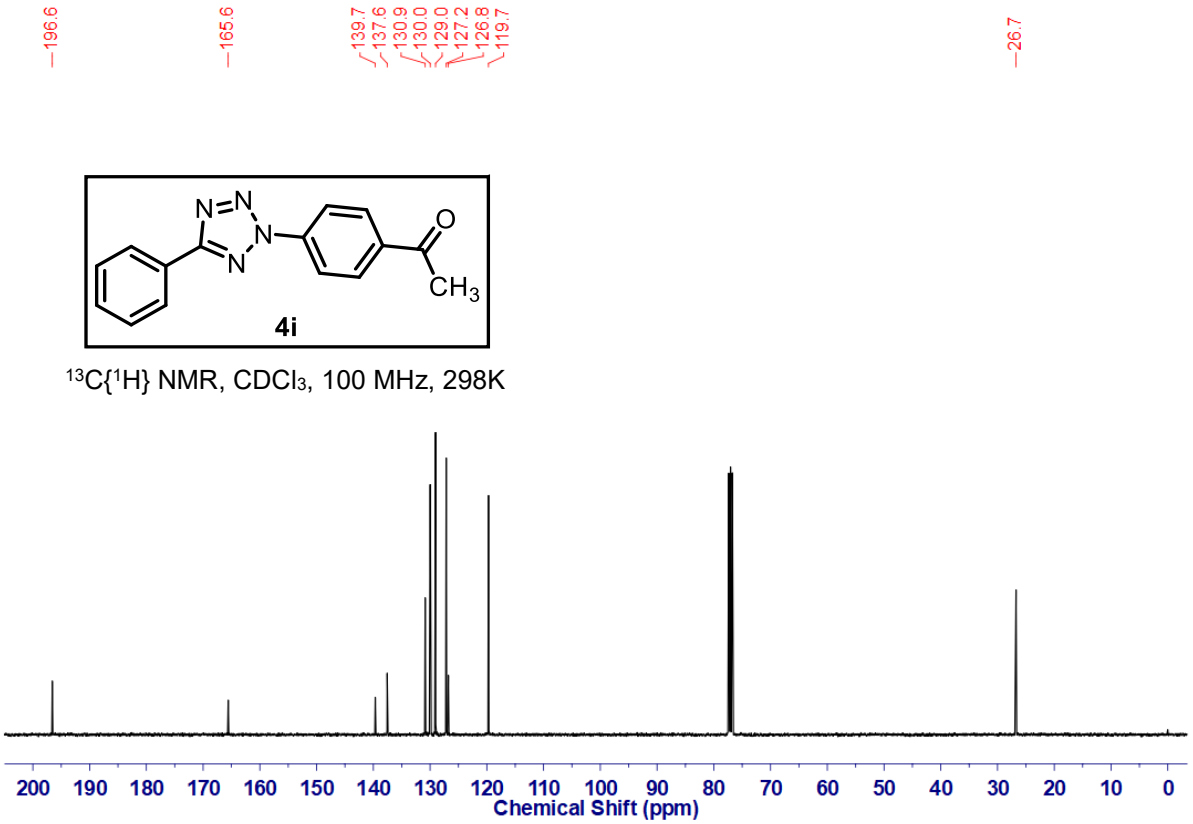
4h

^{19}F NMR, $CDCl_3$, 376 MHz, 298K

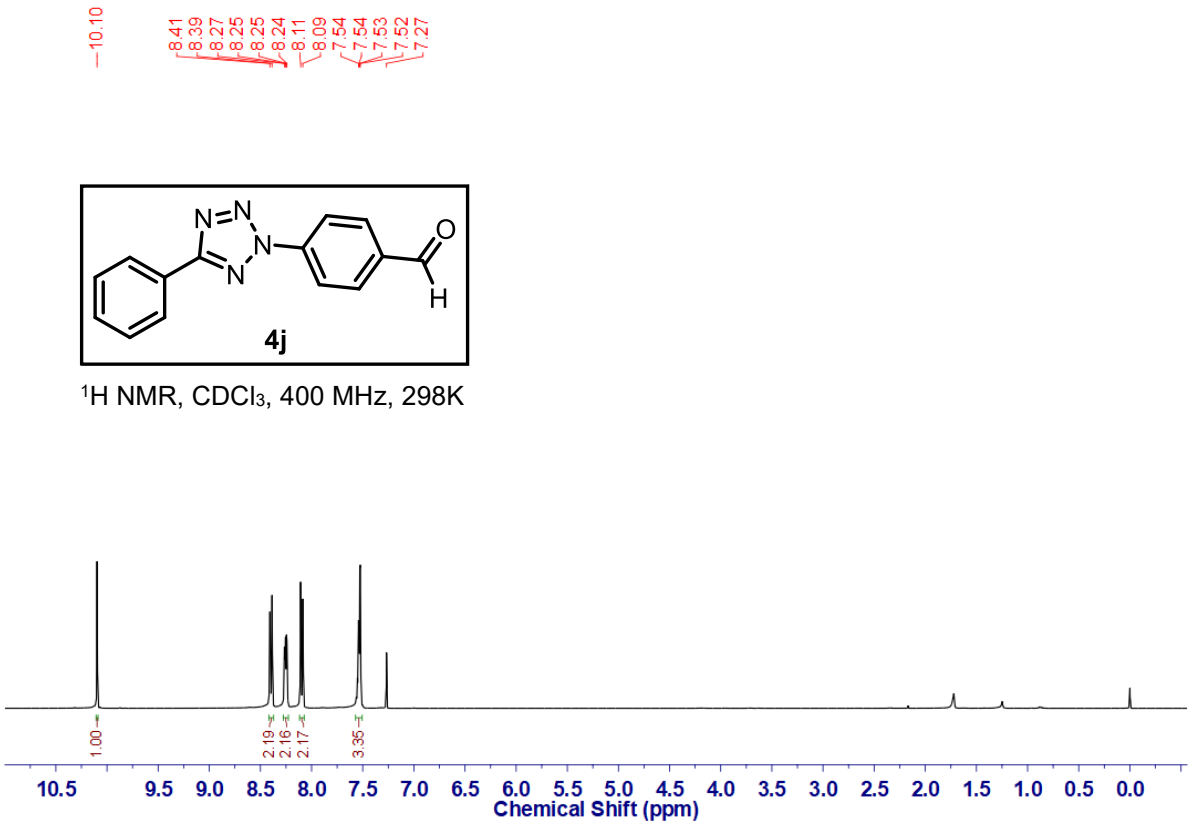


4i

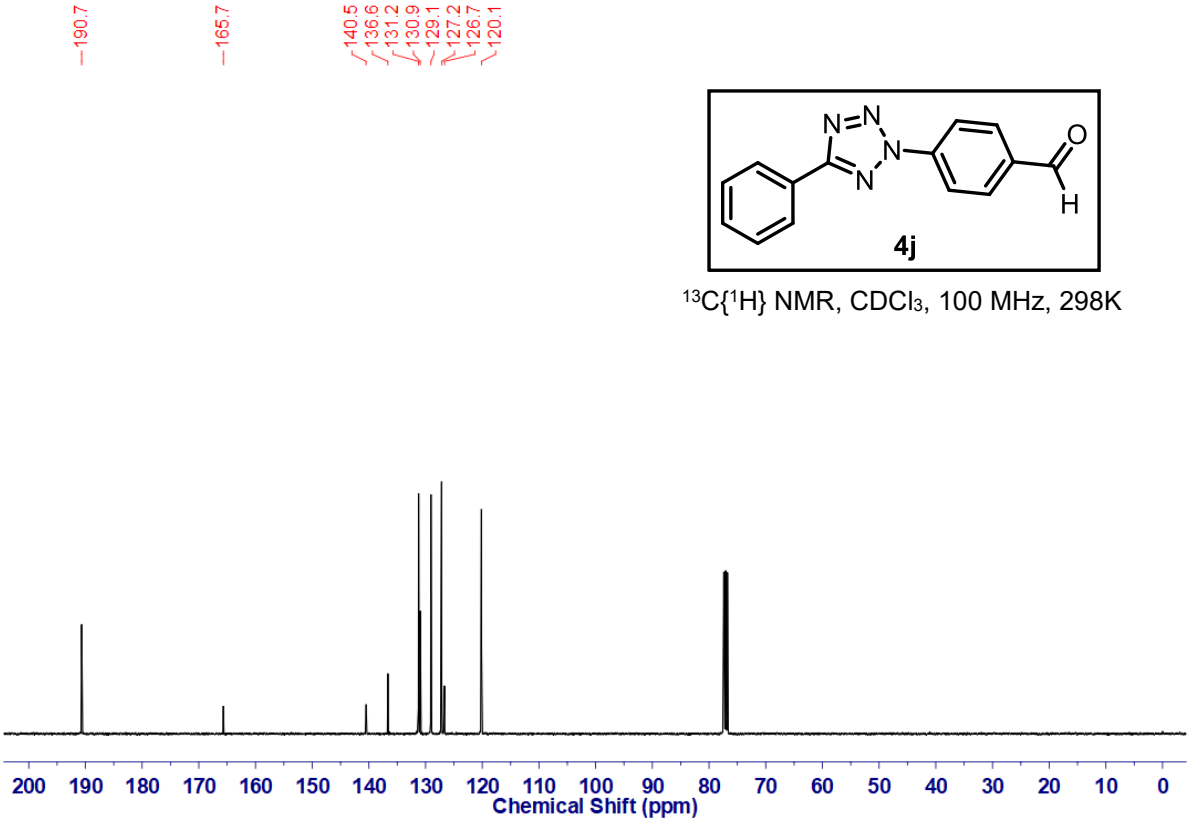
^{1}H NMR, $CDCl_3$, 400 MHz, 298K



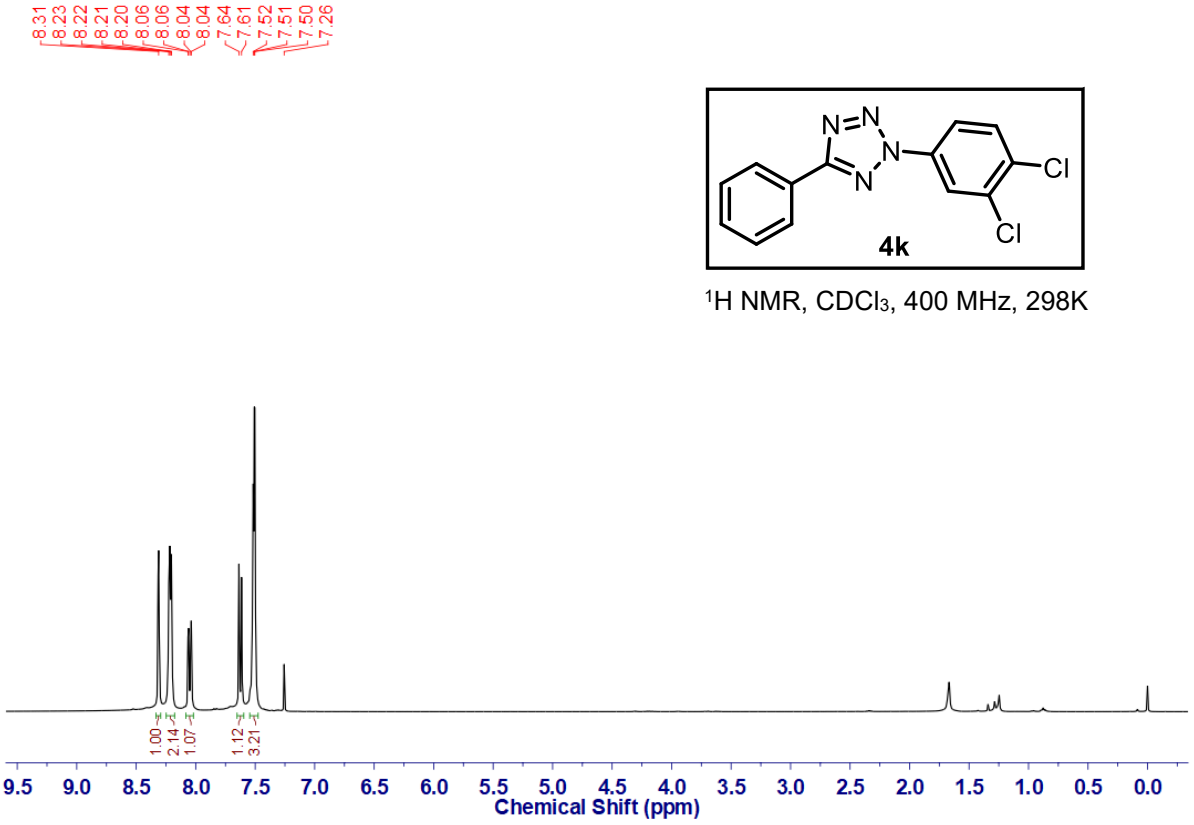
$^{13}C\{^{1}H\}$ NMR, $CDCl_3$, 100 MHz, 298K



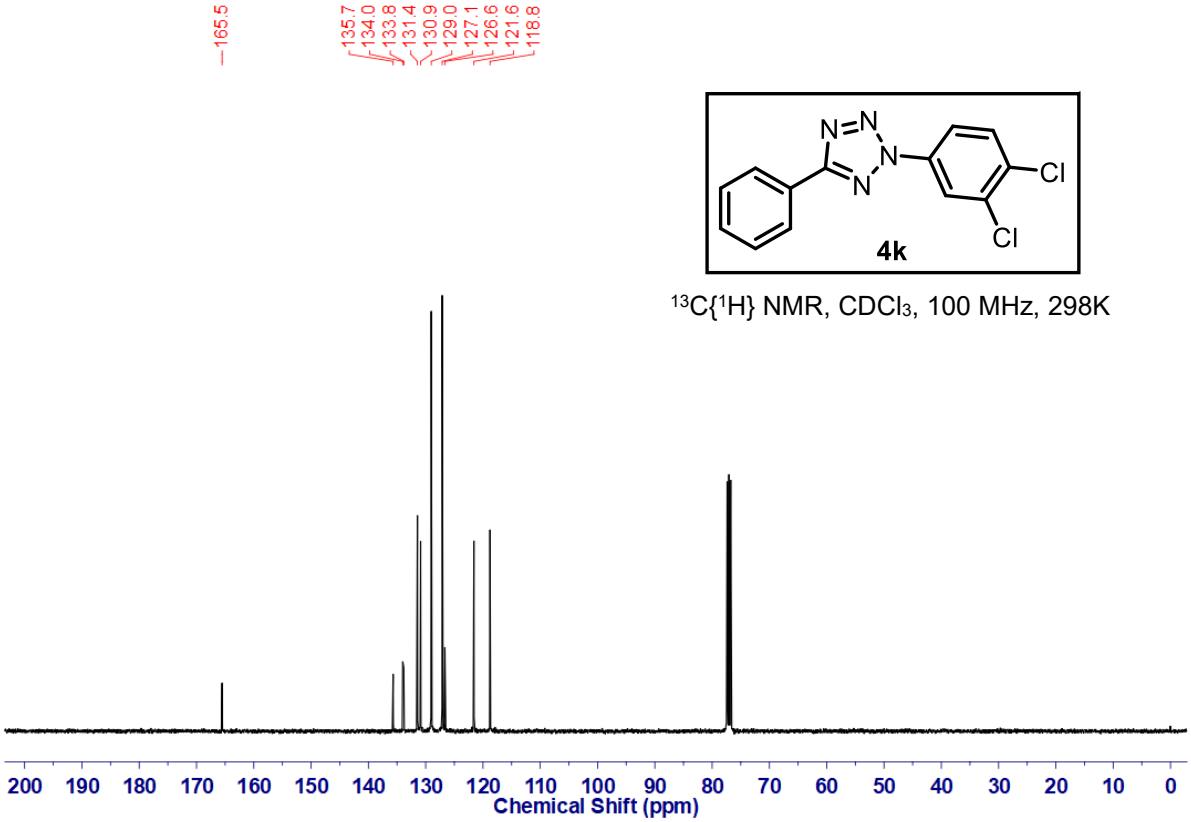
^{1}H NMR, $CDCl_3$, 400 MHz, 298K



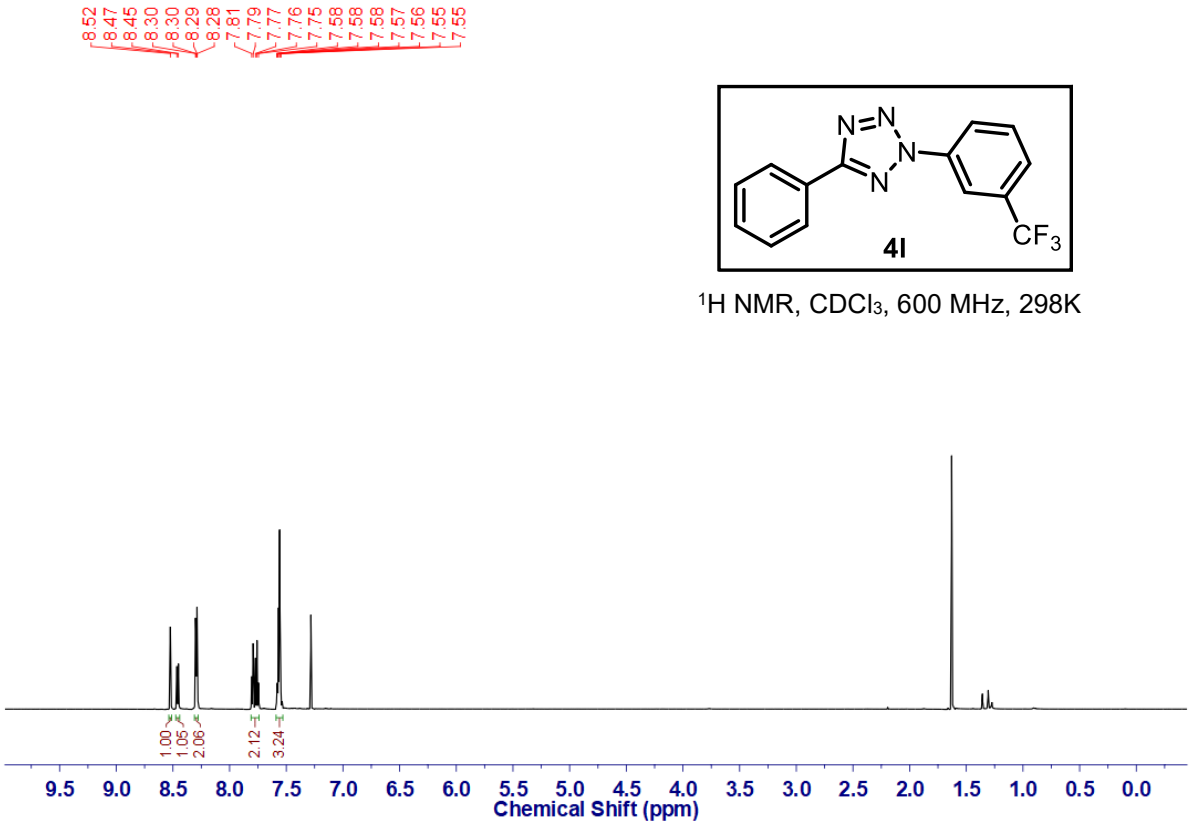
$^{13}C\{^{1}H\}$ NMR, $CDCl_3$, 100 MHz, 298K



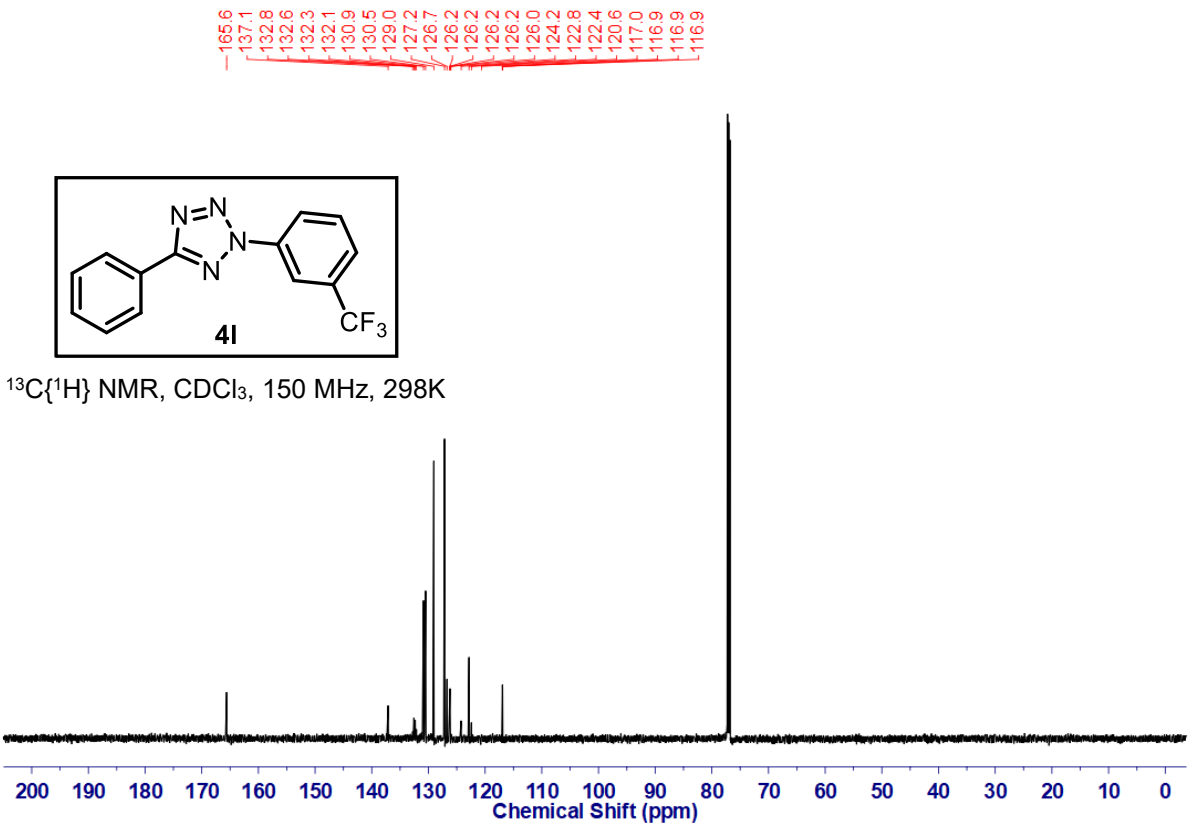
^{1}H NMR, $CDCl_3$, 400 MHz, 298K



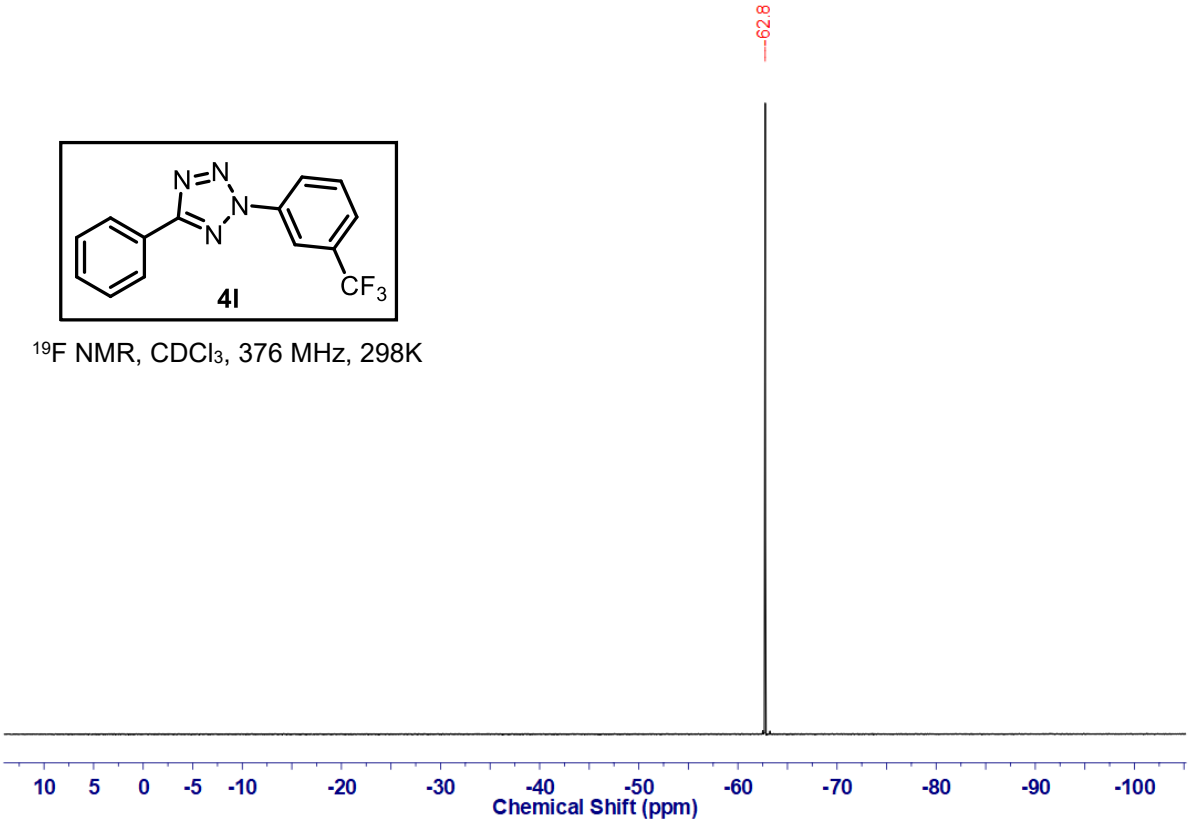
$^{13}C\{^{1}H\}$ NMR, $CDCl_3$, 100 MHz, 298K



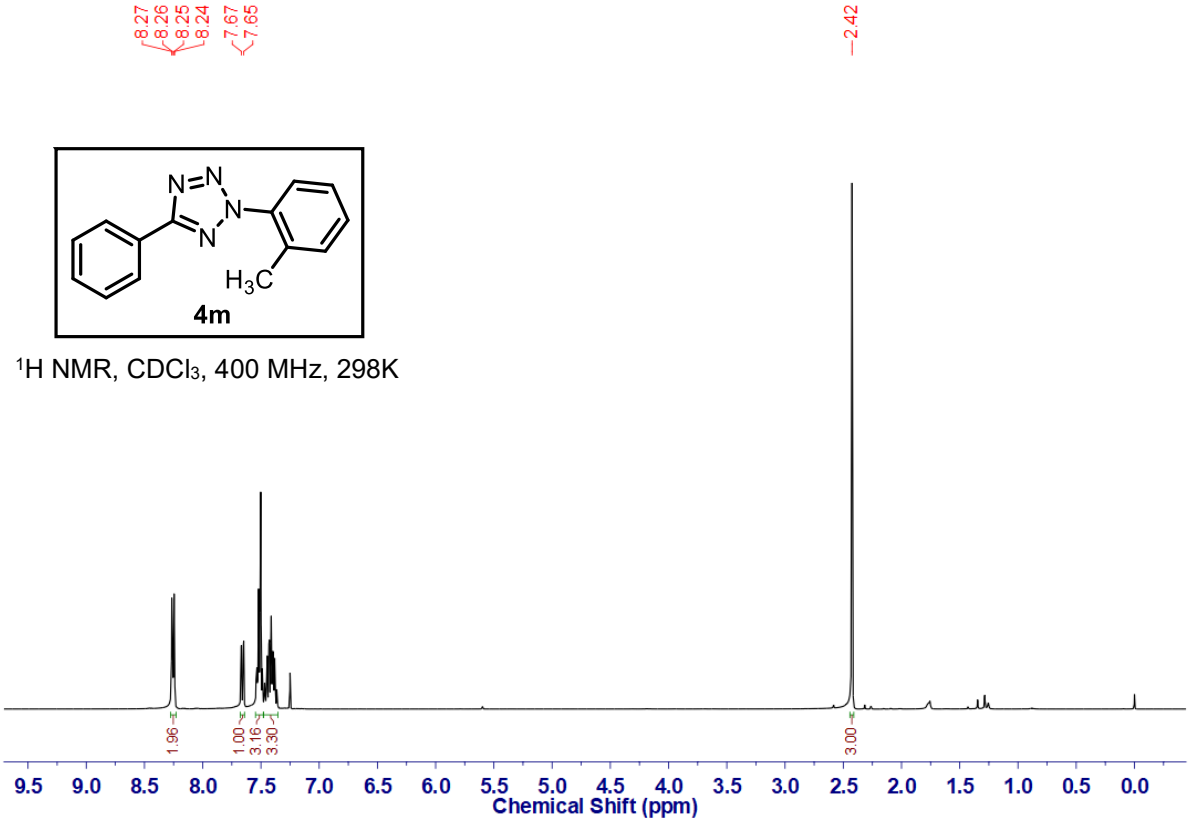
^{1}H NMR, $CDCl_3$, 600 MHz, 298K



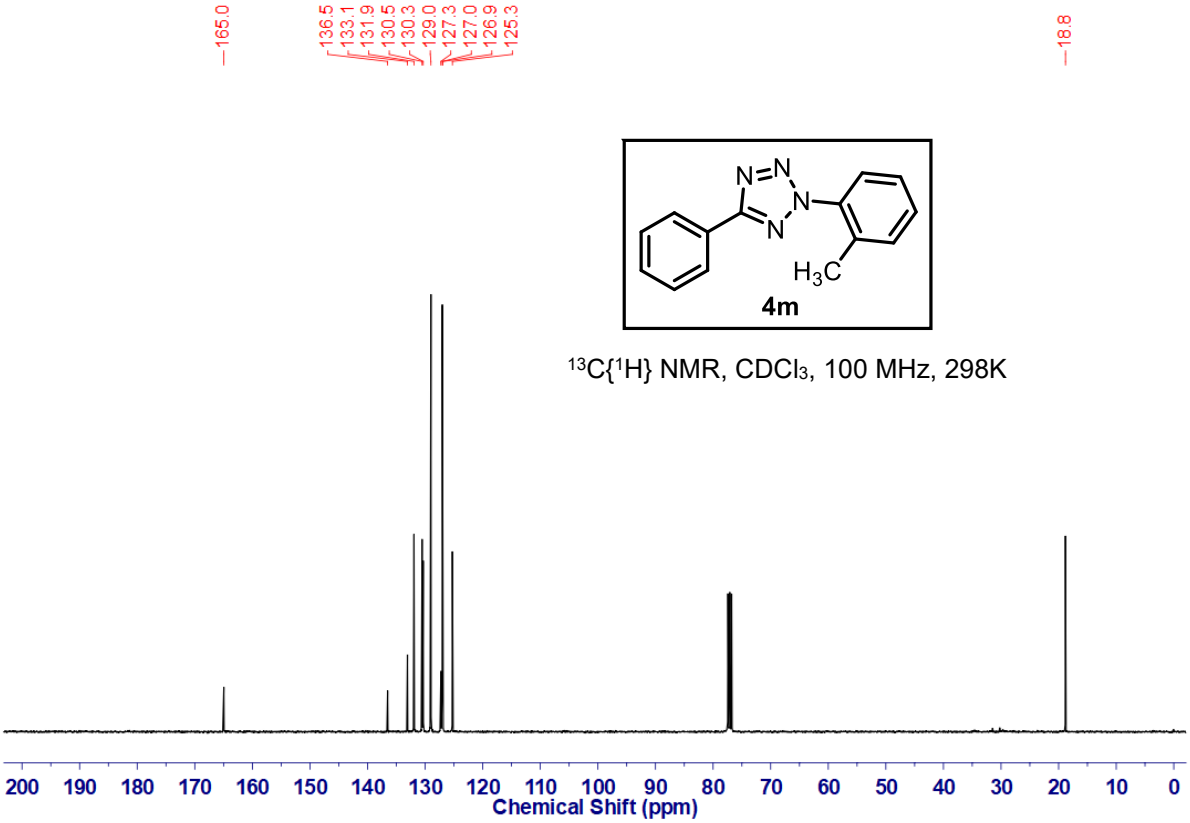
$^{13}C\{^{1}H\}$ NMR, $CDCl_3$, 150 MHz, 298K



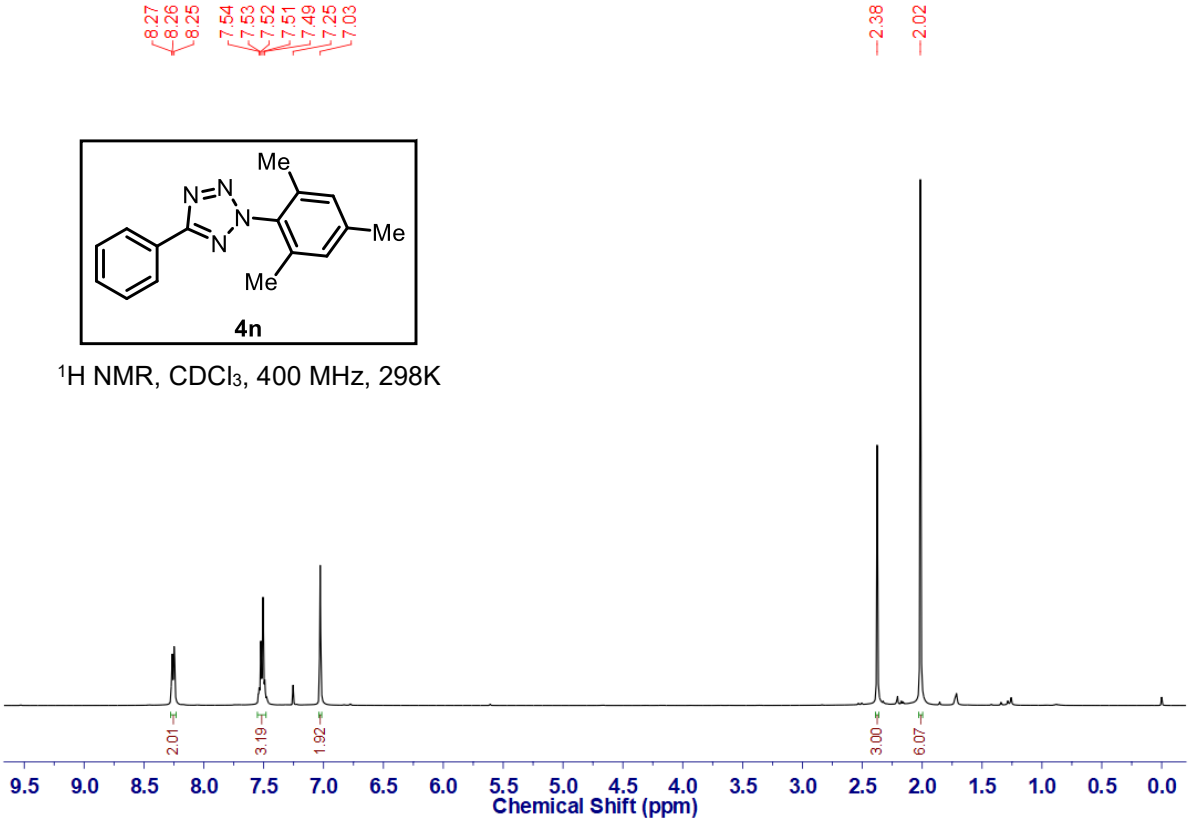
^{19}F NMR, $CDCl_3$, 376 MHz, 298K



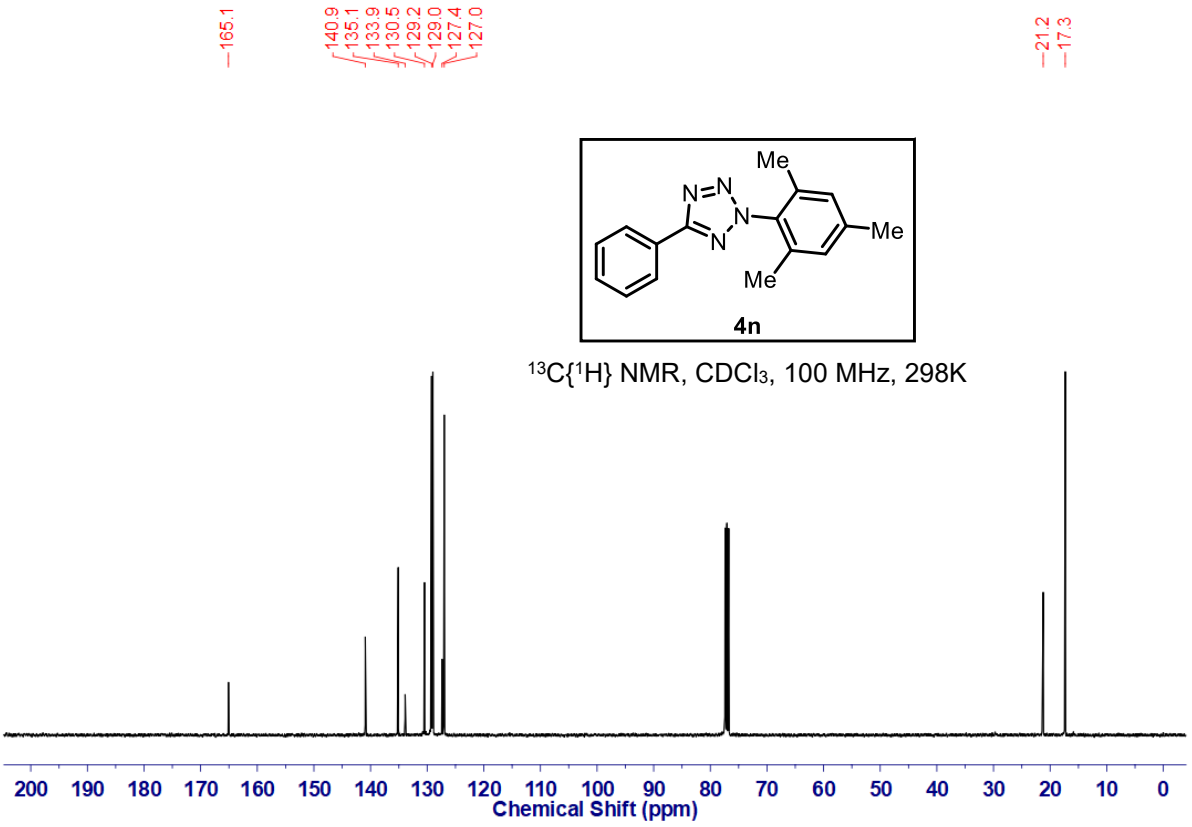
^{1}H NMR, $CDCl_3$, 400 MHz, 298K



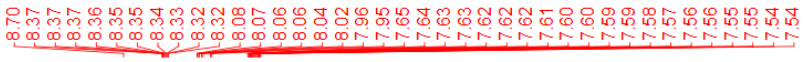
^{13}C{^{1}H} NMR, $CDCl_3$, 100 MHz, 298K

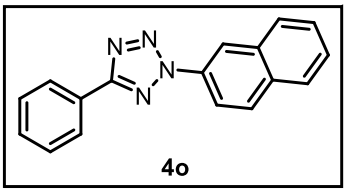


^{1}H NMR, $CDCl_3$, 400 MHz, 298K

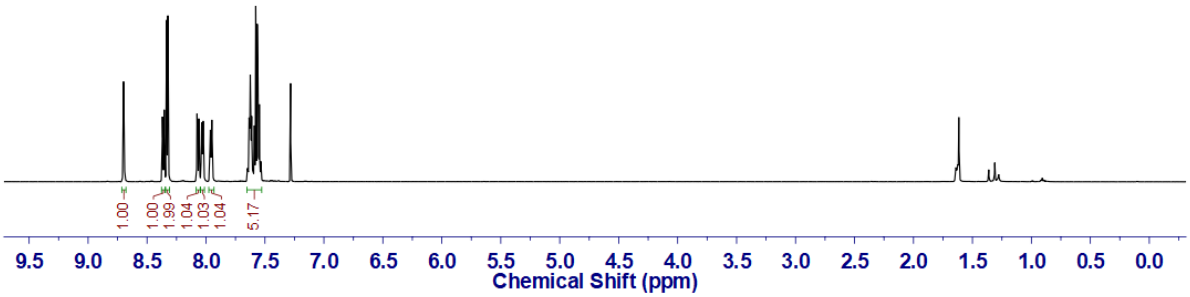


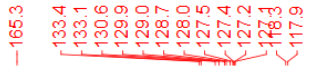
^{13}C{^{1}H} NMR, $CDCl_3$, 100 MHz, 298K

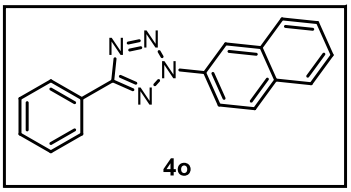




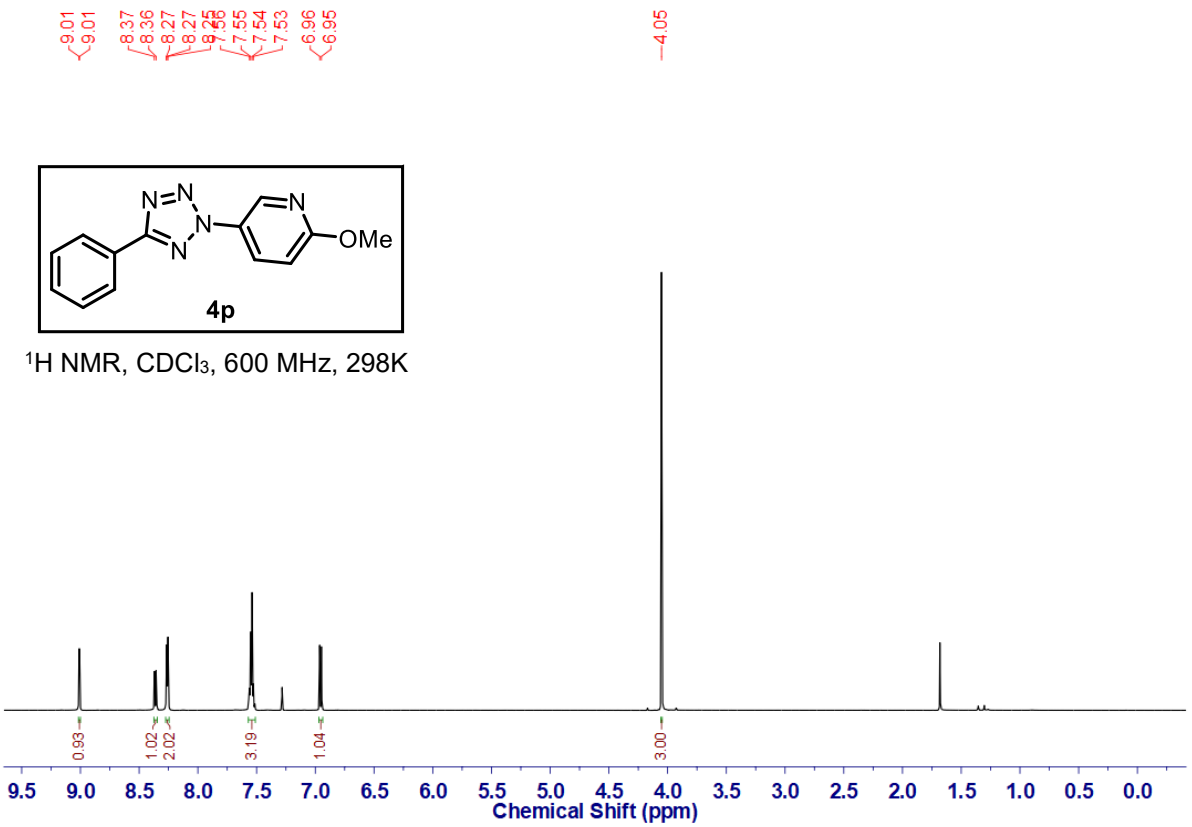
^{1}H NMR, $CDCl_3$, 600 MHz, 298K



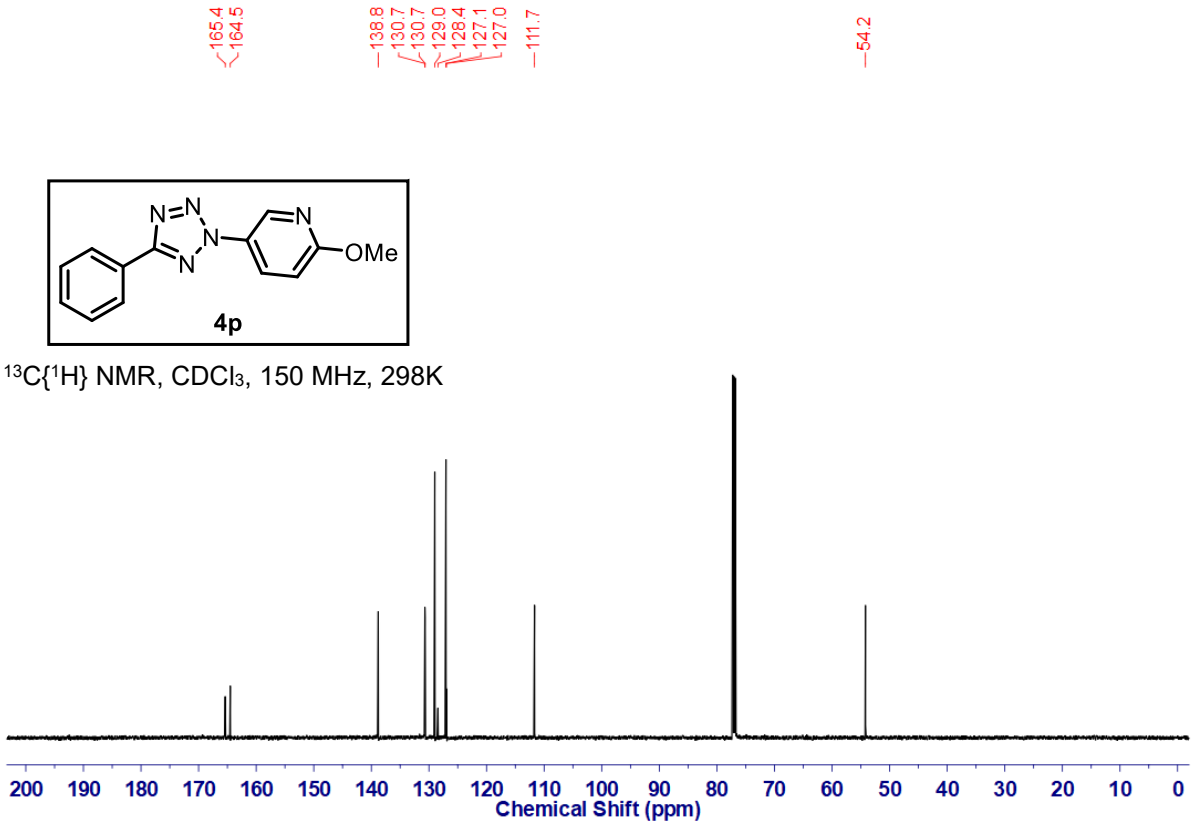




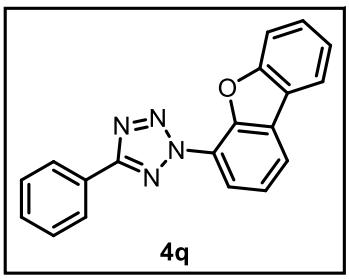
^{13}C{^{1}H} NMR, $CDCl_3$, 150 MHz, 298K



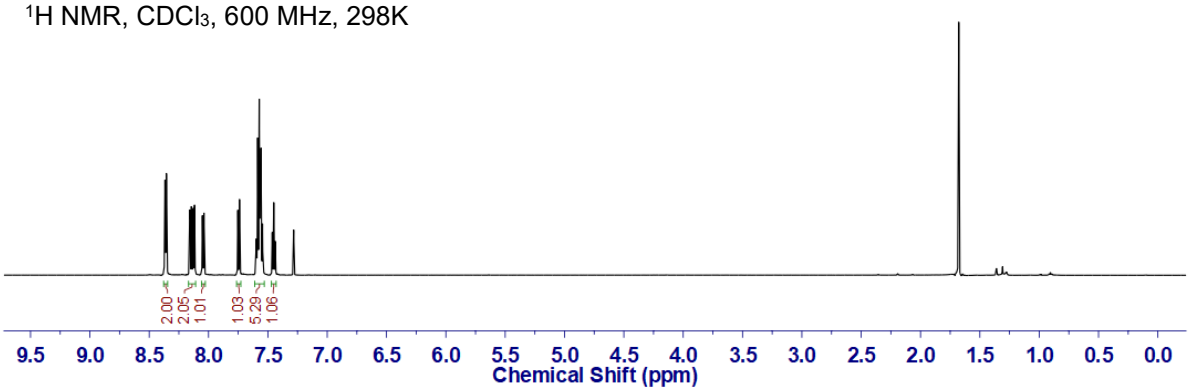
^{1}H NMR, $CDCl_3$, 600 MHz, 298K

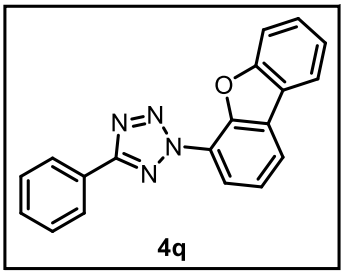


^{13}C{^{1}H} NMR, $CDCl_3$, 150 MHz, 298K



^{1}H NMR, $CDCl_3$, 600 MHz, 298K





$^{13}C\{^{1}H\}$ NMR, $CDCl_3$, 150 MHz, 298K