Supporting Information

n-Bu_4NI-Catalyzed Direct Amination of Ethers with Aryl Tetrazoles and Triazoles *via* Cross-Dehydrogenative Coupling Reaction

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1 General experimental details

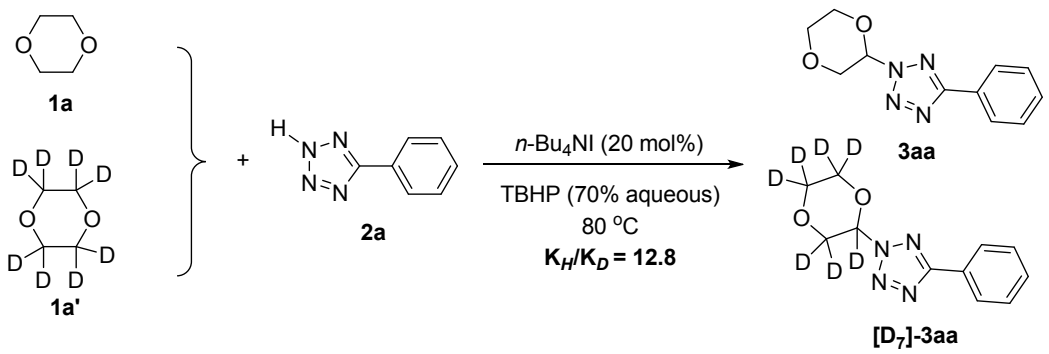
Chemicals were used as received without special purification unless stated otherwise. Aryl tetrazoles and triazoleswere prepared according to the lietrature.[1,2] ^{1}H and ^{13}C NMR were recorded at ambient temperature on a 400 MHz NMR spectrometer. NMR experiments are reported in δ units, parts per million (ppm), and were referenced to $CDCl_3$ (δ 7.26 or 77.0 ppm) as the internal standard. The coupling constants J are given in Hz. Melting points (m.p.) are determined with a MPA 100 apparatus and are not corrected. High-resolution mass spectrometry (HRMS) was performed on a TOF MS instrument with an ESI source.

General procedure for the amination of alkylethers

In a sealed tube, *n*-Bu_4NI (22.1 mg, 0.06 mmol) was added to the mixture of alkyl ethers **1** (1 mL), aryl tetrazole **2** or triazoles **4** (0.3 mmol) and *t*-BuOOH (70% aqueous, 1.5 mmol, 5 equiv) at room temperature. The reaction mixture was stirred at 80 ^{o}C for 12 h. After reaction, the mixture was allowed to cool to room temperature. The solvent was then removed under vacuum, and the residue was purified by silica gel chromatography using a mixture of PE/EA to afford the desired product **3** and **5**.

2 KIE experiment

In a sealed tube, the mixture of **1a** (0.5 mL) and **1a'** (0.5 mL) with **2a** was treated by standard procedures and heated for 12 h. The mixture was concentrated in vacuum and the residue was purified by flash column chromatography on silica gel with petroleum ether-ethyl acetate as eluent to give product **3aa** and **[D_7]-3aa**. The mixture was analyzed using ^{1}H NMR spectrometer. As shown in Scheme S1, the ratio of **3aa** and **[D_7]-3aa** is 12.8.



Scheme S1 KIE experiment.

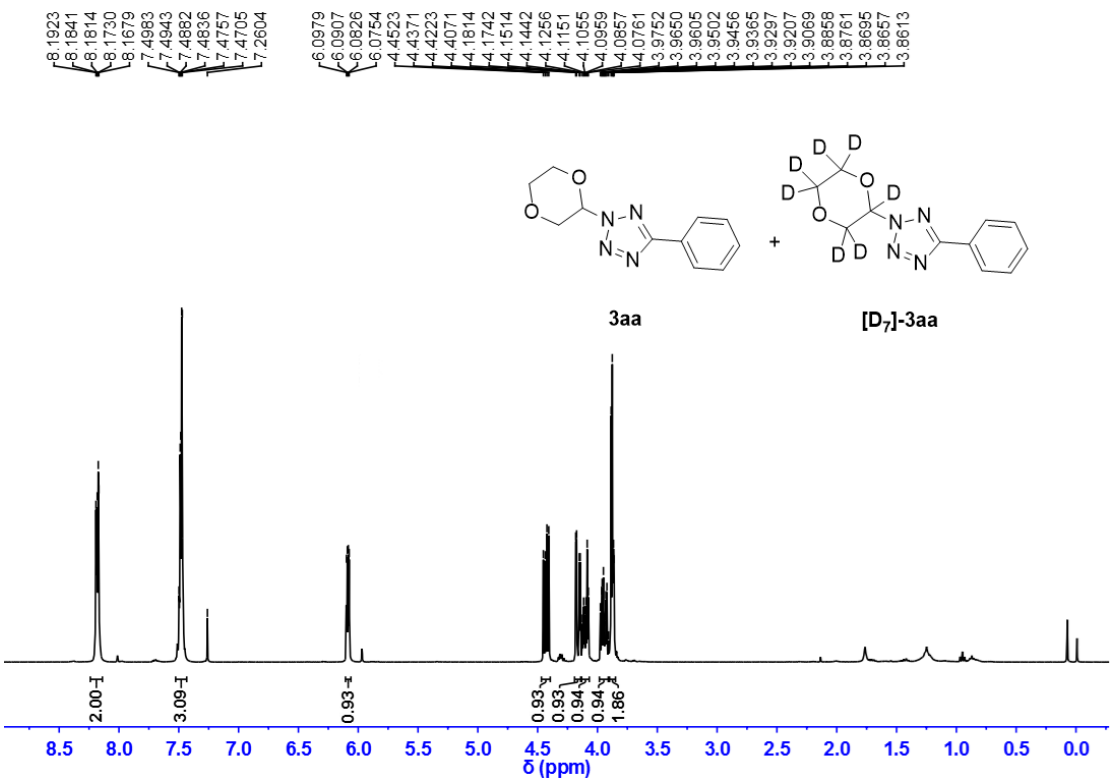
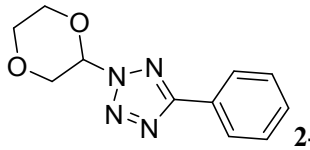


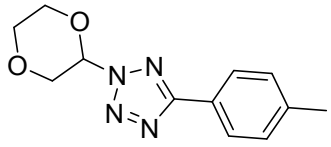
Figure S1 The ^{1}H NMR spectrum of the KIE results

3 Characterization data

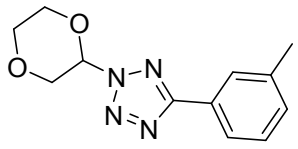


2-(1,4-dioxan-2-yl)-5-phenyl-2*H*-tetrazole (3aa). white solid (54.3 mg, 78%), mp: 51-53 °C; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.24-8.11 (m, 2H), 7.48-7.47 (m, 3H), 6.09 (dd, J = 6.1, 2.9 Hz, 1H), 4.43 (dd, J = 12.0, 6.1 Hz, 1H), 4.16 (dd, J = 12.0, 2.9 Hz, 1H), 4.09 (dd,

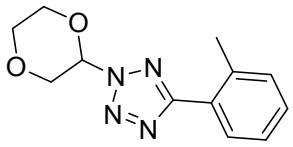
J = 9.8, 5.8 Hz, 1H), 3.98-3.92 (m, 1H), 3.90-3.85 (m, 2H) ppm; ^{13}C NMR ($CDCl_3$,100 MHz) δ 165.2, 130.5, 128.8, 127.0, 126.9, 84.0, 67.1, 65.8, 64.9 ppm; HRMS (ESI): Calcd. for $C_{11}H_{12}N_4NaO_2$ $(M+Na)^+$ 255.0852, found 255.0860.



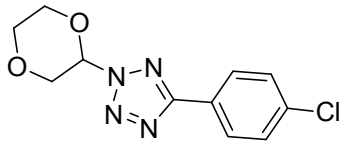
2-(1,4-dioxan-2-yl)-5-(*p*-tolyl)-2*H*-tetrazole (3ab). Light yellow oil (53.2 mg, 72%); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.05 (d, *J* = 8.1 Hz, 2H), 7.28 (d, *J* = 8.0 Hz, 2H), 6.07 (dd, *J* = 6.1, 2.9 Hz, 1H), 4.41 (dd, *J* = 12.0, 6.2 Hz, 1H), 4.19-4.04 (m, 2H), 3.98-3.83 (m, 3H), 2.39 (s, 3H) ppm; ^{13}C NMR ($CDCl_3$,100 MHz) δ 165.3, 140.7, 129.5, 126.9, 124.0, 84.0, 67.0, 65.8, 64.9, 21.4 ppm. HRMS (ESI): Calcd. for $C_{12}H_{14}N_4NaO_2$ $(M+Na)^+$ 269.1009, found 269.1004.



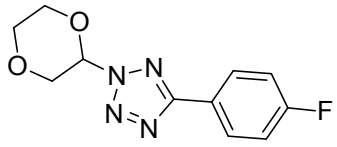
2-(1,4-dioxan-2-yl)-5-(*m*-tolyl)-2*H*-tetrazole (3ac). White solid (48.0 mg, 65%), mp: 54-55 ^{o}C; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.01-7.97 (m, 2H), 7.39-7.27 (m, 2H), 6.09 (dd, *J* = 6.1, 2.8 Hz, 1H), 4.43 (dd, *J* = 12.0, 6.2 Hz, 1H), 4.19-4.10 (m, 2H), 3.98-3.86 (m, 3H), 2.42 (s, 3H) ppm; ^{13}C NMR ($CDCl_3$,100 MHz) δ 165.4, 138.6, 131.3, 128.8, 127.6, 126.8, 124.2, 84.0, 67.1, 65.8, 65.0, 21.3 ppm. HRMS (ESI): Calcd. for $C_{12}H_{14}N_4NaO_2$ $(M+Na)^+$ 269.1009, found 269.1015.



2-(1,4-dioxan-2-yl)-5-(*o*-tolyl)-2*H*-tetrazole (3ad). Light yellow oil (42.8 mg, 58%); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.08-7.92 (m, 2H), 7.39-7.27 (m, 2H), 6.08 (dd, *J* = 6.1, 2.9 Hz, 1H), 4.43 (dd, *J* = 12.0, 6.1 Hz, 1H), 4.21-4.05 (m, 2H), 3.99-3.85 (m, 3H), 2.42 (s, 3H) ppm; ^{13}C NMR ($CDCl_3$,100 MHz) δ 165.4, 138.6, 131.3, 128.8, 127.6, 126.7, 124.1, 84.0, 67.1, 65.8, 65.0, 21.3 ppm. HRMS (ESI): Calcd. for $C_{12}H_{14}N_4NaO_2$ $(M+Na)^+$ 269.1009, found 269.1012.

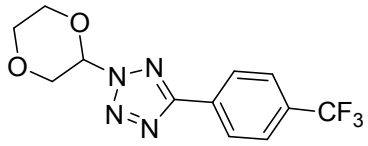


5-(4-chlorophenyl)-2-(1,4-dioxan-2-yl)-2*H*-tetrazole (3ae). White solid (49.5 mg, 62%), mp: 101-103 ^{o}C; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.12 (d, *J* = 8.6 Hz, 2H), 7.47 (d, *J* = 8.6 Hz, 2H), 6.09 (dd, *J* = 6.0, 2.9 Hz, 1H), 4.43 (dd, *J* = 12.0, 6.0 Hz, 1H), 4.20-4.07 (m, 2H), 3.99-3.86 (m, 3H) ppm; ^{13}C NMR ($CDCl_3$,100 MHz) δ 164.4, 136.6, 129.2, 128.3, 125.4, 84.1, 67.1, 65.9, 64.9 ppm. HRMS (ESI): Calcd. for $C_{11}H_{11}ClN_4NaO_2$ $(M+Na)^+$ 289.0463, found 289.0470.

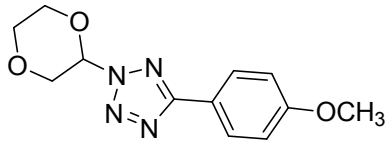


2-(1,4-dioxan-2-yl)-5-(4-fluorophenyl)-2*H*-tetrazole (3af). Light yellow solid (42.0 mg, 56%), mp: 81-83 ^{o}C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.20-8.16 (m, 2H),

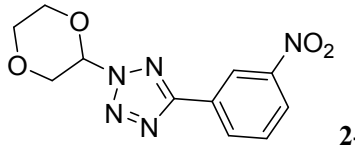
7.19-7.12 (m, 2H), 6.08 (dd, J = 6.0, 2.8 Hz, 1H), 4.42 (dd, J = 12.0, 6.1 Hz, 1H), 4.18-4.10 (m, 2H), 3.99-3.87 (m, 3H) ppm; ^{13}C NMR ($CDCl_3$,100 MHz) δ 165.4, 163.7 (d, J = 157.1 Hz), 129.1 (d, J = 8.5 Hz), 128.6, 116.0 (d, J = 21.9 Hz), 84.1, 67.1, 65.9, 65.0 ppm. HRMS (ESI): Calcd. for $C_{11}H_{11}FN_4NaO_2$ $(M+Na)^+$ 273.0758, found 273.0764.



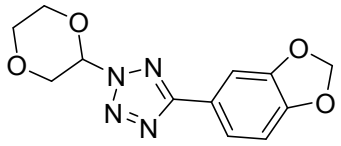
2-(1,4-dioxan-2-yl)-5-(4-(trifluoromethyl)phenyl)-2*H*-tetrazole (3ag). Yellow solid (45.0 mg, 50%), mp: 104-106 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.32 (d, J = 8.2 Hz, 2H), 7.76 (d, J = 8.2 Hz, 2H), 6.12 (dd, J = 5.8, 2.8 Hz, 1H), 4.45 (dd, J = 12.1, 5.8 Hz, 1H), 4.21-4.10 (m, 2H), 4.01-3.89 (m, 3H) ppm; ^{13}C NMR ($CDCl_3$,100 MHz) δ 164.1, 148.6, 132.3 (q, J = 32.6 Hz), 130.3, 127.3, 125.9 (q, J = 3.7 Hz), 123.8 (q, J = 270.6 Hz), 84.3, 67.0, 65.9, 64.9 ppm. HRMS (ESI): Calcd. for $C_{12}H_{11}F_3N_4NaO_2$ $(M+Na)^+$ 323.0726, found 323.0730.



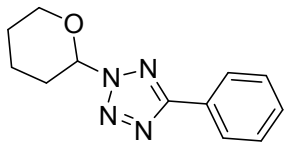
2-(1,4-dioxan-2-yl)-5-(4-methoxyphenyl)-2*H*-tetrazole (3ah). Yellow solid (52.7 mg, 67%), mp: 91-92 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.11 (d, J = 8.8 Hz, 2H), 6.99 (d, J = 8.8 Hz, 2H), 6.06 (dd, J = 6.2, 2.8 Hz, 1H), 4.42 (dd, J = 12.0, 6.3 Hz, 1H), 4.18-4.06 (m, 2H), 3.97-3.87 (m, 3H), 3.85 (s, 3H) ppm; ^{13}C NMR ($CDCl_3$,100 MHz) δ 165.1, 161.4, 128.5, 119.5, 114.2, 83.9, 67.1, 65.8, 65.0, 55.3 ppm. HRMS (ESI): Calcd. for $C_{12}H_{14}N_4NaO_3$ $(M+Na)^+$ 285.0958, found 285.0961.



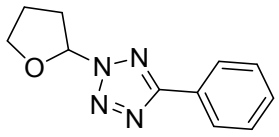
2-(1,4-dioxan-2-yl)-5-(3-nitrophenyl)-2*H*-tetrazole (3ai). Light yellow solid (53.2 mg, 64%), mp: 106-107 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 9.01 (s, 1H), 8.52 (d, J = 7.7 Hz, 1H), 8.32 (d, J = 8.1 Hz, 1H), 7.69 (t, J = 8.0 Hz, 1H), 6.13 (dd, J = 5.3, 2.7 Hz, 1H), 4.45 (dd, J = 12.1, 5.6 Hz, 1H), 4.21-4.10 (m, 2H), 4.00-3.89 (m, 3H) ppm; ^{13}C NMR ($CDCl_3$,100 MHz) δ 163.4, 148.6, 132.6, 130.1, 128.7, 125.1, 122.0, 84.4, 67.0, 65.9, 64.8 ppm. HRMS (ESI): Calcd. for $C_{11}H_{11}N_5NaO_4$ $(M+Na)^+$ 300.0703, found 300.0709.



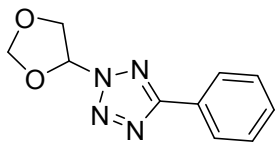
5-(benzo[d][1,3]dioxol-5-yl)-2-(1,4-dioxan-2-yl)-2*H*-tetrazole (3aj). Light yellow solid (58.0 mg, 70%), mp: 104-106 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.74 (d, J = 8.1 Hz, 1H), 7.63 (s, 1H), 6.91 (d, J = 8.1 Hz, 1H), 6.07 (d, J = 3.4 Hz, 1H), 6.04 (s, 2H), 4.42 (dd, J = 11.9, 6.2 Hz, 1H), 4.13 (m, 2H), 4.00-3.85 (m, 3H) ppm; ^{13}C NMR ($CDCl_3$,100 MHz) δ 165.1, 149.6, 148.1, 121.6, 120.9, 108.7, 107.3, 101.5, 84.0, 67.1, 65.9, 65.0 ppm. HRMS (ESI): Calcd. for $C_{12}H_{12}N_4NaO_4$ $(M+Na)^+$ 299.0751, found 299.0760.



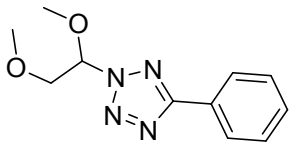
5-phenyl-2-(tetrahydro-2*H*-pyran-2-yl)-2*H*-tetrazole (3ba). Colorless oil (56.6 mg, 82%). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.19-8.17 (m, 2H), 7.47 (dd, J = 5.0, 2.4 Hz, 3H), 6.05 (dd, J = 7.7, 2.8 Hz, 1H), 4.01 (dd, J = 9.6, 5.3 Hz, 1H), 3.83-3.79 (m, 1H), 2.49 (dd, J = 16.7, 8.9 Hz, 1H), 2.18-2.15 (m, 2H), 1.77-1.71 (m, 3H) ppm; ^{13}C NMR ($CDCl_3$, 100 MHz) δ 164.9, 130.3, 128.8, 127.2, 126.9, 87.7, 66.8, 29.0, 24.5, 20.7 ppm. HRMS (ESI): Calcd. for $C_{12}H_{14}N_4NaO$ $(M+Na)^+$ 253.1060, found 253.1054.



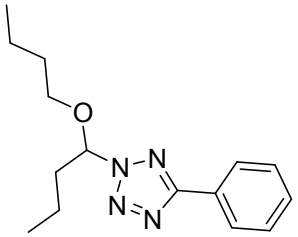
5-phenyl-2-(tetrahydrofuran-2-yl)-2*H*-tetrazole (3ca). Colorless oil (31.8 mg, 49%). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.16 (dd, J = 7.3, 2.1 Hz, 2H), 7.54-7.44 (m, 3H), 6.58 (dd, J = 6.4, 1.9 Hz, 1H), 4.32-4.09 (m, 2H), 2.77-2.64 (m, 1H), 2.58-2.45 (m, 2H), 2.24-2.10 (m, 1H) ppm; ^{13}C NMR ($CDCl_3$,100 MHz) δ 165.1, 130.3, 128.8, 127.3, 126.9, 91.6, 70.2, 31.8, 24.0 ppm. HRMS (ESI): Calcd. for $C_{11}H_{12}N_4NaO$ $(M+Na)^+$ 239.0903, found 239.0910.



2-(1,3-dioxolan-4-yl)-5-phenyl-2*H*-tetrazole (3da). Colorless oil (30.7 mg, 47%). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.17 (d, J = 4.3 Hz, 2H), 7.49 (s, 3H), 6.67 (s, 1H), 5.44 (s, 1H), 5.30 (s, 1H), 4.66 (dd, J = 9.5, 2.4 Hz, 1H), 4.47 (dd, J = 9.4, 6.0 Hz, 1H) ppm; ^{13}C NMR ($CDCl_3$, 100 MHz) δ 165.7, 130.6, 128.9, 127.0, 126.3, 97.1 86.7, 69.6 ppm. HRMS (ESI): Calcd. for $C_{10}H_{10}N_4NaO$ $(M+Na)^+$ 241.0696, found 241.0691.

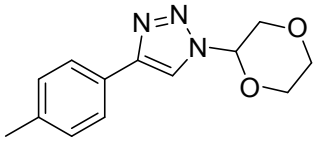


2-(1,2-dimethoxyethyl)-5-phenyl-2*H*-tetrazole (3fa). Colorless oil (38.6 mg, 55%); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.20 (dd, J = 7.4, 2.3 Hz, 2H), 7.51-7.47 (m, 3H), 5.97 (t, J = 6.1 Hz, 1H), 4.05 (d, J = 6.1 Hz, 2H), 3.41 (s, 3H), 3.39 (s, 3H) ppm; ^{13}C NMR ($CDCl_3$, 100 MHz) δ 165.5, 130.5, 128.8, 127.2, 127.0, 91.5, 72.1, 59.5, 57.4 ppm. HRMS (ESI): Calcd. for $C_{11}H_{14}N_4NaO_2$ $(M+Na)^+$ 257.1009, found 257.1017.

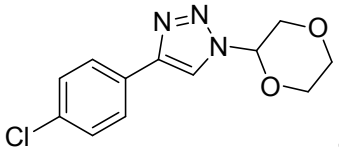


2-(1-butoxybutyl)-5-phenyl-2*H*-tetrazole (3ga). Colorless oil (74.0 mg, 90%). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.20-8.18 (m, 2H), 7.50-7.45 (m, 3H), 5.88 (t, J = 6.7 Hz, 1H), 3.55-3.50 (m, 1H), 3.40-3.34 (m, 1H), 2.33-2.12 (m, 2H), 1.56-1.27 (m, 6H), 0.96 (t, J = 7.4 Hz, 3H), 0.85 (t, J = 7.4 Hz, 3H) ppm; ^{13}C NMR ($CDCl_3$, 100 MHz) δ 165.2, 130.3, 128.8, 127.4, 126.9, 92.6, 69.6, 36.4, 31.0, 19.0, 17.9, 13.6, 13.4 ppm. HRMS (ESI): Calcd. for

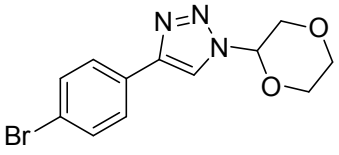
$C_{15}H_{22}N_4NaO$ $(M+Na)^+$ 297.1686, found 297.1679.



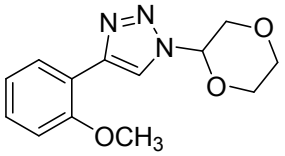
1-(1,4-dioxan-2-yl)-4-(*p*-tolyl)-1*H*-1,2,3-triazole (5aa). Yellow solid (28.7 mg, 39%), mp: 86-87 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.91 (s, 1H), 7.70 (d, J = 8.1 Hz, 2H), 7.23 (d, J = 7.9 Hz, 2H), 5.85 (dd, J = 7.7, 2.8 Hz, 1H), 4.38 (dd, J = 11.7, 7.7 Hz, 1H), 4.13 (dd, J = 11.7, 2.8 Hz, 1H), 4.08-3.93 (m, 2H), 3.85-3.83 (m, 2H), 2.38 (s, 3H) ppm; ^{13}C NMR ($CDCl_3$, 100 MHz) δ 148.8, 138.8, 132.0, 129.5, 126.9, 126.1, 85.1, 67.6, 65.8, 65.7, 21.3 ppm. HRMS (ESI): Calcd. for $C_{13}H_{15}N_3NaO_2$ $(M+Na)^+$ 268.1056, found 268.1062.



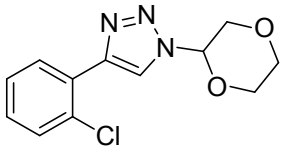
4-(4-chlorophenyl)-1-(1,4-dioxan-2-yl)-1*H*-1,2,3-triazole (5ab). Yellow solid (37.4 mg, 47%), mp: 104-105 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.93 (s, 1H), 7.75 (d, J = 8.5 Hz, 2H), 7.41 (d, J = 8.5 Hz, 2H), 5.85 (dd, J = 7.5, 2.8 Hz, 1H), 4.37 (dd, J = 11.8, 7.5 Hz, 1H), 4.13 (dd, J = 11.8, 2.8 Hz, 1H), 4.07-3.93 (m, 2H), 3.87-3.80 (m, 2H) ppm; ^{13}C NMR ($CDCl_3$, 100 MHz) δ 147.7, 134.7, 132.1, 129.1, 128.3, 127.4, 85.2, 67.6, 65.8, 65.7 ppm. HRMS (ESI): Calcd. for $C_{12}H_{12}ClN_3NaO_2$ $(M+Na)^+$ 288.0510, found 288.0521.



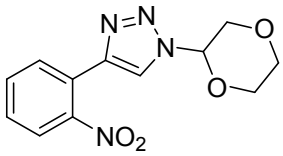
4-(4-bromophenyl)-1-(1,4-dioxan-2-yl)-1*H*-1,2,3-triazole (5ac). Yellow solid (38.0 mg, 41%), mp: 115-117 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.93 (s, 1H), 7.69 (d, J = 8.5 Hz, 2H), 7.56 (d, J = 8.5 Hz, 2H), 5.84 (dd, J = 7.5, 2.8 Hz, 1H), 4.37 (dd, J = 11.7, 7.5 Hz, 1H), 4.12 (dd, J = 11.8, 2.8 Hz, 1H), 4.07-4.02 (m, 1H), 4.00-3.94 (m, 1H), 3.85-3.83 (m, 2H) ppm; ^{13}C NMR ($CDCl_3$, 100 MHz) δ 147.8, 132.0, 130.4, 128.7, 127.7, 122.9, 85.2, 67.5, 65.8, 65.6 ppm. HRMS (ESI): Calcd. for $C_{12}H_{12}BrN_3NaO_2$ $(M+Na)^+$ 332.0005, found 332.0017.



1-(1,4-dioxan-2-yl)-4-(2-methoxyphenyl)-1*H*-1,2,3-triazole (5ad). Yellow oil (25.1 mg, 32%), mp: 50-51 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.17 (s, 1H), 8.03 (dd, J = 7.7, 1.5 Hz, 1H), 7.37- 7.31 (m, 1H), 7.06-6.98 (m, 2H), 5.86 (dd, J = 7.8, 2.8 Hz, 1H), 4.39 (dd, J = 11.7, 7.8 Hz, 1H), 4.12 (dd, J = 11.7, 2.8 Hz, 1H), 4.06-3.95 (m, 2H), 3.93 (s, 3H), 3.85-3.83 (m, 2H) ppm; ^{13}C NMR ($CDCl_3$, 100 MHz) δ 156.8, 145.4, 135.6, 129.8, 128.7, 120.9, 118.7, 111.2, 85.0, 67.7, 65.8, 65.7, 55.4 ppm. HRMS (ESI): Calcd. for $C_{13}H_{15}N_3NaO_3$ $(M+Na)^+$ 284.1006, found 284.1015.

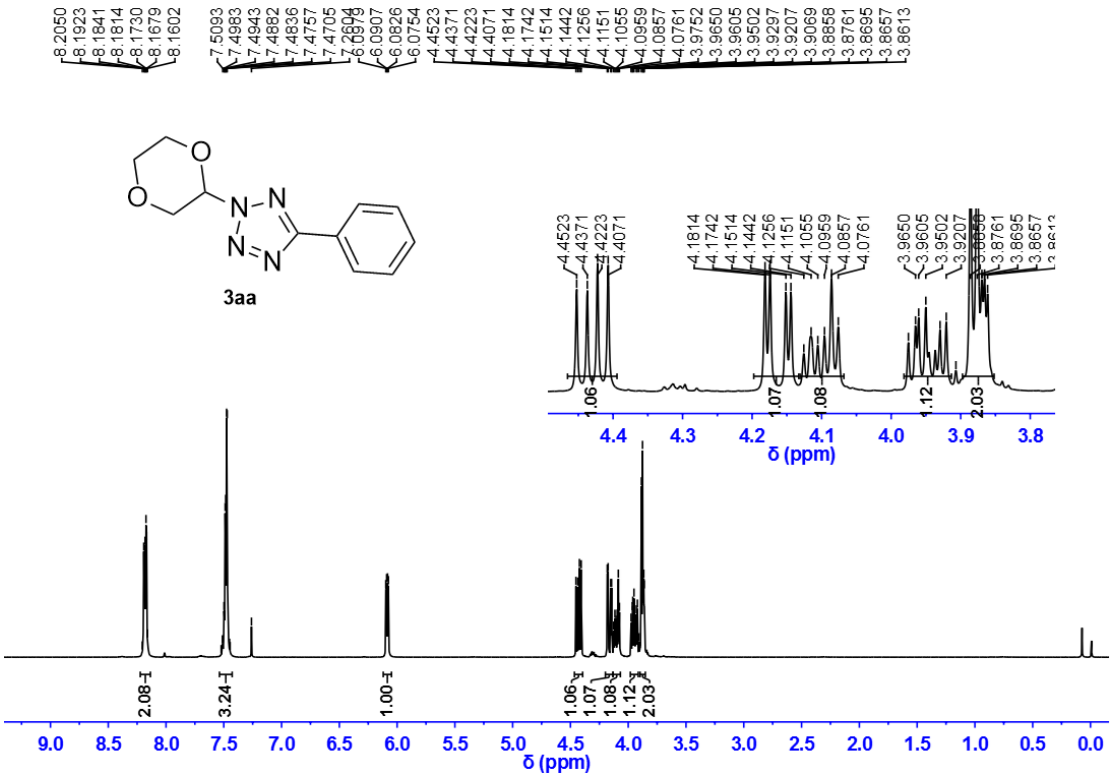


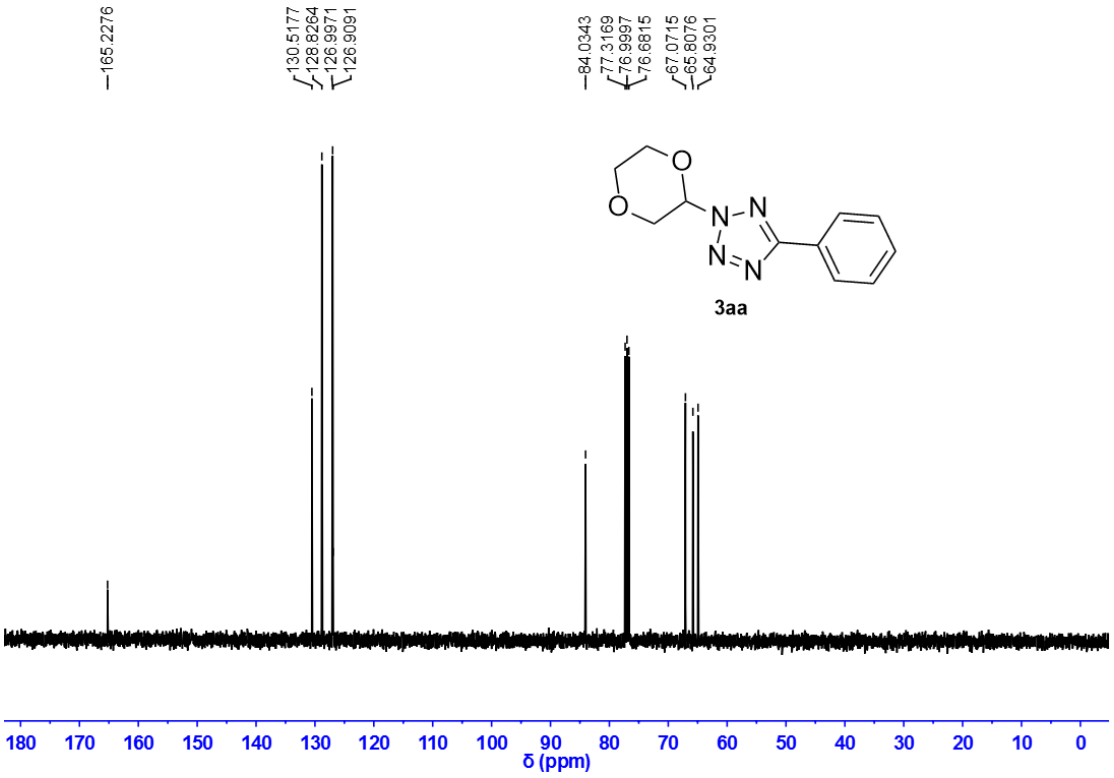
4-(2-chlorophenyl)-1-(1,4-dioxan-2-yl)-1*H*-1,2,3-triazole (5ae). Oil (34.2 mg, 43%), mp: 72-74 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.22 (s, 1H), 7.88 (dd, J = 7.3, 2.1 Hz, 1H), 7.47 (dd, J = 7.3, 1.6 Hz, 1H), 7.37-7.27 (m, 2H), 5.87 (dd, J = 7.5, 2.8 Hz, 1H), 4.39 (dd, J = 11.7, 7.5 Hz, 1H), 4.14 (dd, J = 11.8, 2.7 Hz, 1H), 4.07-3.94 (m, 2H), 3.89-3.84 (m, 2H) ppm; ^{13}C NMR ($CDCl_3$, 100 MHz) δ 146.0, 135.2, 132.3, 130.6, 130.3, 129.8, 128.7, 127.0, 85.1, 67.6, 65.8, 65.6 ppm. HRMS (ESI): Calcd. for $C_{12}H_{12}ClN_3NaO_2$ $(M+Na)^+$ 288.0510, found 288.0517.



1-(1,4-dioxan-2-yl)-4-(2-nitrophenyl)-1*H*-1,2,3-triazole (5af). Oil (38.9 mg, 47%), mp: 97-99 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.87-7.83 (m, 2H), 7.73 (d, J = 7.7 Hz, 1H), 7.64 (t, J = 7.6 Hz, 1H), 7.53-7.51 (m, 1H), 5.84 (dd, J = 7.1, 2.8 Hz, 1H), 4.34 (dd, J = 11.8, 7.1 Hz, 1H), 4.12 (dd, J = 11.8, 2.9 Hz, 1H), 4.05-4.02 (m, 1H), 3.97-3.90 (m, 1H), 3.85-3.81 (m, 2H) ppm; ^{13}C NMR ($CDCl_3$, 100 MHz) δ 148.7, 144.0, 134.1, 132.4, 131.3, 129.6, 124.2, 85.1, 67.4, 65.8, 65.4 ppm. HRMS (ESI): Calcd. for $C_{12}H_{12}N_4NaO_4$ $(M+Na)^+$ 299.0751, found 299.0759.

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

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126.9091
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77.3169
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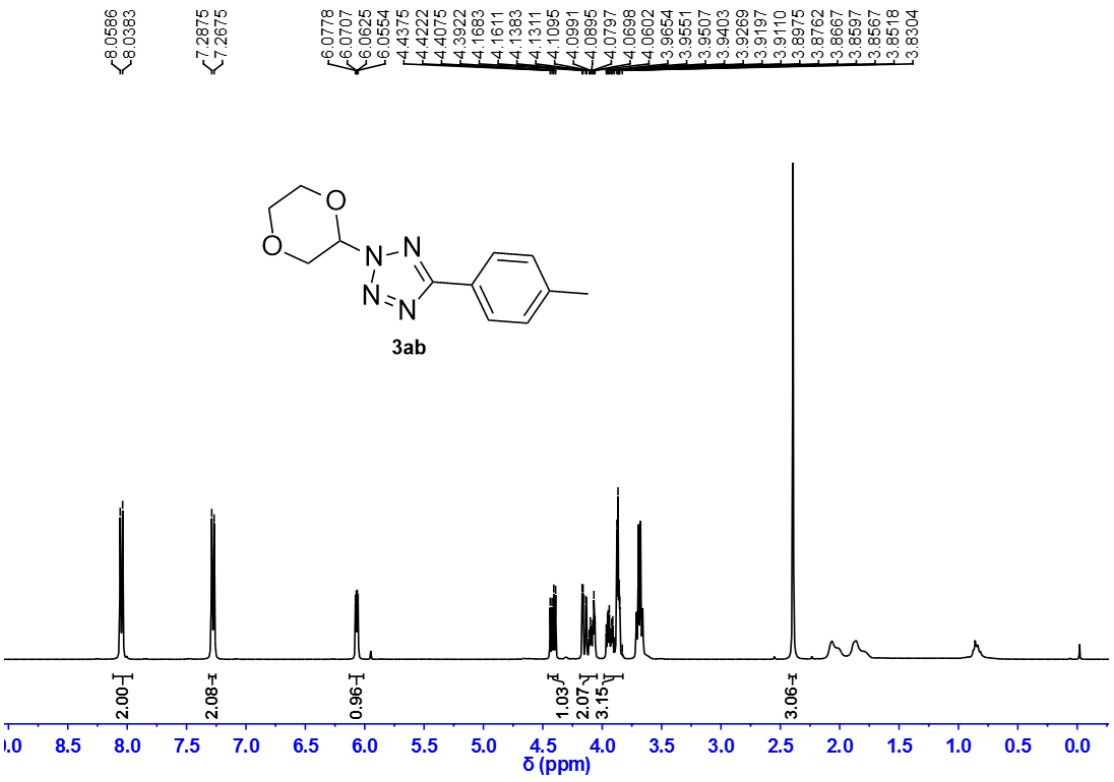
65.8076
64.9301
3aa
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
δ (ppm)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6.0707
6.0625
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4.4375
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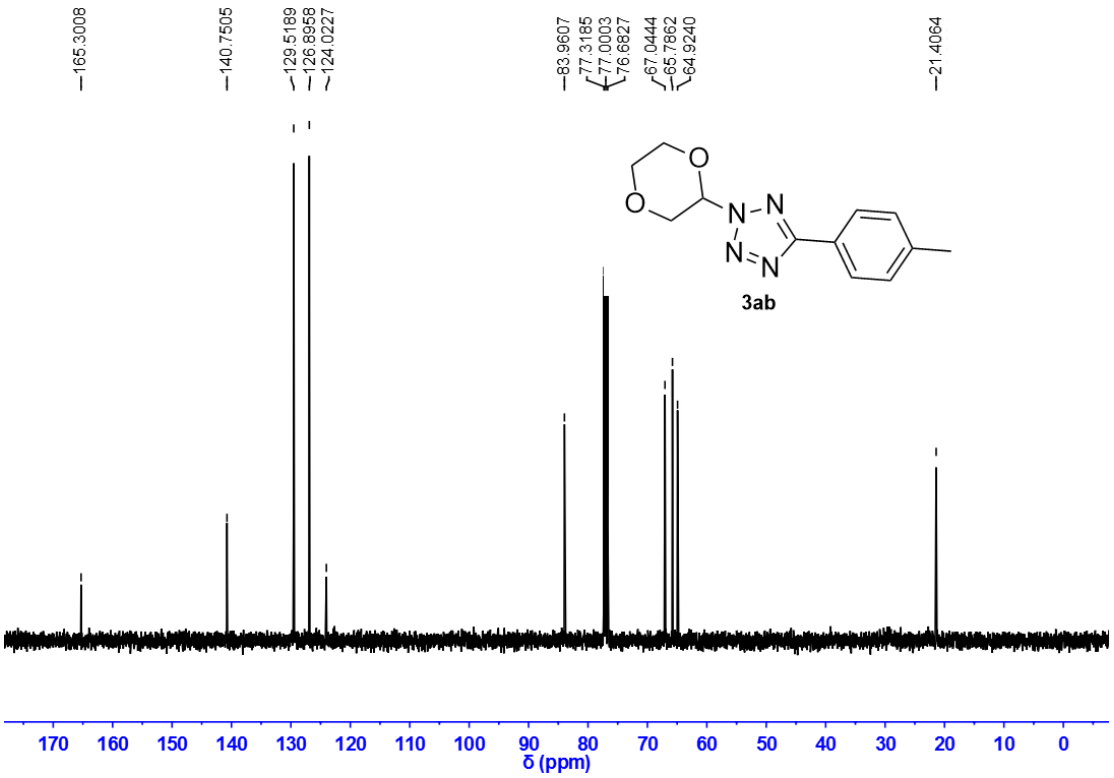
4.4075
4.3922
4.1683
4.1611
4.1383
4.1311
4.1095
4.0991
4.0895
4.0797
4.0698
4.0602
3.9654
3.9551
3.9507
3.9403
3.9269
3.9197
3.9110
3.8975
3.8762
3.8667
3.8597
3.8567
3.8518
3.8304
3ab
2.00
2.08
0.96
1.03
2.07
3.15
3.06
δ (ppm)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129.5189
126.8958
124.0227
83.9607
77.3185
77.0003
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65.7862
64.9240
21.4064
3ab
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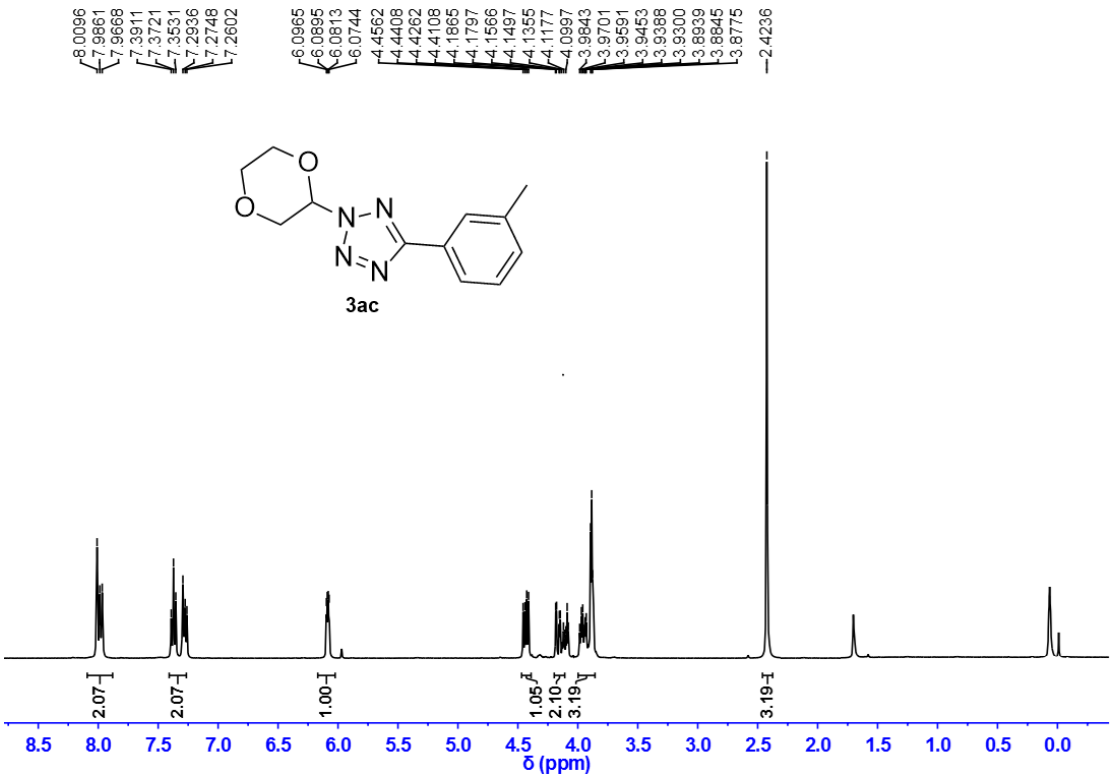
δ (ppm)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7.3531
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7.2602
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6.0813
6.0744
4.4562
4.4408
4.4262
4.4108
4.1965
4.1797
4.1566
4.1497
4.1355
4.1177
4.0997
3.9843
3.9701
3.9591
3.9453
3.9388
3.9300
3.8939
3.8845
3.8775
2.4236
3ac
2.07
2.07
1.00
1.05
2.10
3.19
3.19
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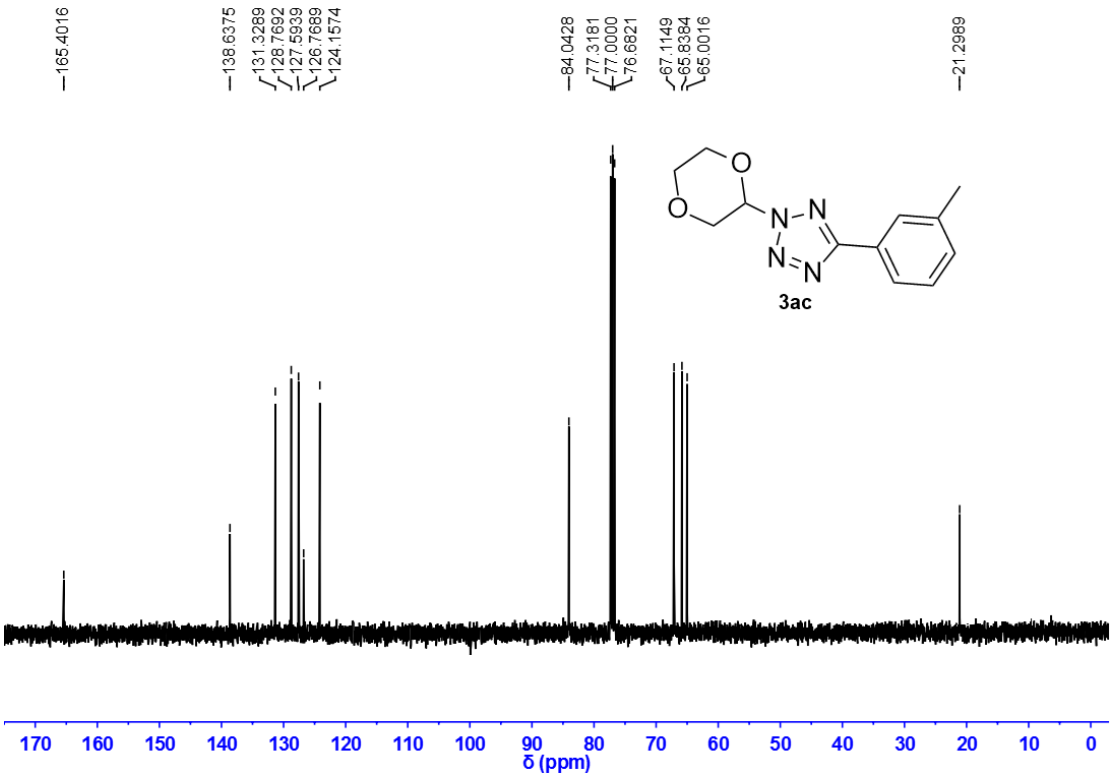
δ (ppm)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77.3181
77.0000
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21.2989
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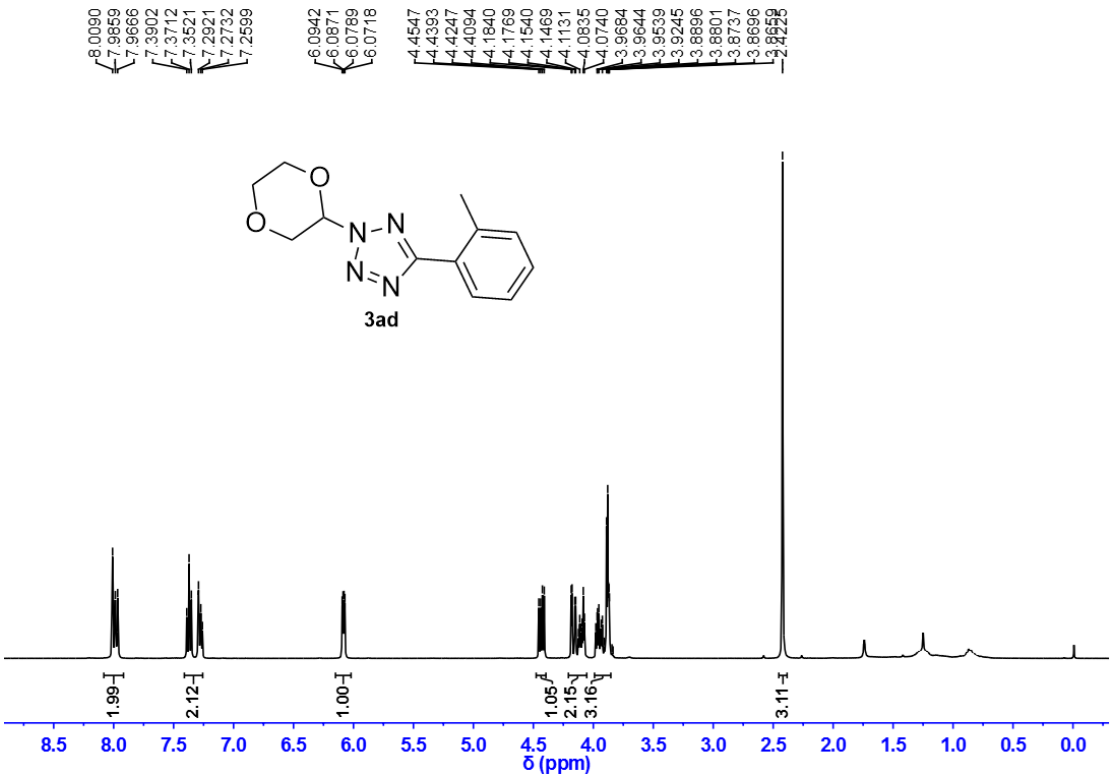
δ (ppm)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6.0718
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4.4393
4.4247
4.4094
4.1840
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4.1540
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4.1131
4.0835
4.0740
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3.9644
3.9539
3.9245
3.8896
3.8801
3.8737
3.8696
3.8659
2.4225
3ad
1.99
2.12
1.00
1.05
2.15
3.16
3.11
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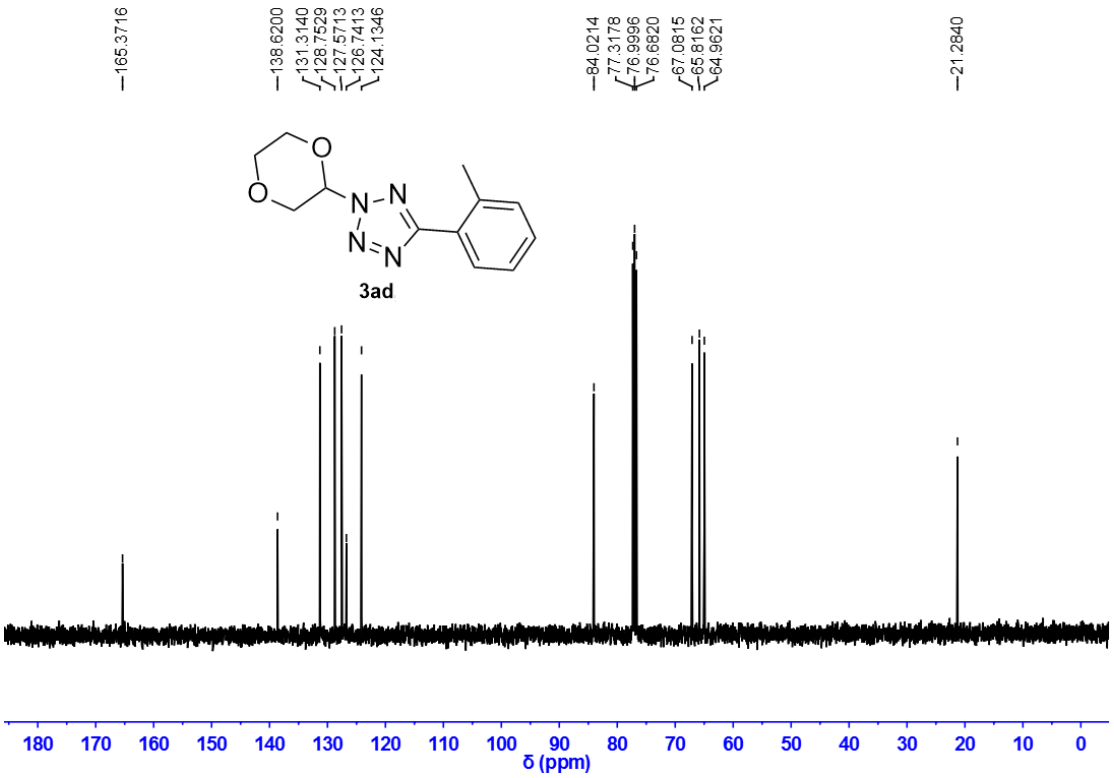
δ (ppm)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77.3178
76.9996
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65.8162
64.9621
21.2840
3ad
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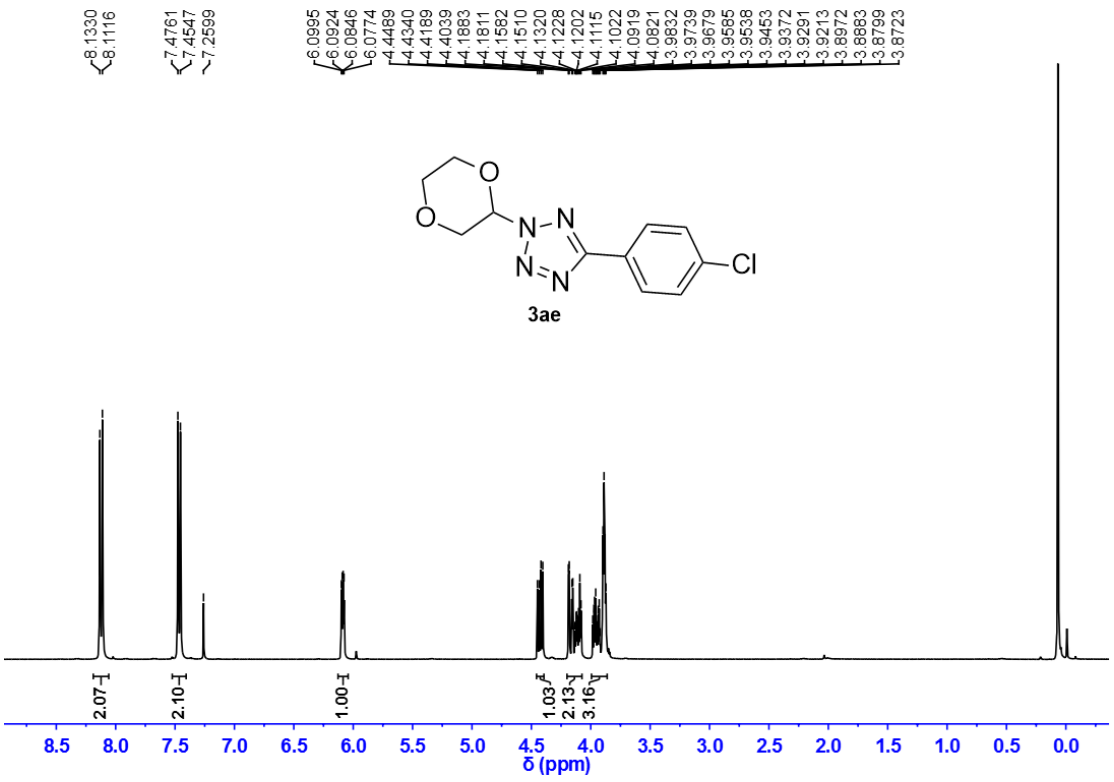
δ (ppm)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7.2599
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6.0924
6.0846
6.0774
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4.4340
4.4189
4.4039
4.1883
4.1811
4.1582
4.1510
4.1320
4.1228
4.1202
4.1115
4.1022
4.0919
4.0821
3.9832
3.9739
3.9679
3.9585
3.9538
3.9453
3.9372
3.9291
3.9213
3.8972
3.8883
3.8799
3.8723
Cl
3ae
2.07
2.10
1.00
1.03
2.13
3.16
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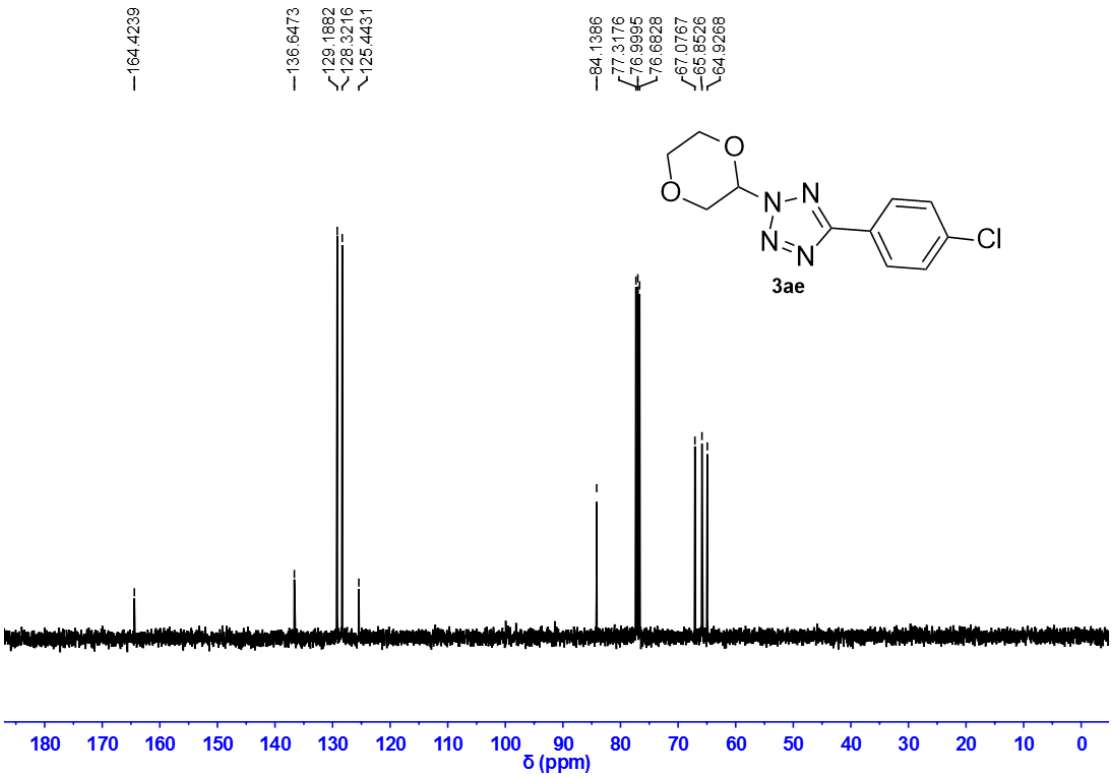
δ (ppm)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67.0767
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64.9268
O
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N-N
N=N
Cl
3ae
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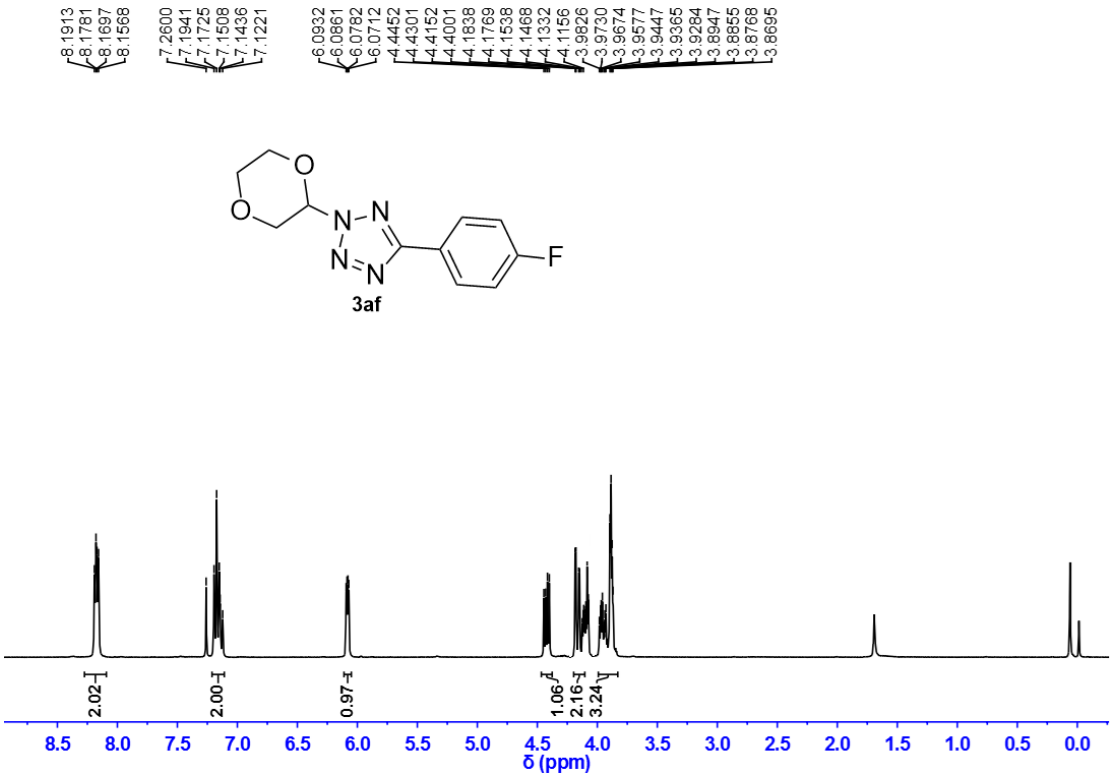
δ (ppm)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6.0932
6.0861
6.0782
6.0712
4.4452
4.4301
4.4152
4.4001
4.1838
4.1769
4.1538
4.1468
4.1332
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3.8947
3.8855
3.8768
3.8695
O
O
N-N
N=N
F
3af
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2.00
0.97
1.06
2.16
3.24
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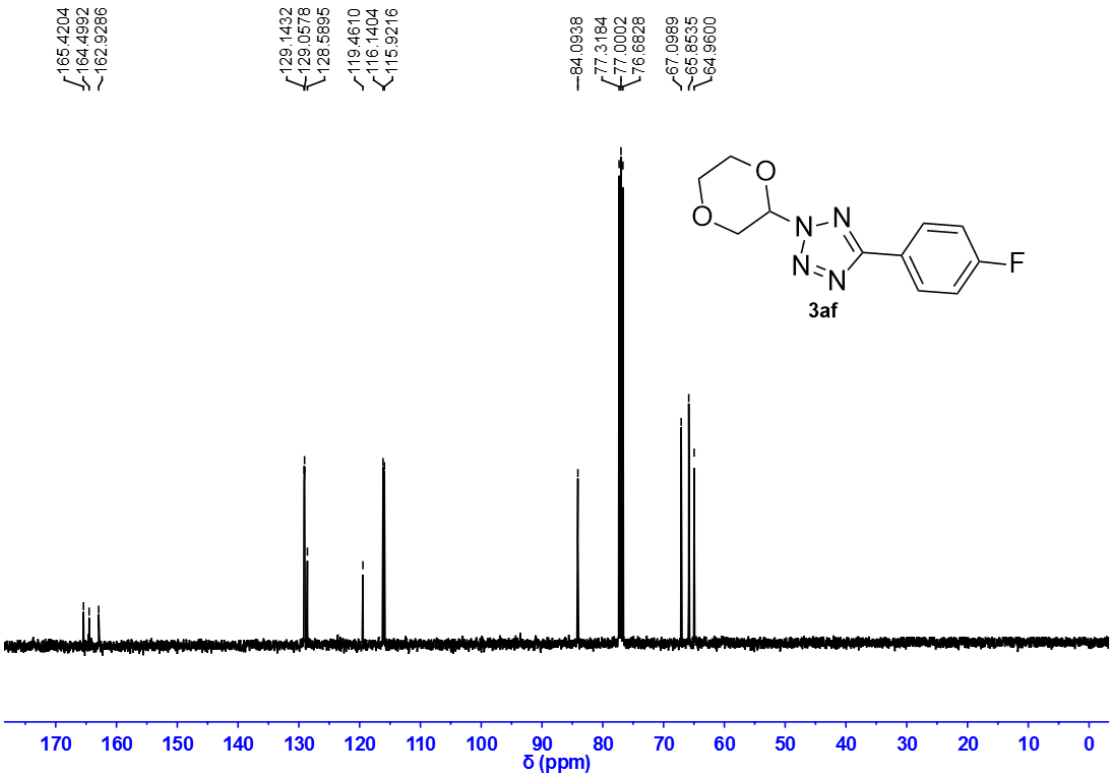
δ (ppm)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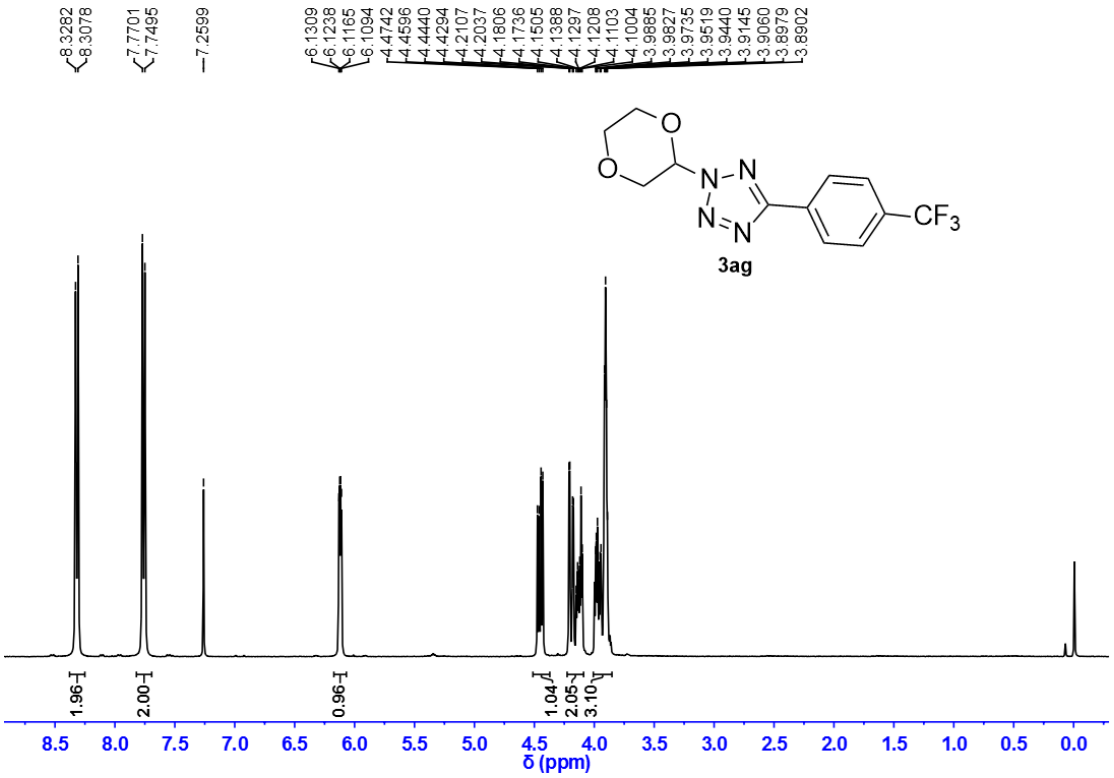
δ (ppm)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4.4440
4.4294
4.2107
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4.1297
4.1208
4.1103
4.1004
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3.9827
3.9735
3.9519
3.9440
3.9145
3.9060
3.8979
3.8902
3ag
1.96
2.00
0.96
1.04
2.05
3.10
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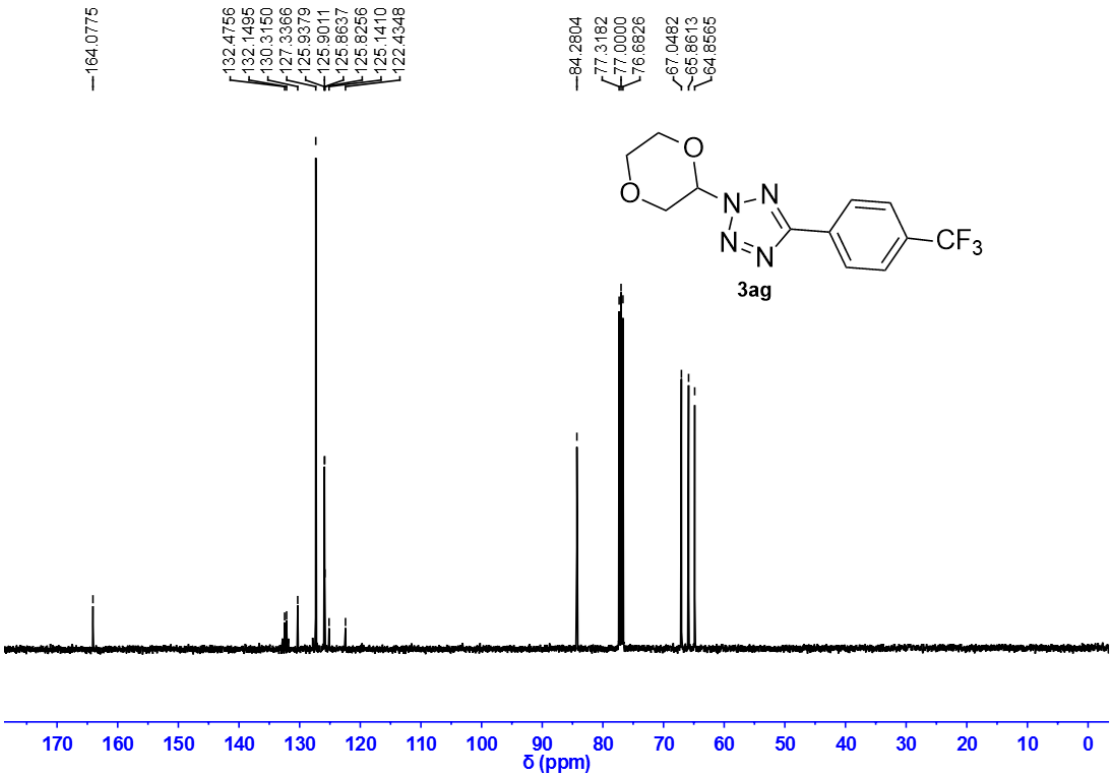
δ (ppm)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84.2804
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64.8565
3ag
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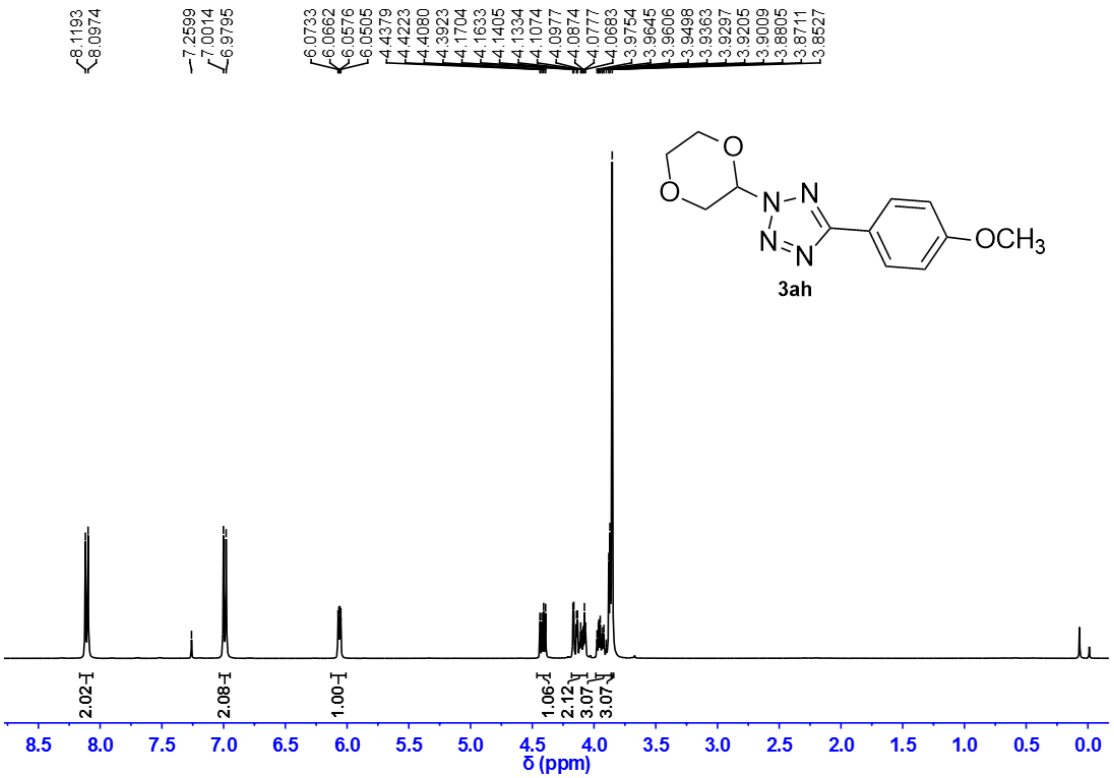
δ (ppm)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4.3923
4.1704
4.1633
4.1405
4.1334
4.1074
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3.8711
3.8527
3ah
2.02
2.08
1.00
1.06
2.12
3.07
3.07
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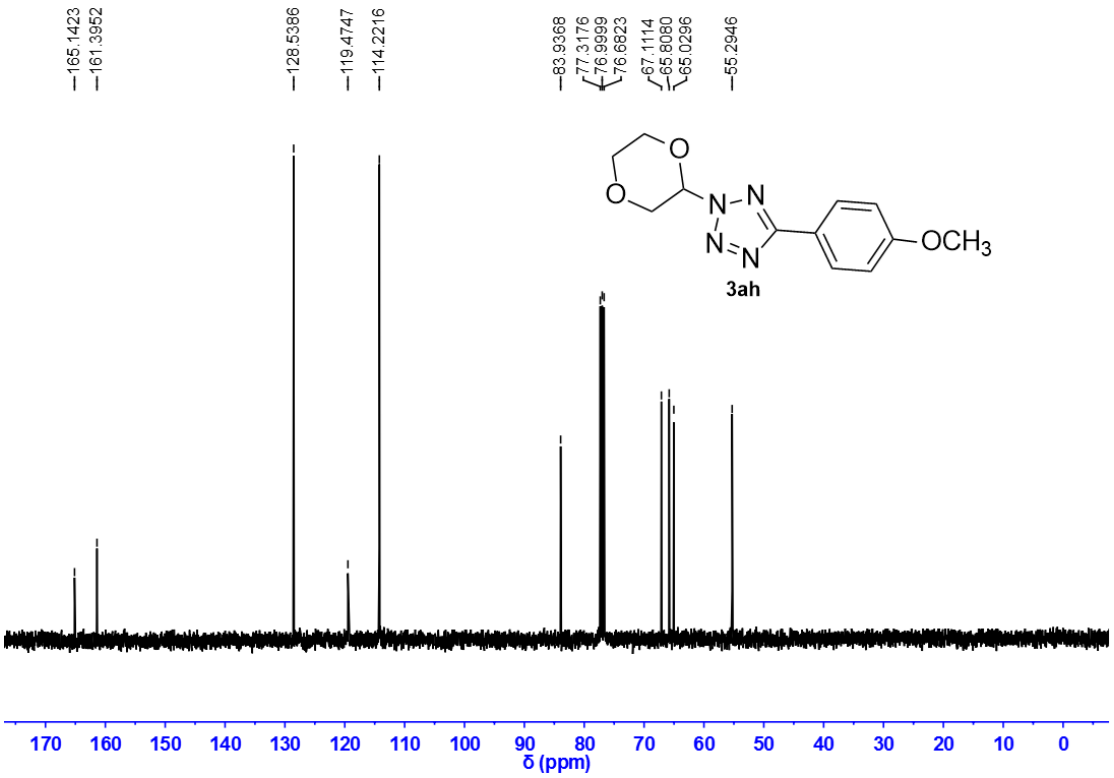
δ (ppm)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OCH3
3ah
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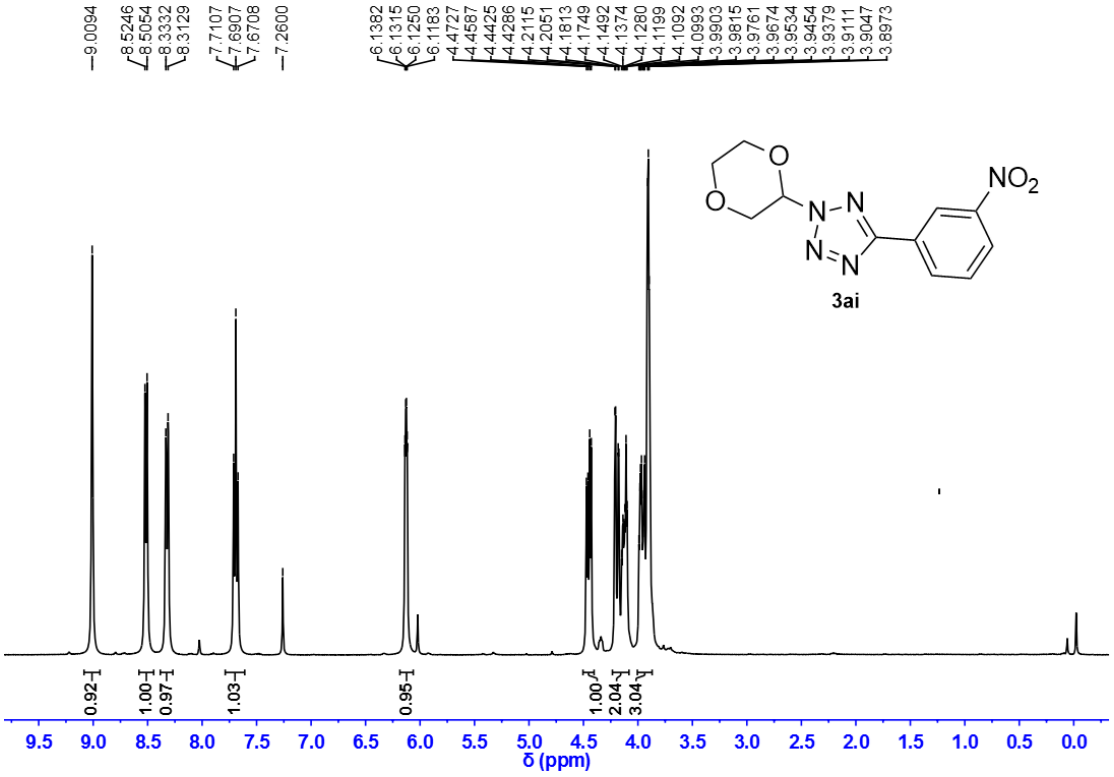
δ (ppm)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6.1250
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3.9903
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NO2
3ai
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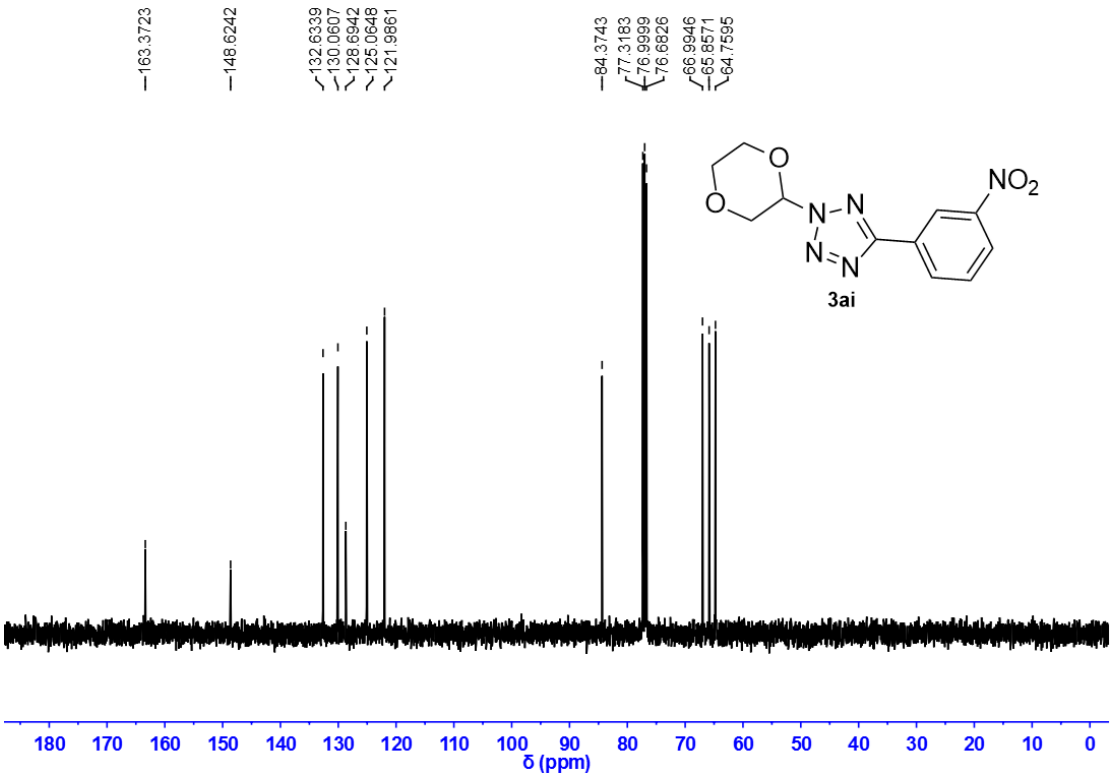
1.00
0.97
1.03
0.95
1.00
2.04
3.04
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
δ (ppm)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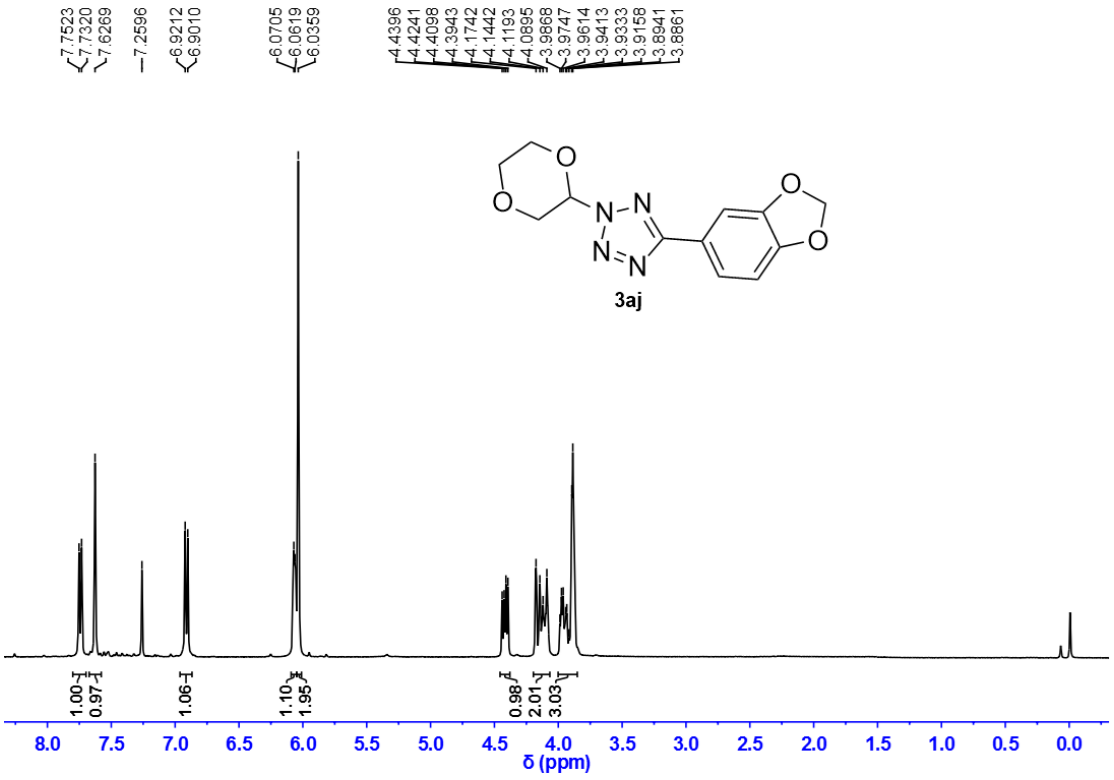
65.8571
64.7595
NO2
3ai
δ (ppm)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6.0619
6.0359
4.4396
4.4241
4.4098
4.3943
4.1742
4.1442
4.1193
4.0895
3.9868
3.9747
3.9614
3.9413
3.9333
3.9158
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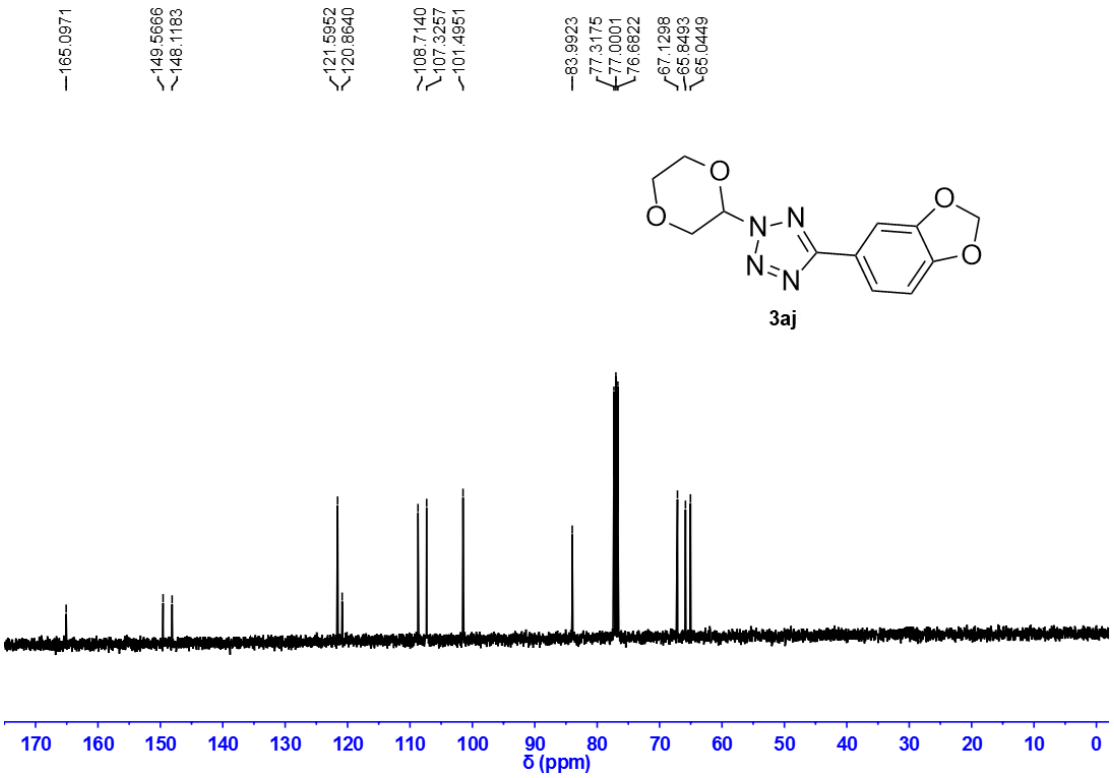
1.95
0.98
2.01
3.03
3aj
δ (ppm)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67.1298
65.8493
65.0449
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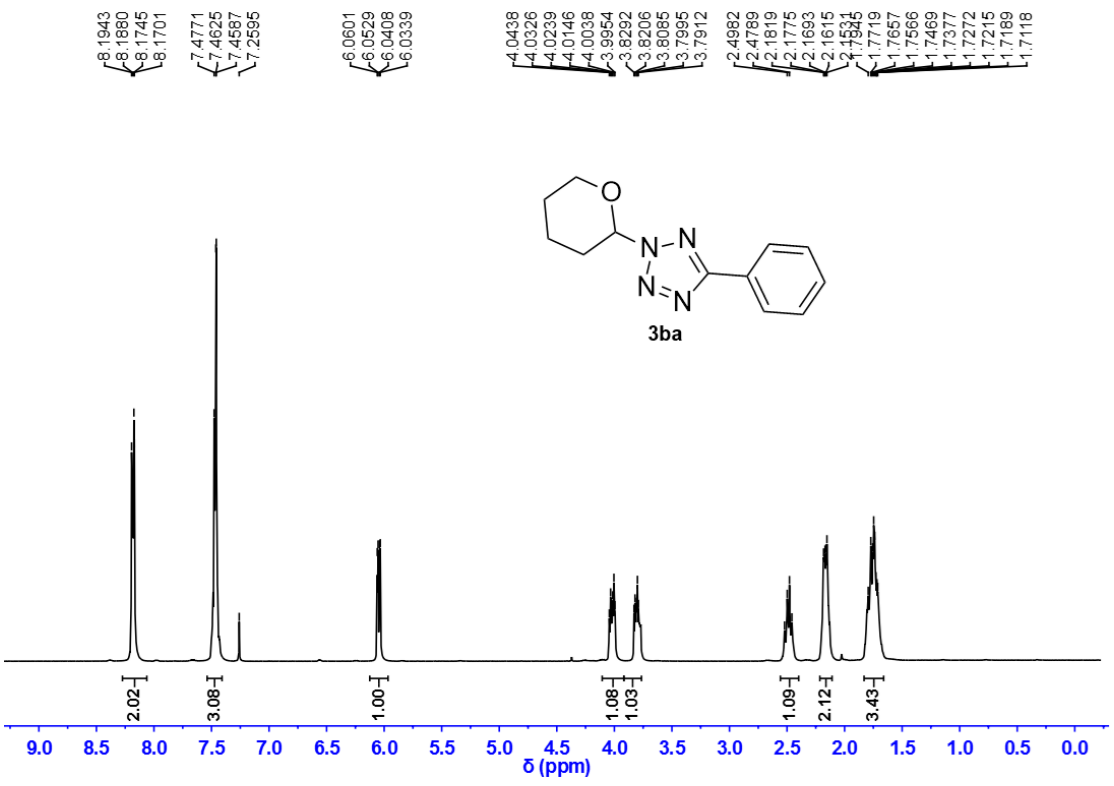
δ (ppm)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4.0146
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3.8206
3.8085
3.7995
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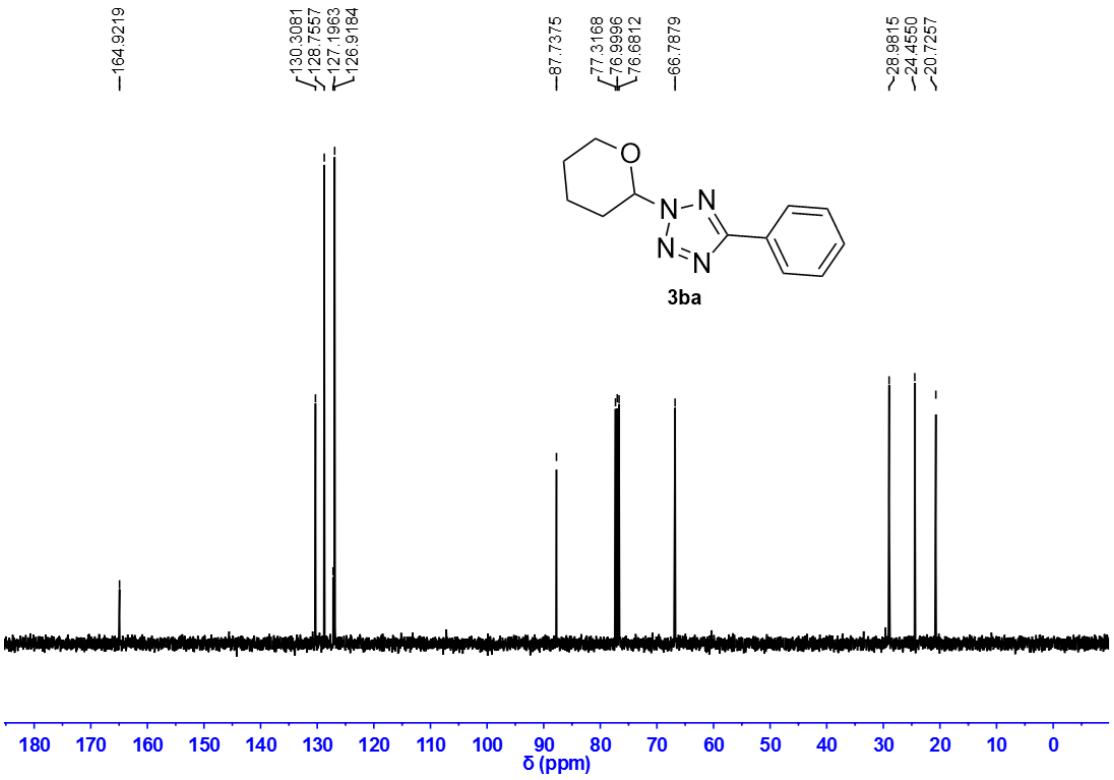
2.4789
2.1819
2.1775
2.1693
2.1615
1.7719
1.7657
1.7566
1.7469
1.7377
1.7272
1.7215
1.7189
1.7118
3ba
2.02
3.08
1.00
1.08
1.03
1.09
2.12
3.43
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
δ (ppm)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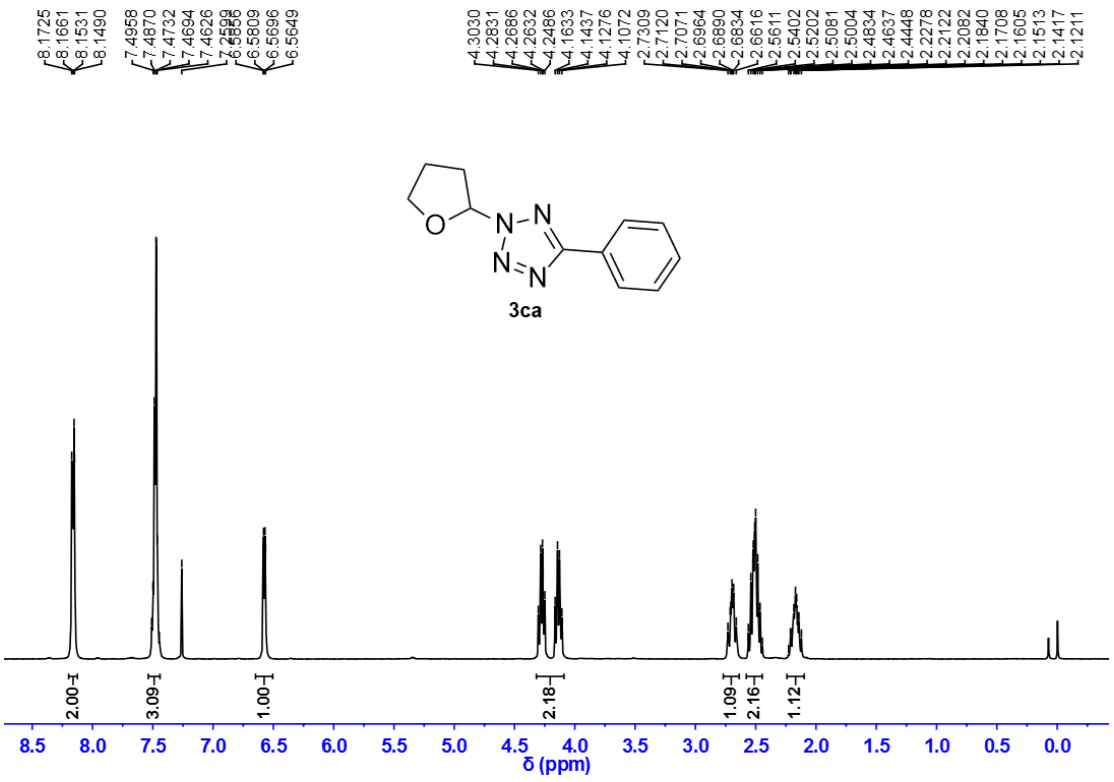
δ (ppm)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6.5649
4.3030
4.2831
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4.2632
4.2486
4.1633
4.1437
4.1276
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2.6834
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2.5611
2.5402
2.5202
2.5081
2.5004
2.4834
2.4637
2.4448
2.2278
2.2122
2.2082
2.1840
2.1708
2.1605
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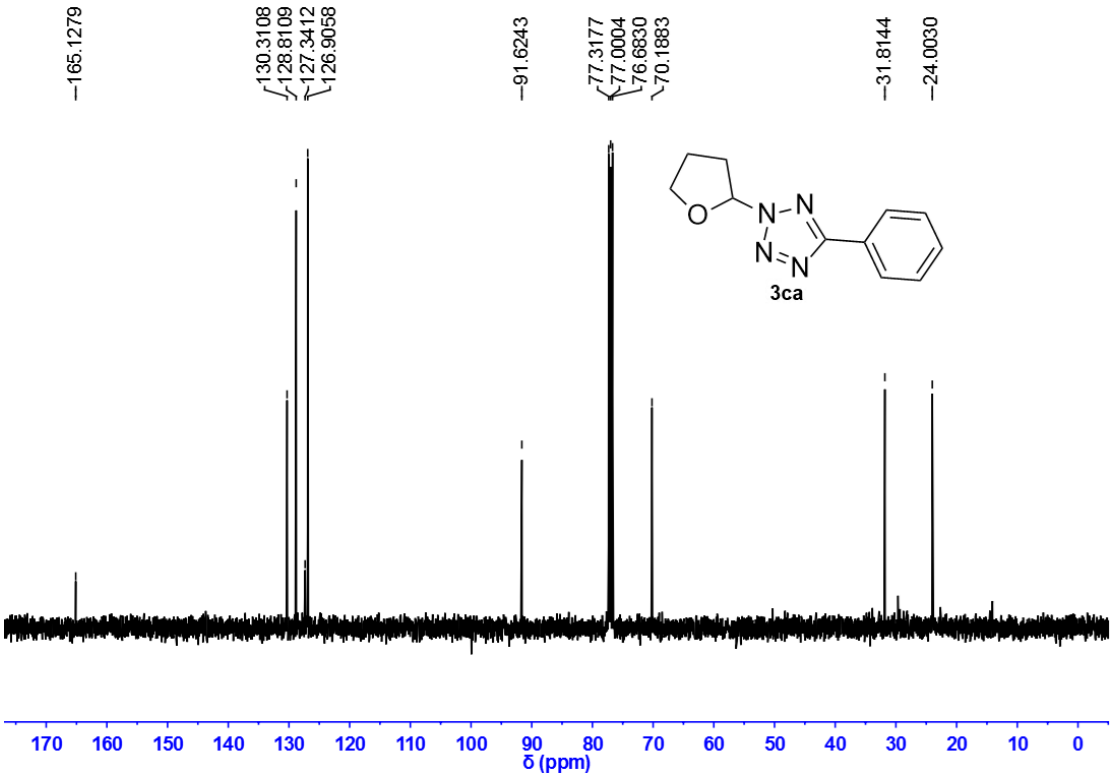
δ (ppm)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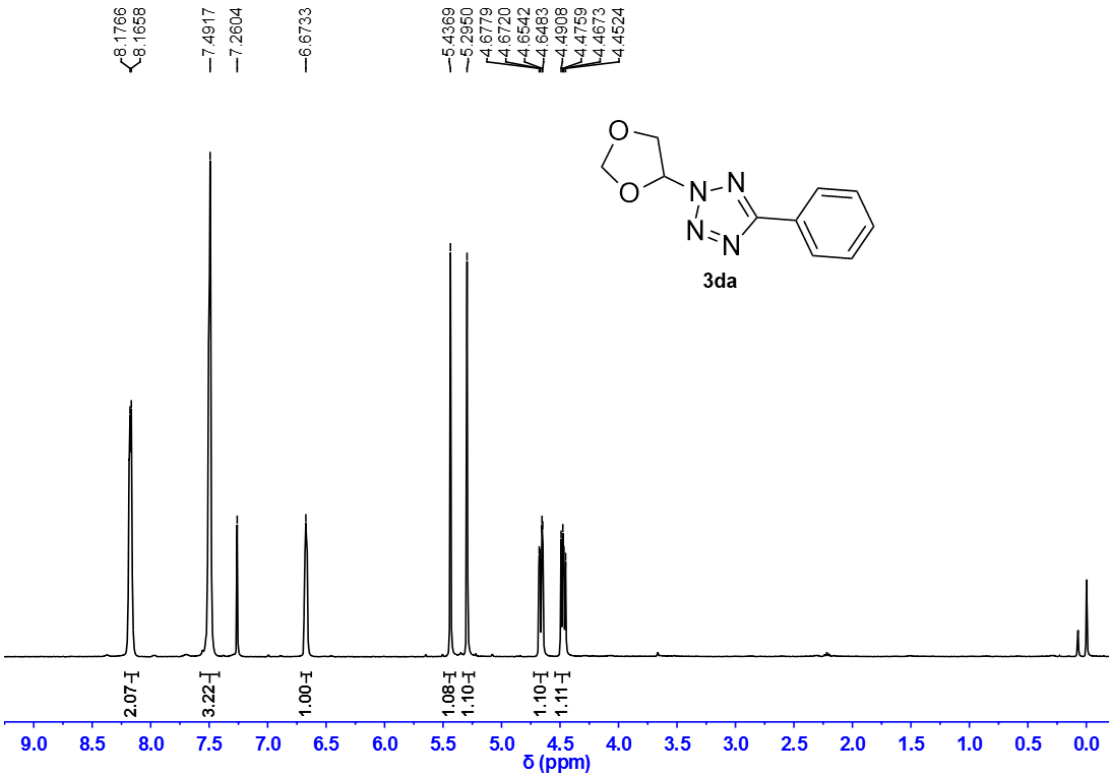
δ (ppm)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4.4759
4.4673
4.4524
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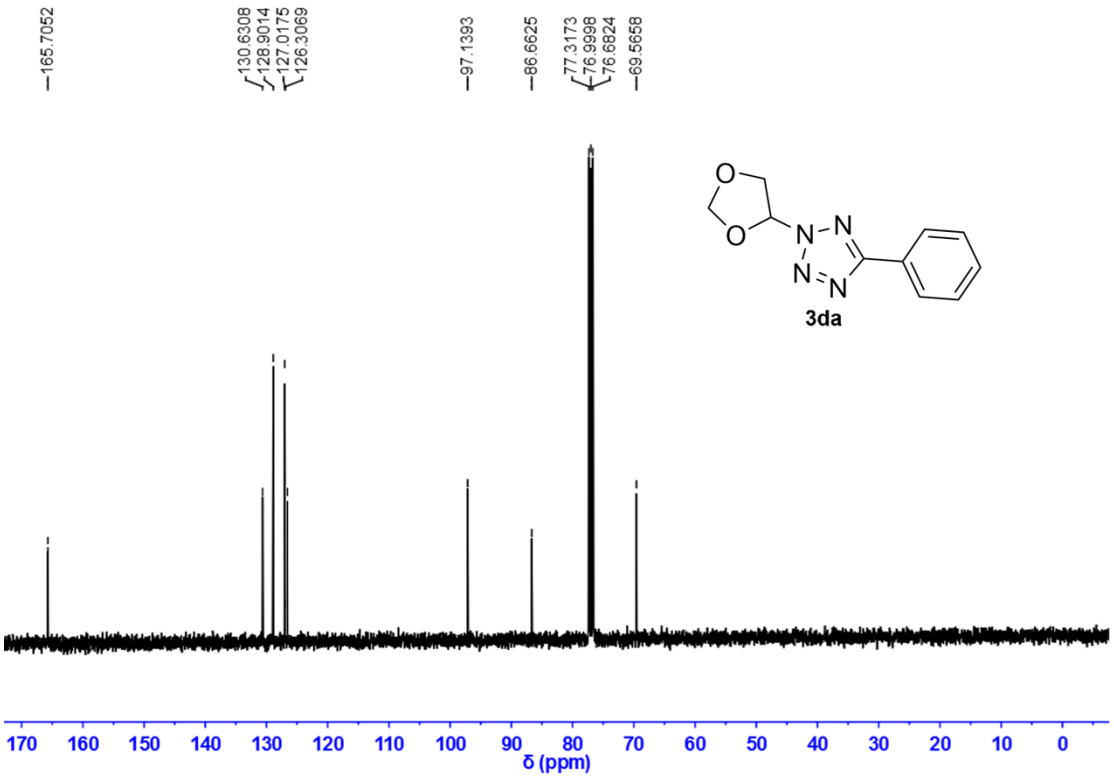
2.07
3.22
1.00
1.08
1.10
1.10
1.11
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
δ (ppm)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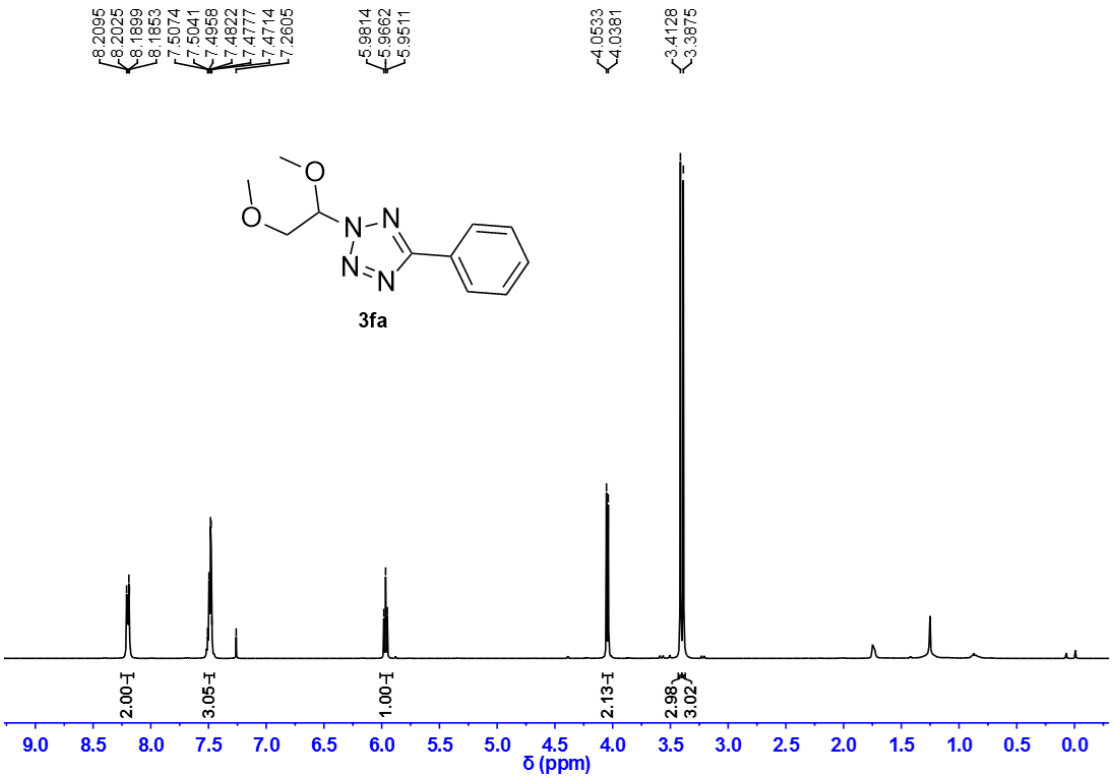
δ (ppm)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7.4777
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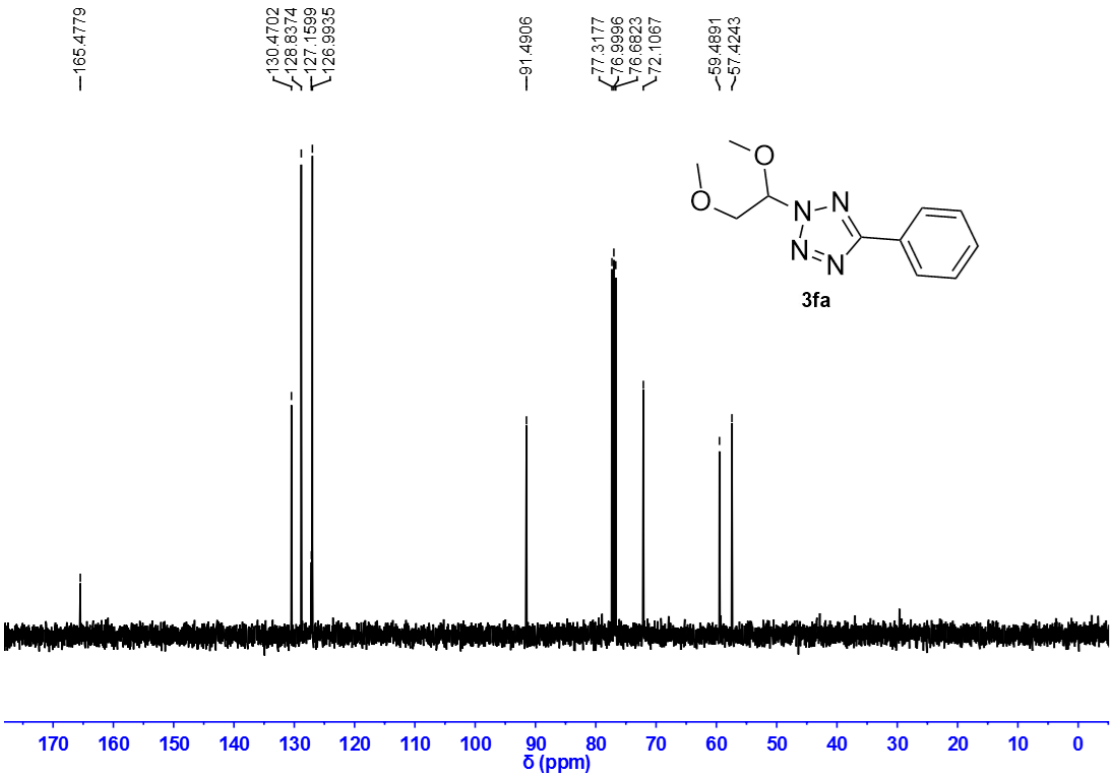
5.9814
5.9662
5.9511
4.0533
4.0381
3.4128
3.3875
3fa
2.00
3.05
1.00
2.13
2.98
3.02
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
δ (ppm)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57.4243
3fa
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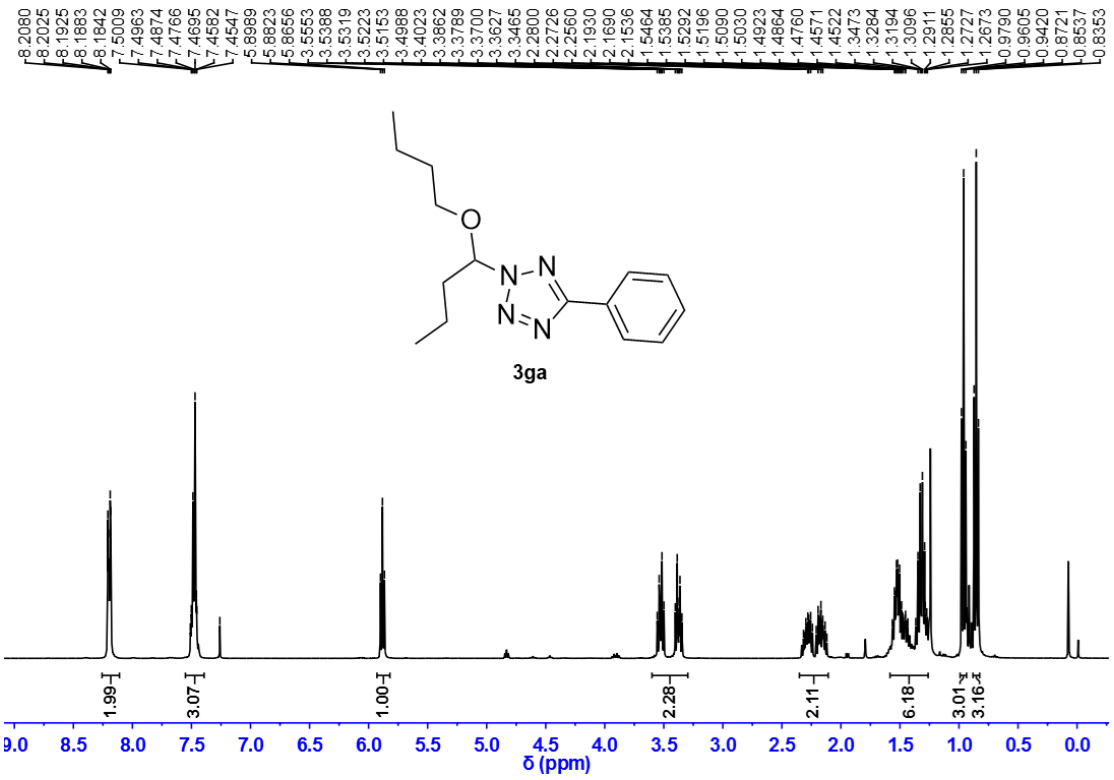
δ (ppm)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3.5319
3.5223
3.5153
3.4988
3.4023
3.3862
3.3789
3.3700
3.3627
3.3465
2.2800
2.2726
2.2560
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2.1690
2.1536
1.5464
1.5385
1.5292
1.5196
1.5090
1.5030
1.4923
1.4864
1.4760
1.4571
1.4522
1.3473
1.3284
1.3194
1.3096
1.2911
1.2855
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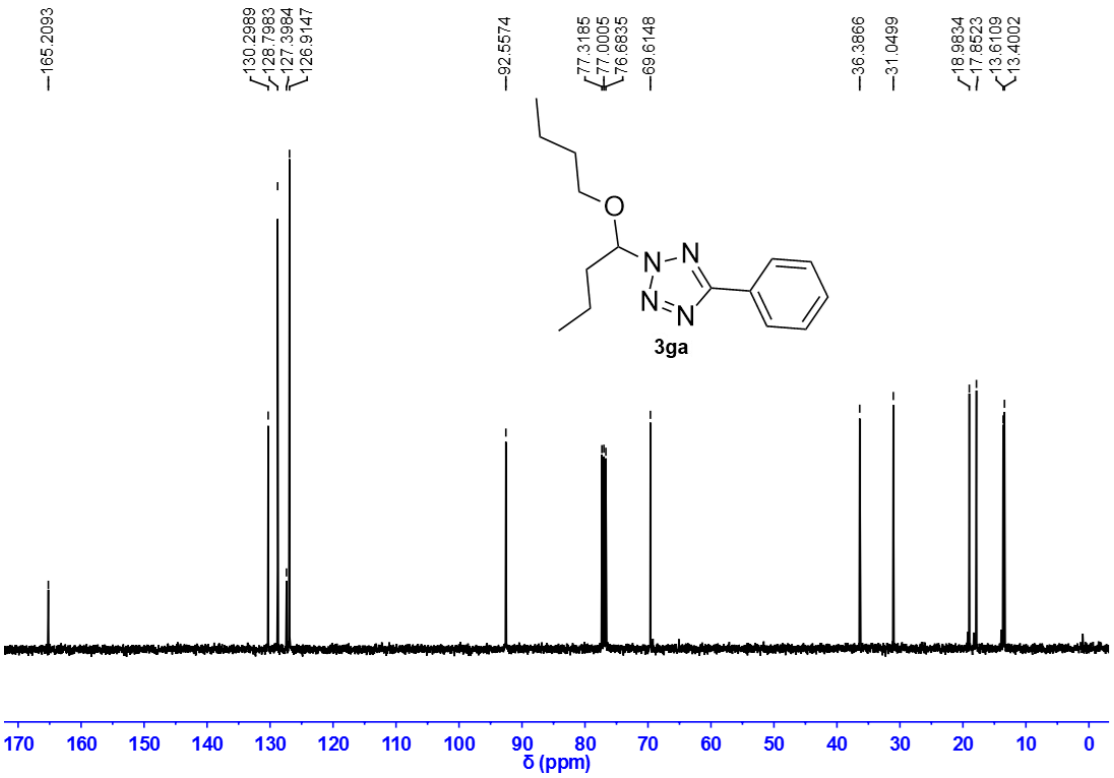
0.8537
0.8353
3ga
1.99
3.07
1.00
2.28
2.11
6.18
3.01
3.16
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
δ (ppm)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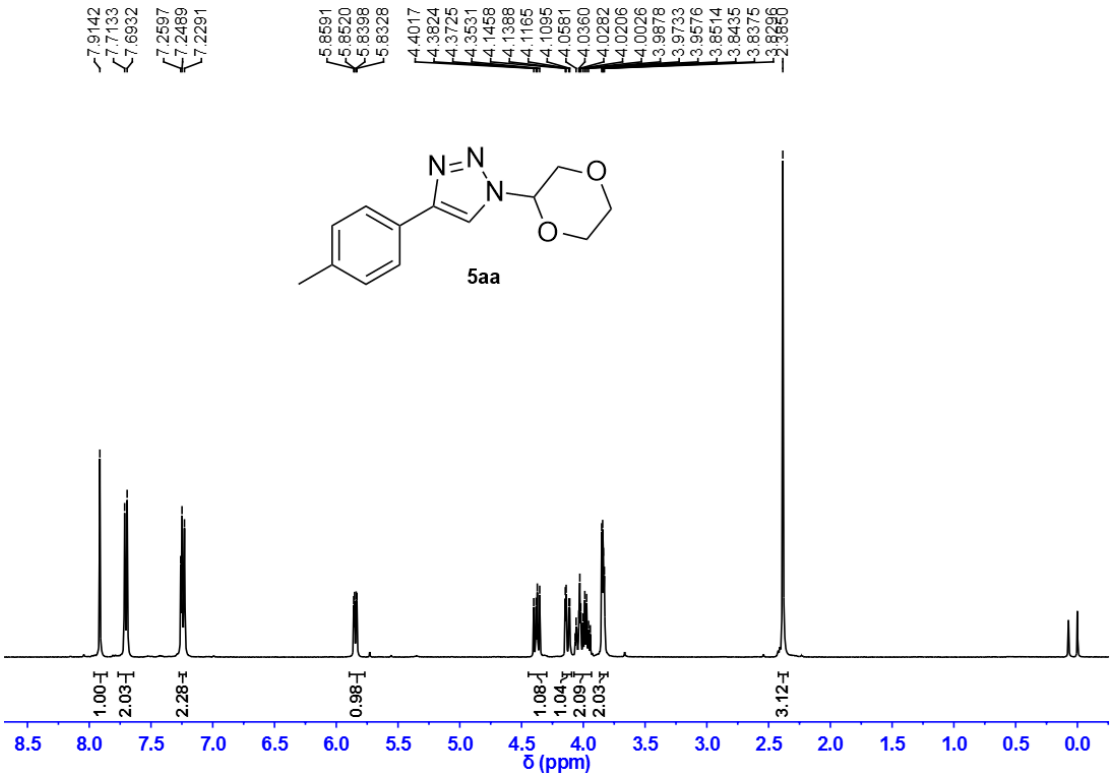
δ (ppm)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4.3824
4.3725
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4.1368
4.1165
4.1095
4.0581
4.0360
4.0282
4.0206
4.0026
3.9878
3.9733
3.9576
3.8514
3.8435
3.8375
2.3850
5aa
1.00
2.03
2.28
0.98
1.08
1.04
2.09
2.03
3.12
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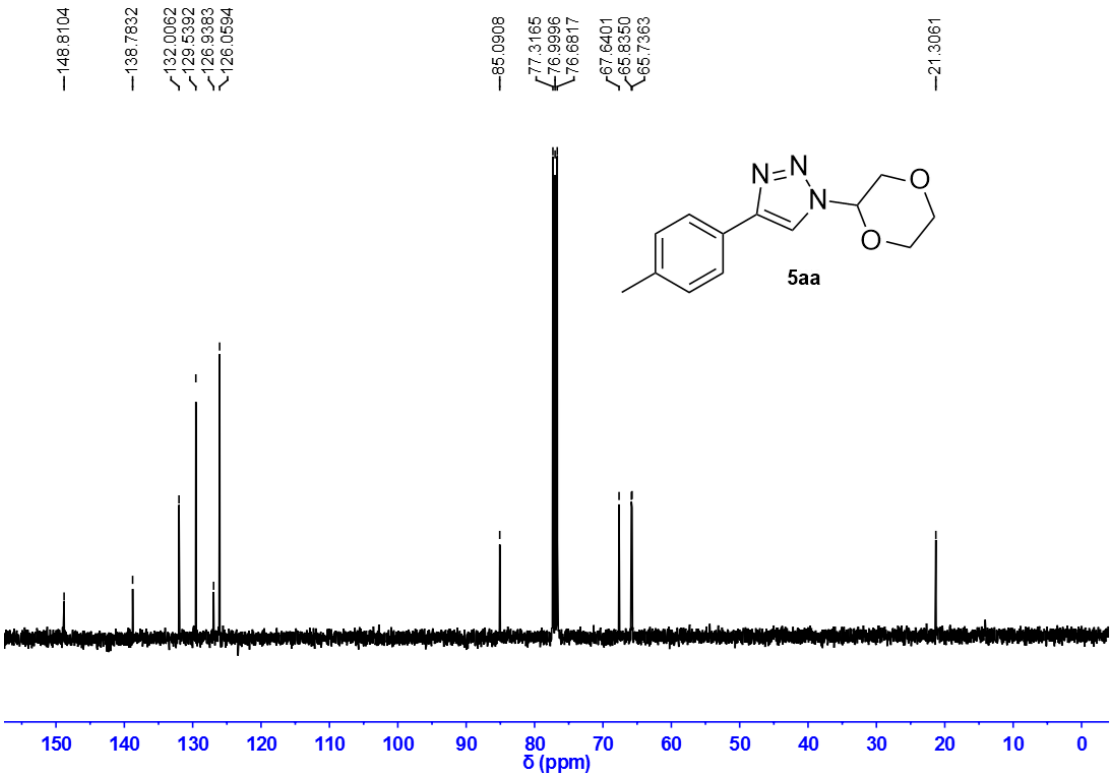
δ (ppm)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65.8350
65.7363
21.3061
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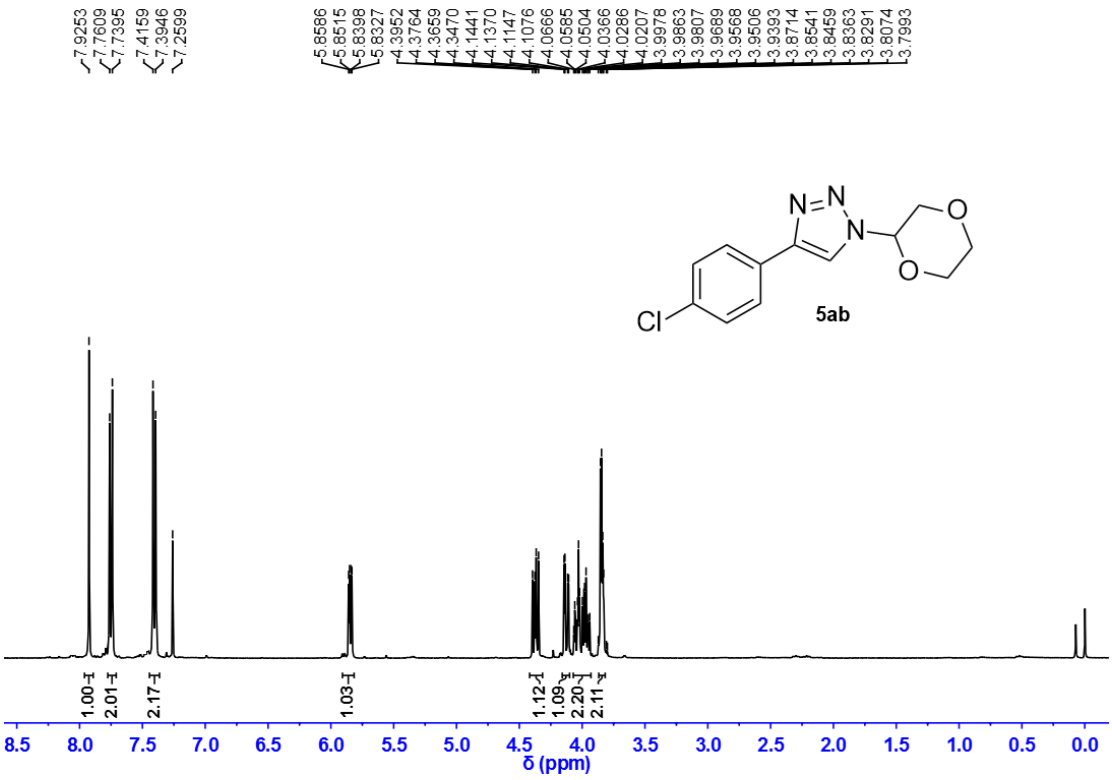
δ (ppm)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4.1147
4.1076
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4.0207
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6.0
5.5
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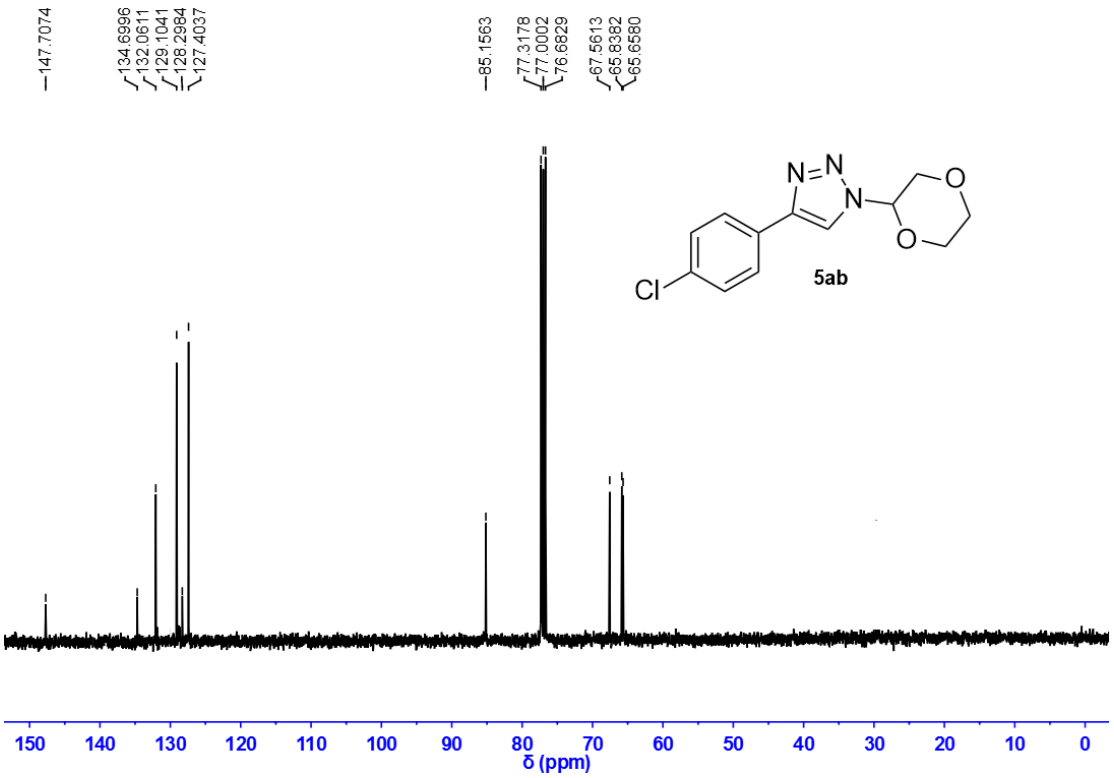
δ (ppm)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Cl
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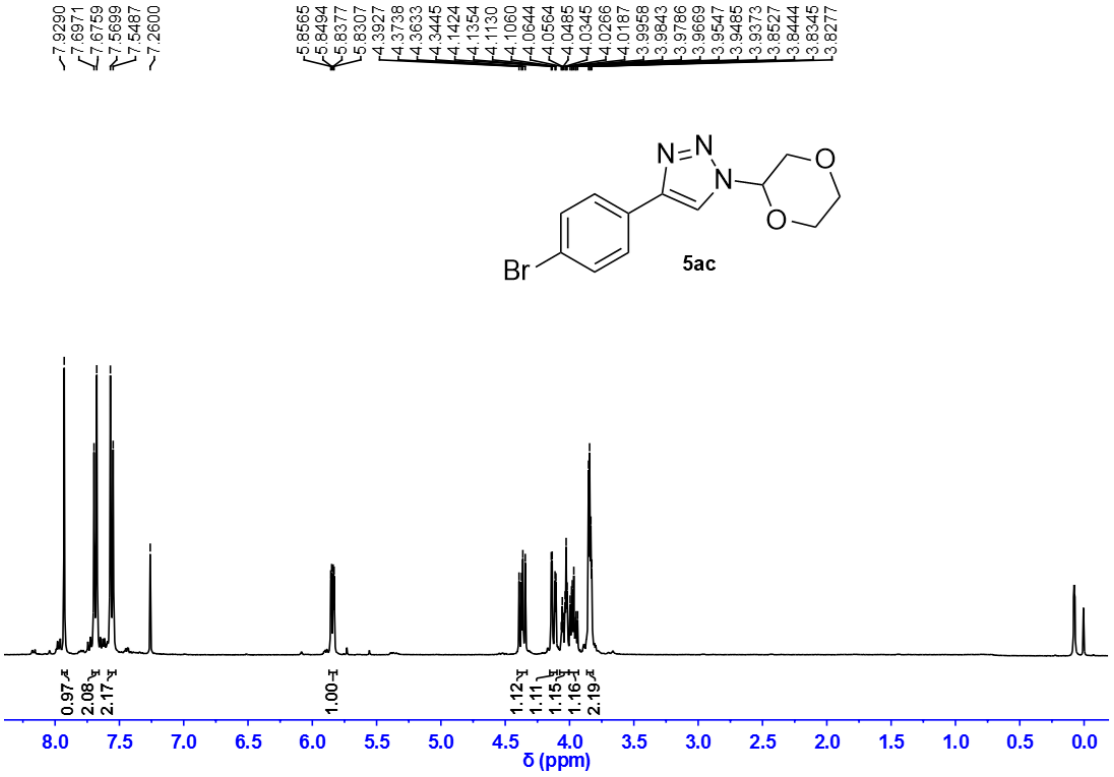
δ (ppm)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1.11
1.15
1.16
2.19
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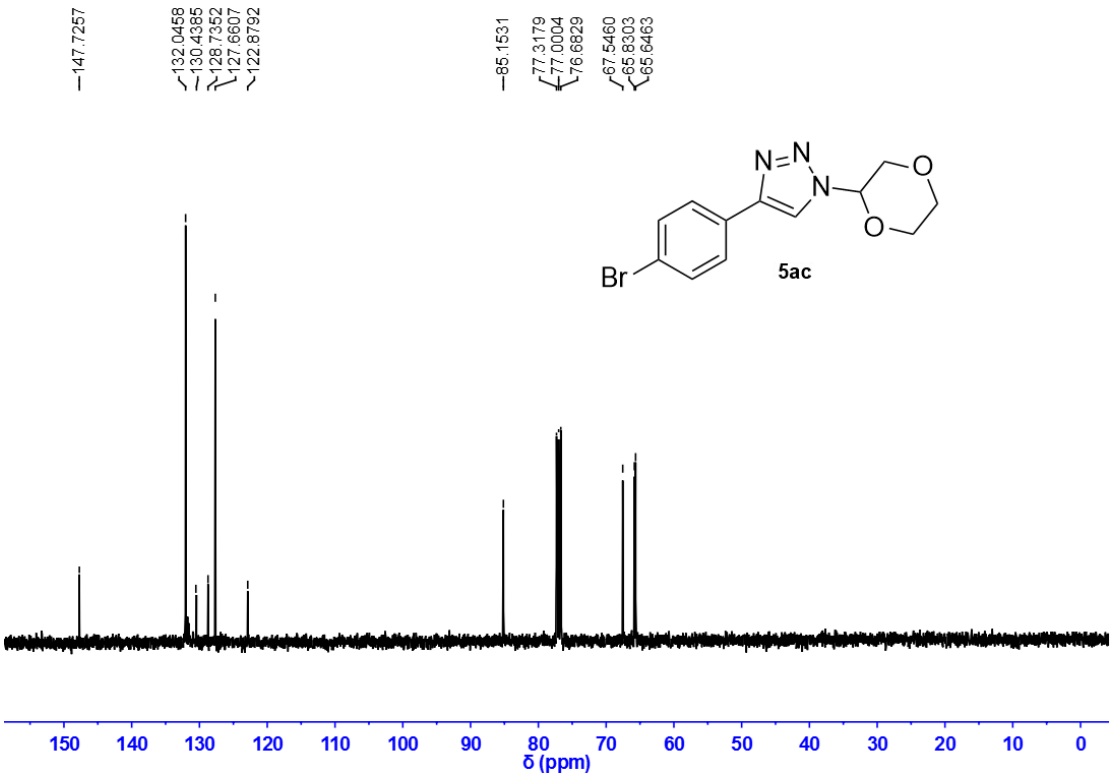
δ (ppm)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65.6463
Br
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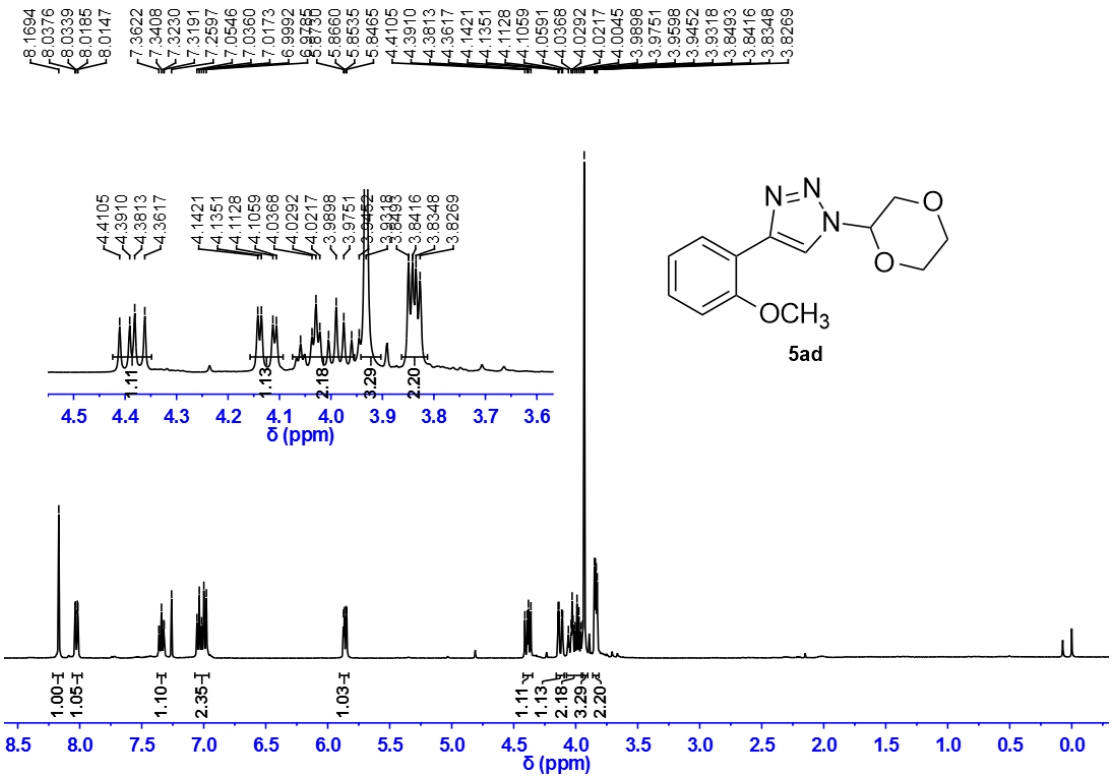
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
δ (ppm)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3.29
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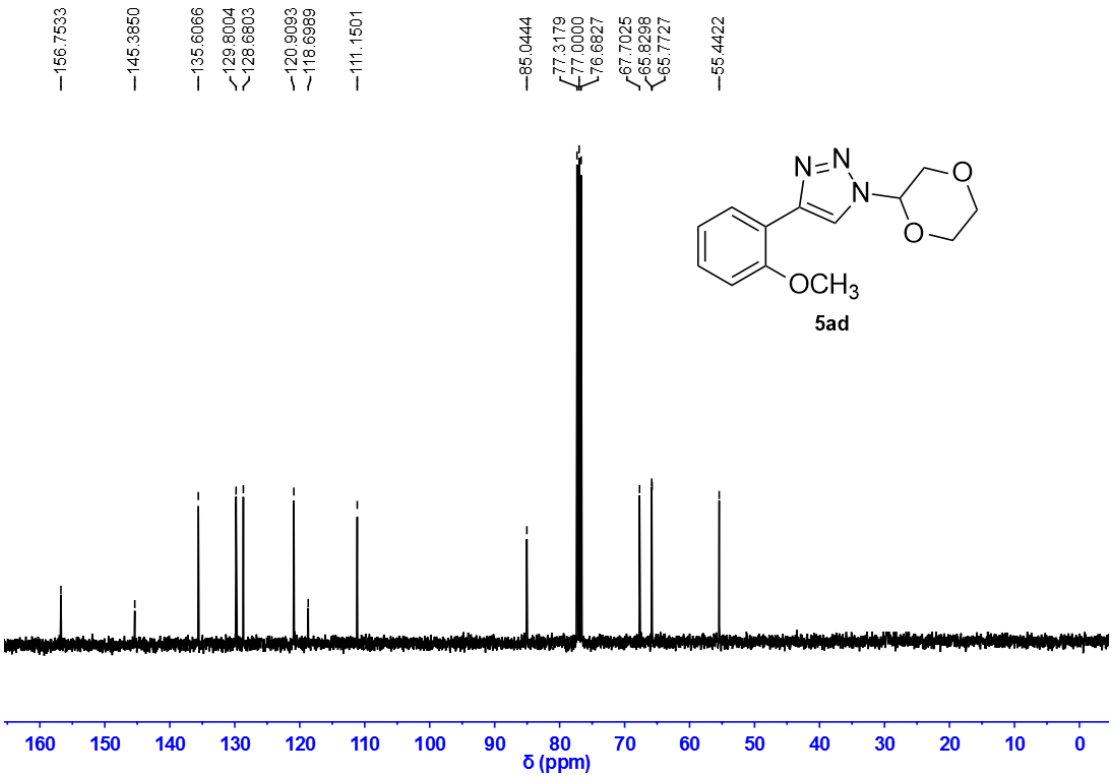
δ (ppm)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OCH3
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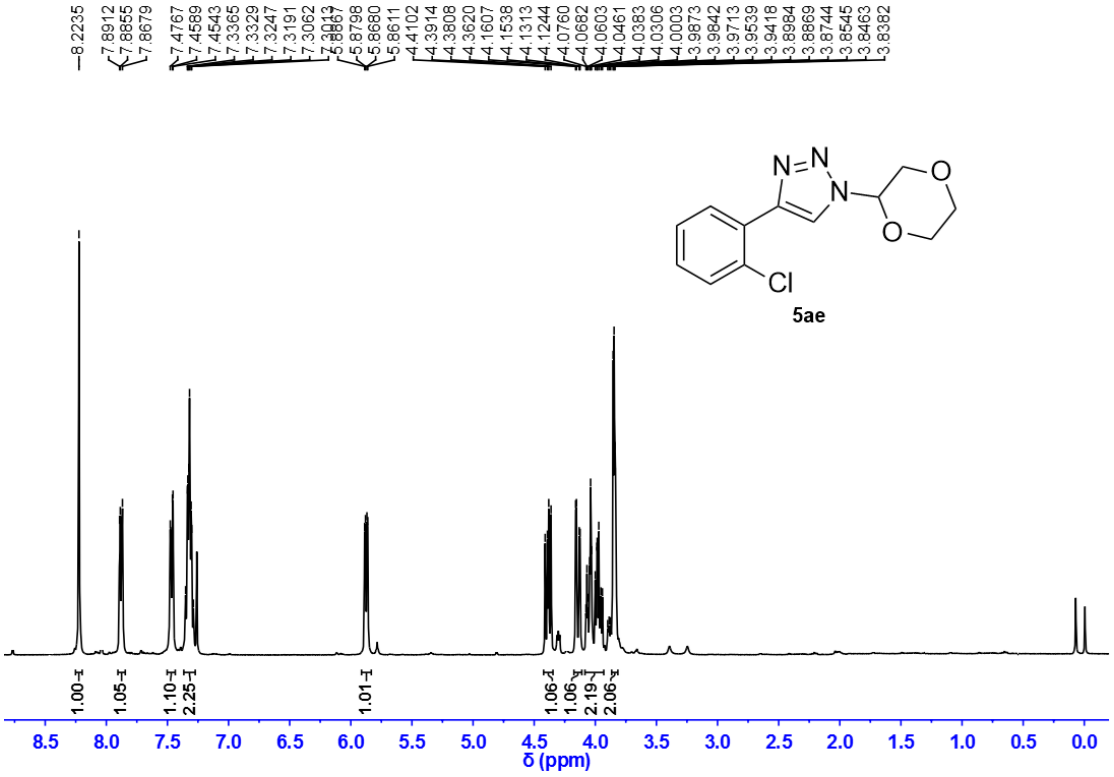
δ (ppm)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3.8744
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Cl
5ae
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1.05
1.10
2.25
1.01
1.06
1.06
2.19
2.06
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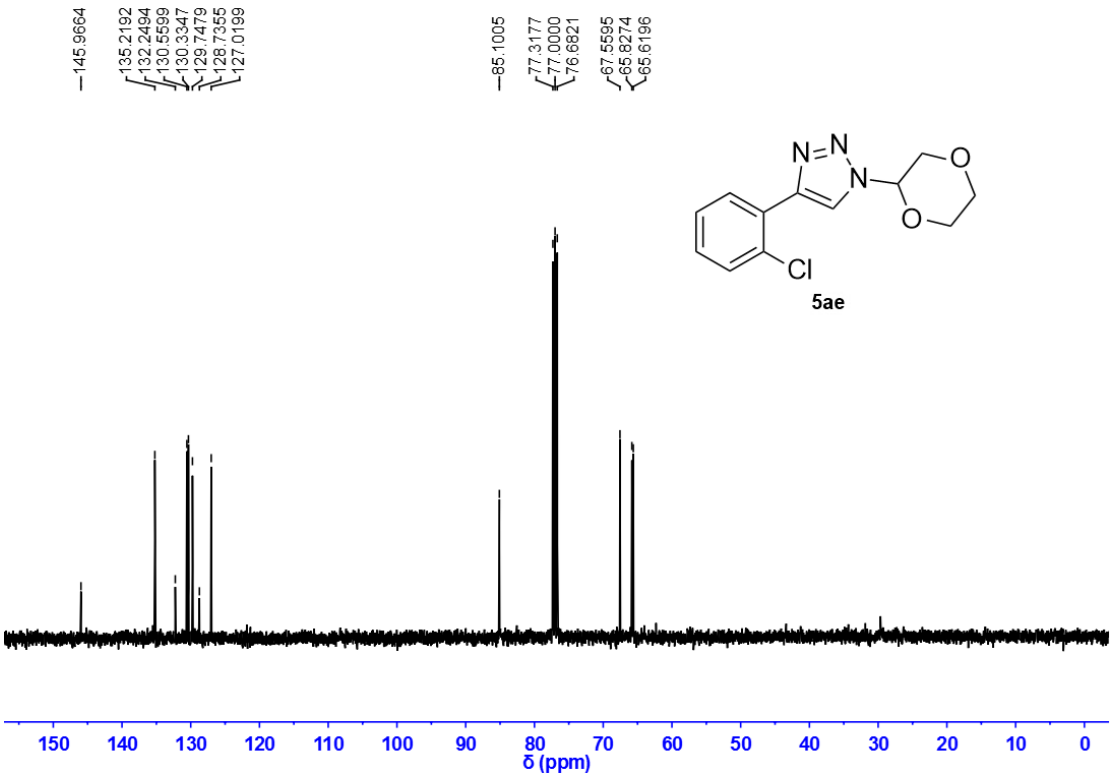
δ (ppm)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N
O
O
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10
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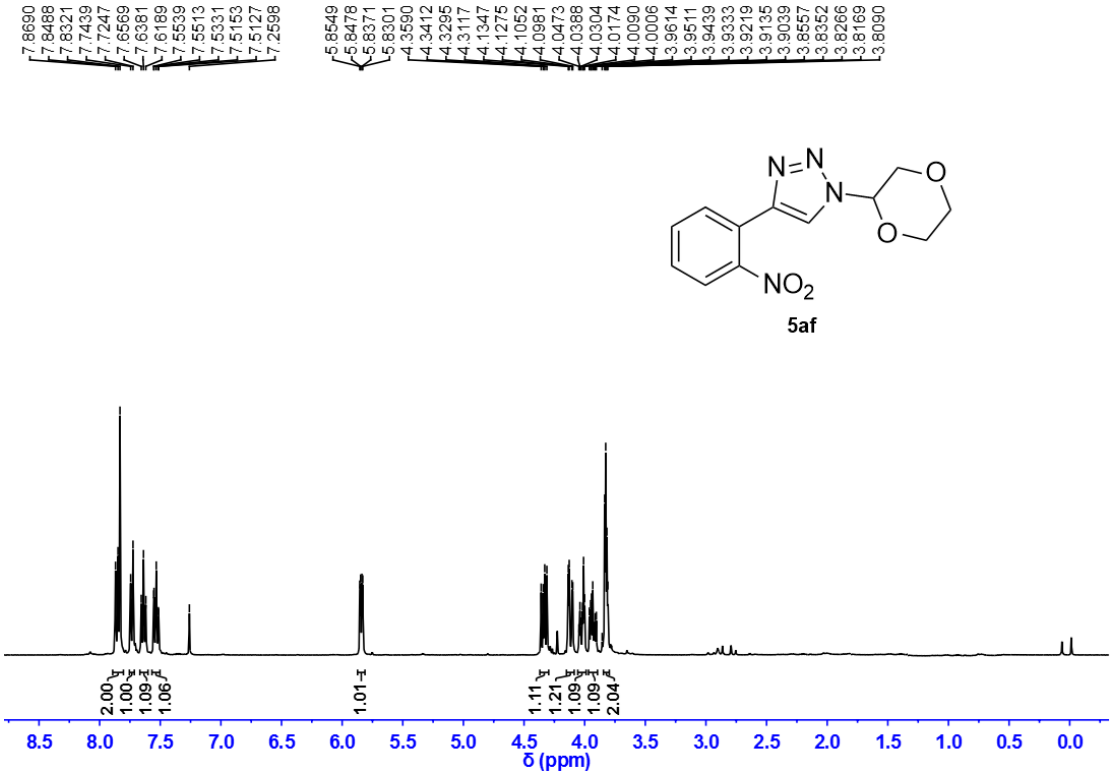
δ (ppm)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3.9333
3.9219
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3.8557
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3.8169
3.8090
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O
O
NO2
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1.06
1.01
1.11
1.21
1.09
1.09
2.04
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7.0
6.5
6.0
5.5
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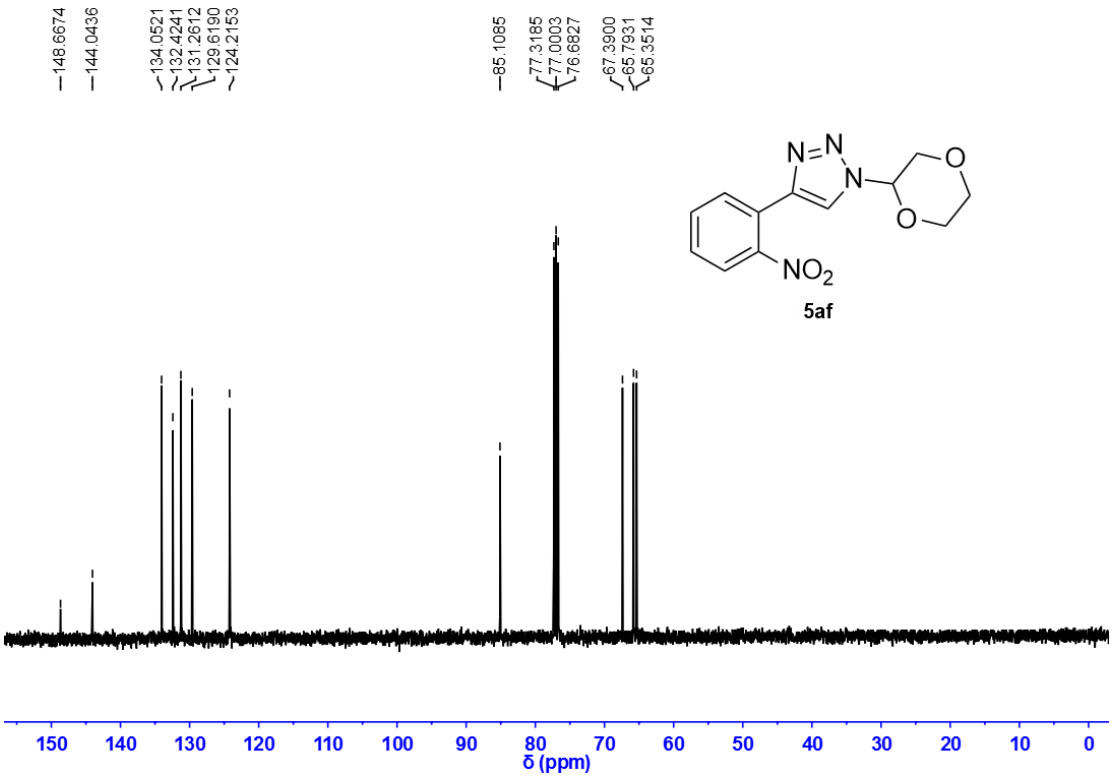
δ (ppm)



5 Reference

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