

Supporting Information

Nanomagnetic Tetraaza (N₄ Donor) Macrocyclic Schiff Base Complex of Copper(II): Synthesis, Characterizations, and Its Catalytic Application in Click Reaction

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Figure S1. ¹H NMR of 5-Phenyltetrazole

Figure S2. ¹H NMR of 5-p-Tolyl-1H-tetrazole.

Figure S3. ¹H NMR of 5-(4-Trifluoromethyl-phenyl)-1H-tetrazole

Figure S4. ¹H NMR of 5-(4-Nitrophenyl)tetrazole.

Figure S5. ¹H NMR of 5-(2-Fluoro-phenyl)-1H-tetrazole

Figure S6. ¹H NMR of 5-(2-Chlorophenyl)tetrazole.

Figure S7. ¹H NMR of 5-(4-Chlorophenyl)tetrazole.

Figure S8. ¹H NMR of 5-(4-Bromo-phenyl)-1H-tetrazole.

Figure S9. ¹H NMR of 4-(1H-Tetrazol-5-yl)-phenol.

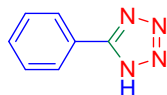
Figure S10. ¹H NMR of 2-(1H-Tetrazol-5-yl)-benzotrile.

Figure S11. The reaction mixture before and after of catalyst separation via a magnetism.

Supporting Information

Spectral Data:

5-Phenyltetrazole (Table 2, entry 1):



Yield = 98%; M.P.= (215-217 °C Found, 211-214°C Reported); $^1\text{H NMR}$ (400 MHz, DMSO- d_6), δ (ppm): 16.92 (s, 1H), 8.03 (dd, J = 6.5, 3.3 Hz, 2H), 7.60 (dd, J = 5.1, 2.1 Hz, 3H).

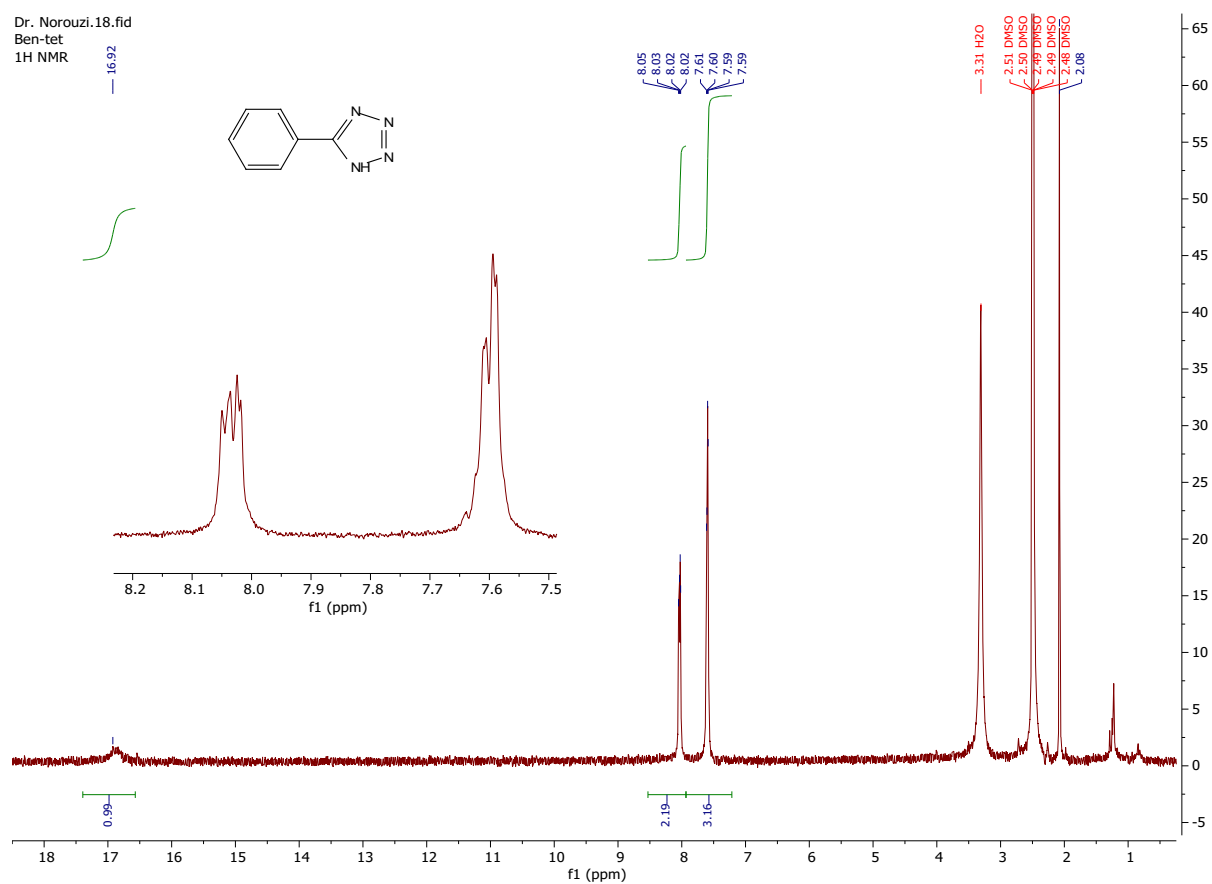
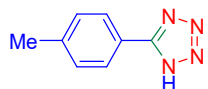


Figure S1. $^1\text{H NMR}$ of 5-Phenyltetrazole.

5-p-Tolyl-1H-tetrazole (Table 2, entry 2):

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Yield = 93%; M.P.= (294-251 °C Found, 252-254°C Reported); ^1H NMR (400 MHz, DMSO- d_6), δ (ppm): 16.68 (s, 1H), 7.93-7.89 (d, J = 8 Hz, 2H), 7.42-7.38 (d, J = 8 Hz, 2H), 2.38 (s, 3H).

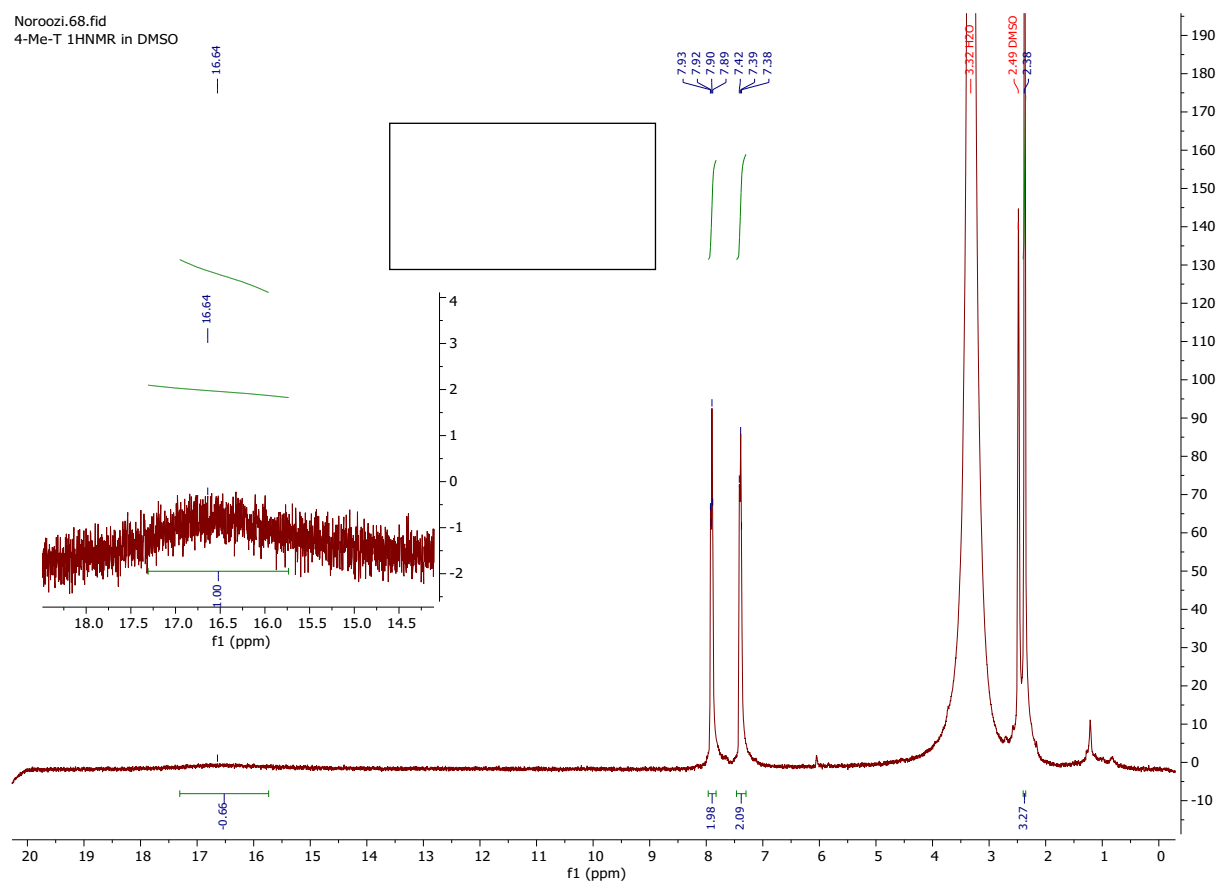
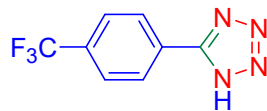


Figure S2. ^1H NMR of 5-p-Tolyl-1H-tetrazole.

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5-(4-Trifluoromethyl-phenyl)-1H-tetrazole (Table 2, entry 3):



Yield = 96%; M.P.= (221-222 °C Found, 218-219°C Reported); ^1H NMR (400 MHz, DMSO- d_6), δ (ppm): 8.35-8.33 (d, J = 8 Hz, 2H), 7.98-7.95 (d, J = 8 Hz, 1H), 7.88-7.83 (t, 1H).

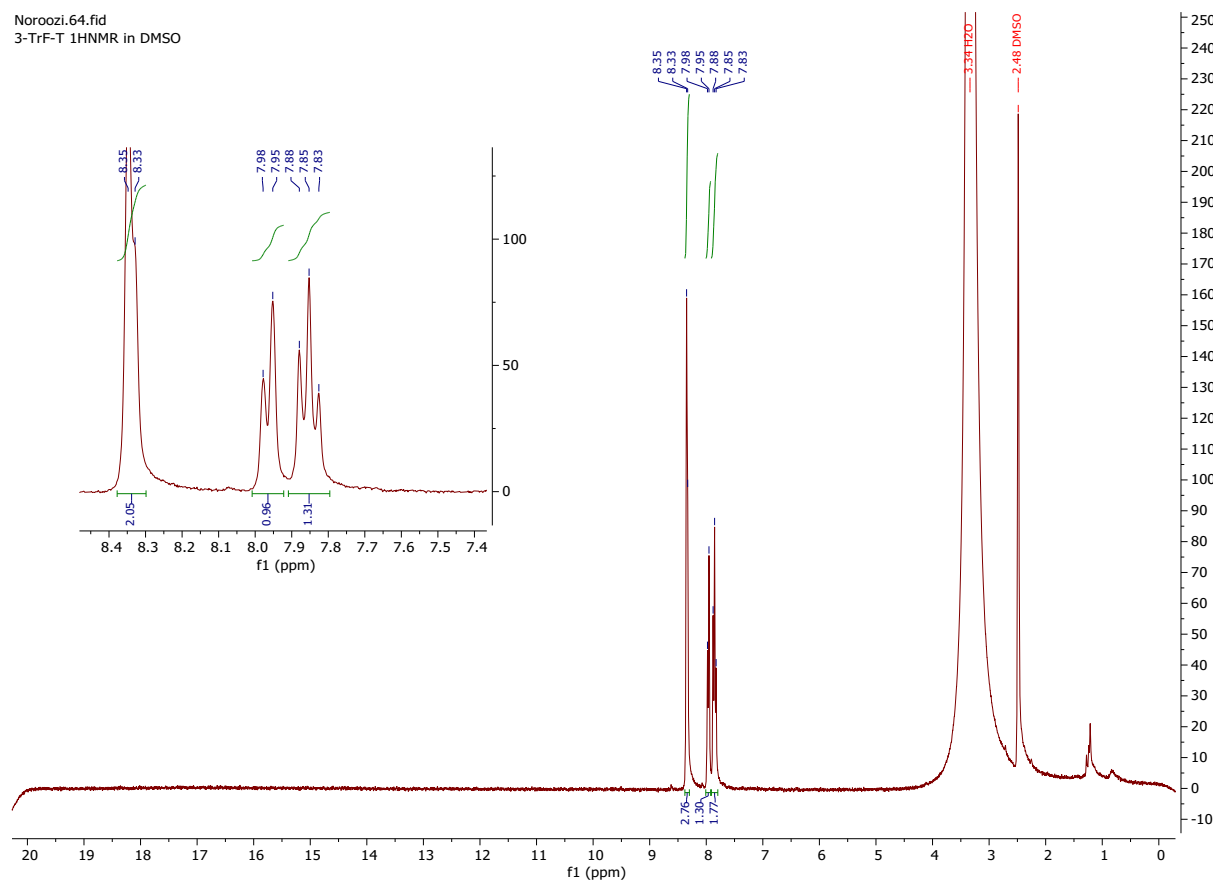
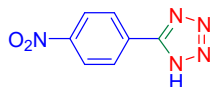


Figure S3. ^1H NMR of 5-(4-Trifluoromethyl-phenyl)-1H-tetrazole

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5-(4-Nitrophenyl)tetrazole (Table 2, entry 5):



Yield = 93%; M.P.= (219-220 °C Found, 217-220°C Reported); ^1H NMR (400 MHz, DMSO- d_6), δ (ppm): 8.46-8.81 (d, $J = 8$ Hz, 2H), 8.52 – 8.33 (m, 2H).

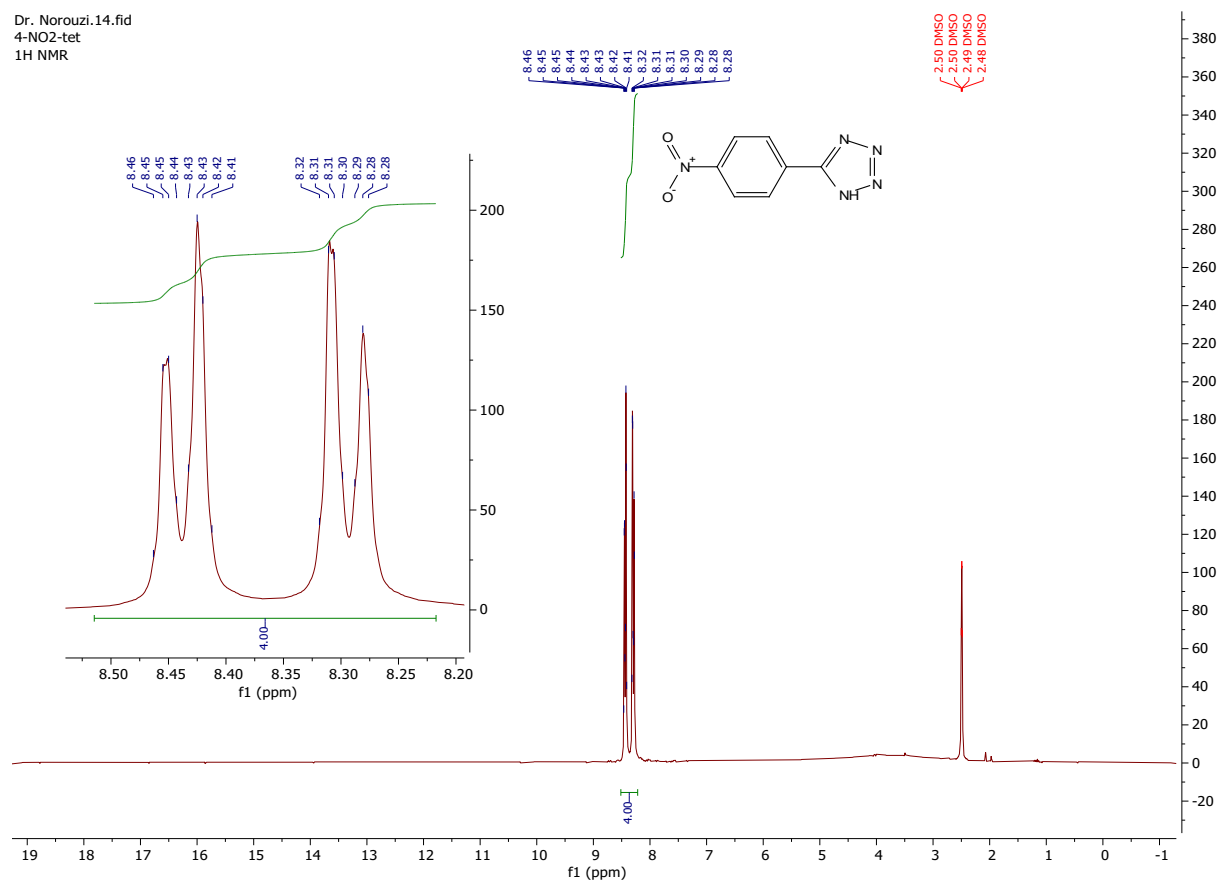
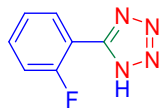


Figure S4. ^1H NMR of 5-(4-Nitrophenyl)tetrazole.

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5-(2-Fluoro-phenyl)-1H-tetrazole (Table 2, entry 6):



Yield = 95%; M.P.= (157-159 °C Found, 158-160°C Reported); ^1H NMR (400 MHz, DMSO- d_6), δ (ppm): 16.86 (b, 1H (N-H)), 8.07 (s, 1H), 7.67-7.64 (d, $J = 8$ Hz, 1H), 7.52-7.41 (m, 2H)

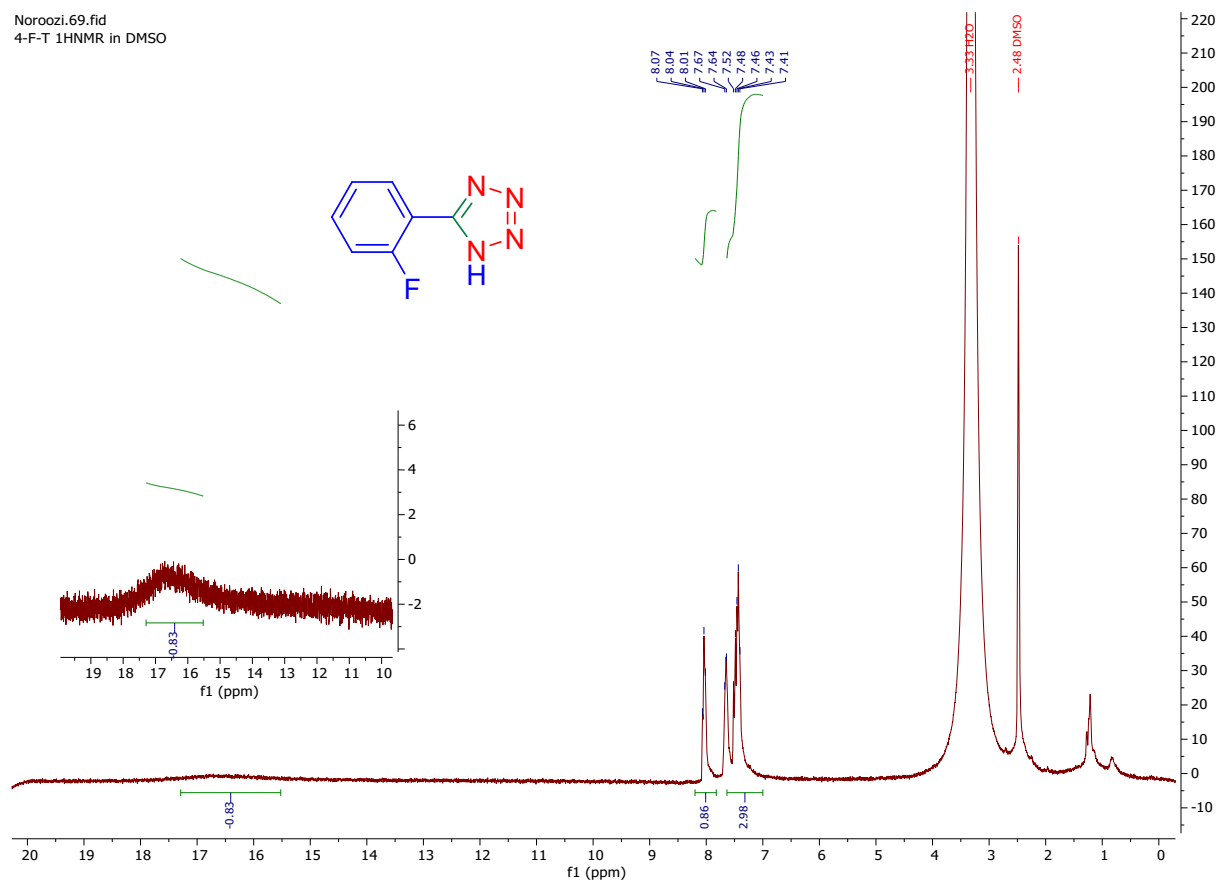
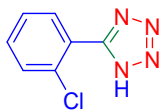


Figure S5. ^1H NMR of 5-(2-Fluoro-phenyl)-1H-tetrazole

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5-(2-Chlorophenyl)tetrazole (Table 2, entry 7):



Yield = 93%; M.P. = (179-180 °C Found, 180-181 °C Reported); $^1\text{H NMR}$ (400 MHz, DMSO- d_6), δ (ppm): 16.88 (b, 1H(N-H)), 8.01 (s, 1H), 7.82-7.79 (d, $J = 8$ Hz, 1H), 7.73-7.72 (d, $J = 8$ Hz, 1H), 7.63- 7.55 (m, 1H).

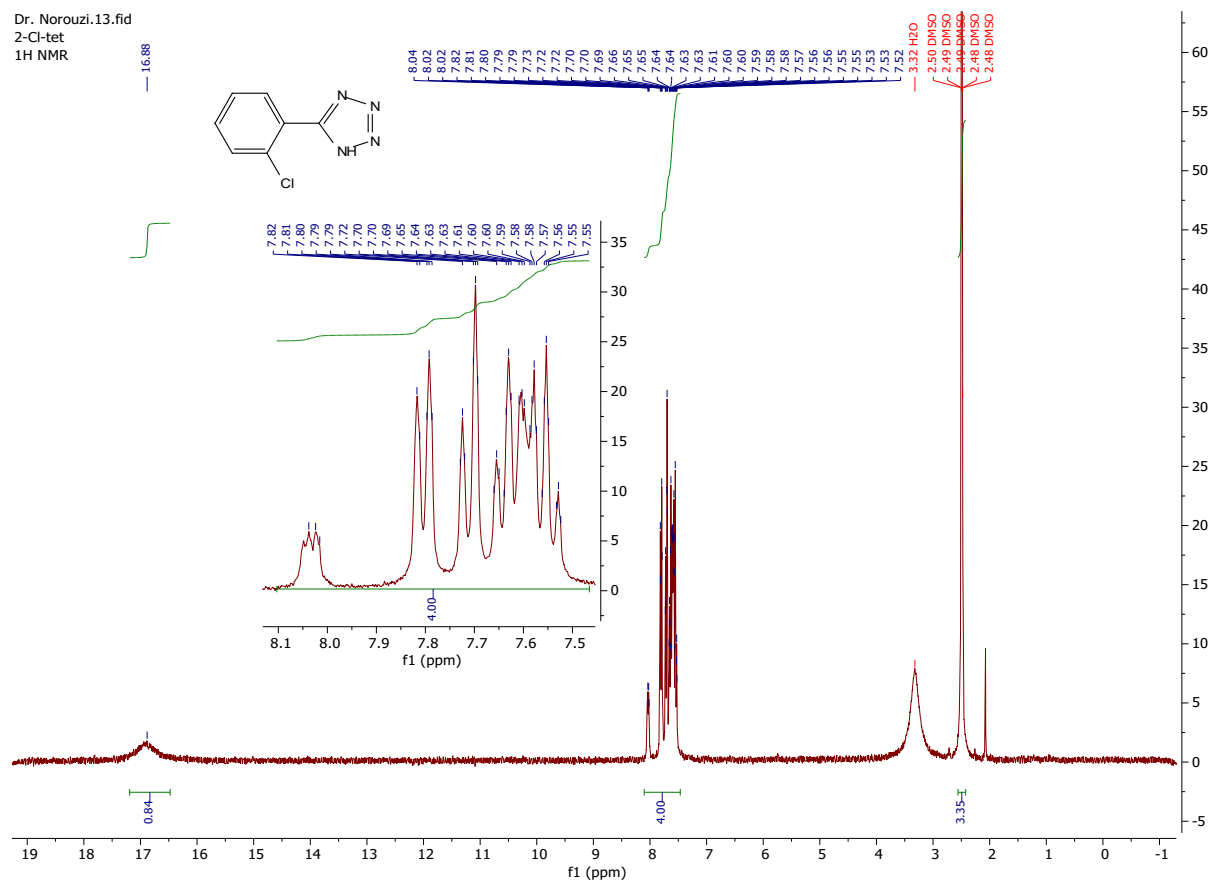
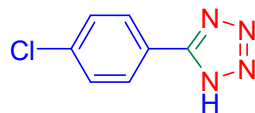


Figure S6. $^1\text{H NMR}$ of 5-(2-Chlorophenyl)tetrazole.

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5-(4-Chloro-phenyl)-1H-tetrazole (Table 2, entry 8):



Yield = 94%; M.P. = (252-254 °C Found, 261-263 °C Reported); ^1H NMR (400 MHz, DMSO- d_6), δ (ppm): 16.89 (b, 1H (N-H)), 8.07 (s, 1H), 8.05-8.02 (d, $J = 8$ Hz, 2H), 7.70-7.66 (d, $J = 8$ Hz, 2H).

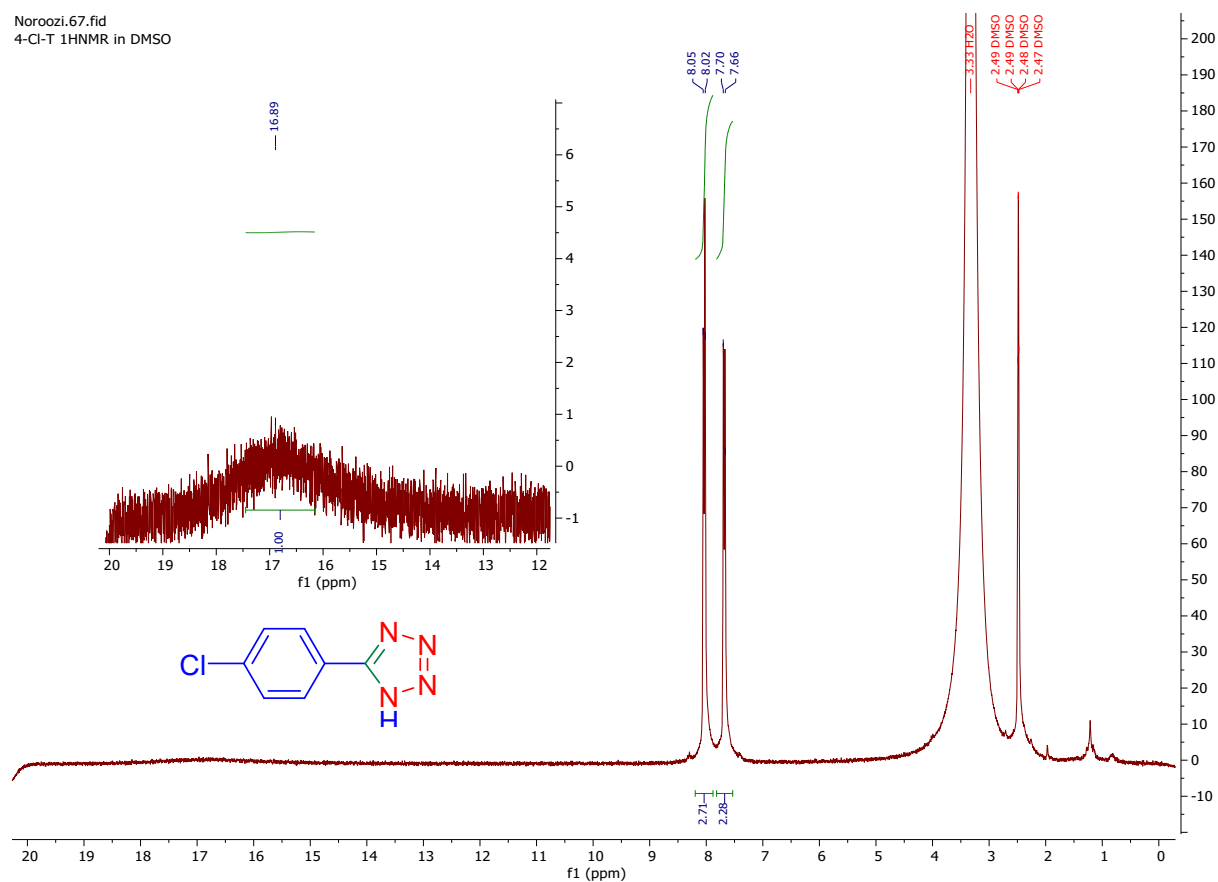
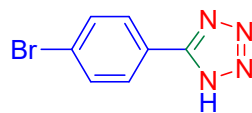


Figure S7. ^1H NMR of 5-(4-Chlorophenyl)tetrazole.

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5-(4-Bromo-phenyl)-1H-tetrazole (Table 2, entry 9):



Yield = 96%; M.P. = (264-266 °C Found, 268-269°C Reported); ^1H NMR (400 MHz, DMSO- d_6), δ (ppm): 7.98-7.95 (d, J = 8 Hz, 2H), 7.83-7.80 (d, J = 8 Hz, 2H).

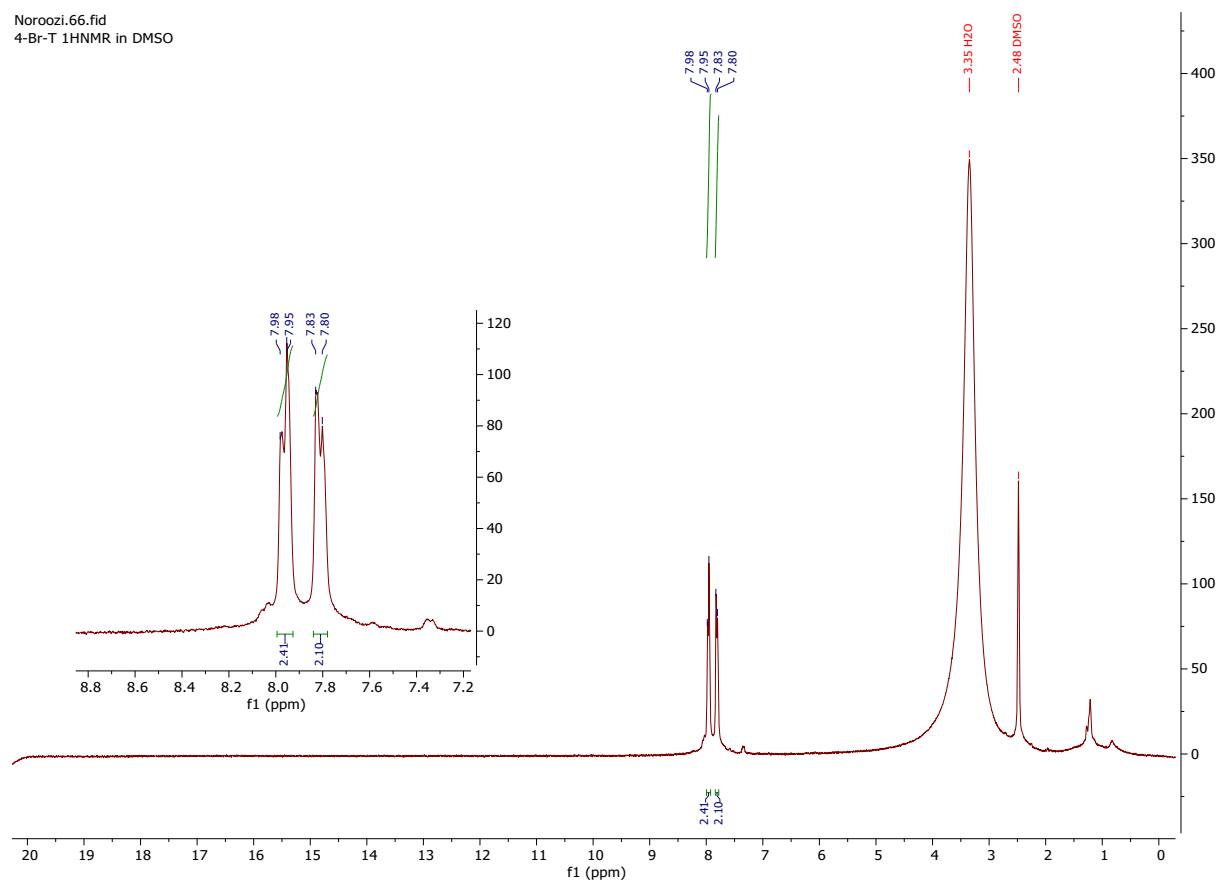
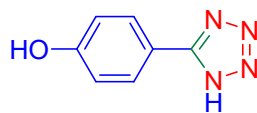


Figure S8. ^1H NMR of 5-(4-Bromo-phenyl)-1H-tetrazole.

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4-(1H-Tetrazol-5-yl)-phenol (Table 2, entry 11):



Yield = 95%; M.P. = (234-236 °C Found, 233-235 °C Reported); ^1H NMR (400 MHz, DMSO- d_6), δ (ppm): 10 (br, 1H, OH), 7.86-7.83 (d, J = 8 Hz, 2H), 6.95-6.98 (d, J = 8 Hz, 2H).

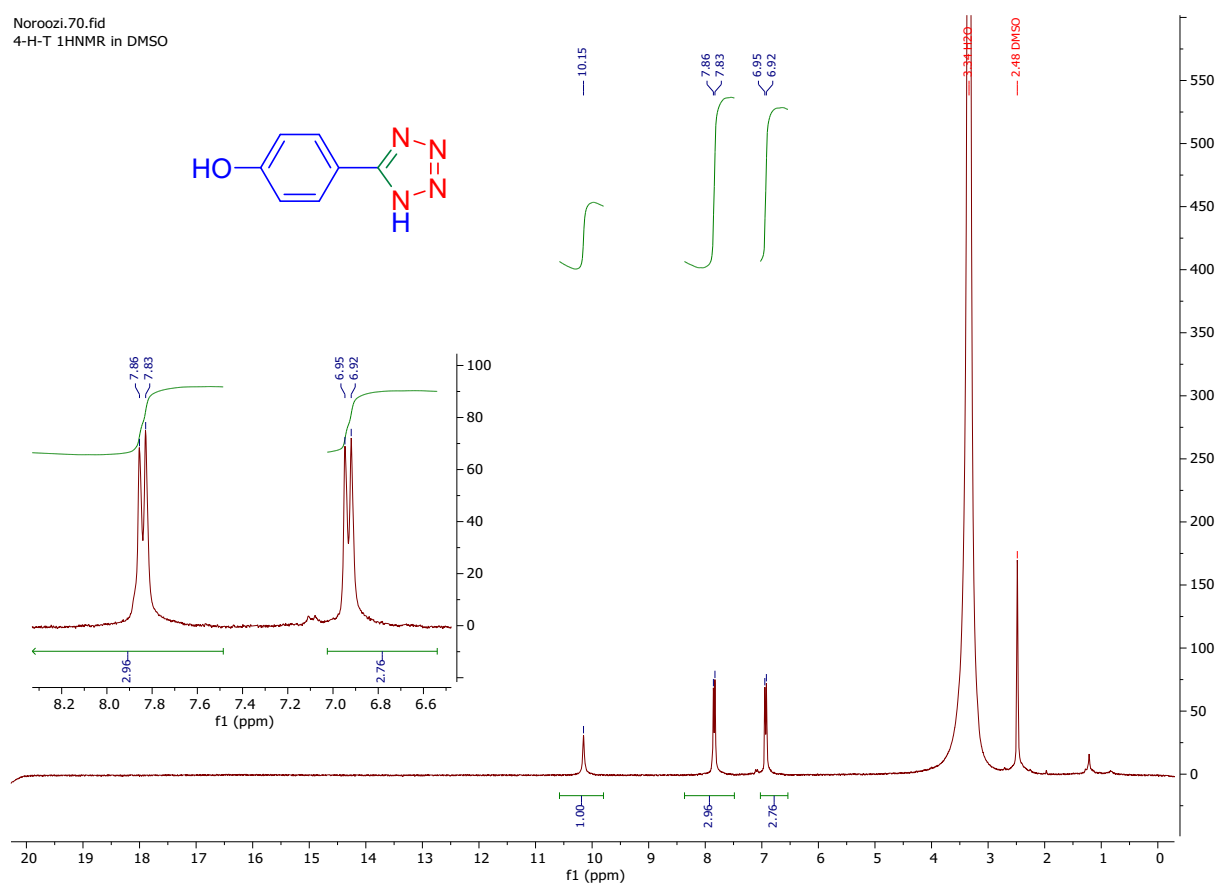
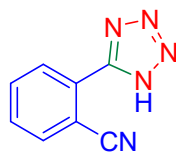


Figure S9. ^1H NMR of 4-(1H-Tetrazol-5-yl)-phenol.

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2-(1H-Tetrazol-5-yl)-benzonitrile (Table 2, entry 12):



Yield = 94%; M.P.= (211-213 °C Found, 209-211°C Reported); ^1H NMR (400 MHz, DMSO- d_6), δ (ppm): 8.19- 8.06 (m, 2H), 7.95-7.90 (t, J = 8 Hz, 1H), 7.80-7.75 (t, J = 8 Hz, 1H).

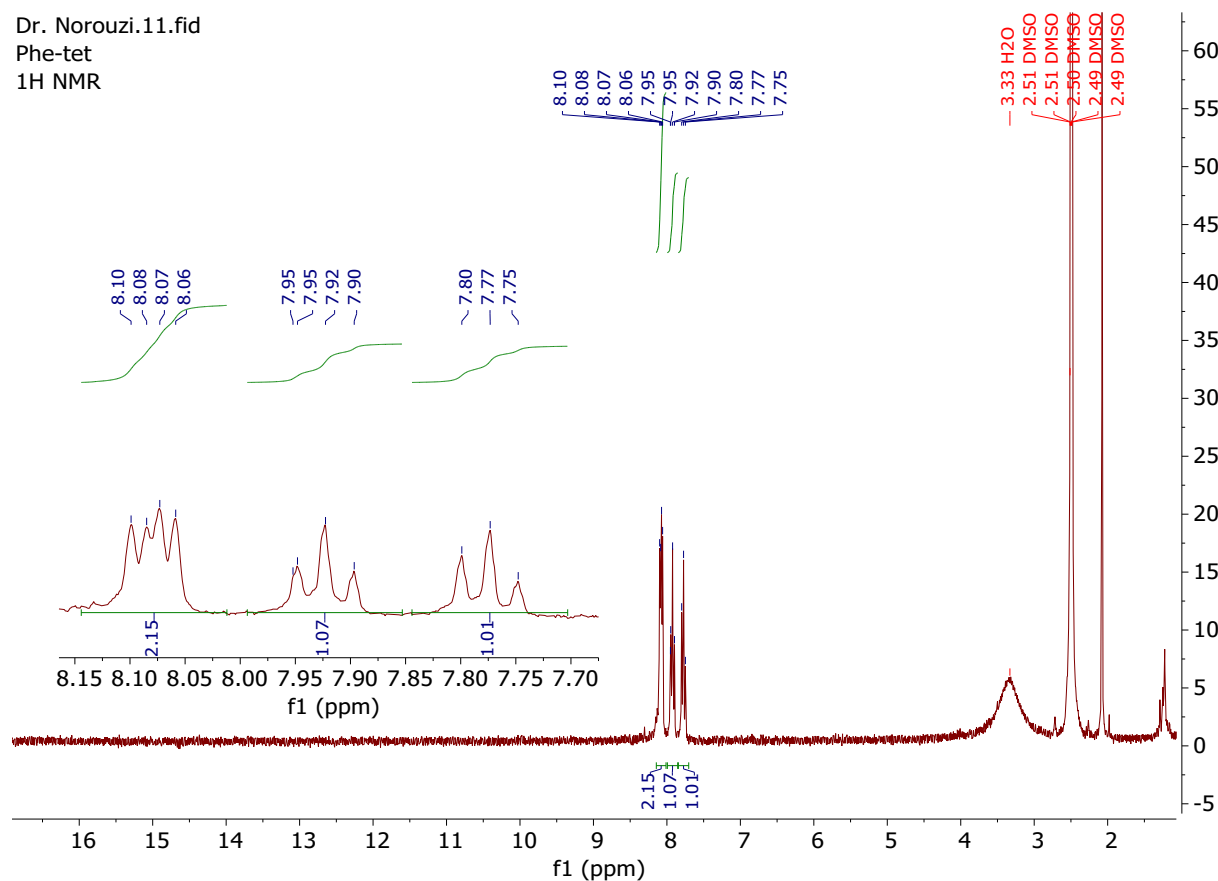


Figure S10. ^1H NMR of 2-(1H-Tetrazol-5-yl)-benzonitrile.

Supporting Information

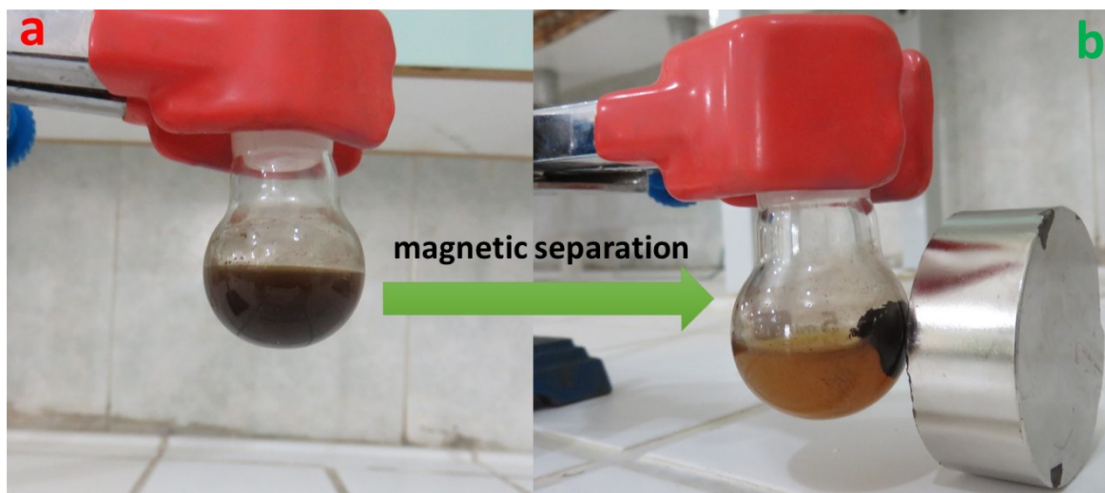


Figure S11. The reaction mixture a) before and b) after of catalyst separation via a magnetism.