Supporting Information

An Efficient CuI/DBU-Catalyzed One-pot Protocol for Synthesis of 1,4-Disubstituted 1,2,3-Triazoles

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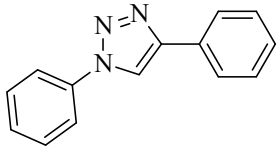
I. General Information:

All reagents were purchased from commercial sources and used without further treatment, unless otherwise indicated. The products were characterized using ^{1}H NMR and ^{13}C NMR (Bruker Avance 400 MHz or Bruker AVANCE III HD 600) which used $CDCl_3$ or DMSO-d_6 as the solvent and TMS as internal standard. Data is represented as follows: chemical shift, integration, multiplicity (s = singlet, d = doublet, dd = double of doublets, t = triplet, q = quartet, m = multiplet, br = broad) and coupling constants (*J*) in Hertz (Hz).

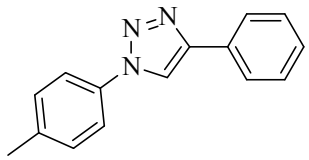
II. General procedure for the synthesis of triazoles

A mixture of aryl iodides (1.0 mmol), sodium azide (1.2 mmol), DBU (0.3 mmol) and CuI (0.2 mmol) in DMSO (5.0 mL) in a sealed tube was heated to 95 ºC for 0.5-5.0 h until the reaction was completed as judged by TLC. After cooling the resulting reaction mixture to room temperature, phenylacetaldehyde derivatives (1.0 mmol) or alkynes (1.0 mmol) was added and stirred for another 0.5-2.0 h. After the reaction was completed, the cooled mixture was poured into water (50 mL) containing several drops of ammonia. The resulting aqueous phase was extracted with dichloromethane for three times. The combined organic phases were washed with brine, dried over anhydrous Na_2SO_4, and concentrated in vacuo. The residue was loaded on a silica gel column and eluted with petroleum ether/ethyl acetate to afford the product.

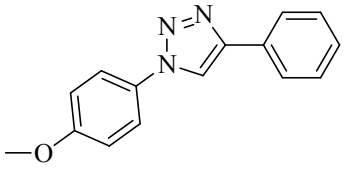
III. ^{1}H and ^{13}C NMR Data of Triazoles



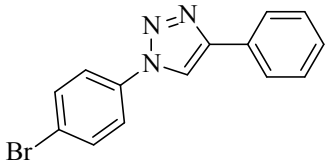
1,4-diphenyl-1*H*-1,2,3-triazole (**Table 2,** entry 1): ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.20 (s, 1H), 7.95-7.89 (m, 2H), 7.82-7.77 (m, 2H), 7.55 (t, J = 7.7Hz, 2H), 7.50-7.43 (m, 3H), 7.38 (t, J = 7.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 148.4, 137.1, 130.3, 129.8, 128.9, 128.4, 125.9, 120.5, 117.6.



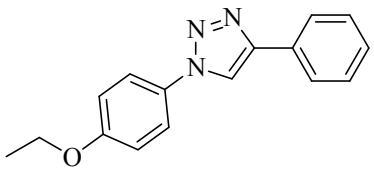
4-phenyl-1-(p-tolyl)-1*H*-1,2,3-triazole (**Table 2,** entry 2): ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.16 (s, 1H), 7.91 (d, J = 7.1 Hz, 2H), 7.66 (d, J = 8.4 Hz, 2H), 7.46 (t, J = 7.5 Hz, 2H), 7.35 (dd, J = 16.8, 7.9 Hz, 3H), 2.43 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 148.3, 138.9, 134.8, 130.3, 130.3, 128.9, 128.4, 125.9, 120.4, 117.7, 21.1.



1-(4-methoxyphenyl)-4-phenyl-1*H*-1,2,3-triazole (**Table 2,** entry 3): ^{1}H NMR (600 MHz, $CDCl_3$) δ: 8.11 (s, 1H), 7.91 (d, J = 7.8 Hz, 2H), 7.69 (d, J = 8.8 Hz, 2H), 7.46 (t, J = 7.1 Hz, 2H), 7.37 (t, J = 7.4 Hz, 1H), 7.04 (d, J = 8.6 Hz, 2H), 3.88 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ: 159.9, 148.2, 130.4, 128.9, 128.4, 125.8, 122.2, 117.9, 114.8, 55.7.

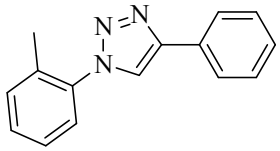


1-(4-bromophenyl)-4-phenyl-1*H*-1,2,3-triazole (**Table 2,** entry 4): ^{1}H NMR (600 MHz, DMSO-d_6) δ: 9.34 (s, 1H), 7.94 (d, J = 8.7 Hz, 4H), 7.86 (d, J = 8.7 Hz, 2H), 7.51 (t, J = 7.6 Hz, 2H), 7.40 (t, J = 7.4 Hz, 1H). ^{13}C NMR (150 MHz, DMSO- d_6) δ: 148.0, 136.3, 133.3, 130.6, 129.5, 128.8, 125.8, 122.4, 121.8, 120.1.

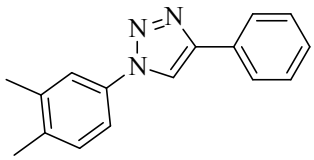


1-(4-ethoxyphenyl)-4-phenyl-1*H*-1,2,3-triazole (**Table 2,** entry 5): ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.03 (s, 1H), 7.82 (d, J = 7.1 Hz, 2H), 7.59 (d, J = 9.0 Hz, 2H), 7.37 (t, J = 7.5 Hz, 2H), 7.29 (d, J = 7.4 Hz, 1H), 6.94 (d, J = 9.0 Hz, 2H), 4.01 (q, J = 7.0

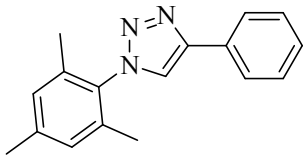
Hz, 2H), 1.38 (t, J = 7.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 159.2, 148.2, 130.4, 128.9, 128.3, 125.8, 122.2, 117.8, 115.3, 63.9, 14.7.



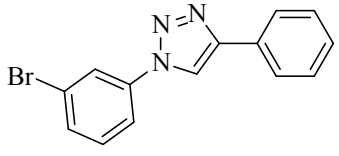
4-phenyl-1-(o-tolyl)-1*H*-1,2,3-triazole (**Table 2,** entry 6): ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.97 (s, 1H), 7.94-7.91 (m, 2H), 7.40-7.35 (m, 7H), 2.28 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 147.6, 136.5, 133.8, 131.6, 130.4, 130.0, 129.0, 128.4, 126.9, 125.9, 121.2, 18.0.



1-(3,4-dimethylphenyl)-4-phenyl-1*H*-1,2,3-triazole (**Table 2,** entry 7): ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.07 (s, 1H), 7.83 (d, J = 7.1 Hz, 2H), 7.49 (s, 1H), 7.38 (dd, J = 13.7, 7.8 Hz, 3H), 7.29 (d, J = 7.5 Hz, 1H), 7.19 (d, J = 8.3 Hz, 1H), 2.28 (s, 3H), 2.25 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 148.2, 138.4, 137.6, 135.0, 130.6, 130.4, 128.9, 128.3, 125.8, 121.7, 117.8, 117.7, 19.9, 19.5.

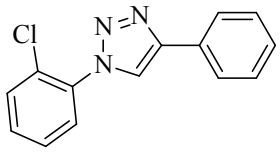


1-mesityl-4-phenyl-1*H*-1,2,3-triazole (**Table 2,** entry 8): ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.95-7.91 (m, 2H), 7.84 (s, 1H), 7.46 (t, J = 7.6 Hz, 2H), 7.40-7.33 (m, 1H), 7.01 (s, 2H), 2.37 (s, 3H), 2.02 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 147.6, 140.1, 135.1, 133.5, 130.5, 129.0, 128.3, 125.8, 121.5, 21.2, 17.4.

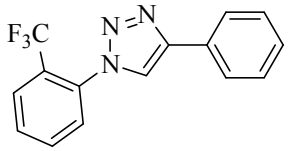


1-(3-bromophenyl)-4-phenyl-1*H*-1,2,3-triazole (**Table 2,** entry 9): ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.11 (s, 1H), 7.91 (s, 1H), 7.83 (d, J = 7.1 Hz, 2H), 7.68 (d, J = 10.1 Hz, 1H), 7.51 (d, J = 8.8 Hz, 1H), 7.39 (t, J = 7.5 Hz, 2H), 7.36-7.29 (m, 2H). ^{13}C

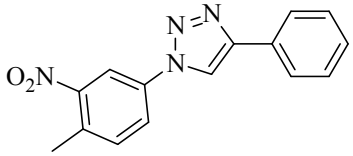
NMR (100 MHz, $CDCl_3$) δ: 148.7, 131.8, 131.1, 129.9, 129.0, 128.6, 126.7, 125.9, 123.5, 123.3, 119.0, 117.4.



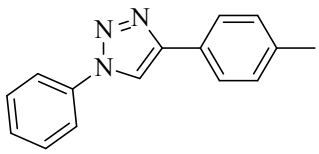
1-(2-chlorophenyl)-4-phenyl-1*H*-1,2,3-triazole (**Table 2,** entry 10): ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.21 (s, 1H), 7.95-7.90 (m, 2H), 7.68 (dd, J = 6.1, 3.4 Hz, 1H), 7.62-7.57 (m, 1H), 7.50-7.43 (m, 4H), 7.37 (t, J = 7.4 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 147.6, 134.9, 130.8, 130.2, 129.0, 128.5, 128.0, 127.8, 125.9, 121.6.



4-phenyl-1-(2-(trifluoromethyl)phenyl)-1*H*-1,2,3-triazole (**Table 2,** entry 11): ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.06 (s, 1H), 7.90 (dd, J = 11.3, 8.3 Hz, 3H), 7.73 (dt, J = 27.0, 7.5 Hz, 2H), 7.62 (d, J = 7.6 Hz, 1H), 7.47 (t, J = 7.5 Hz, 2H), 7.38 (t, J = 7.4 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 147.8, 134.9, 133.1, 130.5, 130.0, 129.0 (d, J = 5.2 Hz), 128.5, 127.4 (q, J = 5.0 Hz), 126.4, 125.9, 124.0, 122.2, 121.3.

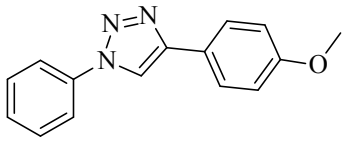


1-(4-methyl-3-nitrophenyl)-4-phenyl-1*H*-1,2,3-triazole (**Table 2,** entry 12): ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.41 (s, 1H), 8.26 (s, 1H), 8.05 (d, J = 10.5 Hz, 1H), 7.92 (d, J = 8.4 Hz, 2H), 7.56 (d, J = 8.3 Hz, 1H), 7.48 (t, J = 7.5 Hz, 2H), 7.40 (t, J = 7.4 Hz, 1H), 2.70 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 134.4, 134.0, 129.0, 128.8, 125.9, 124.4, 117.2, 116.2, 20.3.

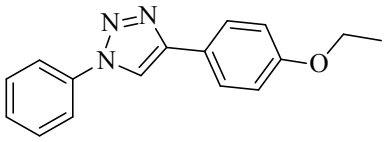


1-phenyl-4-(p-tolyl)-1*H*-1,2,3-triazole (**Table 2,** entry 13): ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.16 (s, 1H), 7.80 (dd, J = 6.0 Hz, 7.6 Hz, 4H), 7.57-7.26 (m, 5H), 2.40 (s,

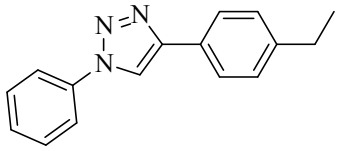
3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 148.5, 138.3, 137.1, 129.8, 129.6, 128.7, 127.4, 125.8, 120.5, 117.3, 21.3.



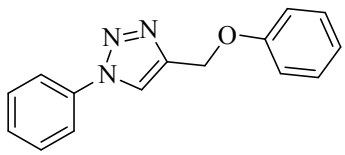
4-(4-methoxyphenyl)-1-phenyl-1*H*-1,2,3-triazole (Table 2, entry 14**)**: ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.11 (s, 1H), 7.82 (d, J = 8.7 Hz, 2H), 7.77 (d, J = 7.7 Hz, 2H), 7.52 (t, J = 7.8 Hz, 2H), 7.42 (t, J = 7.4 Hz, 1H), 6.97 (d, J = 8.7 Hz, 2H), 3.83 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 159.8, 148.3, 137.1, 129.8, 128.7, 127.2, 122.9, 120.4, 116.8, 114.3, 55.3.



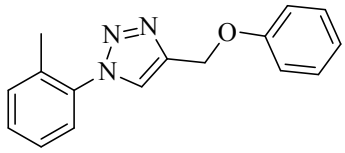
4-(4-ethoxyphenyl)-1-phenyl-1*H*-1,2,3-triazole (Table 2, entry 15**)**: ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.12 (s, 1H), 7.81 (dd, J = 8.4 Hz, J = 8 Hz, 4H), 7.55 (t, J = 7.6 Hz, 2H), 7.45 (t, J = 7.6 Hz, 1H), 6.98 (d, J = 8.4 Hz, 2H), 4.09 (q, J = 7.6 Hz, 2H), 1.45 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 159.2, 148.3, 137.1, 129.8, 128.7, 127.2, 122.8, 120.5, 116.7, 114.9, 63.5, 14.8.



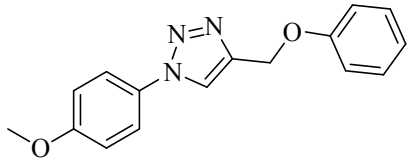
4-(4-ethylphenyl)-1-phenyl-1*H*-1,2,3-triazole (**Table 3,** entry 16): ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.16 (s, 1H), 7.81 (dd, J = 8.4 Hz, J = 8.0 Hz, 4H), 7.54 (t, J = 7.2 Hz, 2H), 7.44 (t, J = 7.6 Hz, 1H), 7.29 (d, J = 8.0 Hz, 2H), 2.69 (q, J = 7.6 Hz, 2H), 1.27 (t, J = 7.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 148.5, 144.7, 137.1, 129.7, 128.7, 128.4, 127.6, 125.8, 120.5, 117.2, 28.7, 15.5.



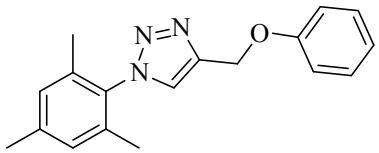
4-(phenoxymethyl)-1-phenyl-1*H*-1,2,3-triazole (**Table 3,** entry 17): ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.06 (s, 1H), 7.74 (d, J = 7.6 Hz, 2H), 7.54-7.43 (m, 3H), 7.32 (t, J = 8.0 Hz, 2H), 7.04-6.98 (m, 3H), 5.31 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 158.2, 145.1, 137.0, 129.8, 129.6, 128.9, 121.4, 120.9, 120.6, 114.8, 62.0.



4-(phenoxymethyl)-1-(o-tolyl)-1*H*-1,2,3-triazole (**Table 3,** entry 18): ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.81 (s, 1H), 7.44-7.30 (m, 6H), 7.04-6.97 (m, 3H), 5.32 (s, 2H), 2.22 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 158.2, 144.1, 136.4, 133.7, 131.5, 130.0, 129.6, 126.9, 126.0, 124.3, 121.4, 114.8, 62.1, 17.9.

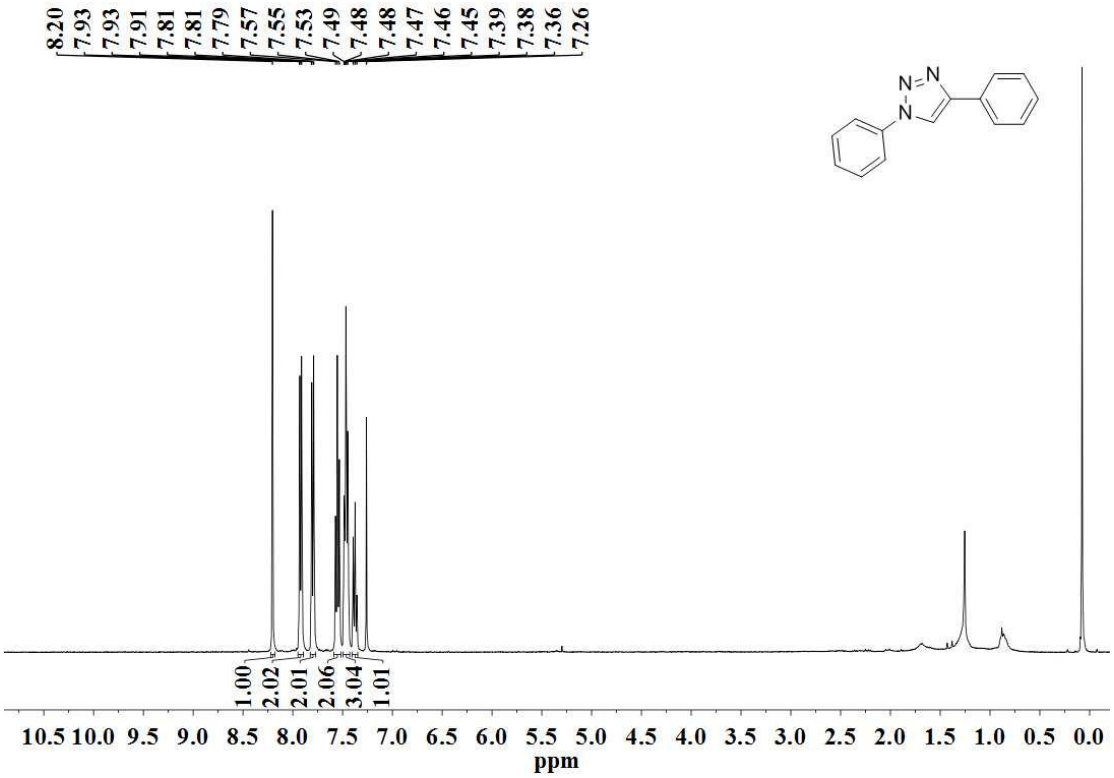


1-(4-methoxyphenyl)-4-(phenoxymethyl)-1*H*-1,2,3-triazole (**Table 3,** entry 19): ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.97 (s, 1H), 7.64-7.60 (m, 2H), 7.33-7.29 (m, 2H), 7.03-6.99 (m, 5H), 5.28 (s, 2H), 3.85 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 159.9, 158.2, 144.8, 130.4, 129.6, 122.3, 121.3, 121.1, 114.8, 114.8, 62.0, 55.6.

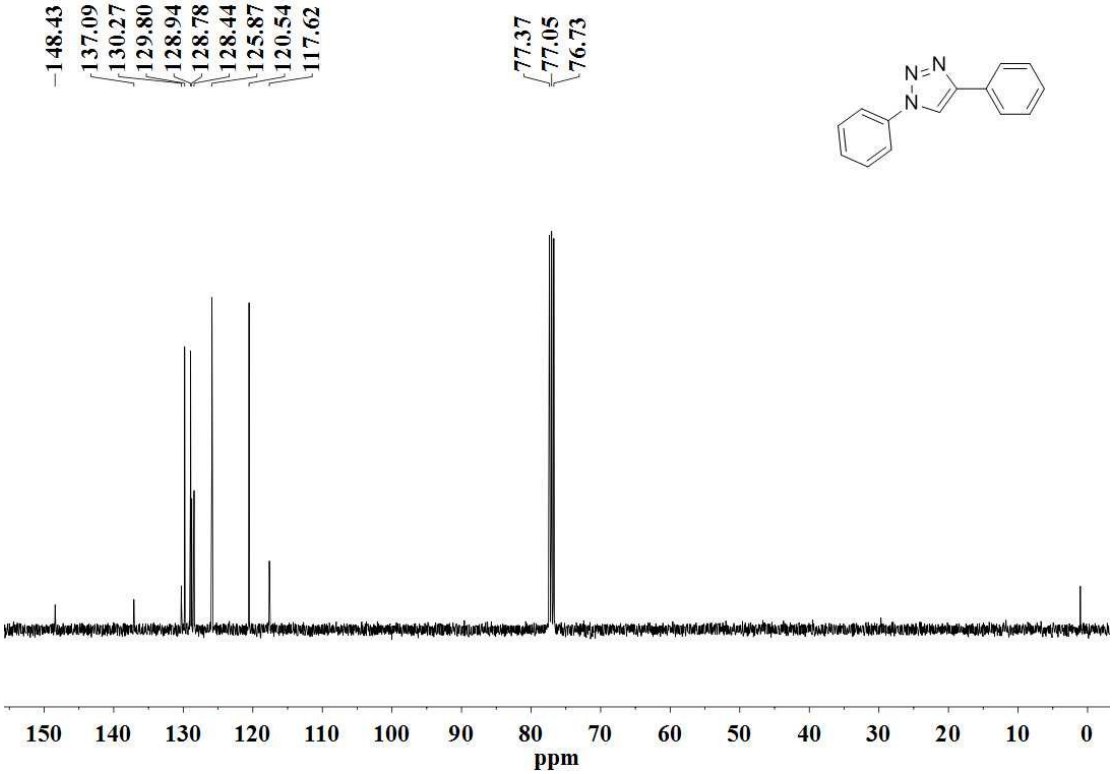


1-mesityl-4-(phenoxymethyl)-1*H*-1,2,3-triazole (**Table 3,** entry 20): ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.65 (s, 1H), 7.63 (t, J = 7.6 Hz, 2H), 7.03-6.97 (m, 5H), 5.34 (s, 2H), 2.35 (s, 3H), 1.95 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 158.2, 144.2, 140.1, 135.1, 133.4, 129.5, 129.1, 124.6, 121.4, 115.0, 62.3, 21.1, 17.3.

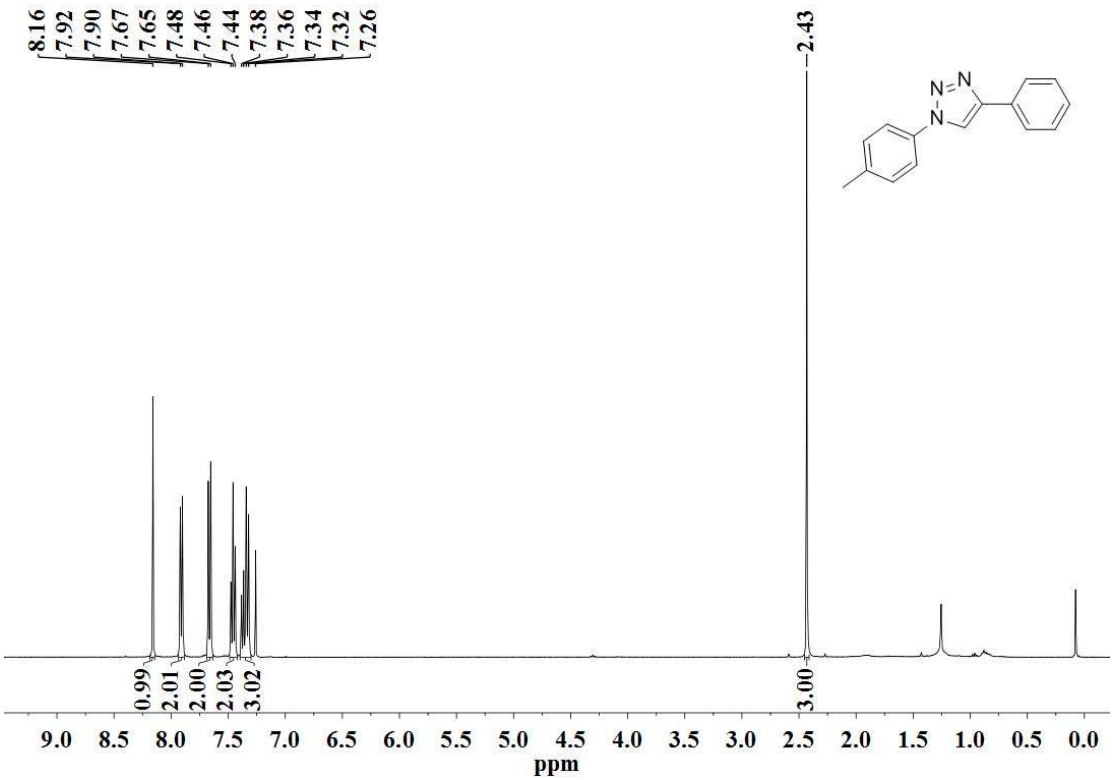
IV. ^{1}H and ^{13}C NMR Spectra of Triazoles



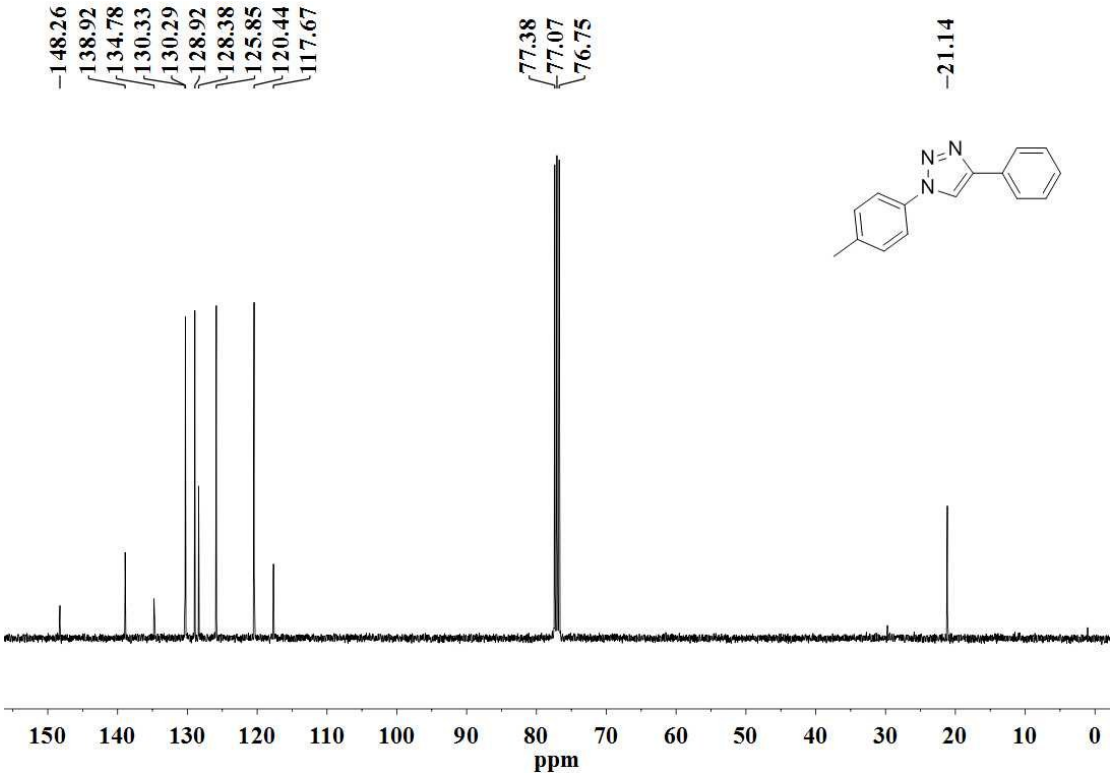
SI Fig. 1. ^{1}H NMR spectrum for 1,4-diphenyl-1*H*-1,2,3-triazole.



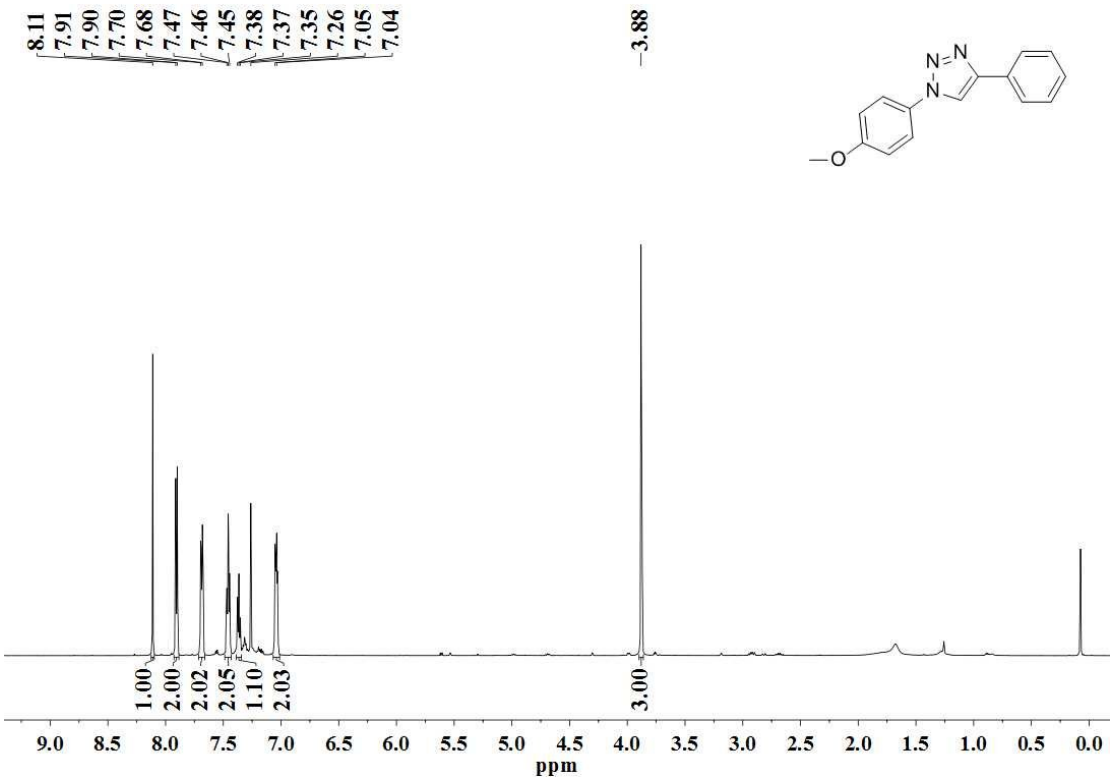
SI Fig. 2. ^{13}C NMR spectrum for 1,4-diphenyl-1*H*-1,2,3-triazole.



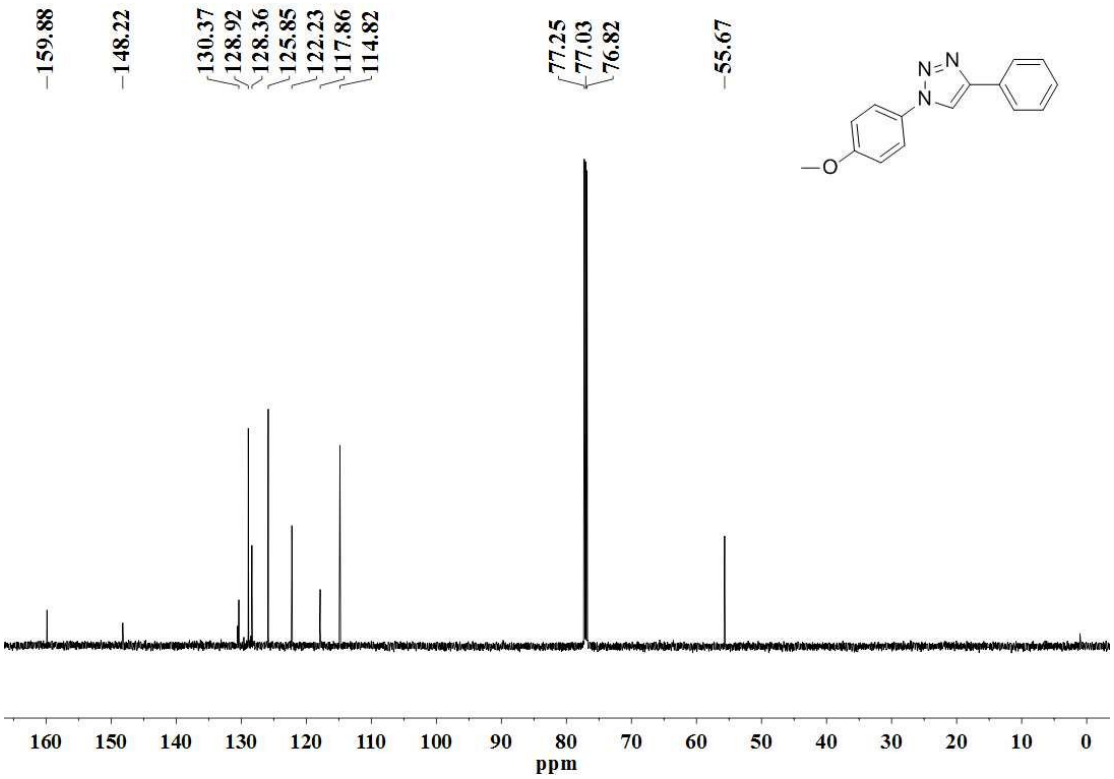
SI Fig. 3. [1]H NMR spectrum for 4-phenyl-1-(p-tolyl)-1*H*-1,2,3-triazole.



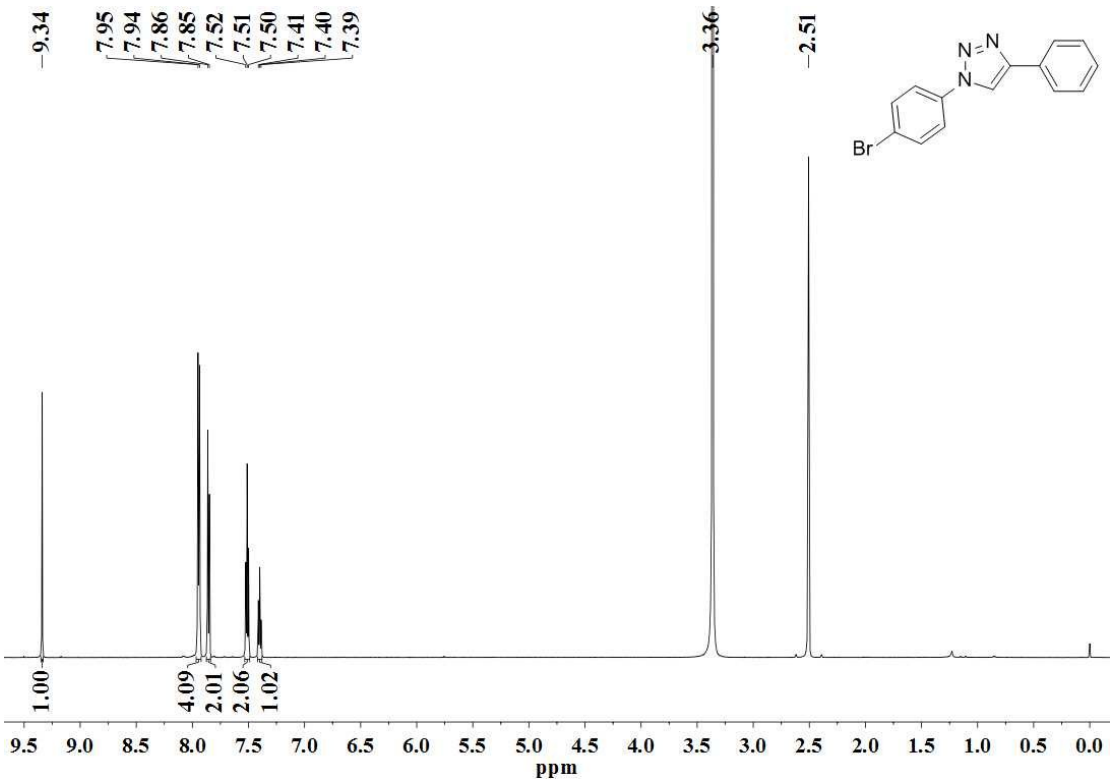
SI Fig. 4. [13]C NMR spectrum for 4-phenyl-1-(p-tolyl)-1*H*-1,2,3-triazole.



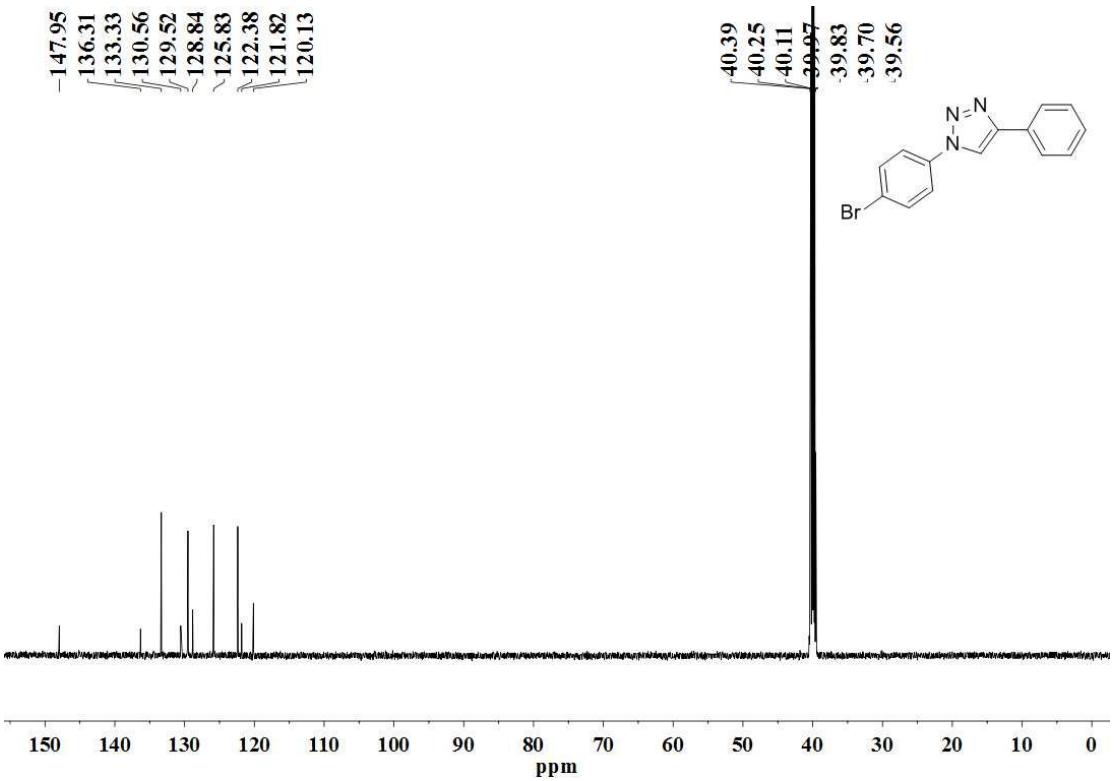
SI Fig. 5. ^{1}H NMR spectrum for 1-(4-methoxyphenyl)-4-phenyl-1*H*-1,2,3-triazole.



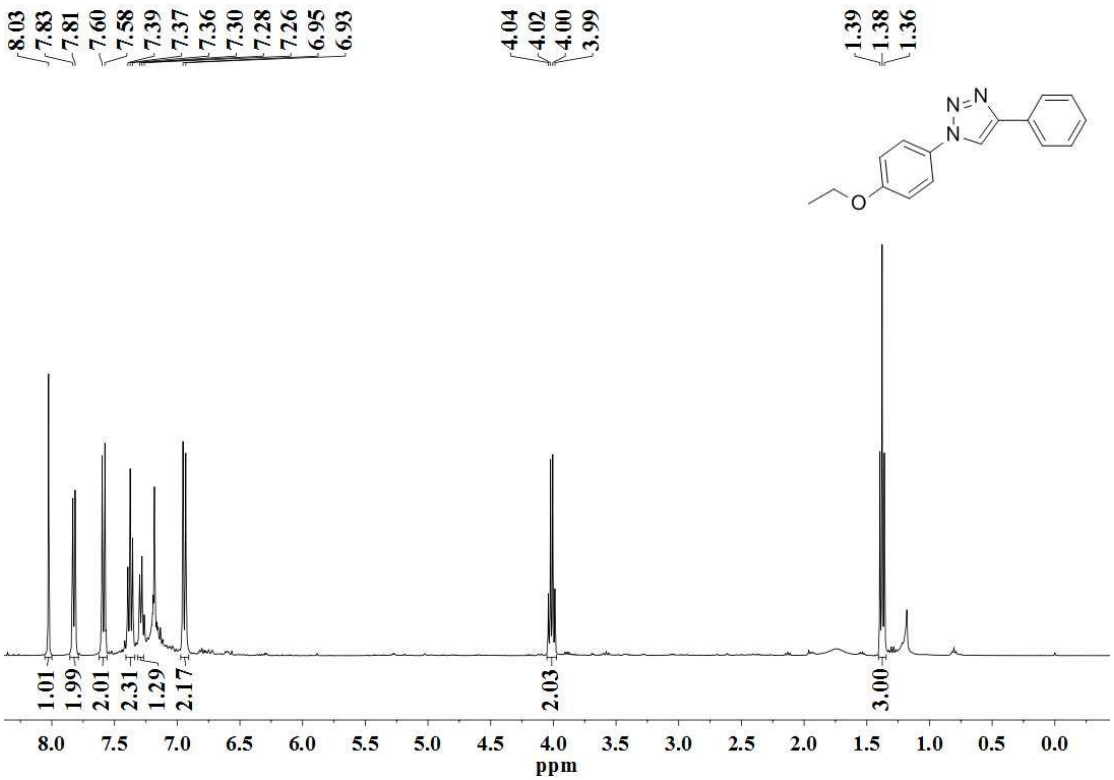
SI Fig. 6. ^{13}C NMR spectrum for 1-(4-methoxyphenyl)-4-phenyl-1*H*-1,2,3-triazole.



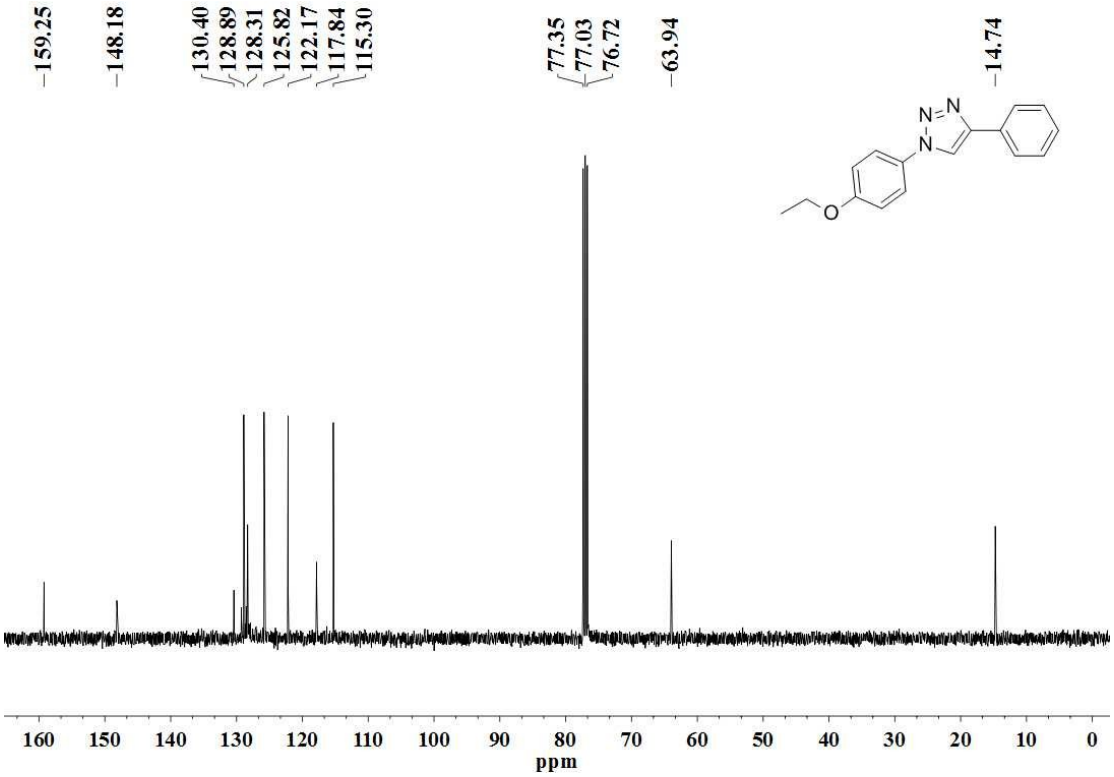
SI Fig. 7. ^{1}H NMR spectrum for 1-(4-bromophenyl)-4-phenyl-1*H*-1,2,3-triazole.



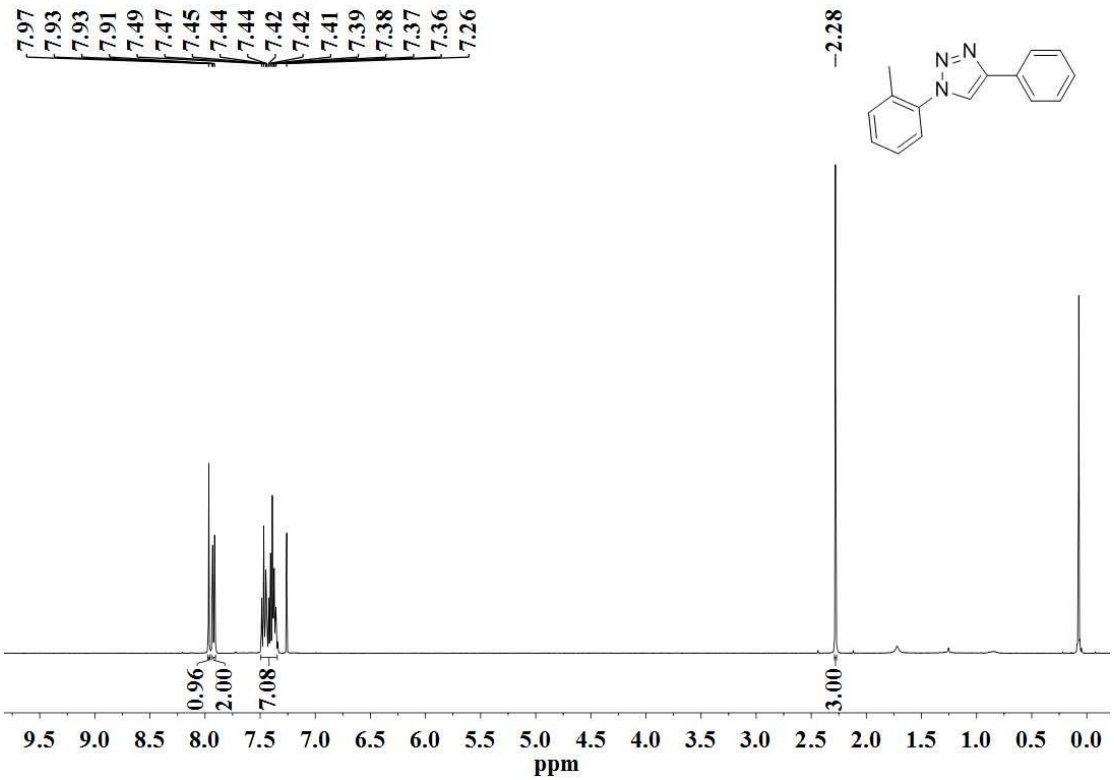
SI Fig. 8. ^{13}C NMR spectrum for 1-(4-bromophenyl)-4-phenyl-1*H*-1,2,3-triazole.



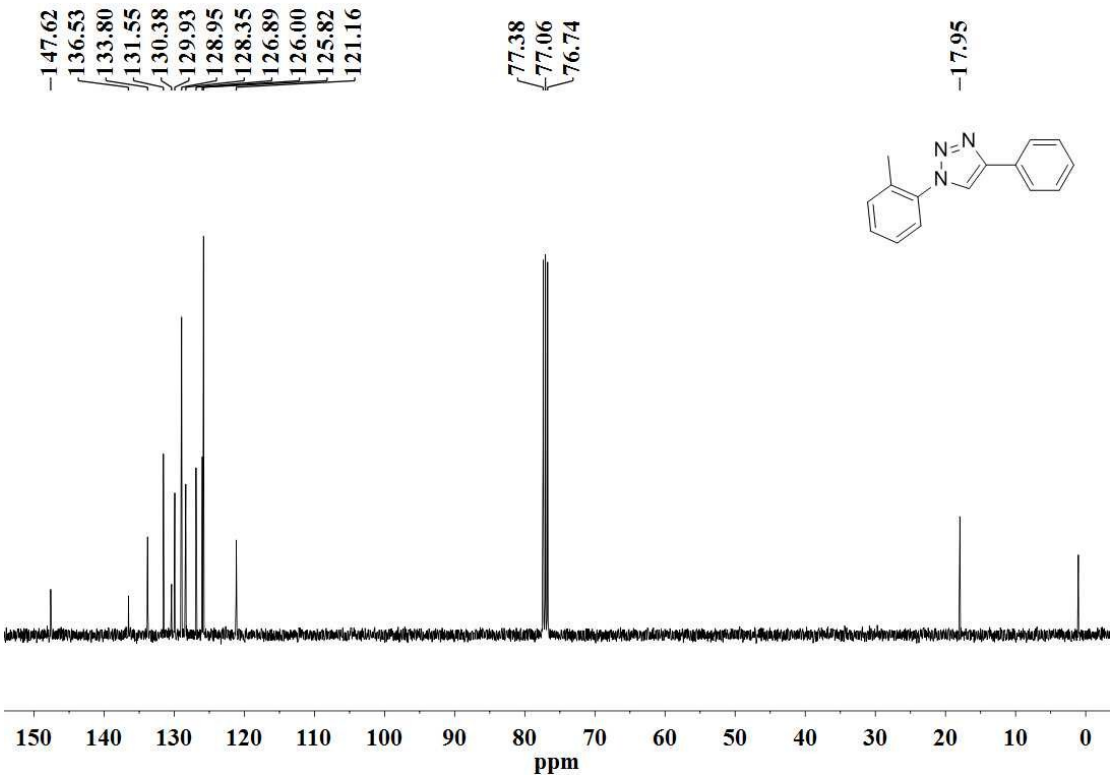
SI Fig. 9. ^{1}H NMR spectrum for 1-(4-ethoxyphenyl)-4-phenyl-1*H*-1,2,3-triazole.



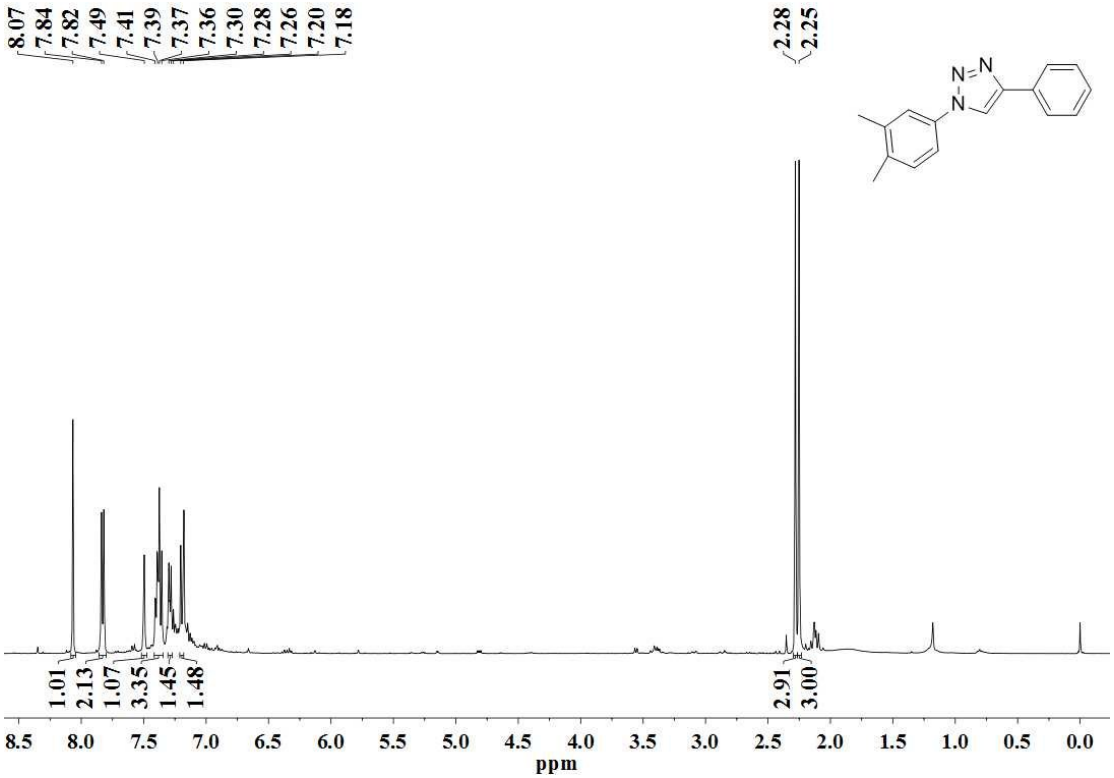
SI Fig. 10. ^{13}C NMR spectrum for 1-(4-ethoxyphenyl)-4-phenyl-1*H*-1,2,3-triazole.



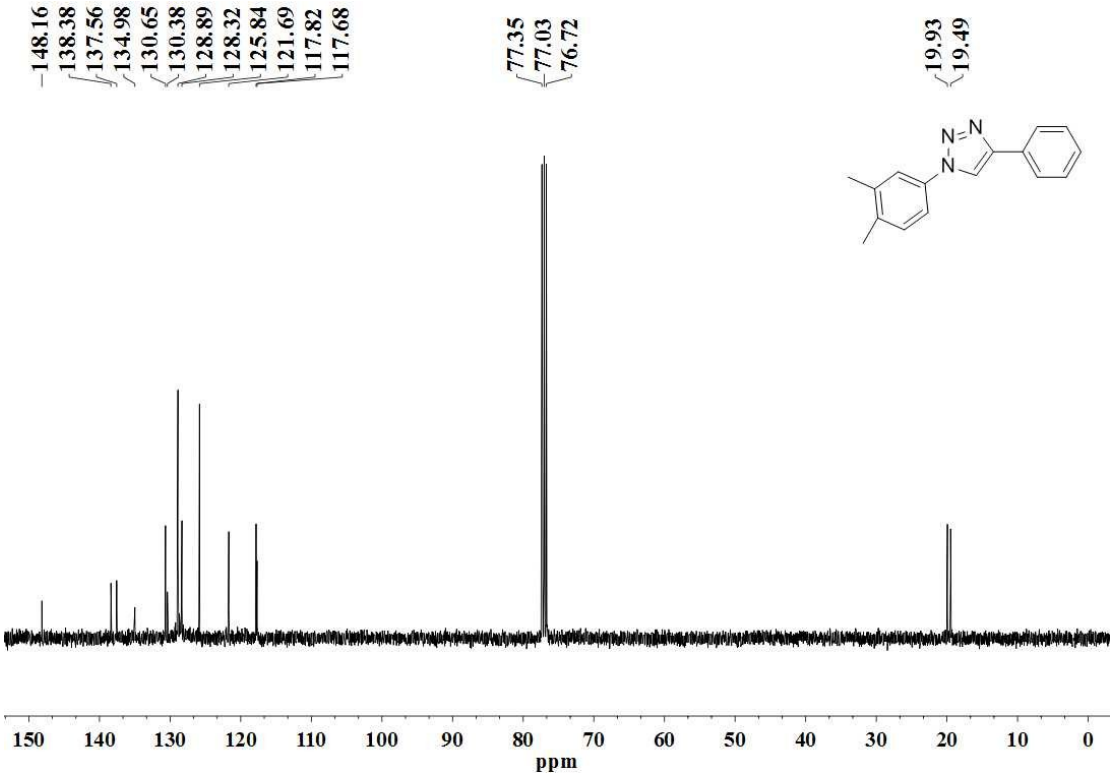
SI Fig. 11. [1]H NMR spectrum for 4-phenyl-1-(o-tolyl)-1*H*-1,2,3-triazole.



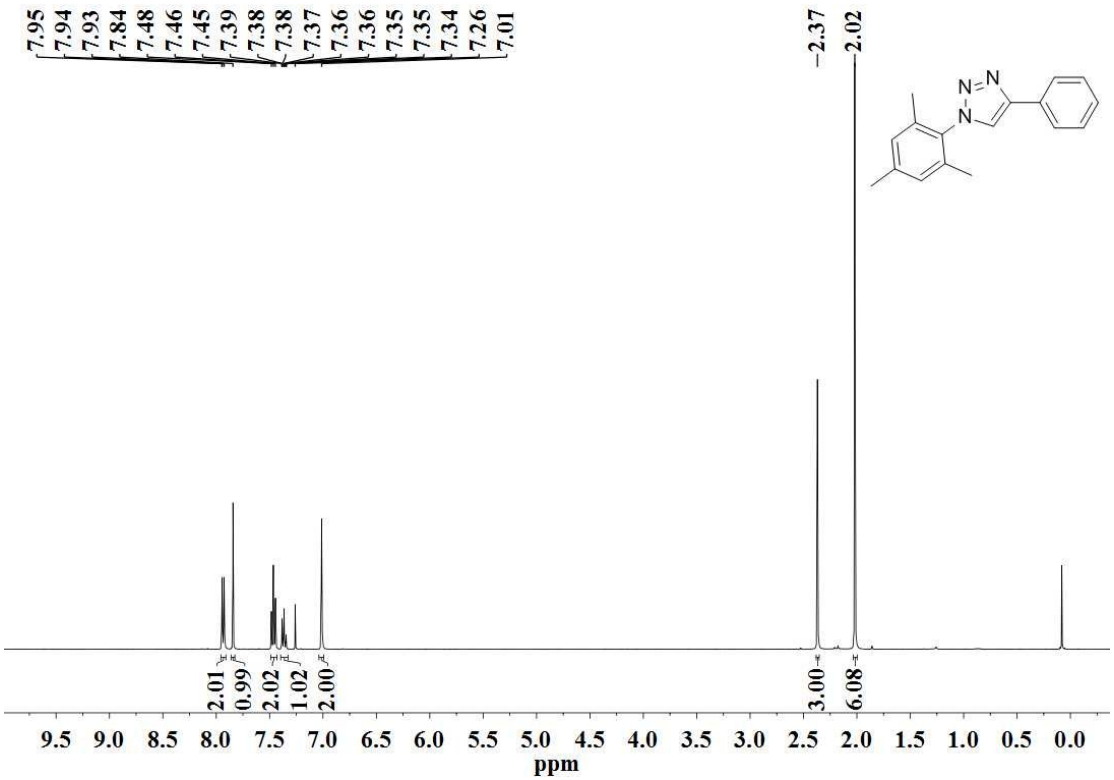
SI Fig. 12. [13]C NMR spectrum for 4-phenyl-1-(o-tolyl)-1*H*-1,2,3-triazole.



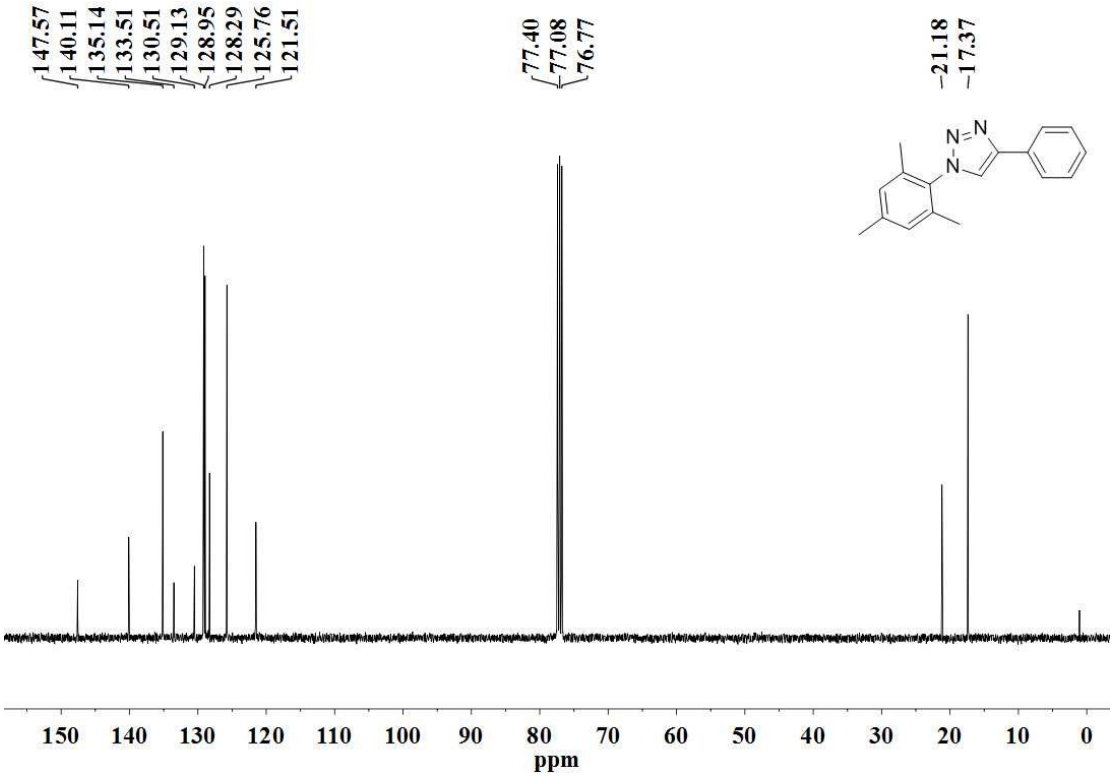
SI Fig. 13. ^{1}H NMR spectrum for 1-(3,4-dimethylphenyl)-4-phenyl-1*H*-1,2,3-triazole.



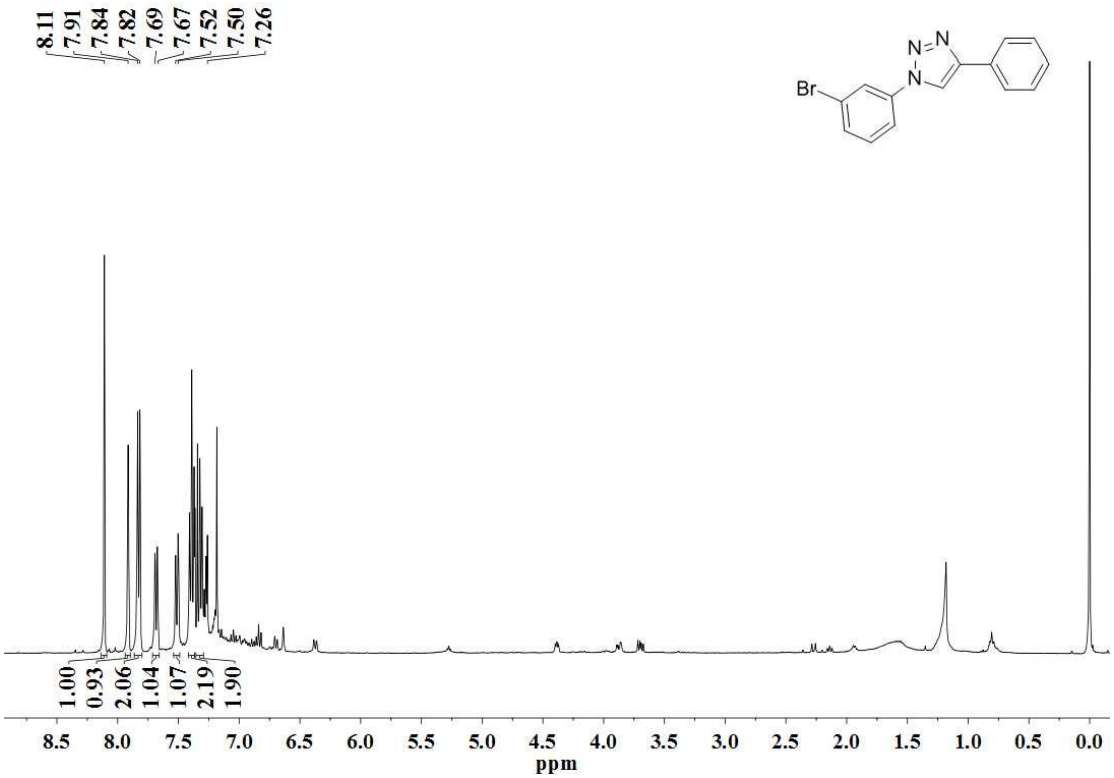
SI Fig. 14. ^{13}C NMR spectrum for 1-(3,4-dimethylphenyl)-4-phenyl-1*H*-1,2,3-triazole.



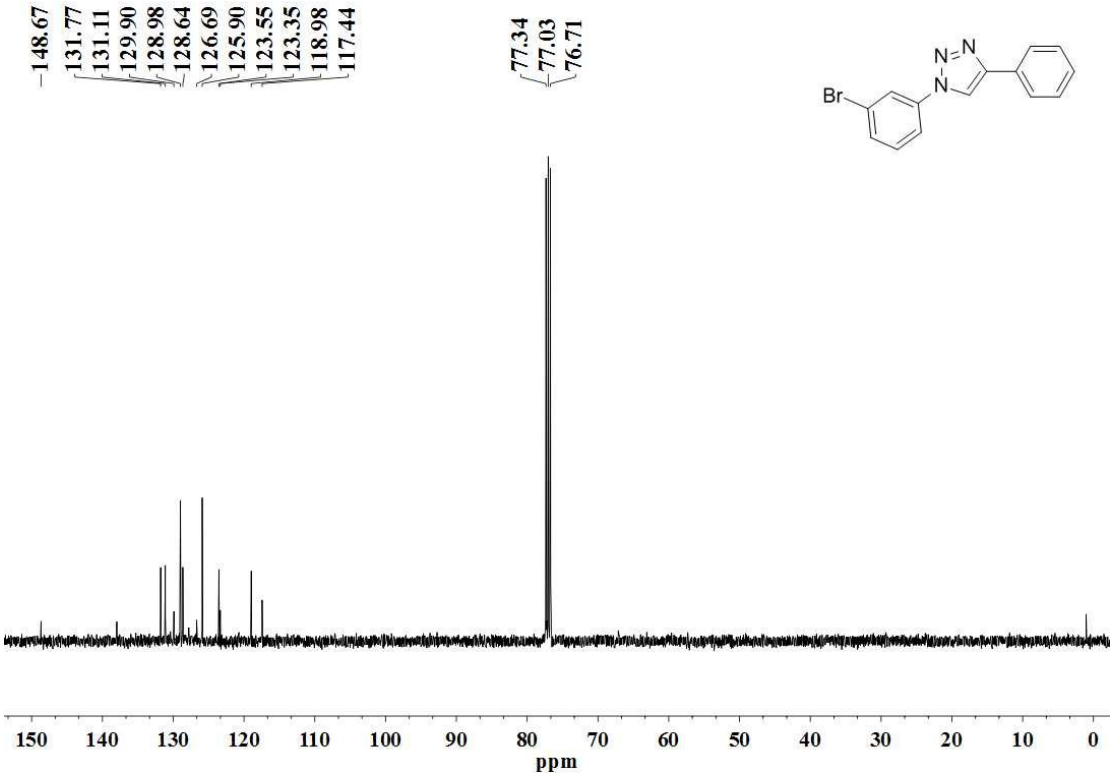
SI Fig. 15. ^{1}H NMR spectrum for 1-mesityl-4-phenyl-1*H*-1,2,3-triazole.



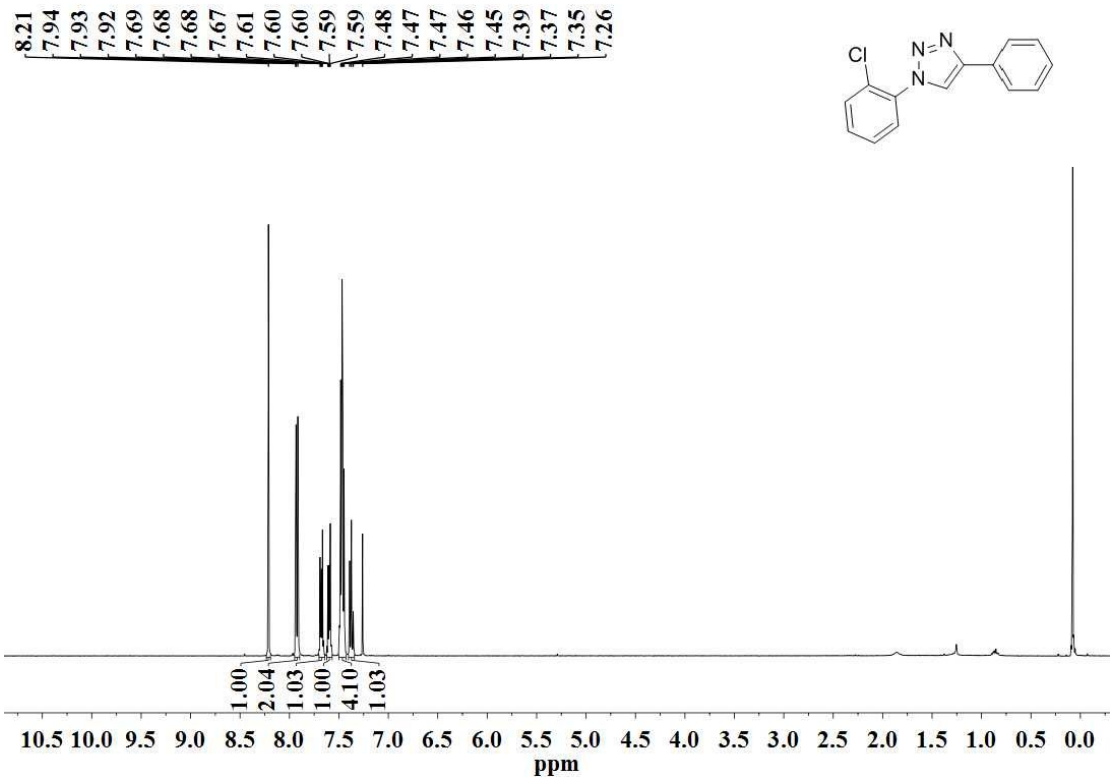
SI Fig. 16. ^{13}C NMR spectrum for 1-mesityl-4-phenyl-1*H*-1,2,3-triazole.



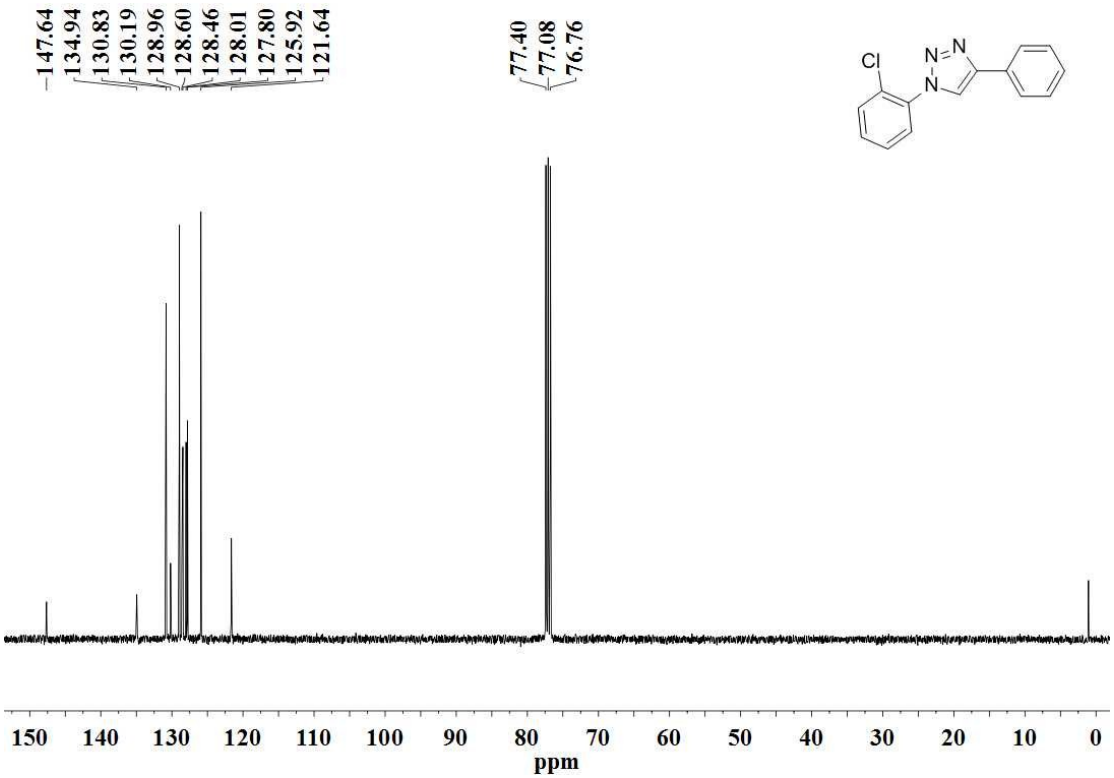
SI Fig. 17. ^{1}H NMR spectrum for 1-(3-bromophenyl)-4-phenyl-1*H*-1,2,3-triazole.



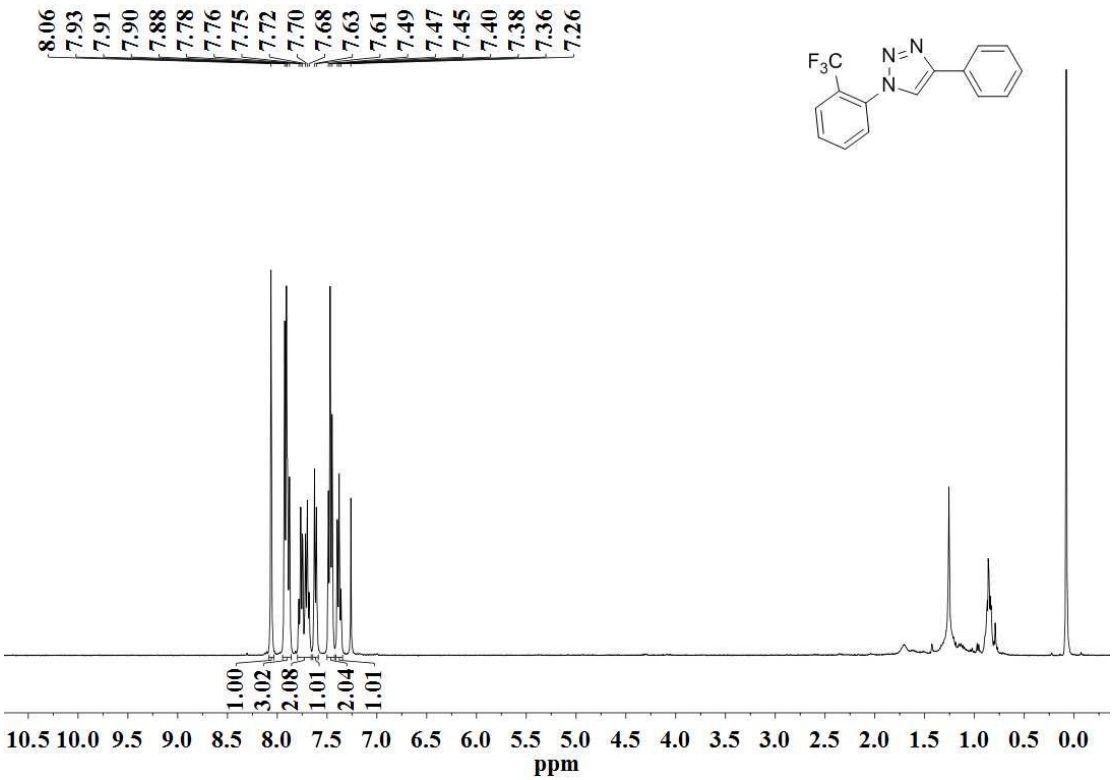
SI Fig. 18. ^{13}C NMR spectrum for 1-(3-bromophenyl)-4-phenyl-1*H*-1,2,3-triazole.



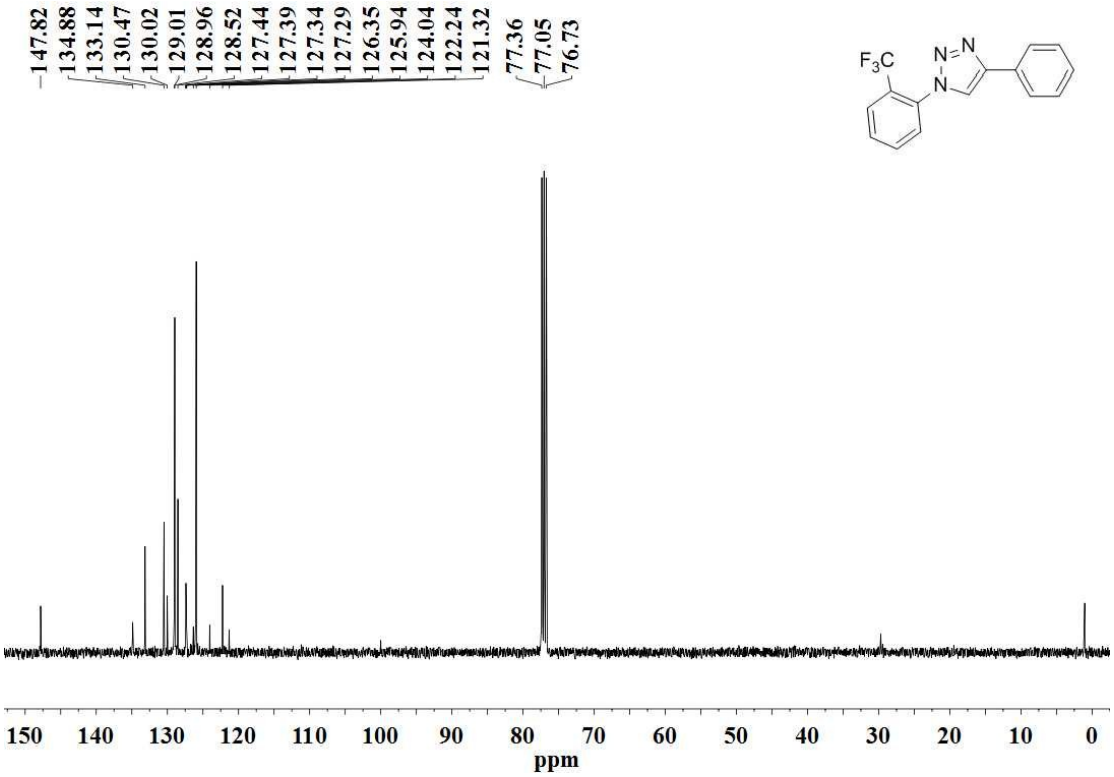
SI Fig. 19. ^{1}H NMR spectrum for 1-(2-chlorophenyl)-4-phenyl-1*H*-1,2,3-triazole.



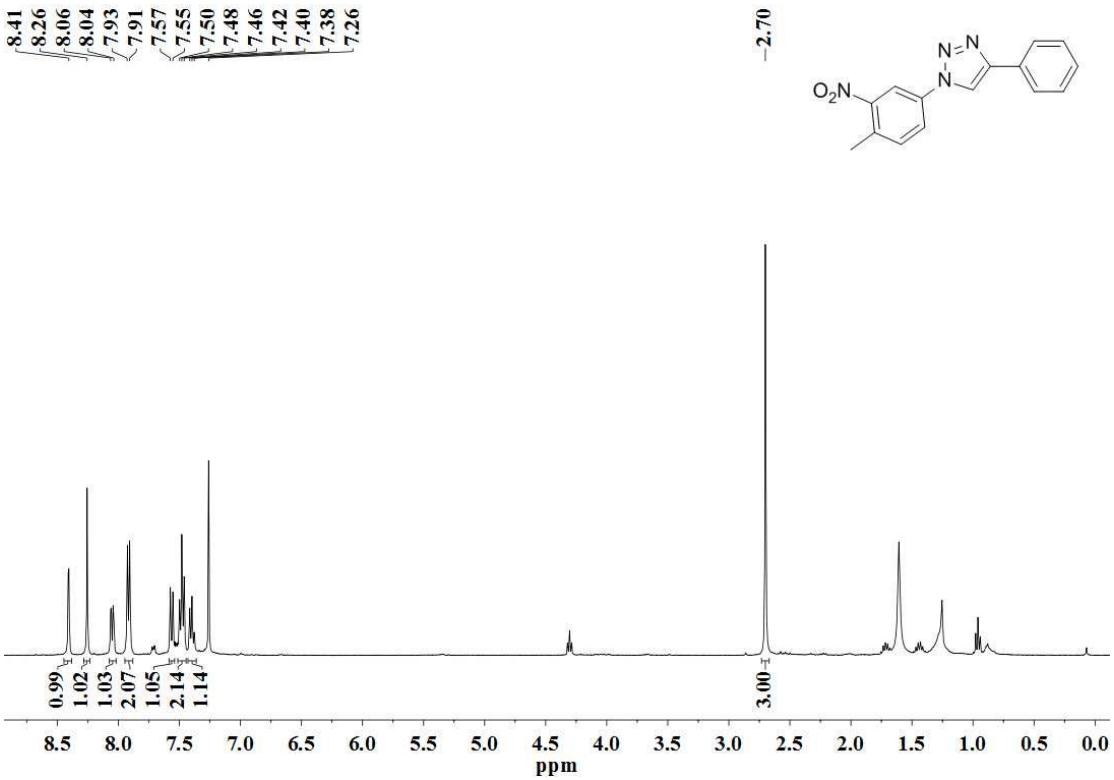
SI Fig. 20. ^{13}C NMR spectrum for 1-(2-chlorophenyl)-4-phenyl-1*H*-1,2,3-triazole.



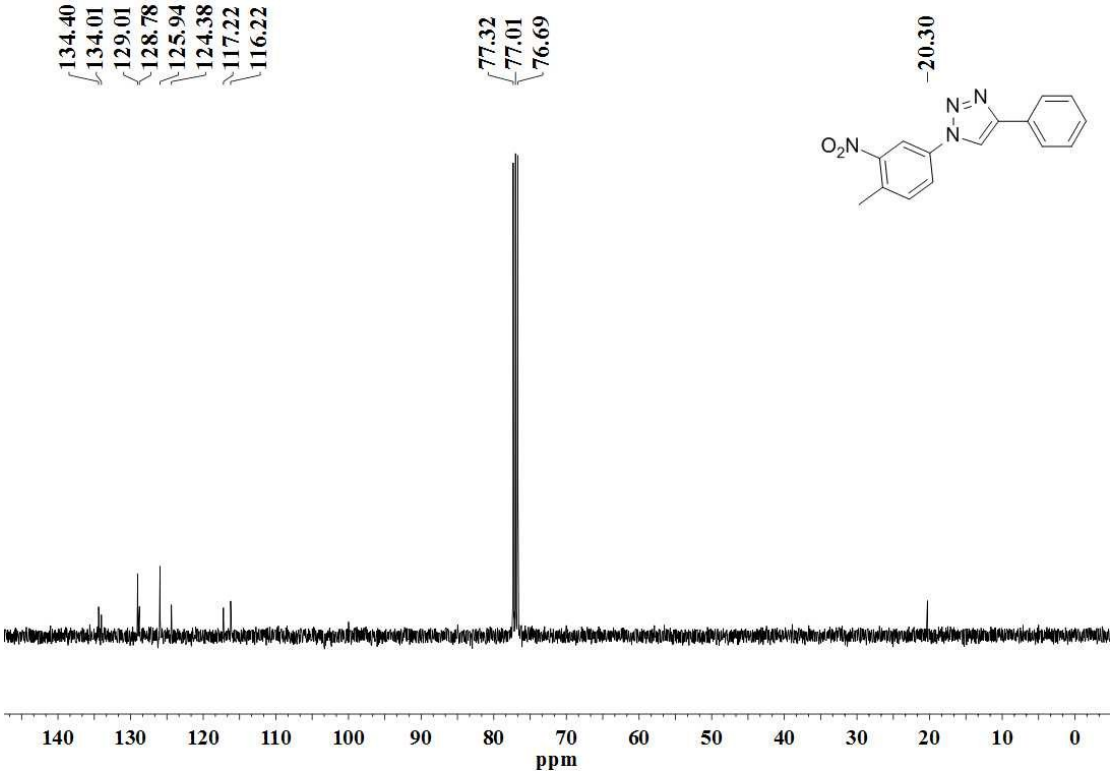
SI Fig. 21. ^{1}H NMR spectrum for 4-phenyl-1-(2-(trifluoromethyl)phenyl)-1*H*-1,2,3-triazole.



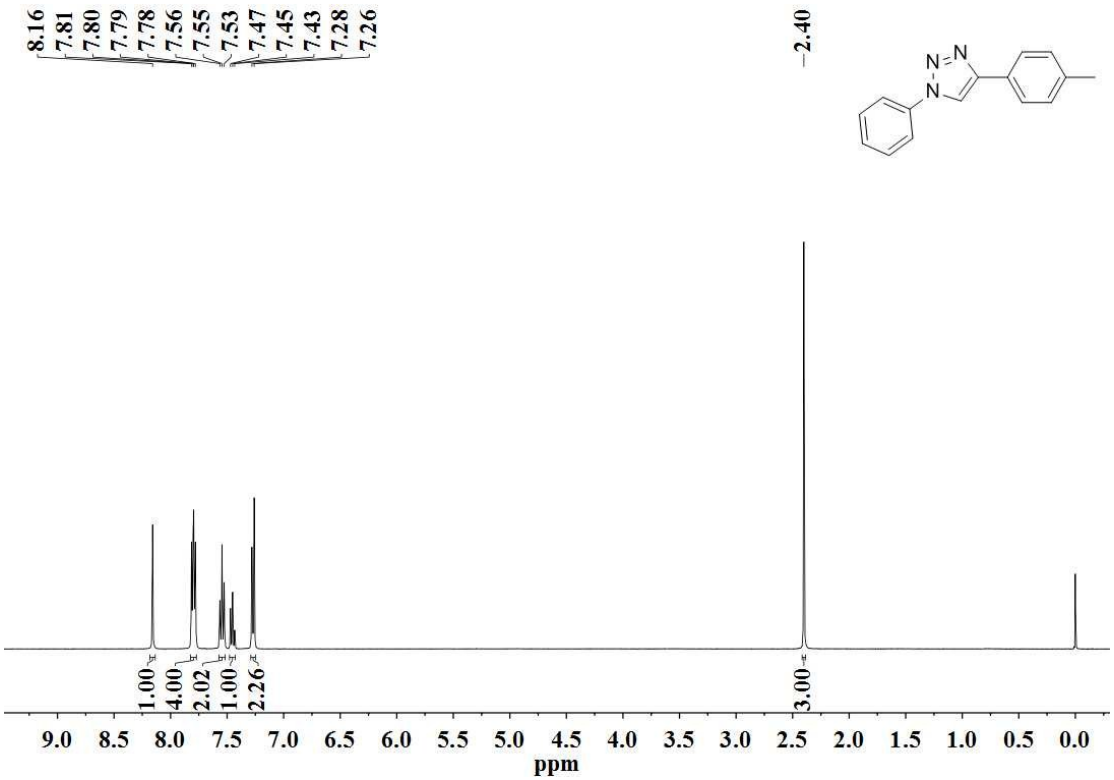
SI Fig. 22. ^{13}C NMR spectrum for 4-phenyl-1-(2-(trifluoromethyl)phenyl)-1*H*-1,2,3-triazole.



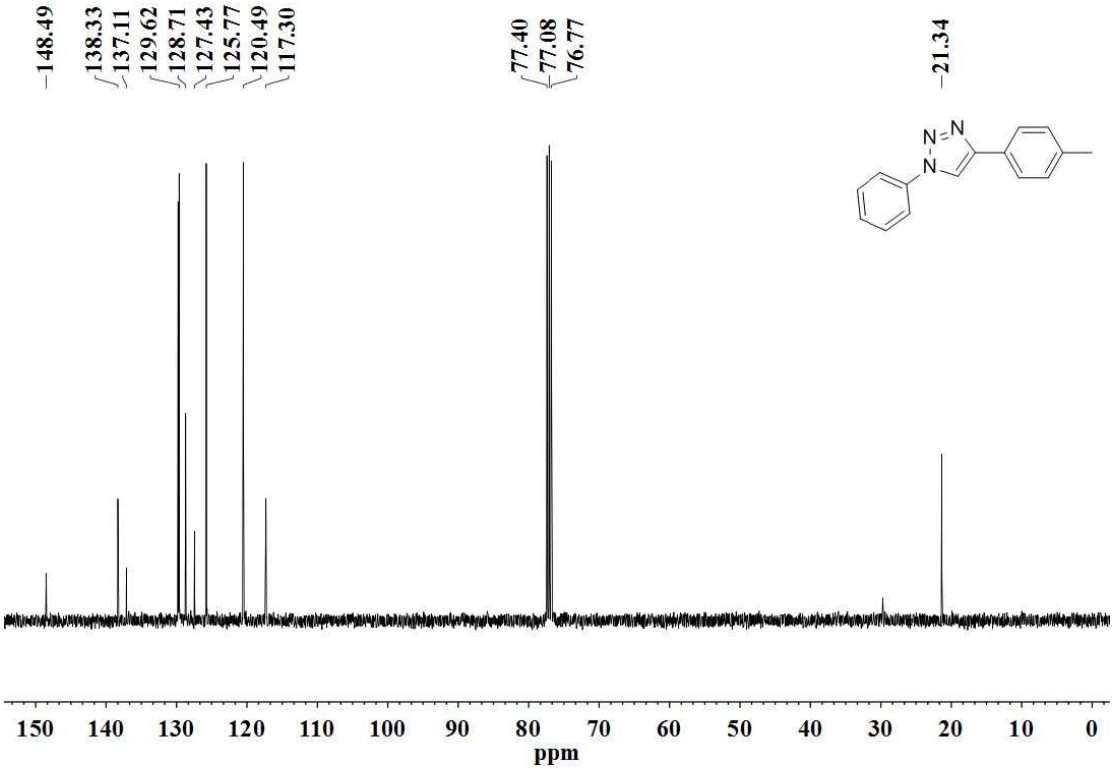
SI Fig. 23. [1]H NMR spectrum for 1-(4-methyl-3-nitrophenyl)-4-phenyl-1*H*-1,2,3-triazole.



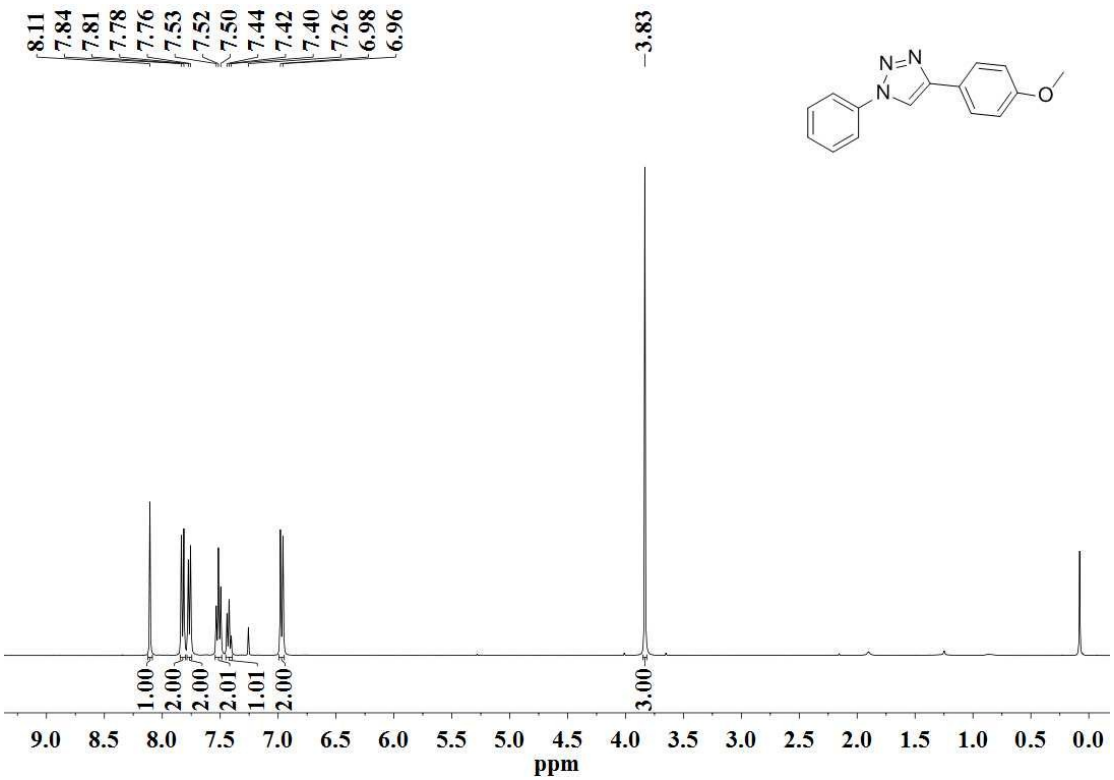
SI Fig. 24. [13]C NMR spectrum for 1-(4-methyl-3-nitrophenyl)-4-phenyl-1*H*-1,2,3-triazole.



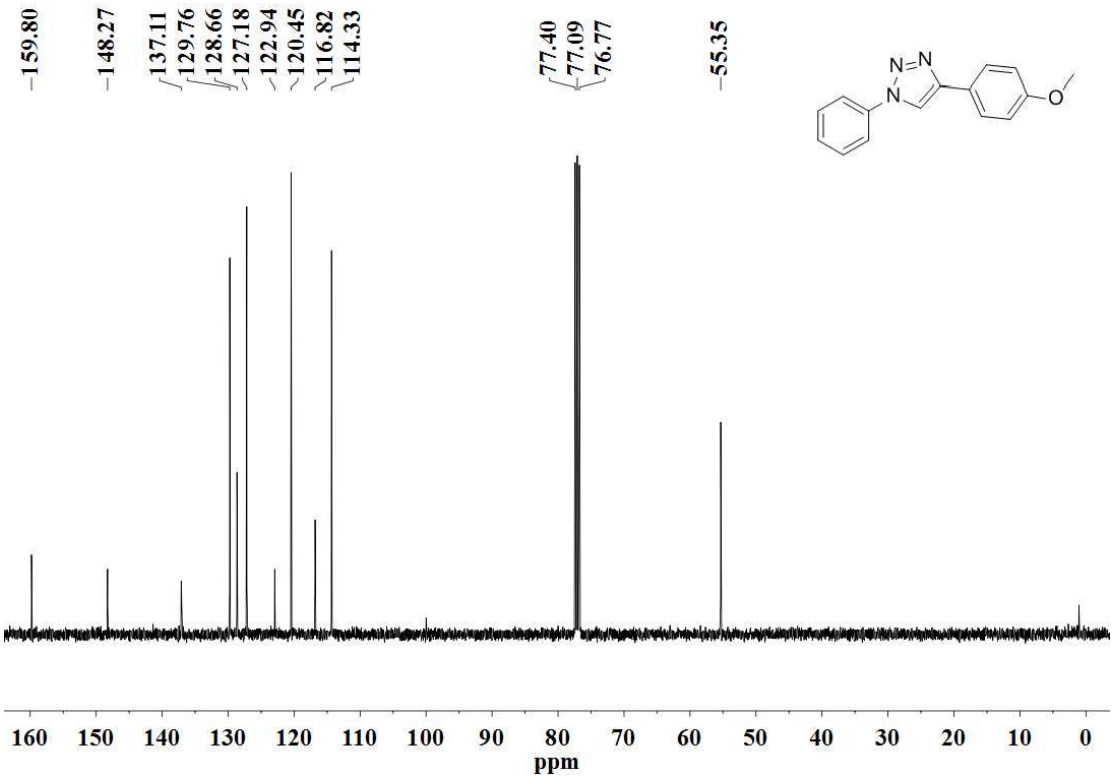
SI Fig. 25. [1]H NMR spectrum for 1-phenyl-4-(p-tolyl)-1*H*-1,2,3-triazole.



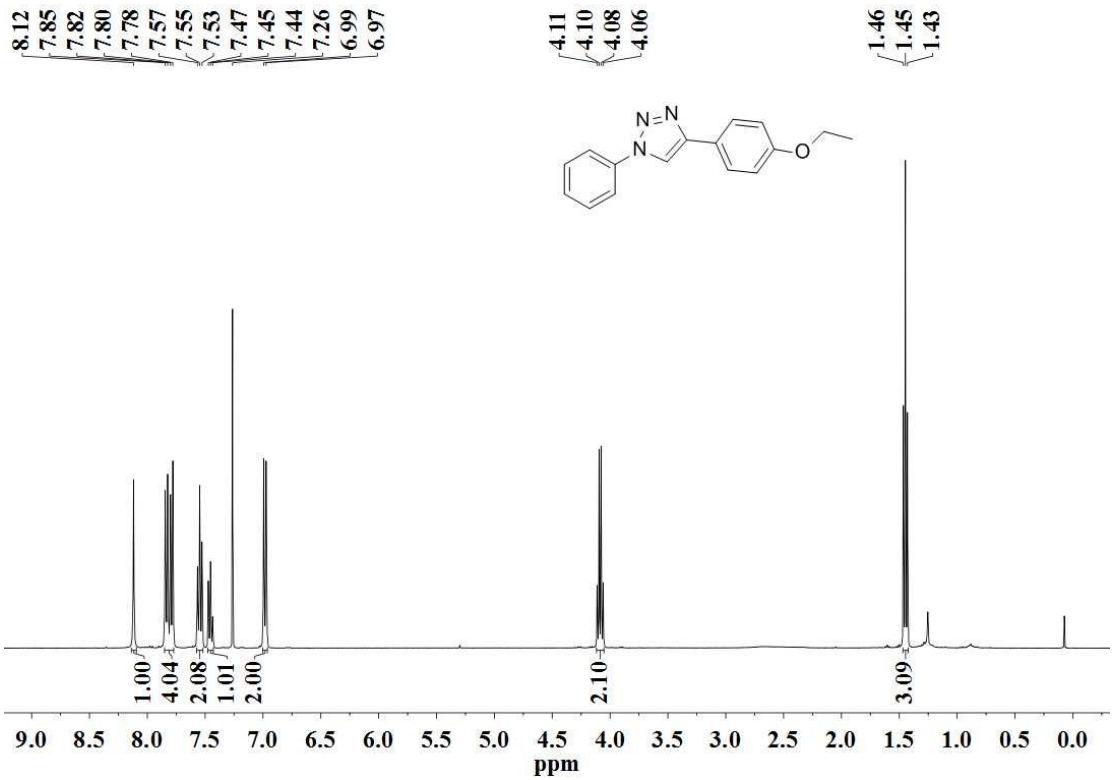
SI Fig. 26. [13]C NMR spectrum for 1-phenyl-4-(p-tolyl)-1*H*-1,2,3-triazole.



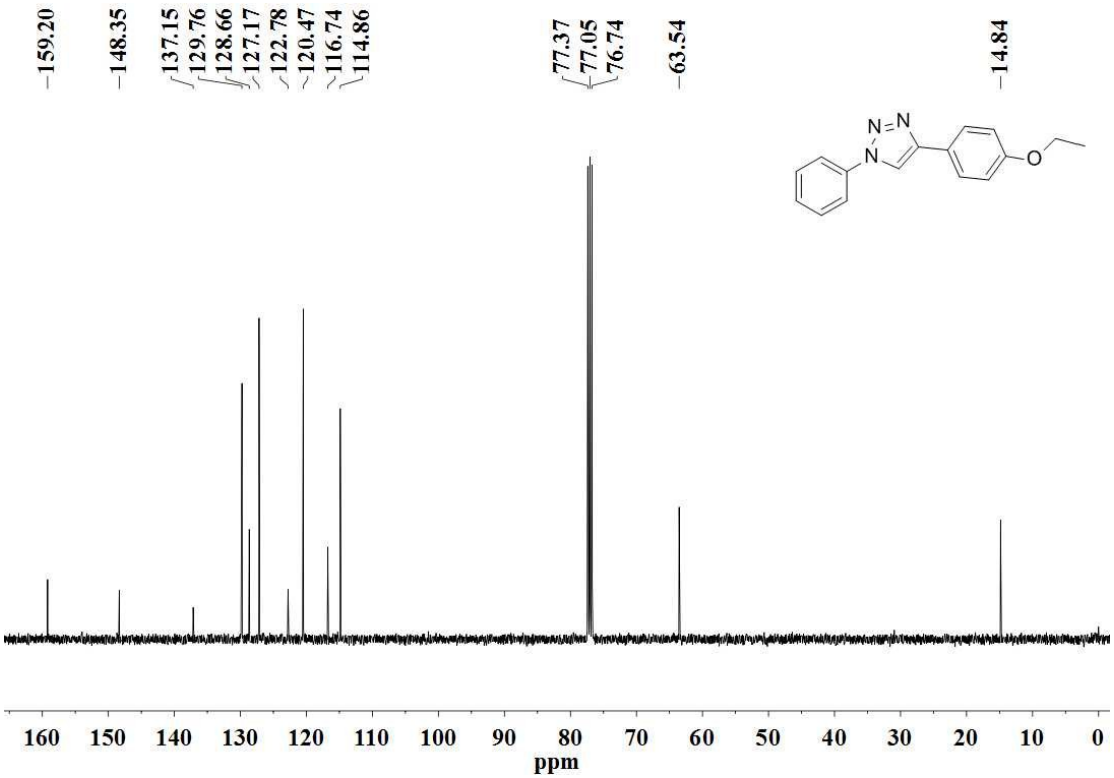
SI Fig. 27. ^{1}H NMR spectrum for 4-(4-methoxyphenyl)-1-phenyl-1*H*-1,2,3-triazole.



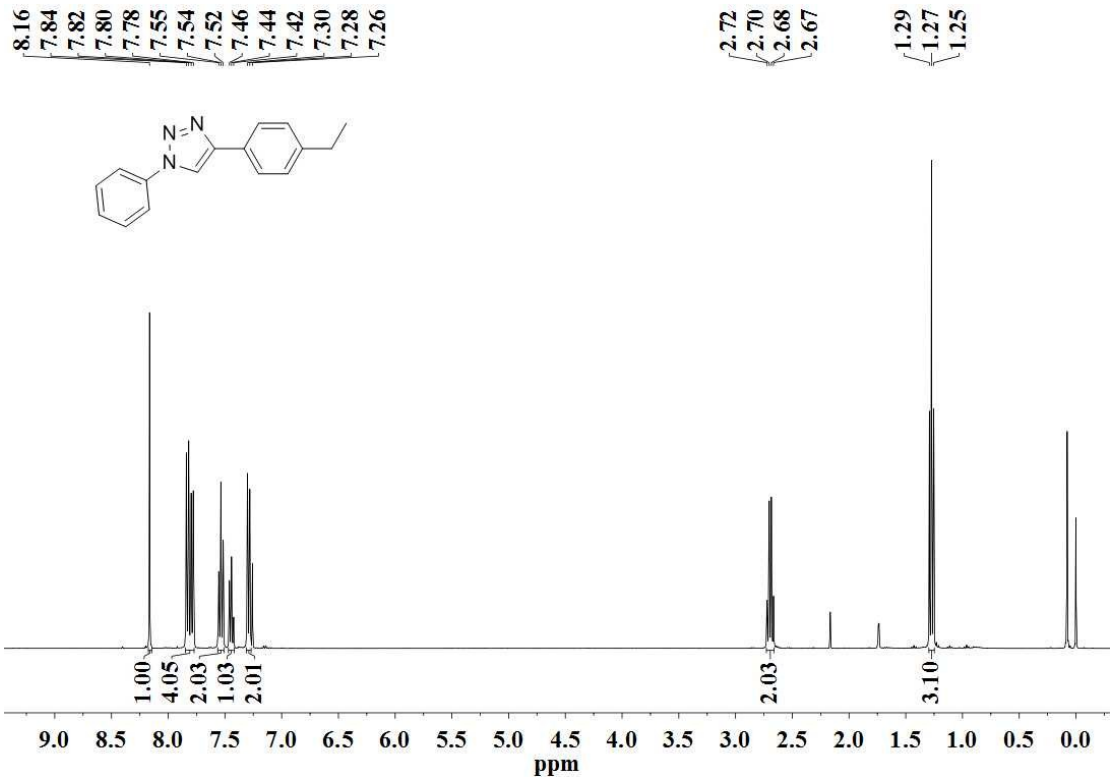
SI Fig. 28. ^{13}C NMR spectrum for 4-(4-methoxyphenyl)-1-phenyl-1*H*-1,2,3-triazole.



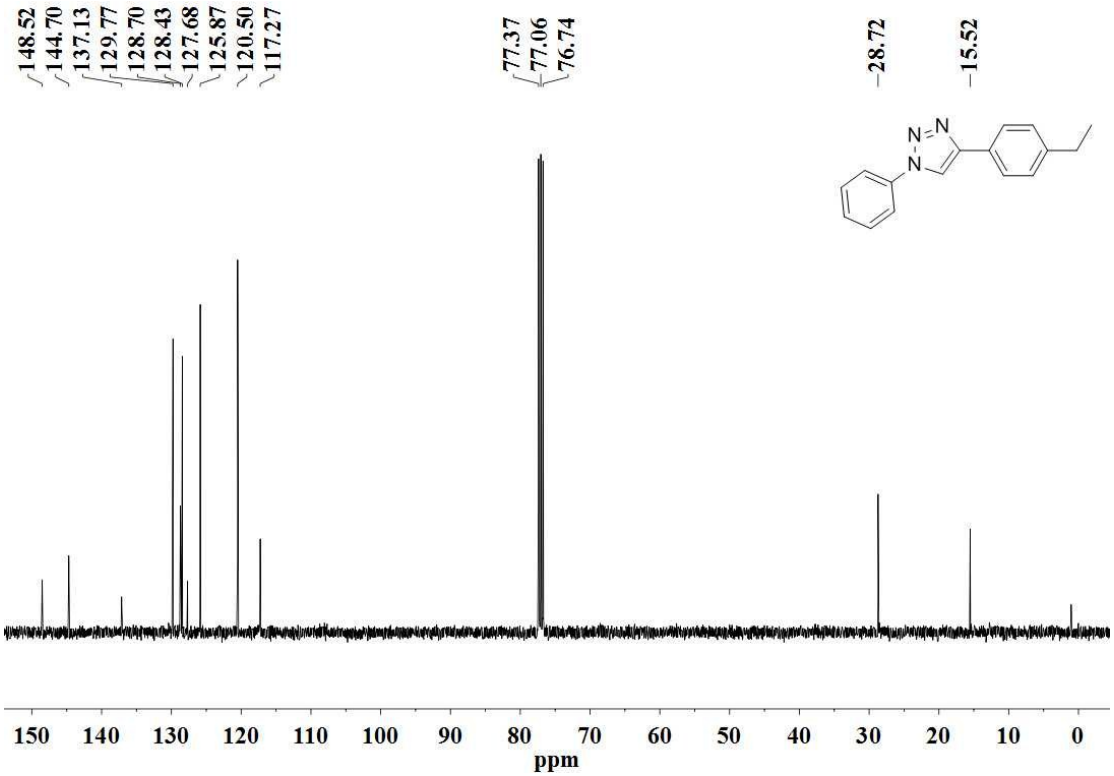
SI Fig. 29. ^{1}H NMR spectrum for 4-(4-ethoxyphenyl)-1-phenyl-1*H*-1,2,3-triazole.



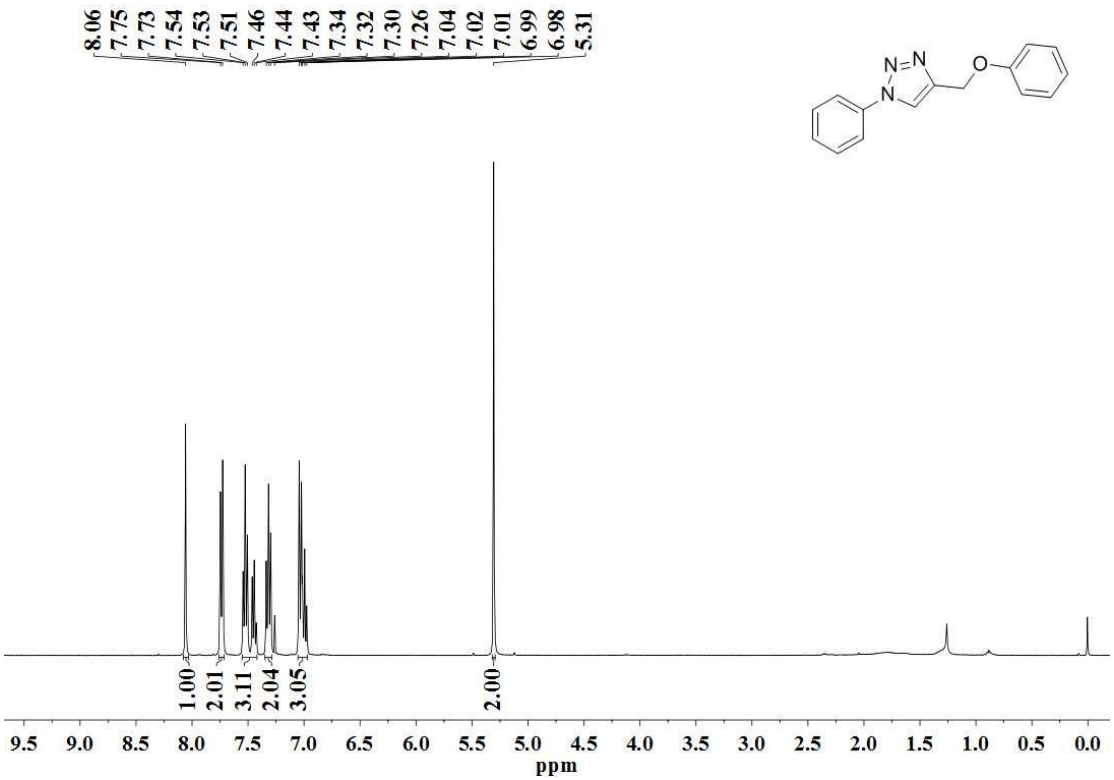
SI Fig. 30. ^{13}C NMR spectrum for 4-(4-ethoxyphenyl)-1-phenyl-1*H*-1,2,3-triazole.



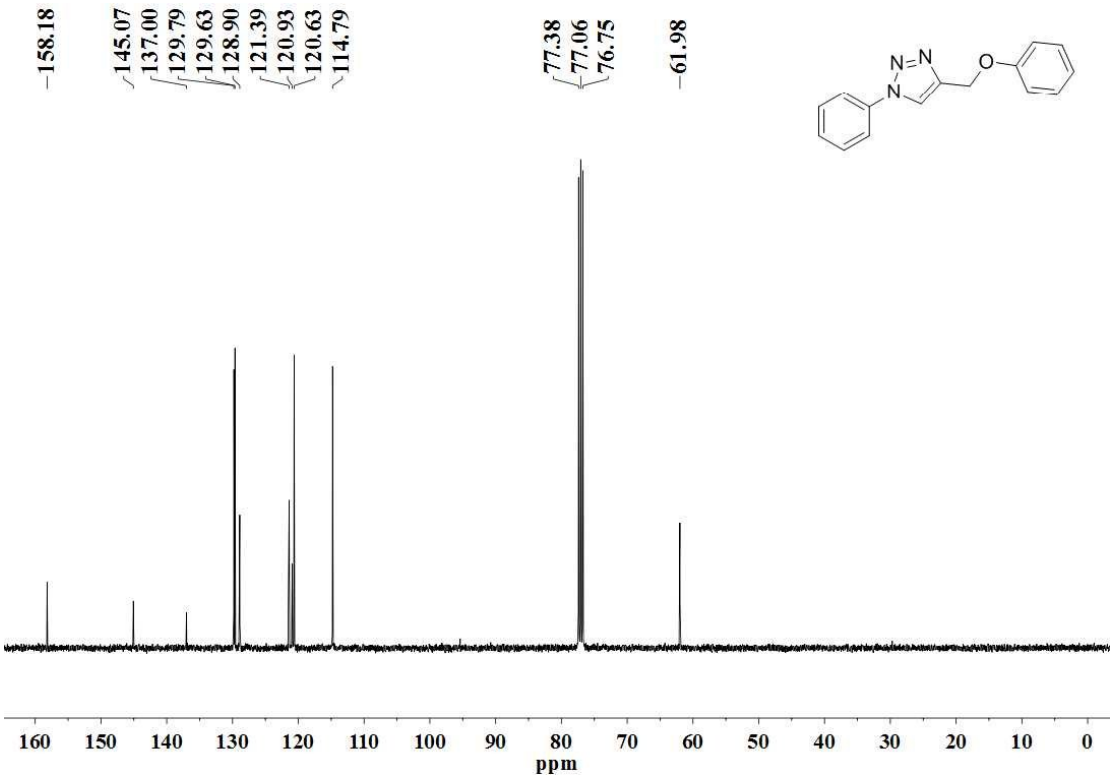
SI Fig. 31. [1]H NMR spectrum for 4-(4-ethylphenyl)-1-phenyl-1*H*-1,2,3-triazole.



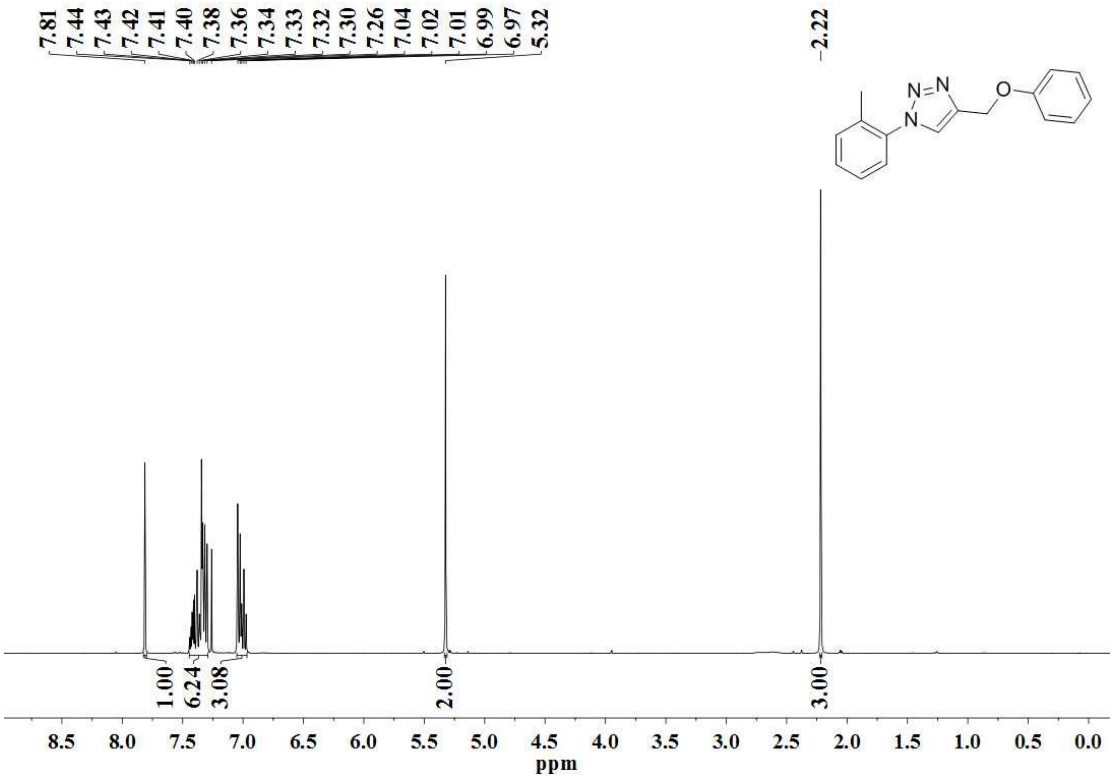
SI Fig. 32. [13]C NMR spectrum for 4-(4-ethylphenyl)-1-phenyl-1*H*-1,2,3-triazole.



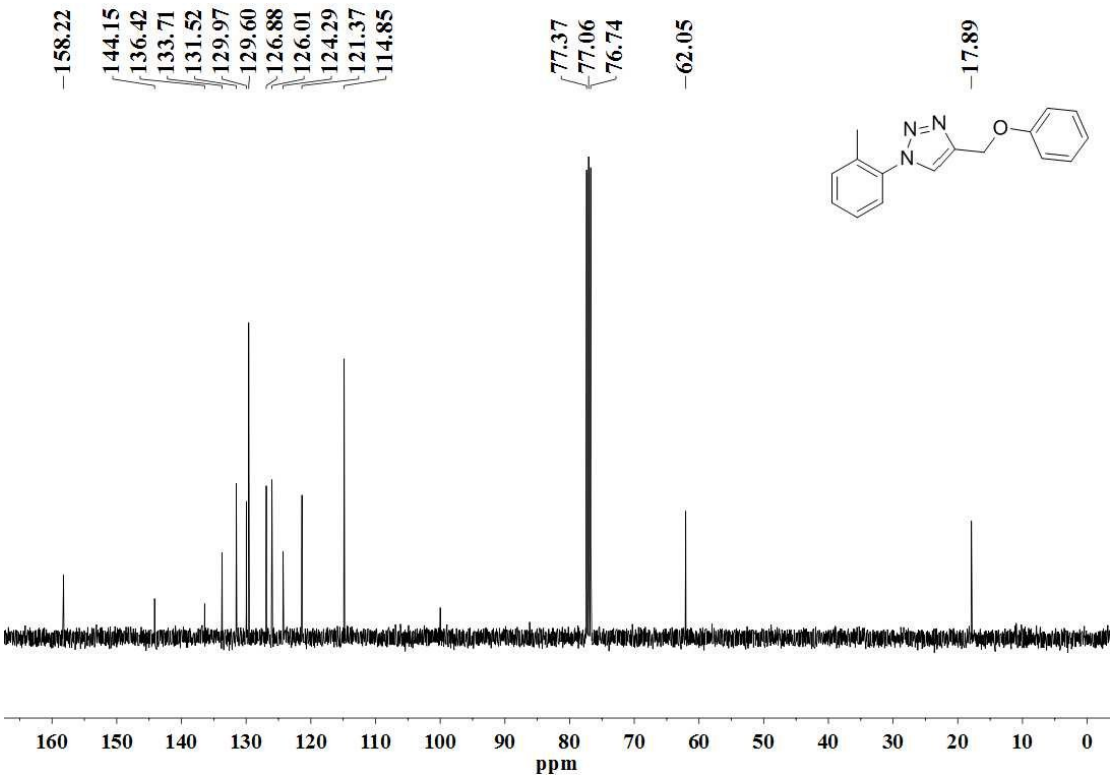
SI Fig. 33. ^{1}H NMR spectrum for 4-(phenoxymethyl)-1-phenyl-1*H*-1,2,3-triazole.



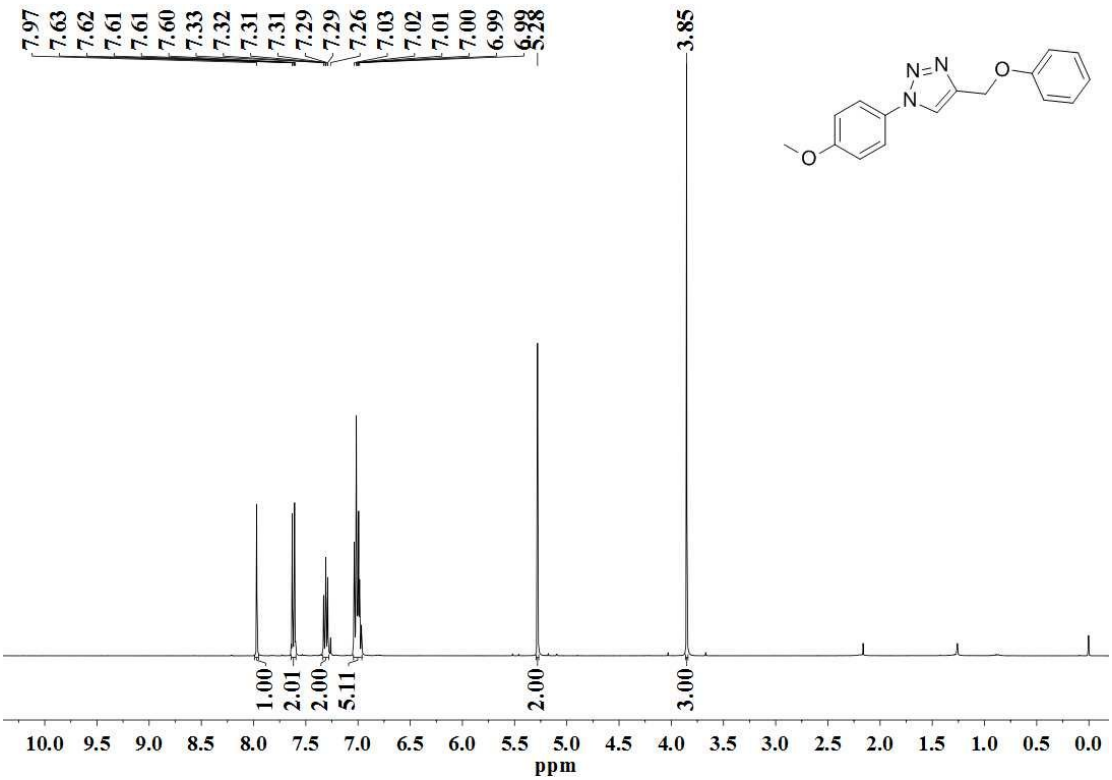
SI Fig. 34. ^{13}C NMR spectrum for 4-(phenoxymethyl)-1-phenyl-1*H*-1,2,3-triazole.



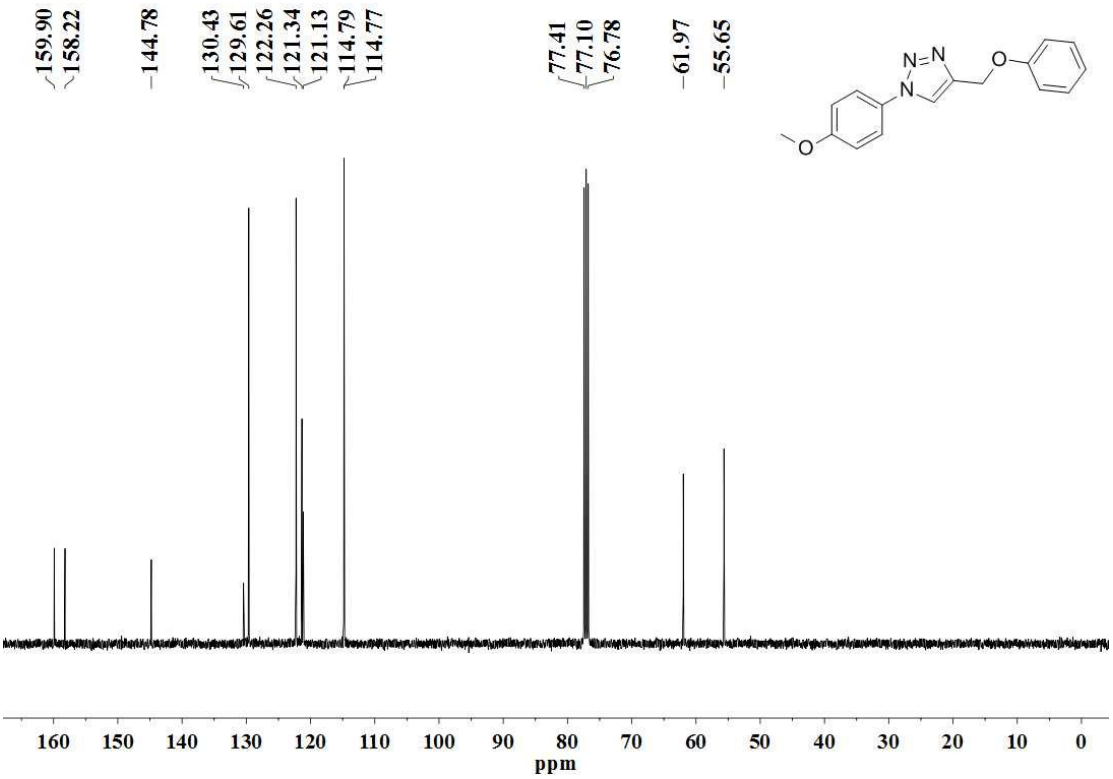
SI Fig. 35. [1]H NMR spectrum for 4-(phenoxymethyl)-1-(o-tolyl)-1*H*-1,2,3-triazole.



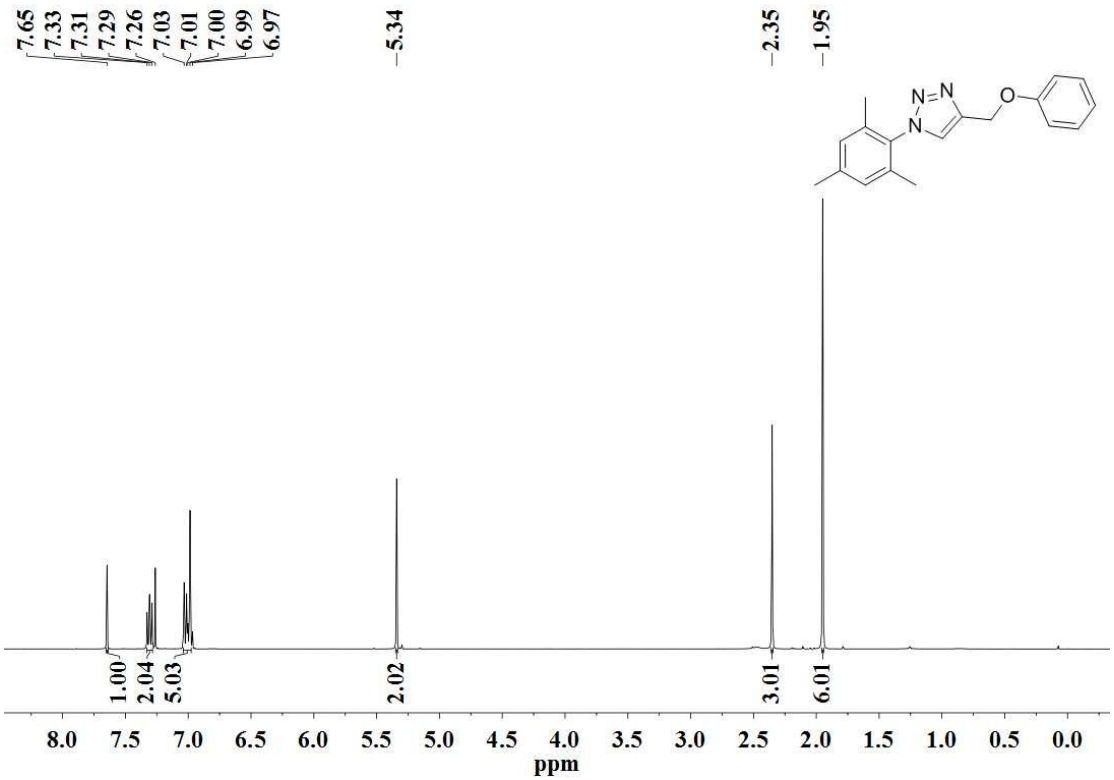
SI Fig. 36. [1]H NMR spectrum for 4-(phenoxymethyl)-1-(o-tolyl)-1*H*-1,2,3-triazole.



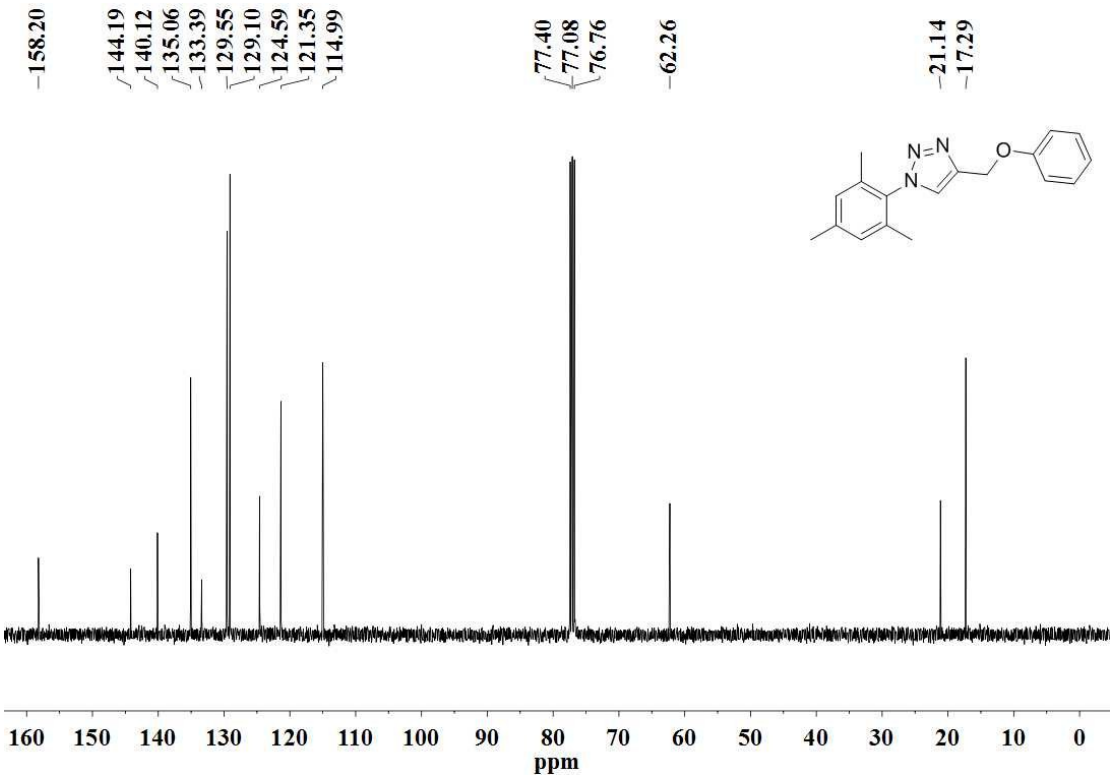
SI Fig. 37. ^{1}H NMR spectrum for 1-(4-methoxyphenyl)-4-(phenoxymethyl)-1*H*-1,2,3-triazole.



SI Fig. 38. ^{1}H NMR spectrum for 1-(4-methoxyphenyl)-4-(phenoxymethyl)-1*H*-1,2,3-triazole.



SI Fig. 39. ^{1}H NMR spectrum for 1-mesityl-4-(phenoxymethyl)-1*H*-1,2,3-triazole.



SI Fig. 40. ^{13}C NMR spectrum for 1-mesityl-4-(phenoxymethyl)-1*H*-1,2,3-triazole.