Synthesis

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Supporting Information

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Supporting Information

(3 + 2) Cycloadditions of Vinyl Sulfonyl Fluorides with Ethyl Diazoacetate or Azides: Metal-Free Synthesis of Pyrazole and Triazole Scaffolds *via* SO_2 Elimination

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Crystallographic data for compound 3g and 7ac

The compounds **3g** and **7ac** were recrystallized from ethyl acetate-hexane mixture (ca 4:1 v/v). Single crystal X-ray data for crystal of compounds **3g** and **7ac** was collected on an X-ray diffractometer using Mo-Kα (λ = 0.71073 Å) radiation after mounting on glass fiber inside a brass pin in open air. The structure was solved by direct methods and refined by full matrix least squares method using standard procedures; absorption corrections were done using SADABS program, where applicable.[1] In general, all non-hydrogen atoms were refined anisotropically; hydrogen atoms were fixed by geometry or located by a Difference Fourier map and refined isotropically. CCDC numbers 2141604-2141605.

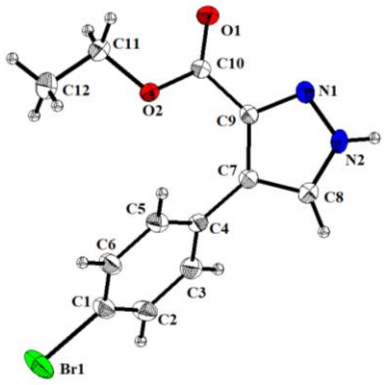

Figure S1. ORTEP (ellipsoid contour probability 50%) of compound **3g** (CCDC no. 2141604). ORTEP view of Ethyl 4-(4-bromophenyl)-1*H*-pyrazole-5-carboxylate with 30% probability of ellipsoids. Crystal data: $C_{12}H_{11}BrN_2O_2$, M = 295.14, Monoclinic, Space group P 1 21/n 1, a = 12.6702(9), b = 7.6733(4), c = 13.3160(6) Å, β = 113.360(7)^o, V = 1188.49(12) Å^3, Z = 4, μ = 3.449 mm^{-1}, data/restraints/parameters: 2090/0/158, R indices (I> 2sigma(I)): R1 = 0.0505, wR2 (all data) = 0.1427.

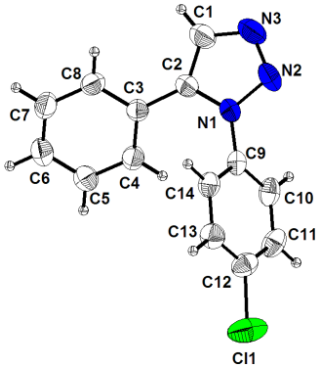

Figure S2. ORTEP (ellipsoid contour probability 50%) of compound **7ac** (CCDC no. 2141605). ORTEP view of 1-(4-Chlorophenyl)-5-phenyl-1H-1,2,3-triazole with 30% probability of ellipsoids. Crystal data: $C_{14}H_{10}N_3Cl$, M = 255.70, Monoclinic, Space group P 1 21/n 1, a = 9.1767(4), b = 14.6009(7), c = 9.7541(5) Å, β = 103.867(4)^o, V = 1268.84(10) Å^3, Z = 4, μ = 0.285 mm^{-1}, data/restraints/parameters: 2217/0/164, R indices (I> 2sigma(I)): R1 = 0.0513, wR2 (all data) = 0.1625.

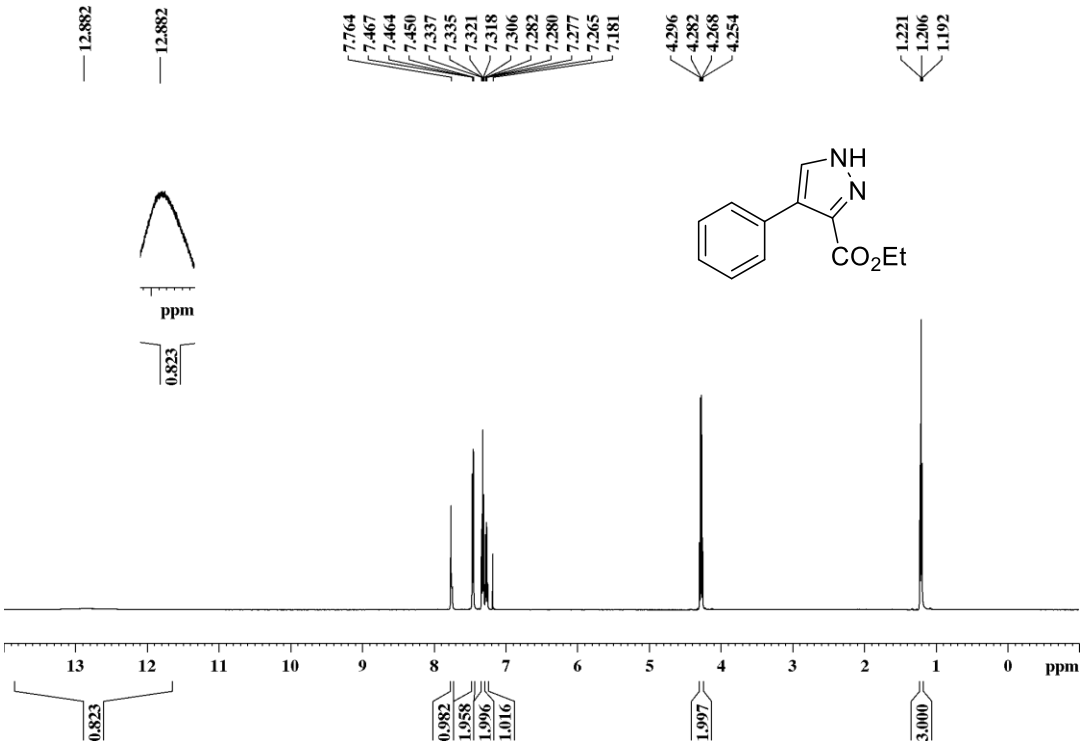

Figure S3. ^{1}H NMR spectrum of compound 3a

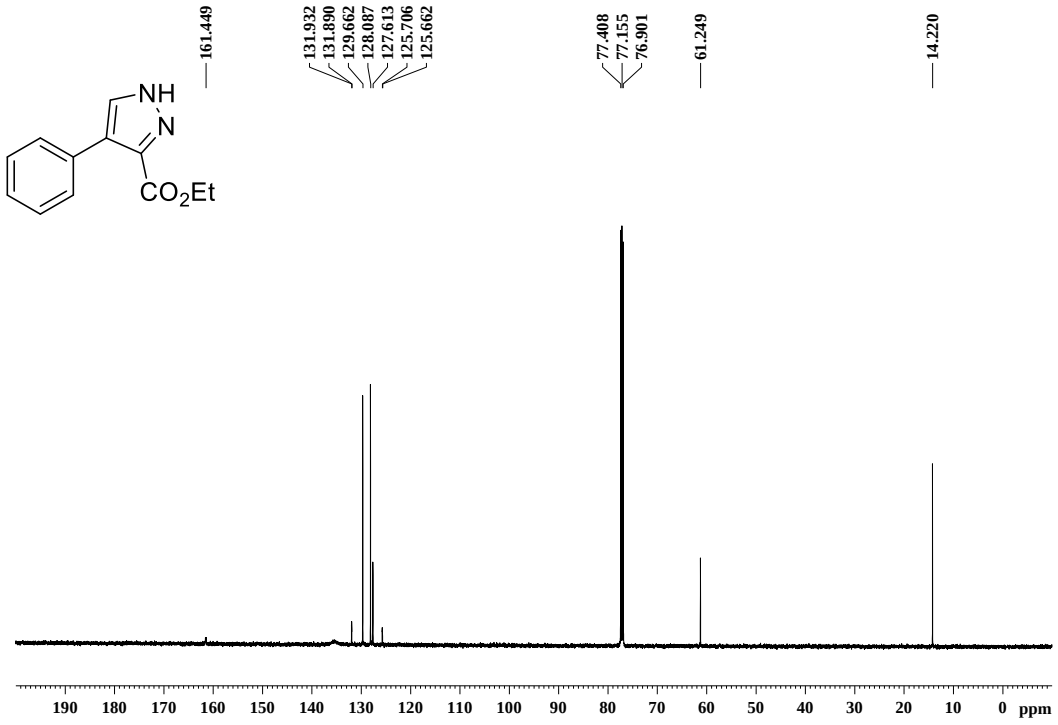

Figure S4. ^{13}C{^{1}H} NMR spectrum of compound 3a

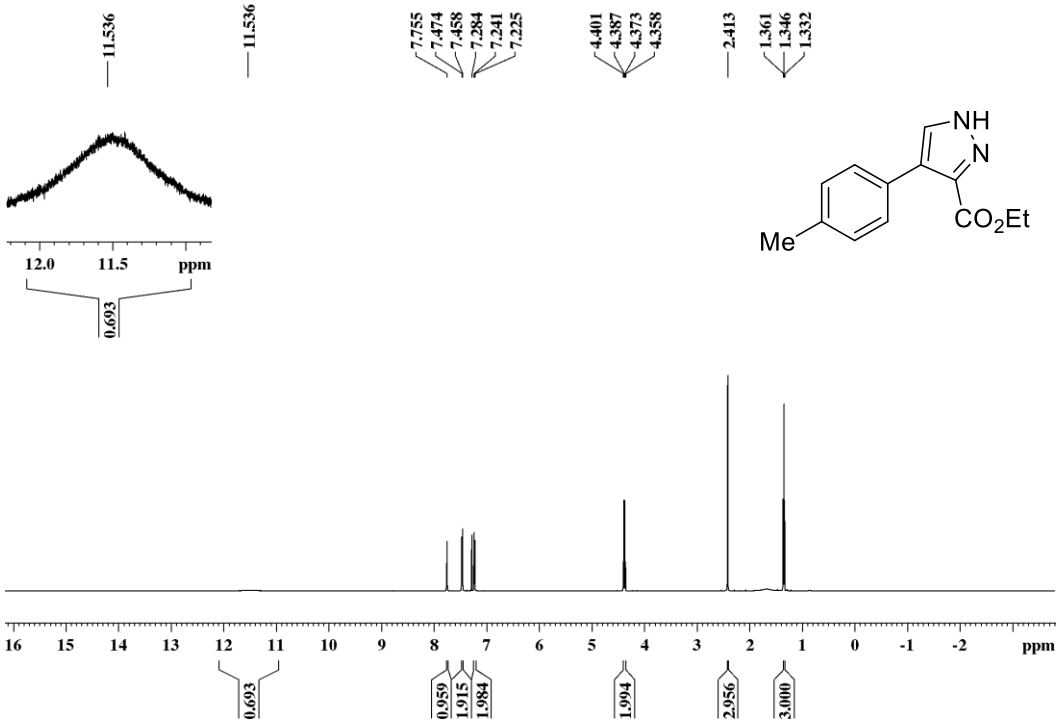

Figure S5. ^{1}H NMR spectrum of compound 3b

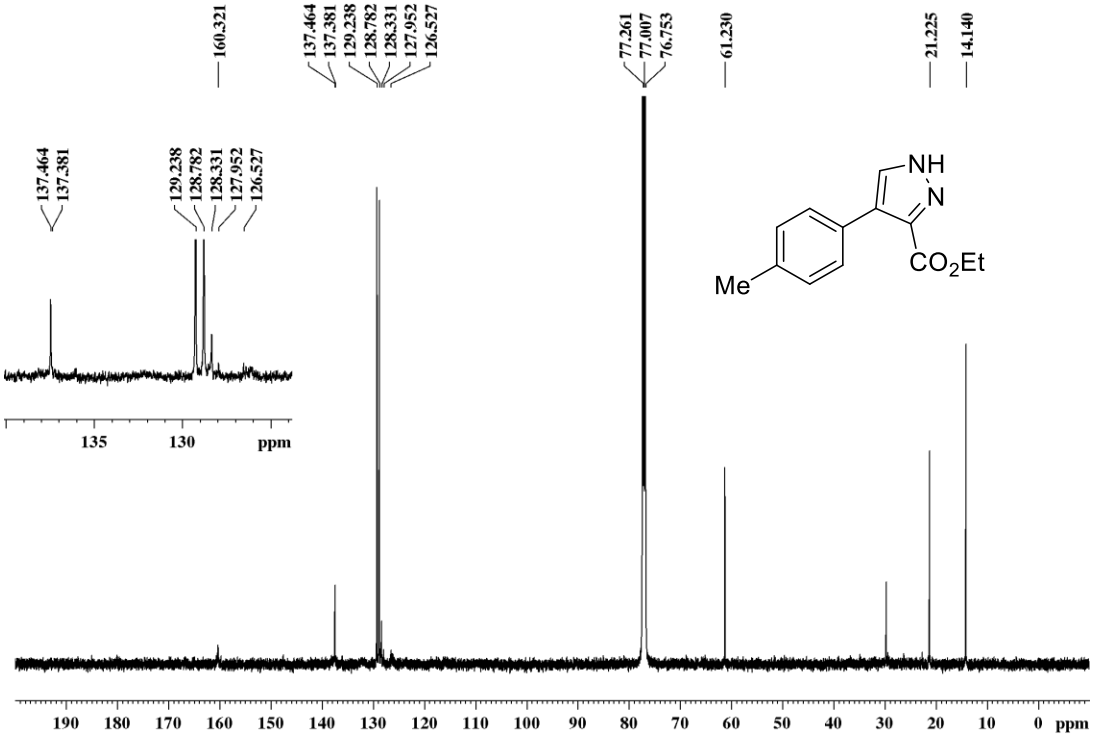

Figure S6. ^{13}C{^{1}H} NMR spectrum of compound 3b

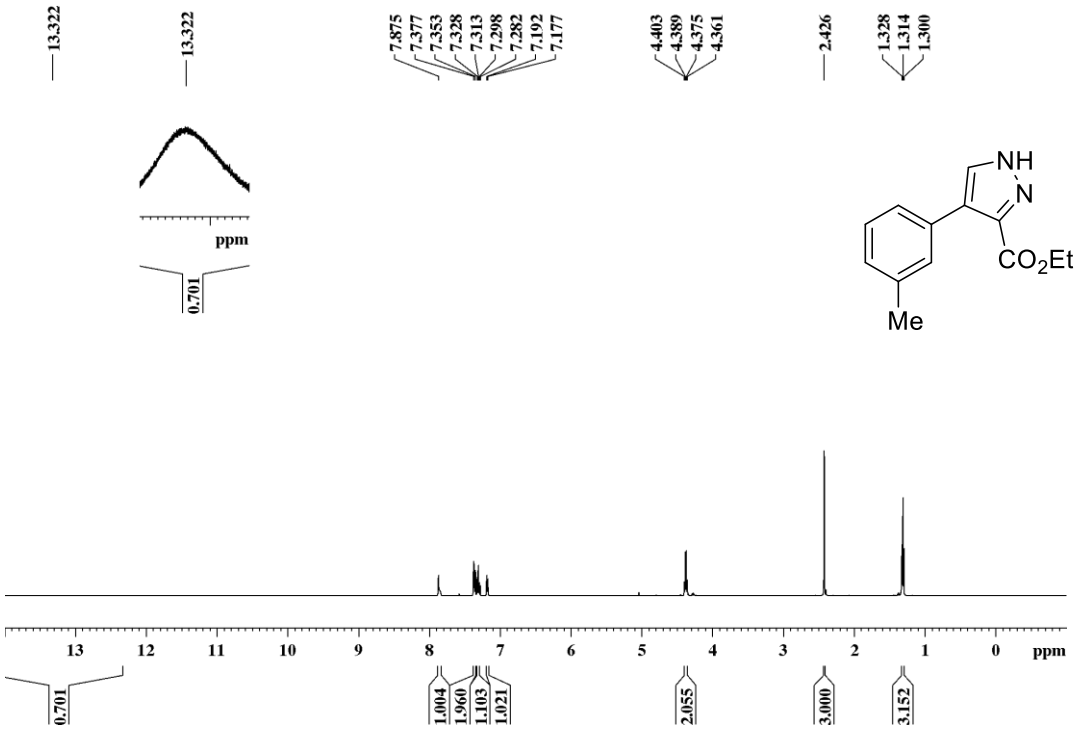

Figure S7. ^{1}H NMR spectrum of compound 3c

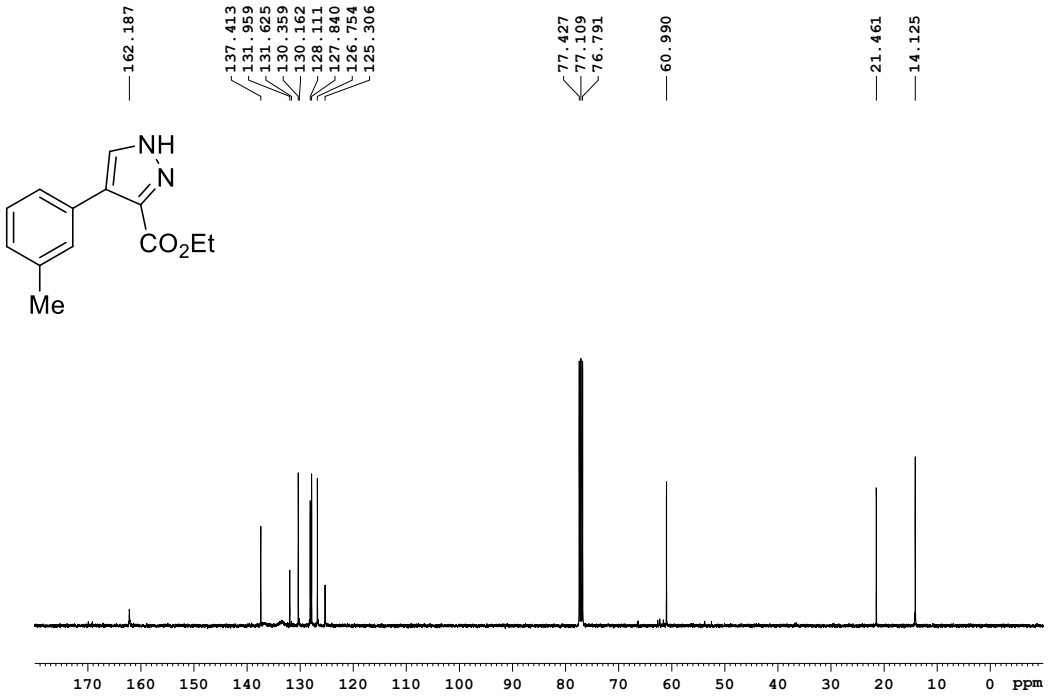

Figure S8. ^{13}C{^{1}H} NMR spectrum of compound 3c

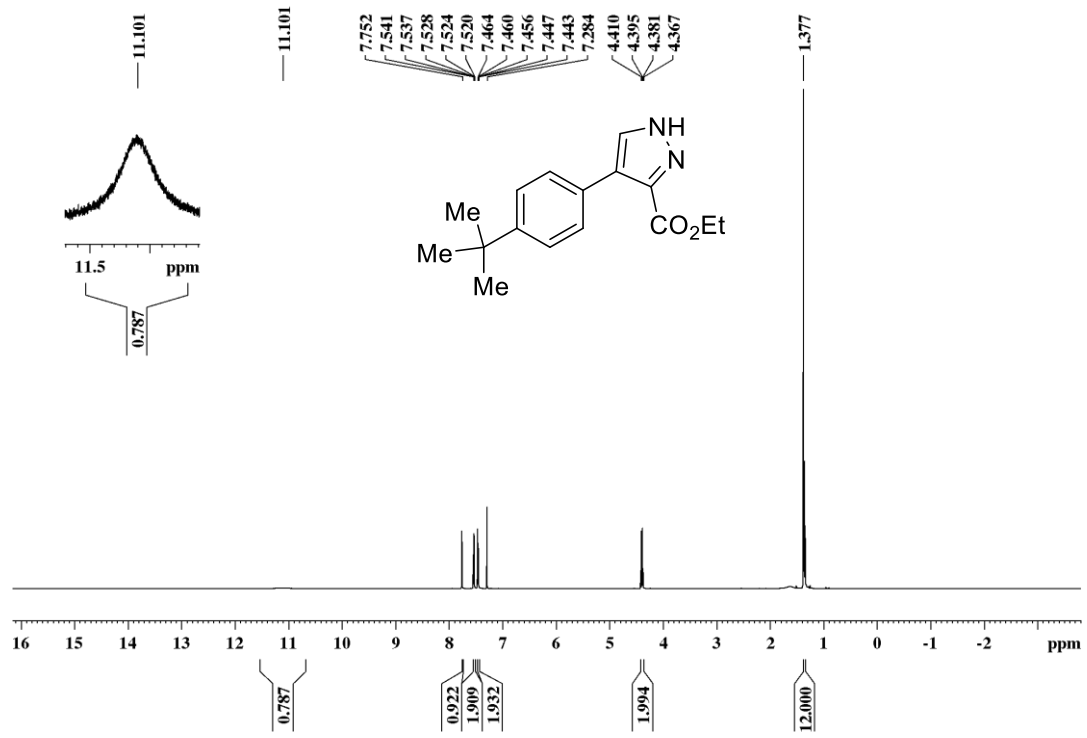

Figure S9. ^{1}H NMR spectrum of compound 3d

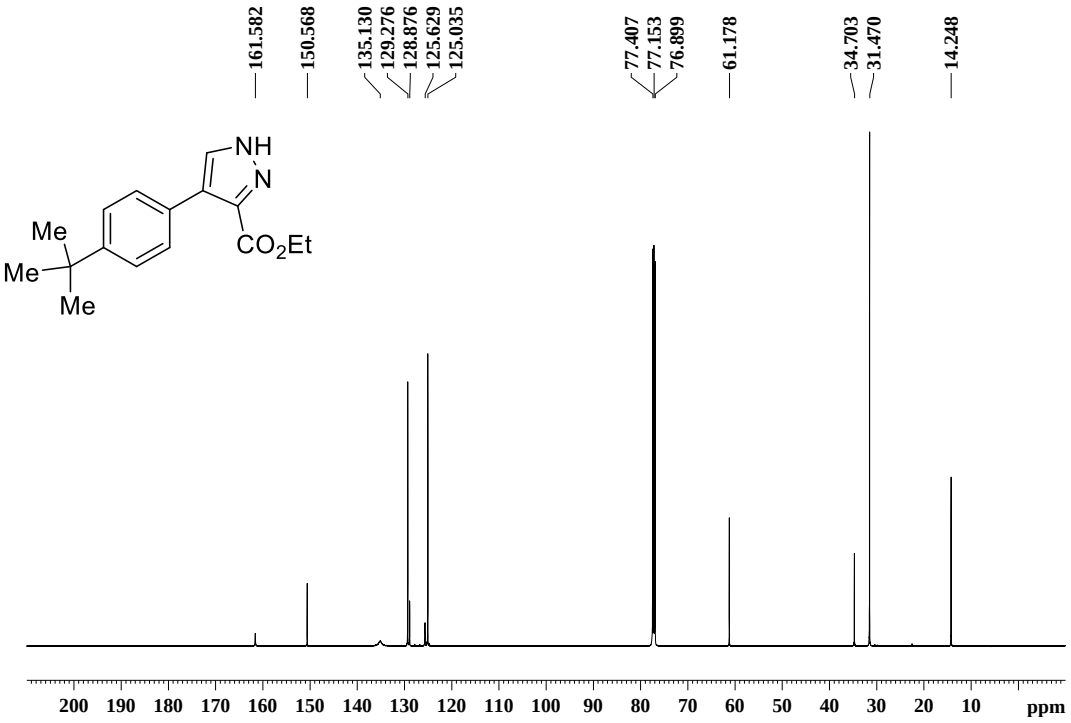

Figure S10. ^{13}C{^{1}H} NMR spectrum of compound 3d

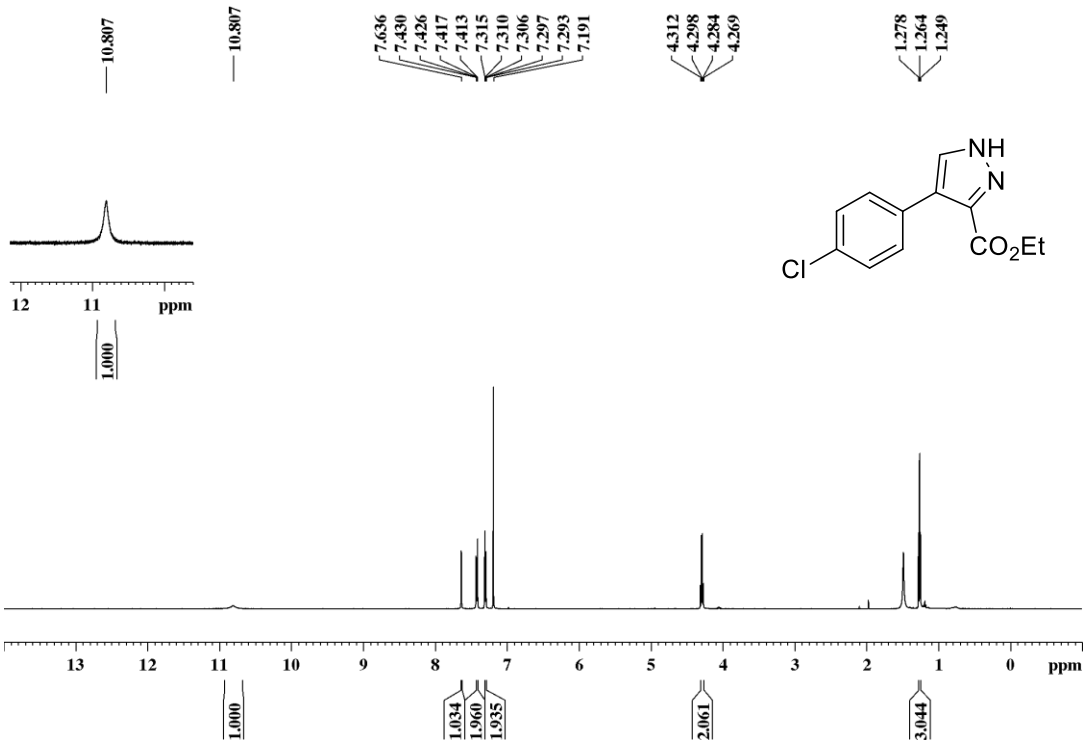

Figure S11. ^{1}H NMR spectrum of compound 3e

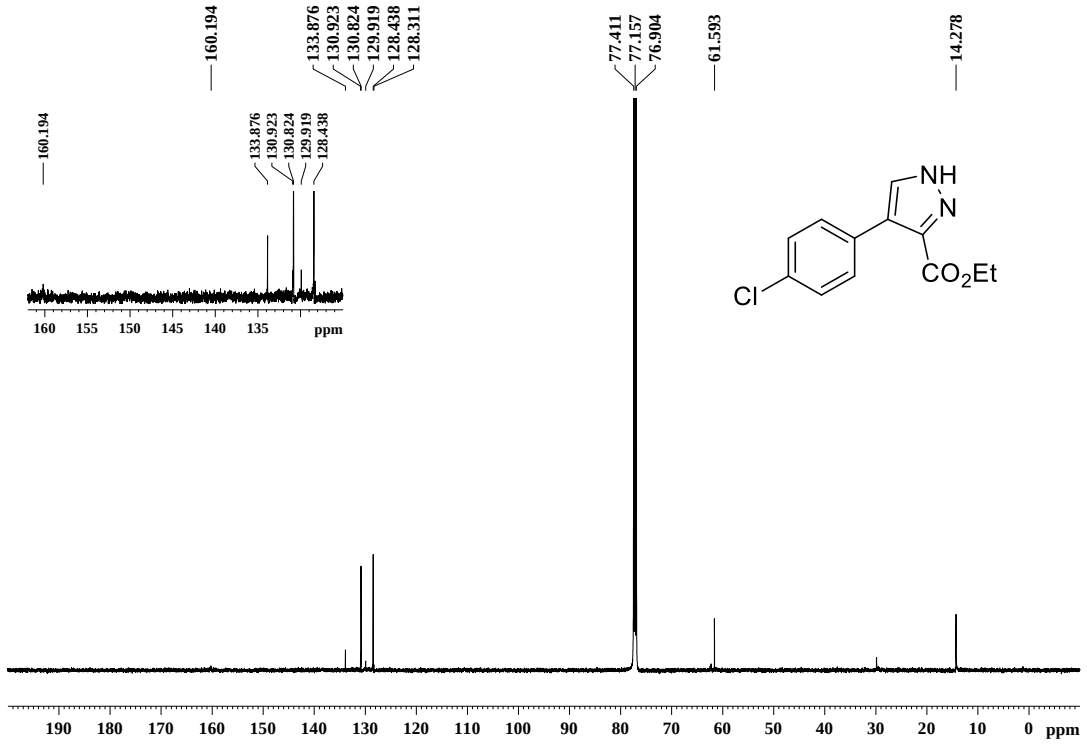

Figure S12. ^{13}C{^{1}H} NMR spectrum of compound 3e

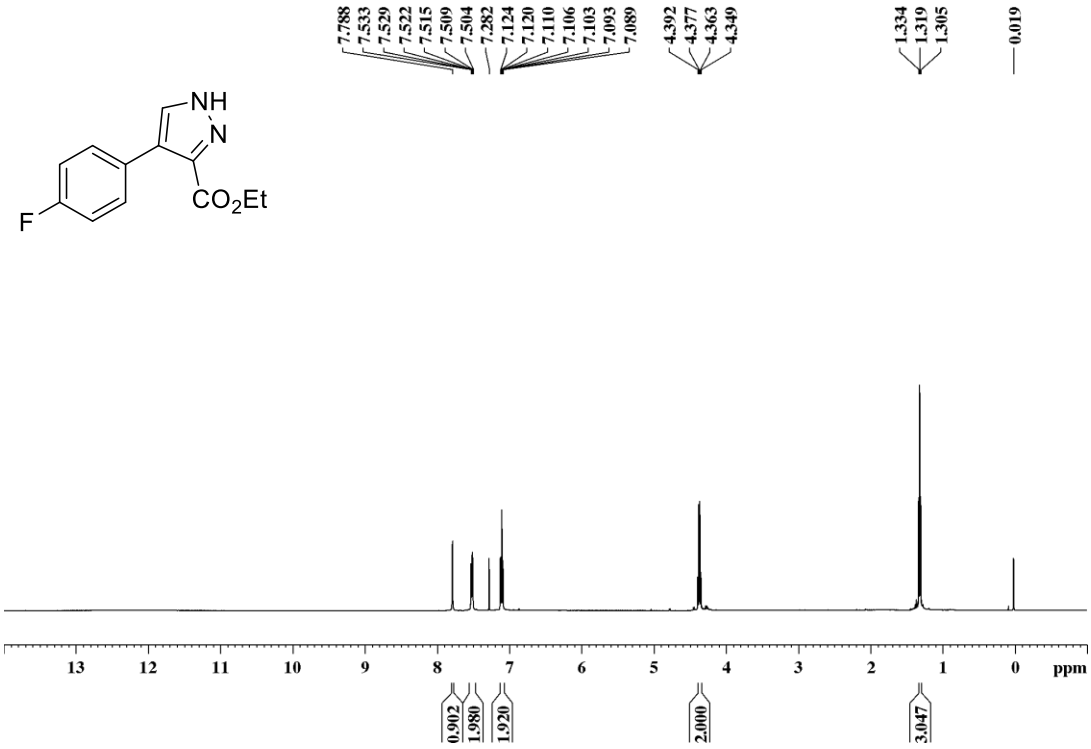

Figure S13. ^{1}H NMR spectrum of compound 3f

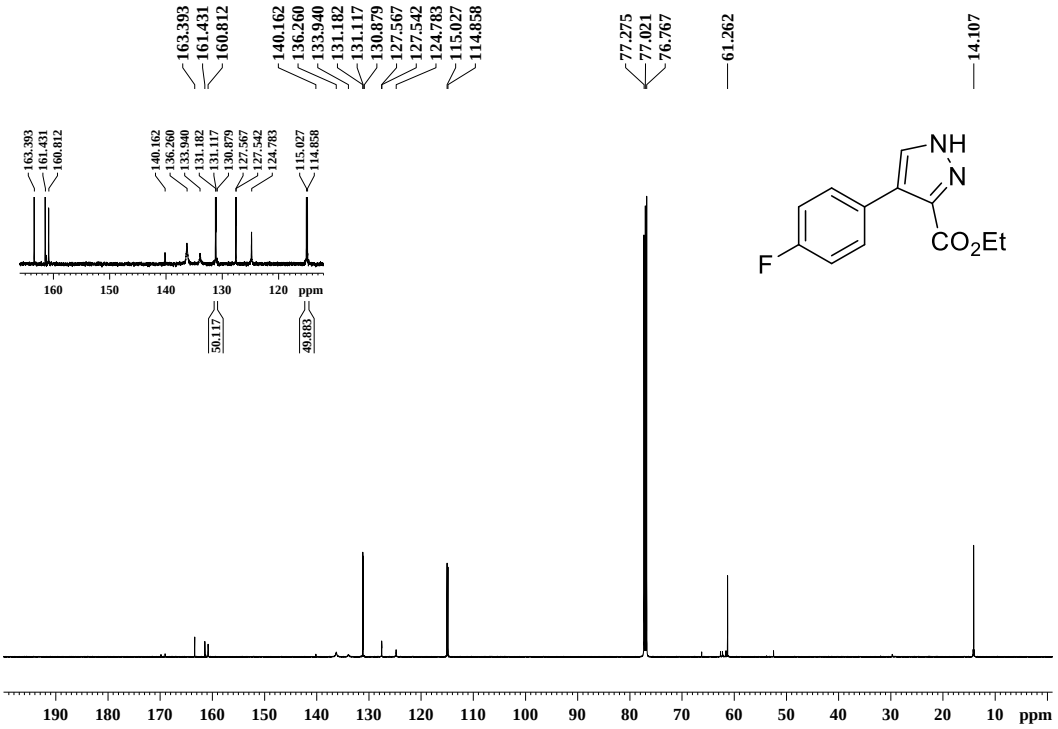

Figure S14. ^{13}C{^{1}H} NMR spectrum of compound 3f

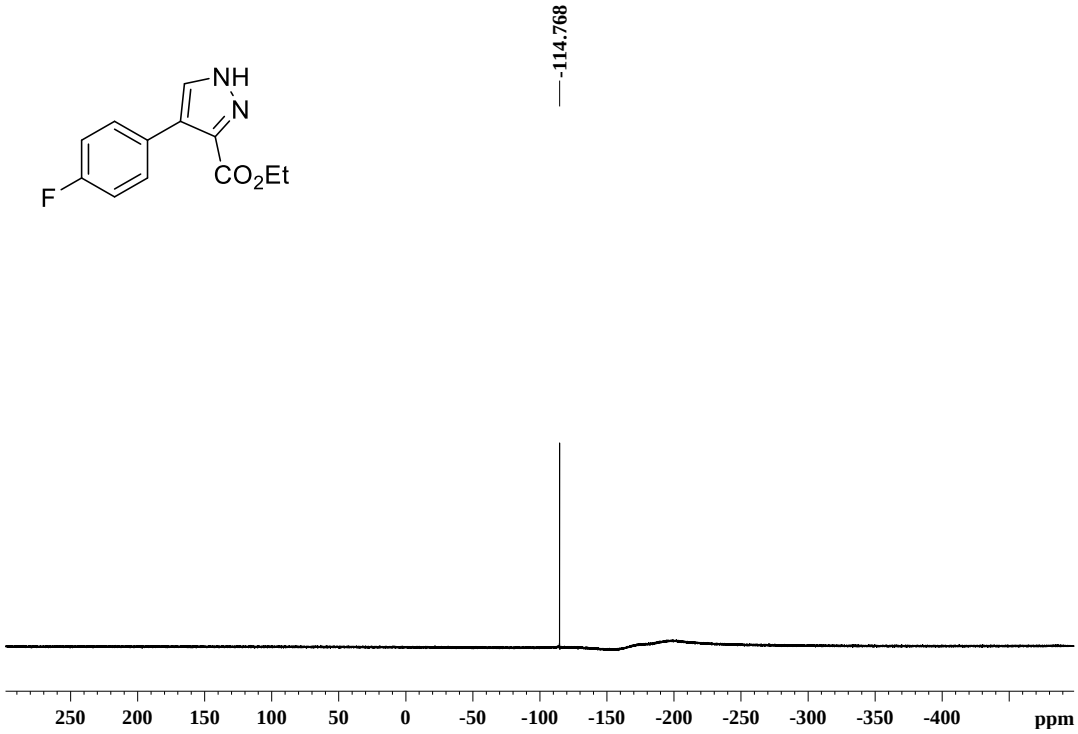

Figure S15. $^{13}C\{^{1}H\}$ NMR spectrum of compound 3f

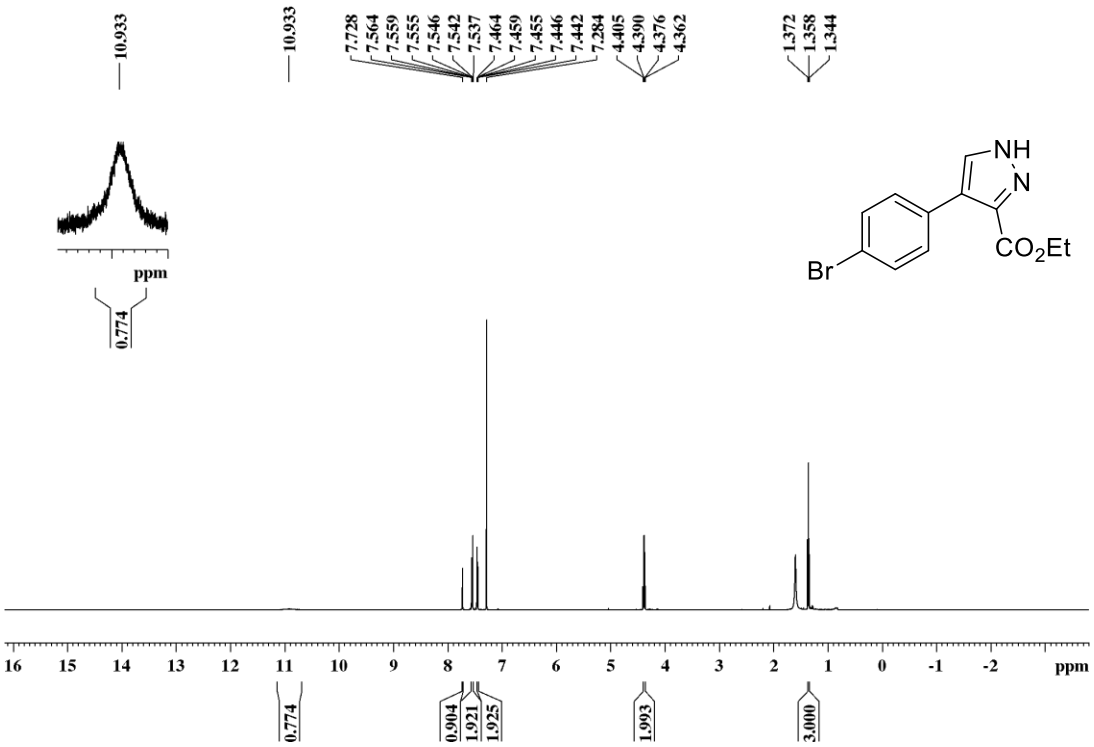

Figure S16. ^{1}H NMR spectrum of compound 3g

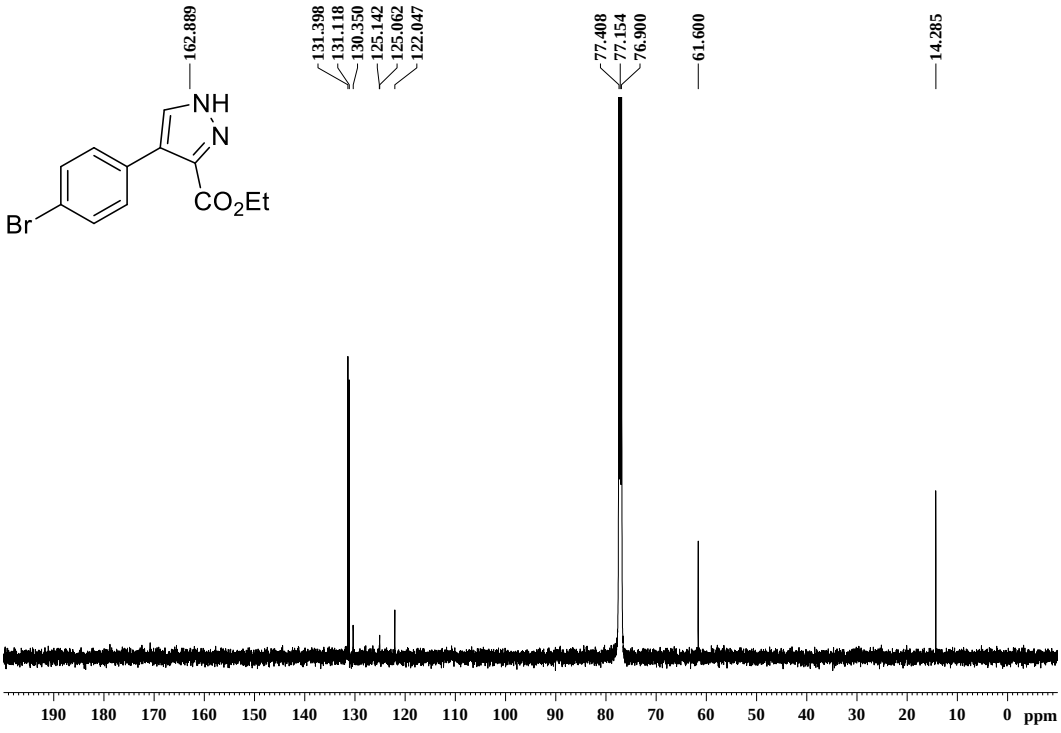

Figure S17. ^{13}C{^{1}H} NMR spectrum of compound 3g

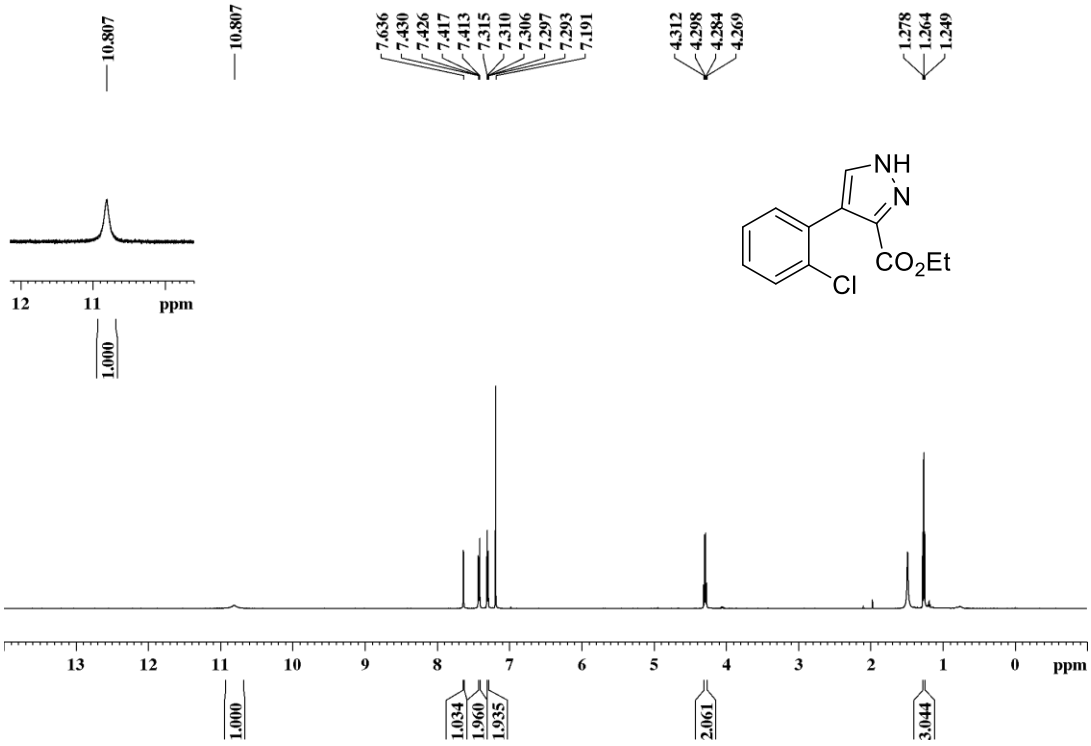

Figure S18. ^{1}H NMR spectrum of compound 3h

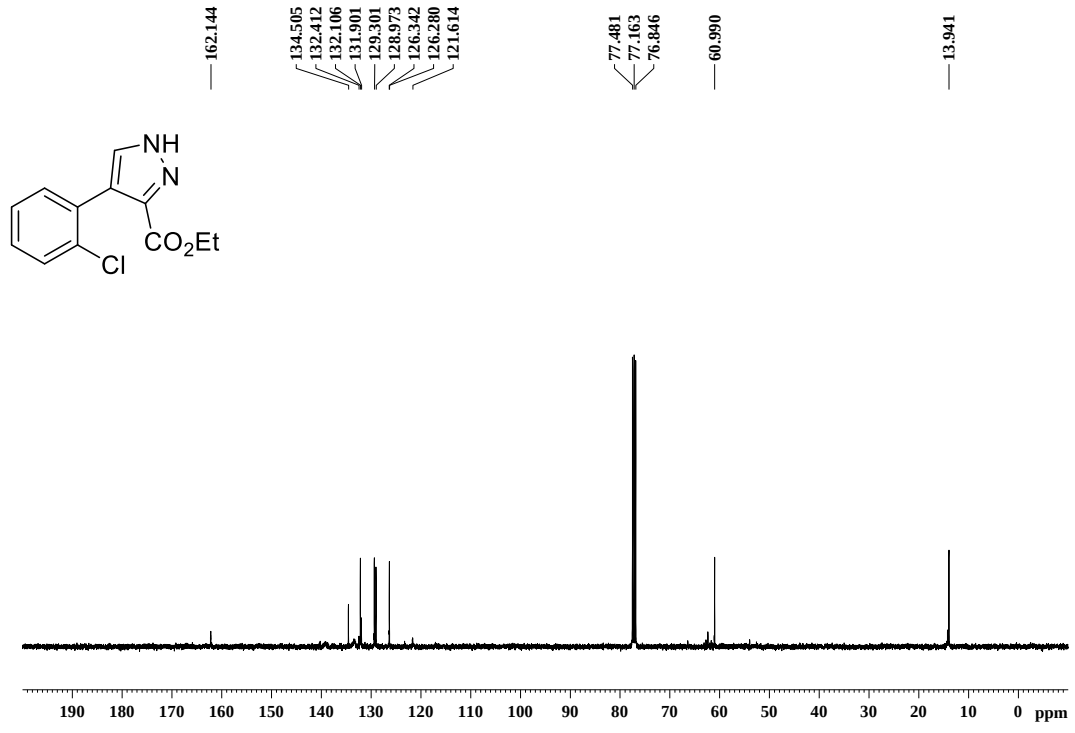

Figure S19. ^{13}C{^{1}H} NMR spectrum of compound 3h

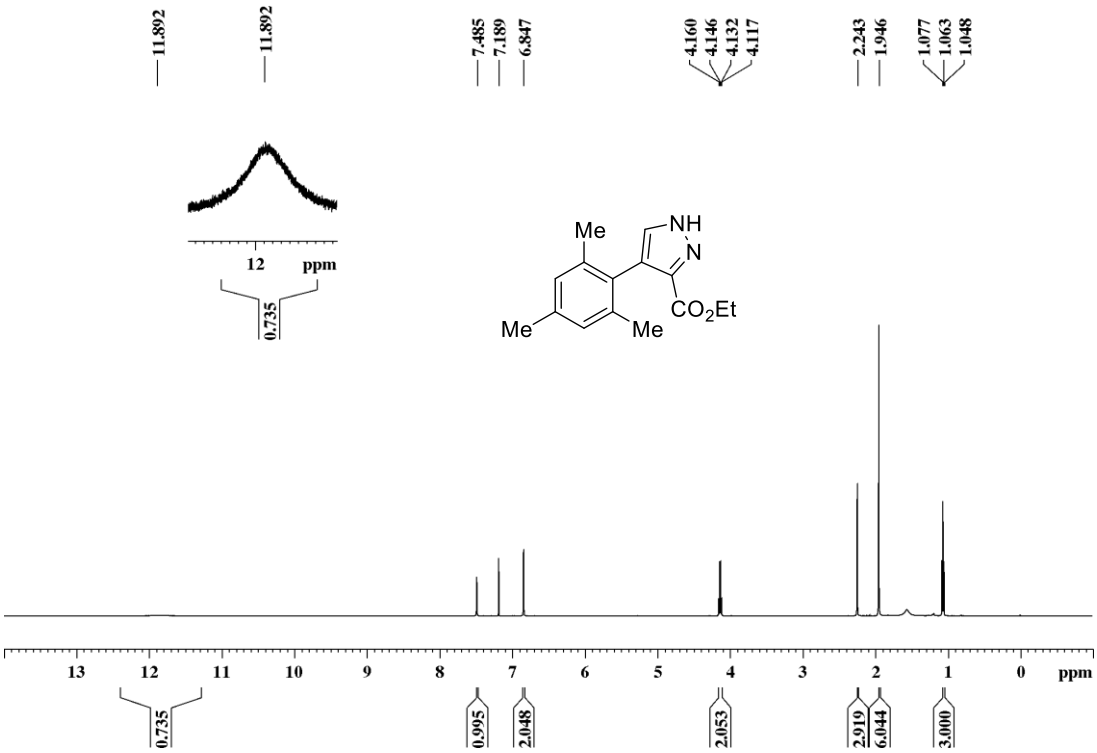

Figure S20. ^{1}H NMR spectrum of compound 3i

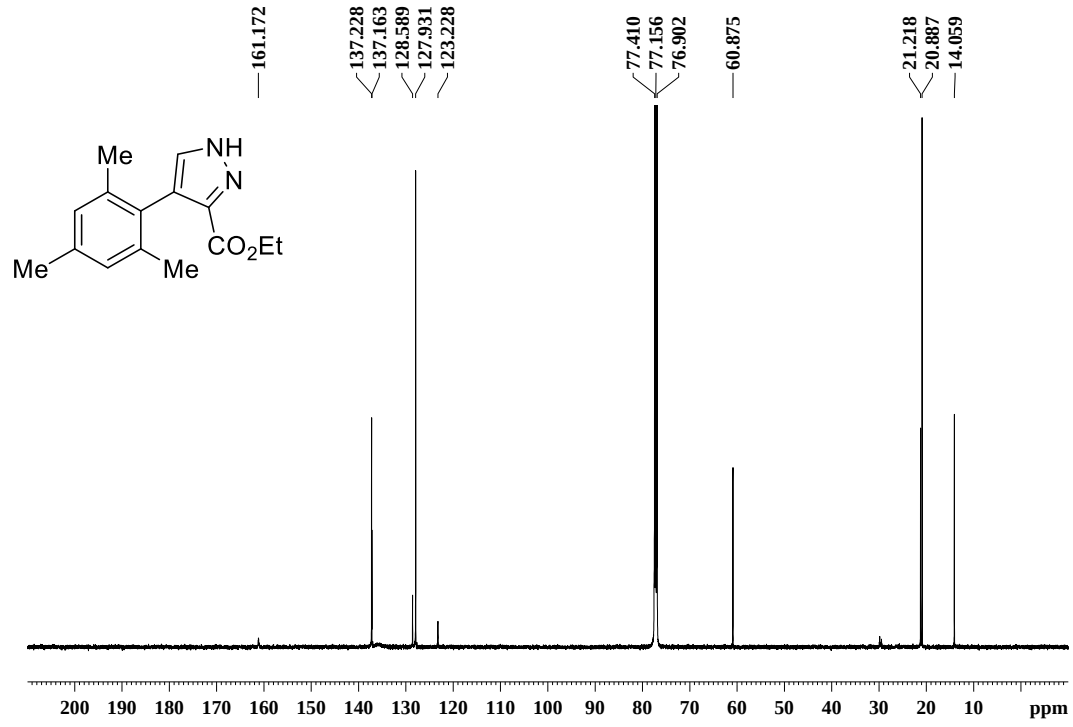

Figure S21. ^{13}C{^{1}H} NMR spectrum of compound 3i

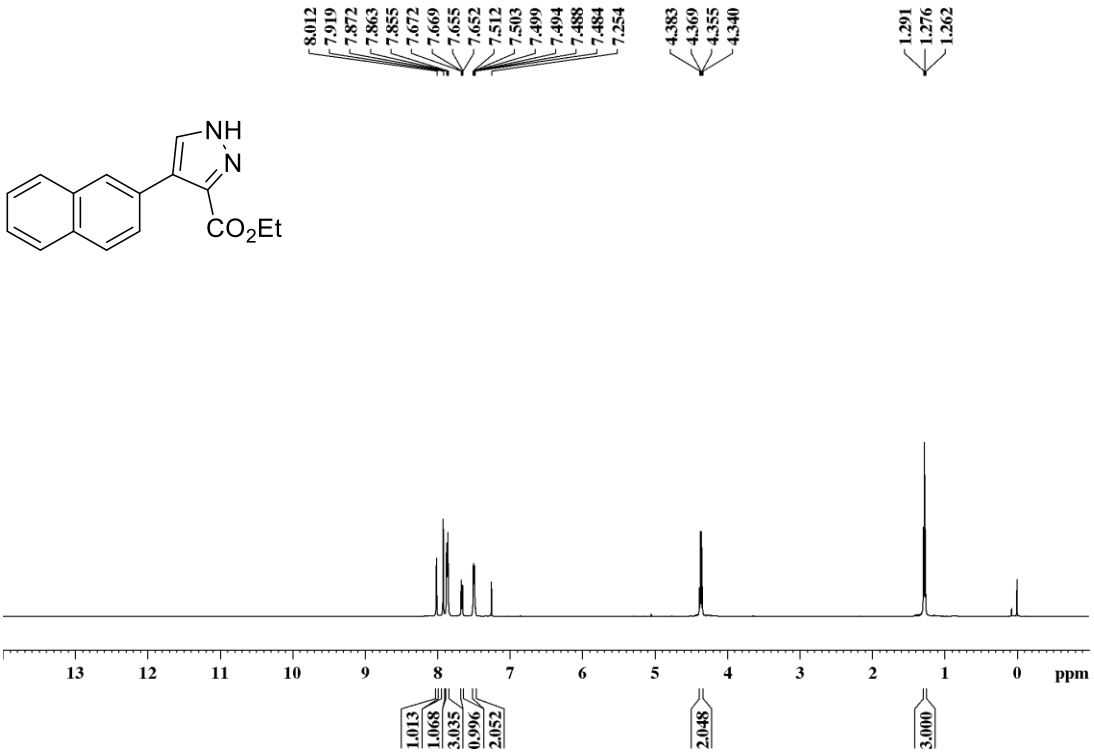

Figure S22. ^{1}H NMR spectrum of compound 3j

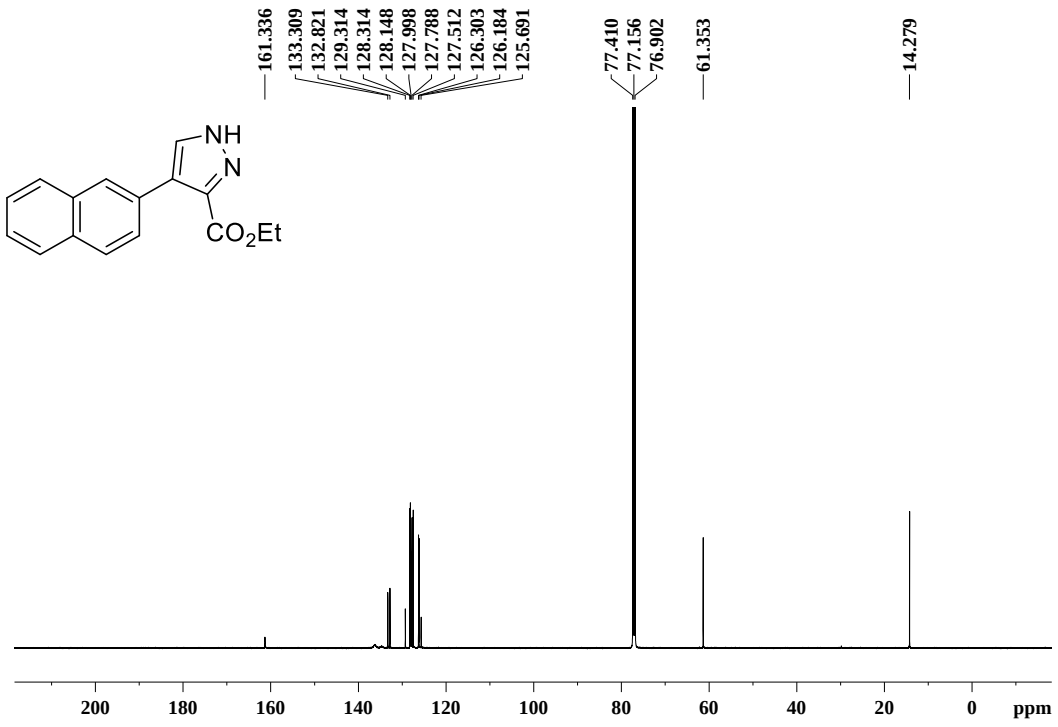

Figure S23. ^{13}C{^{1}H} NMR spectrum of compound 3j

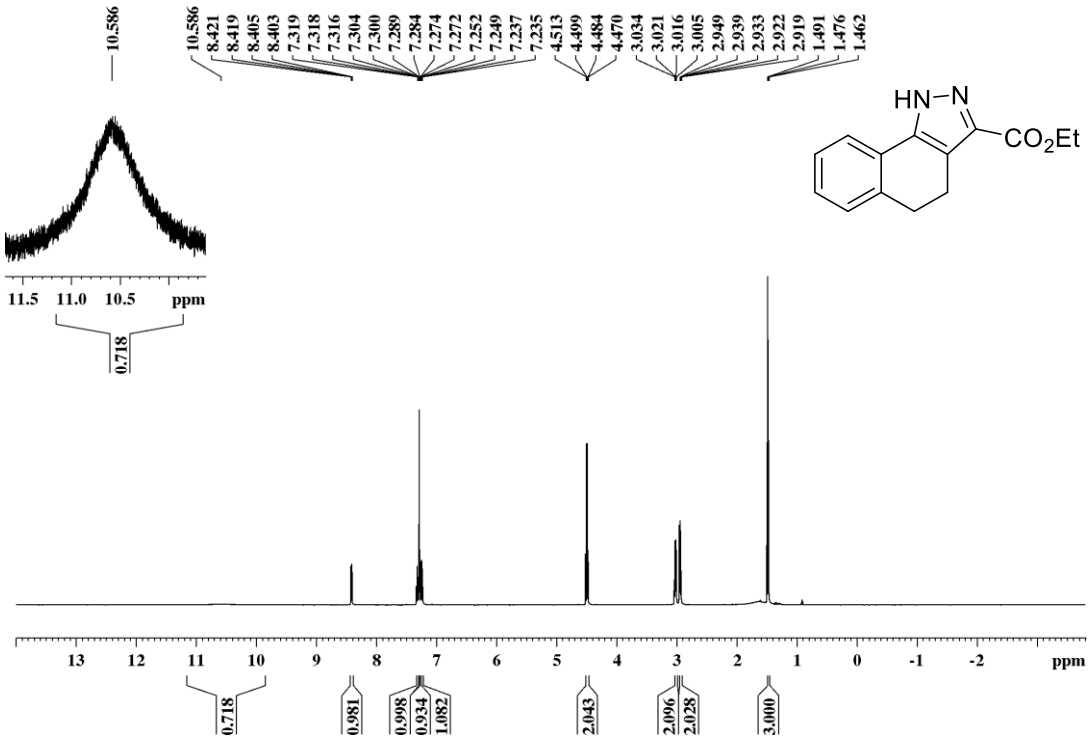

Figure S24. ^{1}H NMR spectrum of compound 3k

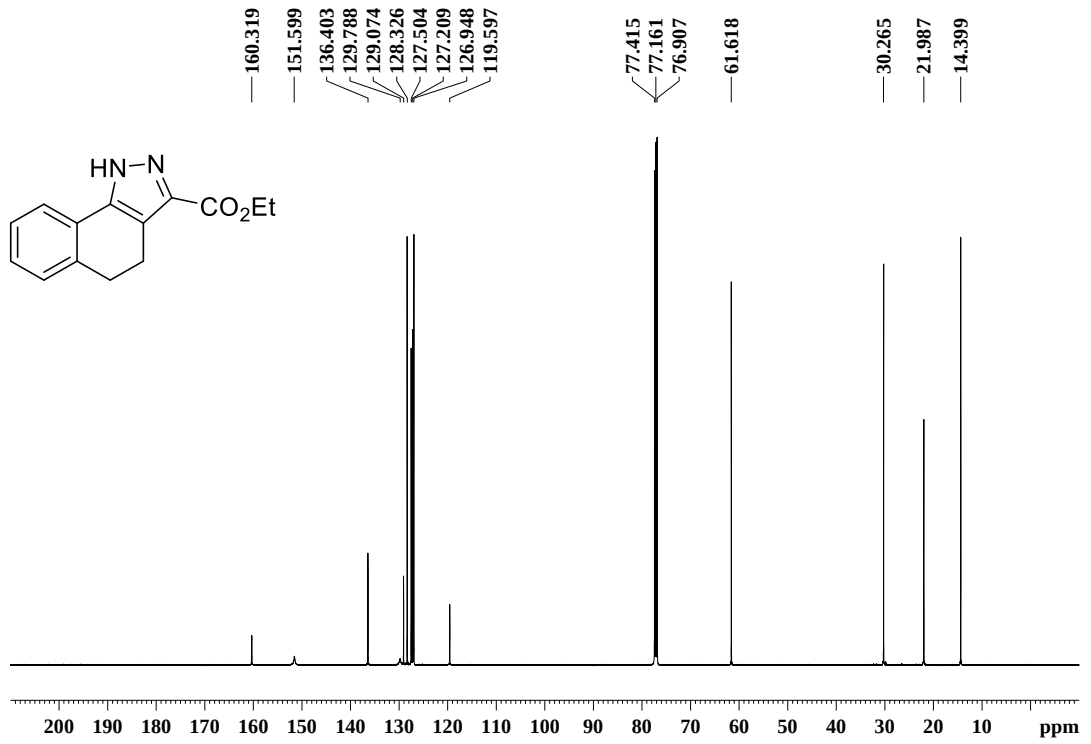

Figure S25. ^{13}C{^{1}H} NMR spectrum of compound 3k

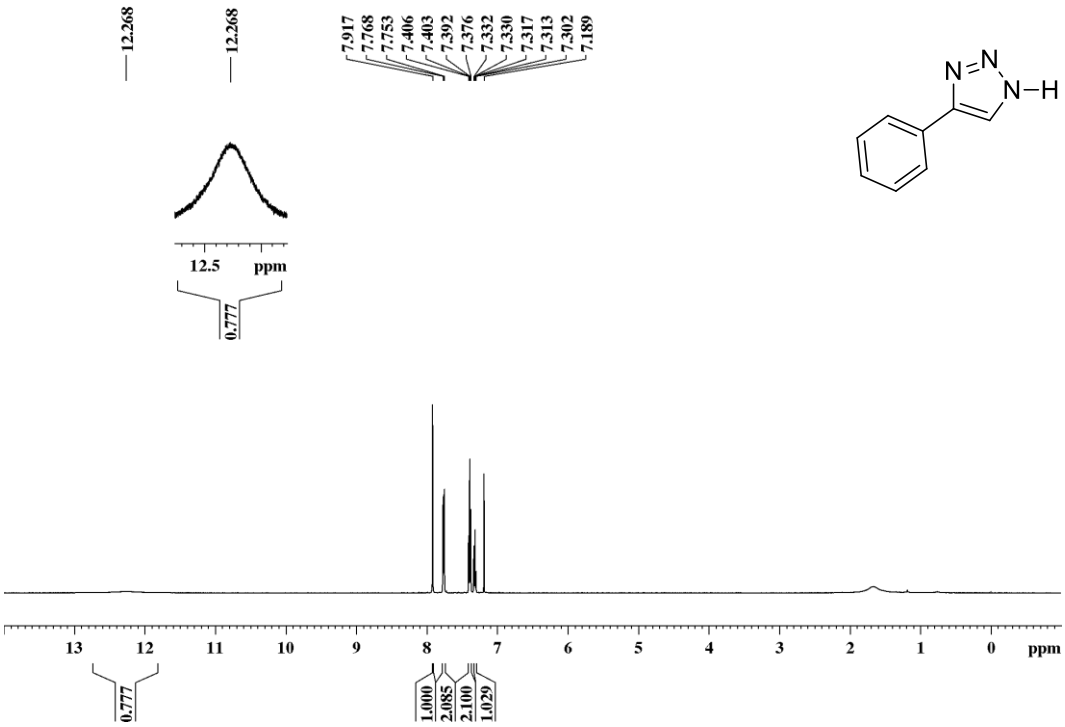

Figure S26. ^{1}H NMR spectrum of compound 5a

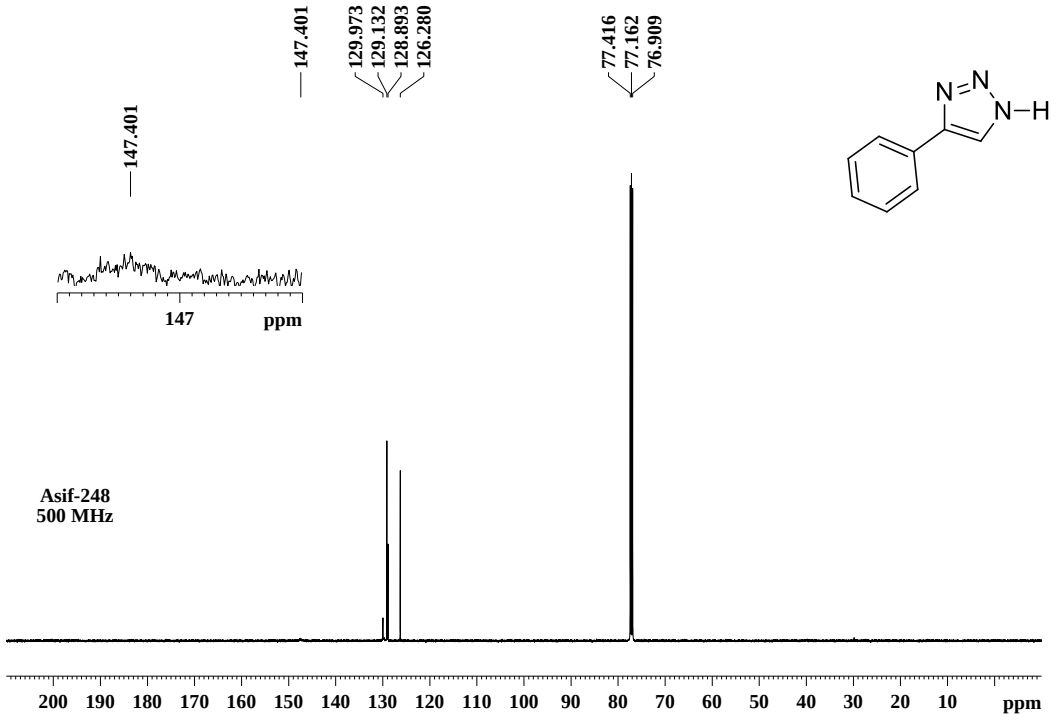

Figure S27. ^{13}C{^{1}H} NMR Spectrum of compound 5a

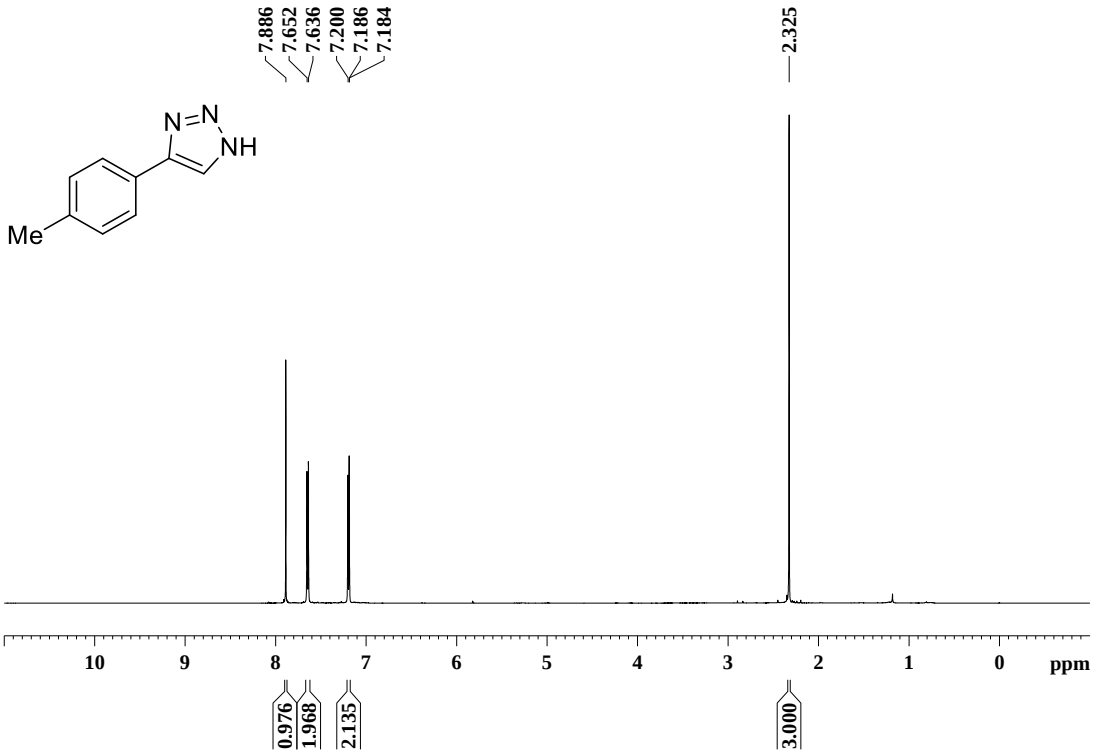

Figure S28. ^{1}H NMR spectrum of compound 5b

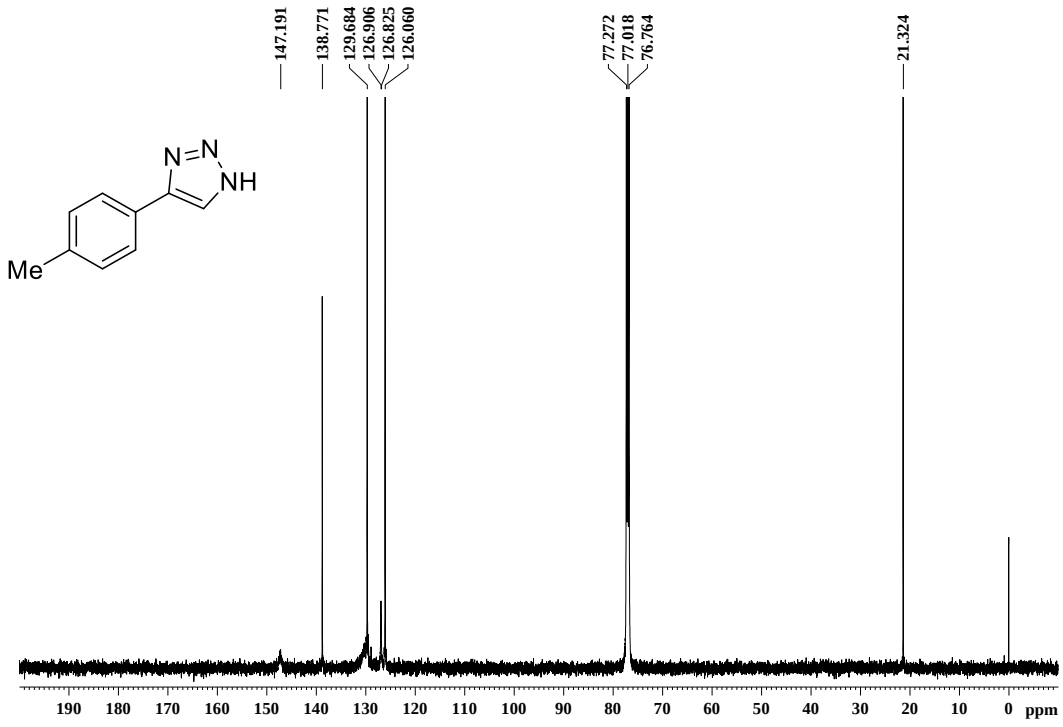

Figure S29. ^{13}C{^{1}H} NMR spectrum of compound 5b

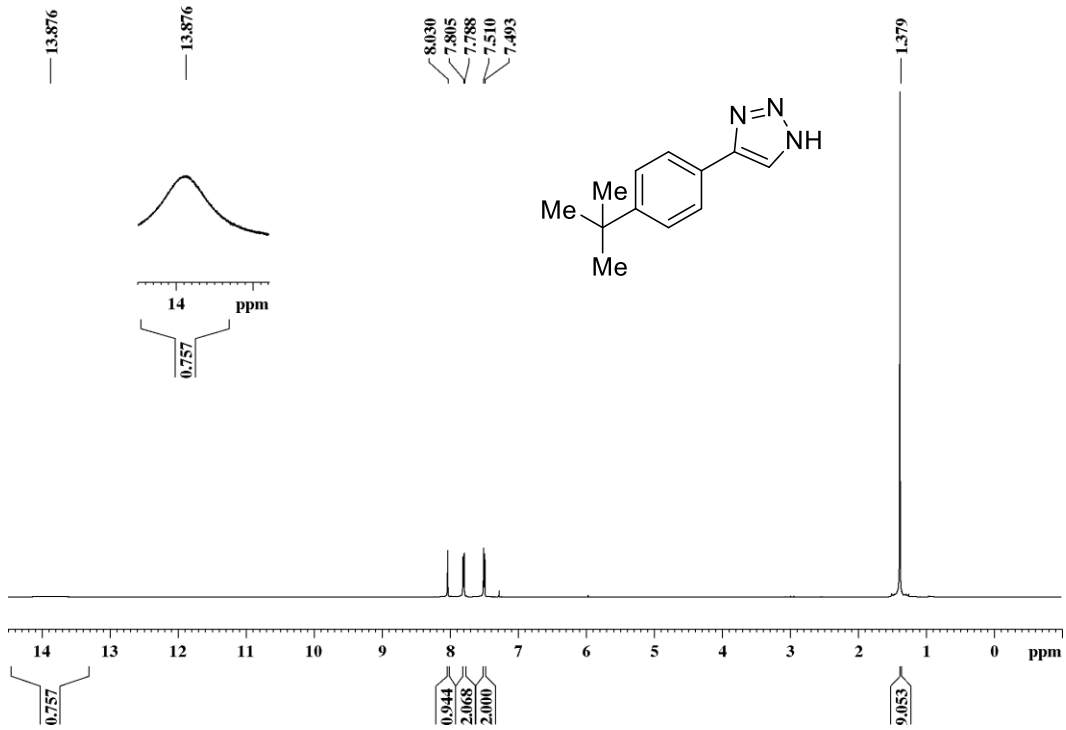

Figure S30. ^{1}H NMR spectrum of compound 5d

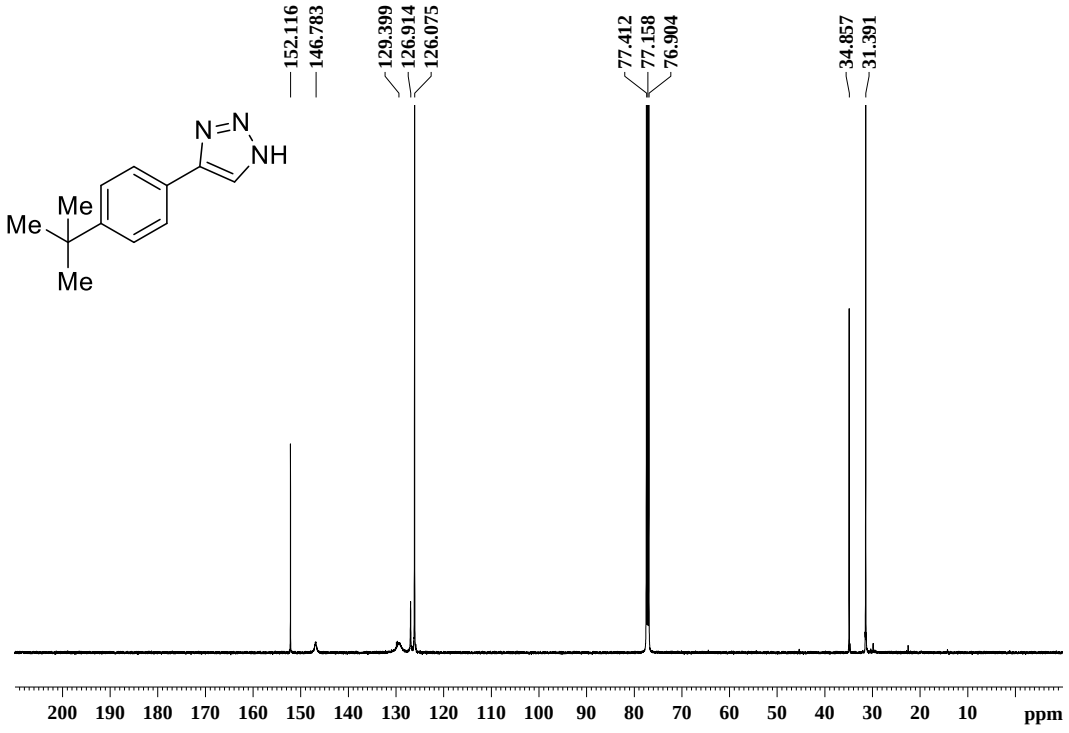

Figure S31. ^{13}C{^{1}H} NMR spectrum of compound 5d

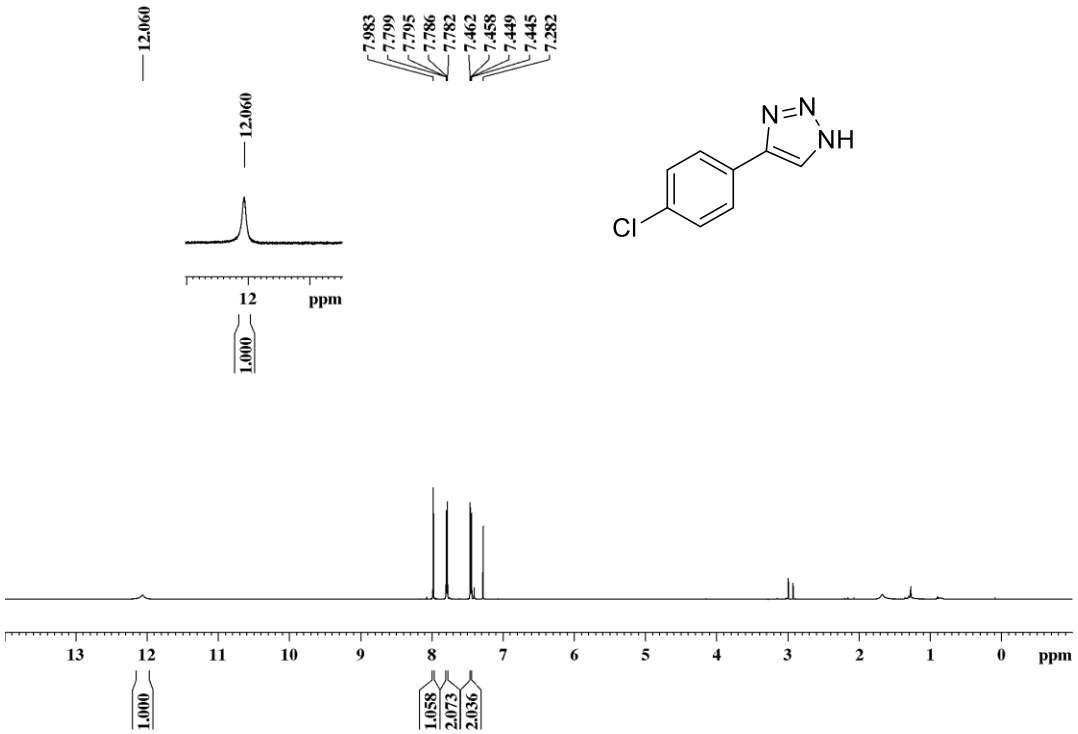

Figure S32. ^{1}H NMR spectrum of compound 5e

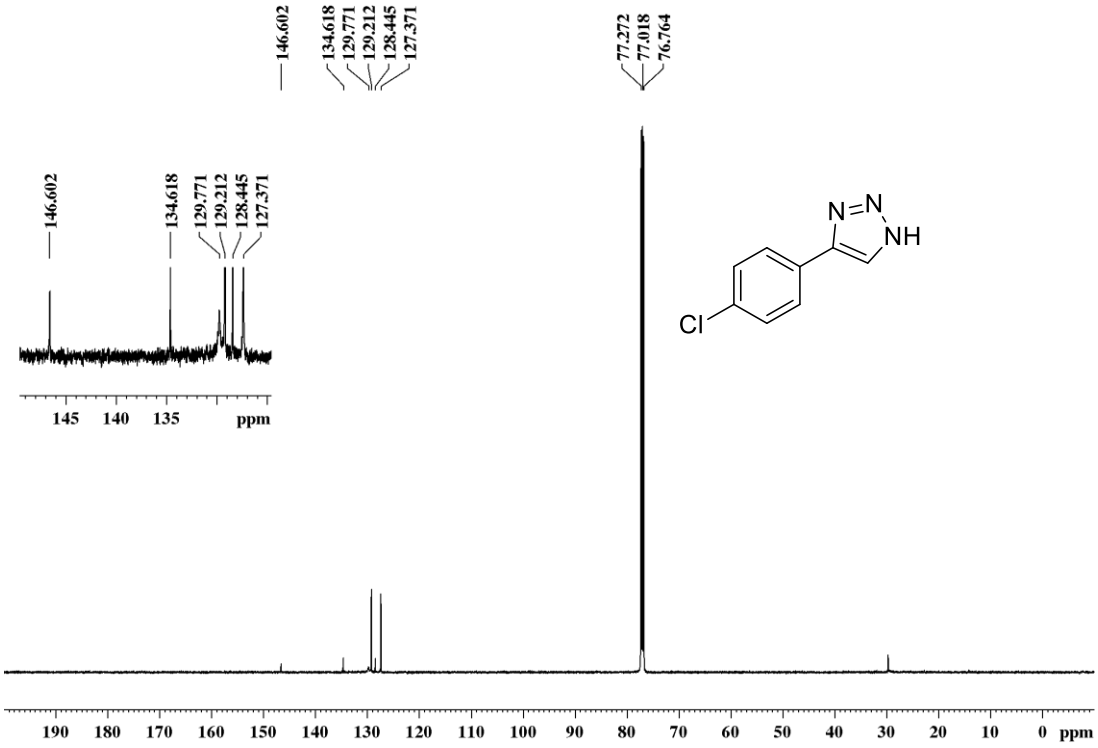

Figure S33. ^{13}C{^{1}H} NMR spectrum of compound 5e

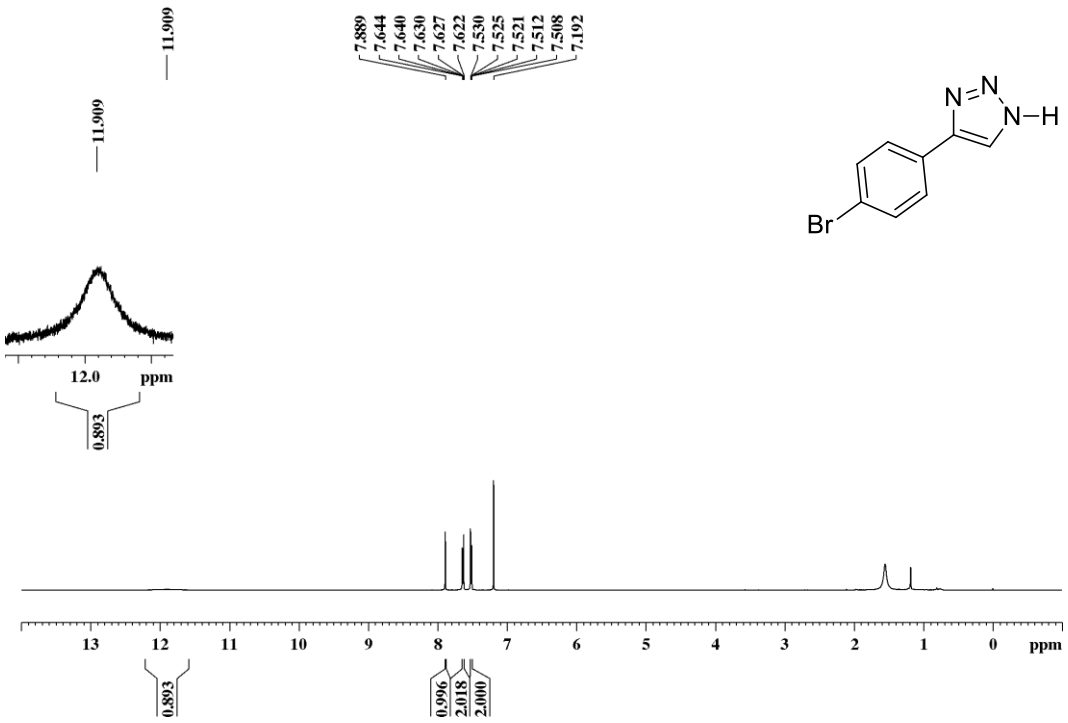

Figure S34. ^{1}H NMR Spectrum of compound 5g

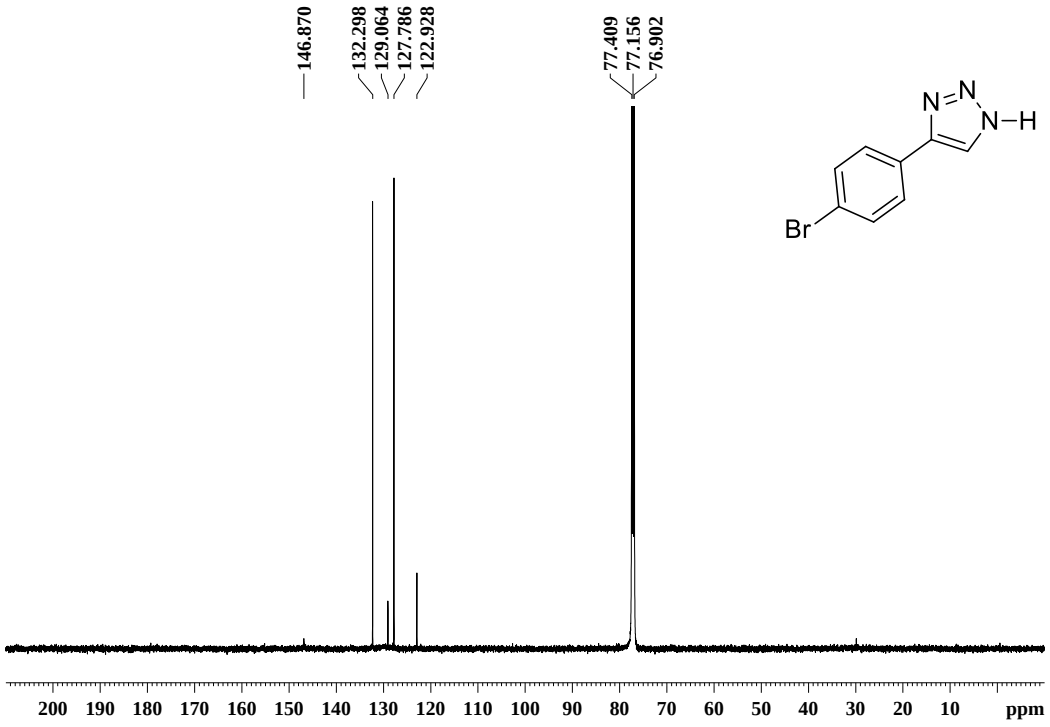

Figure S35. ^{13}C{^{1}H} NMR Spectrum of compound 5g

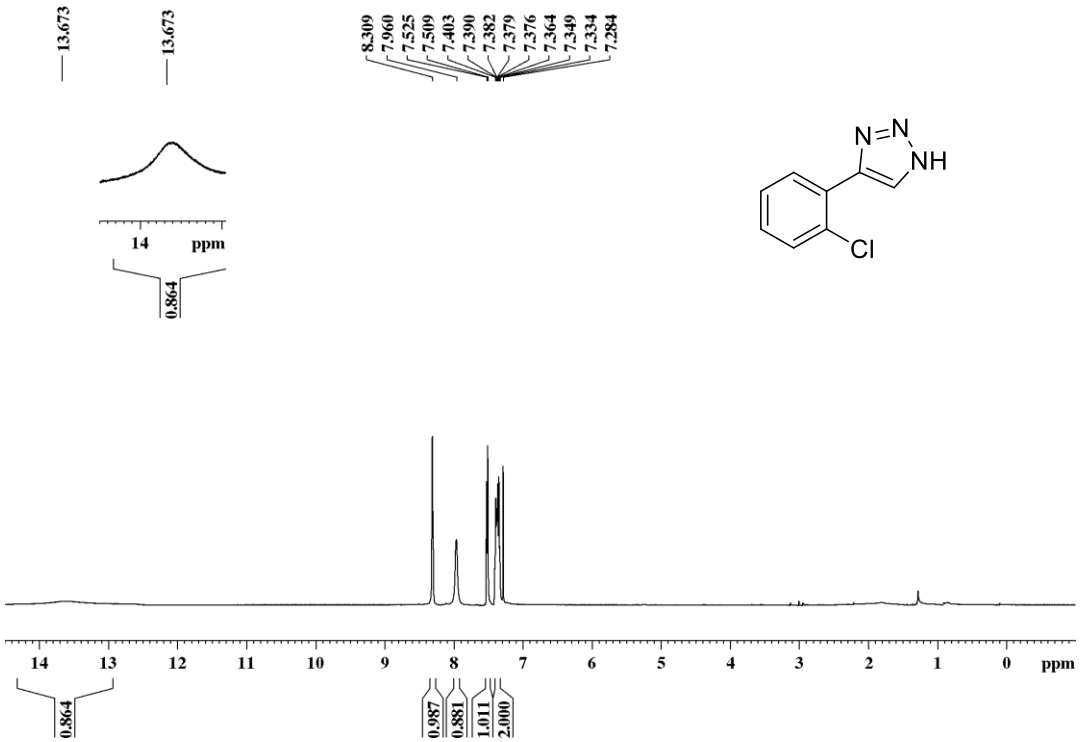

Figure S36. ^{1}H NMR spectrum of compound 5h

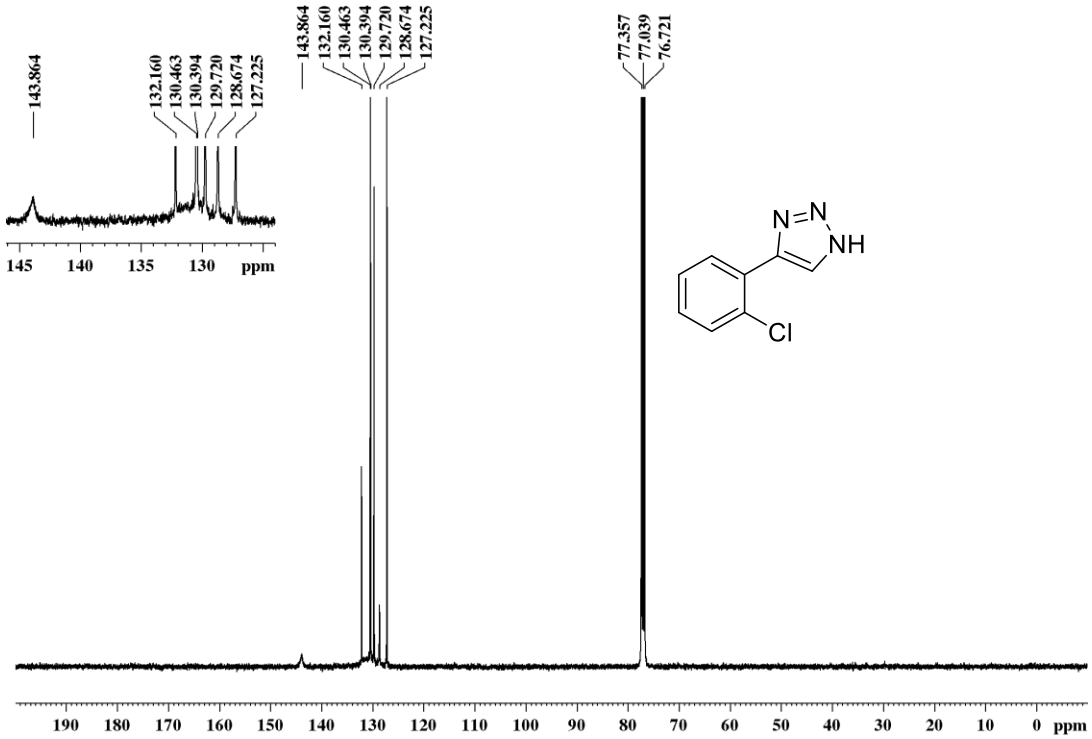

Figure S37. ^{13}C{^{1}H} NMR spectrum of compound 5h

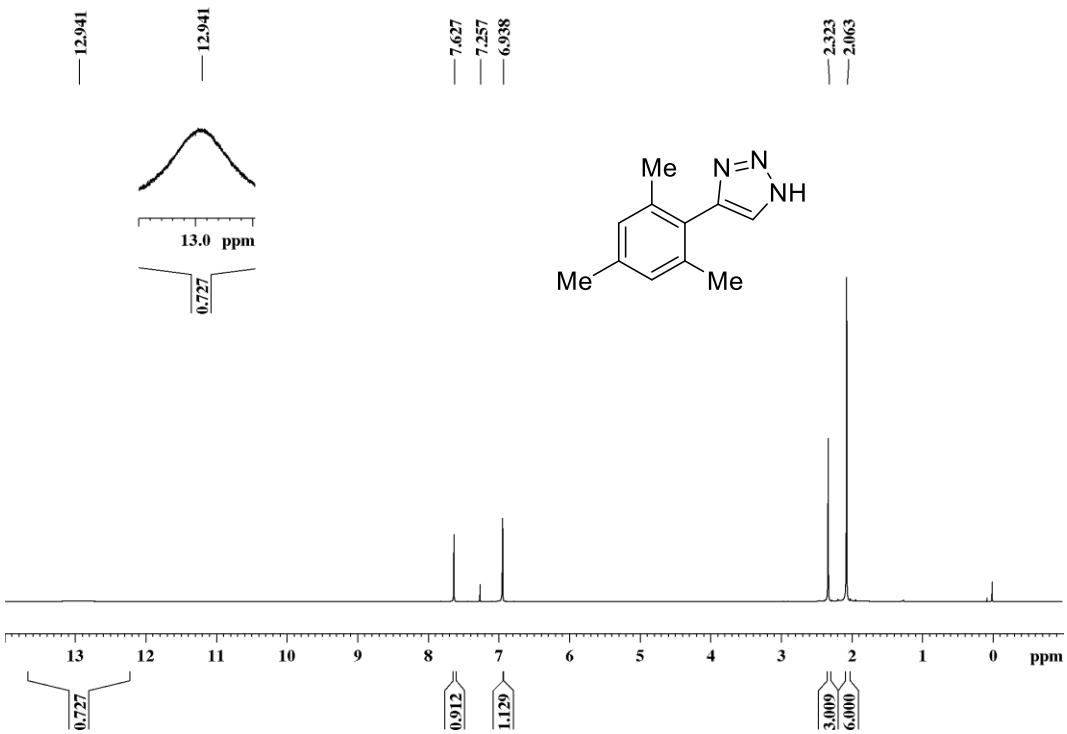

Figure S38. ^{1}H NMR spectrum of compound 5i

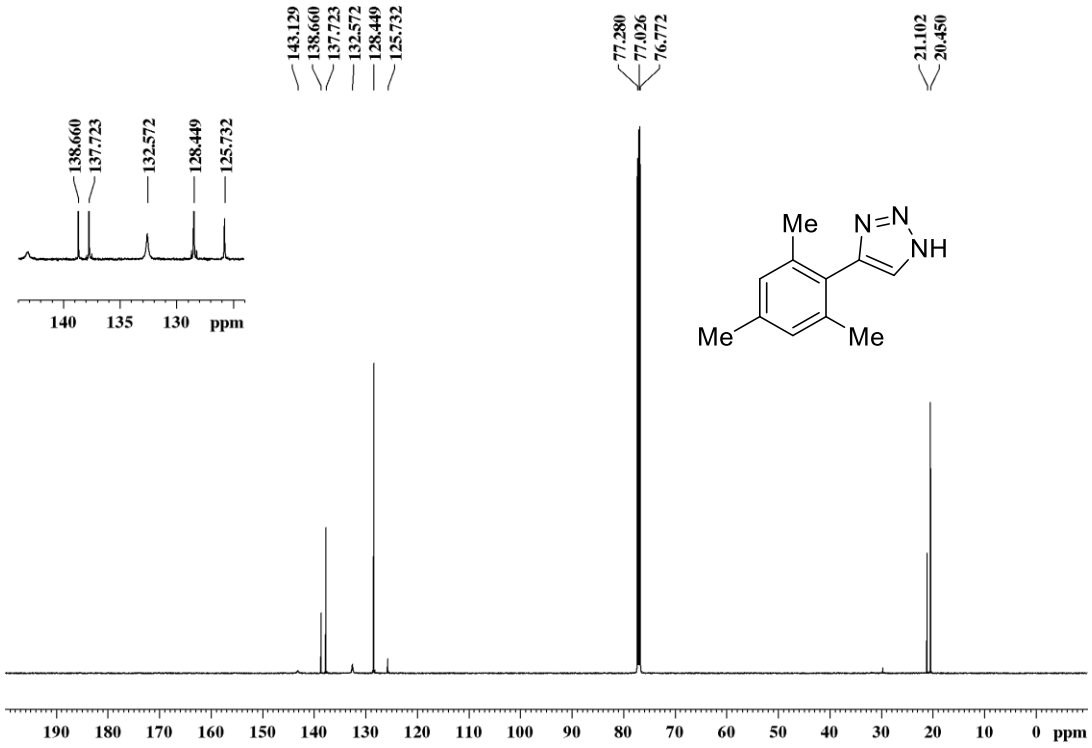

Figure S39. ^{13}C{^{1}H} NMR spectrum of compound 5i

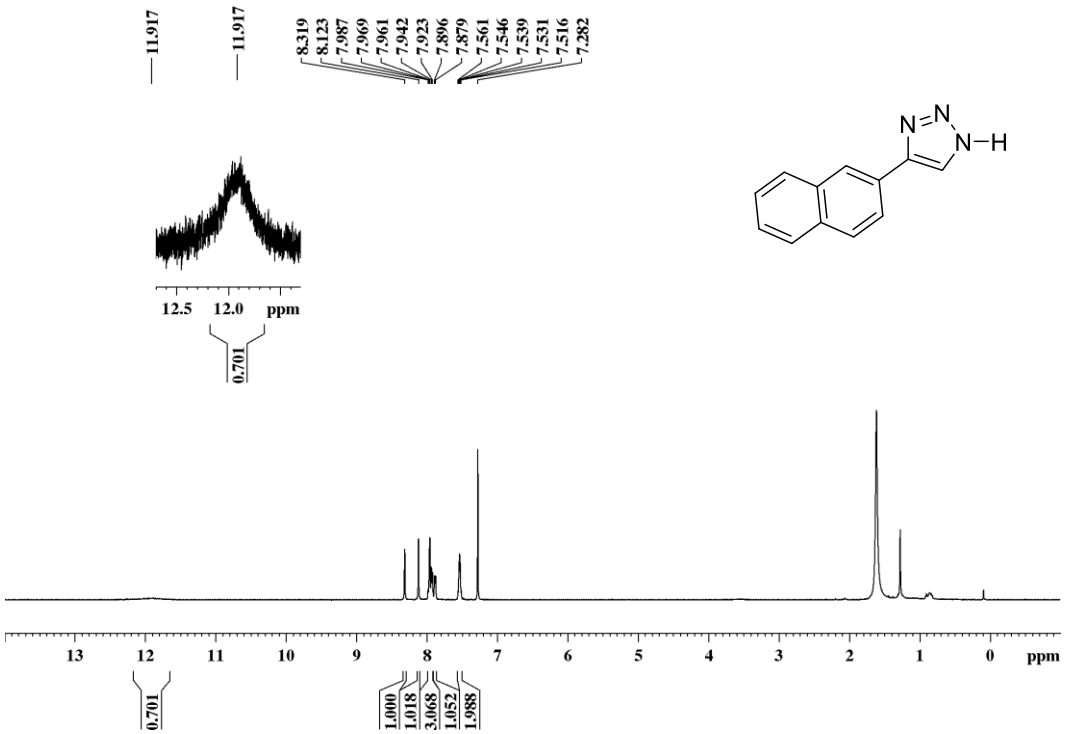

Figure S40. ^{1}H NMR spectrum of compound 5j

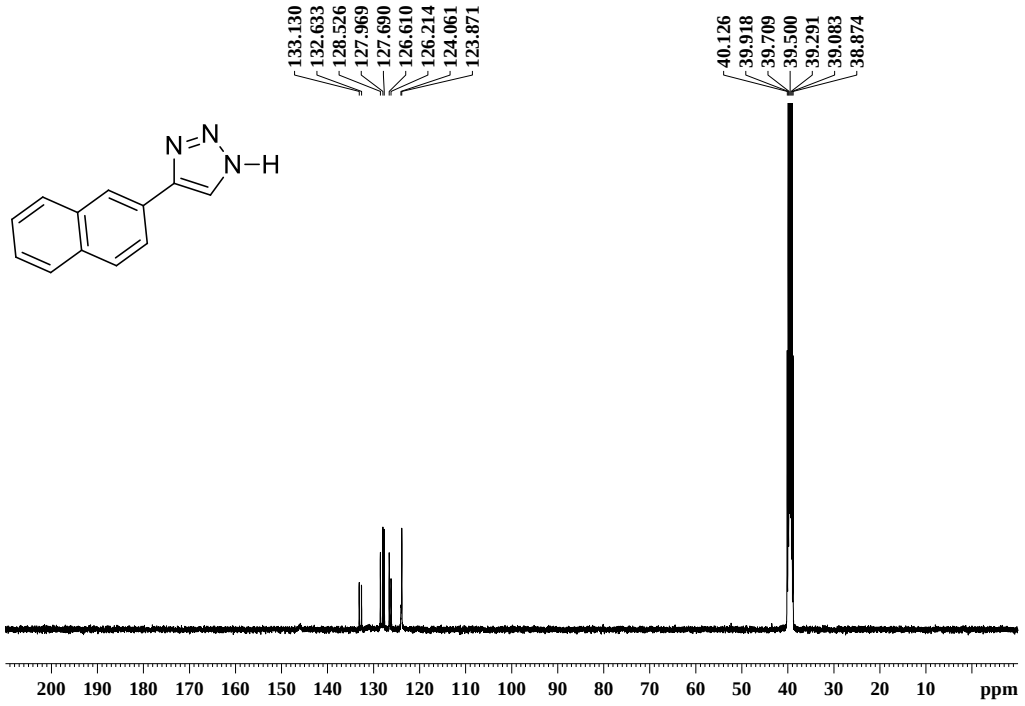

Figure S41. ^{13}C{^{1}H} NMR spectrum of compound 5j

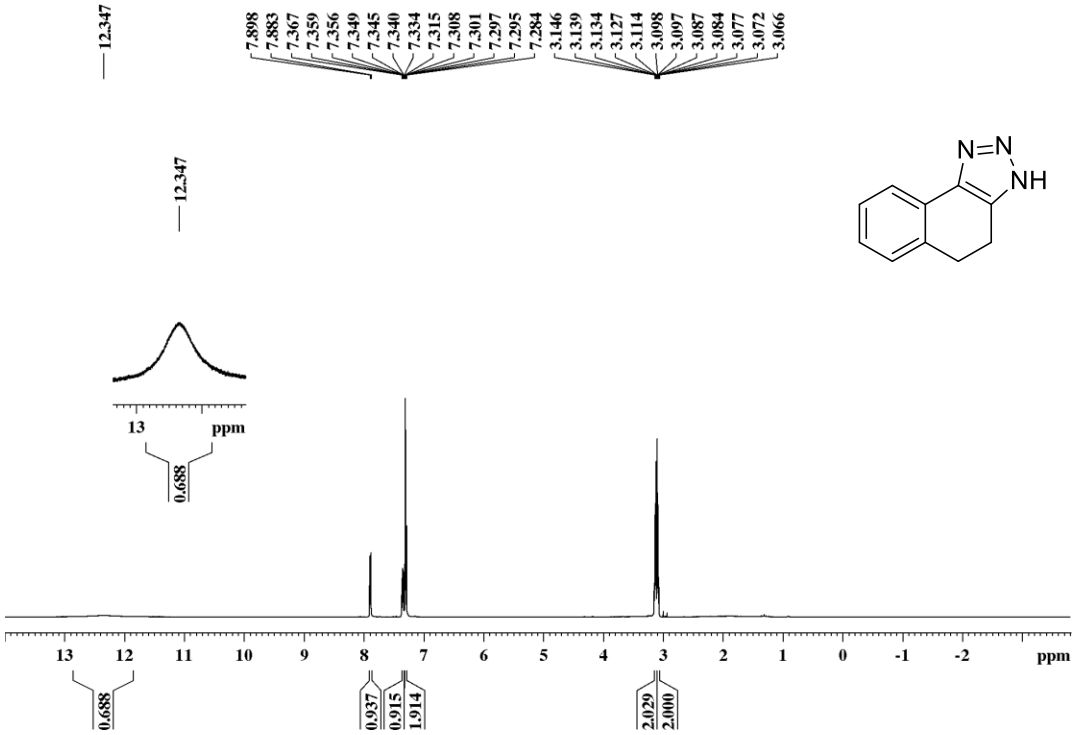

Figure S42. ^{1}H NMR spectrum of compound 5k

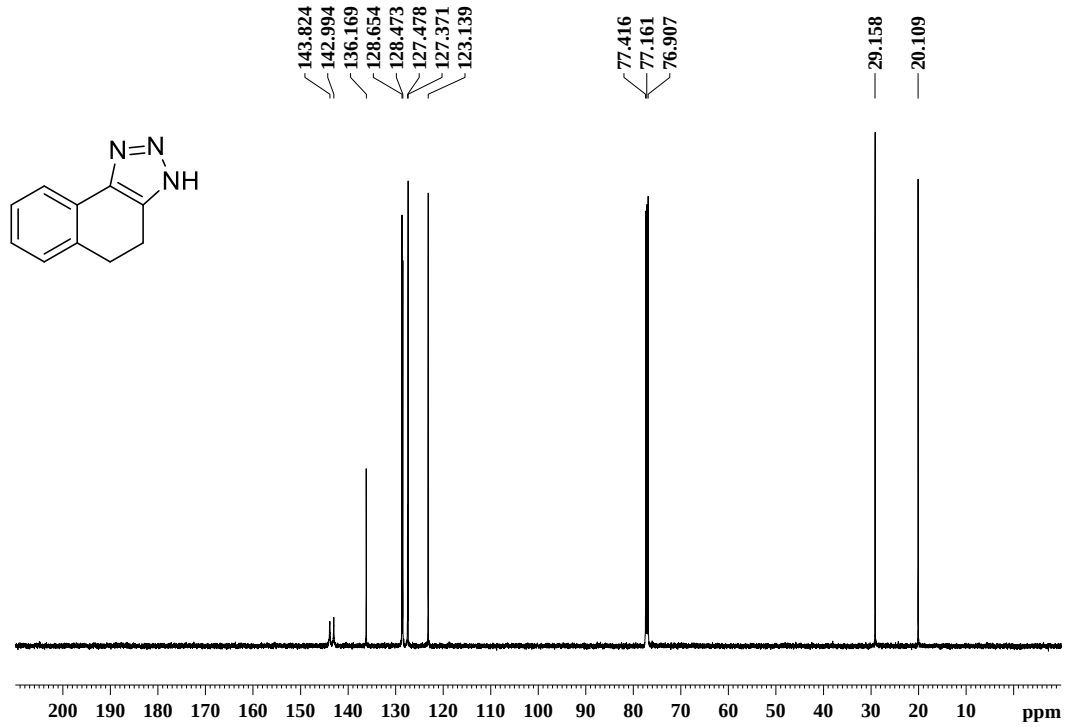

Figure S43. ^{13}C{^{1}H} NMR spectrum of compound 5k

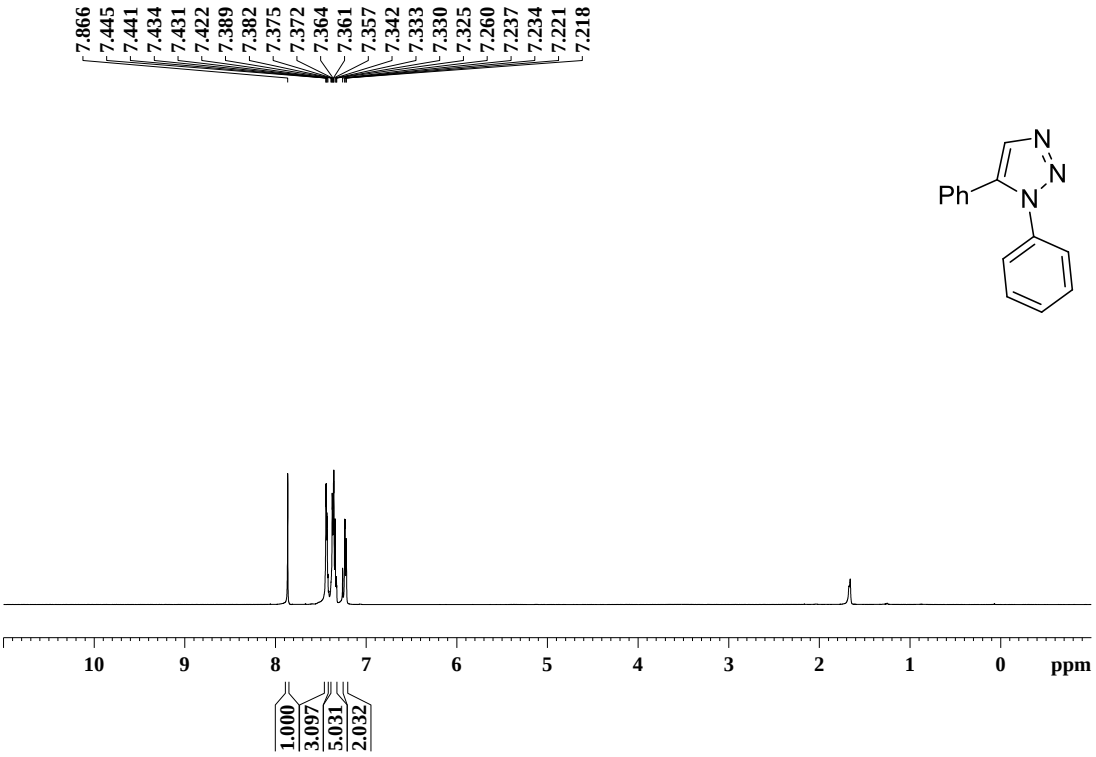

Figure S44. ^{1}H NMR spectrum of compound 7aa

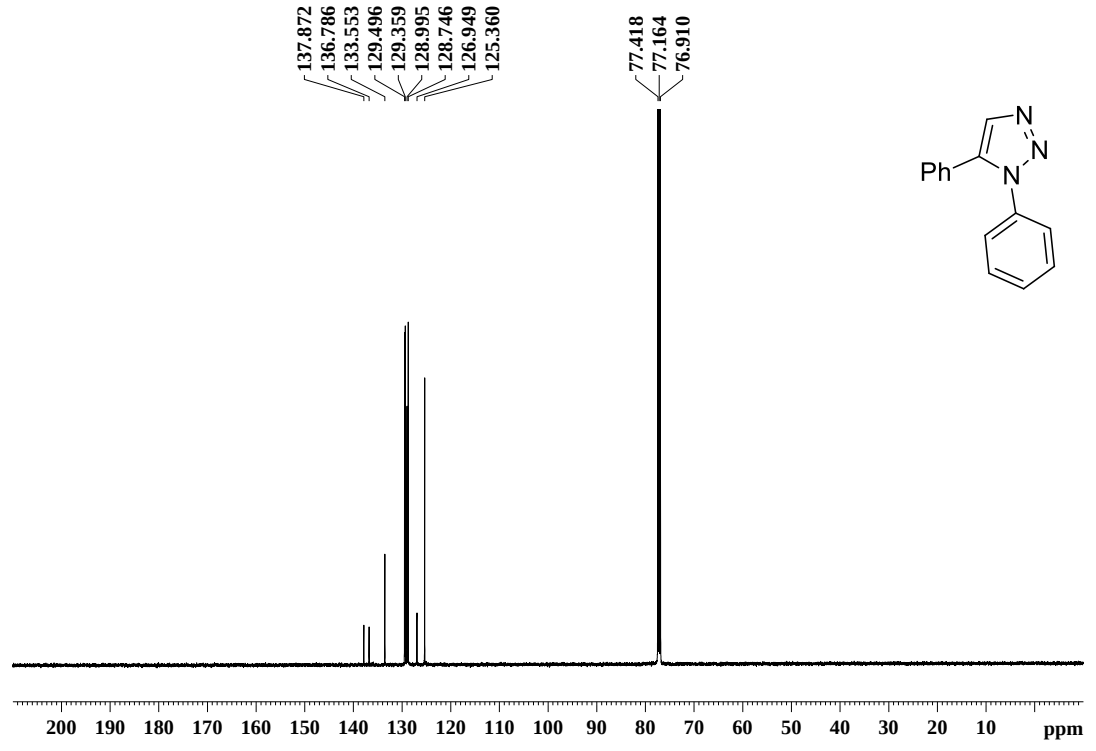

Figure S45. ^{13}C{^{1}H} NMR spectrum of compound 7aa

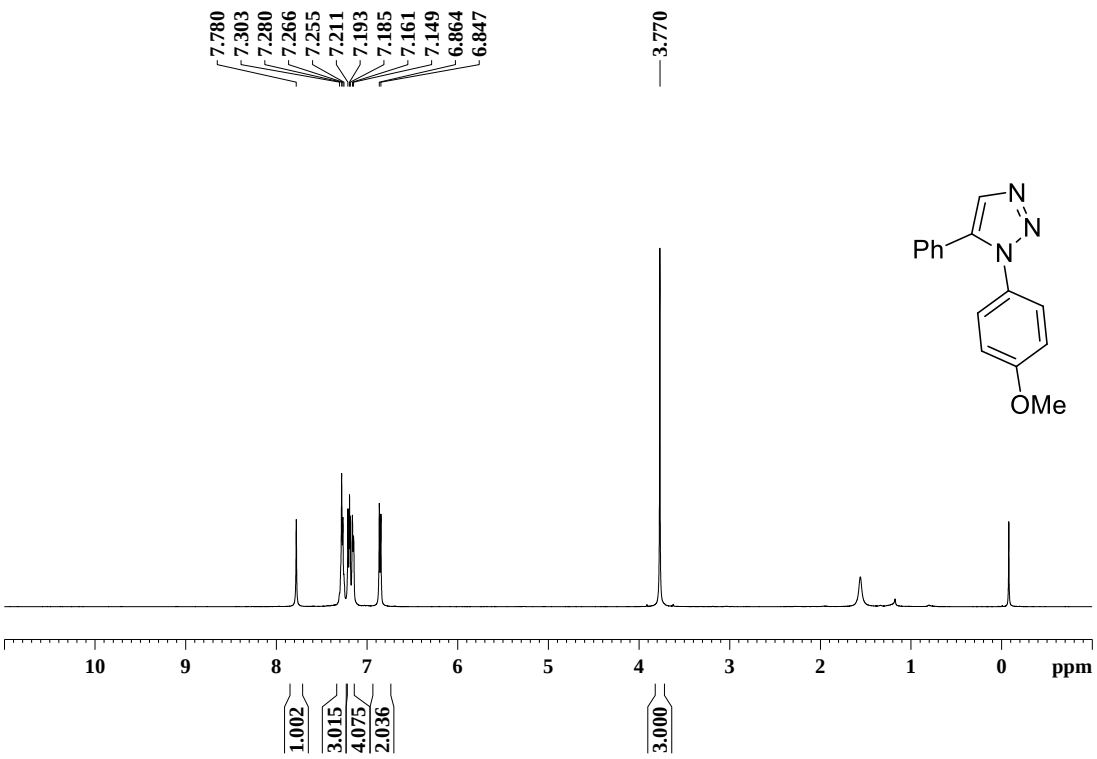

Figure S46. ^{1}H NMR spectrum of compound 7ab

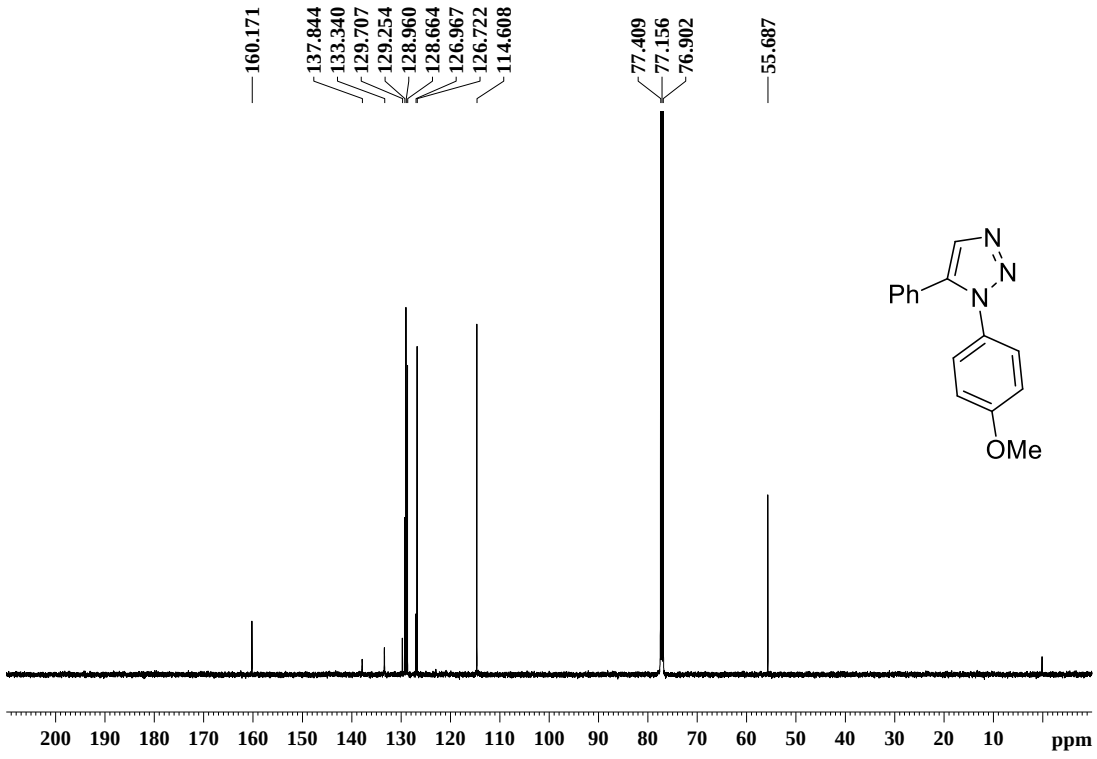

Figure S47. ^{13}C{^{1}H} NMR spectrum of compound 7ab

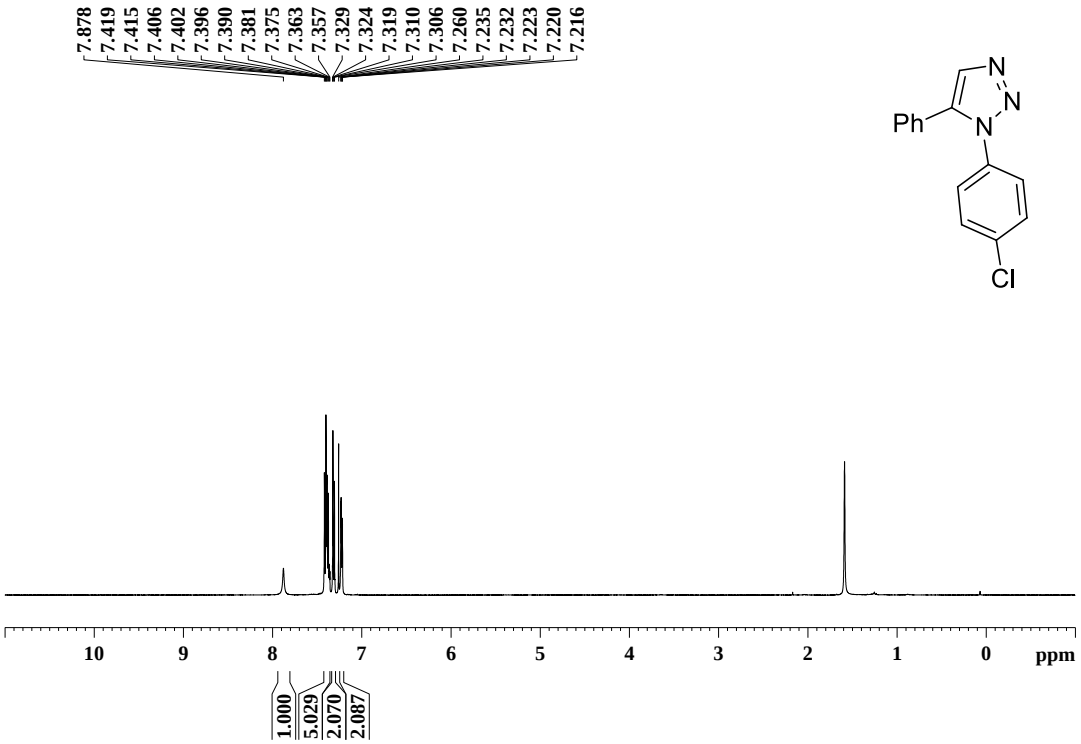

Figure S48. ^{1}H NMR spectrum of compound 7ac

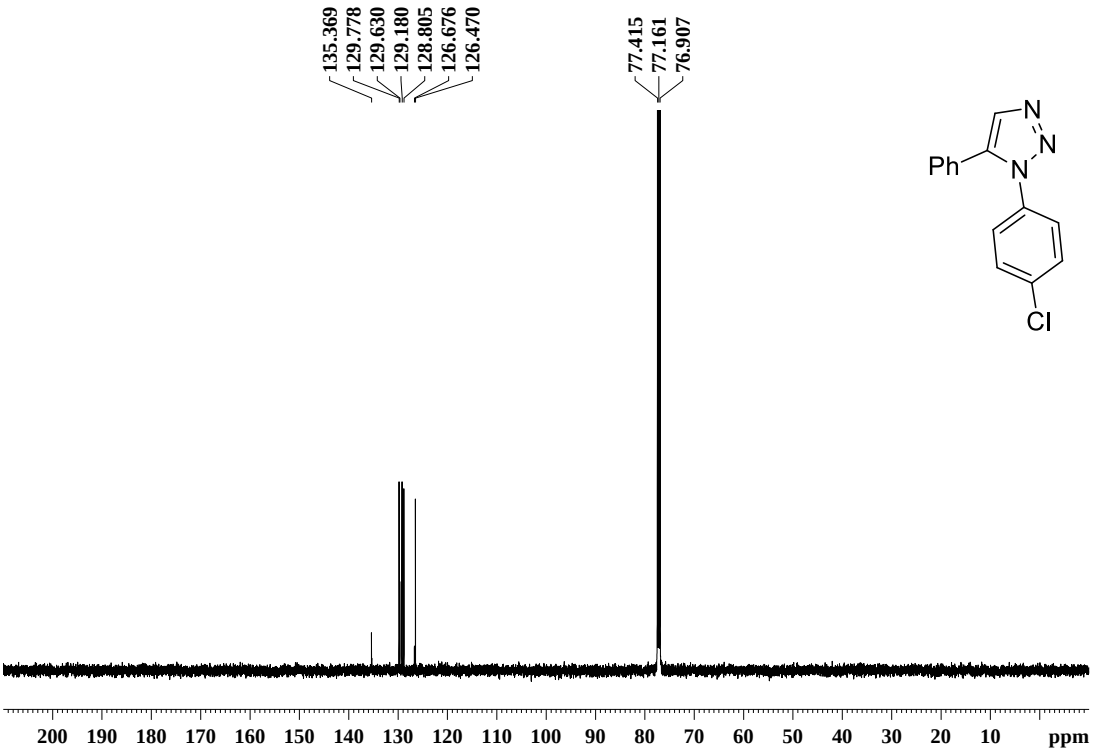

Figure S49. ^{13}C{^{1}H} NMR spectrum of compound 7ac

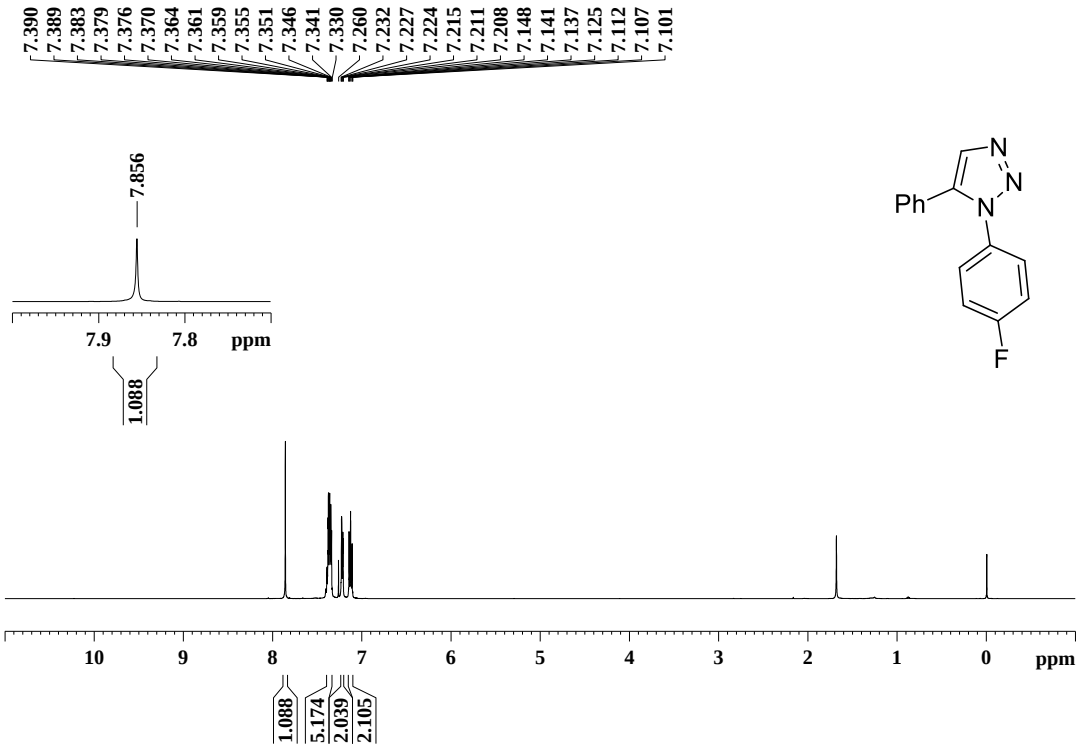

Figure S50. ^{1}H NMR spectrum of compound 7ad

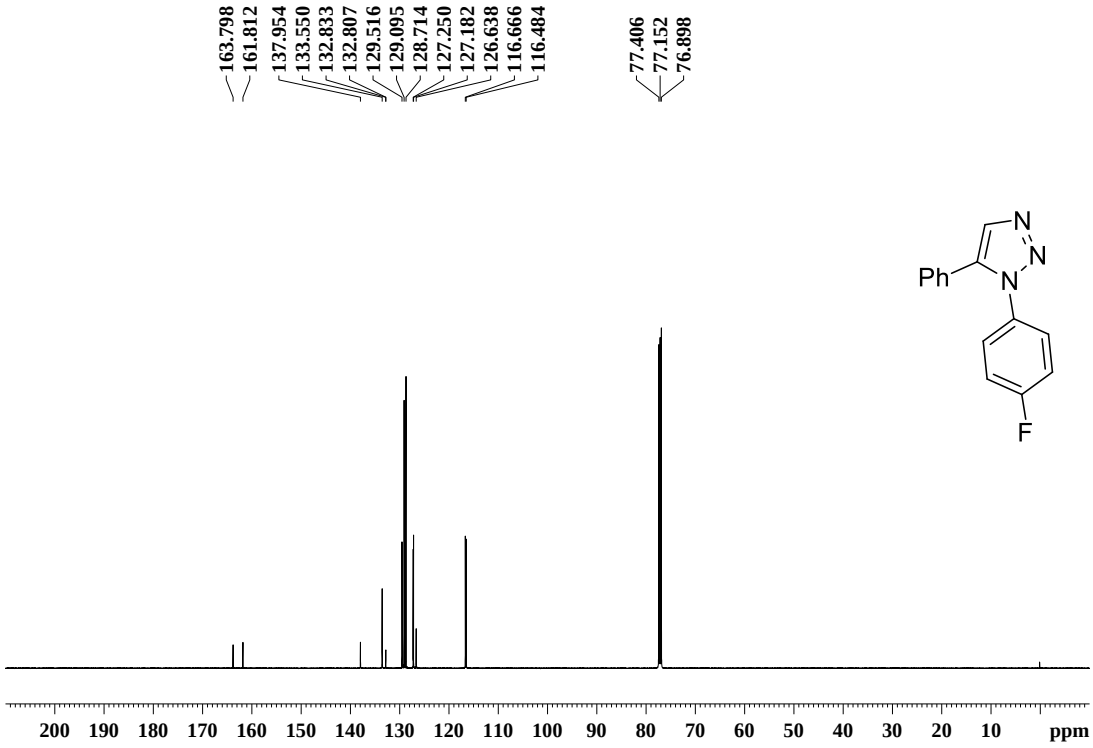

Figure S51. ^{13}C{^{1}H} NMR spectrum of compound 7ad

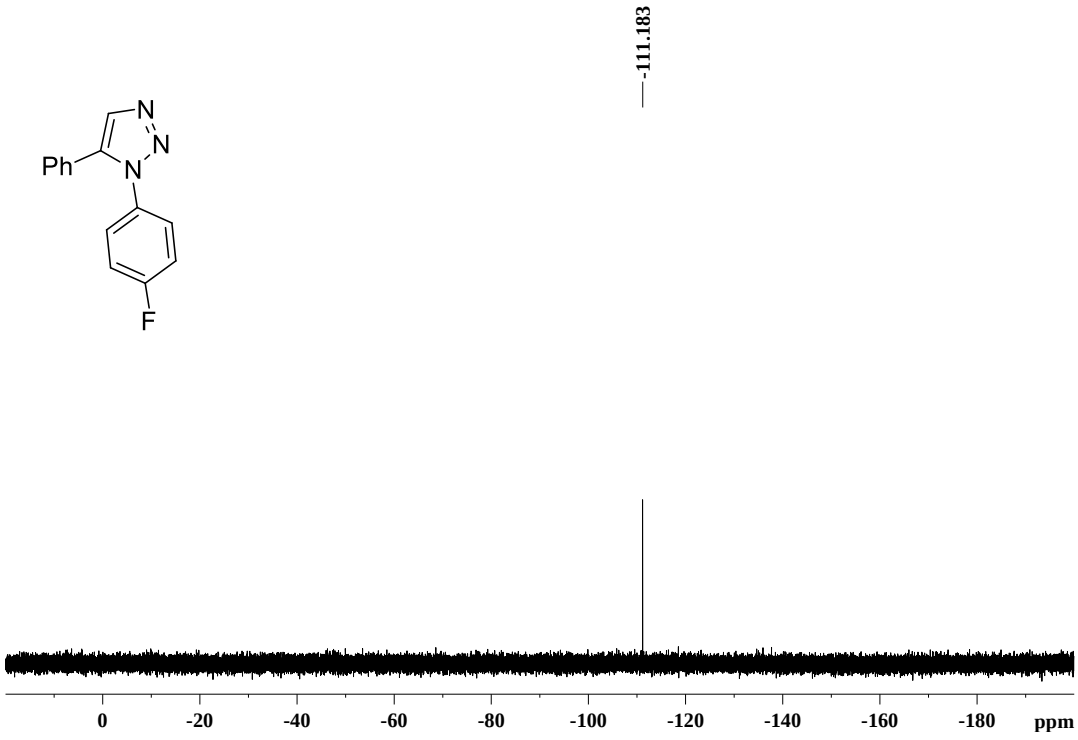

Figure S52. $^{19}F\{^{1}H\}$ NMR spectrum of compound 7ad

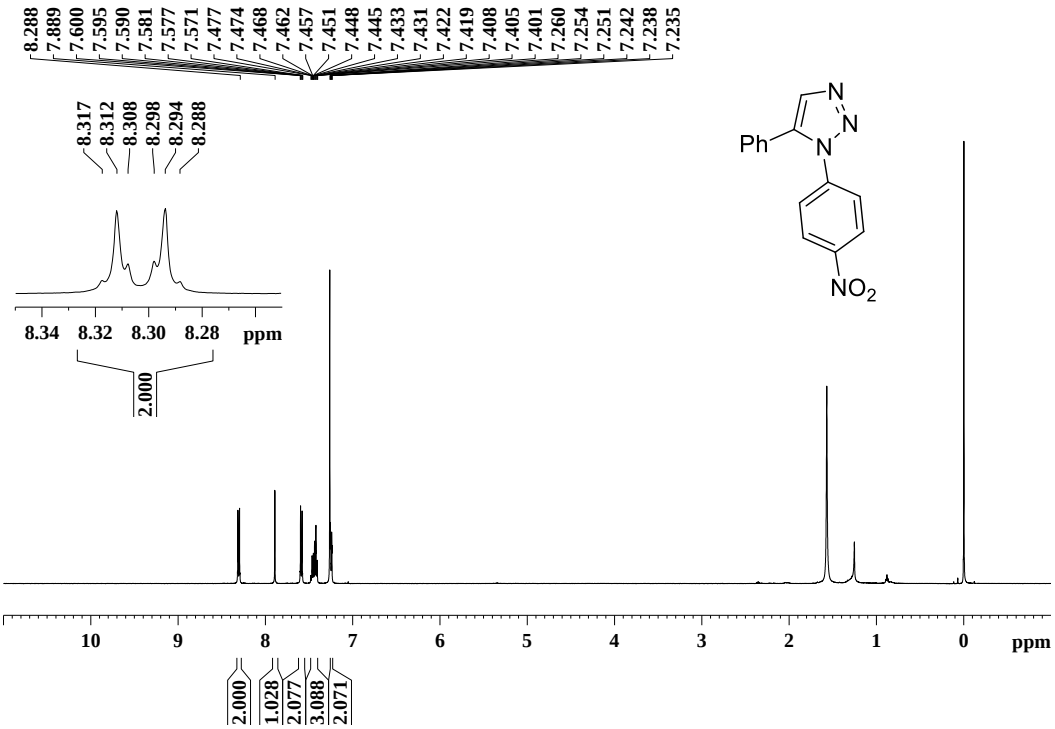

Figure S53. ^{1}H NMR spectrum of compound 7ae

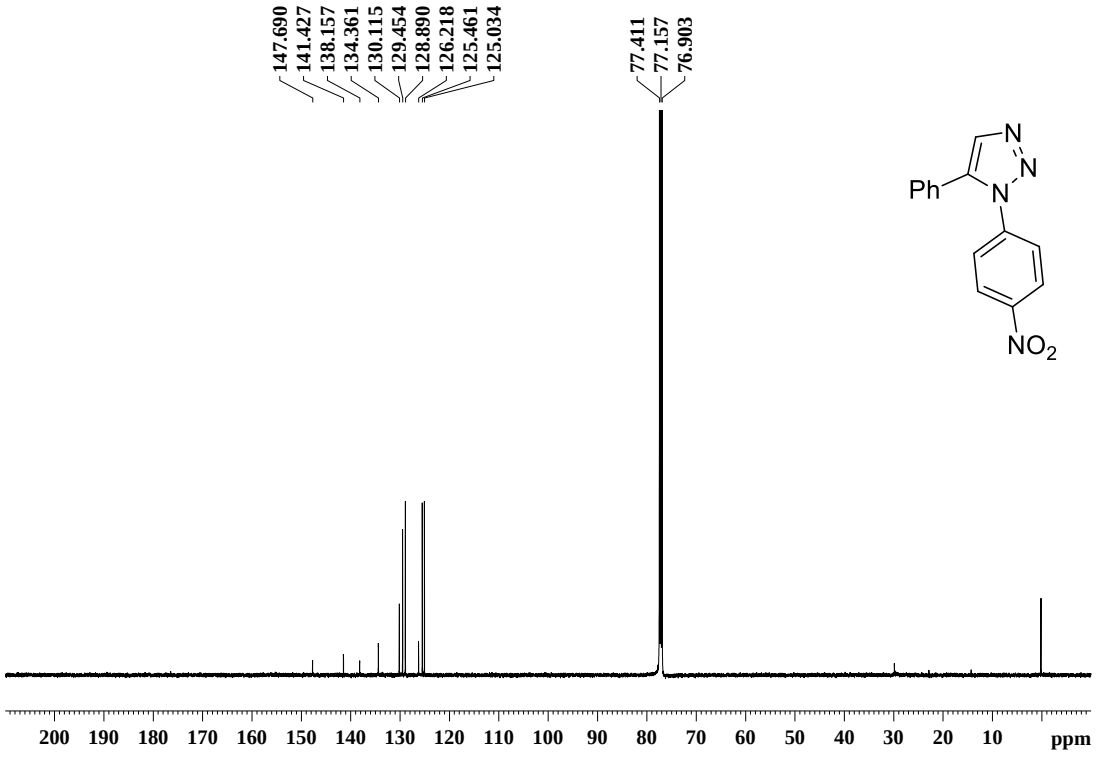

Figure S54. ^{13}C{^{1}H} NMR spectrum of compound 7ae

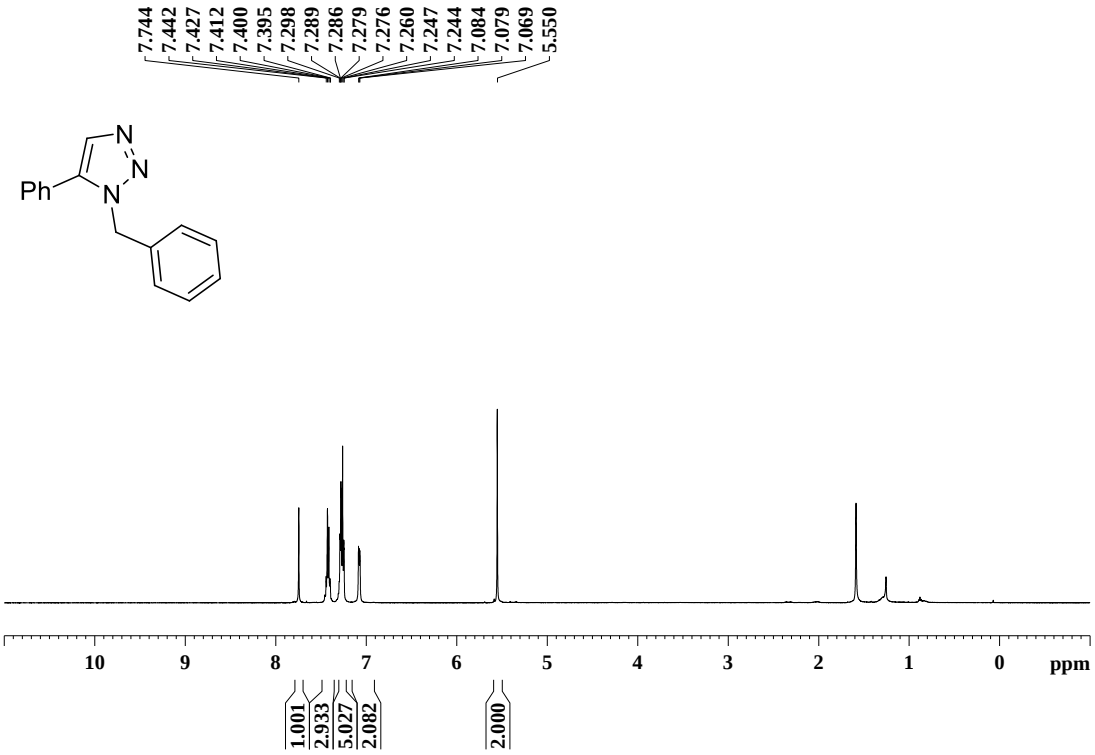

Figure S55. ^{1}H NMR spectrum of compound 7af

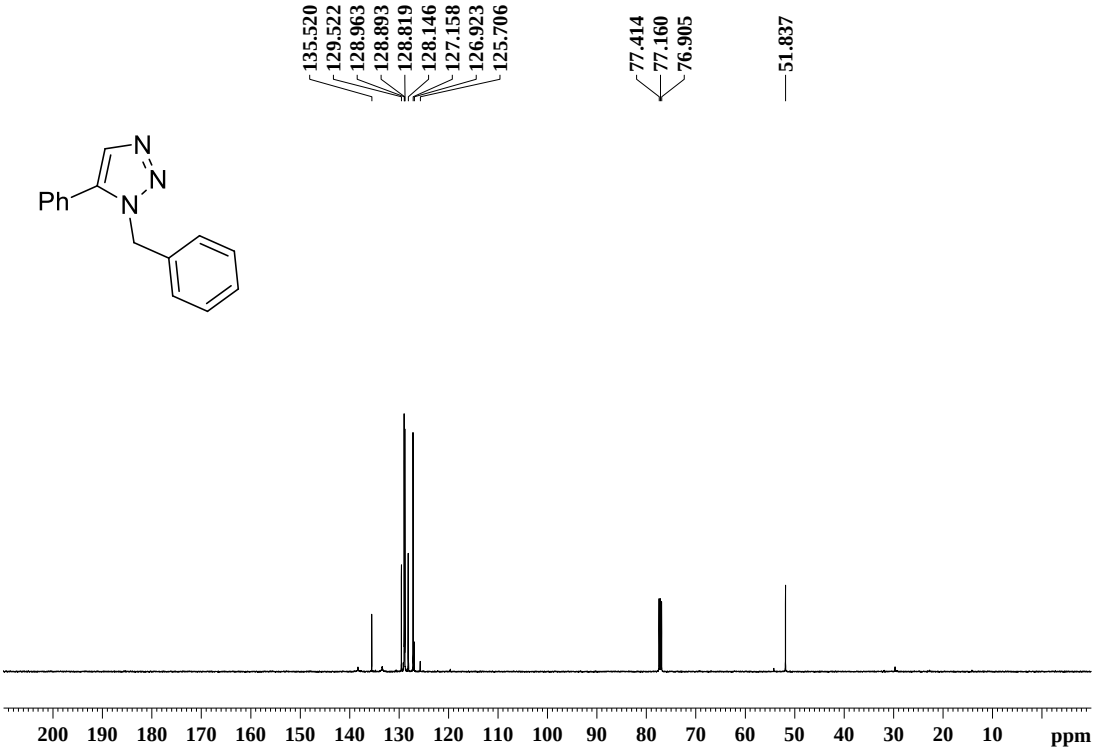

Figure S56. ^{13}C{^{1}H} NMR spectrum of compound 7af

Reference:

1. (a) Sheldrick, G. M. SADABS, Siemens Area Detector Absorption Correction, University of Gottingen, Germany, 1996; (b) Sheldrick, G. M. SHELX97- A program for crystal structure solution and refinement, University of Gottingen, 1997; (c) Sheldrick, G. M. SHELXTL NT Crystal Structure Analysis Package, Bruker AXS, Analytical X-ray System, WI, USA, 1999, version 5.10.