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Supplementary Information

A Novel Approach for the Synthesis of 5-Substituted-1*H*-tetrazoles

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Experimental

General

The products were purified by column chromatography. The purity determinations of the products were accomplished by TLC on silica gel polygram STL G/UV 254 plates. The melting points of products were determined with an Electrothermal Type 9100 melting point apparatus. The FT-IR spectra were recorded on an Avatar 370 FT-IR Therma Nicolet spectrometer. The NMR spectra were provided on a Brucker Avance 100 and 400 MHz instrument in DMSO. All of the products were known compounds and characterized by the IR, ^{1}H NMR and ^{13}C NMR spectra and comparison of their melting points with known compounds. Elemental analyses were performed using a Elementar, Vario EL III and Thermofinnigan Flash EA 1112 Series instrument. Mass spectra were recorded with Shimadzu GC-MS-QP5050A and Aglien Technology (HP) 5973 Network Mass Selective Detector instruments at 70 eV; in *m/z* (rel %).

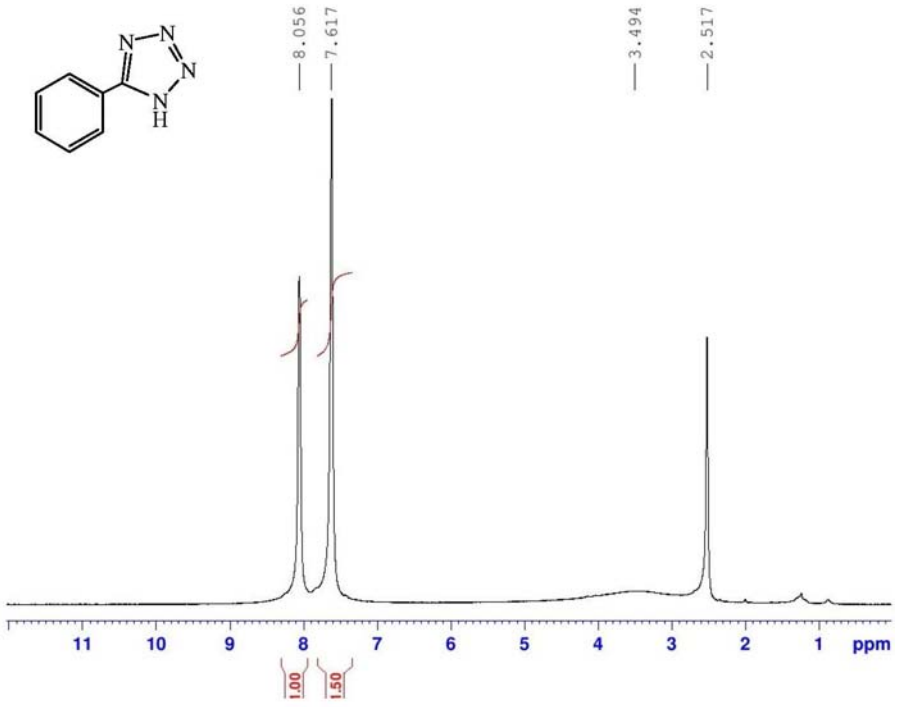

Figure S1. ^{1}H NMR (400 MHz, DMSO-d_6) of 5-phenyl-1*H*-tetrazole (**1**).

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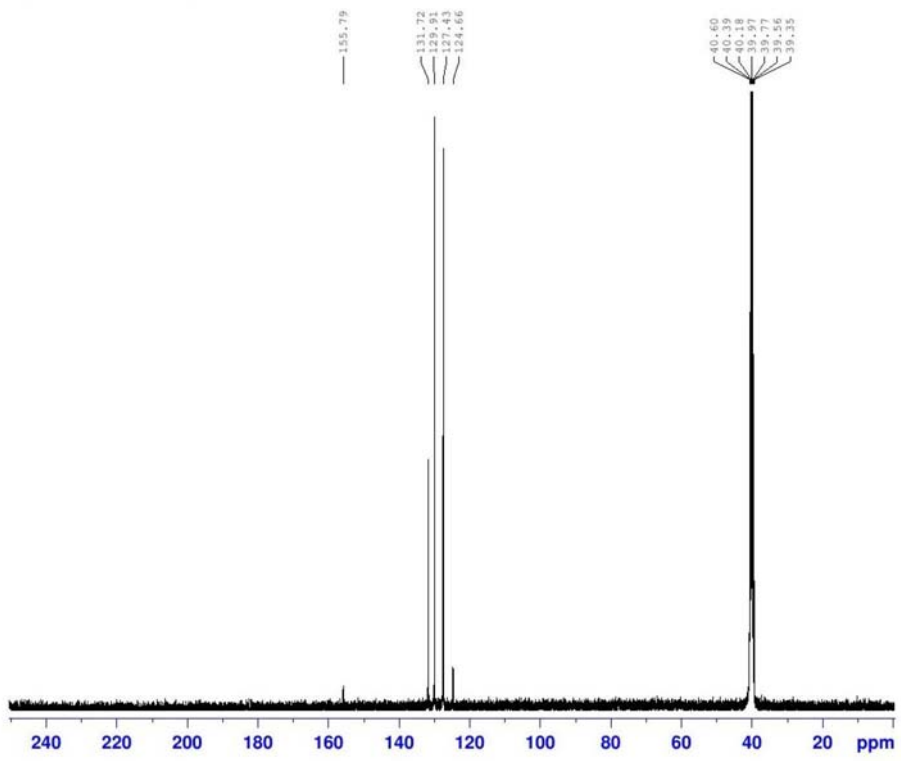

Figure S2. ^{13}C NMR (100 MHz, DMSO-d_6) of 5-phenyl-1*H*-tetrazole (**1**).

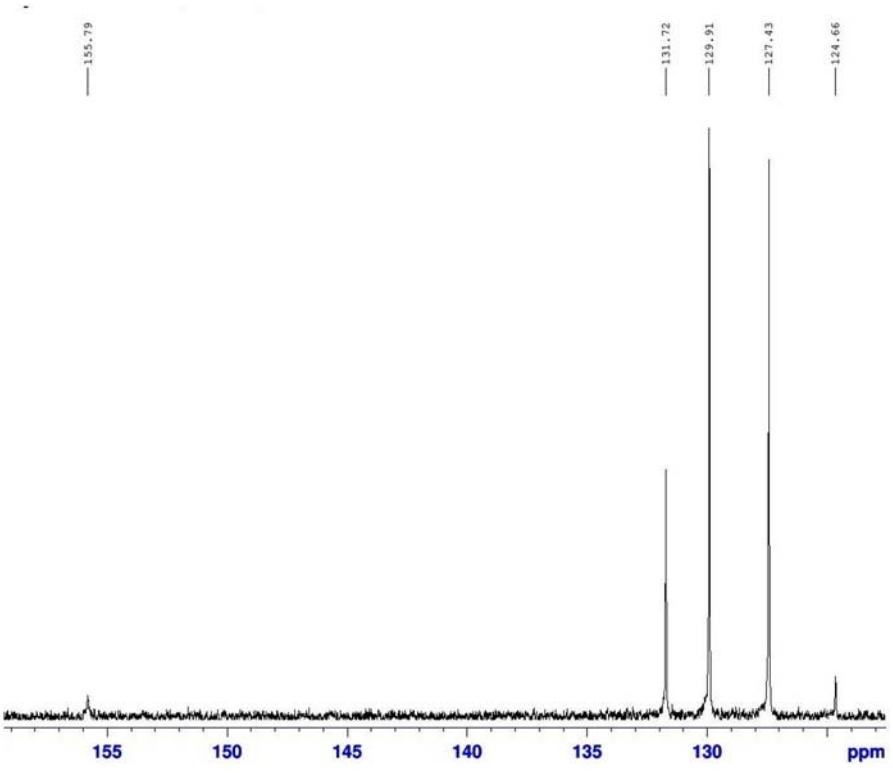

Figure S3. ^{13}C NMR (100 MHz, DMSO-d_6) of 5-phenyl-1*H*-tetrazole (**1**) expanded.

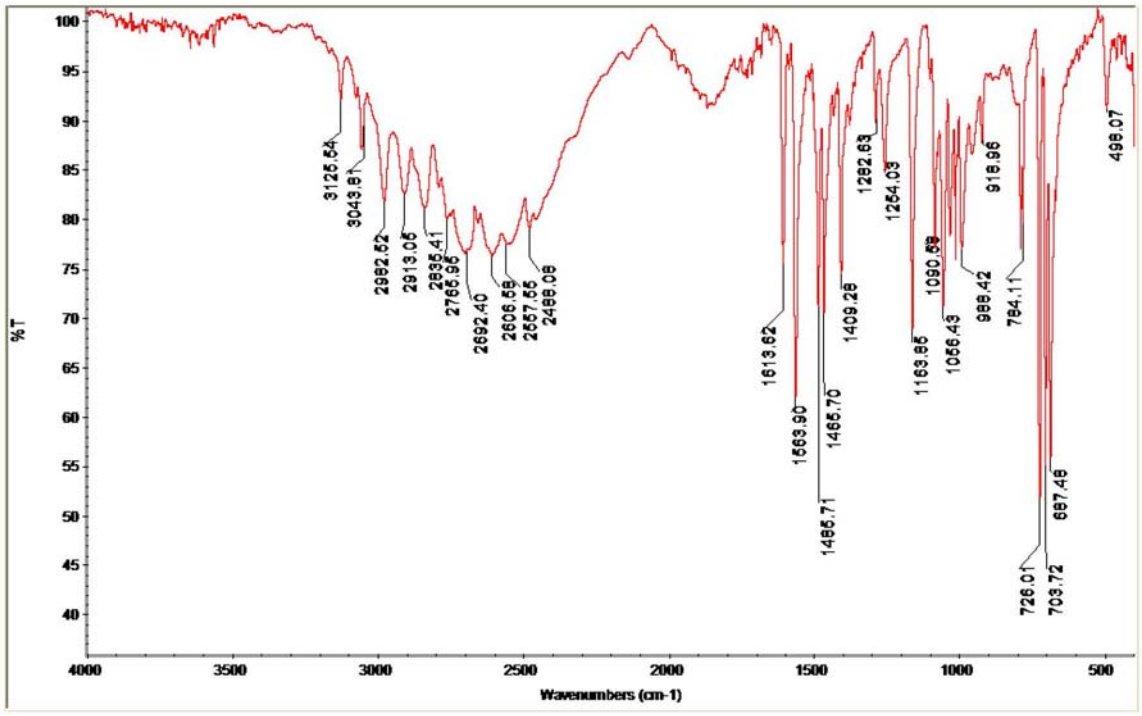

Figure S4. FT-IR (KBr) of 5-phenyl-1*H*-tetrazole (**1**).

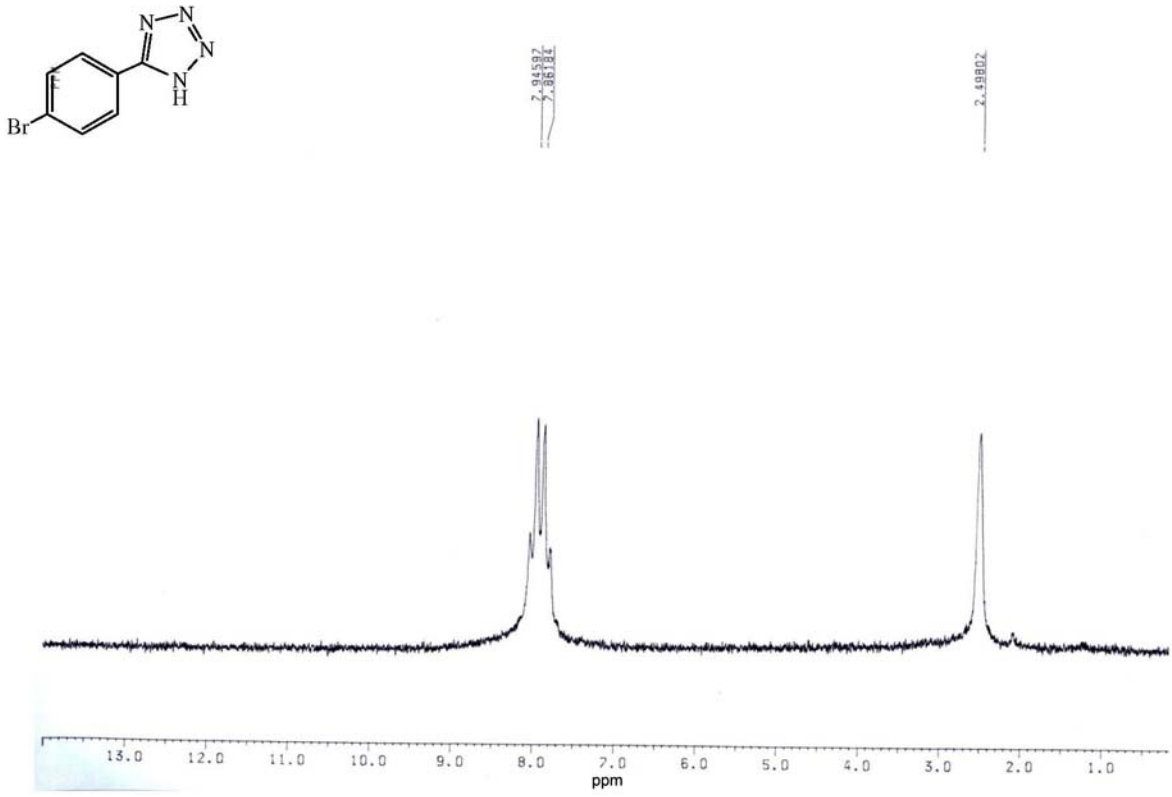

Figure S5. ^{1}H NMR (100 MHz, DMSO-d_6) of 5-(4-bromophenyl)-1*H*-tetrazole (**2**).

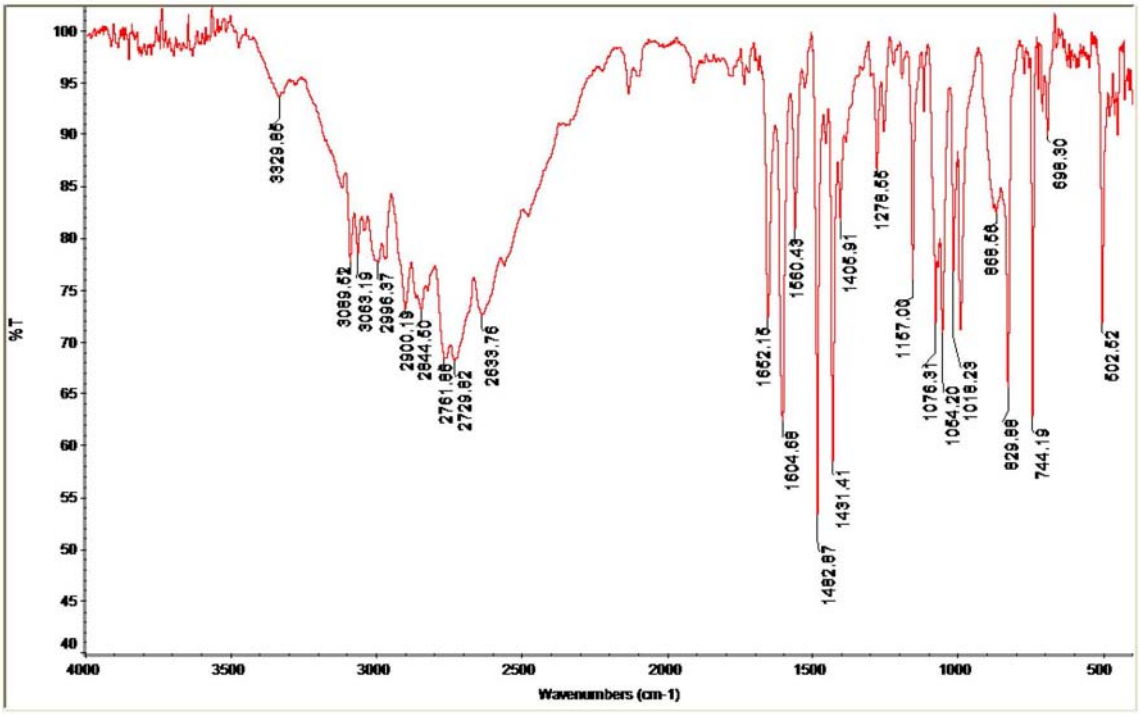

Figure S6. FT-IR (KBr) of 5-(4-bromophenyl)-1*H*-tetrazole (**2**).

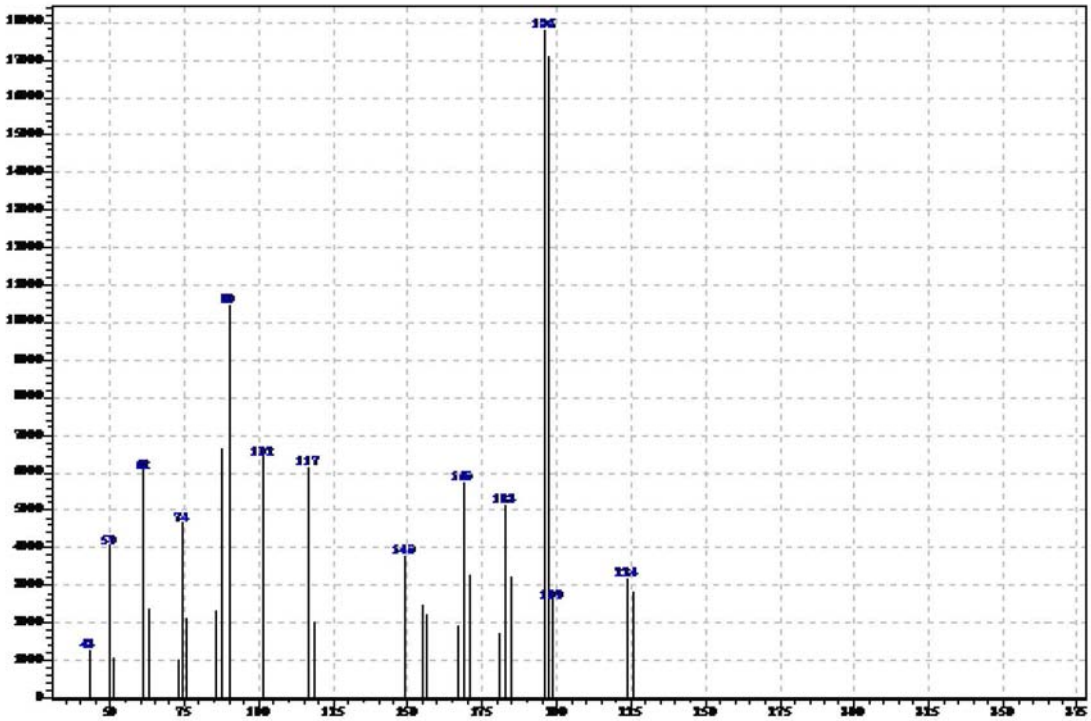

Figure S7. Mass spectrum of 5-(4-bromophenyl)-1*H*-tetrazole (**2**).

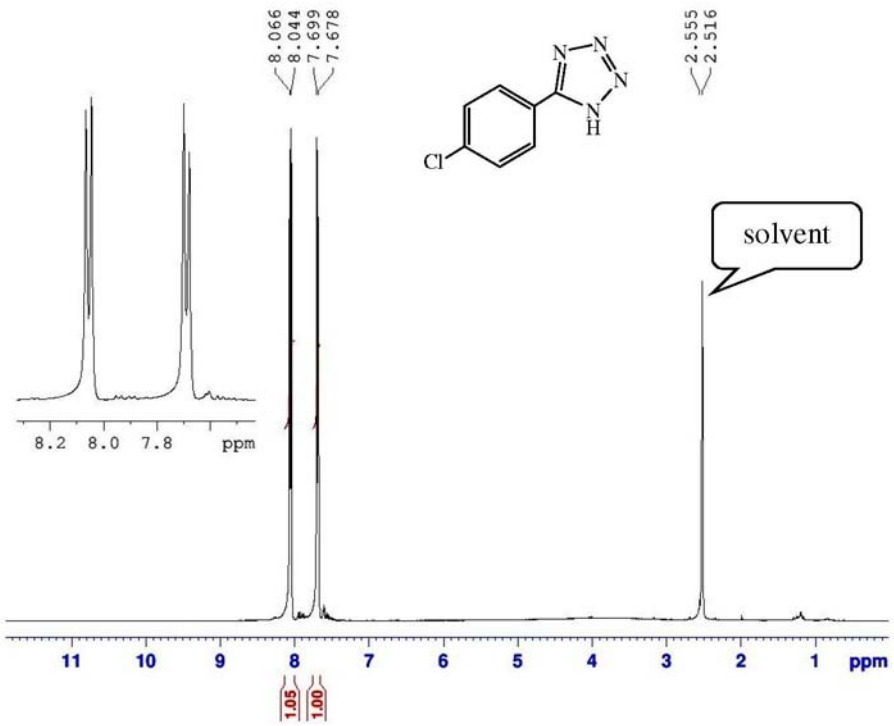

Figure S8. [1]H NMR (400 MHz, DMSO-d_6) of 5-(4-chlorophenyl)-1*H*-tetrazole (**3**).

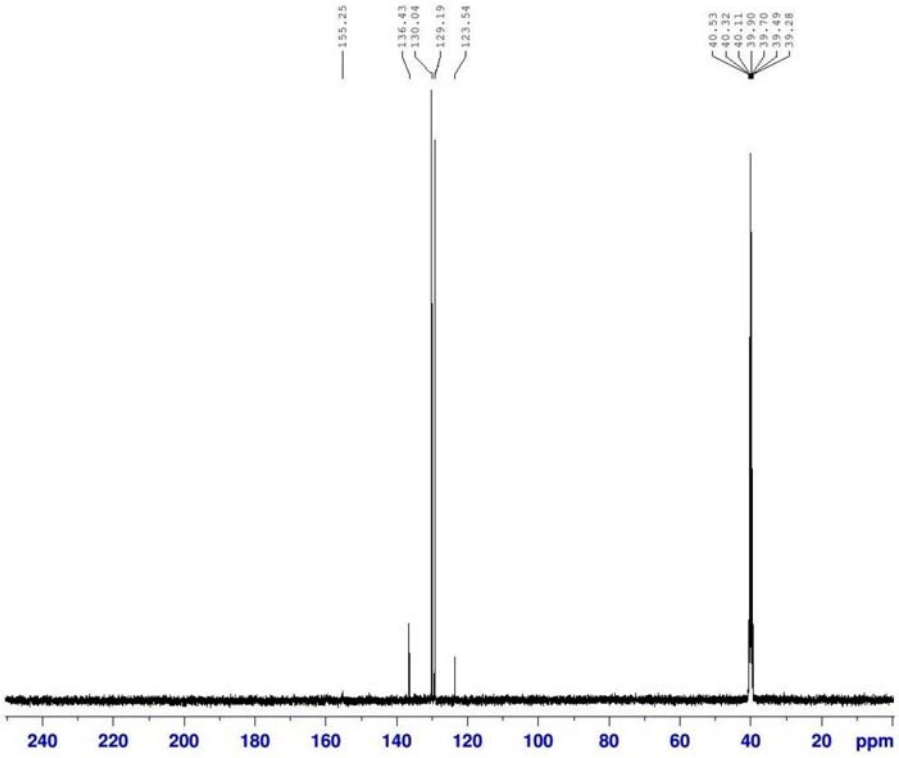

Figure S9. [13]C NMR (100 MHz, DMSO-d_6) of 5-(4-chlorophenyl)-1*H*-tetrazole (**3**).

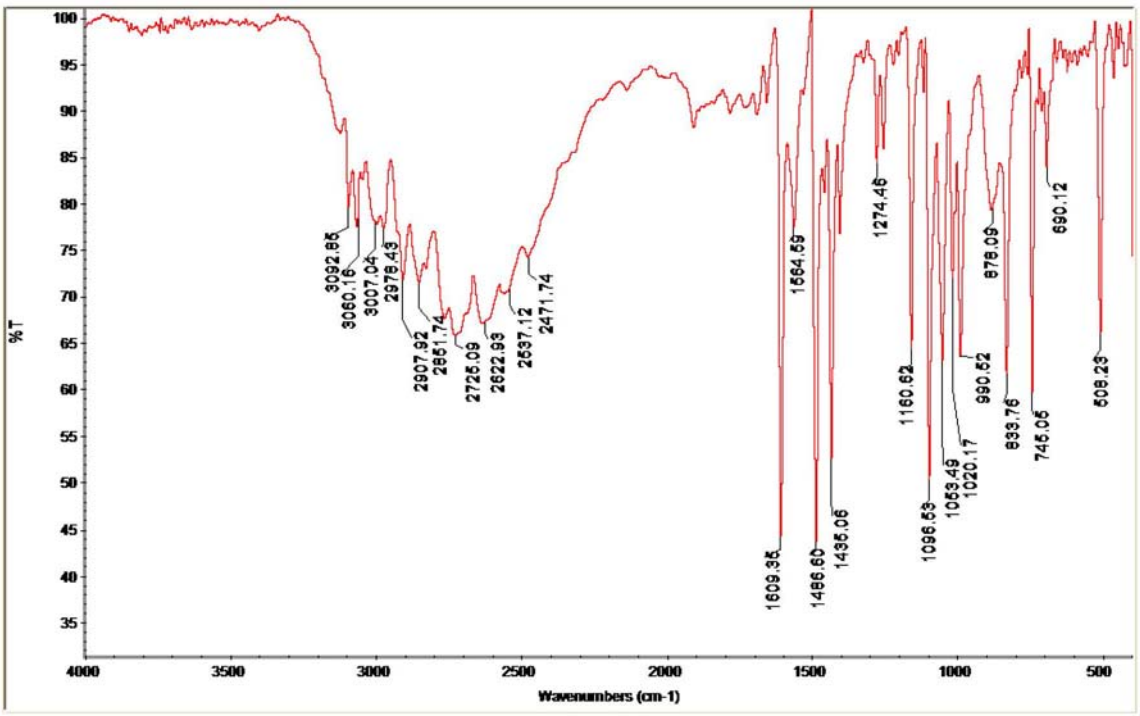

Figure S10. FT-IR (KBr) of 5-(4-chlorophenyl)-1*H*-tetrazole (**3**).

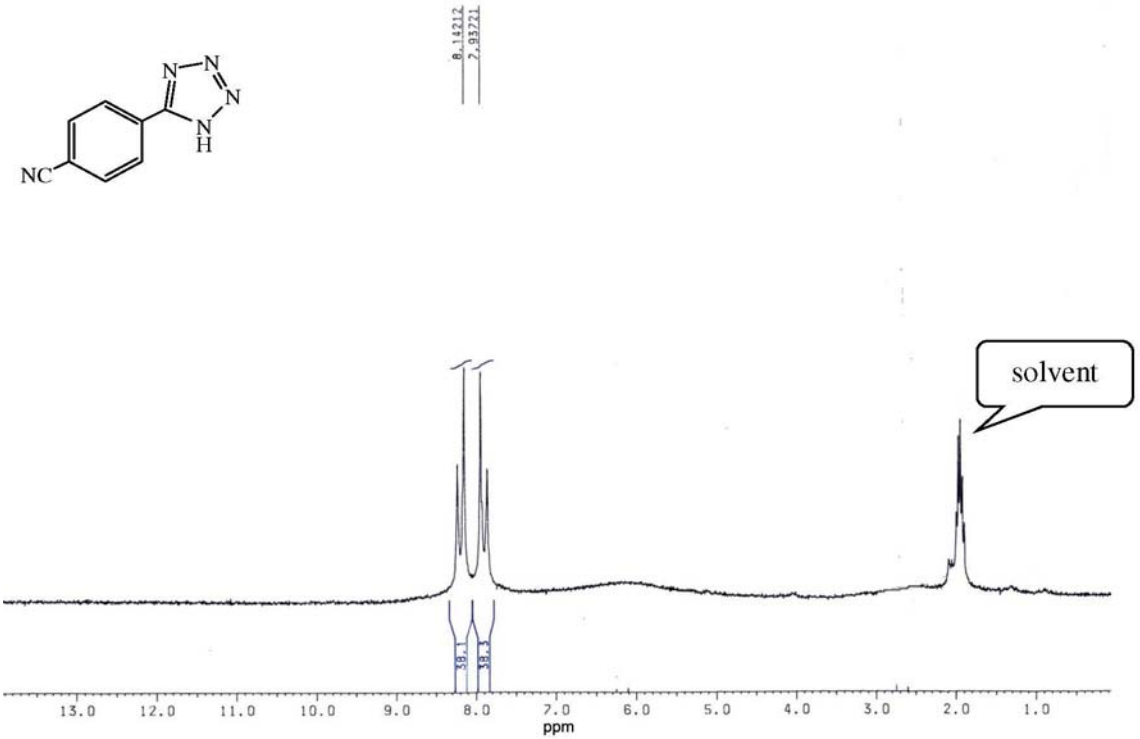

Figure S11. ^{1}H NMR (100 MHz, CD_3CN) of 4-(1*H*-tetrazol-5-yl)benzonitrile (**4**).

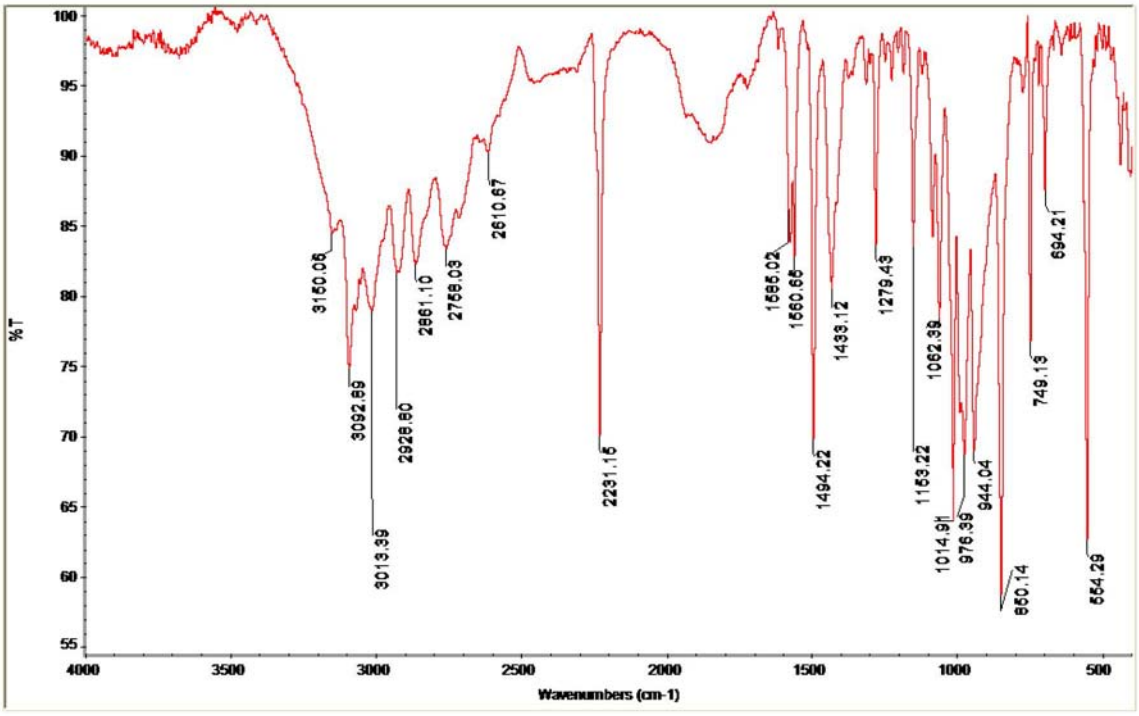

Figure S12. FT-IR (KBr) of 4-(1*H*-tetrazol-5-yl)benzonitrile (**4**).

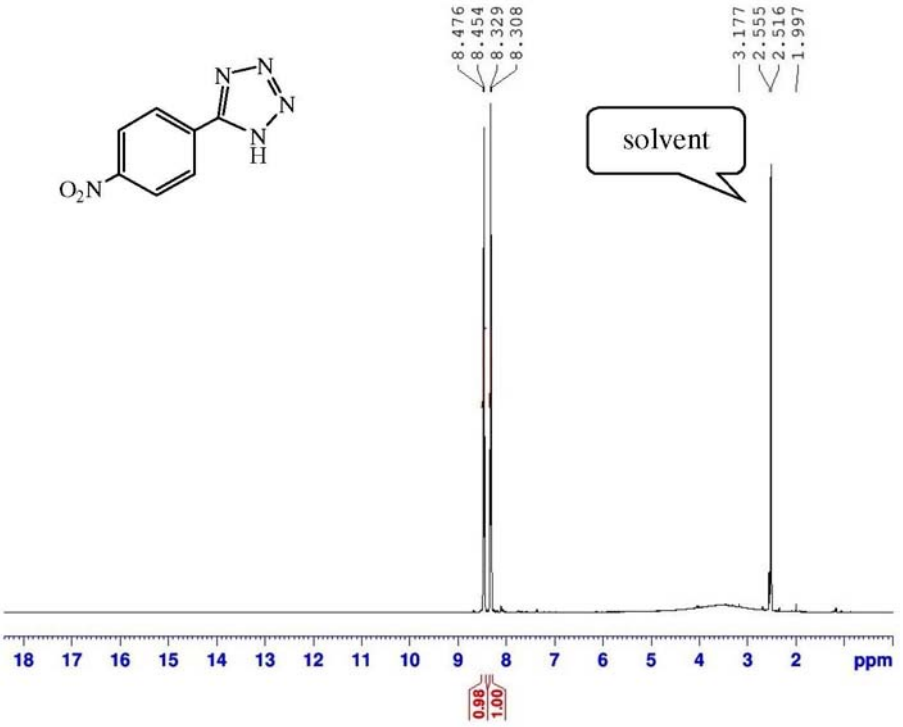

Figure S13. ^{1}H NMR (400 MHz, DMSO-d_6) of 5-(4-nitrophenyl)-1*H*-tetrazole (**5**).

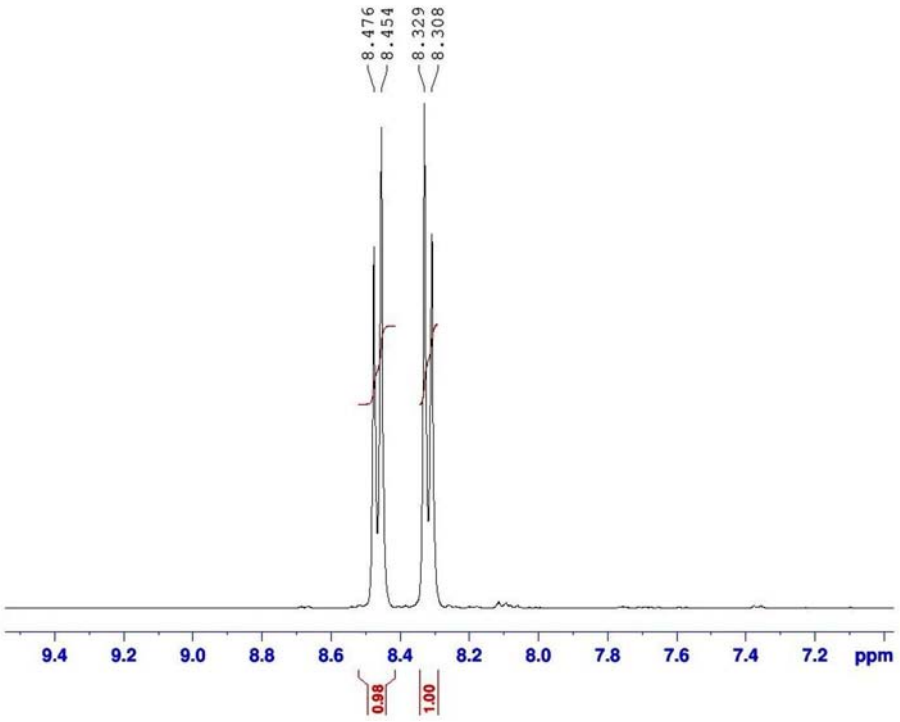

Figure S14. [1]H NMR (400 MHz, DMSO-d_6) of 5-(4-nitrophenyl)-1*H*-tetrazole (**5**) expanded.

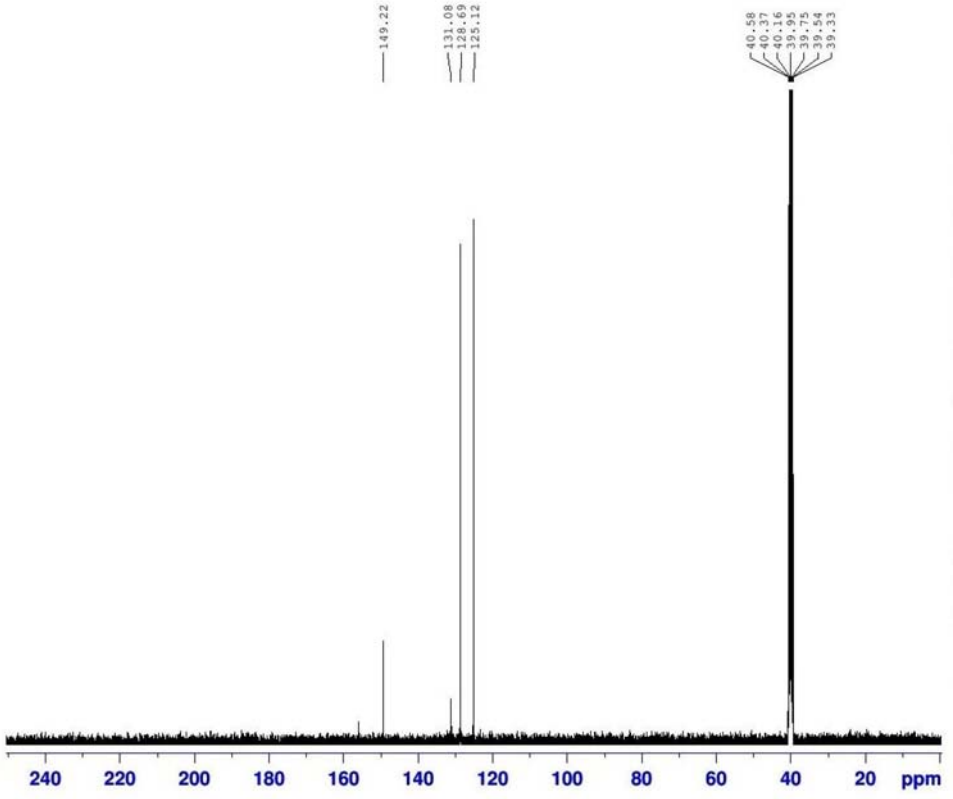

Figure S15. [13]C NMR (100 MHz, DMSO-d_6) of 5-(4-nitrophenyl)-1*H*-tetrazole (**5**).

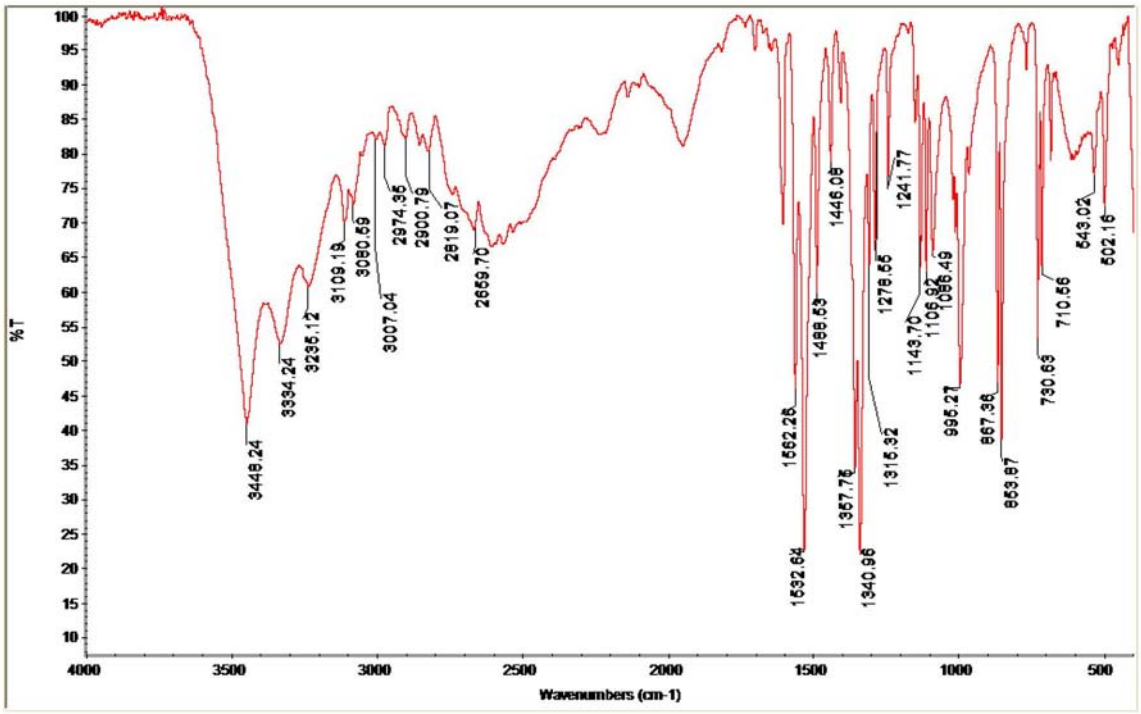

Figure S16. FT-IR (KBr) of 5-(4-nitrophenyl)-1*H*-tetrazole (**5**).

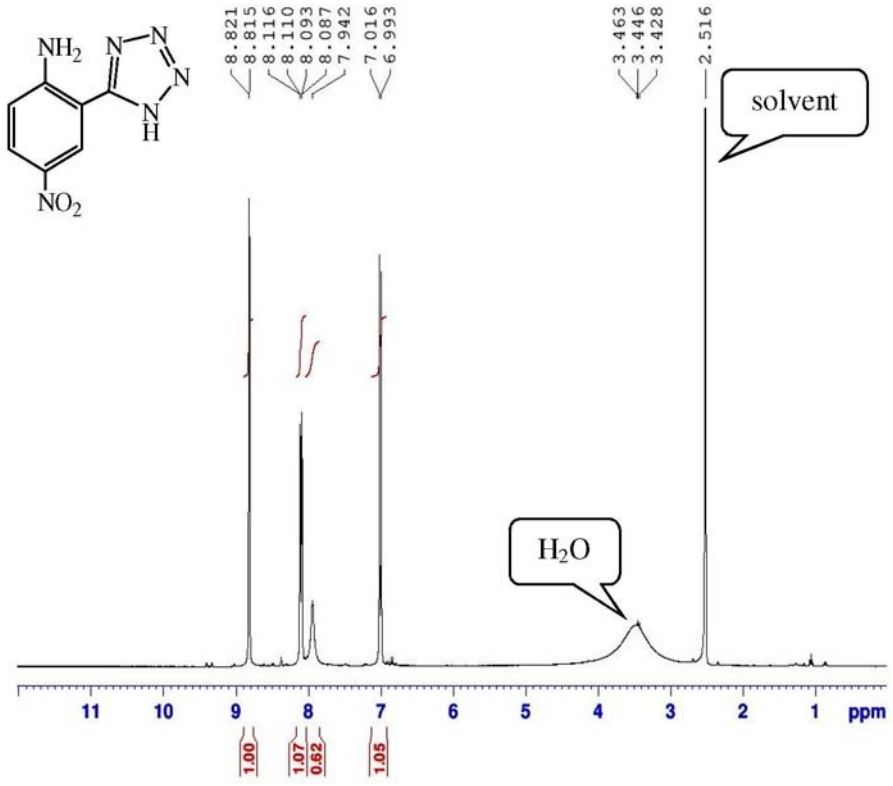

Figure S17. ^{1}H NMR (400 MHz, DMSO-d_6) of 4-nitro-2-(1*H*-tetrazol-5-yl)benzenamine (**6**).

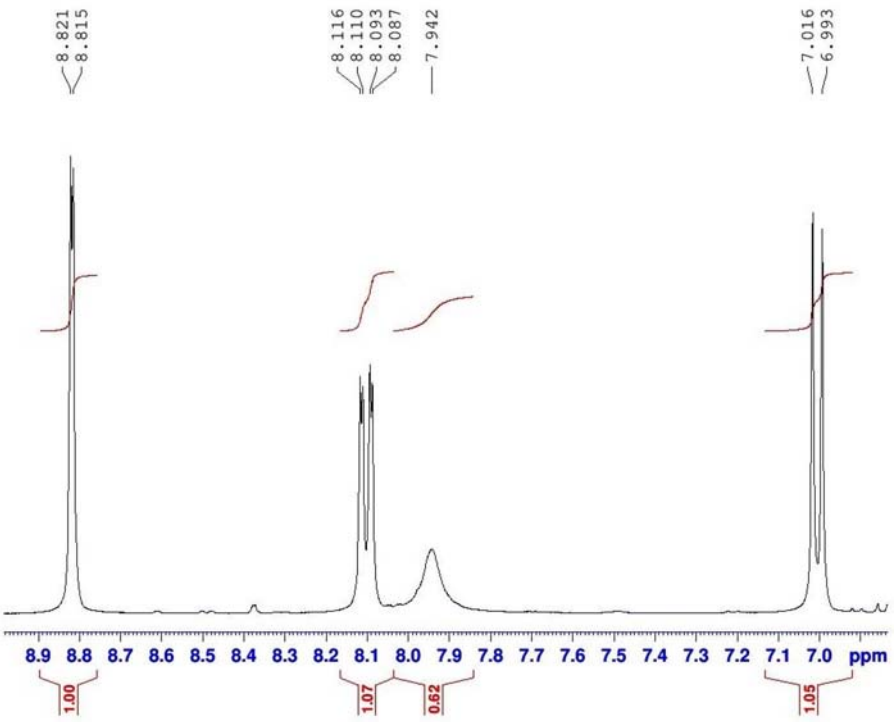

Figure S18. ^{1}H NMR (400 MHz, DMSO-d_6) of 4-nitro-2-(1*H*-tetrazol-5-yl)benzenamine (**6**) expanded.

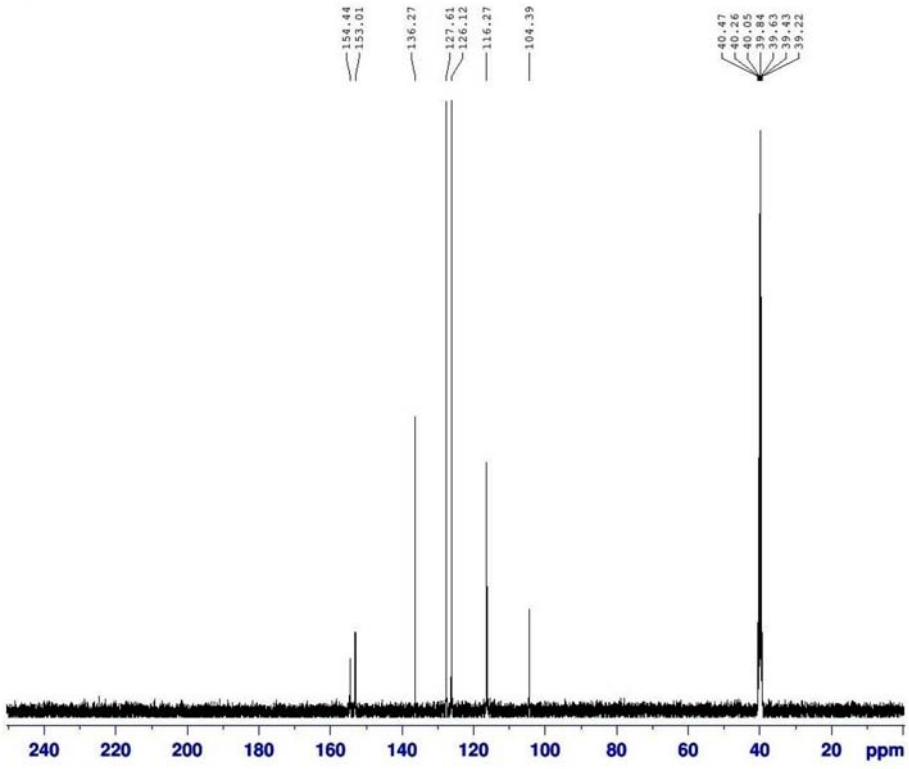

Figure S19. ^{13}C NMR (100 MHz, DMSO-d_6) of 4-nitro-2-(1*H*-tetrazol-5-yl)benzenamine (**6**).

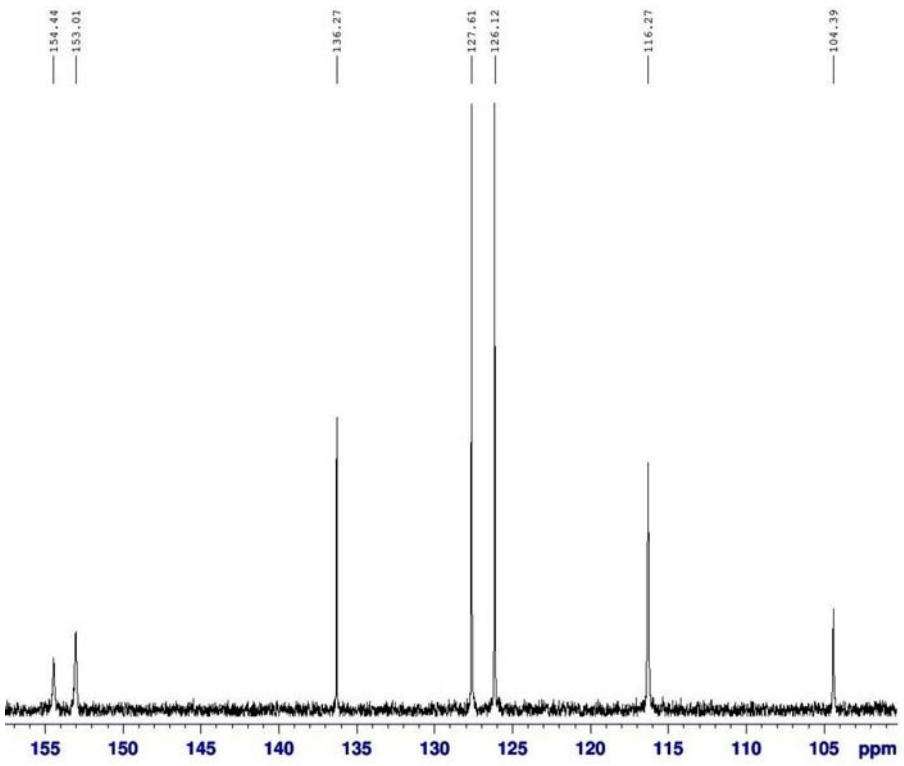

Figure S20. ^{13}C NMR (100 MHz, DMSO-d_6) of 4-nitro-2-(1*H*-tetrazol-5-yl)benzenamine (**6**) expanded.

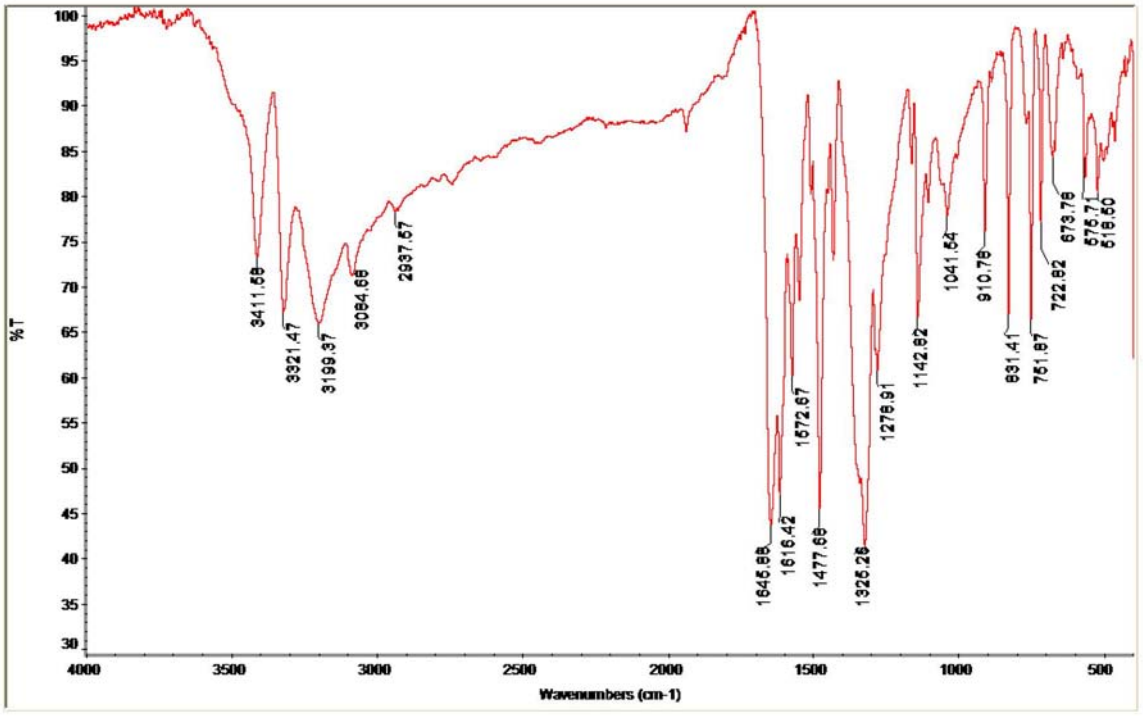

Figure S21. FT-IR (KBr) of 4-nitro-2-(1*H*-tetrazol-5-yl)benzenamine (**6**).

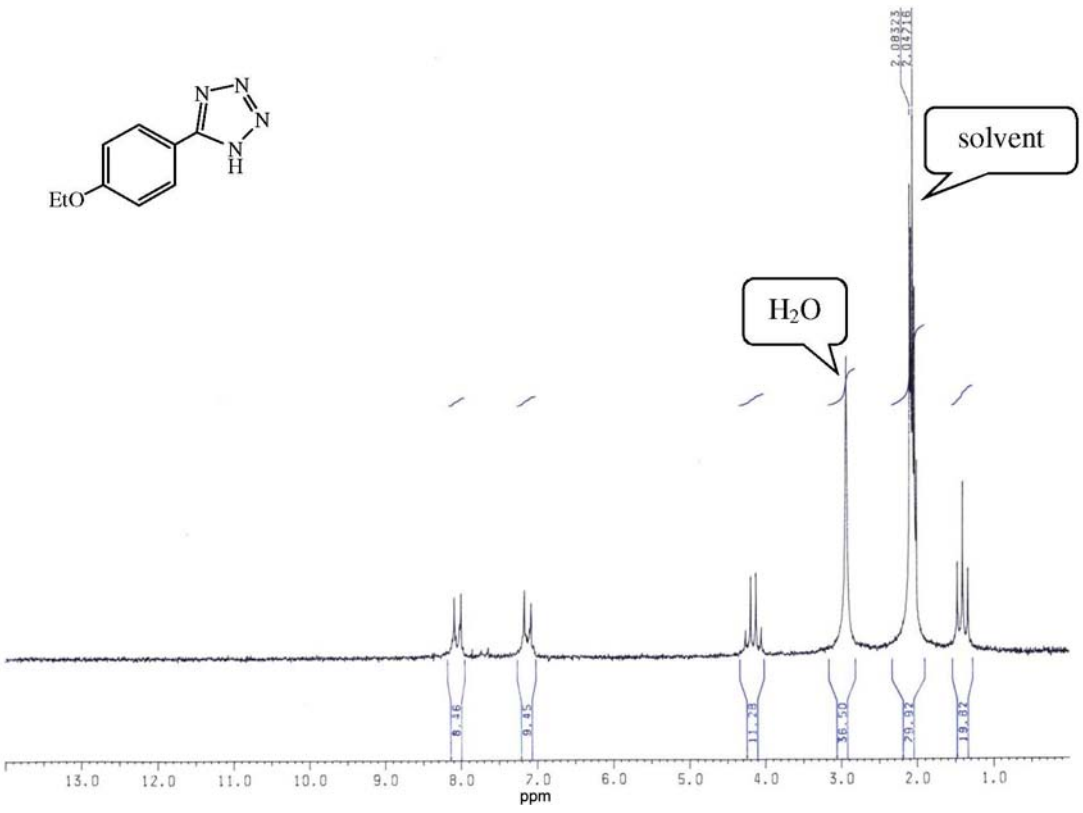

Figure S22. ^{1}H NMR (100 MHz, acetone-d_6) of 5-(4-ethoxyphenyl)-1*H*-tetrazole (**7**).

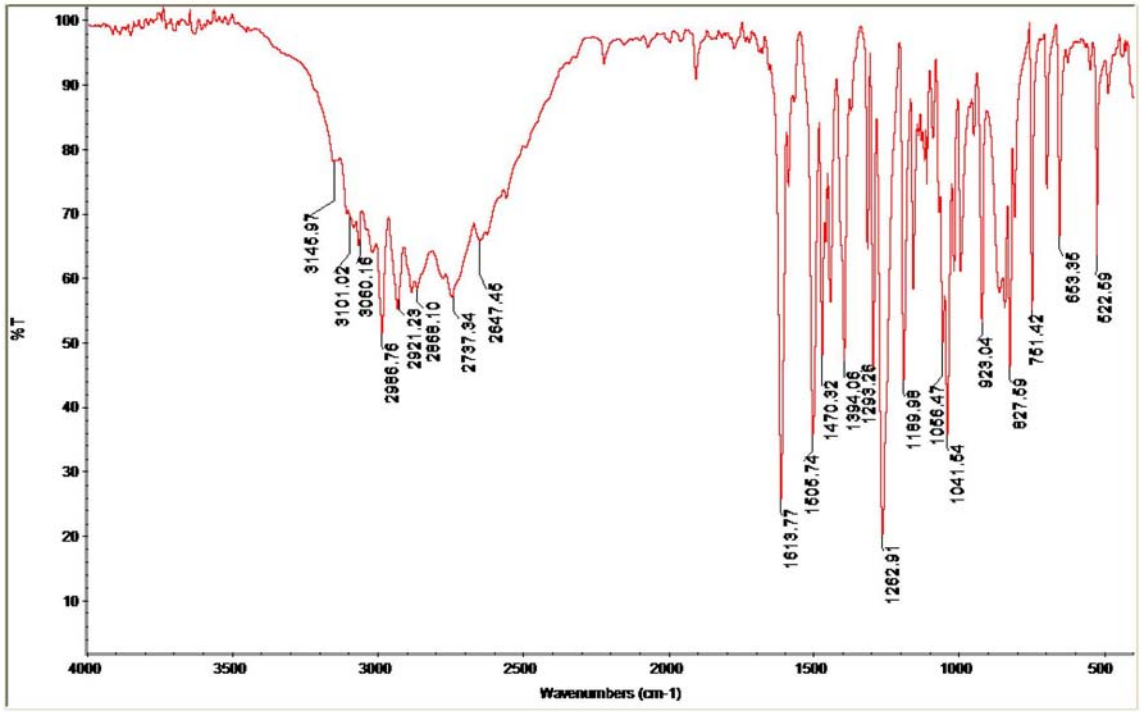

Figure S23. FT-IR (KBr) of 5-(4-ethoxyphenyl)-1*H*-tetrazole (**7**).

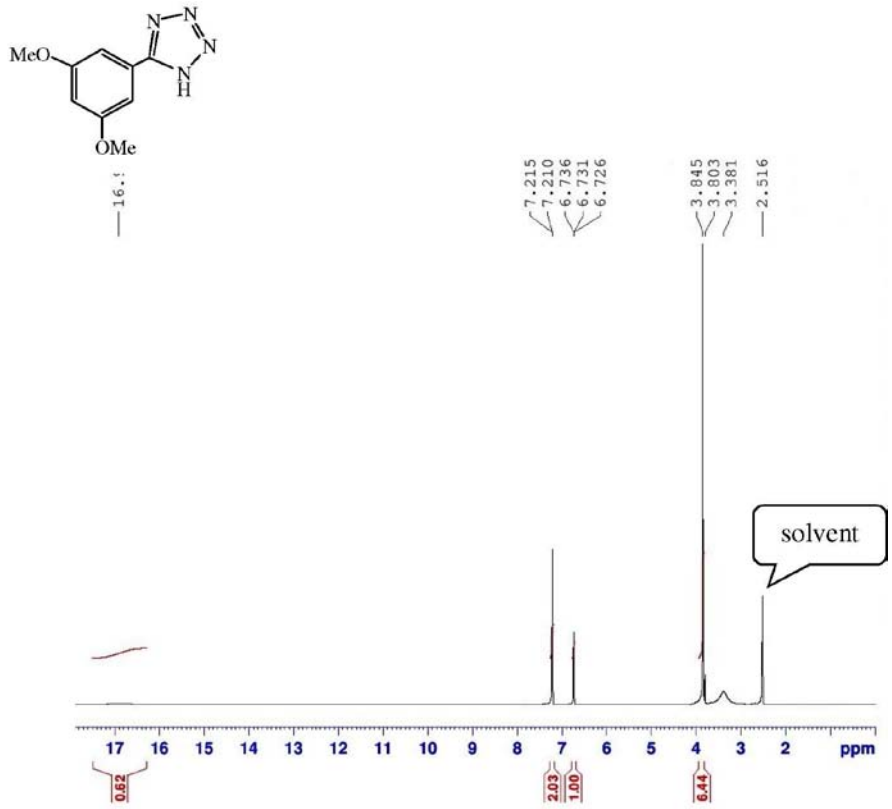

Figure S24. [1]H NMR (400 MHz, DMSO-d_6) of 5-(3,5-dimethoxyphenyl)-1*H*-tetrazole (**8**).

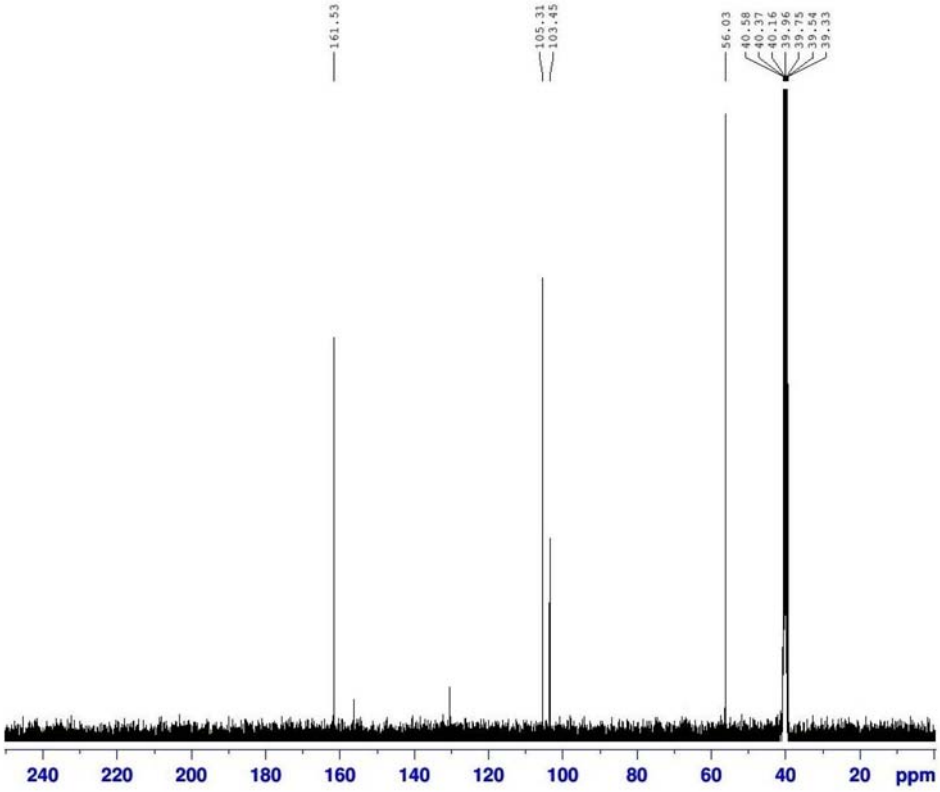

Figure S25. [13]C NMR (100 MHz, DMSO-d_6) of 5-(3,5-dimethoxyphenyl)-1*H*-tetrazole (**8**).

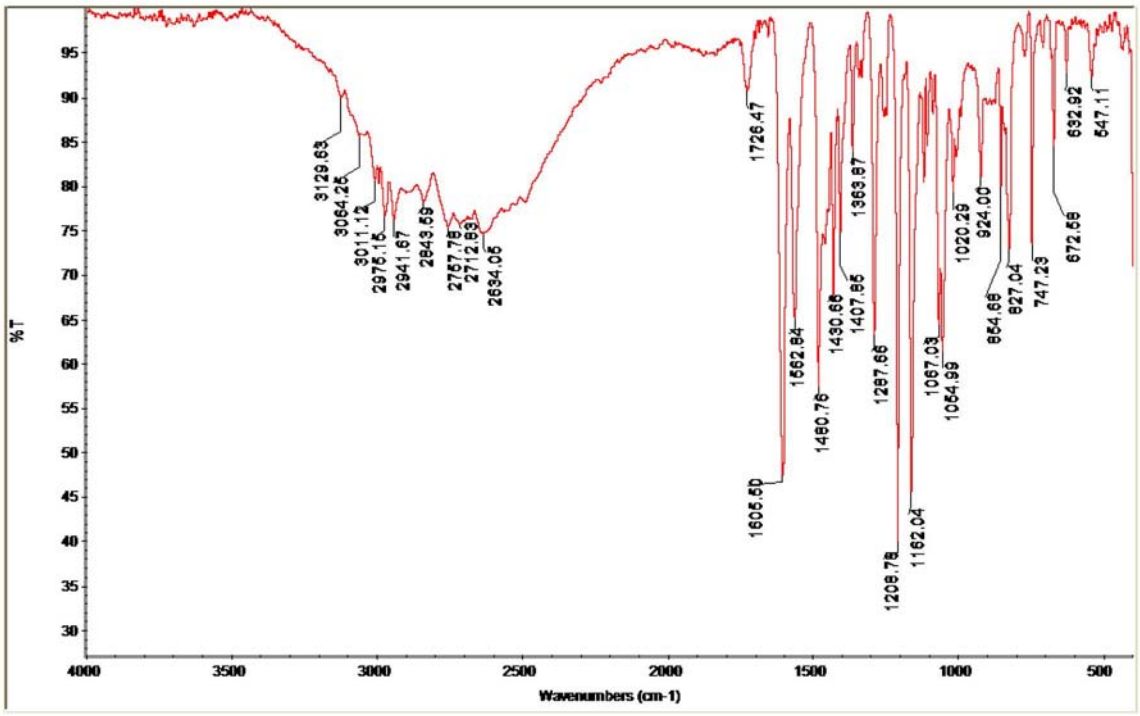

Figure S26. FT-IR (KBr) of 5-(3,5-dimethoxyphenyl)-1*H*-tetrazole (**8**).

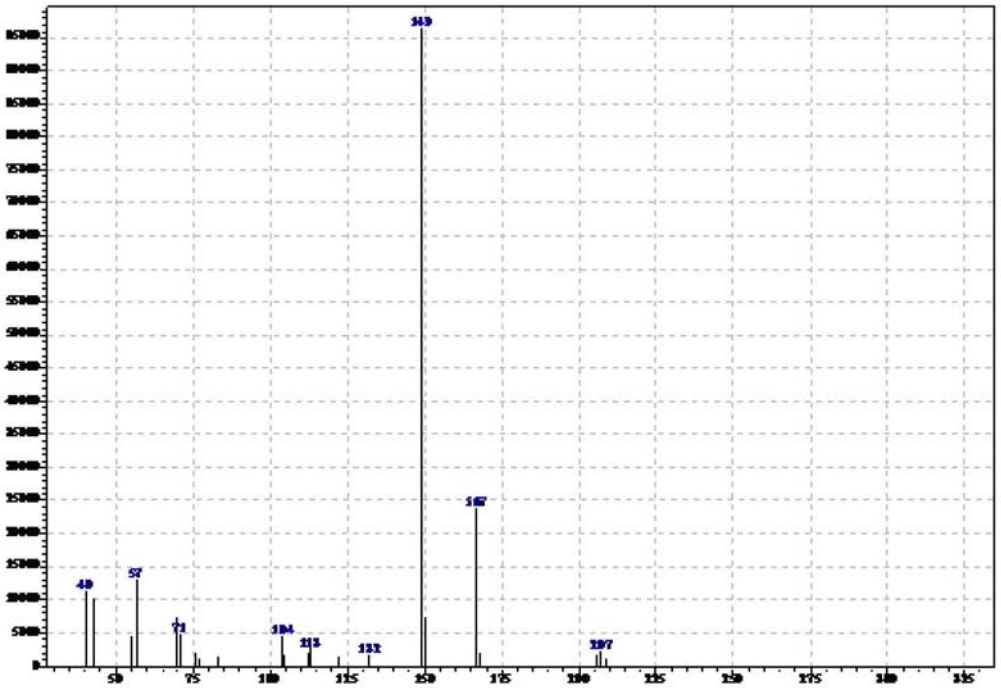

Figure S27. Mass spectrum of 5-(3,5-dimethoxyphenyl)-1*H*-tetrazole (**8**).

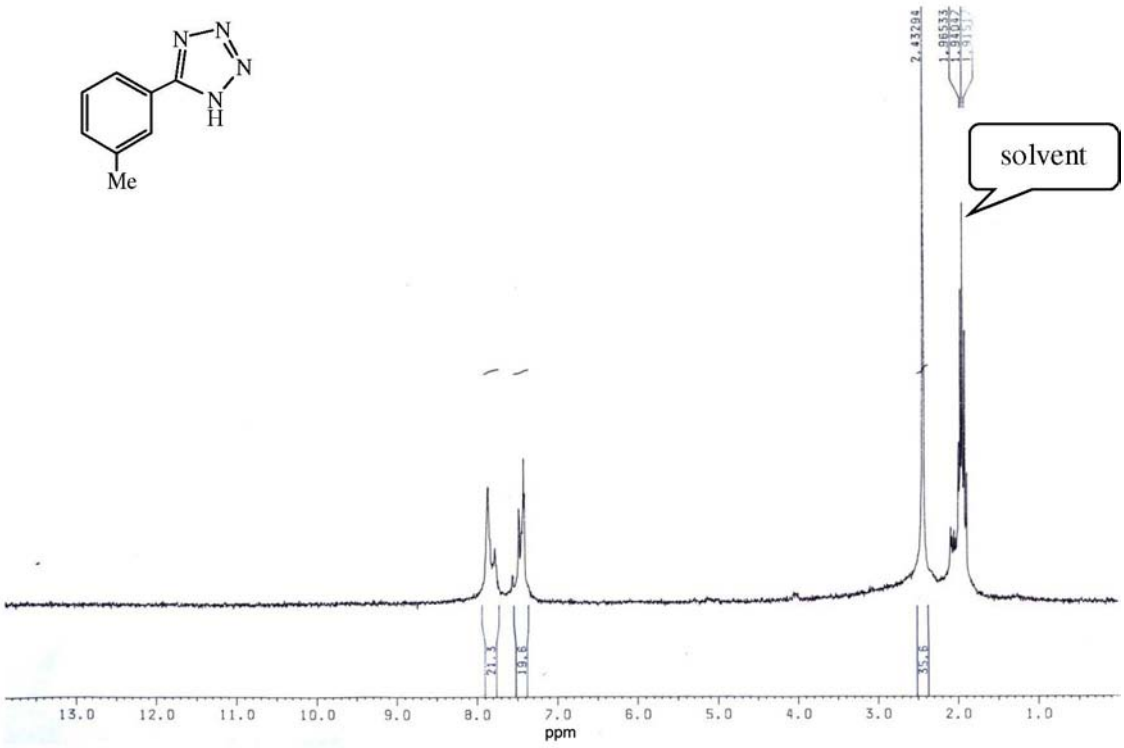

Figure S28. ^{1}H NMR (100 MHz, CD_3CN) of 5-*m*-tolyl-1*H*-tetrazole (**9**).

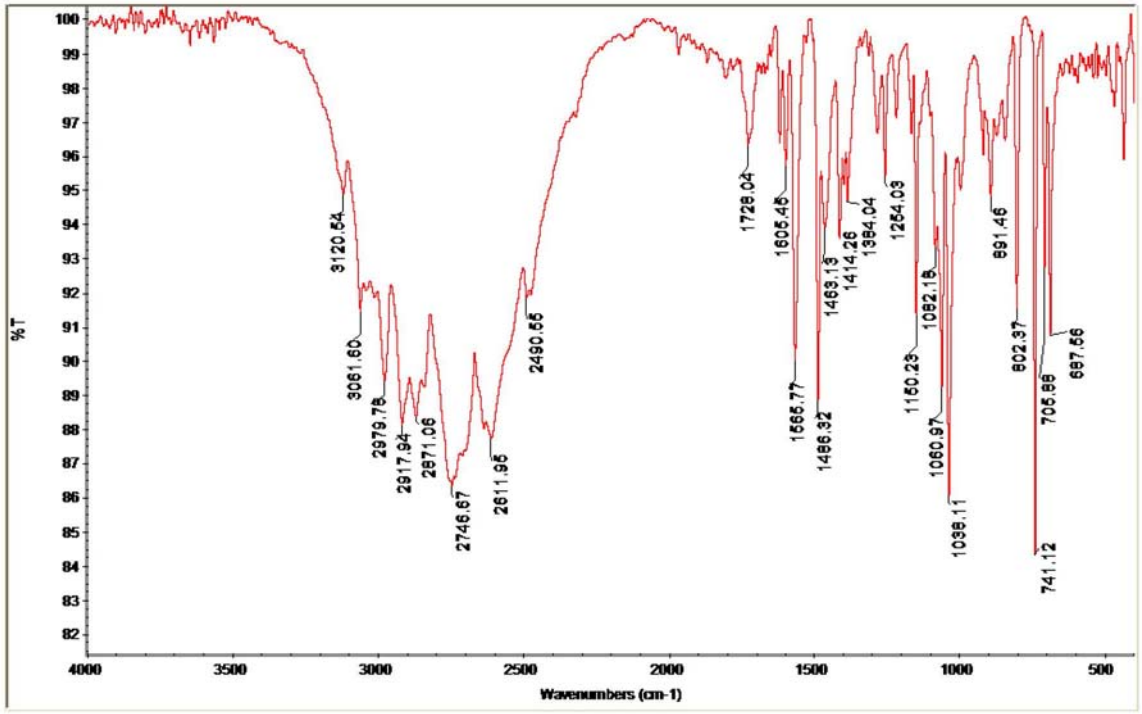

Figure S29. FT-IR (KBr) of 5-*m*-tolyl-1*H*-tetrazole (**9**).

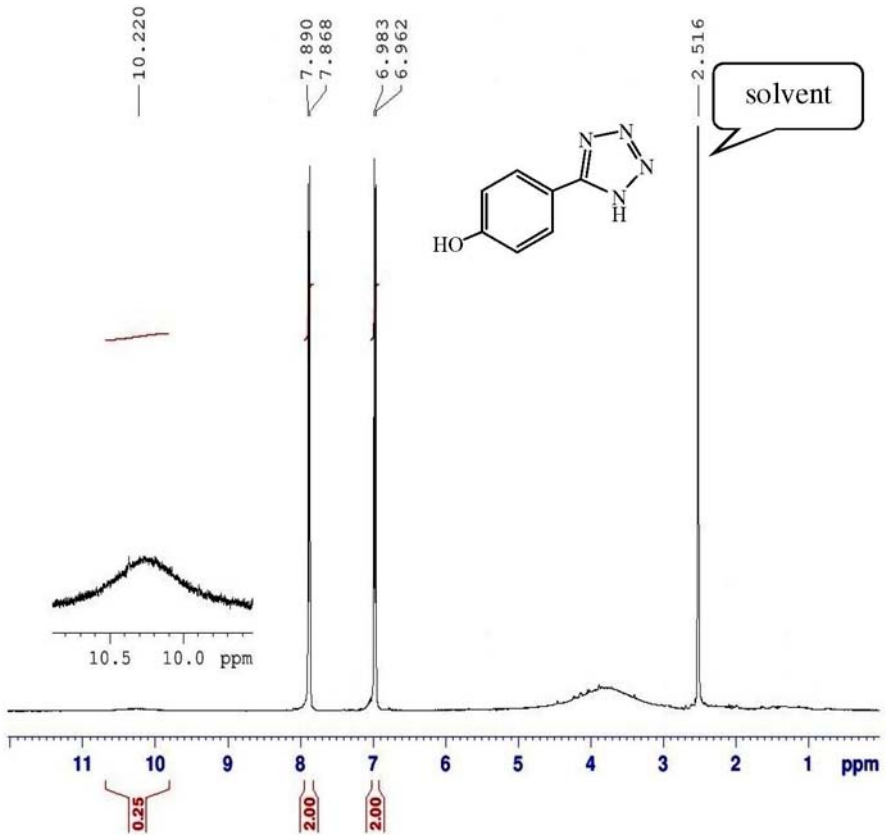

Figure S30. [1]H NMR (400 MHz, DMSO-d_6) of 4-(1*H*-tetrazol-5-yl) phenol (**10**).

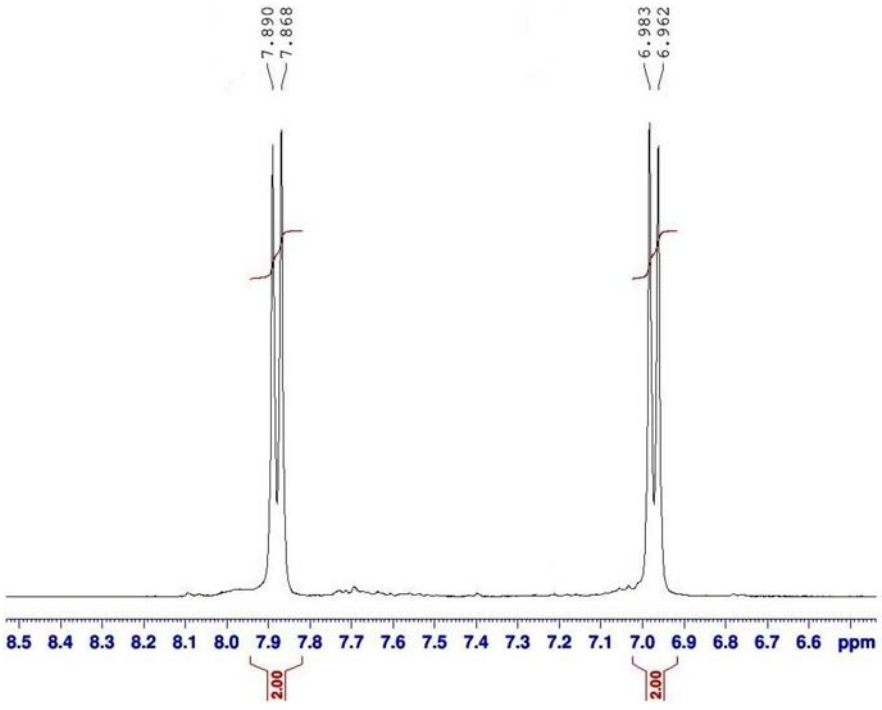

Figure S31. [1]H NMR (400 MHz, DMSO-d_6) of 4-(1*H*-tetrazol-5-yl)phenol (**10**) expanded.

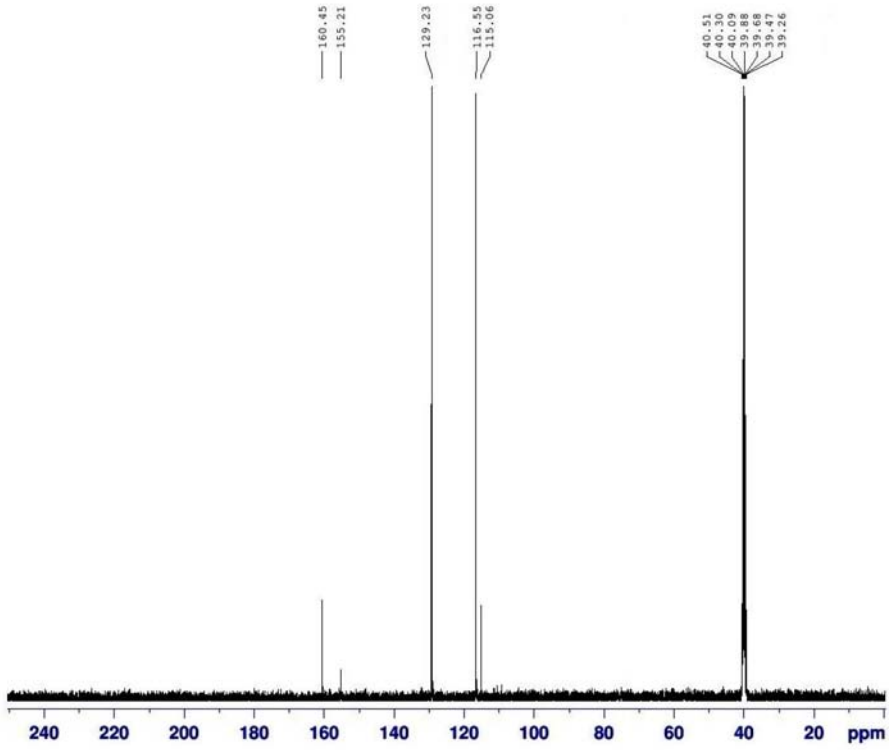

Figure S32. ^{13}C NMR (100 MHz, DMSO-d_6) of 4-(1*H*-tetrazol-5-yl) phenol (**10**).

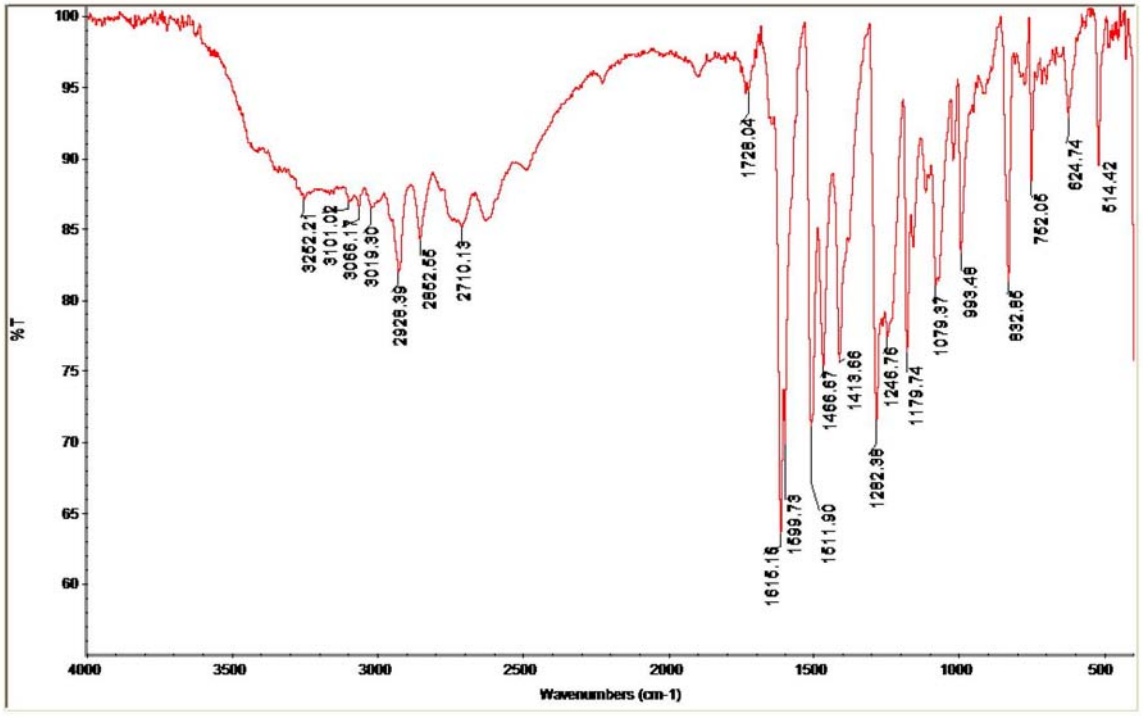

Figure S33. FT-IR (KBr) of 4-(1*H*-tetrazol-5-yl) phenol (**10**).

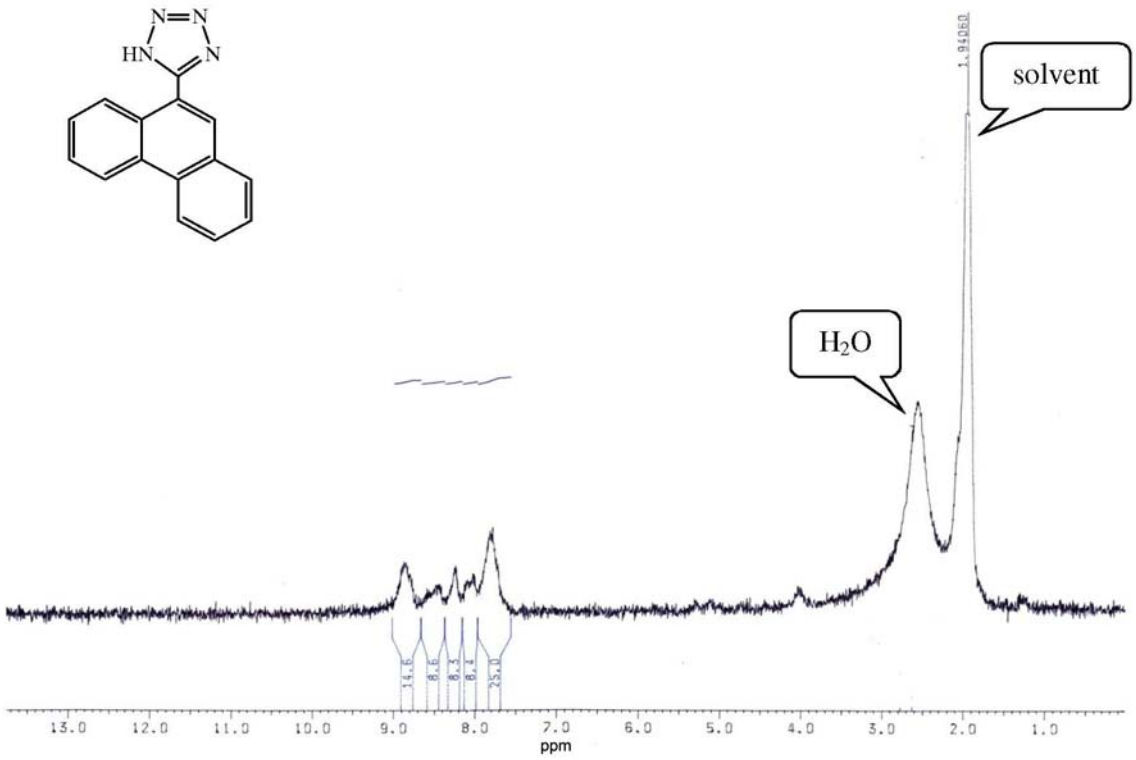

Figure S34. ^{1}H NMR (100 MHz, DMSO-d_6) of 5-(phenanthren-9-yl)-1*H*-tetrazole (**11**).

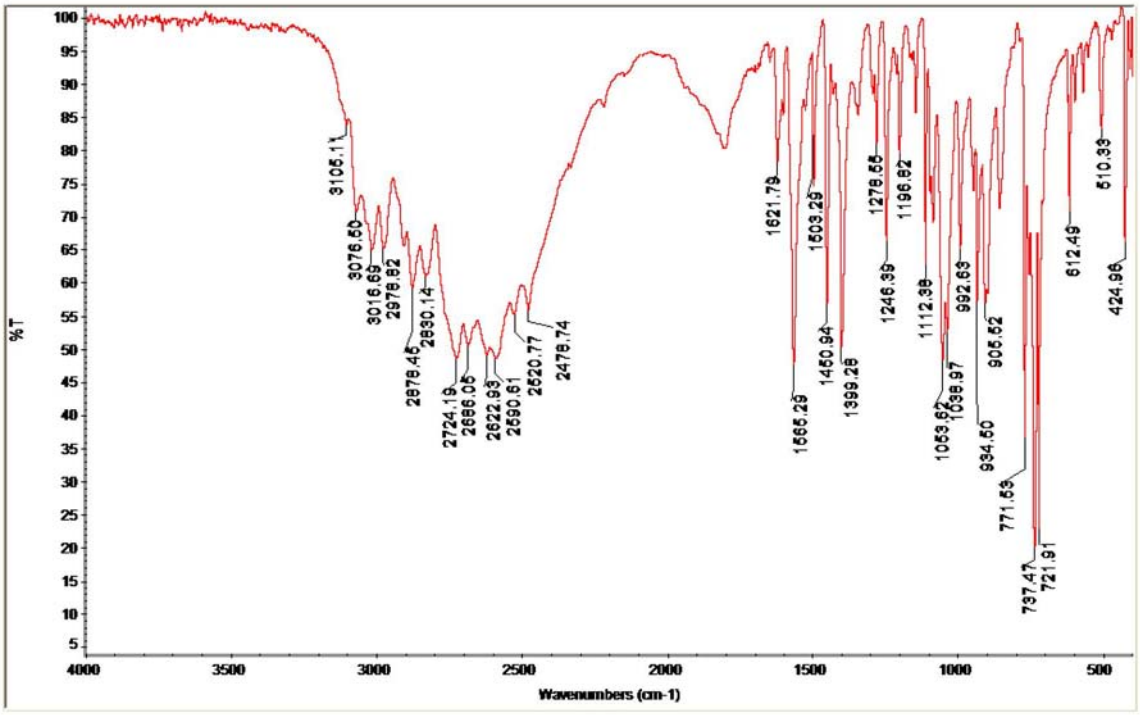

Figure S35. FT-IR (KBr) of 5-(phenanthren-9-yl)-1*H*-tetrazole (**11**).

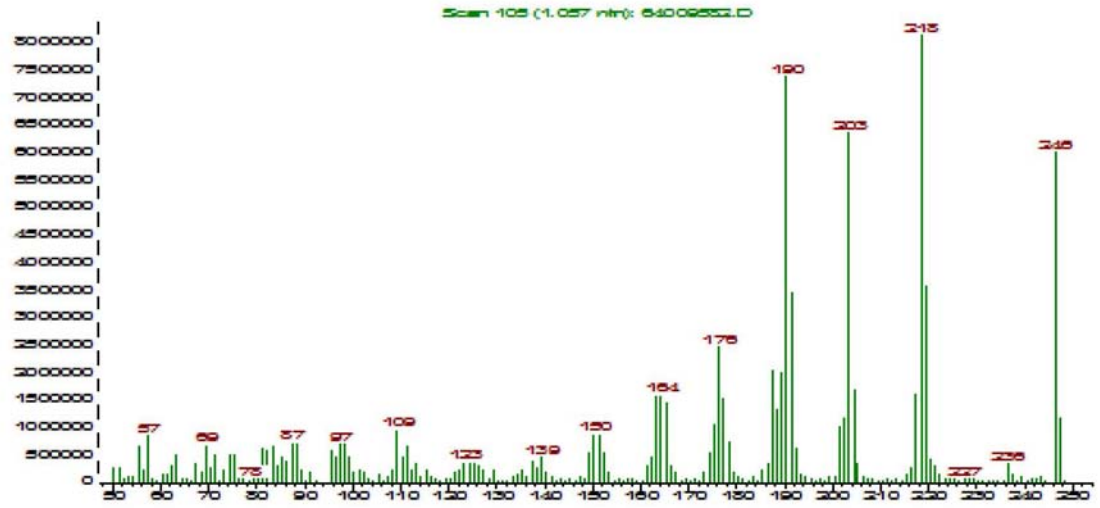

Figure S36. Mass spectrum of 5-(phenanthren-9-yl)-1*H*-tetrazole (**11**).

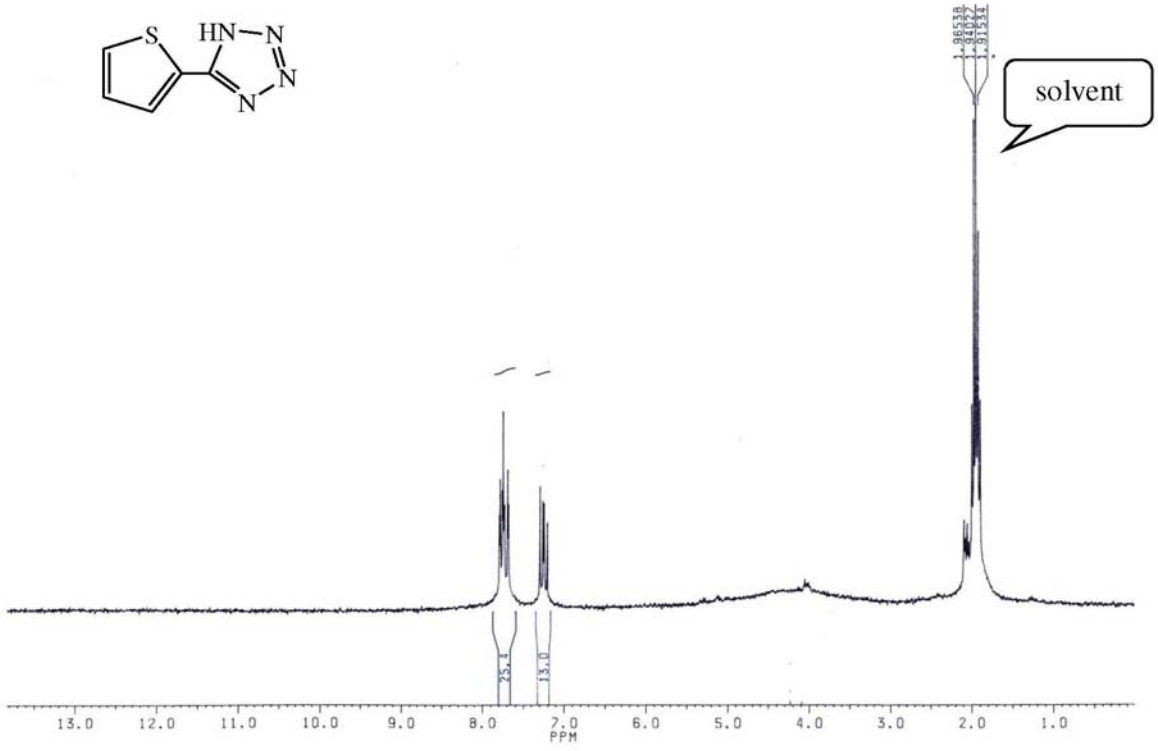

Figure S37. ^{1}H NMR (100 MHz, CD_3CN) of 5-(thiophen-2-yl)-1*H*-tetrazole (**12**).

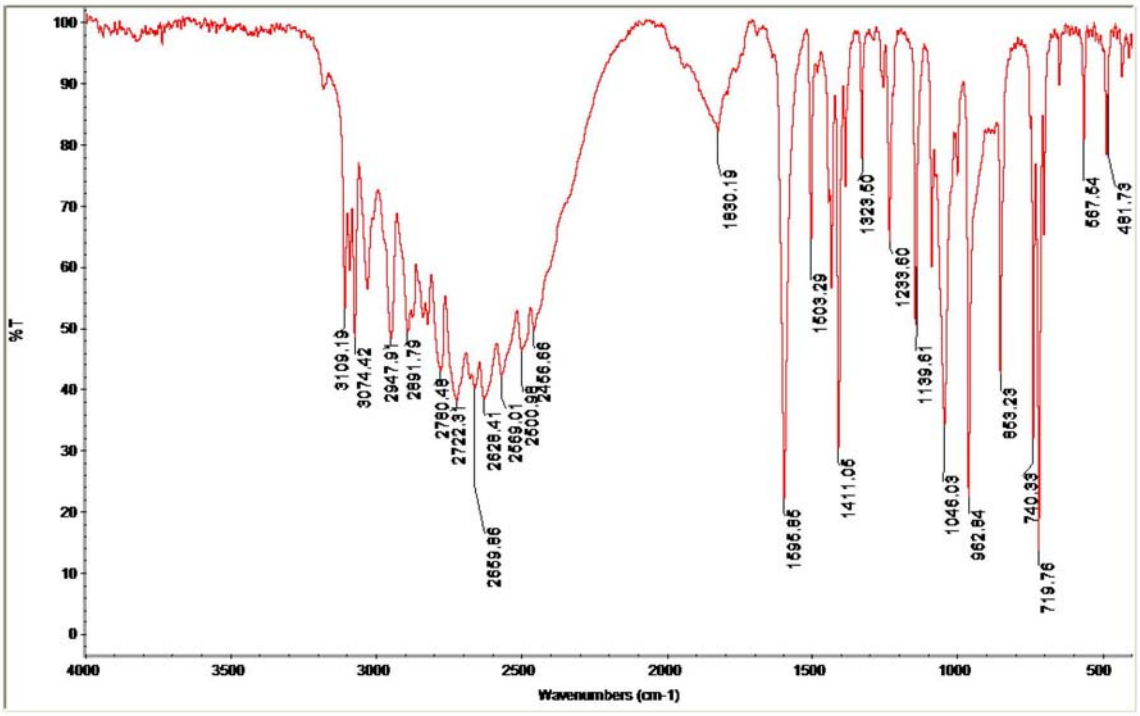

Figure S38. FT-IR (KBr) of 5-(thiophen-2-yl)-1*H*-tetrazole (**12**).

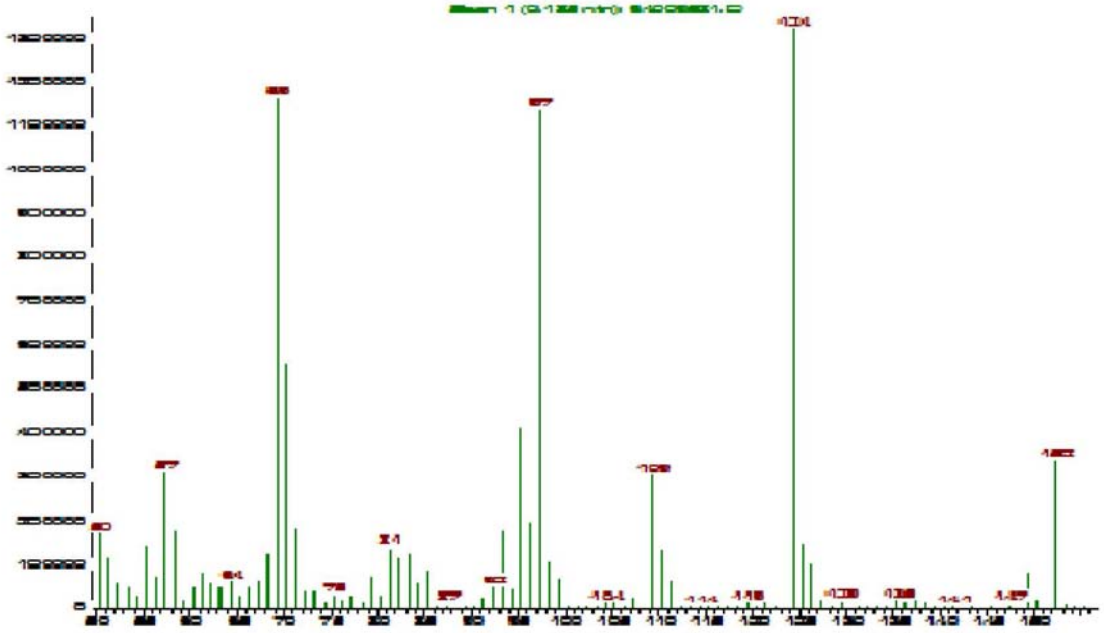

Figure S39. Mass spectrum of 5-(thiophen-2-yl)-1*H*-tetrazole (**12**).

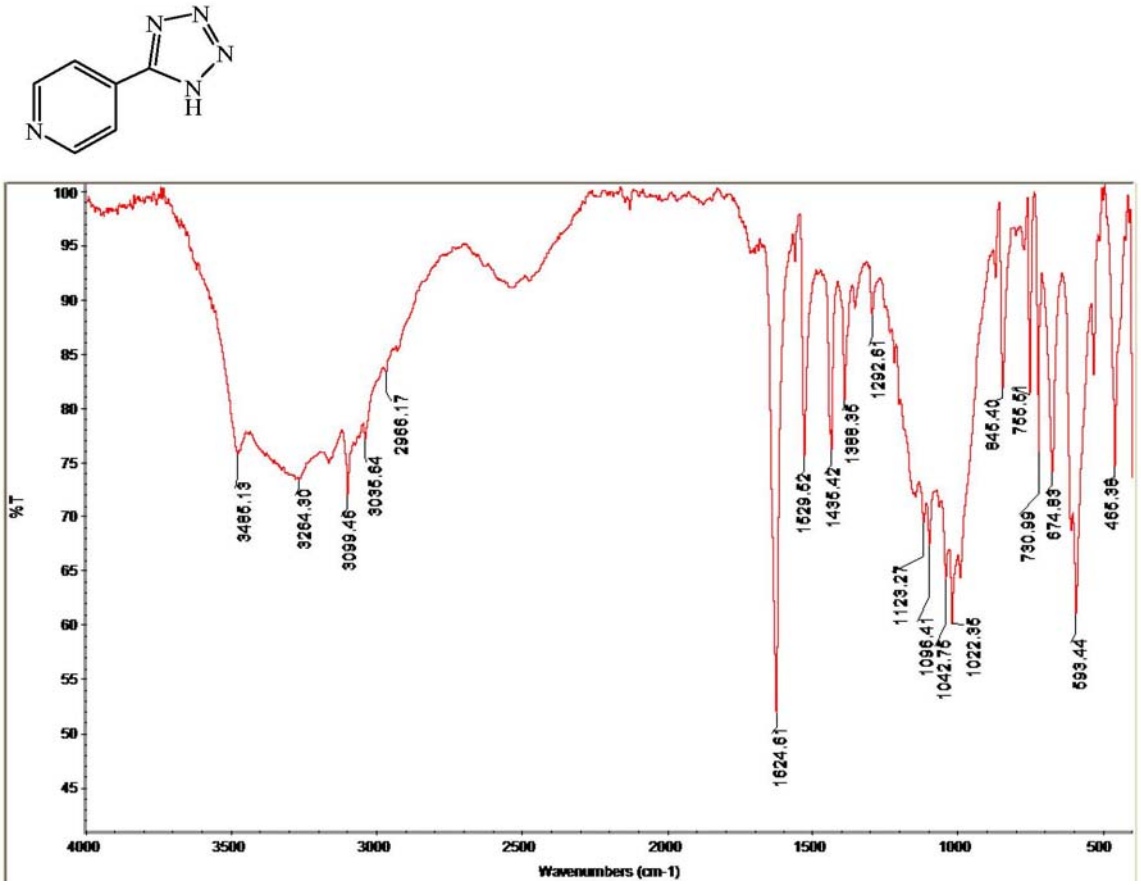

Figure S40. FT-IR (KBr) of 4-(1*H*-tetrazol-5-yl) pyridine (**13**).

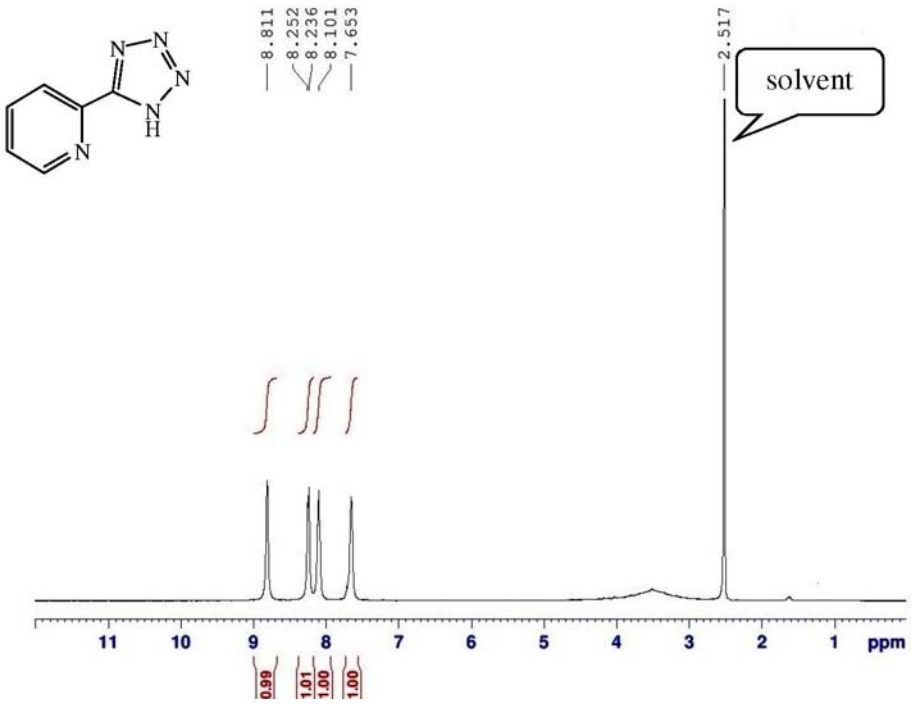

Figure S41. ^{1}H NMR (400 MHz, DMSO-d_6) of 2-(1*H*-tetrazol-5-yl)pyridine (**14**).

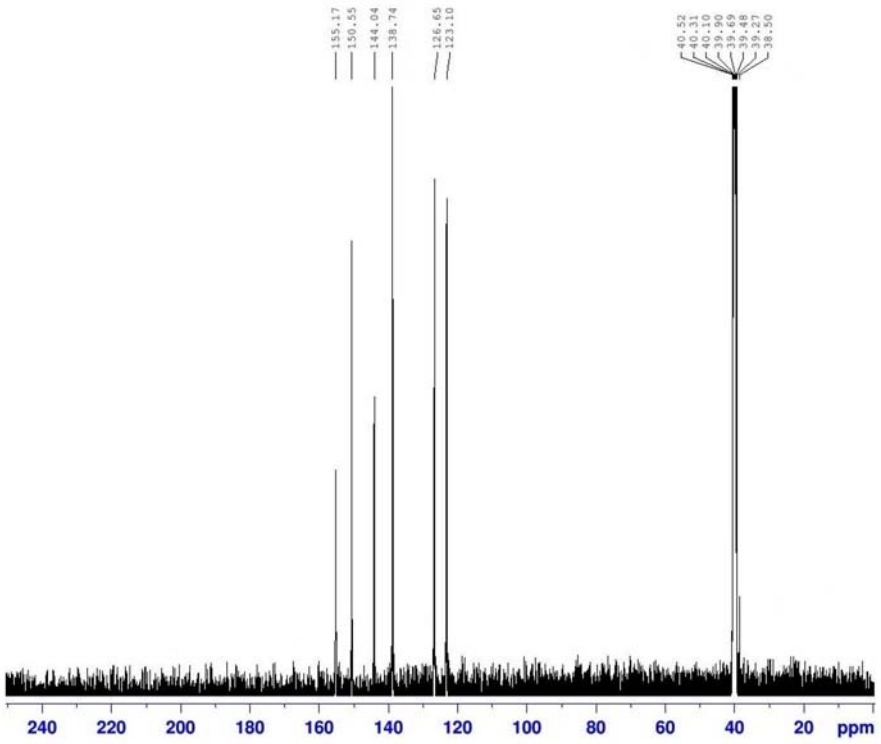

Figure S42. ^{13}C NMR (100 MHz, DMSO-d_6) of 2-(1*H*-tetrazol-5-yl) pyridine (**14**).

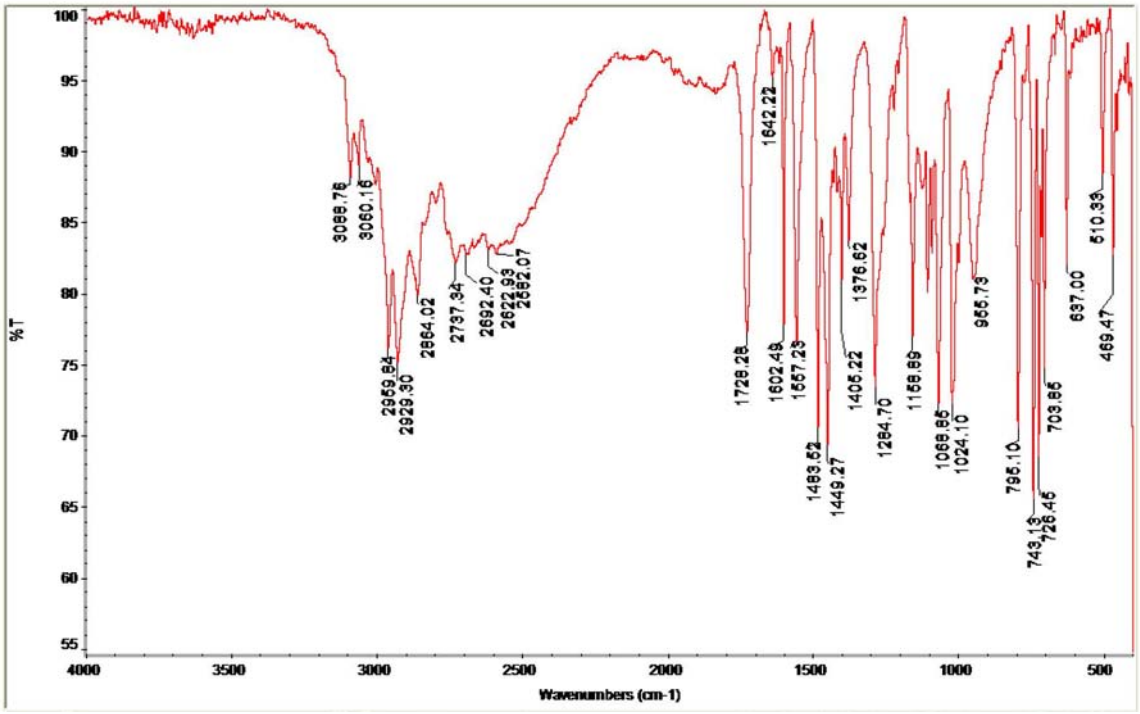

Figure S43. FT-IR of 2-(1*H*-tetrazol-5-yl) pyridine (**14**).

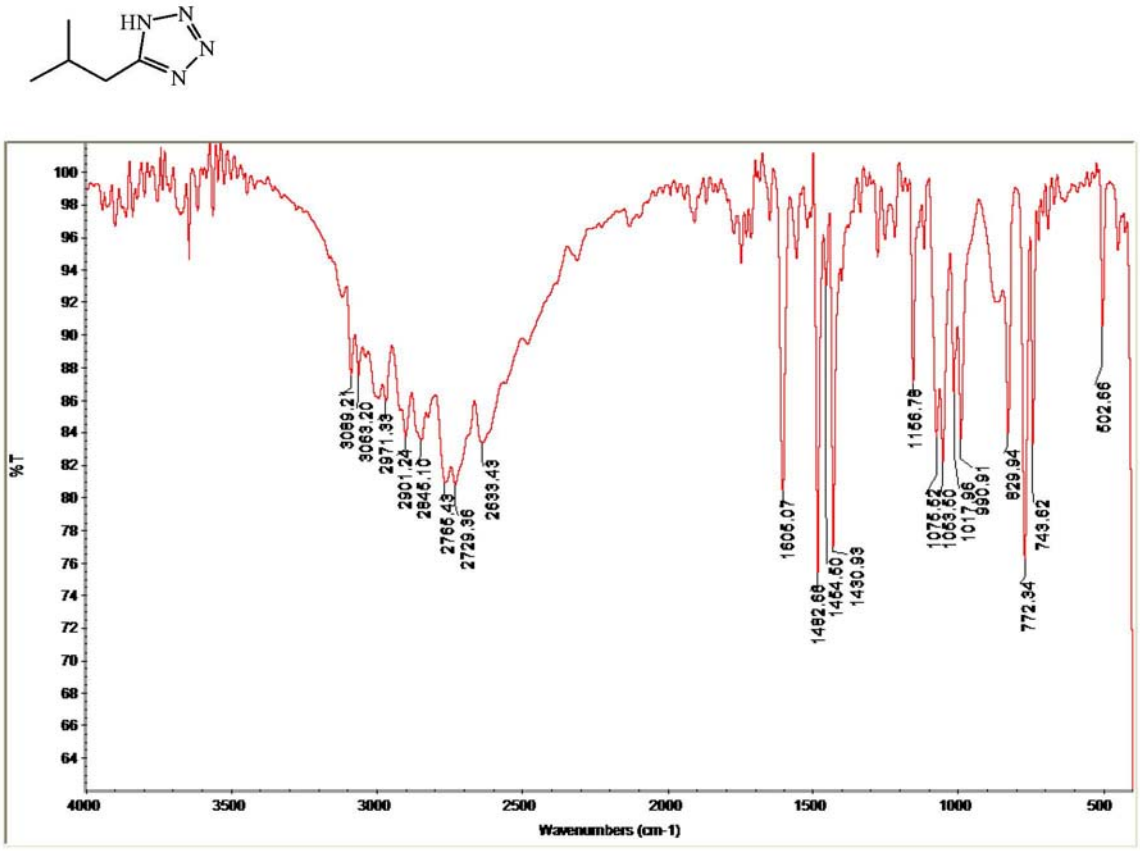

Figure S44. FT-IR of 5-isobutyl-1*H*-tetrazole (**15**).

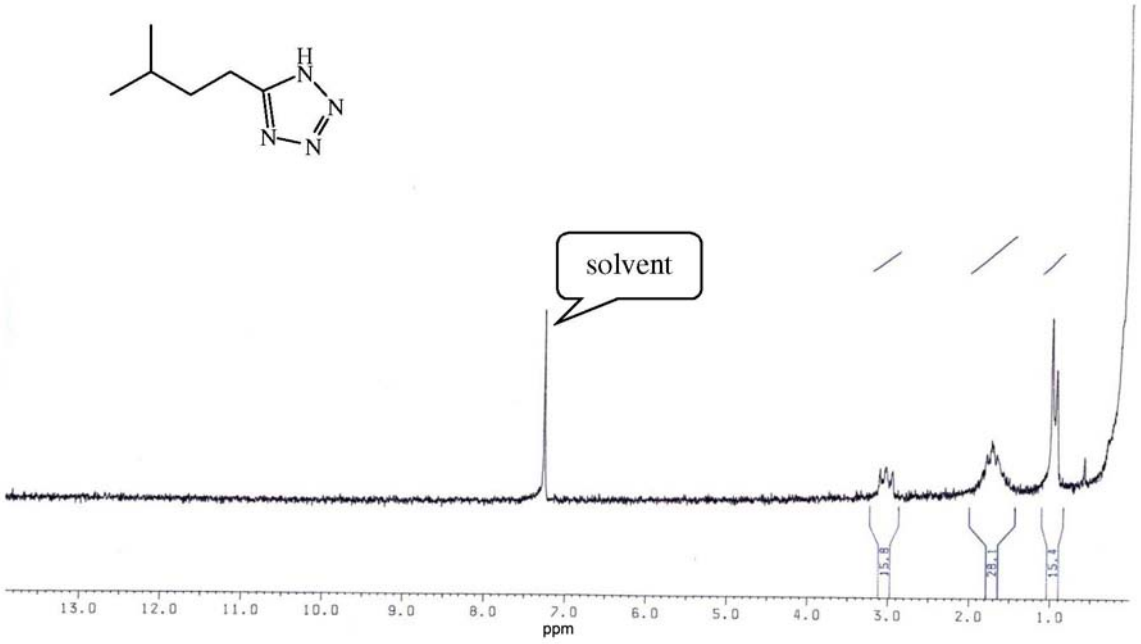

Figure S45. ^{1}H NMR (100 MHz, $CDCl_3$) of 5-isopentyl-1*H*-tetrazole (**16**).

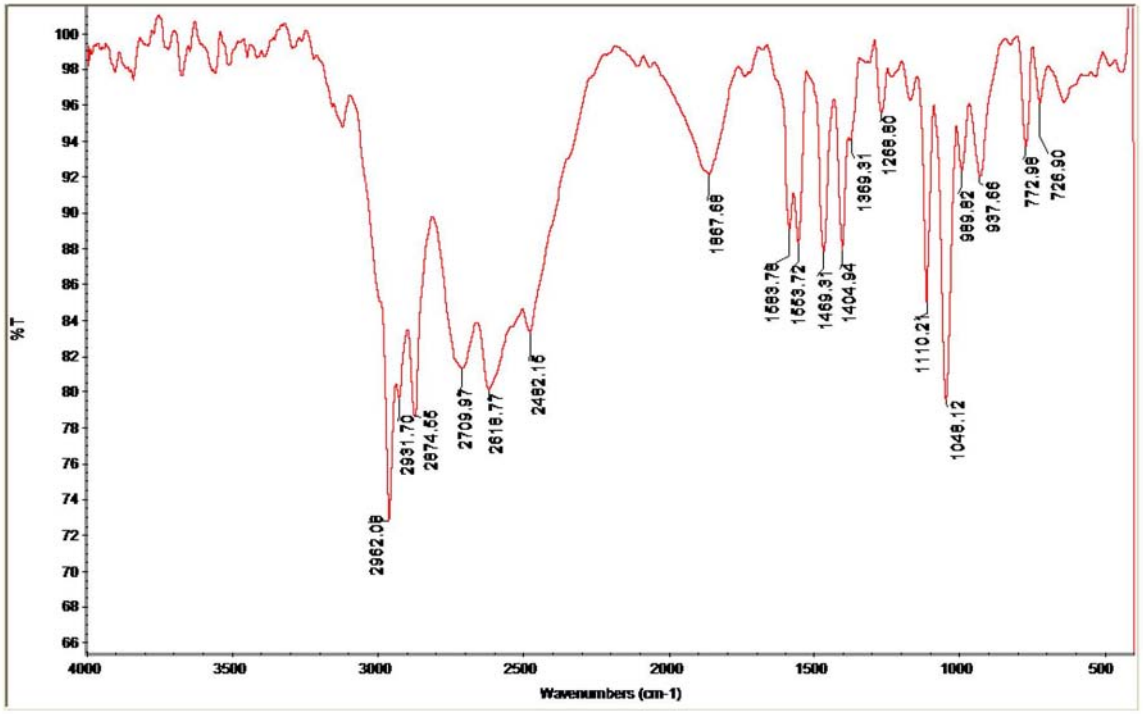

Figure S46. FT-IR of 5-isopentyl-1*H*-tetrazole (**16**).

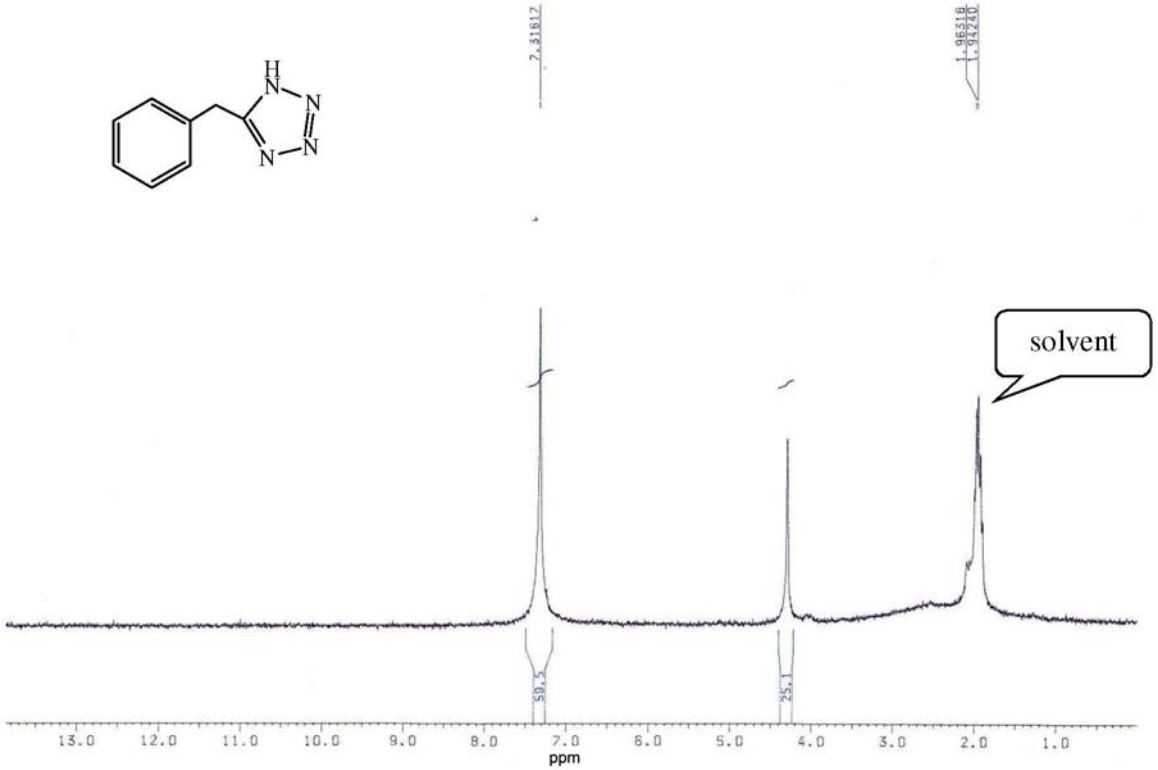

Figure S47. ^{1}H NMR (100 MHz, CD_3CN) of 5-benzyl-1*H*-tetrazole (**17**).

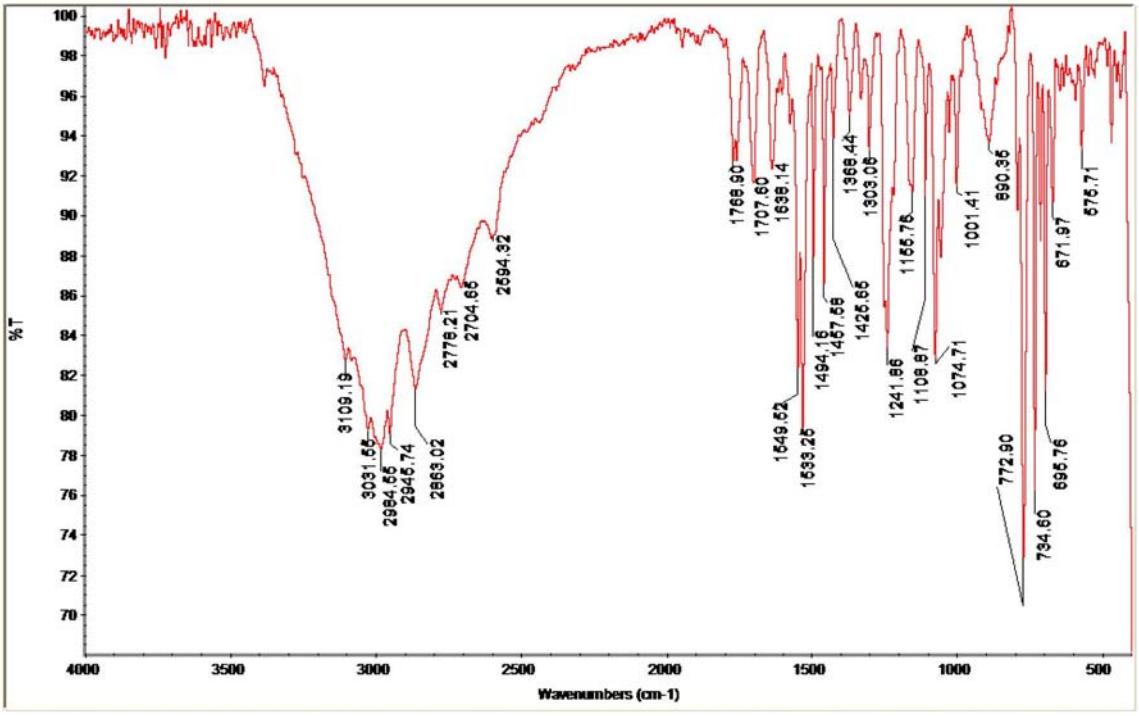

Figure S48. FT-IR of 5-benzyl-1*H*-tetrazole (**17**).