

Supplementary Material

N,N-Dialkyl-*N'*-Chlorosulfonyl Chloroformamidines in Heterocyclic Synthesis. Part X. The First Pyrazolo[1,5-*b*][1,2,4,6]thiatriazine Derivatives and their Unusual Reactions with Acylating Agents.

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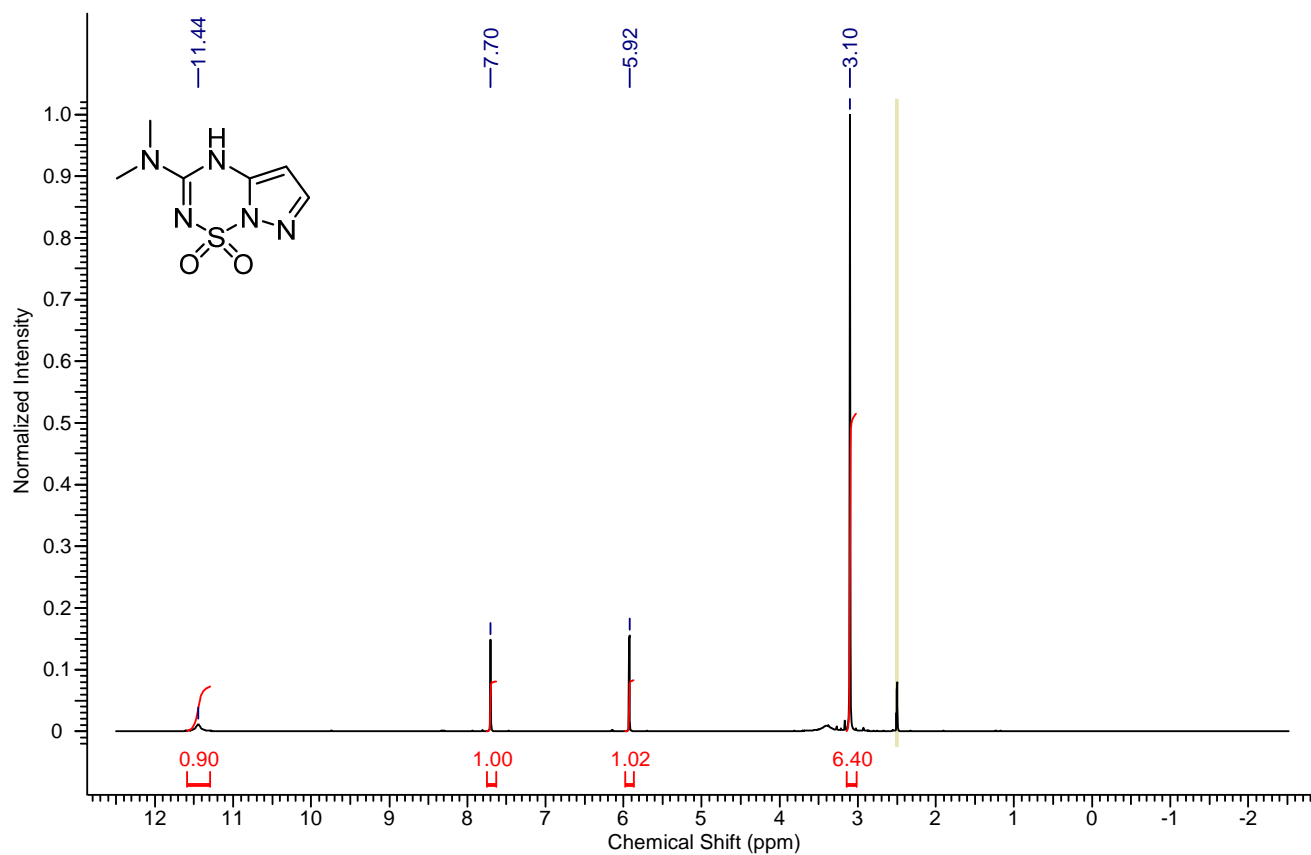
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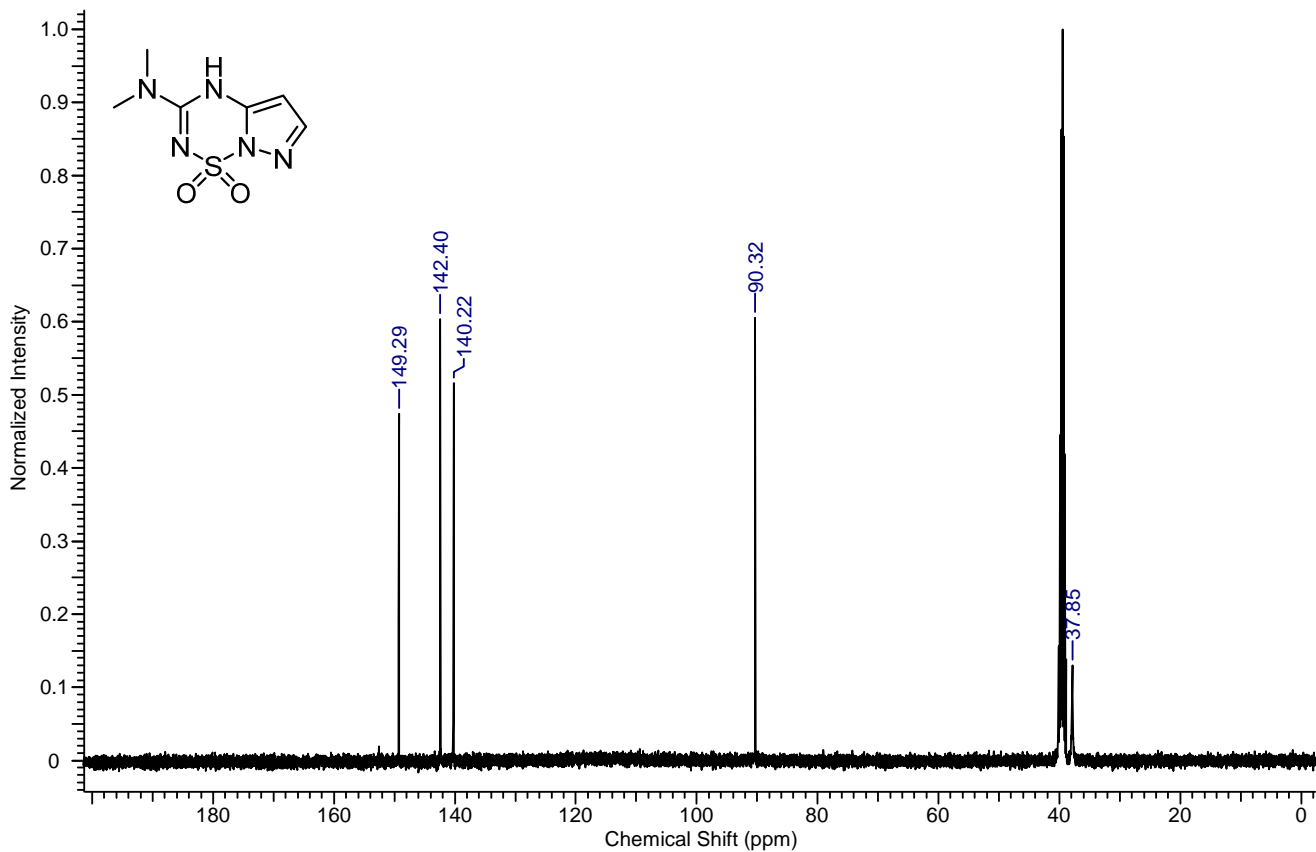
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| Pages S2-S13 | ¹ H NMR and ¹³ C NMR spectra of pyrazolo[1,5- <i>b</i>][1,2,4,6]thiatriazines 3 |
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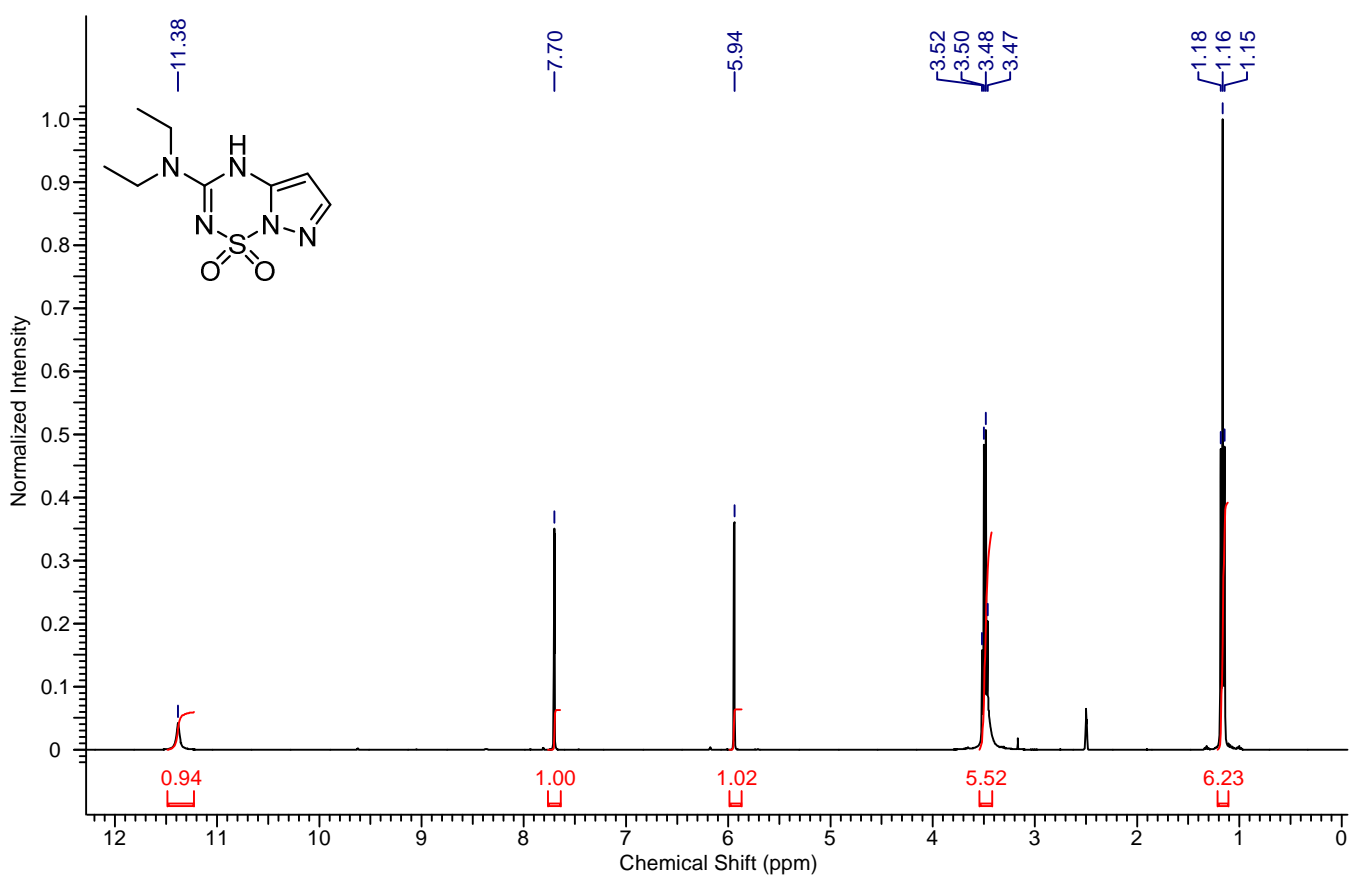
^1H NMR spectrum of **3a** ($\text{DMSO-}d^6$)



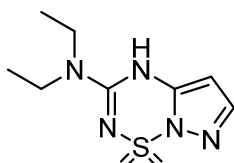
^{13}C NMR spectrum of **3a** ($\text{DMSO-}d^6$)

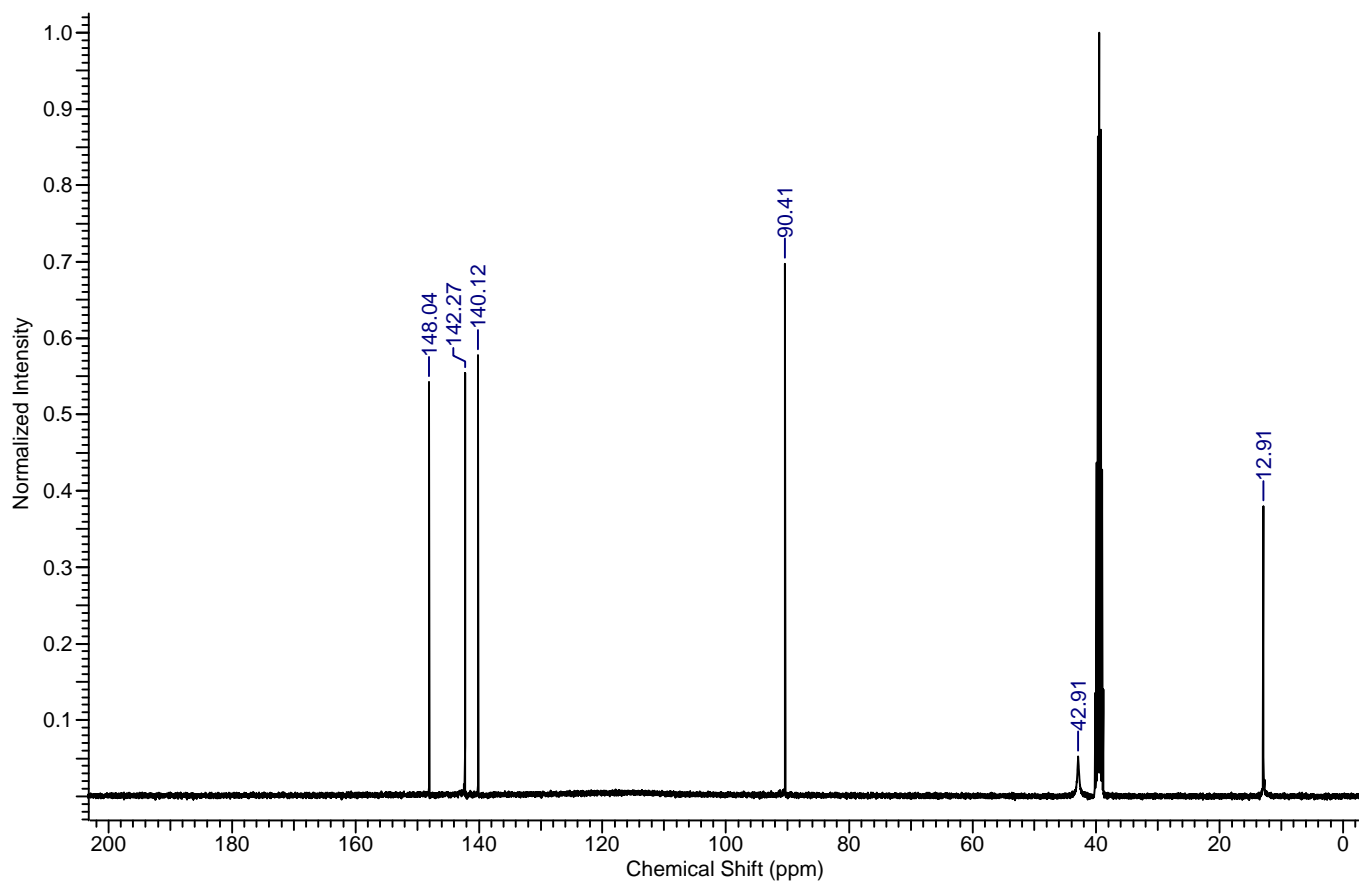


¹H NMR spectrum of **3b (DMSO-*d*₆)**

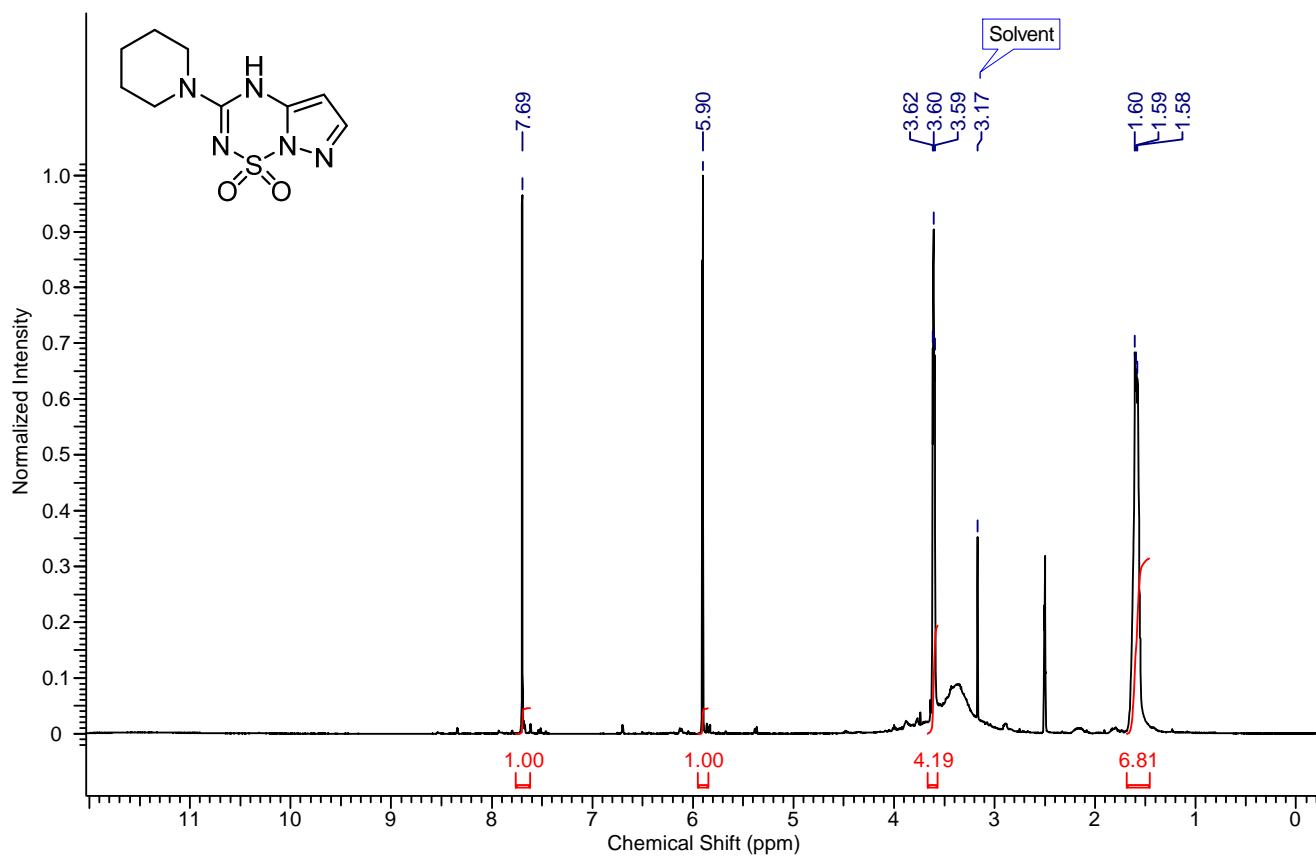


¹³C NMR spectrum of **3b (DMSO-*d*₆)**

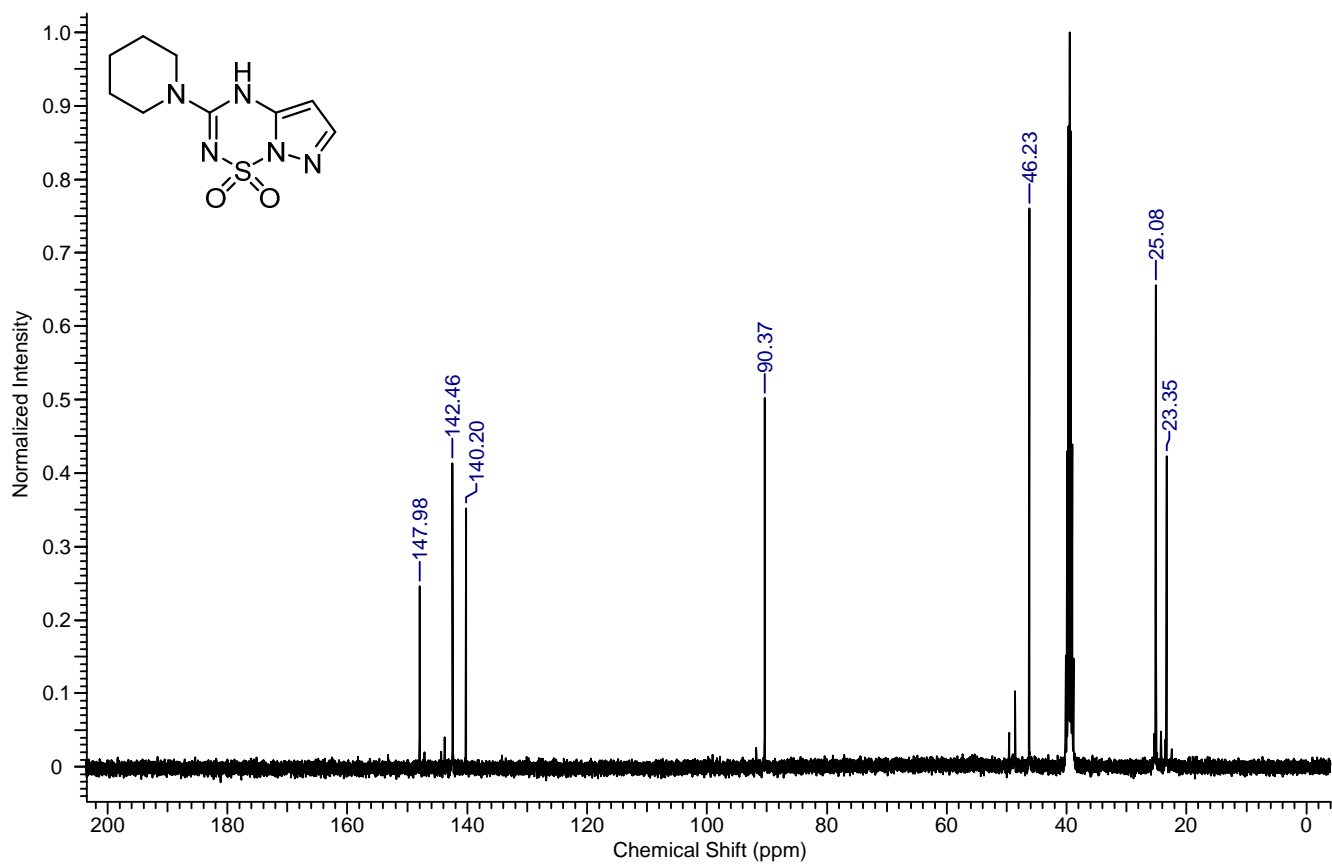




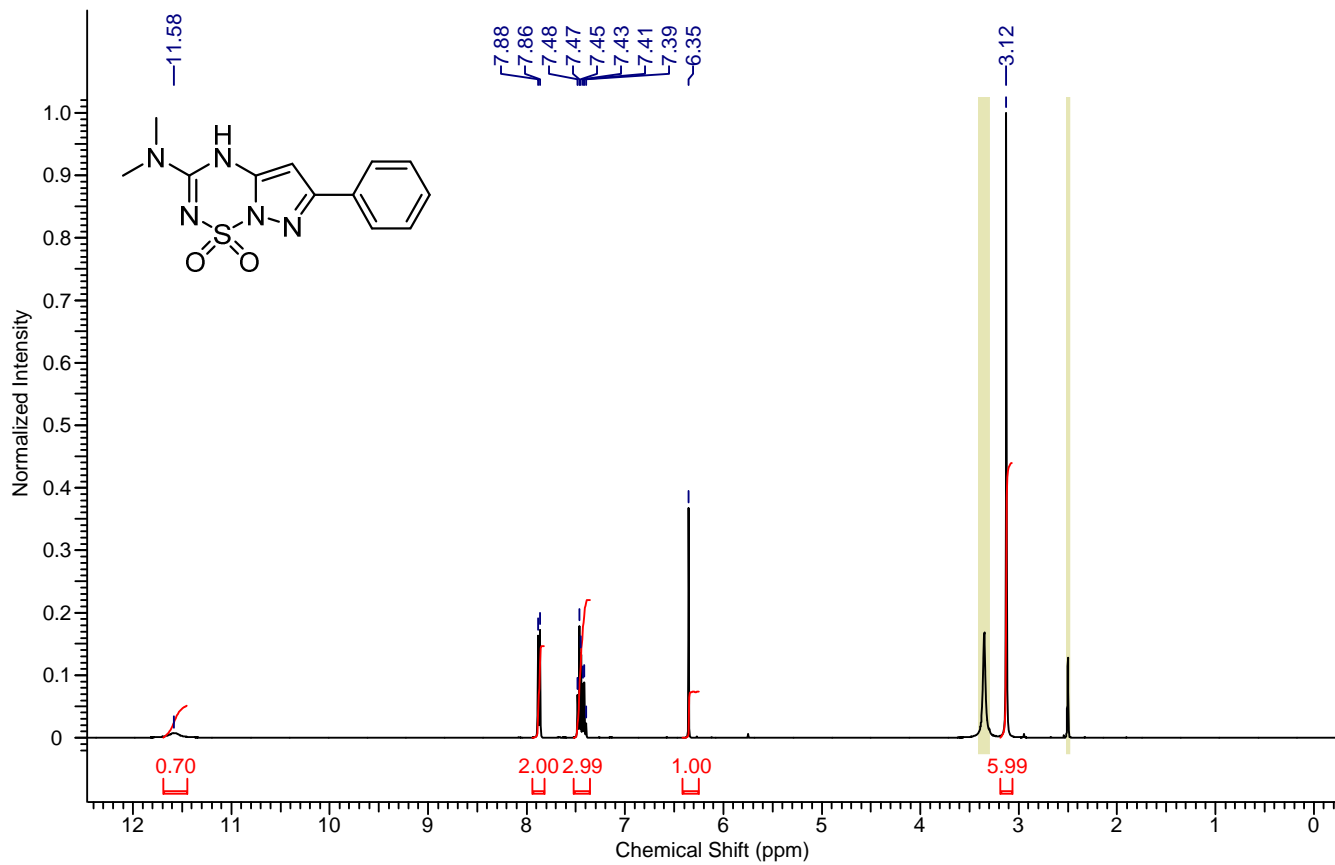
^1H NMR spectrum of **3c** (DMSO- d_6)



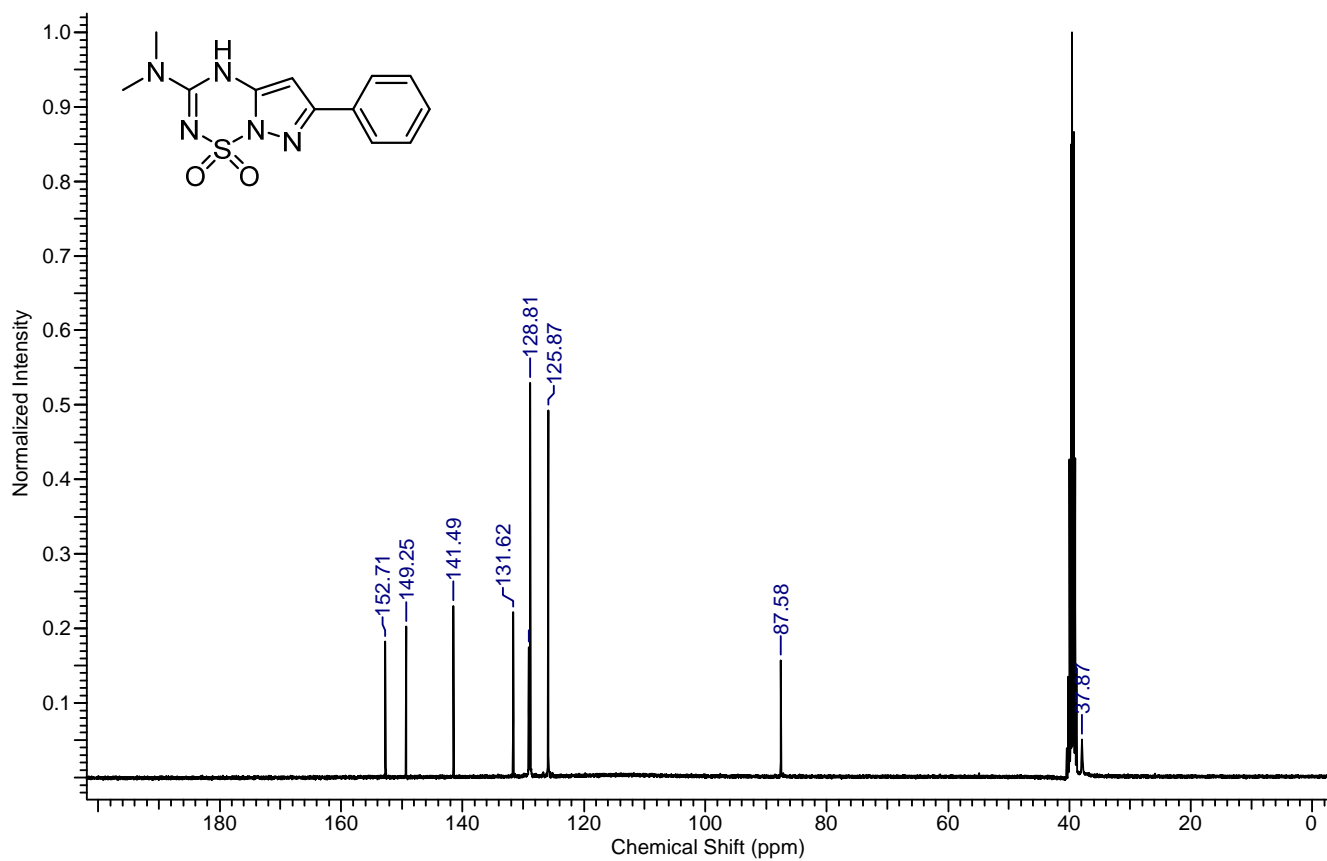
^{13}C NMR spectrum of **3c** (DMSO- d_6)



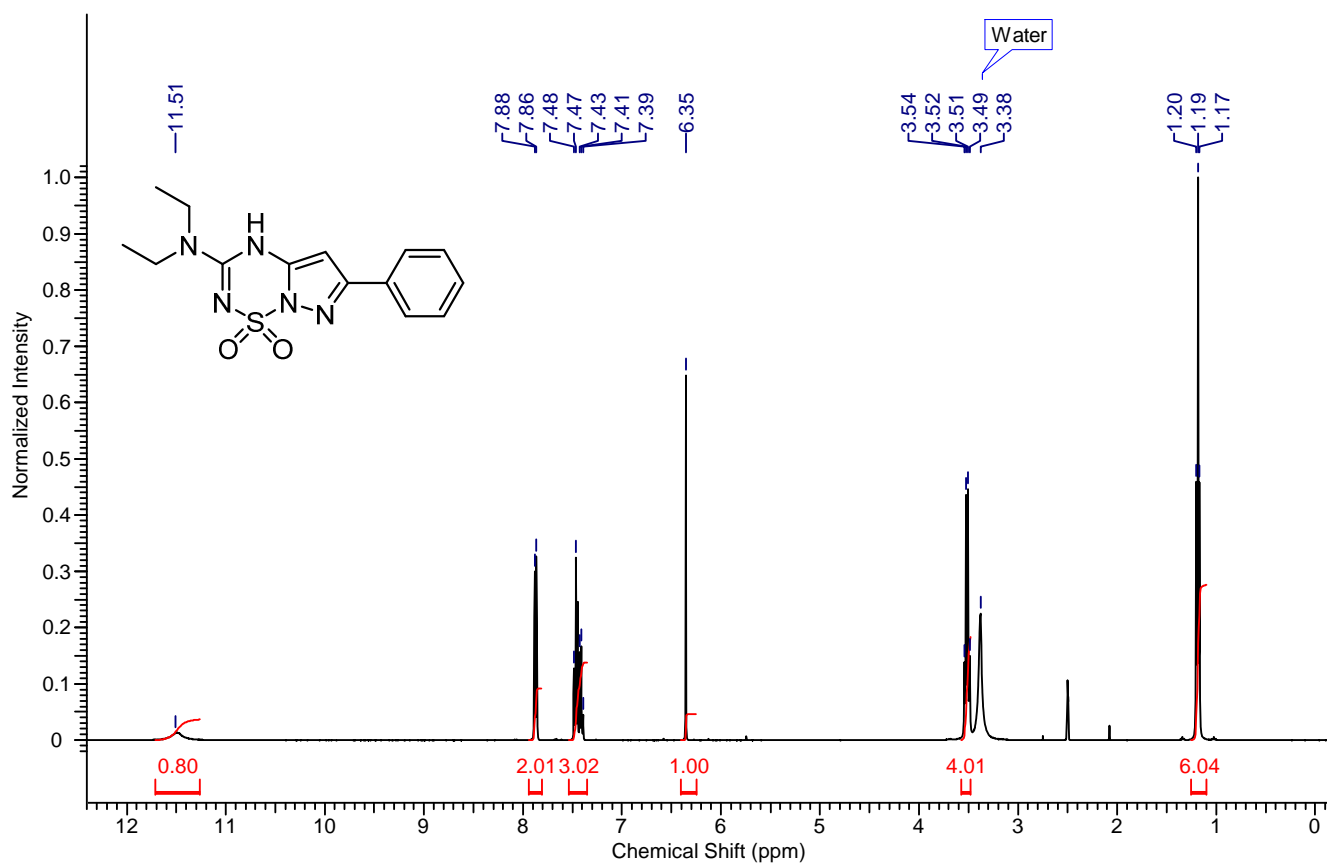
¹H NMR spectrum of **3d (DMSO-*d*⁶)**



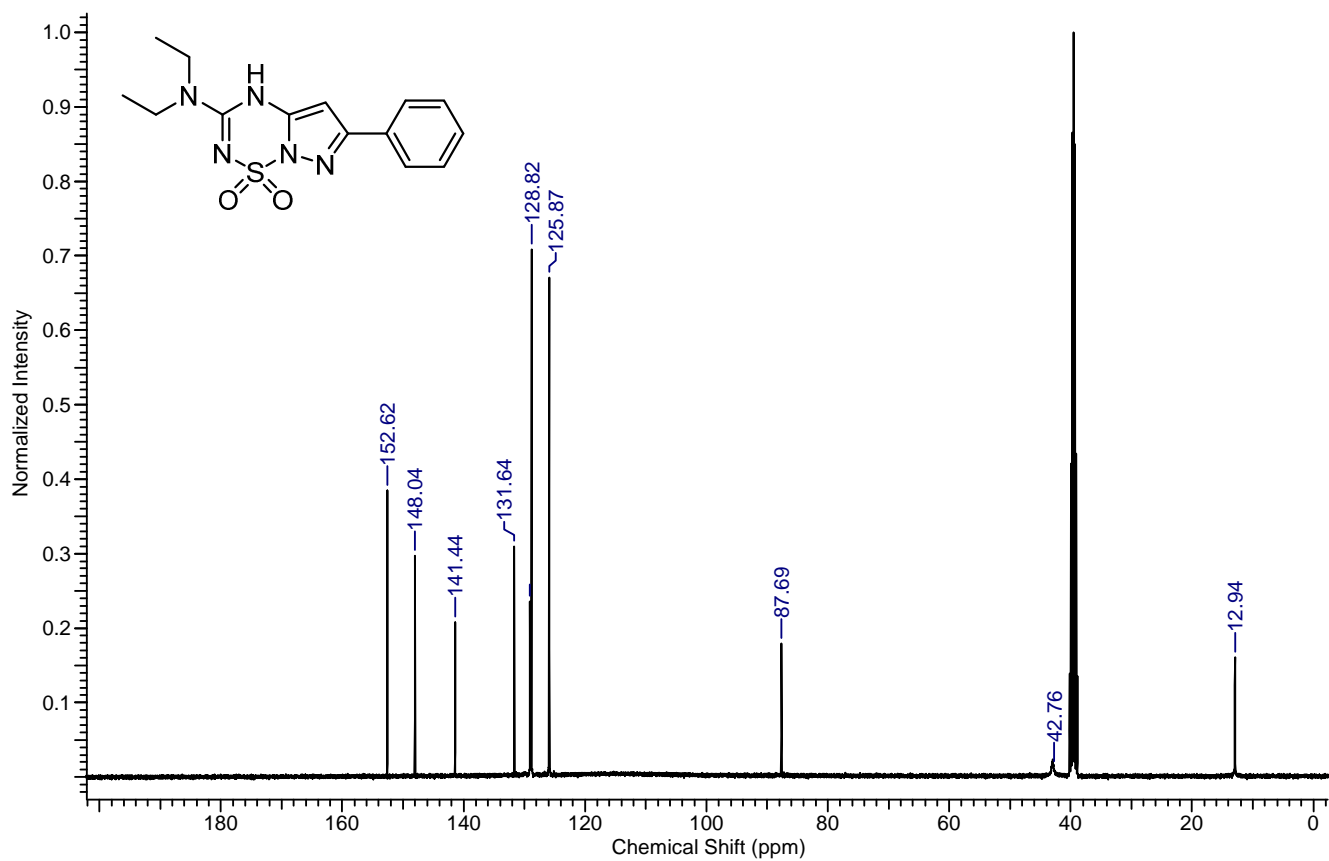
¹³C NMR spectrum of **3d (DMSO-*d*⁶)**



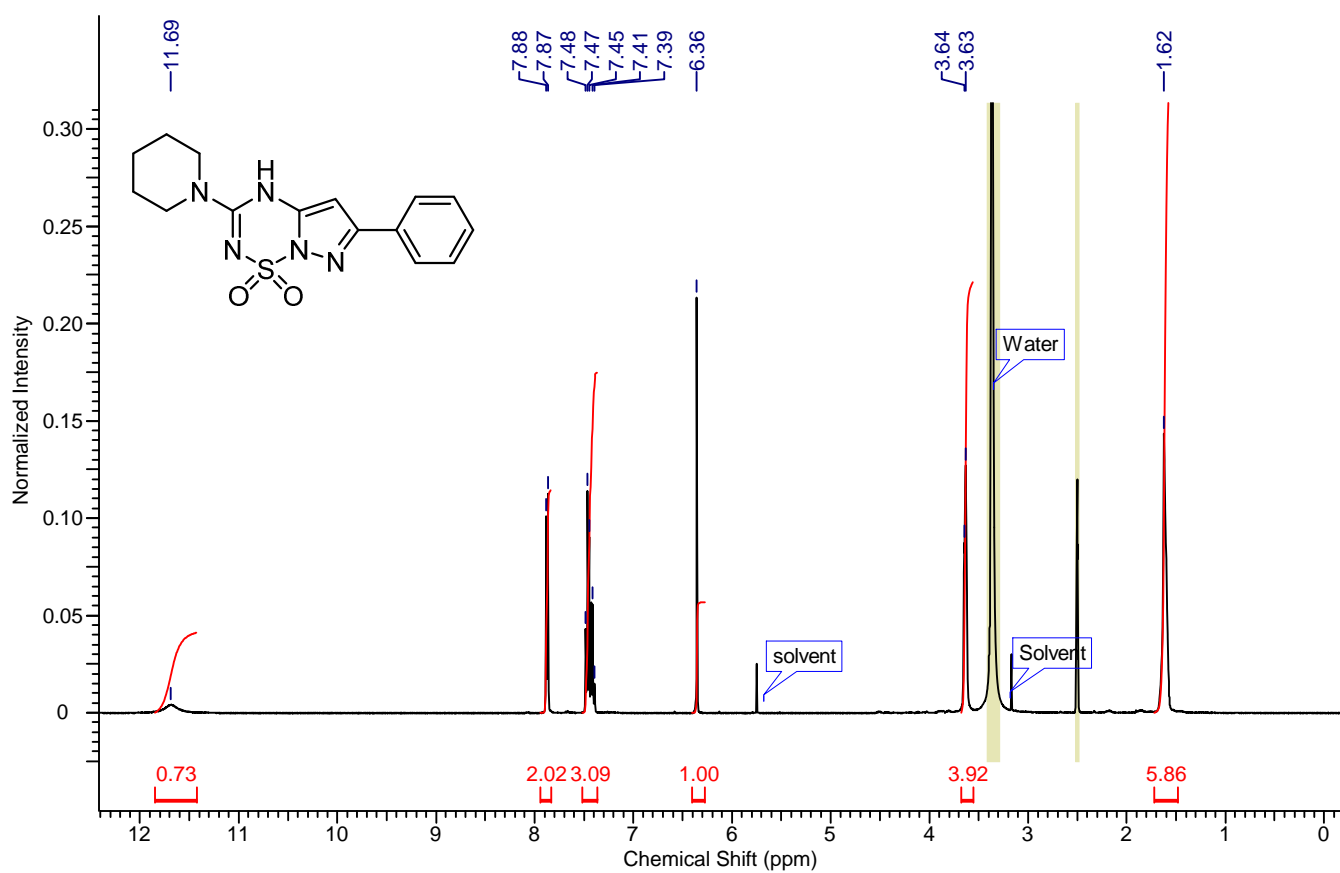
¹H NMR spectrum of **3e (DMSO-*d*₆)**



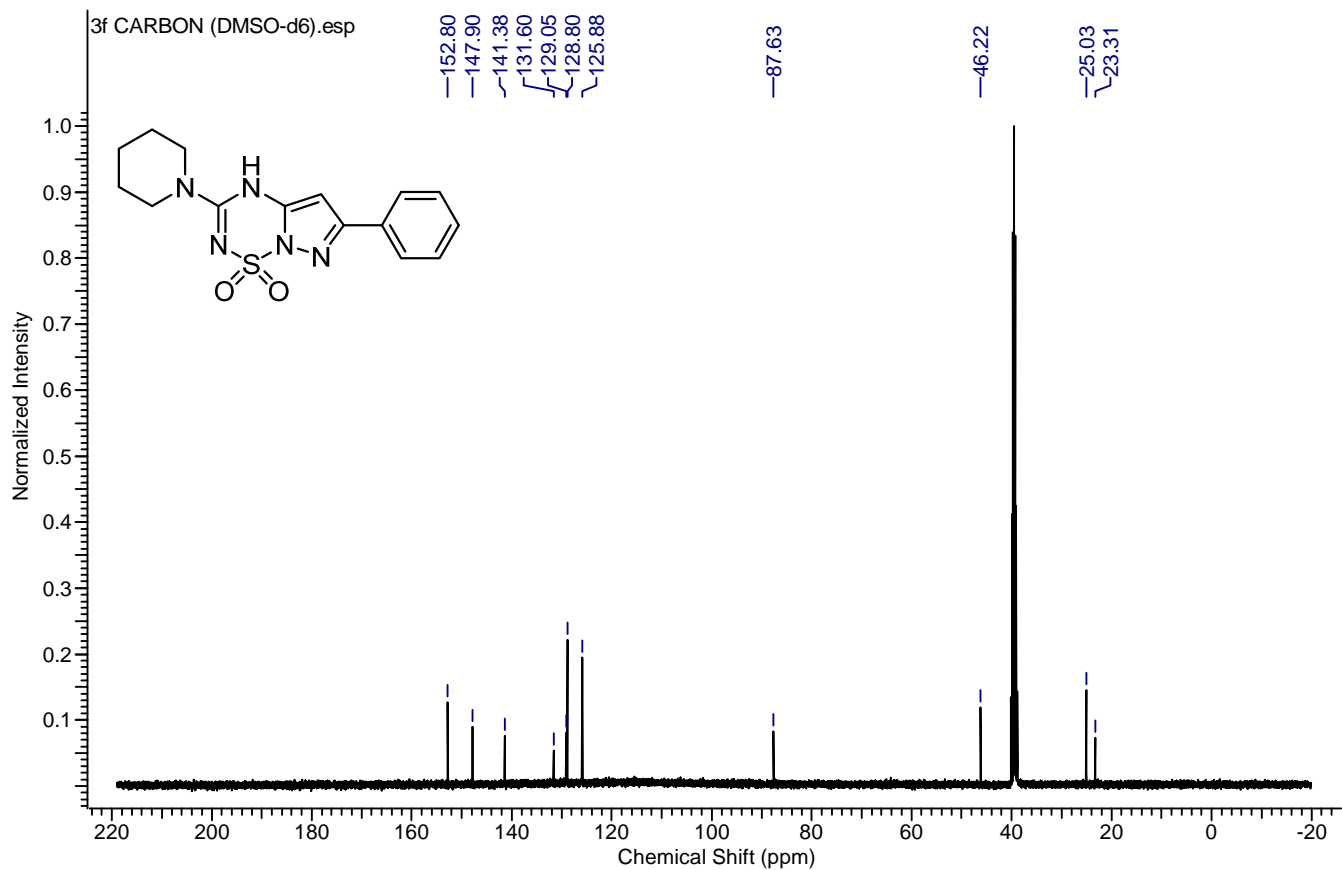
¹³C NMR spectrum of **3e (DMSO-*d*₆)**



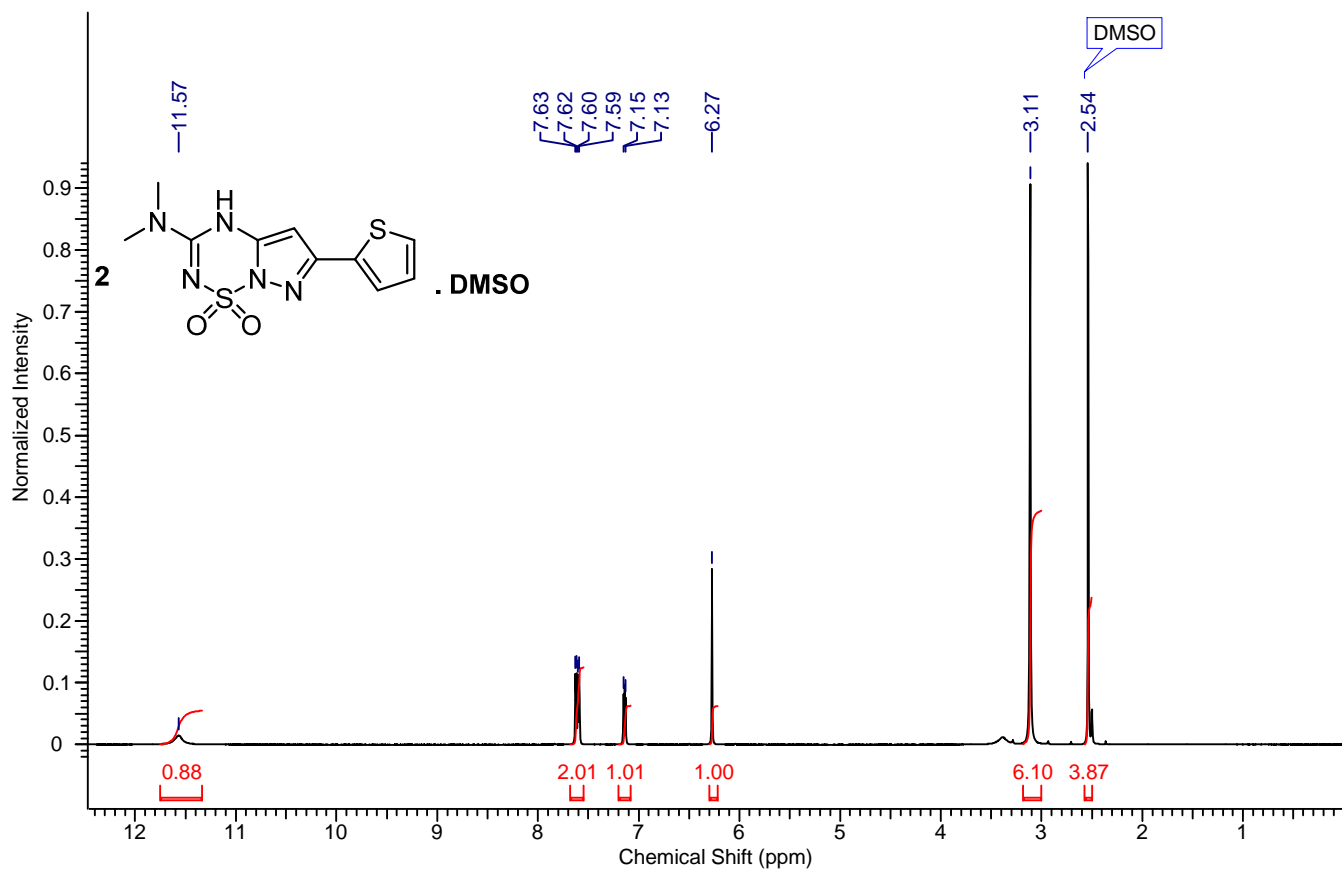
¹H NMR spectrum of **3f (DMSO-*d*₆)**



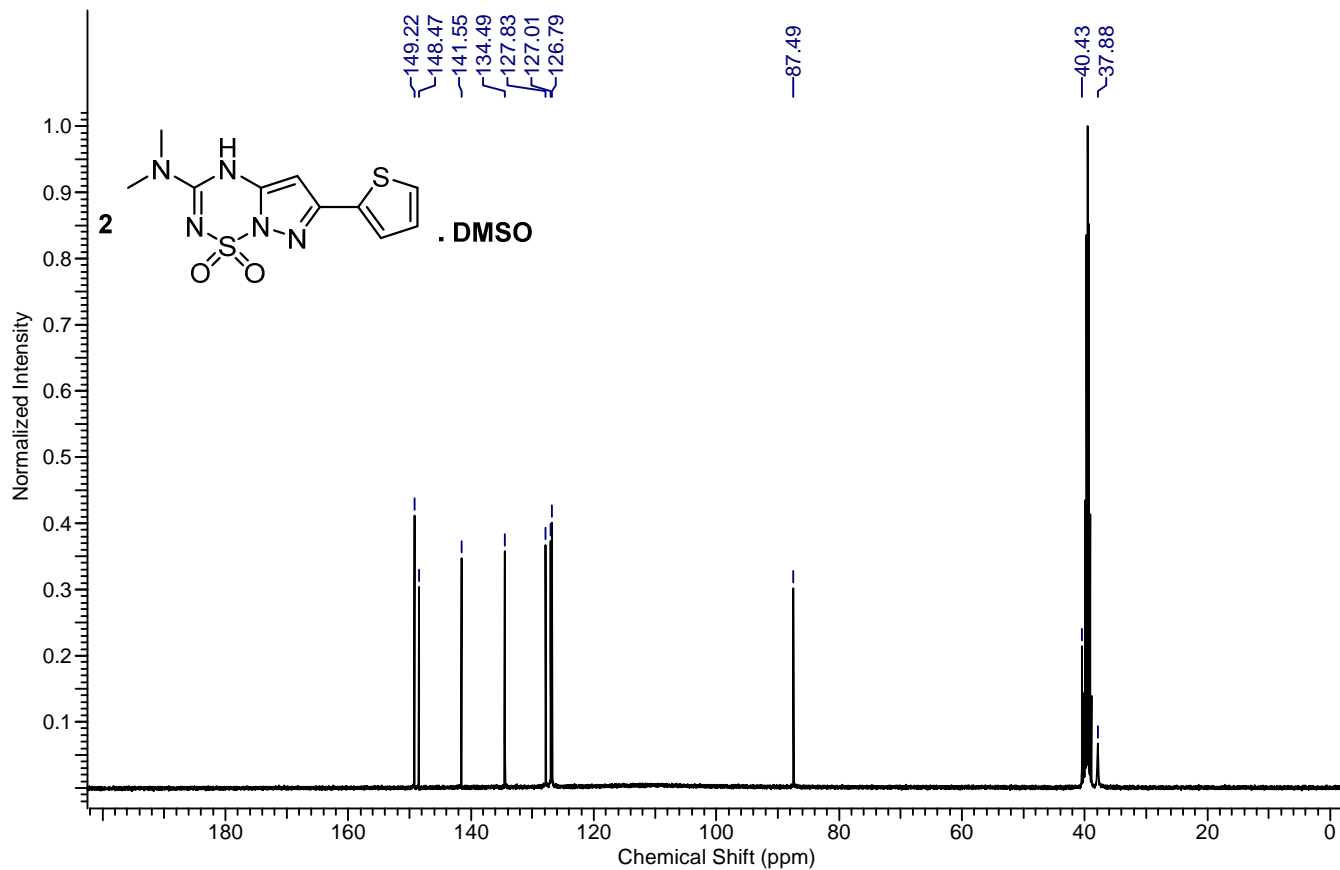
¹³C NMR spectrum of **3f (DMSO-*d*₆)**



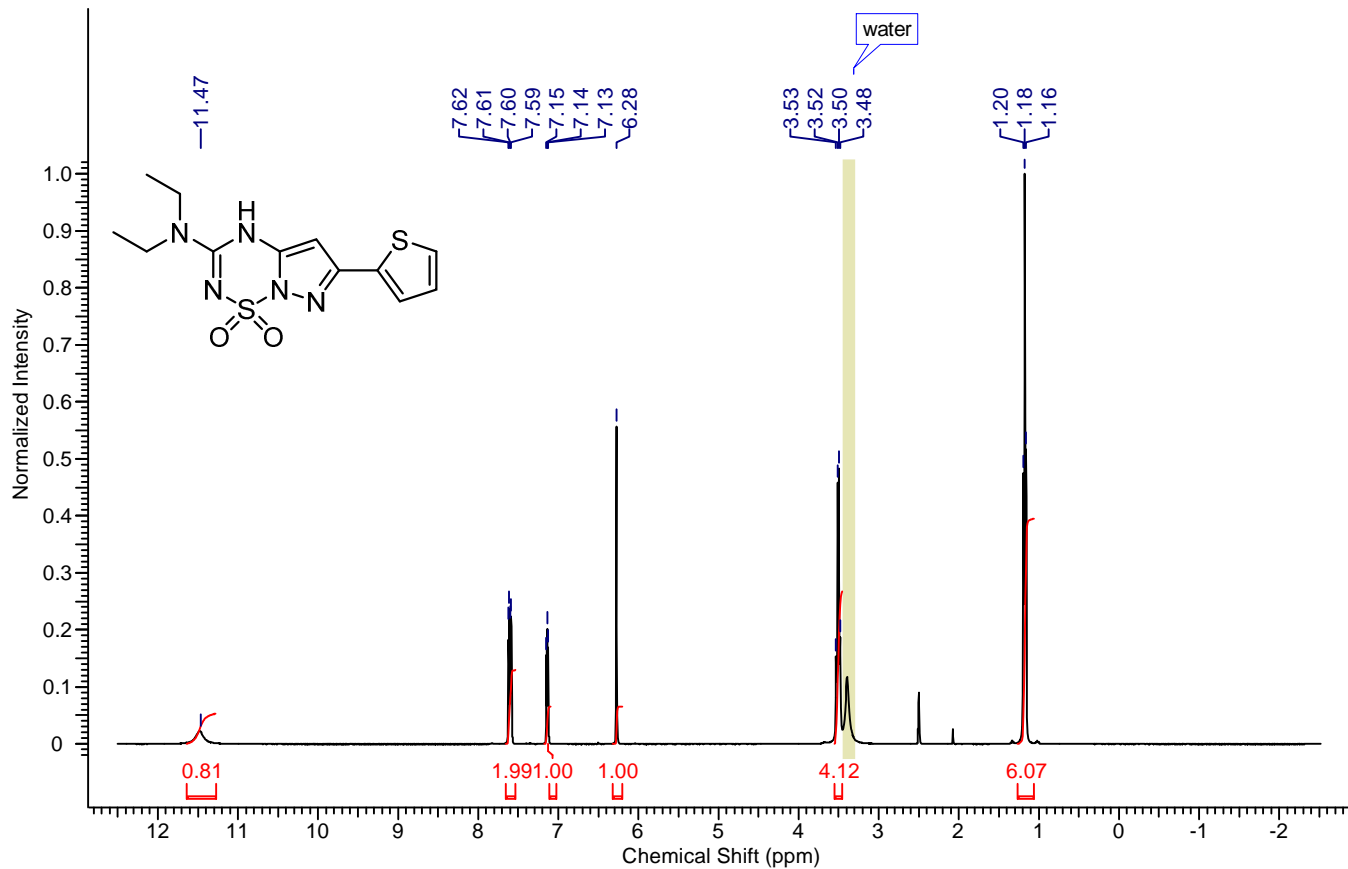
^1H NMR spectrum of **3g** (DMSO- d^6)



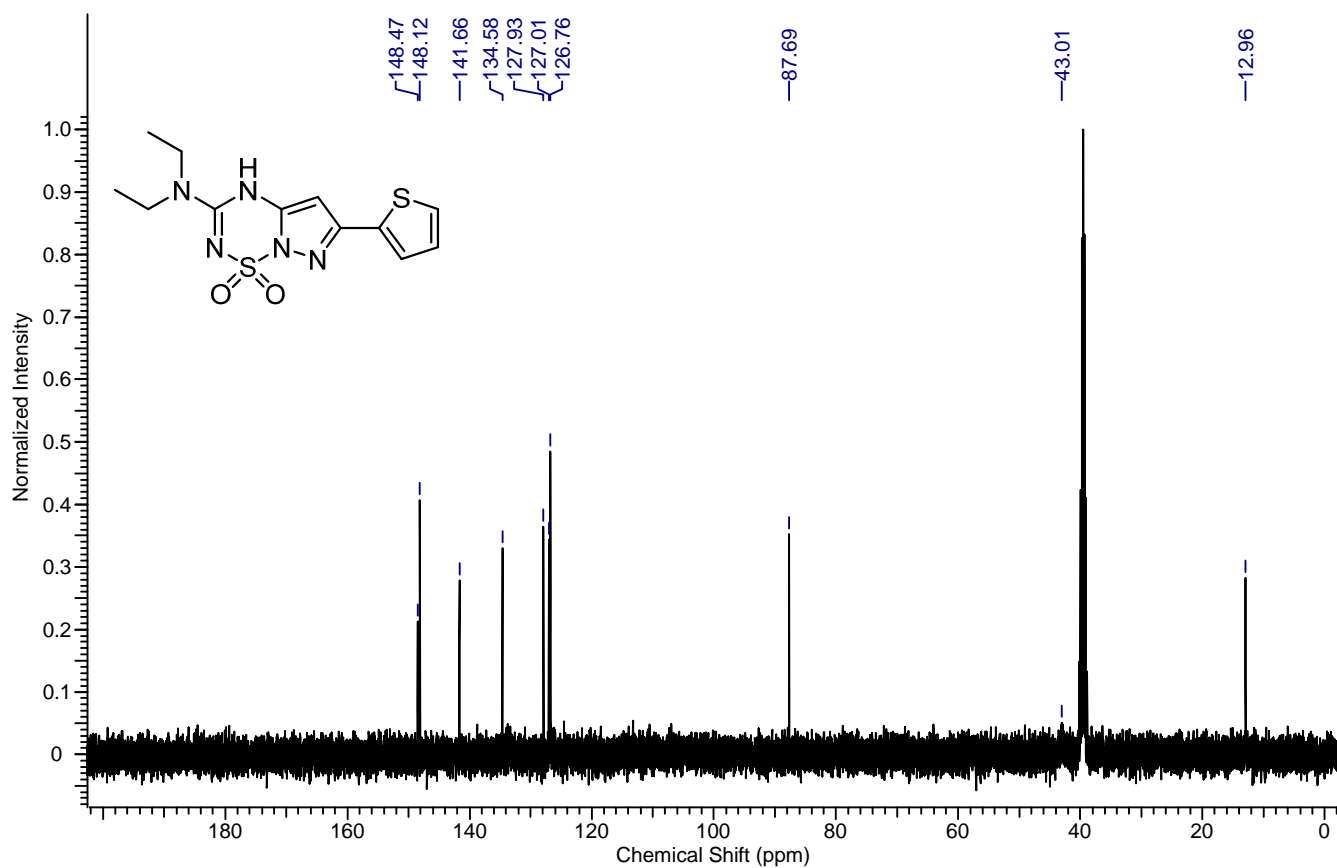
^{13}C NMR spectrum of **3g** (DMSO- d^6)



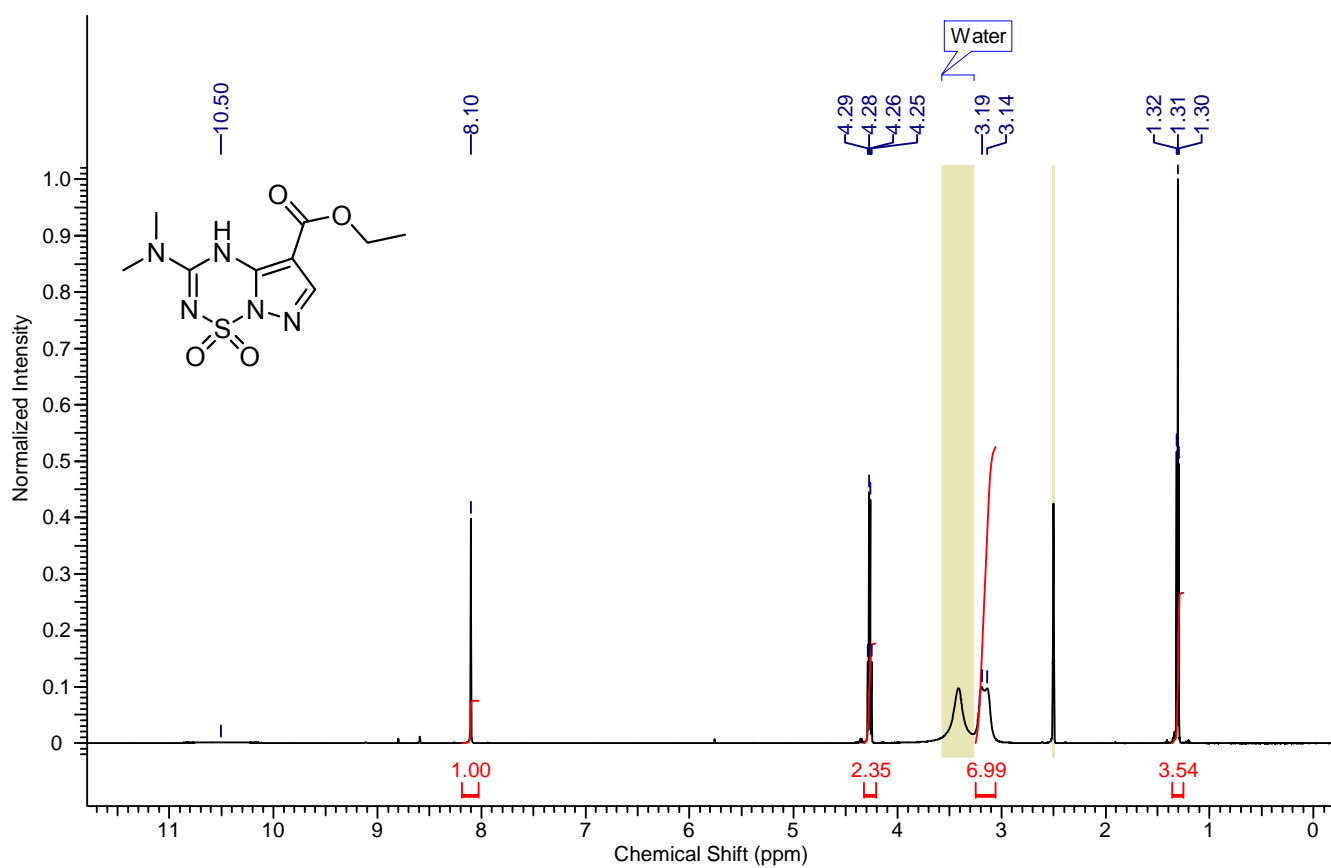
^1H NMR spectrum of **3h** ($\text{DMSO-}d^6$)



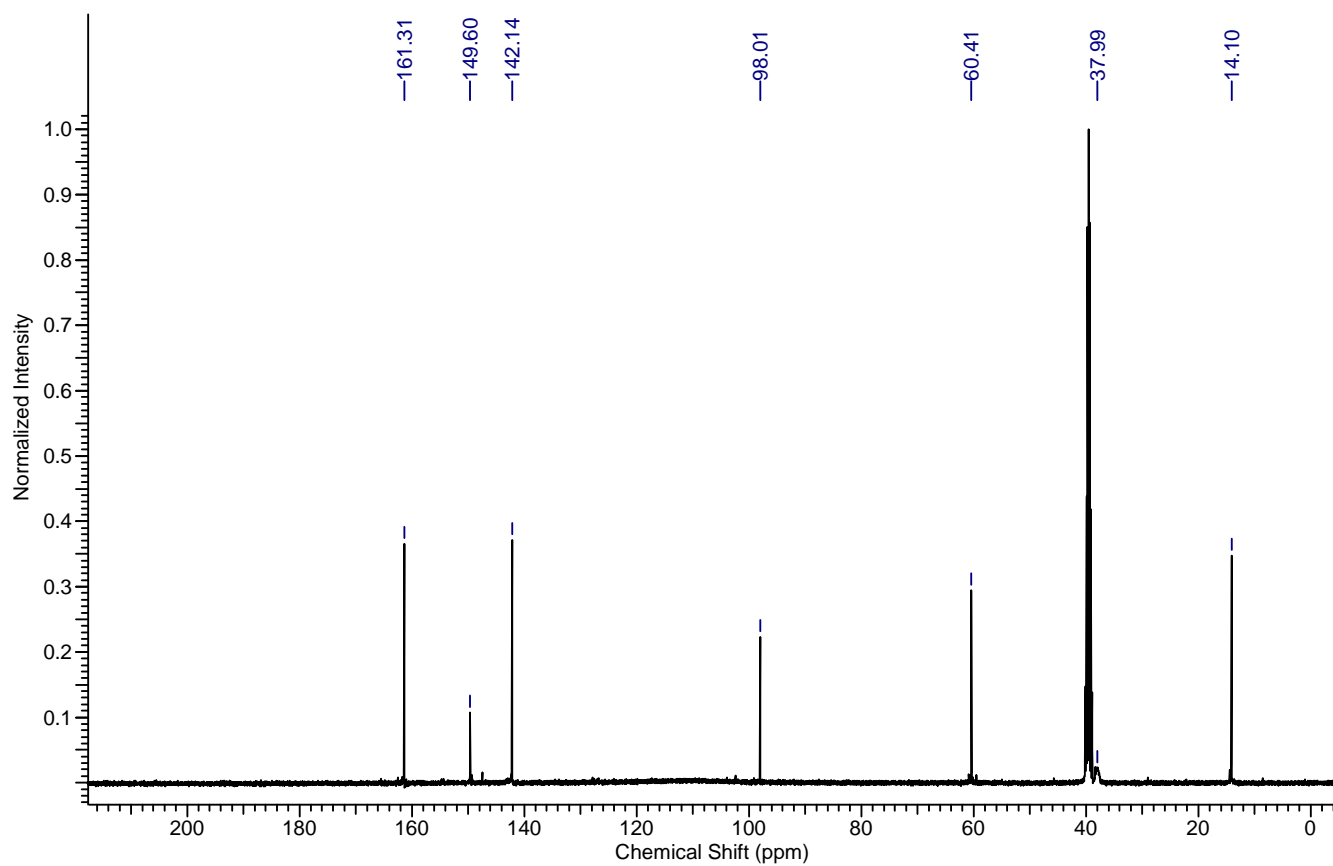
^{13}C NMR spectrum of **3h** ($\text{DMSO-}d_6$)



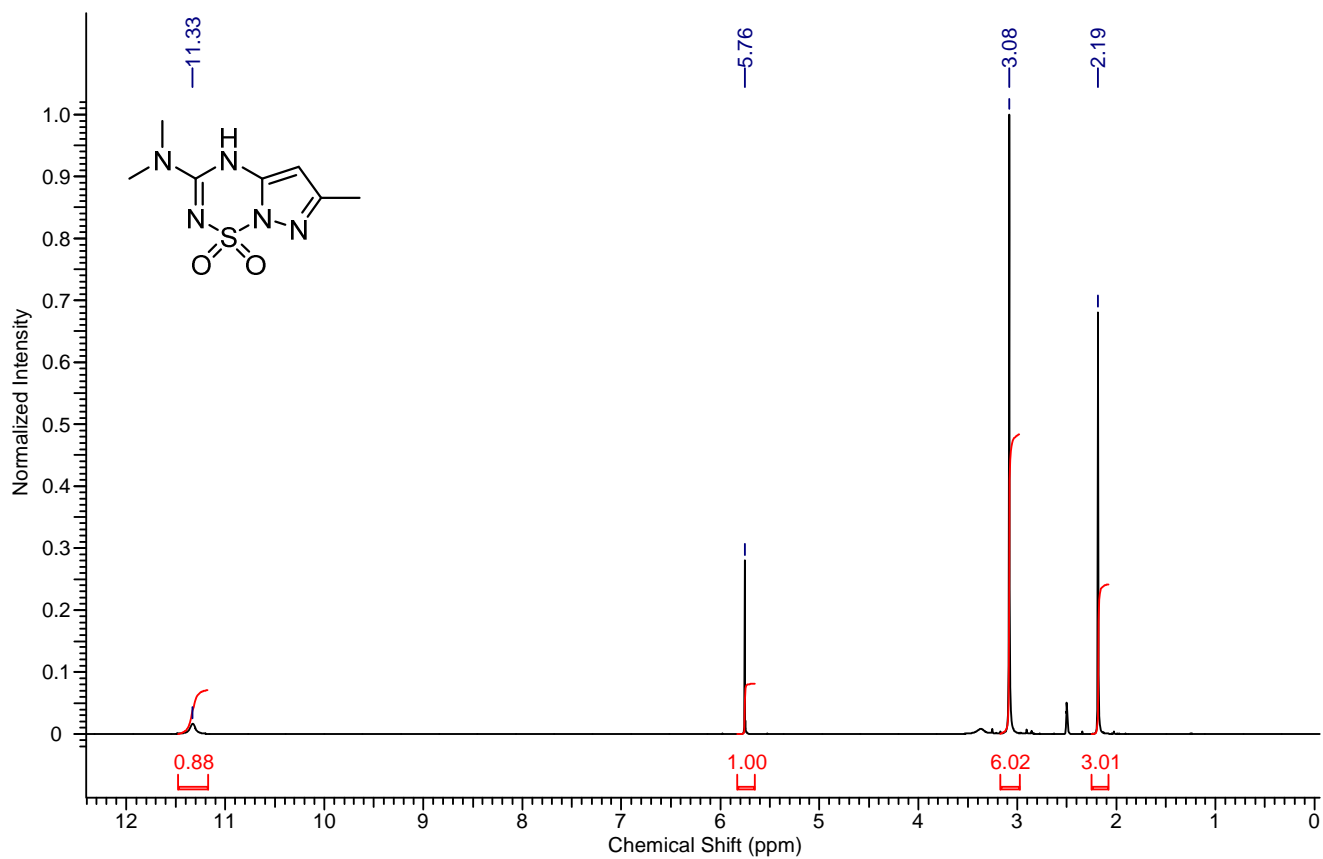
^1H NMR spectrum of **3i** ($\text{DMSO-}d_6$)



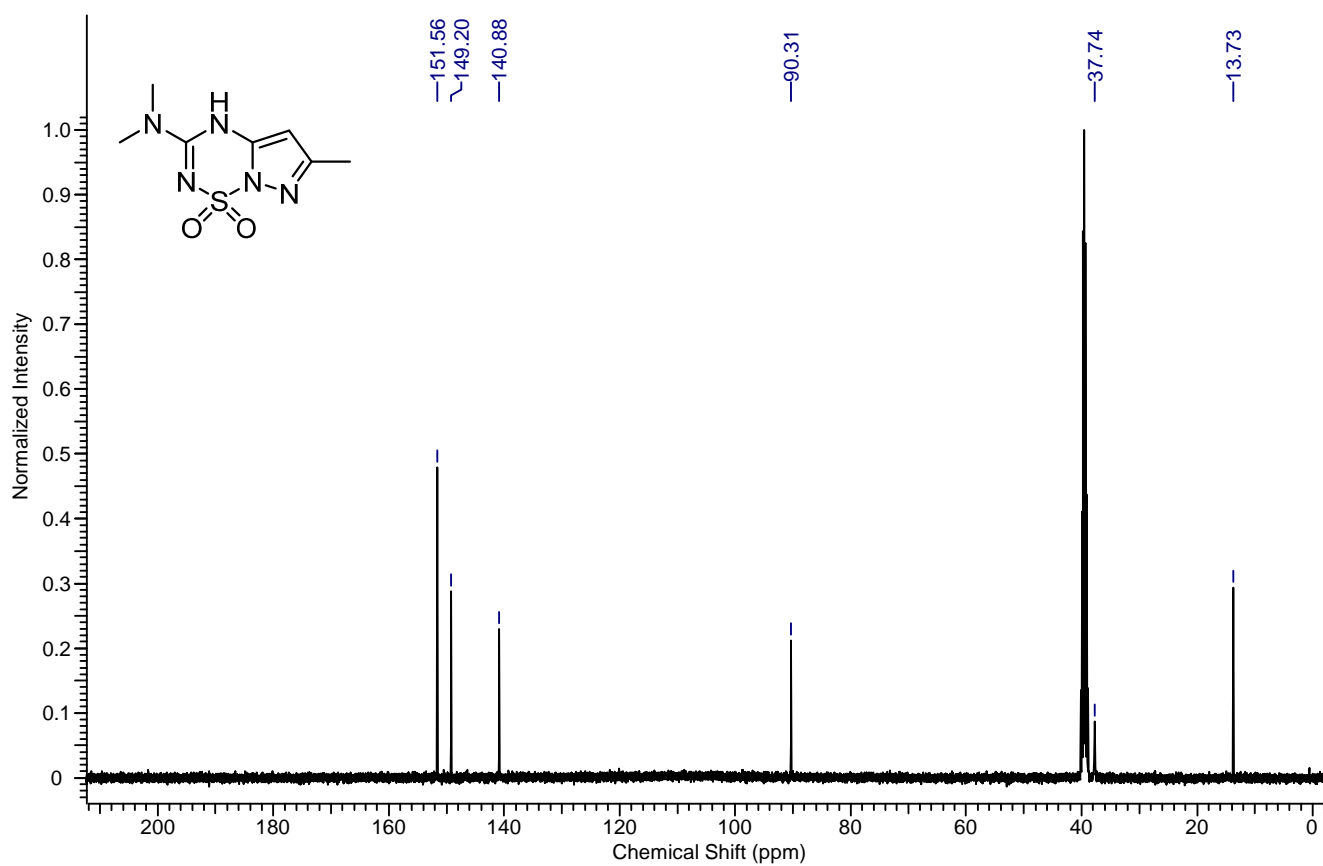
^{13}C NMR spectrum of **3i** ($\text{DMSO-}d_6$)



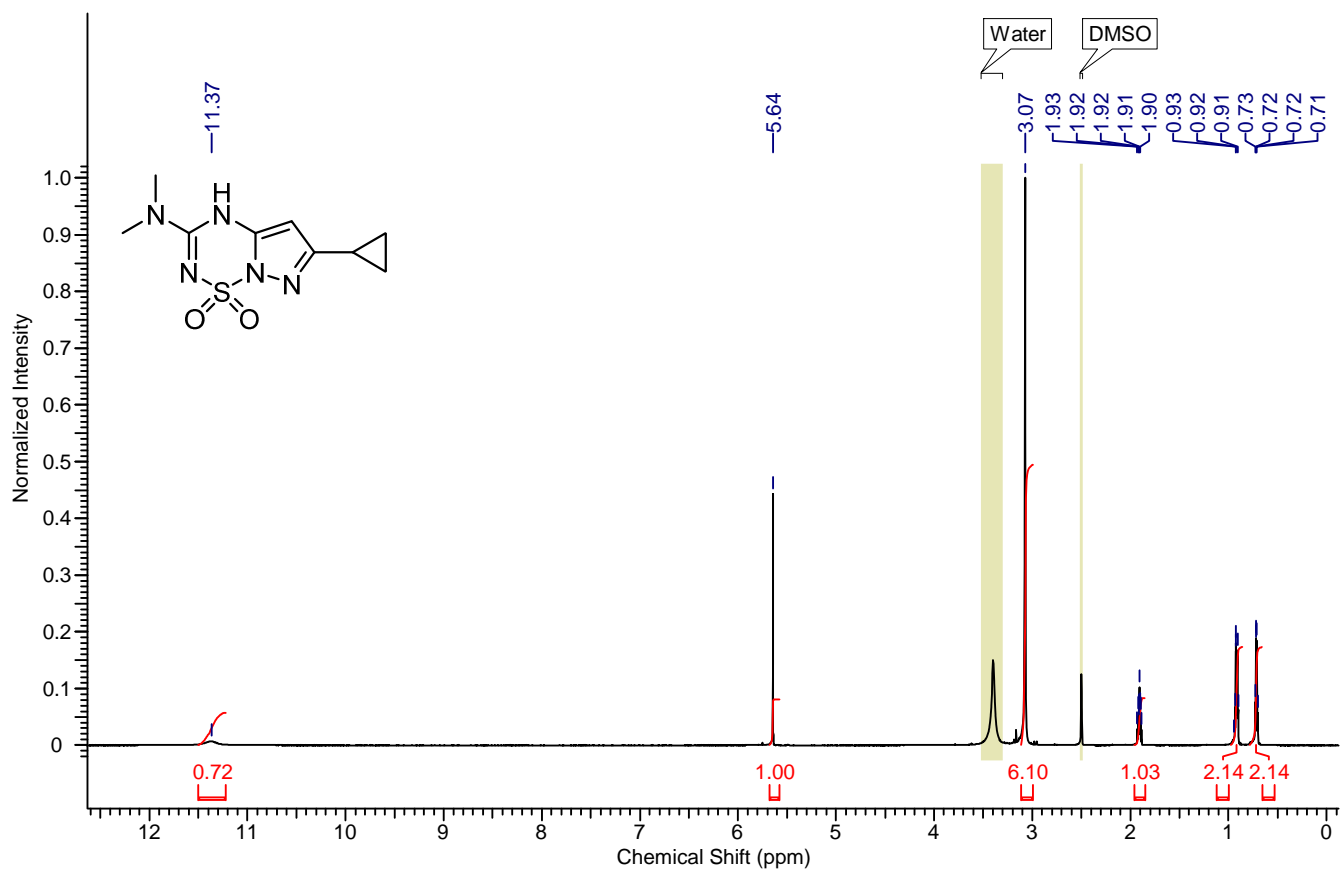
^1H NMR spectrum of **3j** ($\text{DMSO-}d_6$)



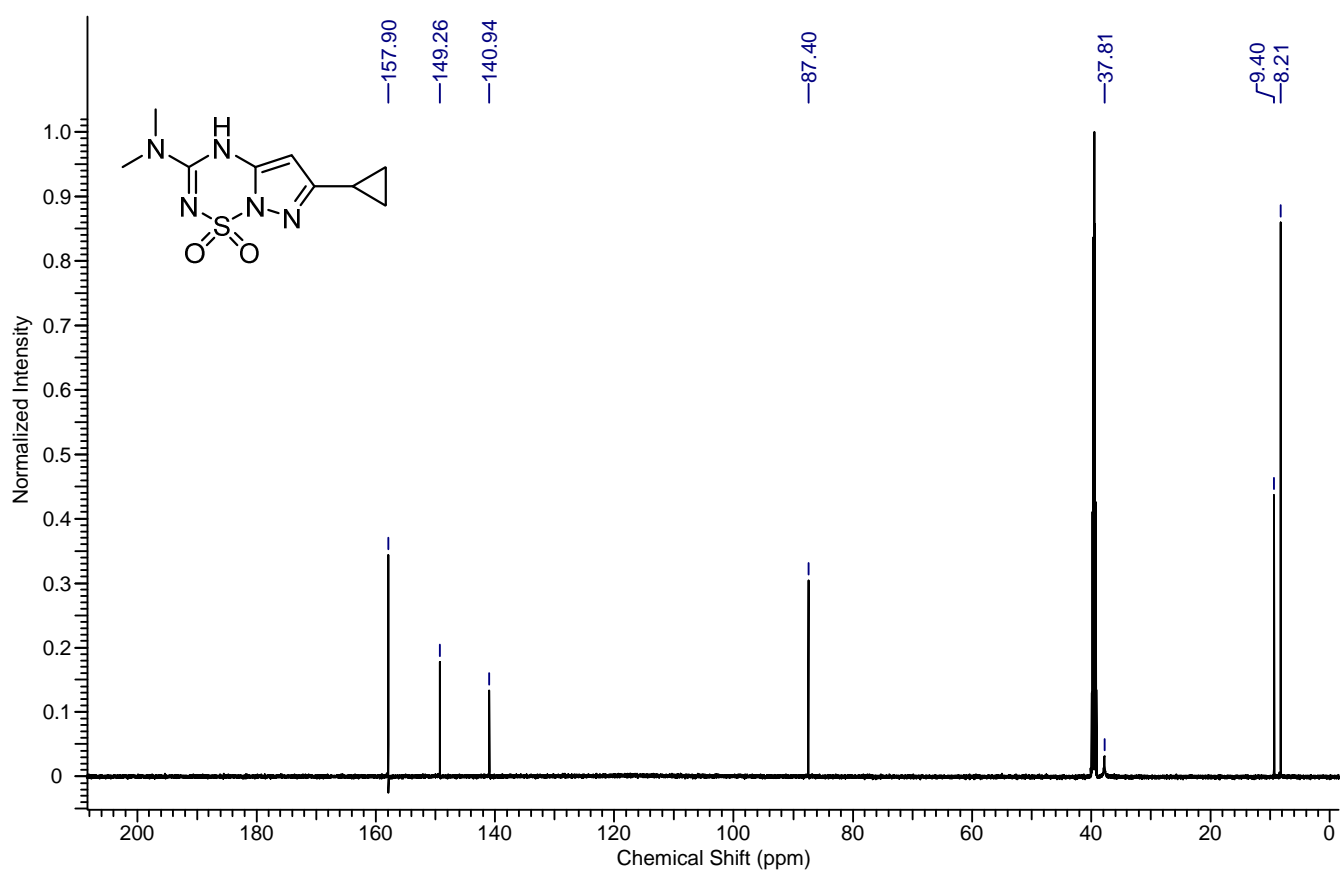
¹³C NMR spectrum of **3j** (DMSO-*d*₆)



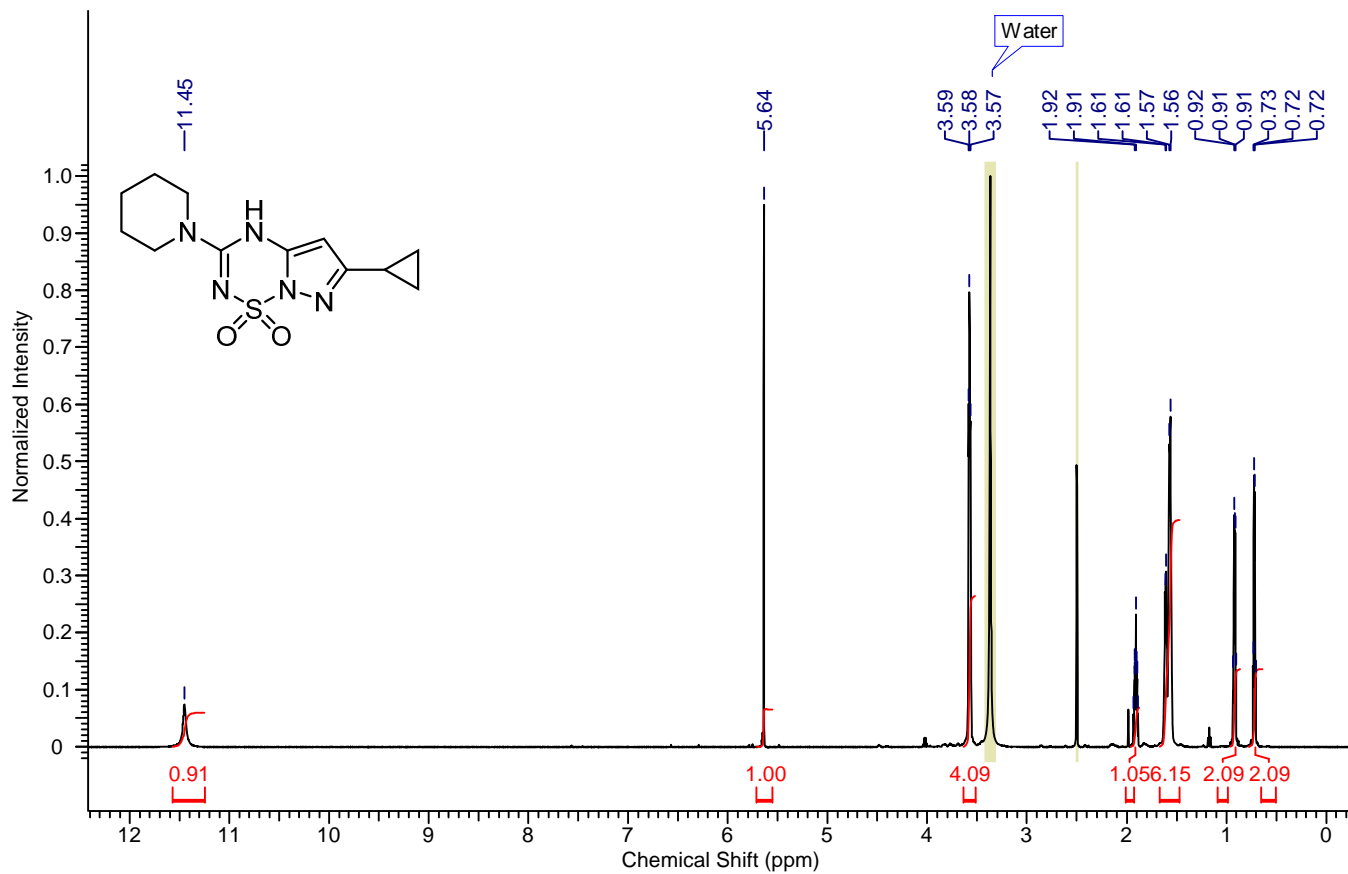
¹H NMR spectrum of **3k** (DMSO-*d*₆)



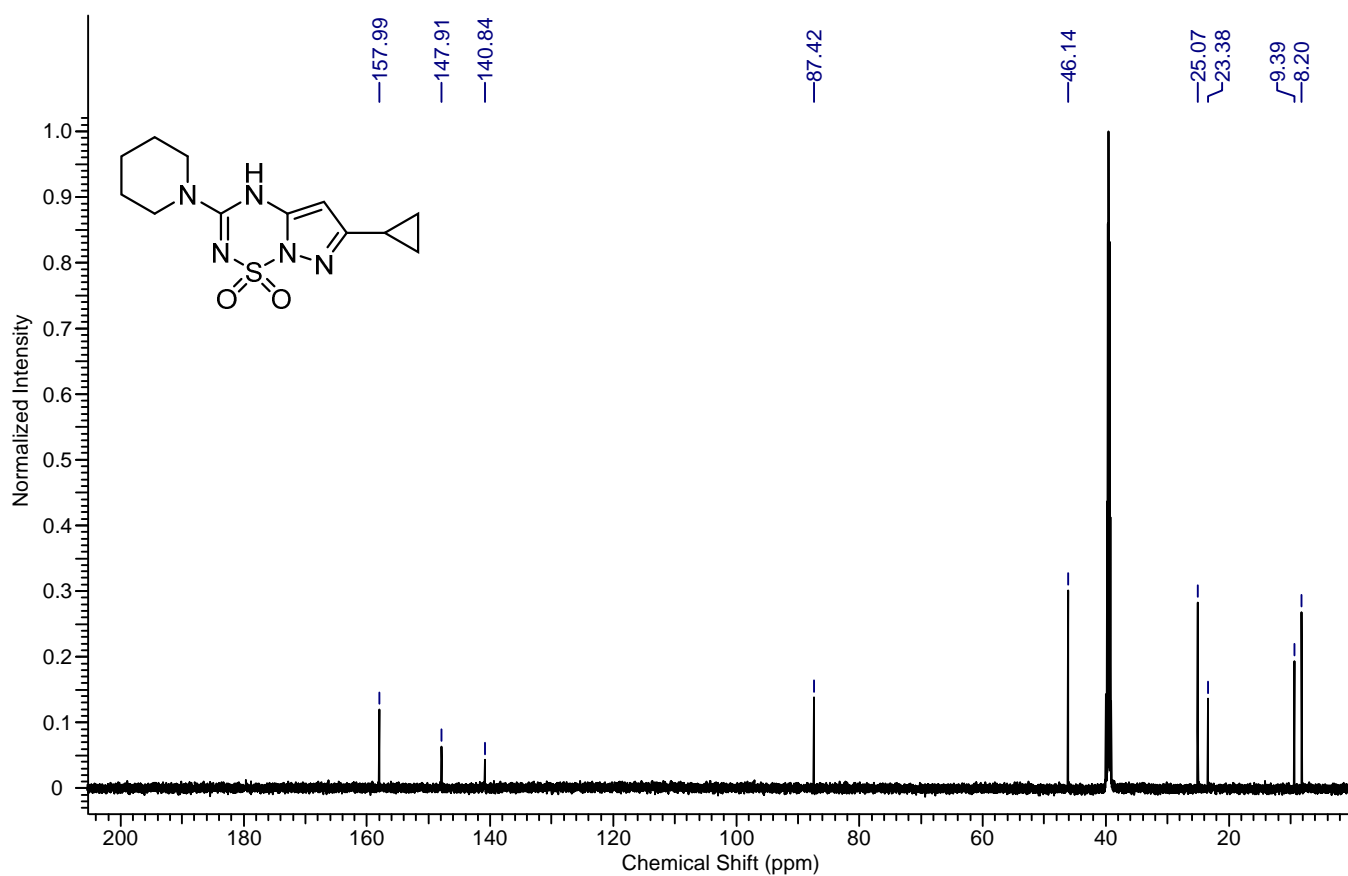
¹³C NMR spectrum of **3k (DMSO-*d*⁶)**



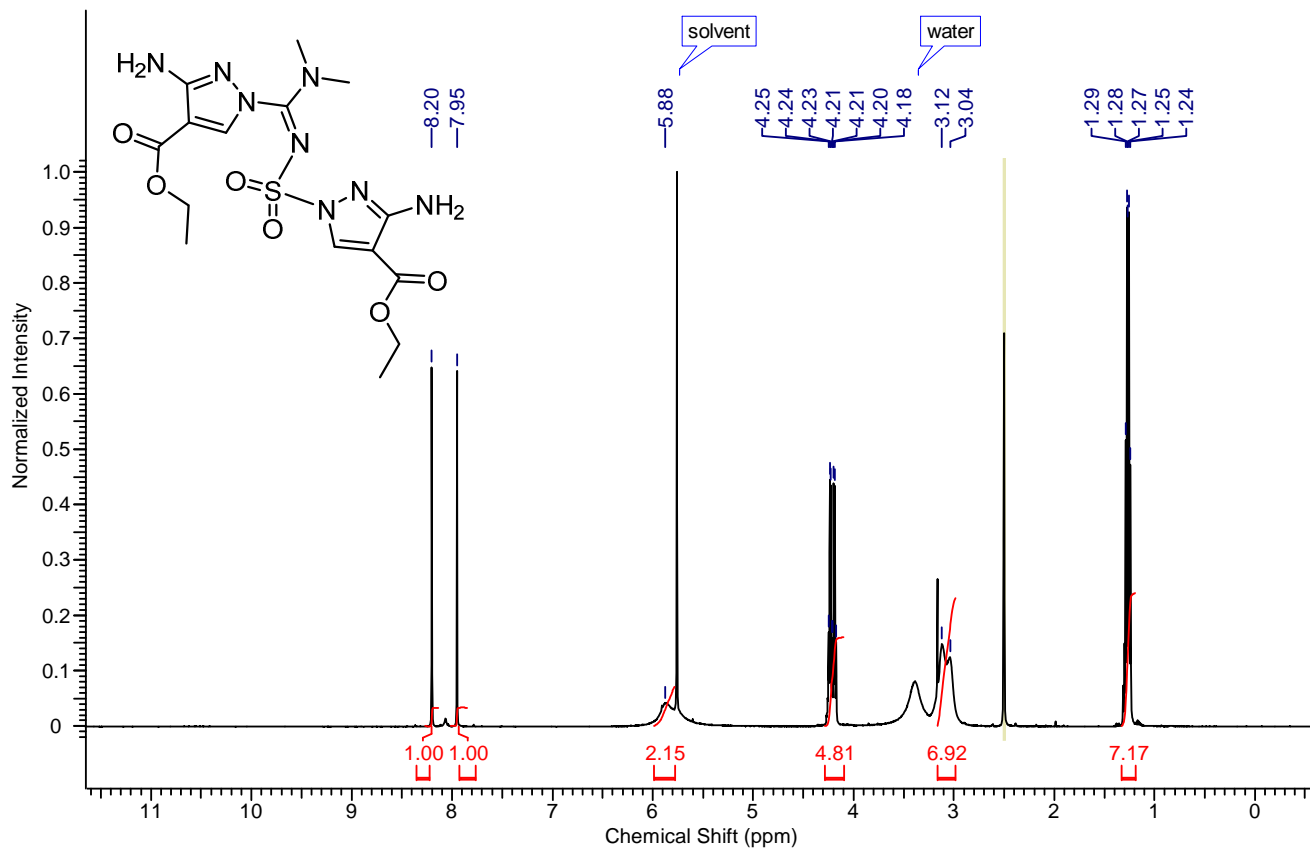
¹H NMR spectrum of **3l (DMSO-*d*⁶)**



¹³C NMR spectrum of **31 (DMSO-*d*₆)**

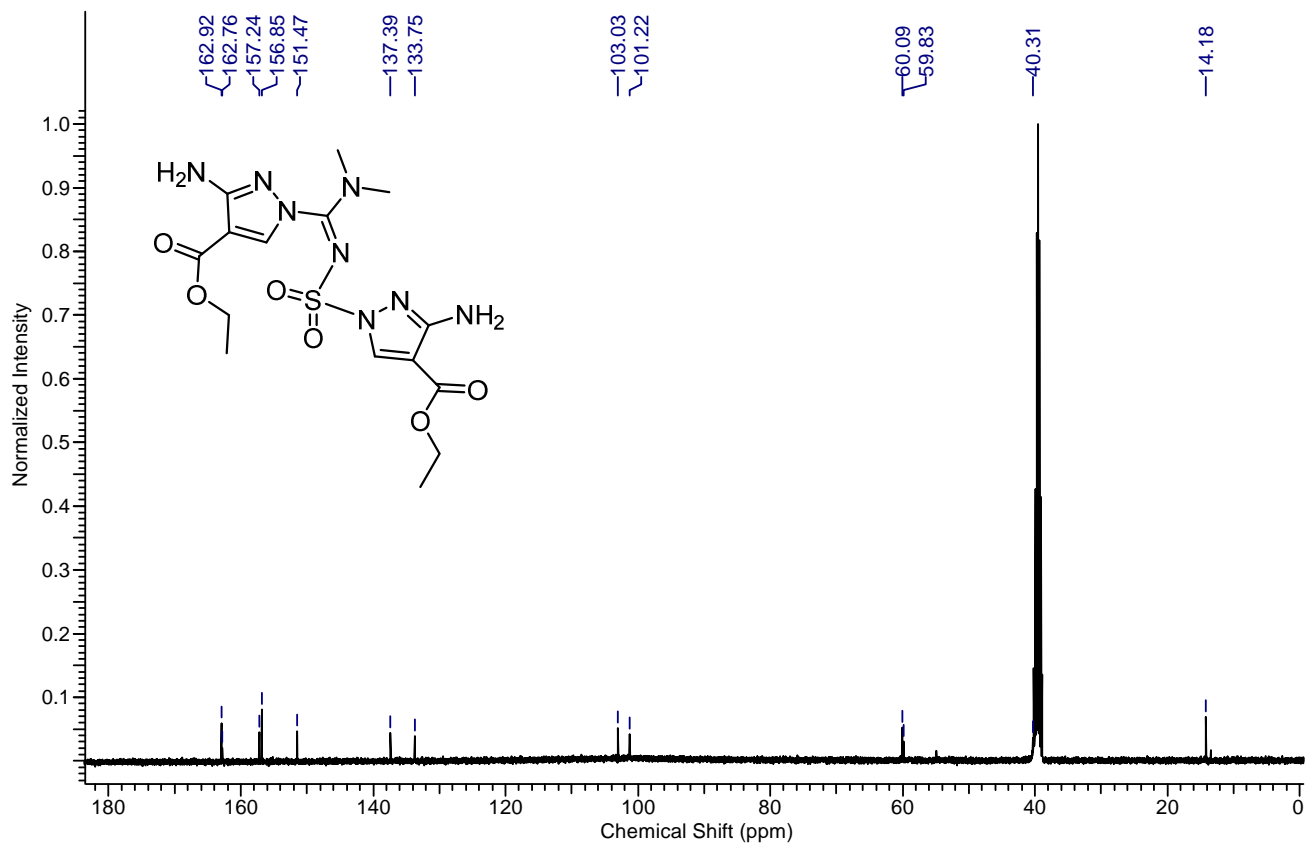


¹H NMR spectrum of bis adduct **5a* (DMSO-*d*₆)**

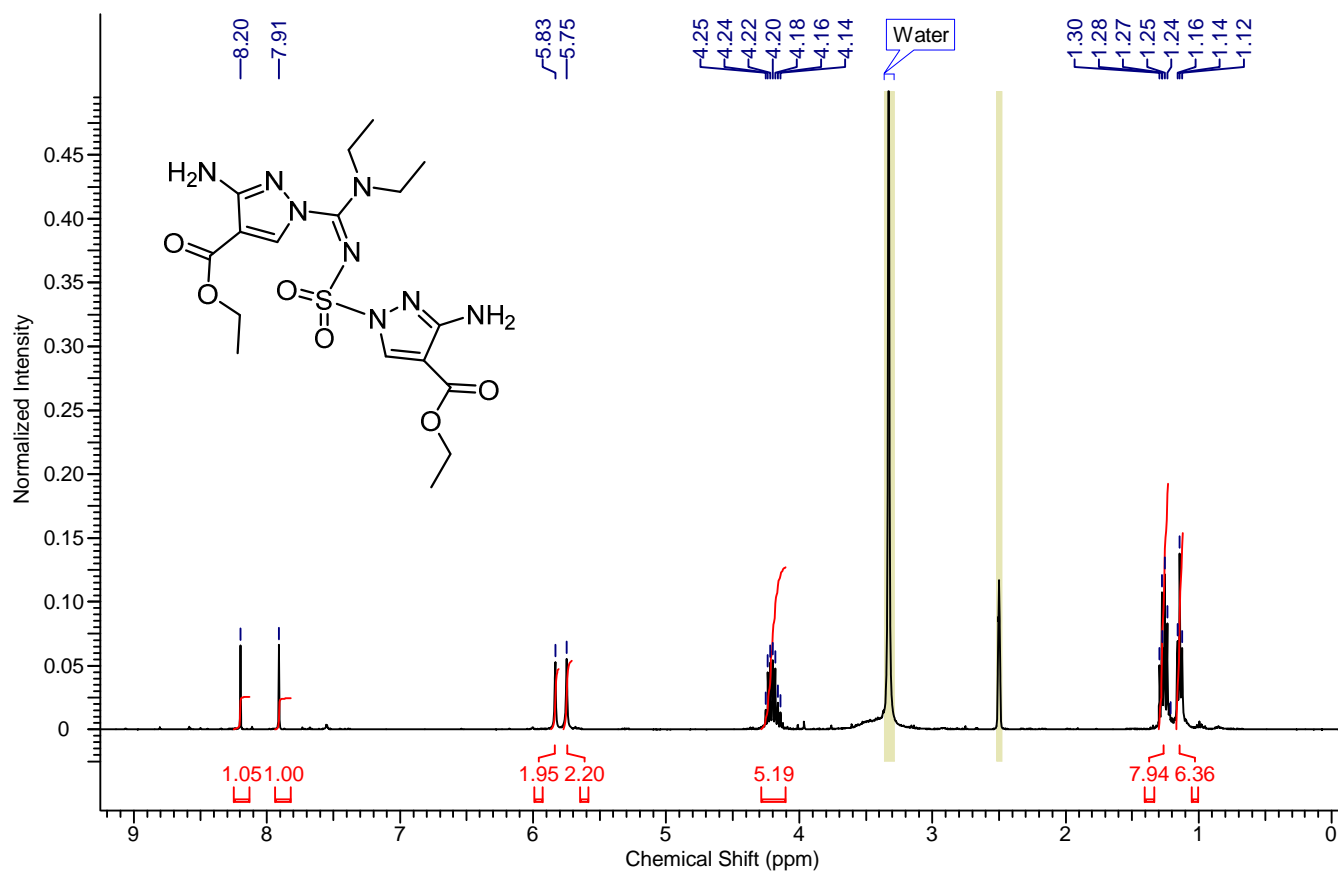


* crystallises with CH_2Cl_2 . Please see notes on X-ray structure.

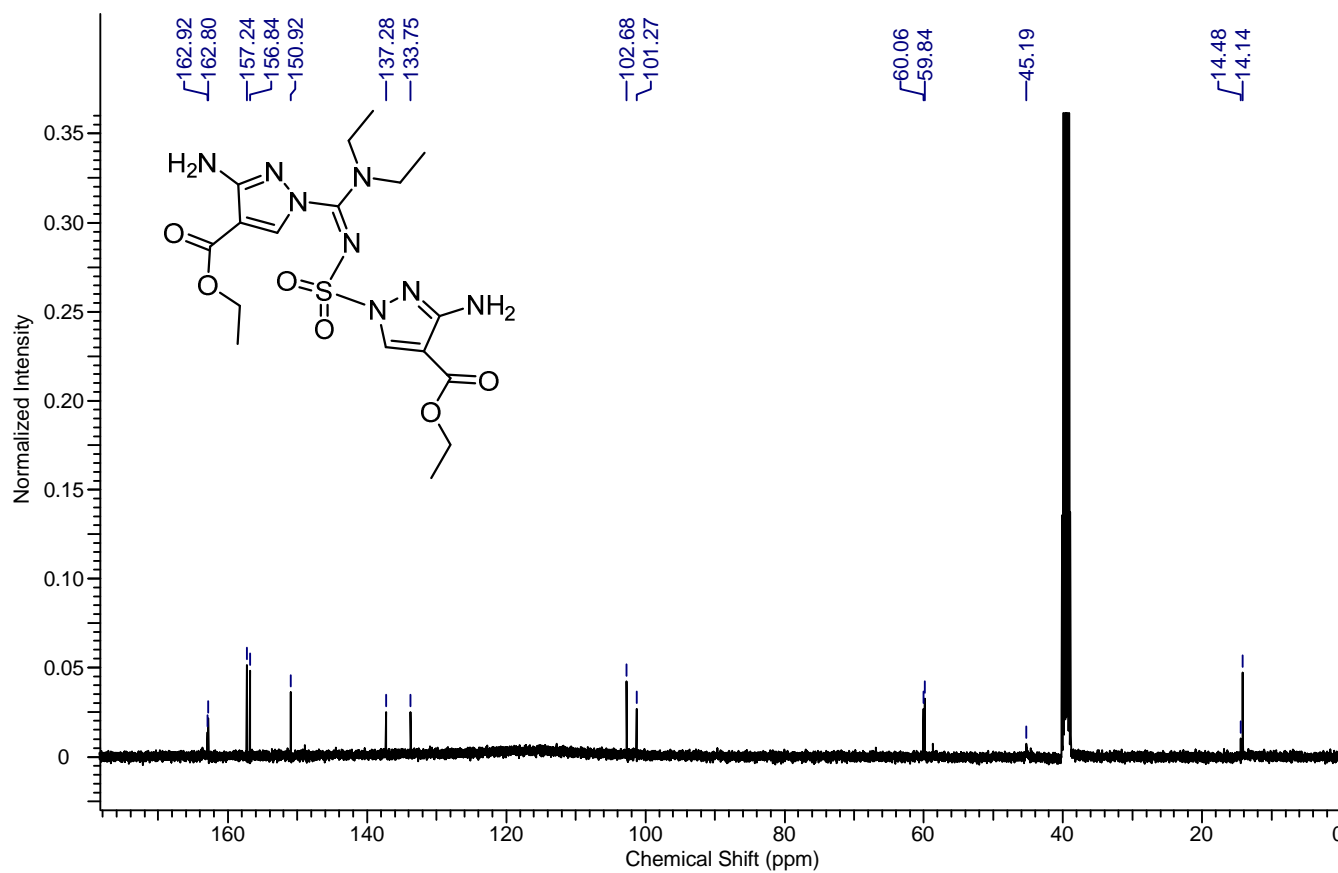
^{13}C NMR spectrum of bis adduct **5a*** ($\text{DMSO}-d_6$)



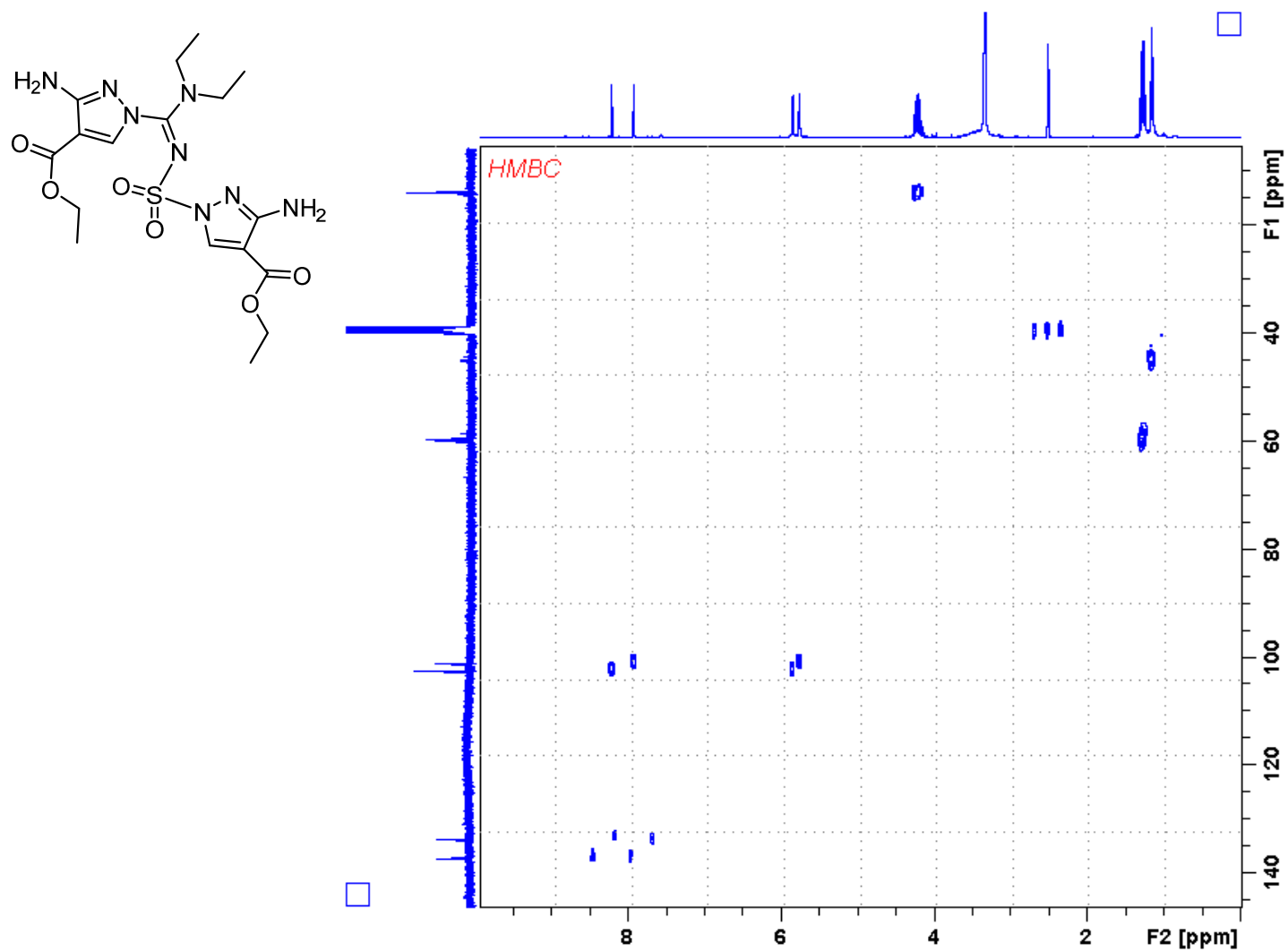
^1H NMR spectrum of bis adduct **5b** ($\text{DMSO-}d_6$)



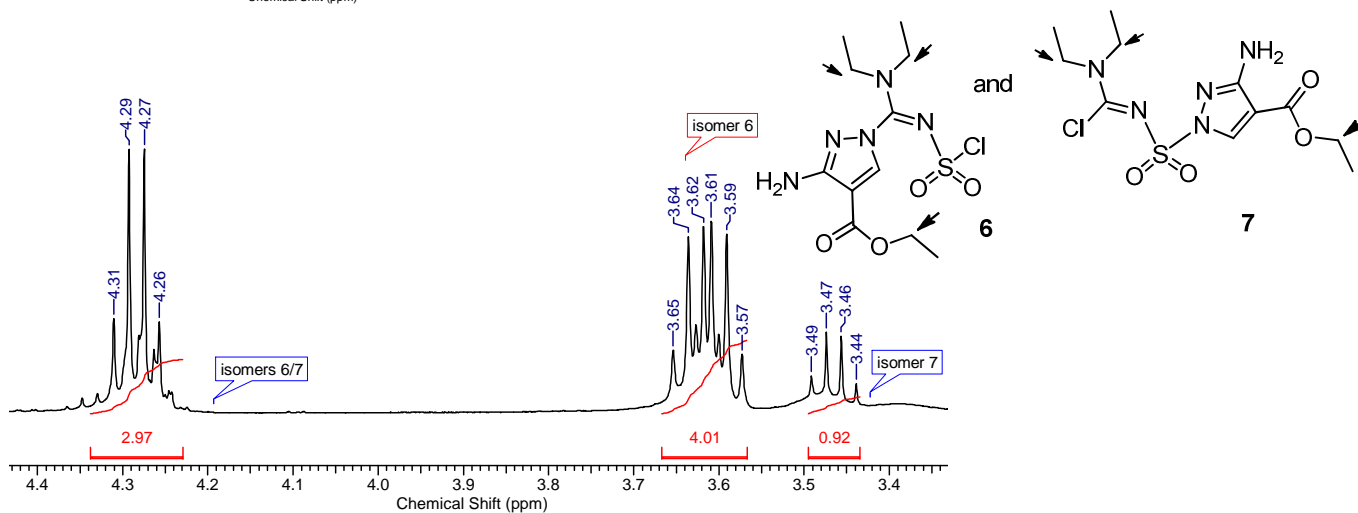
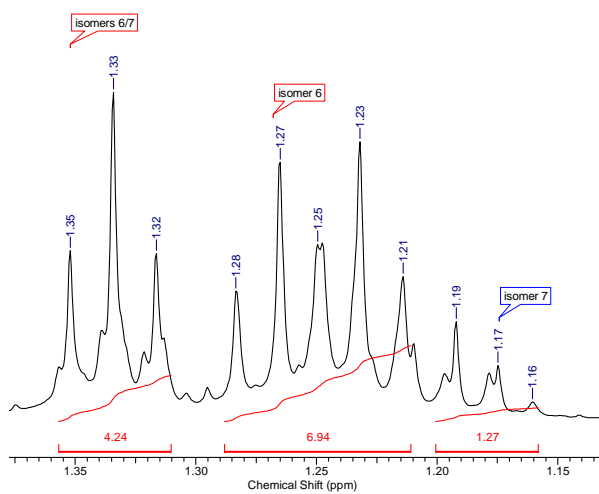
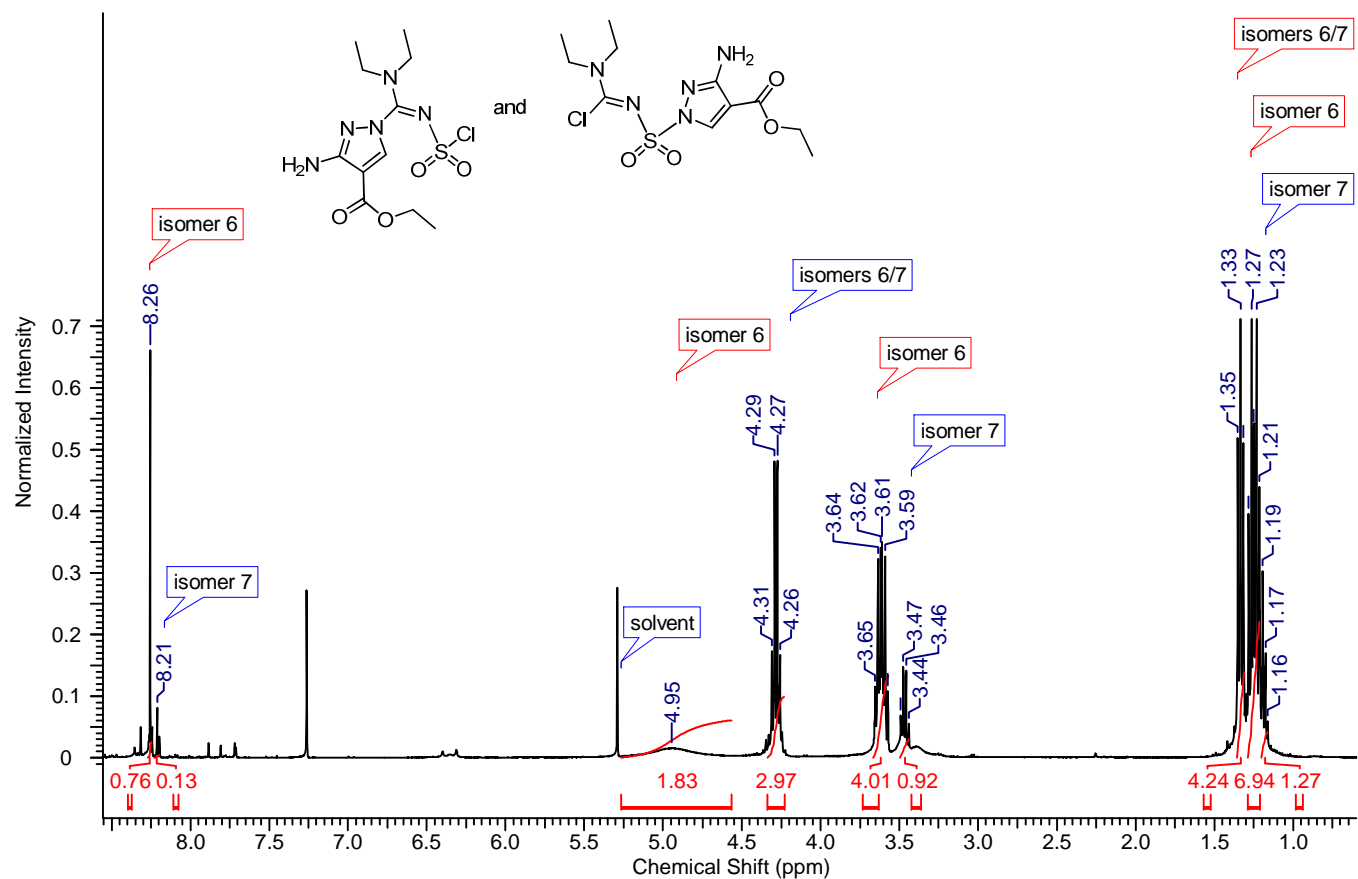
^{13}C NMR spectrum of bis adduct **5b** ($\text{DMSO-}d_6$)

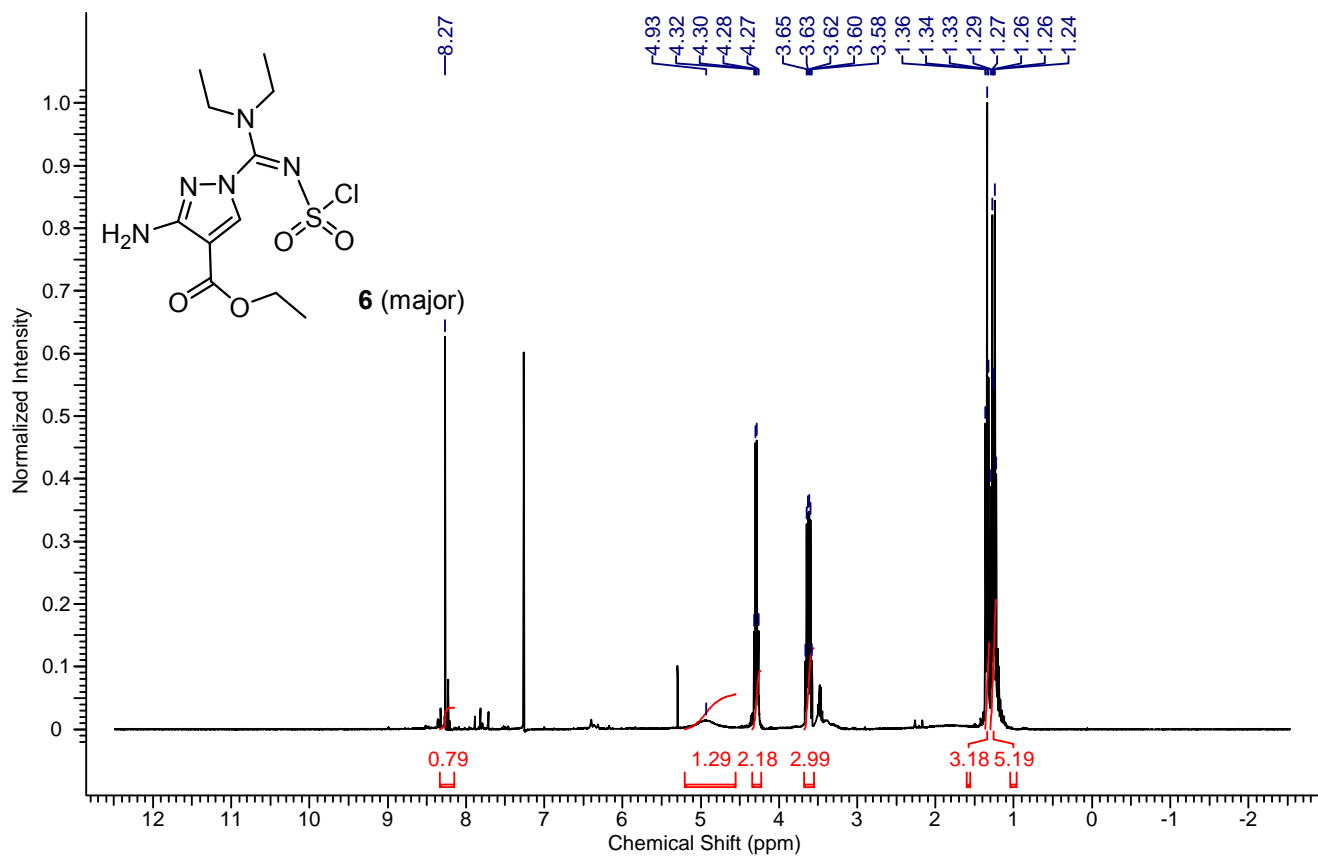


Long range correlation HMBC spectrum of bis-adduct **5b** (DMSO-d⁶)

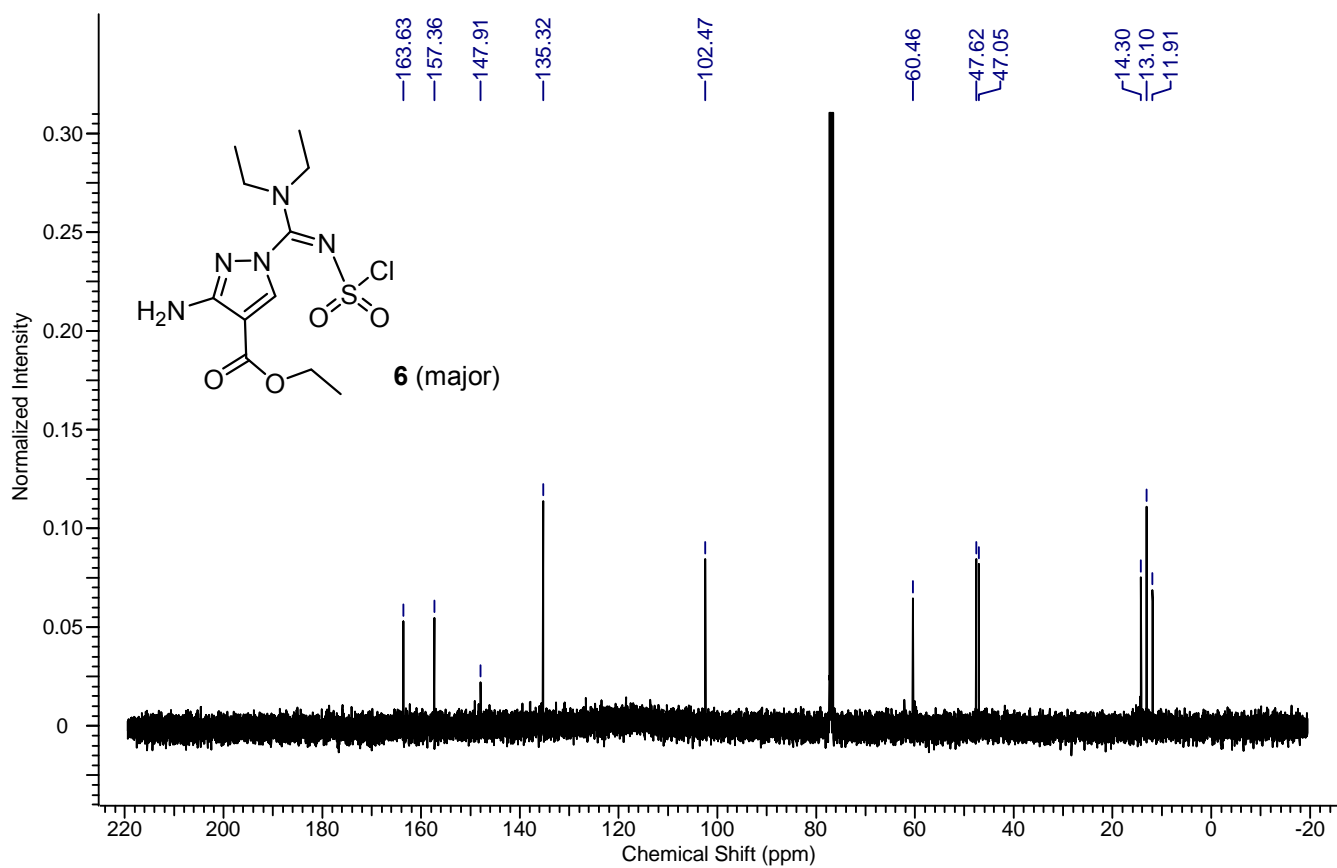


^1H NMR spectrum of unstable chlorides **6/7** (CDCl_3)

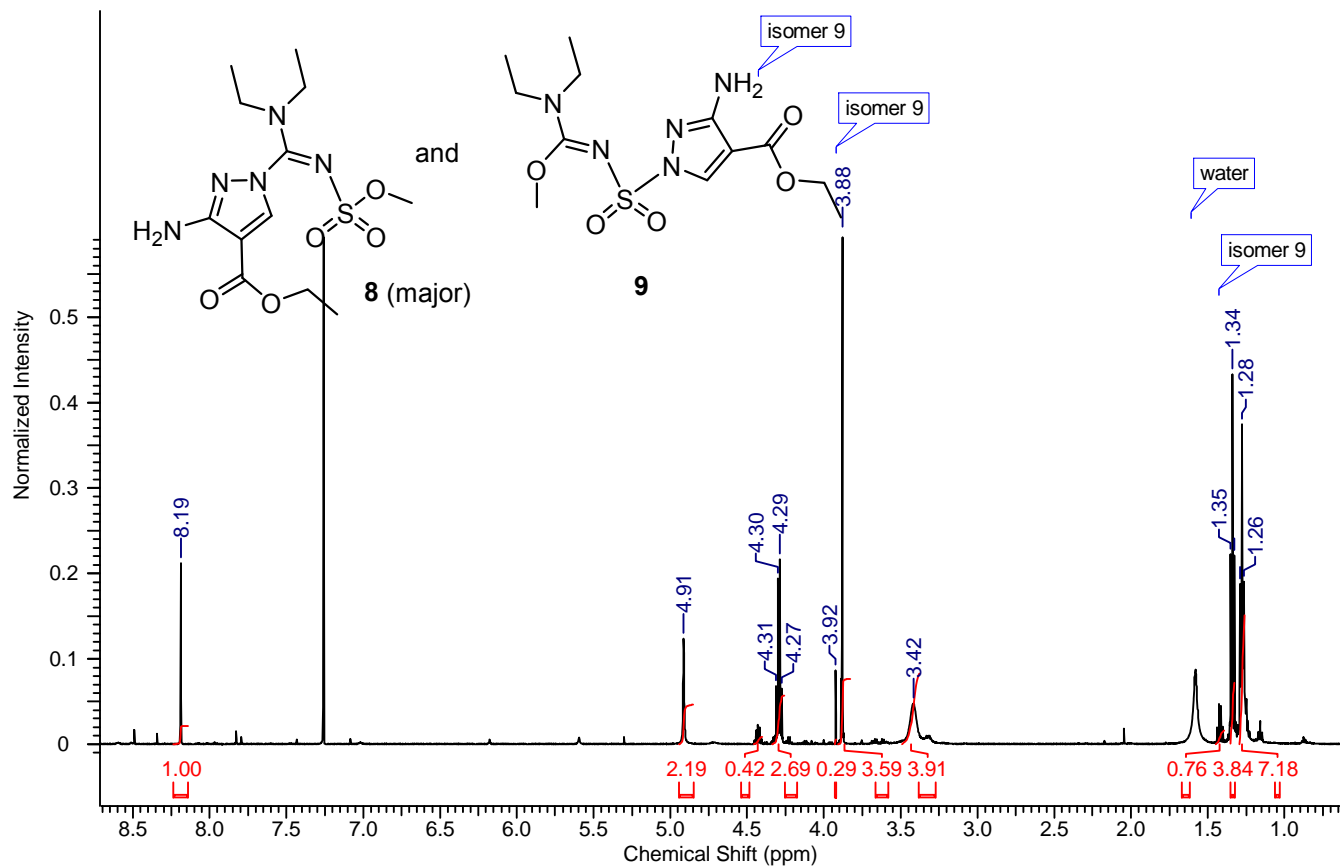




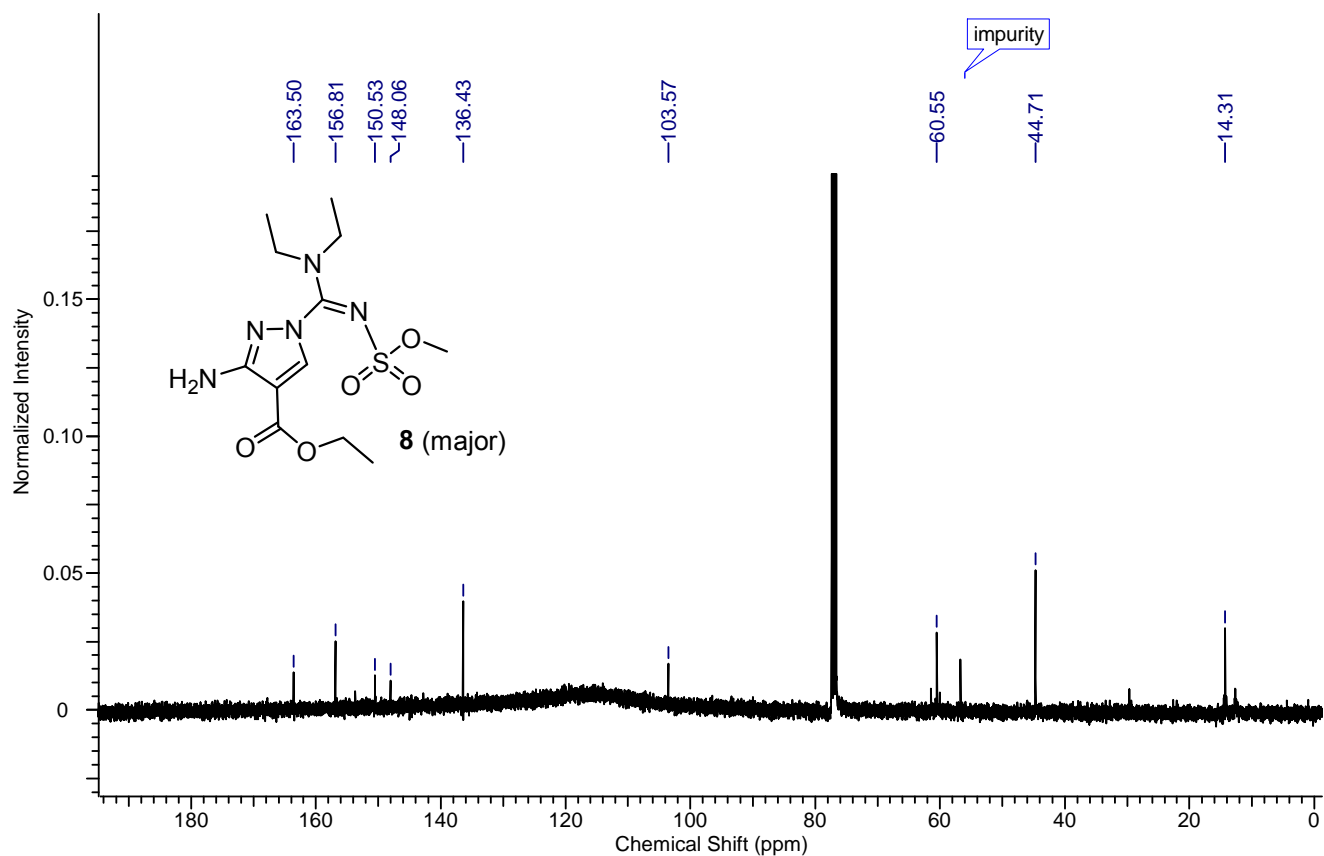
¹³C NMR spectrum of unstable chlorides **6/7** (CDCl₃)



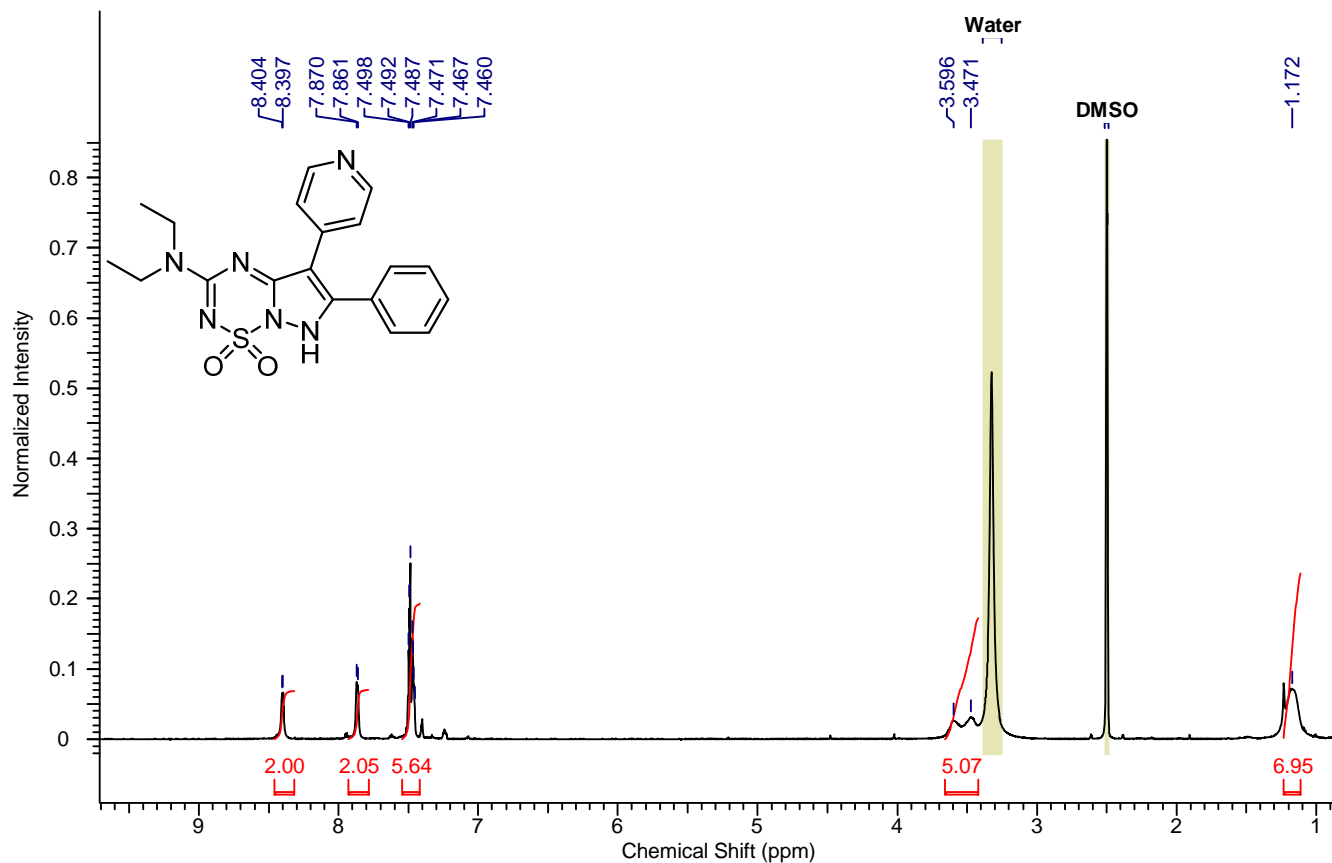
^1H NMR spectrum of unstable methyl sulfonates **8/9** (CDCl_3)



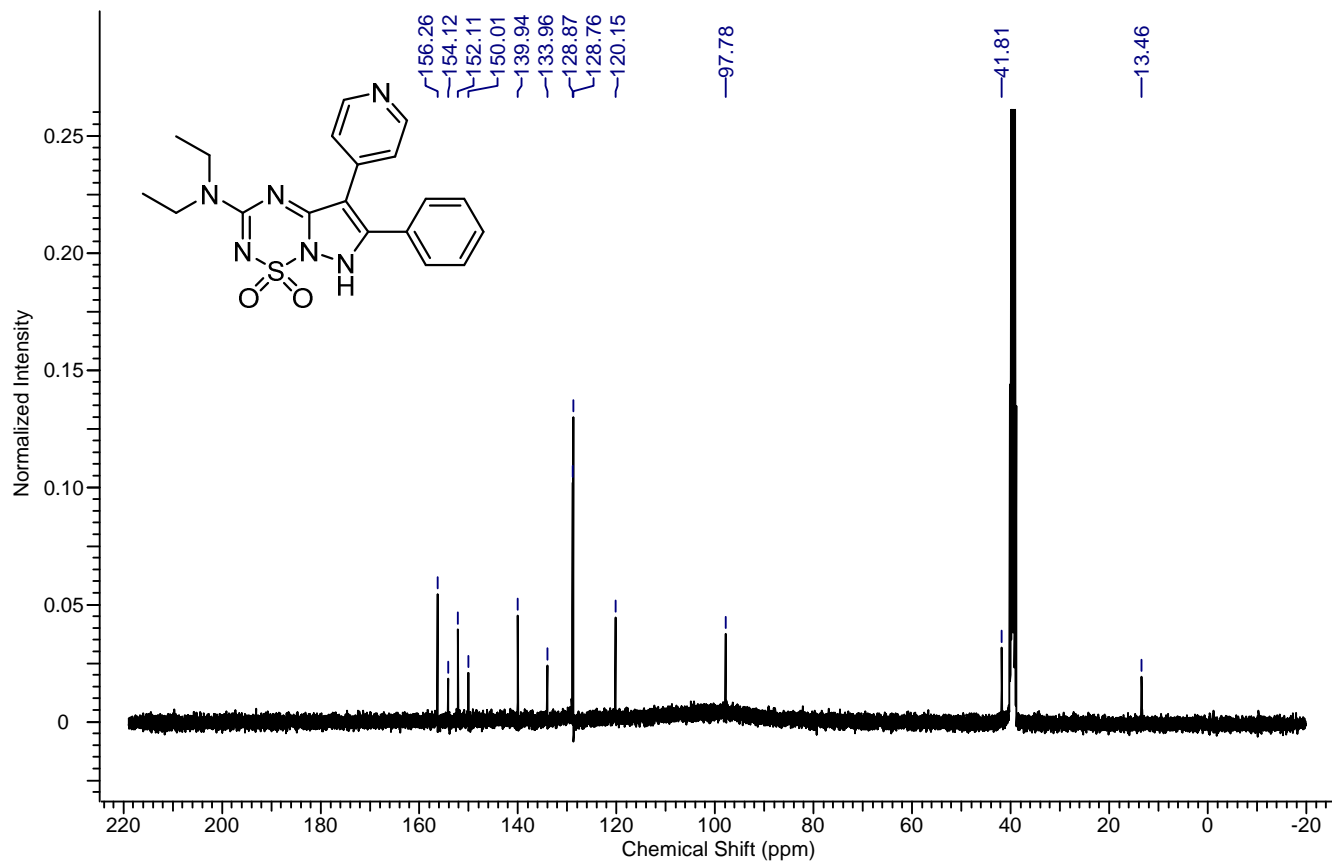
^{13}C NMR spectrum of unstable methyl sulfonates **8/9** (CDCl_3)



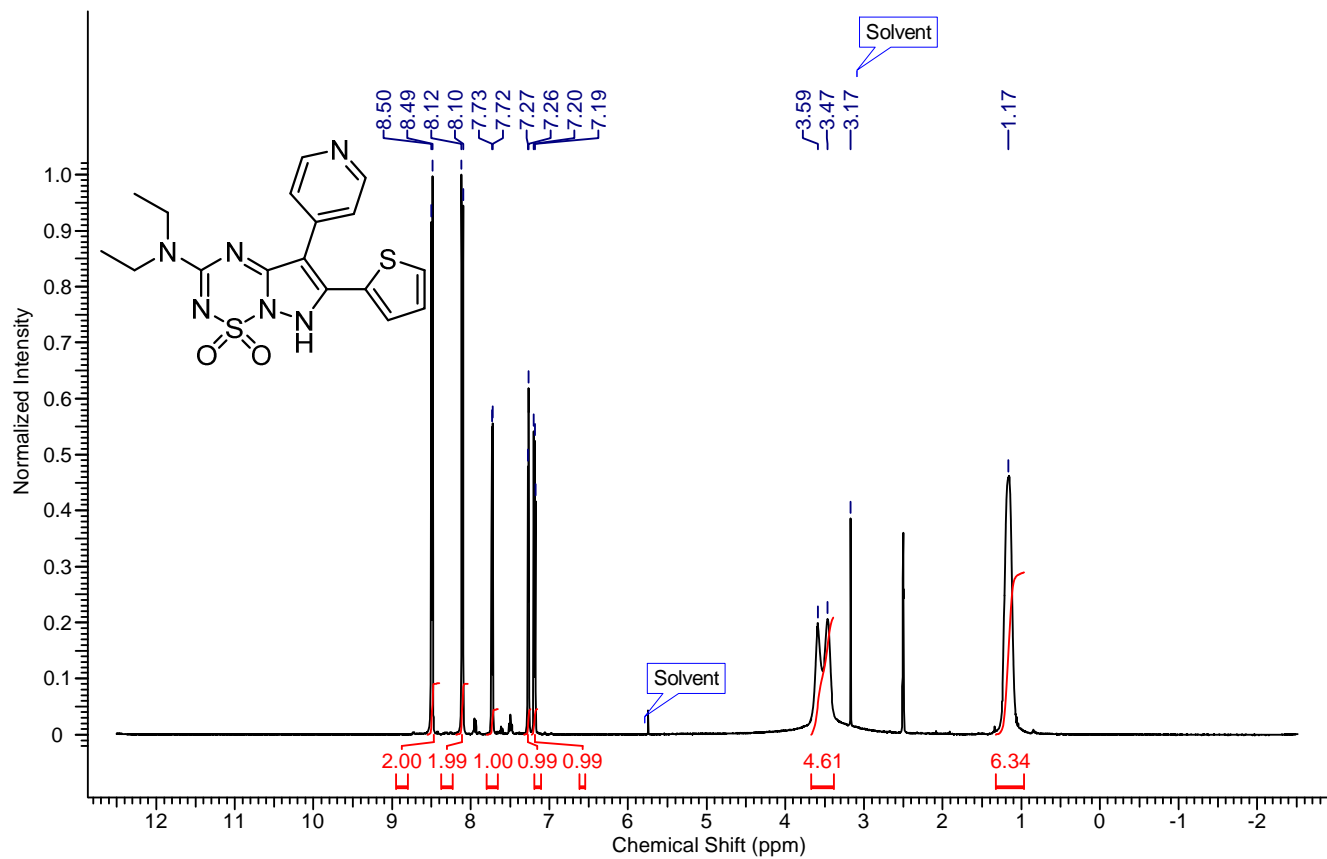
^1H NMR spectrum of pyridine adduct **11a** (DMSO-d^6)



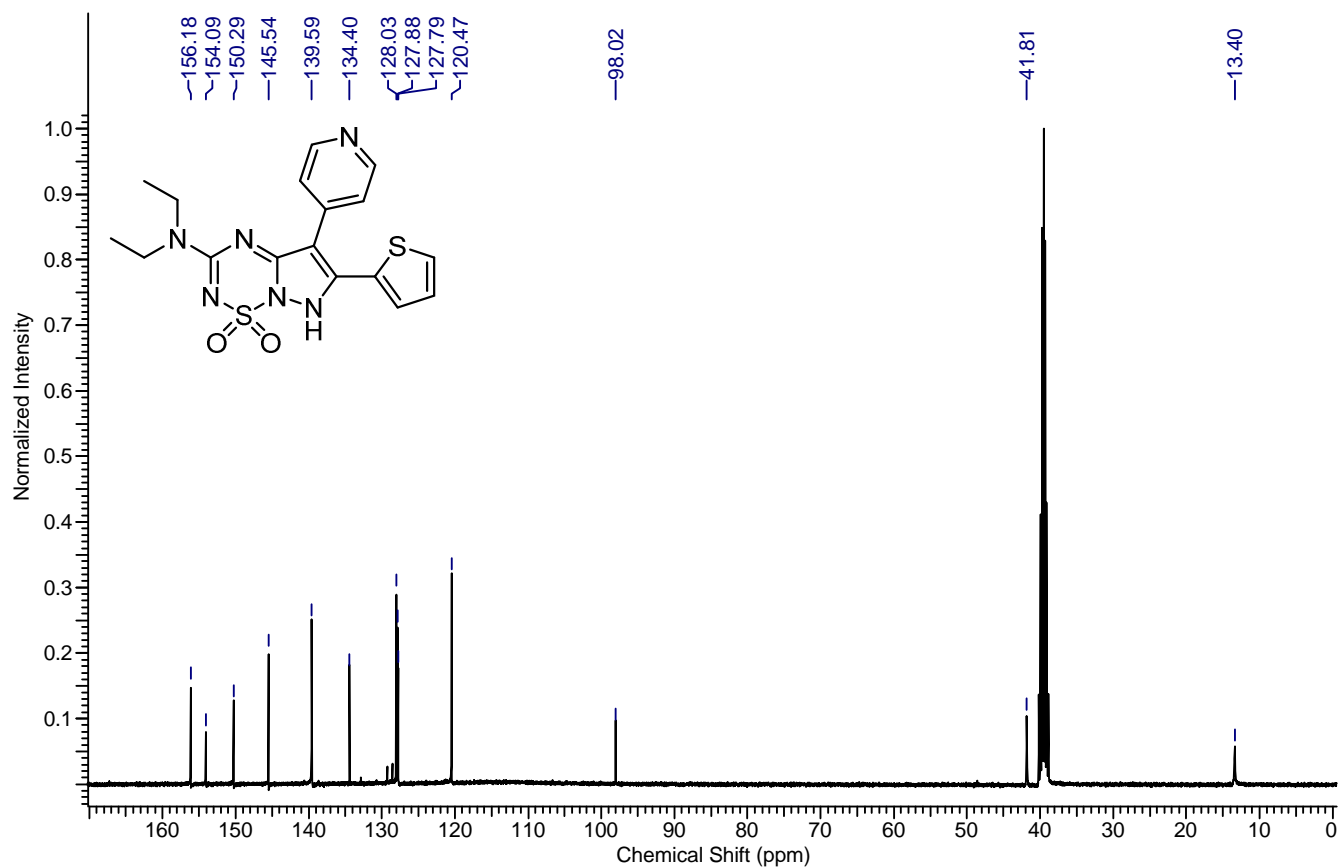
^{13}C NMR spectrum of pyridine adduct **11a** (DMSO-d^6)



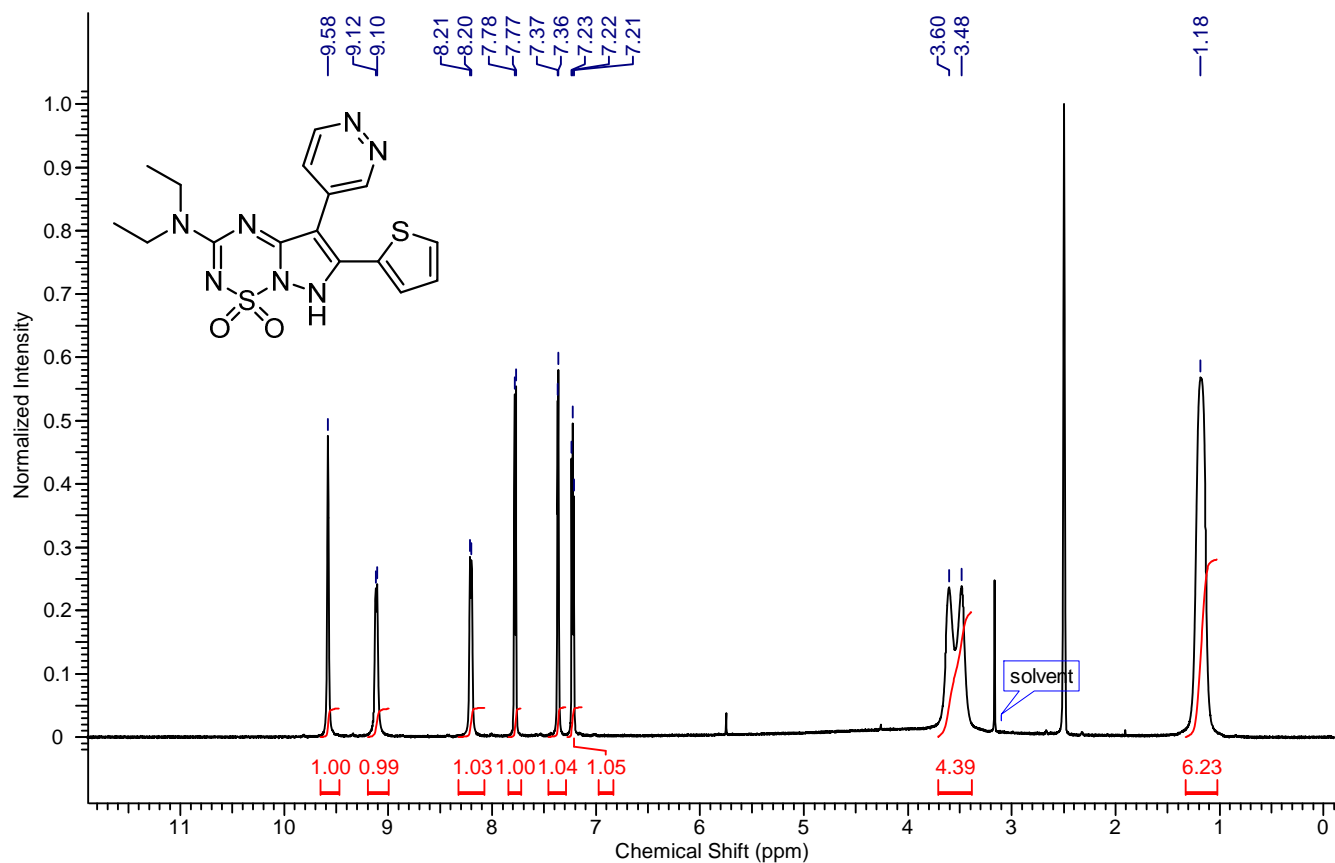
^1H NMR spectrum of pyridine adduct **11b** (DMSO- d_6)



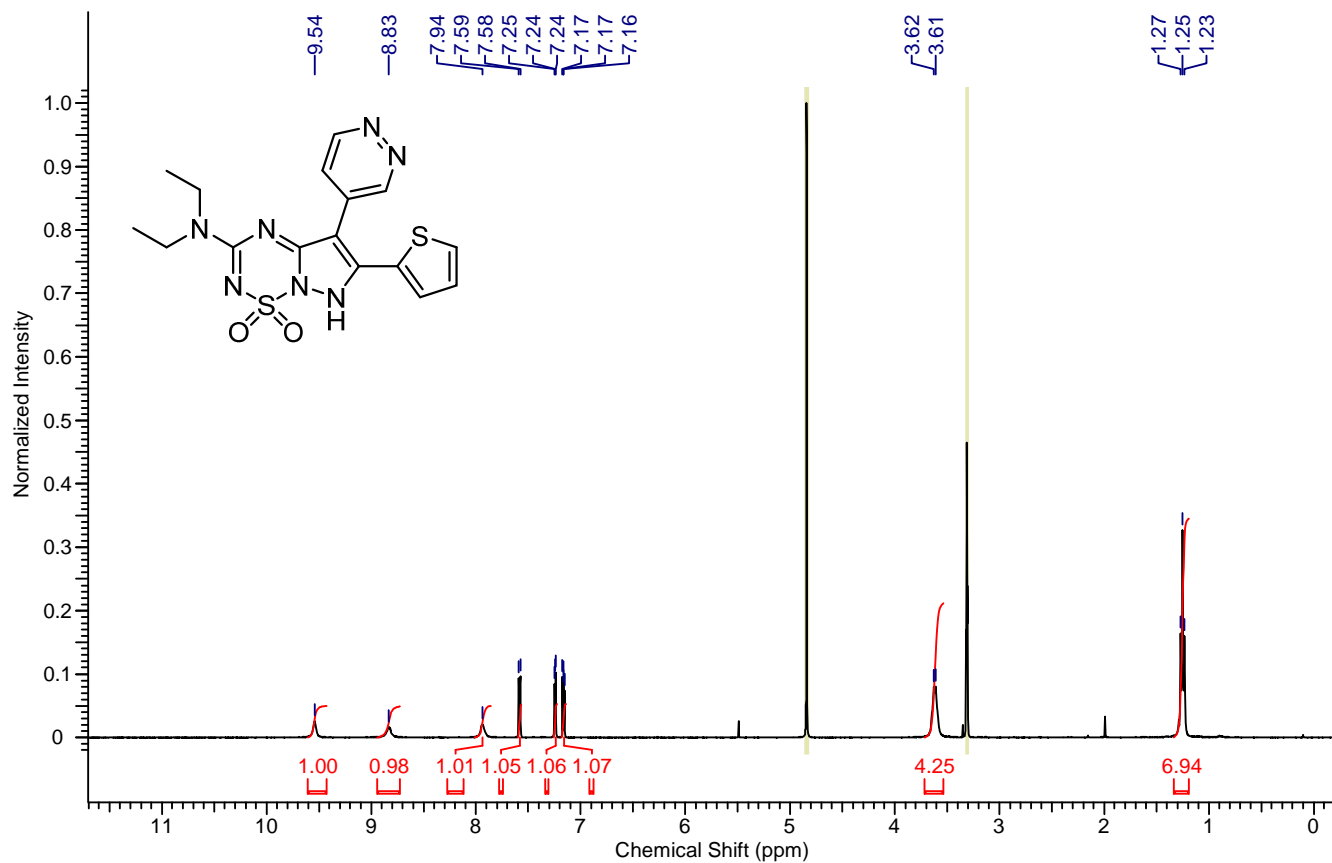
^{13}C NMR spectrum of pyridine adduct **11b** (DMSO- d_6)



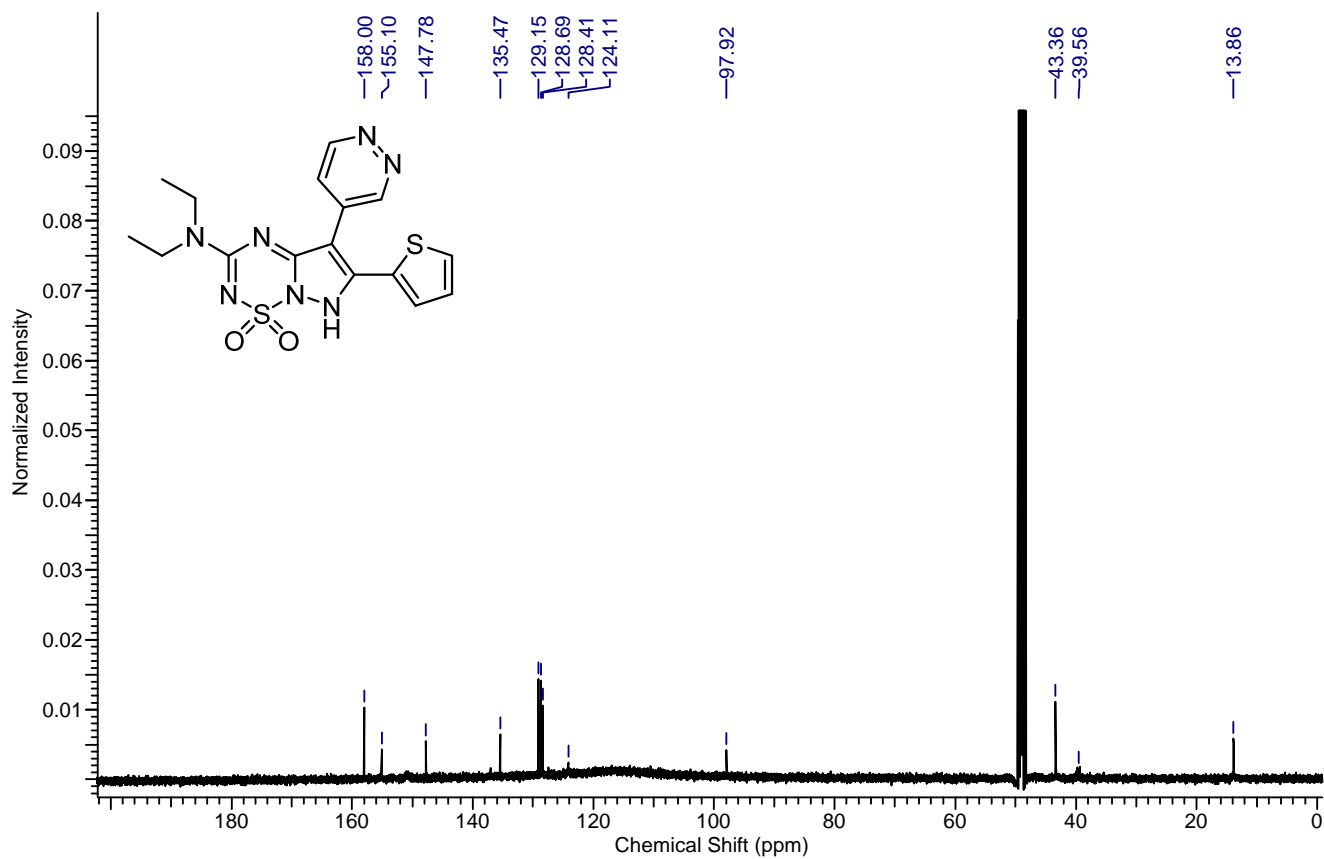
^1H NMR spectrum of pyridazine adduct **11c** (DMSO-d_6)



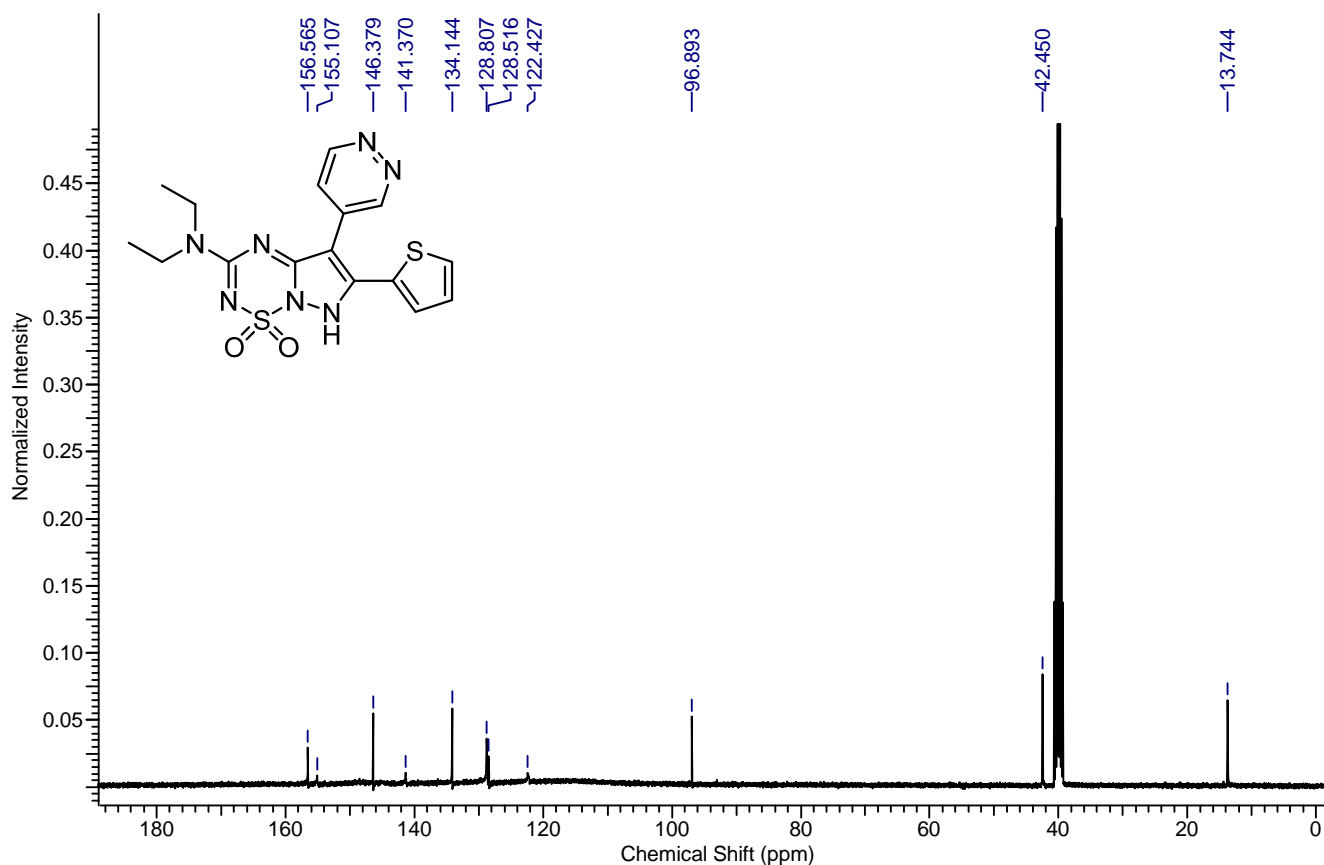
^1H NMR spectrum of pyridazine adduct **11c** (methanol-d_4)



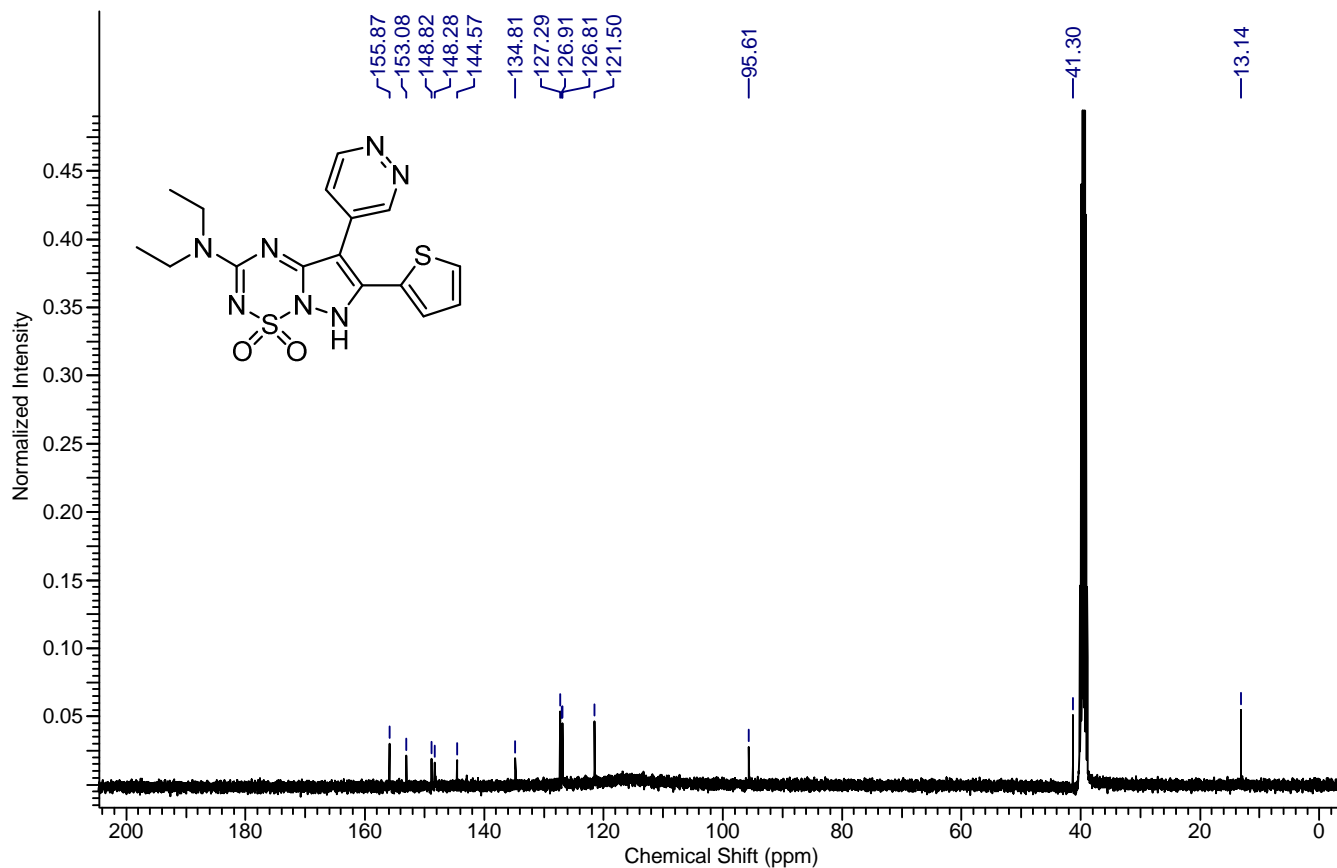
^{13}C NMR spectrum of pyridazine adduct **11c** (methanol- d^4)



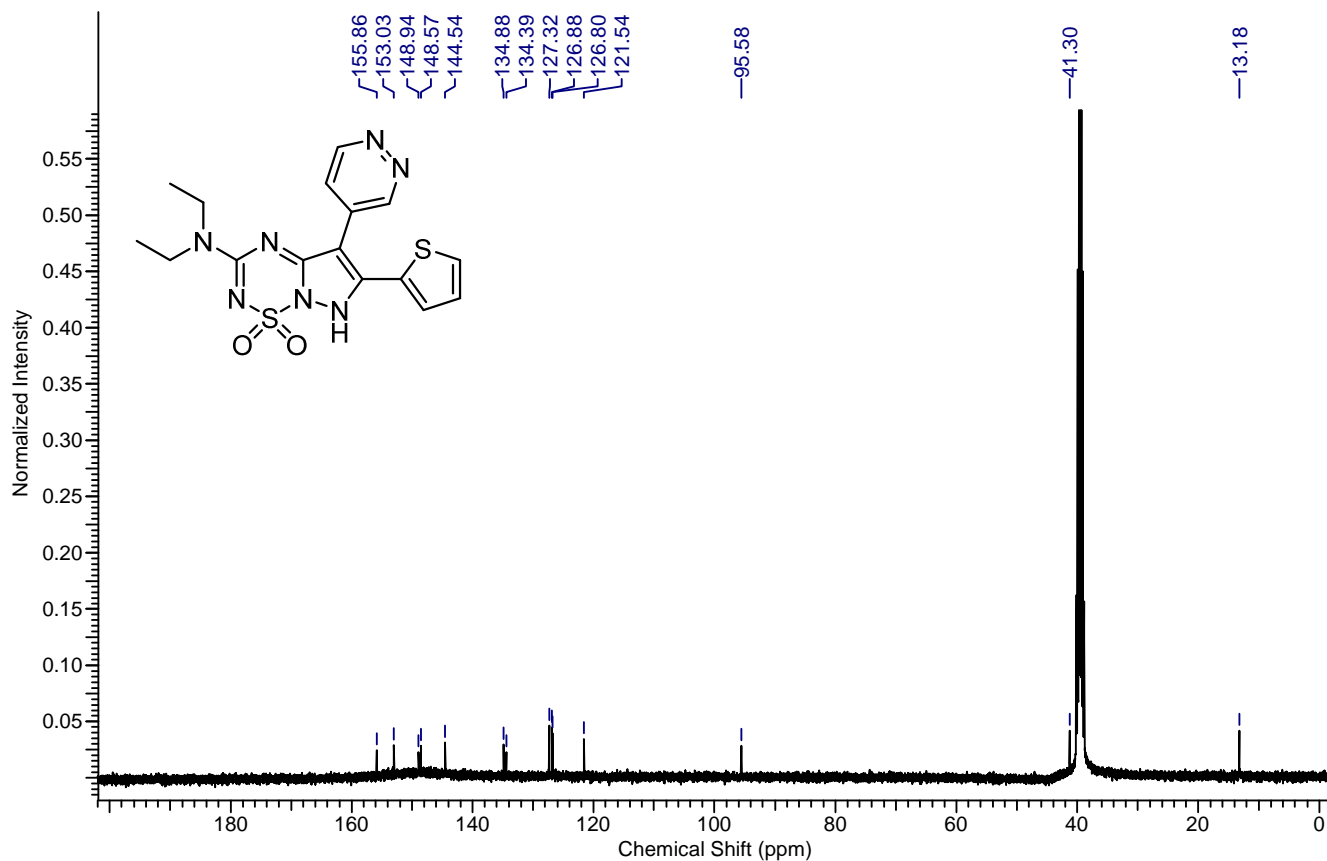
^{13}C NMR spectrum of pyridazine adduct **11c** (DMSO- d^6) 26°C d1=2



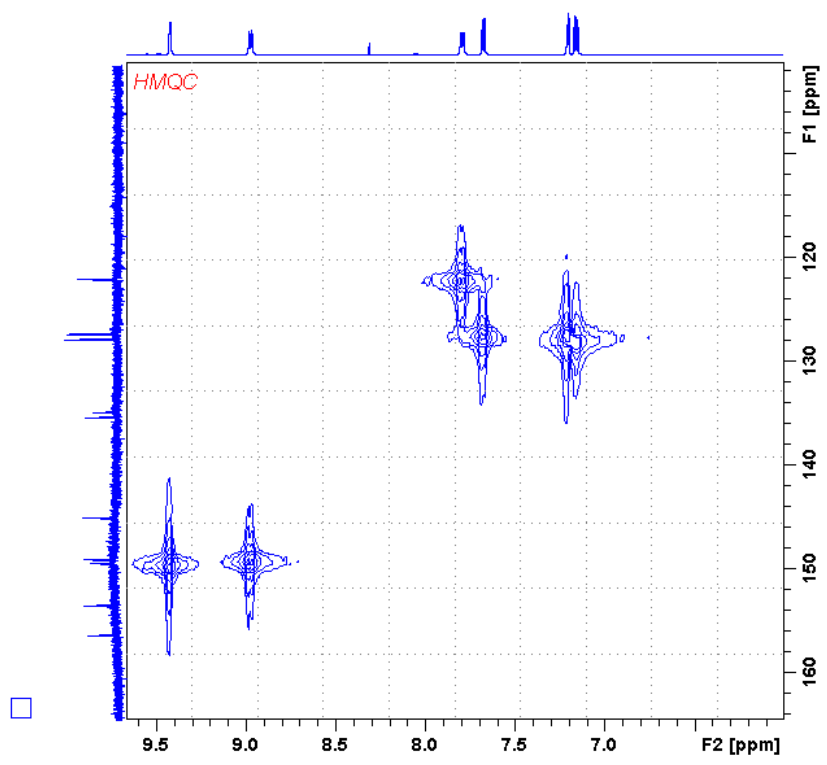
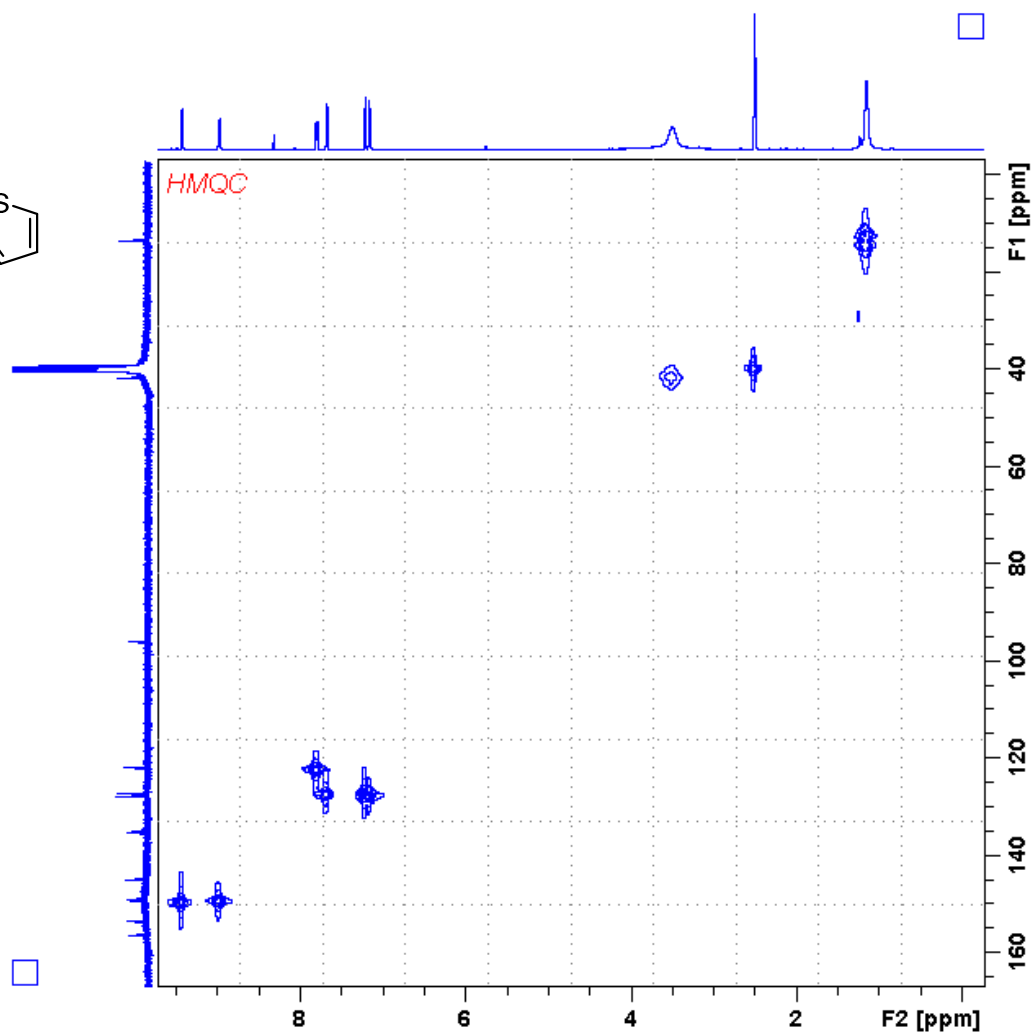
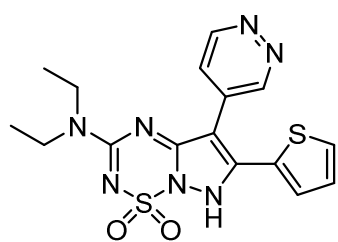
^{13}C NMR spectrum of pyridazine adduct **11c** (DMSO- d_6) 70°C d1=2



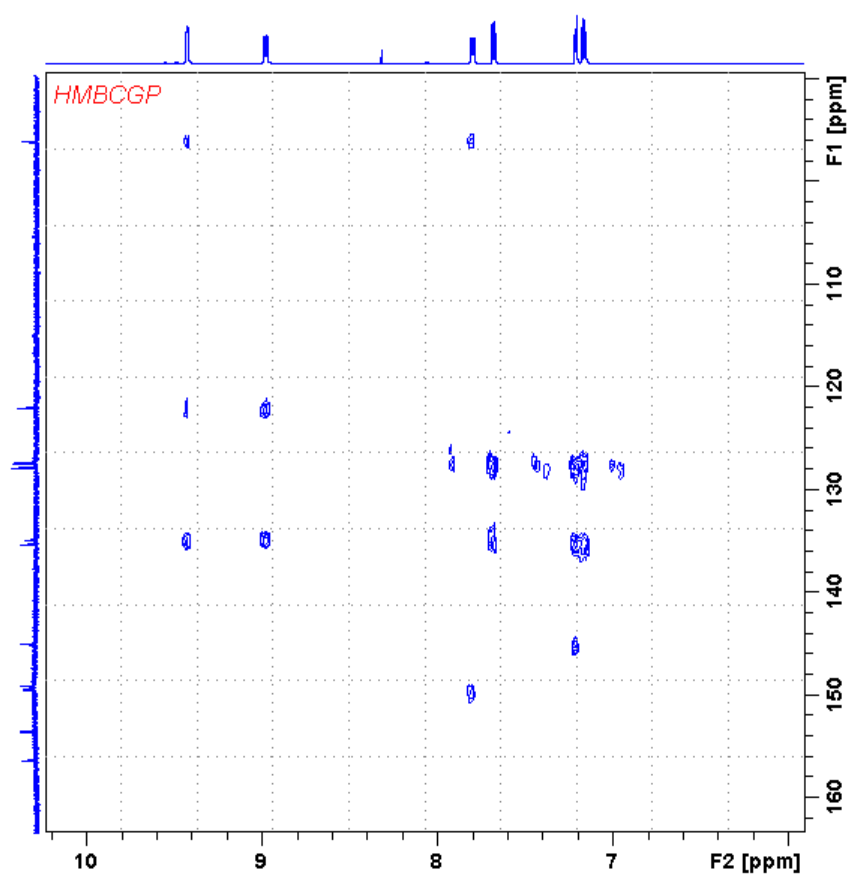
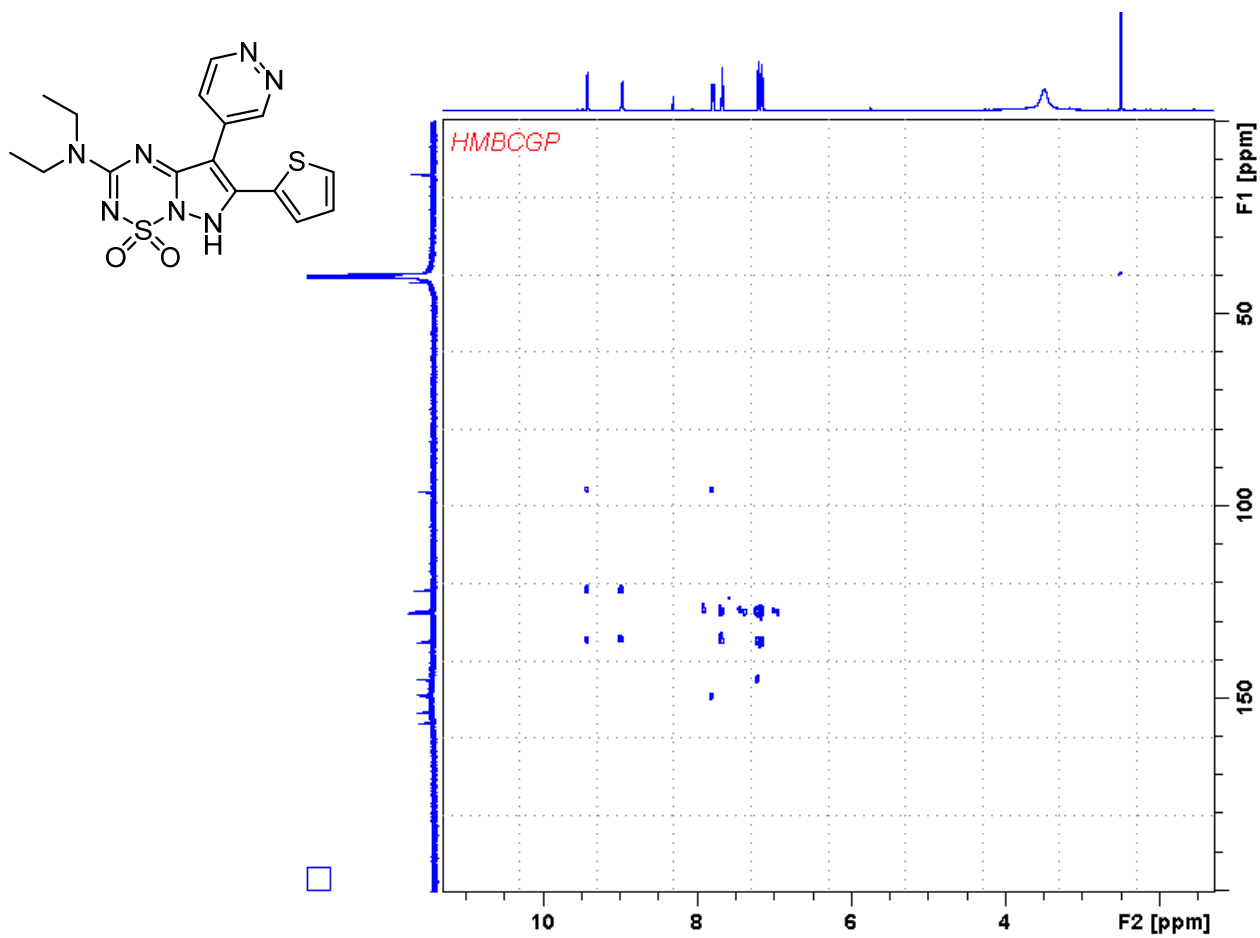
^{13}C NMR spectrum of pyridazine adduct **11c** (DMSO- d_6) 65°C d1=5



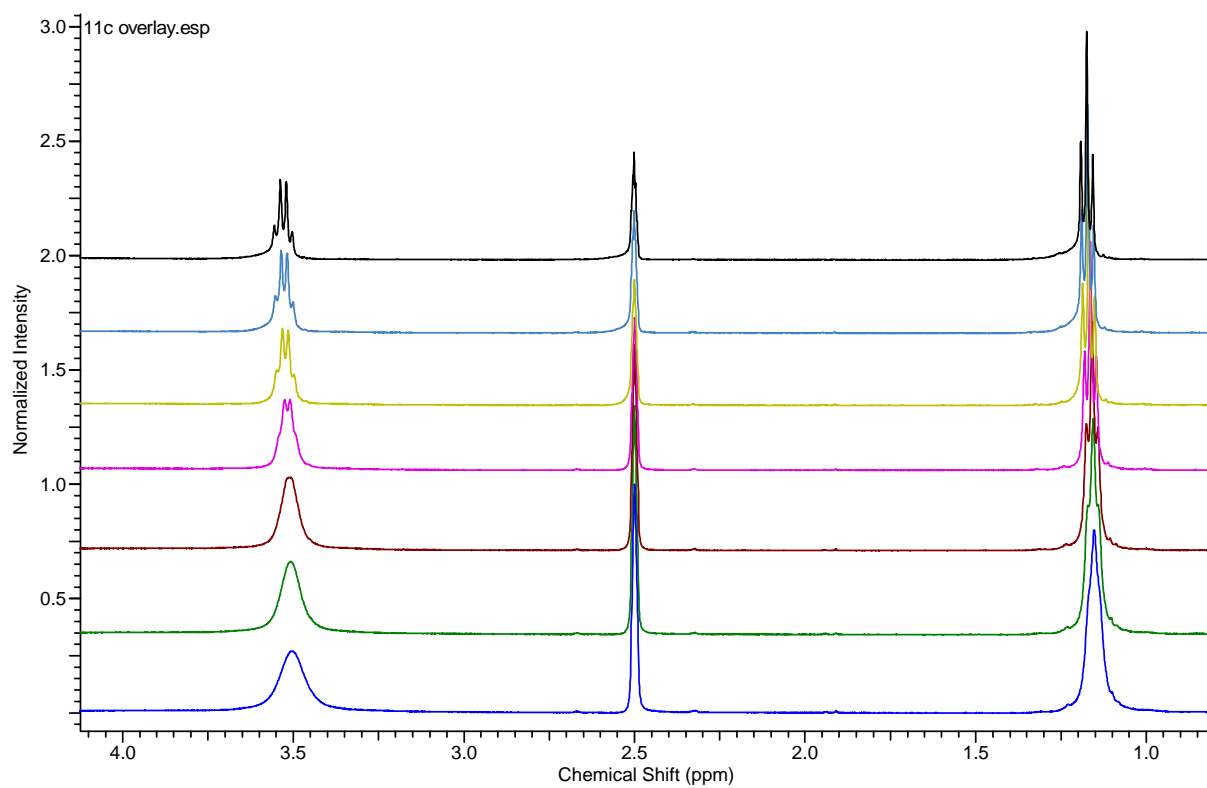
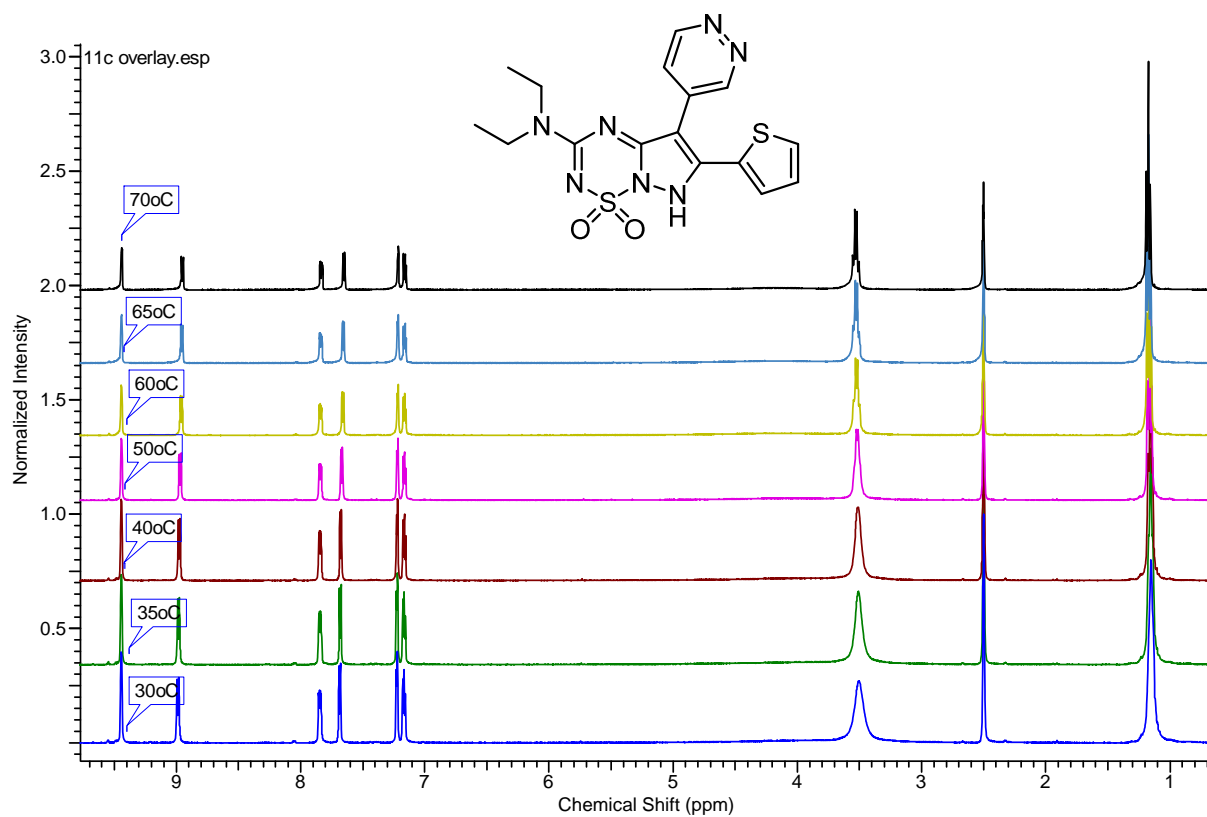
Short range correlation HMQC spectrum of pyridazine adduct **11c** (DMSO- d^6)



Long range correlation HMBC spectrum of pyridazine adduct **11c** (DMSO- d^6)



Variable temperature ^1H NMR spectra of pyridazine adduct **11c** ($\text{DMSO-}d_6$)



ORTEP diagrams of pyridine adduct **11a** generated in *Mercury -version 3.0* showing H-bonding between pyridine ring NH and N7 (pyrazole ring) of an adjacent molecule (upper left); packing within the crystal lattice (upper right, below).

