

Supplementary Material

N,N-Dialkyl-*N'*-Chlorosulfonyl Chloroformamidines in Heterocyclic Synthesis. Part XII. Synthesis and Reactivity of the Pyrazolo[3,4-*e*][1,2,4]thiadiazine Ring System.

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^A School of Chemical and Physical Sciences, Flinders University, Bedford Park, SA 5042, Australia.

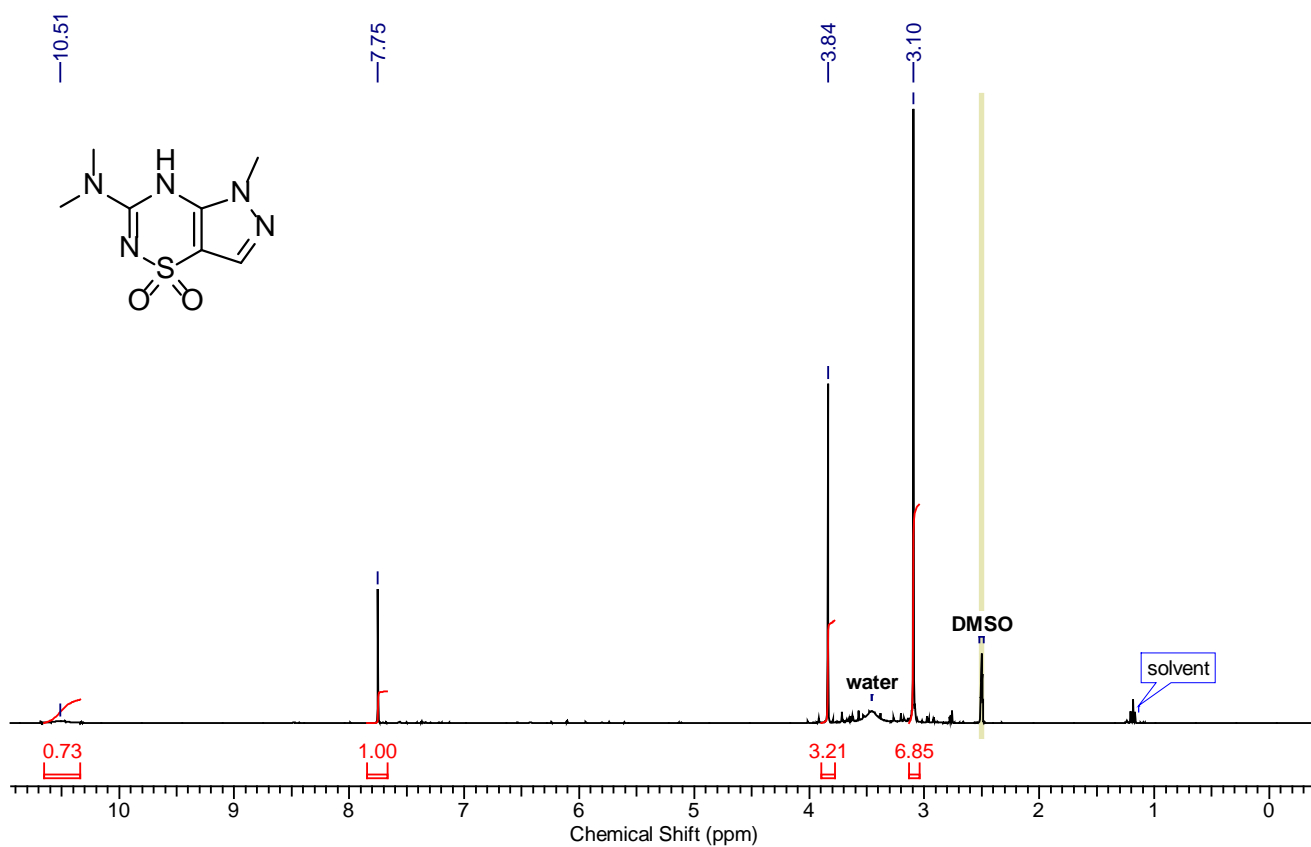
^B CSIRO Manufacturing Flagship, Clayton, VIC 3168, Australia.

^C Corresponding author. Email: craig.francis@csiro.au

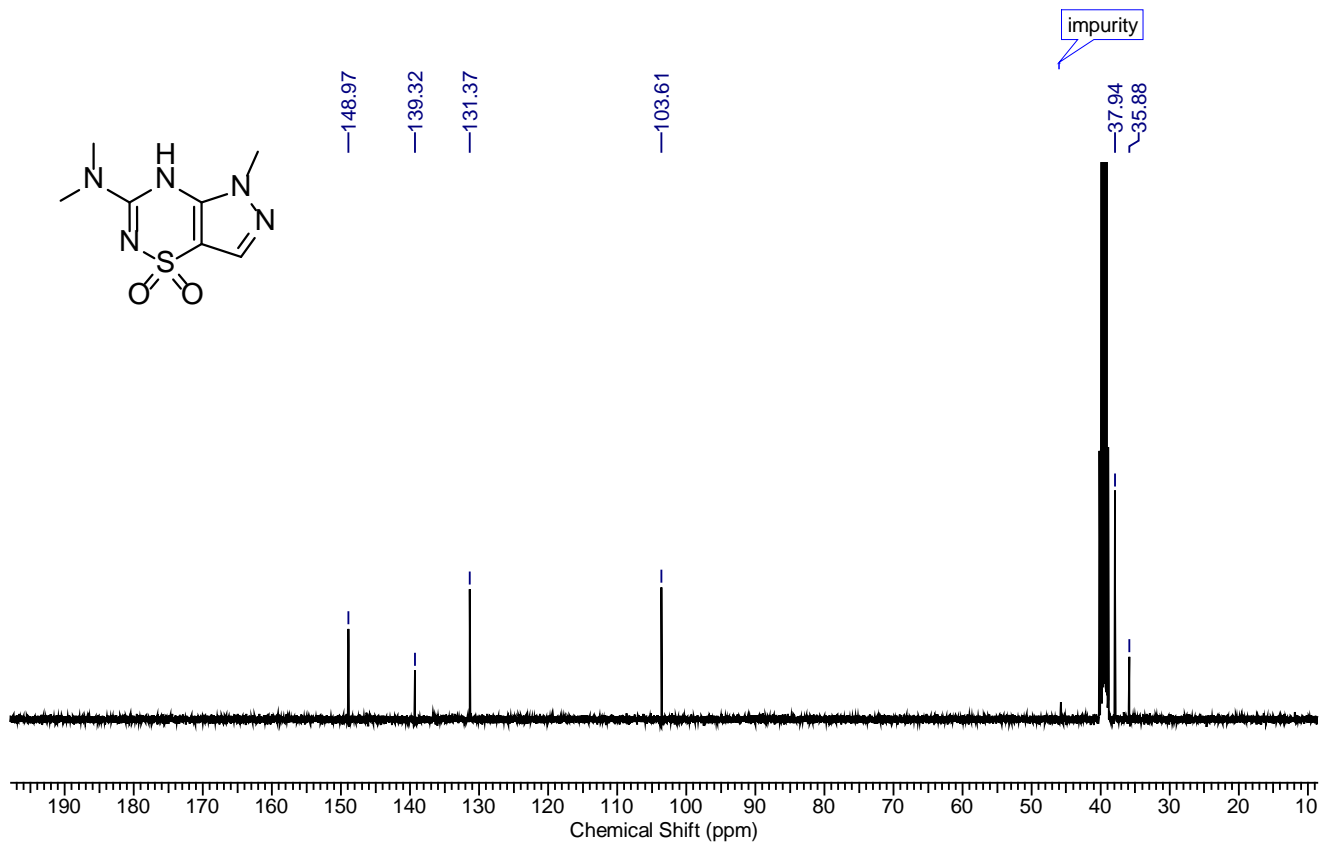
SO

S1-S10	¹ H NMR and ¹³ C NMR spectra fused pyrazolo-thiadiazines 3a-j
S11	¹ H NMR and ¹³ C NMR spectra of bis-pyrazole compound 6
S12-S23	¹ H NMR and ¹³ C NMR spectra of alkylated pyrazolo-thiadiazines 7a-10d
S24-S30	¹ H NMR and ¹³ C NMR spectra of alkylated pyrazolo-thiadiazines 11 and 14 and pyrimido-thiadiazines 13
S31-S38	2D NOESY, short and long range HETCOR (HMOC and HMBC) spectra of alkylated pyrazolo-thiadiazines 7-11 and 14 and pyrimido-thiadiazines 13

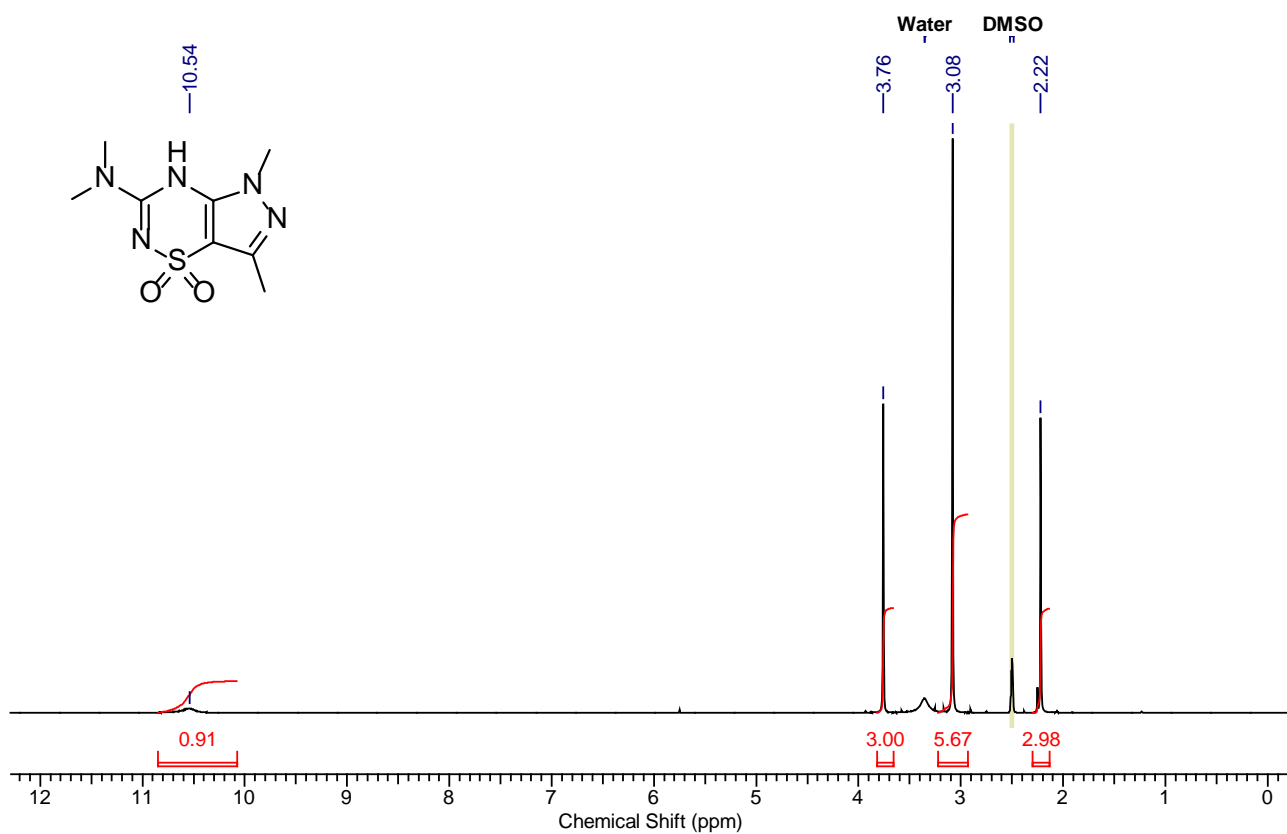
^1H NMR spectrum of **3a** 400MHz (DMSO- d_6) 26°C



S1 ^{13}C NMR spectrum of **3a** 100MHz (DMSO- d_6) 36°C

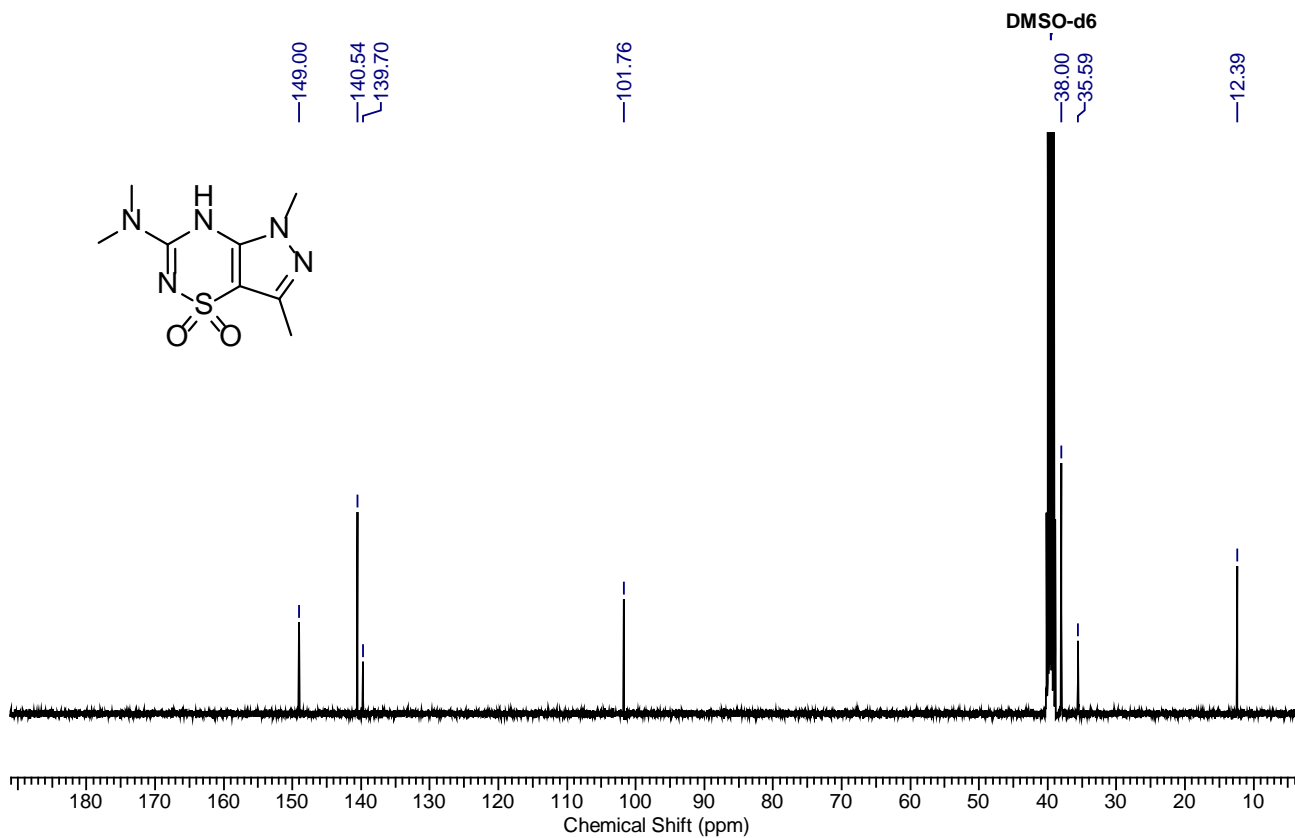


^1H NMR spectrum of **3b** 400MHz (DMSO- d_6) 26°C

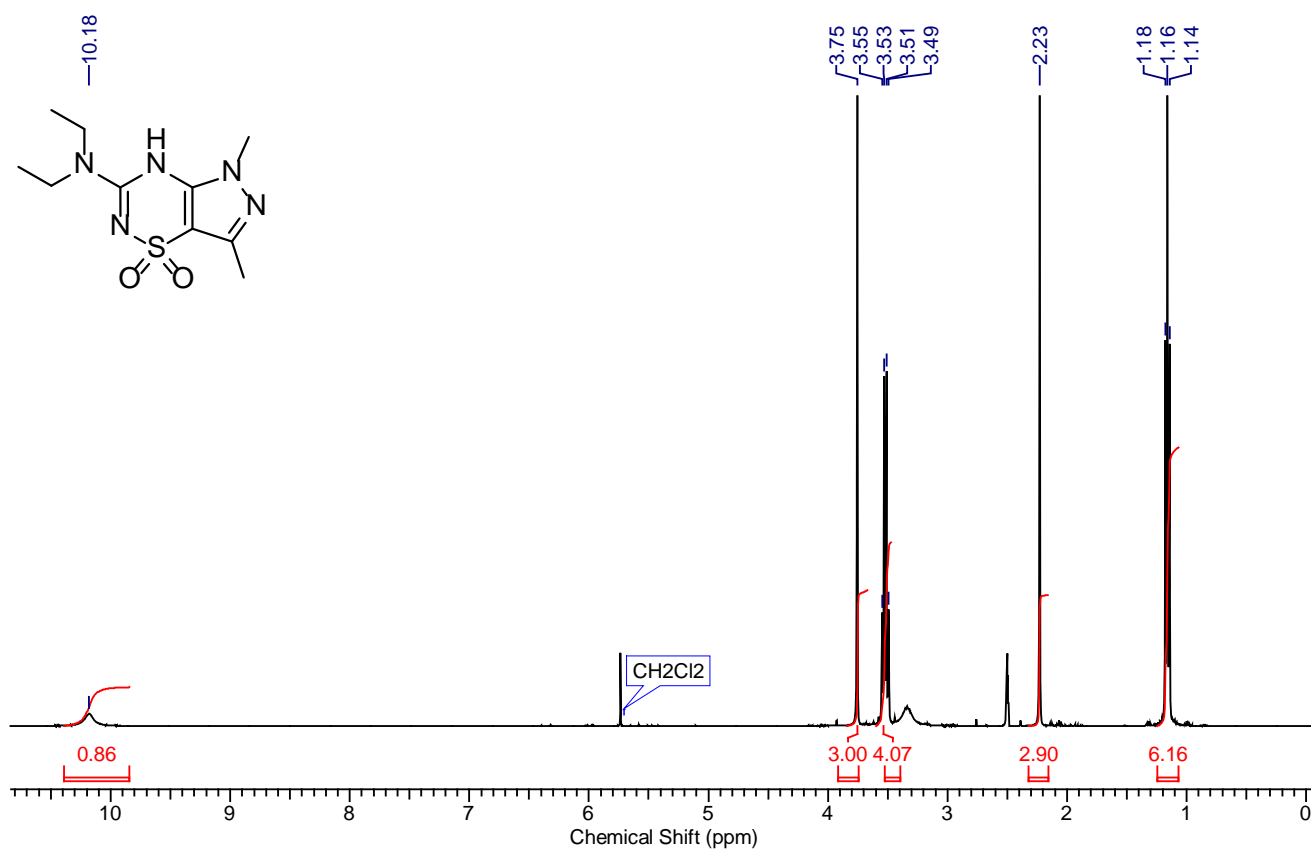


^{13}C NMR spectrum of **3b** 100MHz (DMSO- d_6) 26°C

S2

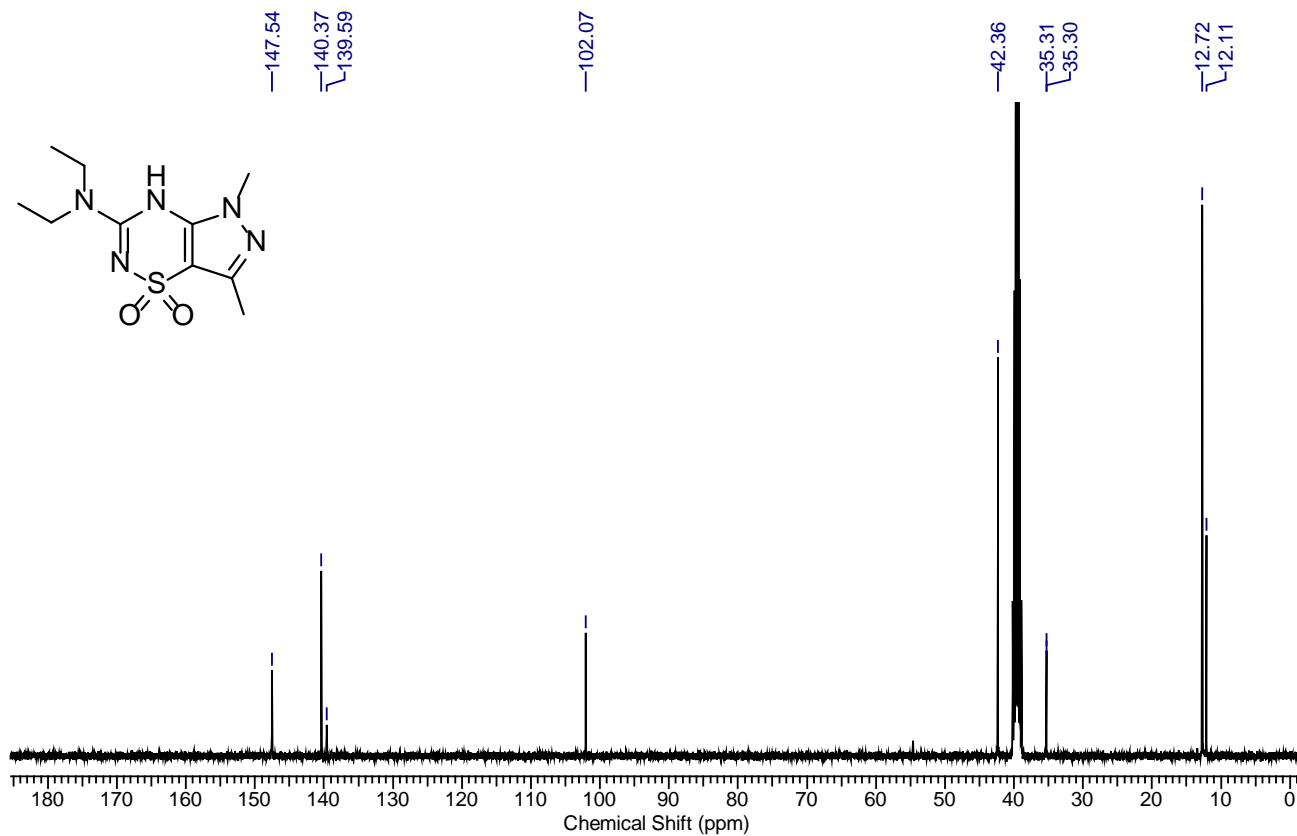


¹H NMR spectrum of **3c** 400MHz (DMSO-d⁶) 36°C

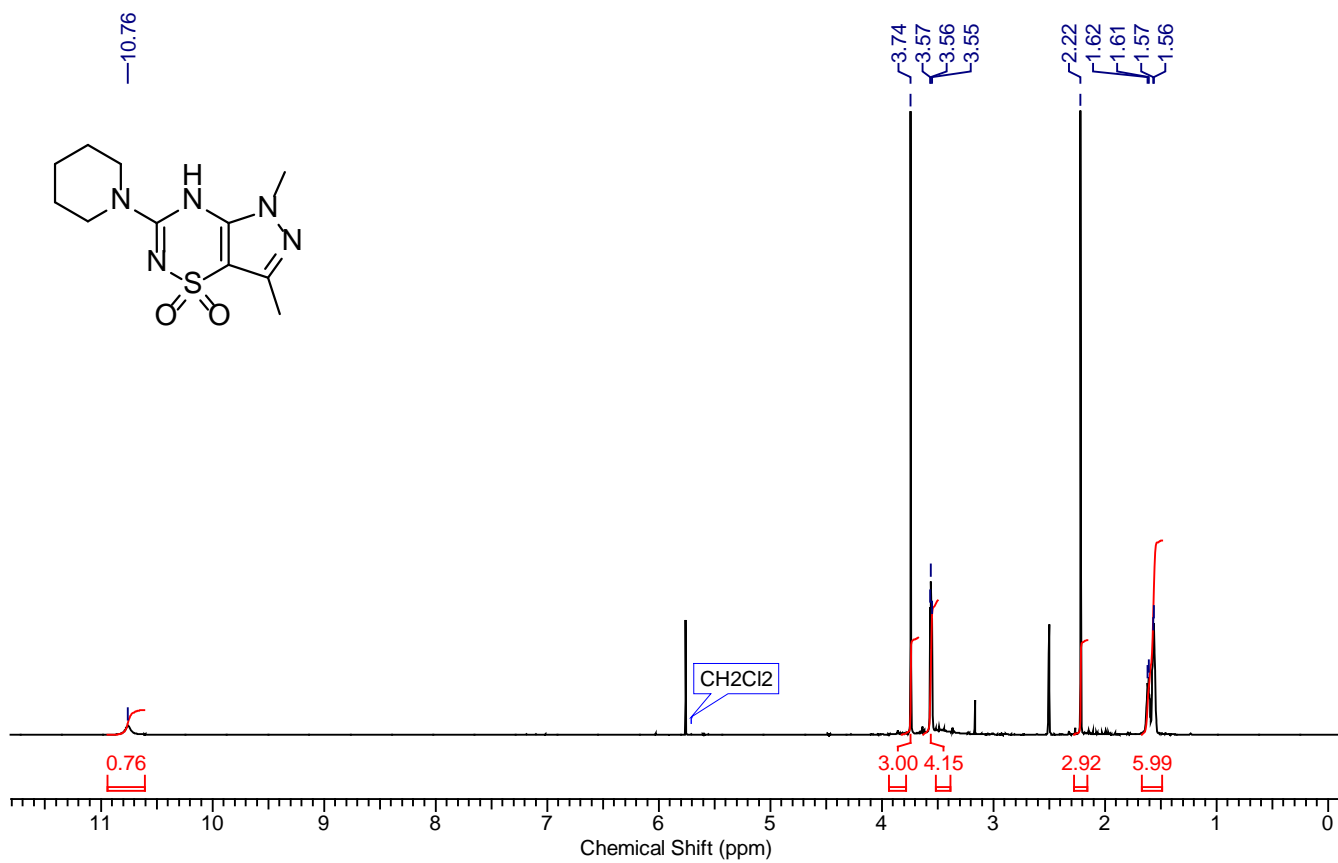


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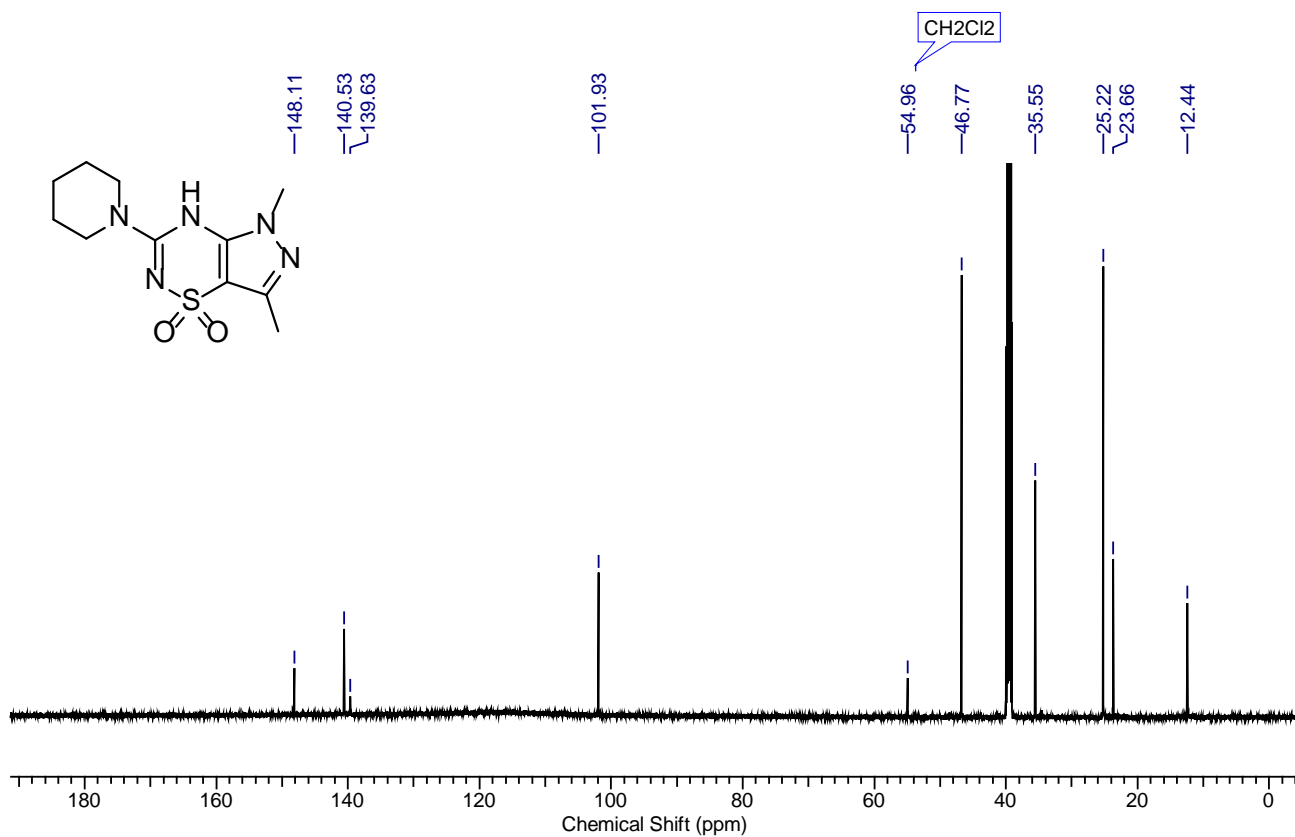
¹³C NMR spectrum of **3c** 100MHz (DMSO-d⁶) 56°C



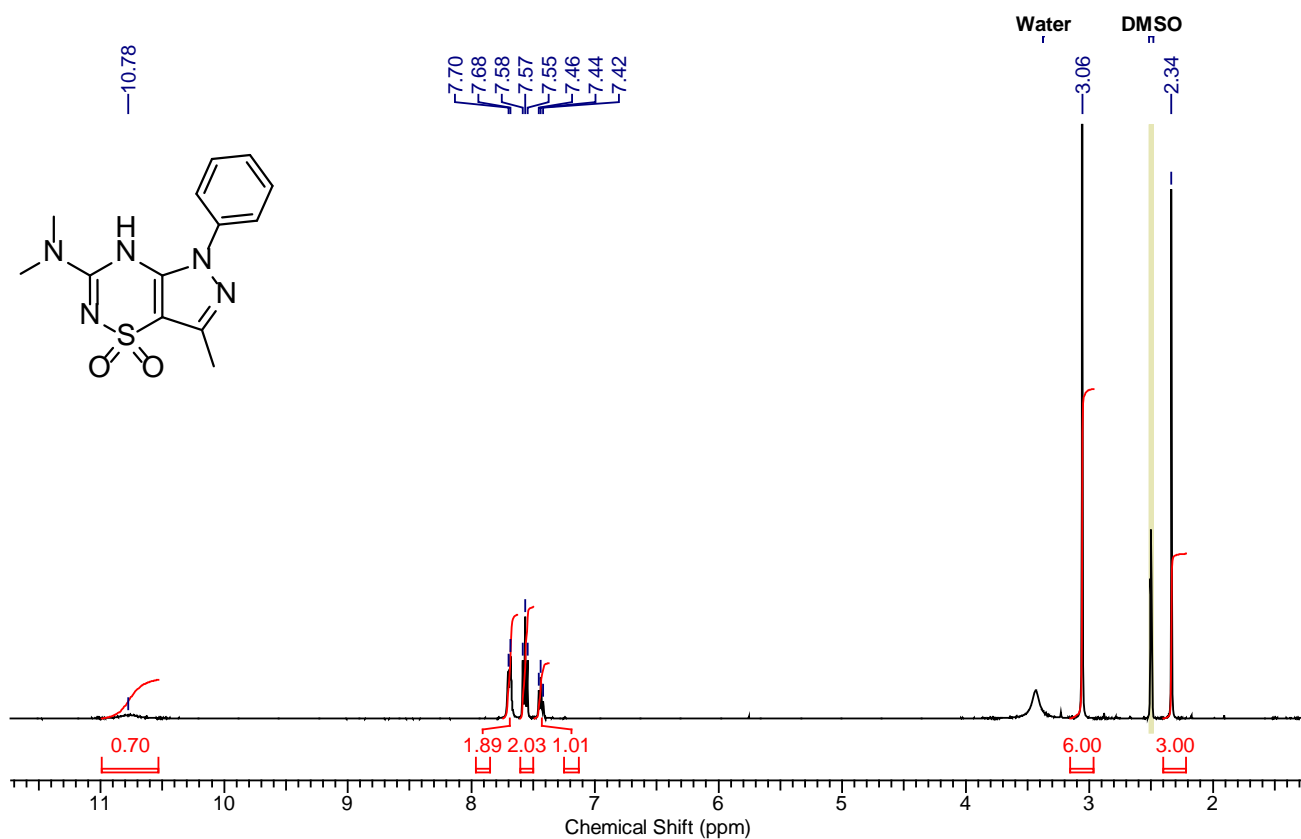
^1H NMR spectrum of **3d** 600MHz (DMSO- d_6) 20°C



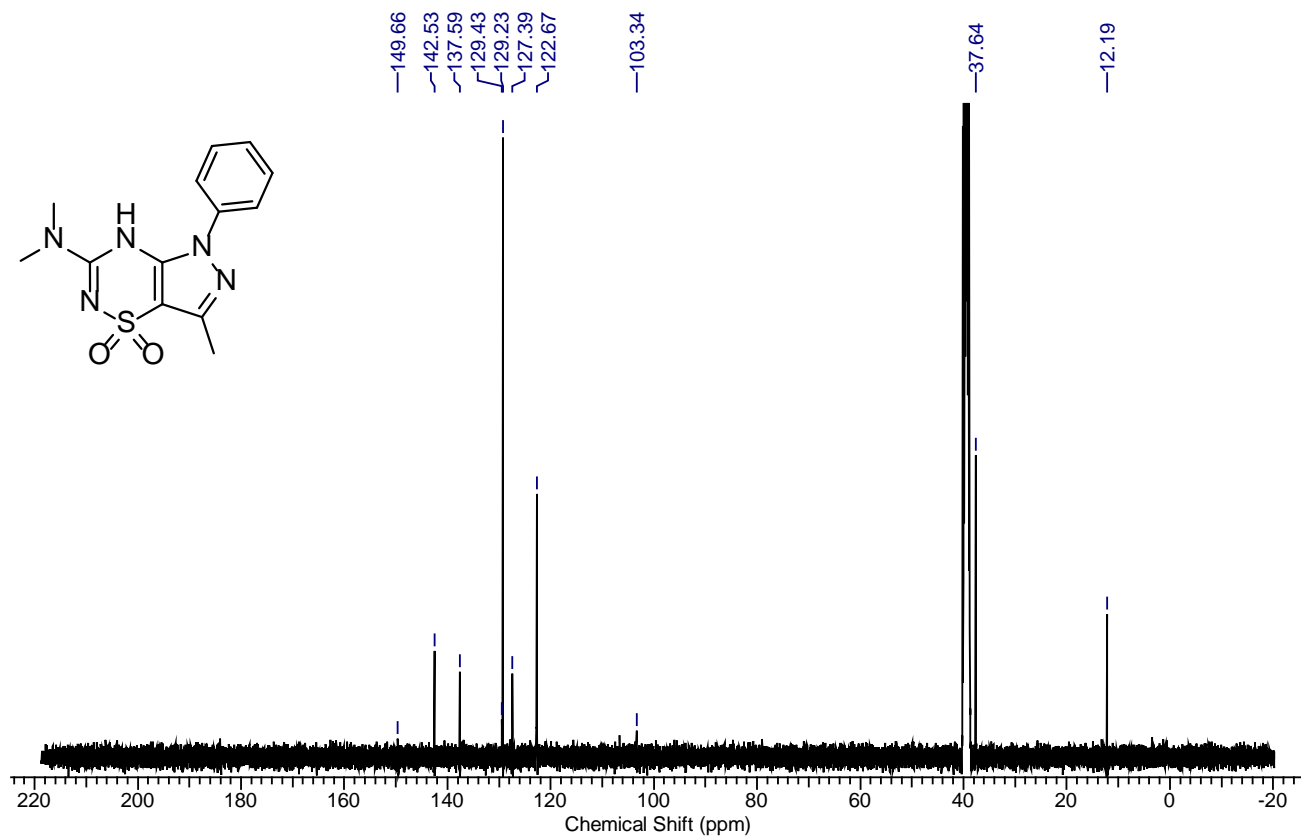
S4 ^{13}C NMR spectrum of **3d** 150MHz (DMSO- d_6) 20°C



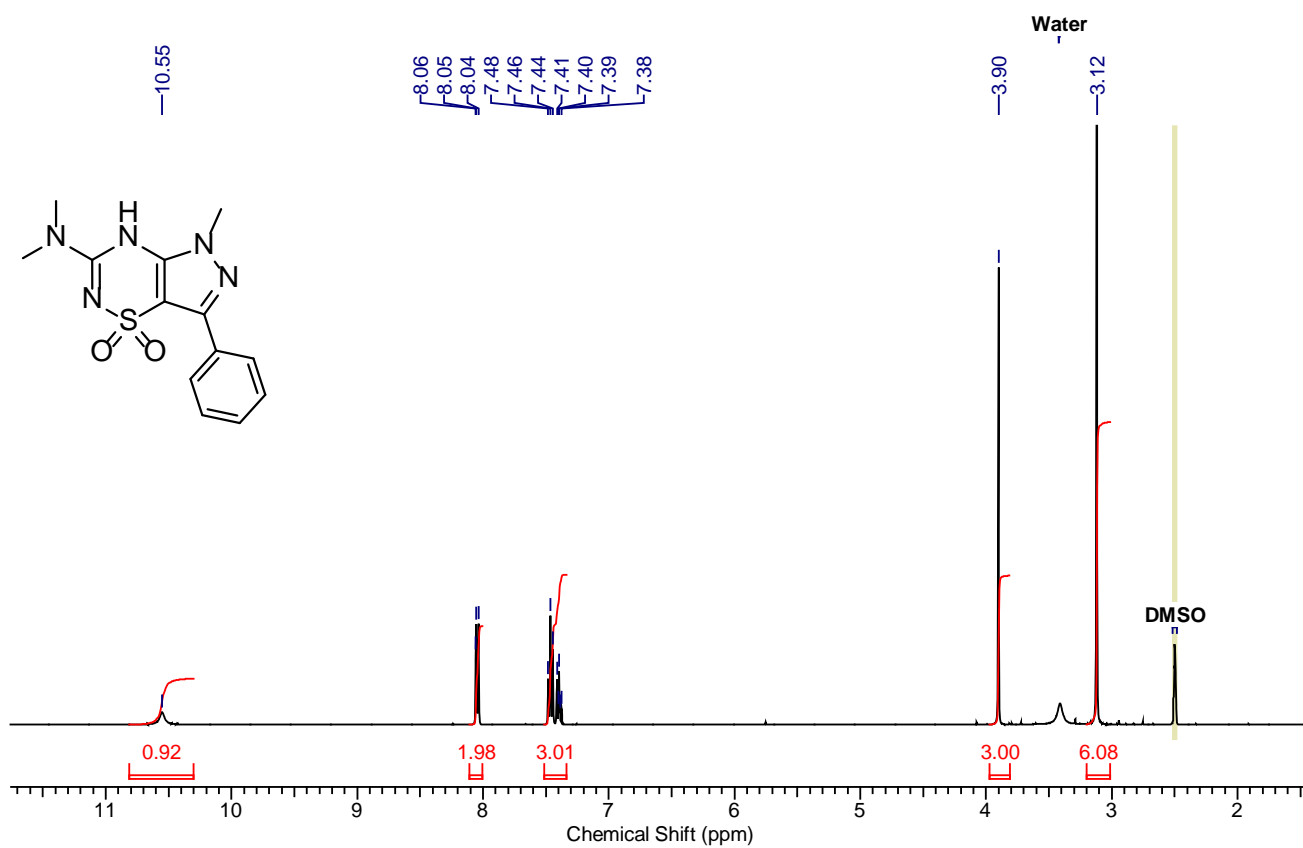
^1H NMR spectrum of **3e** 400MHz (DMSO- d_6) 26°C



^{13}C NMR spectrum of **3e** 100MHz (DMSO- d_6) 56°C

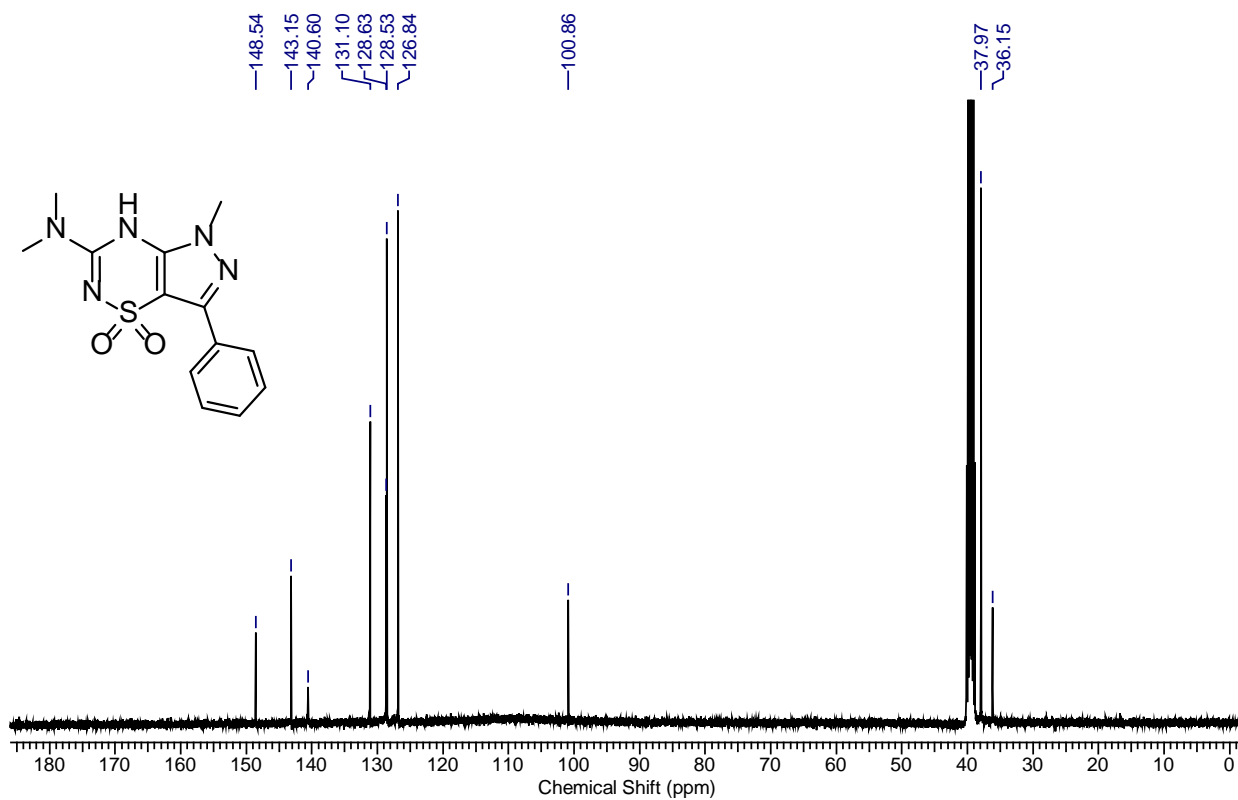


^1H NMR spectrum of **3f** 400MHz (DMSO- d_6) 26°C

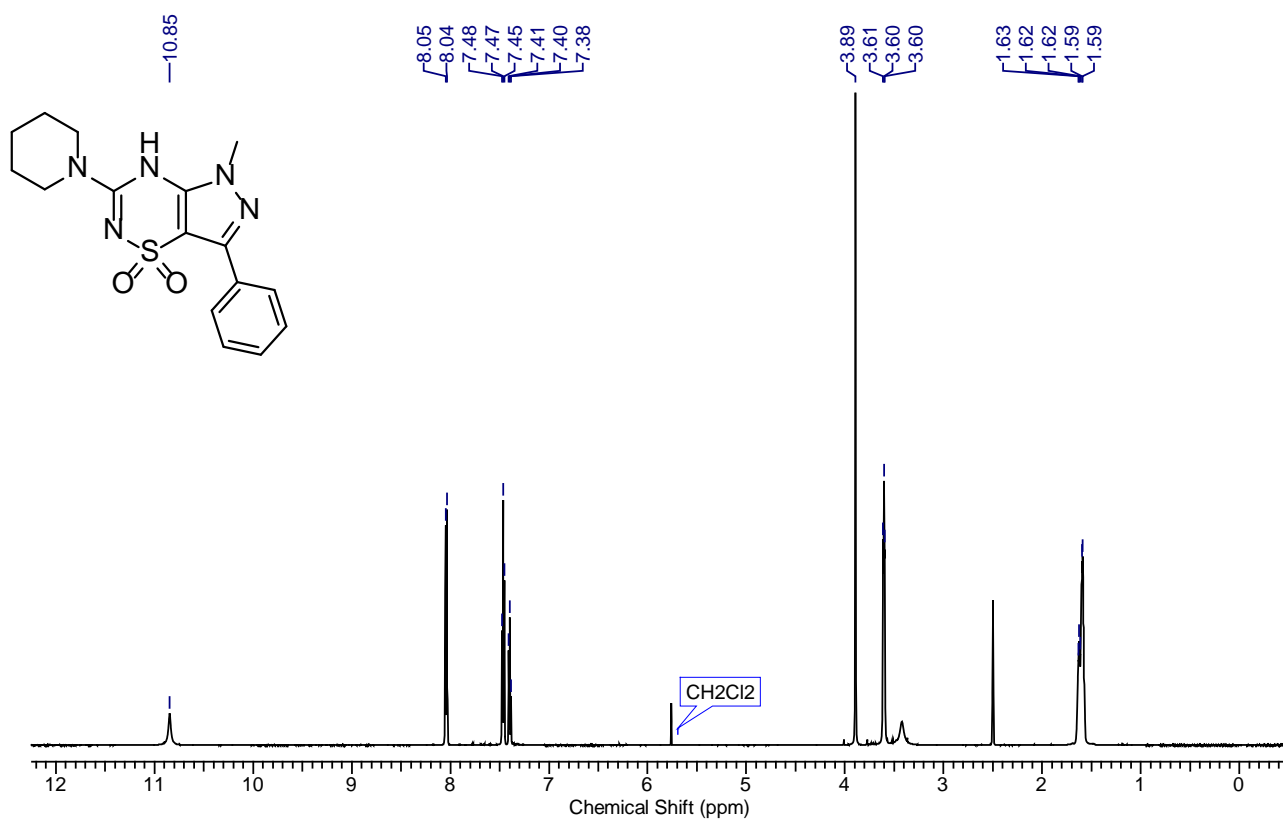


S6

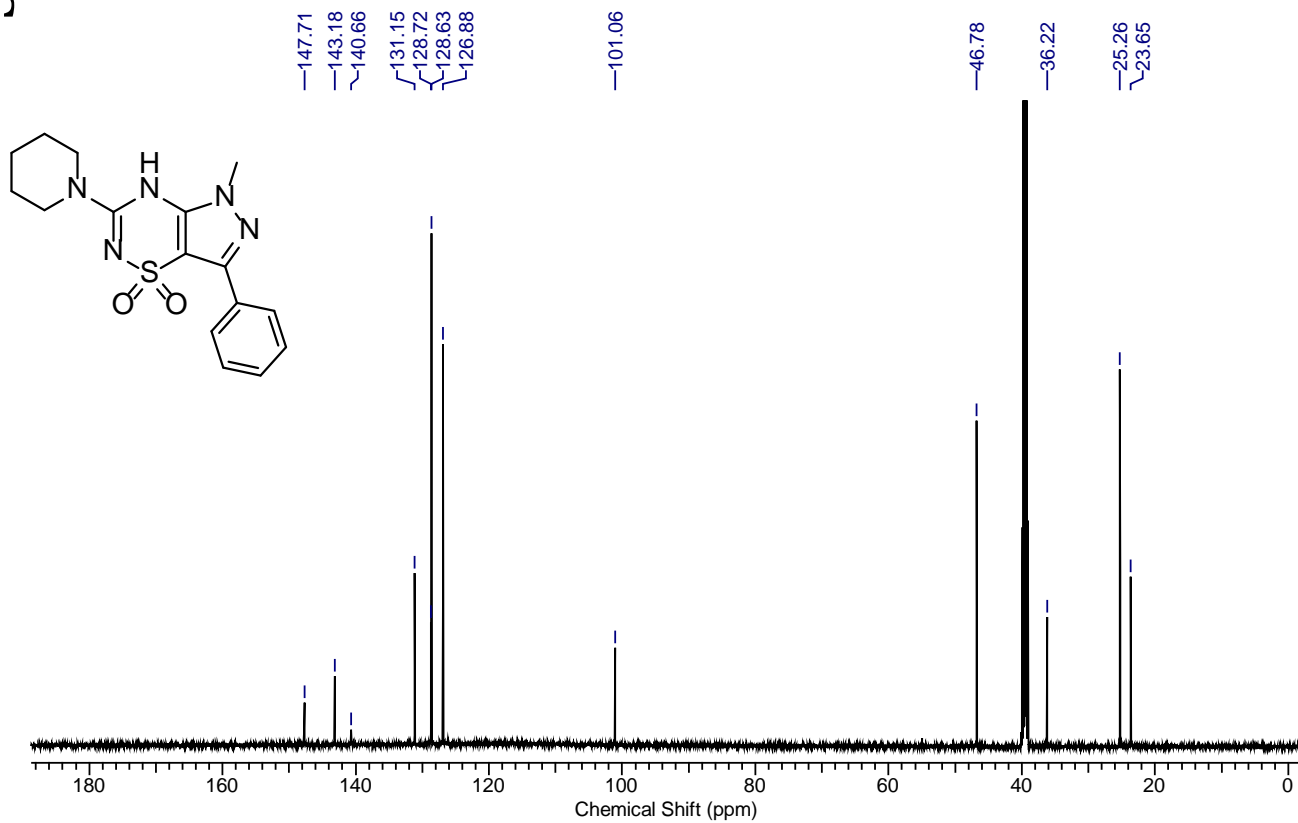
^{13}C NMR spectrum of **3f** 100MHz (DMSO- d_6) 26°C



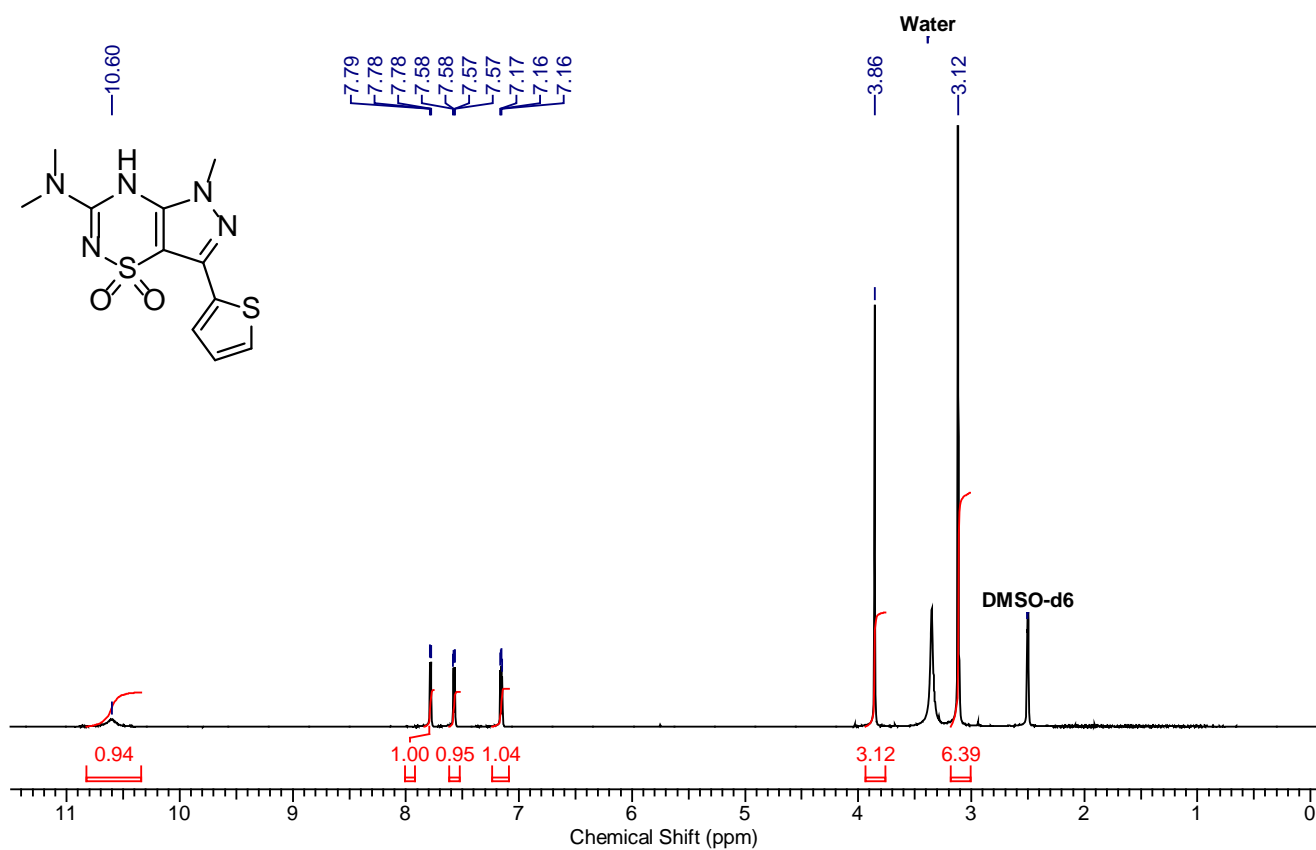
^1H NMR spectrum of **3g** 600MHz (DMSO- d_6) 20°C



S7 ^{13}C NMR spectrum of **3g** 150MHz (DMSO- d_6) 20°C

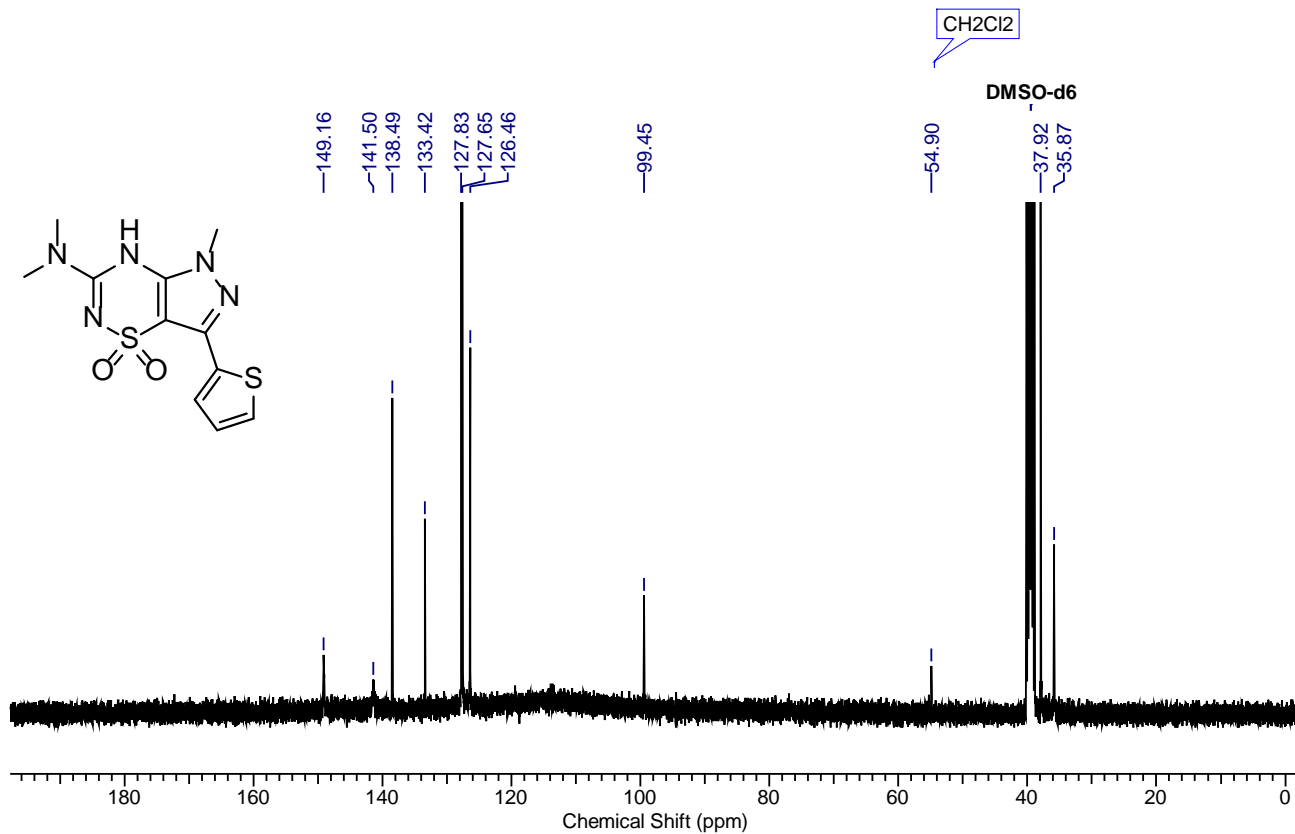


^1H NMR spectrum of **3h** 400MHz (DMSO- d_6) 26°C

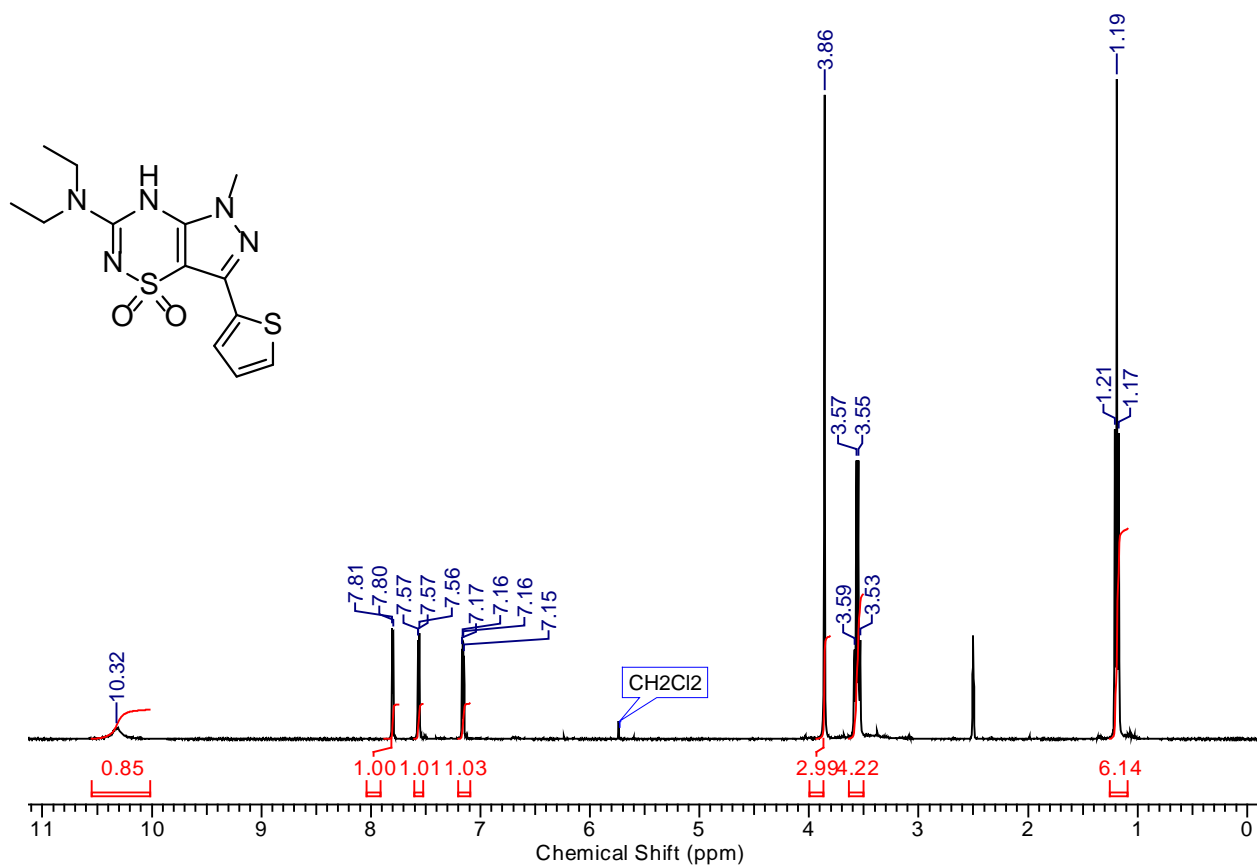


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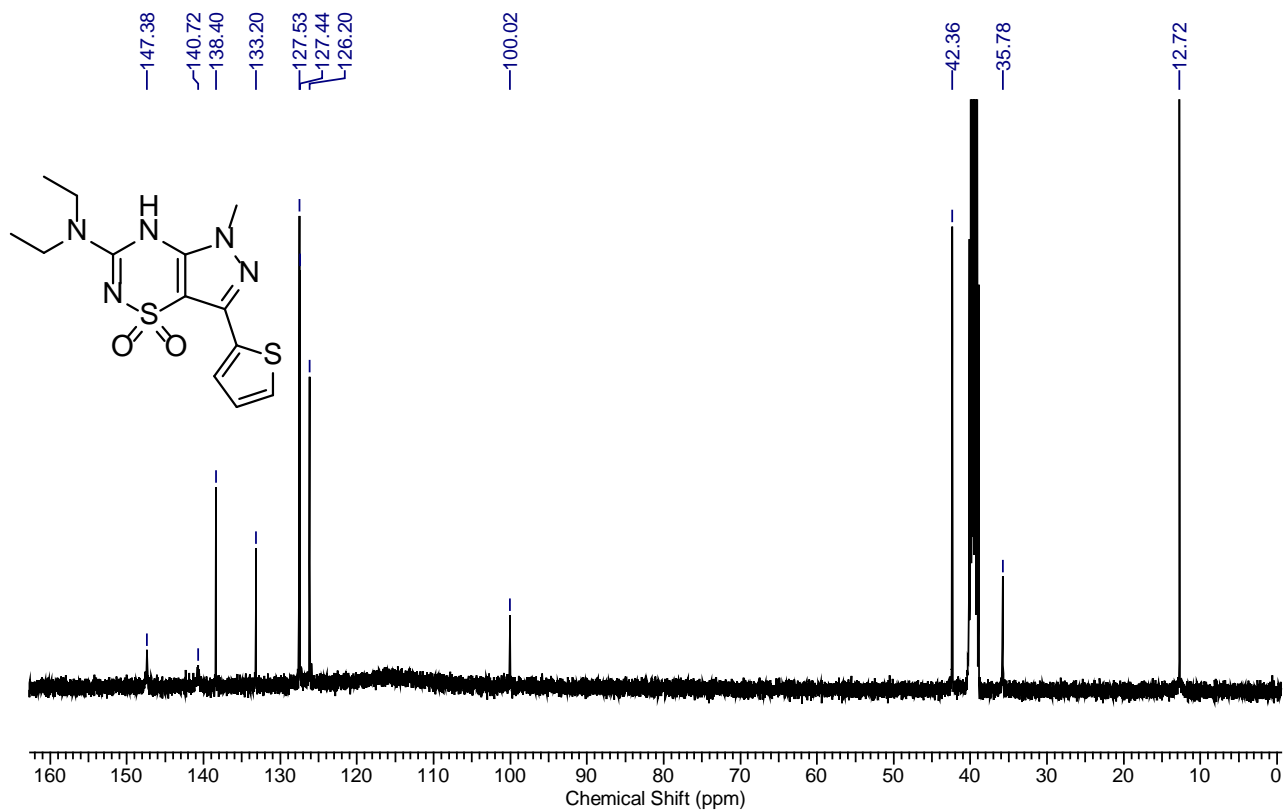
^{13}C NMR spectrum of **3h** 100MHz (DMSO- d_6) 26°C



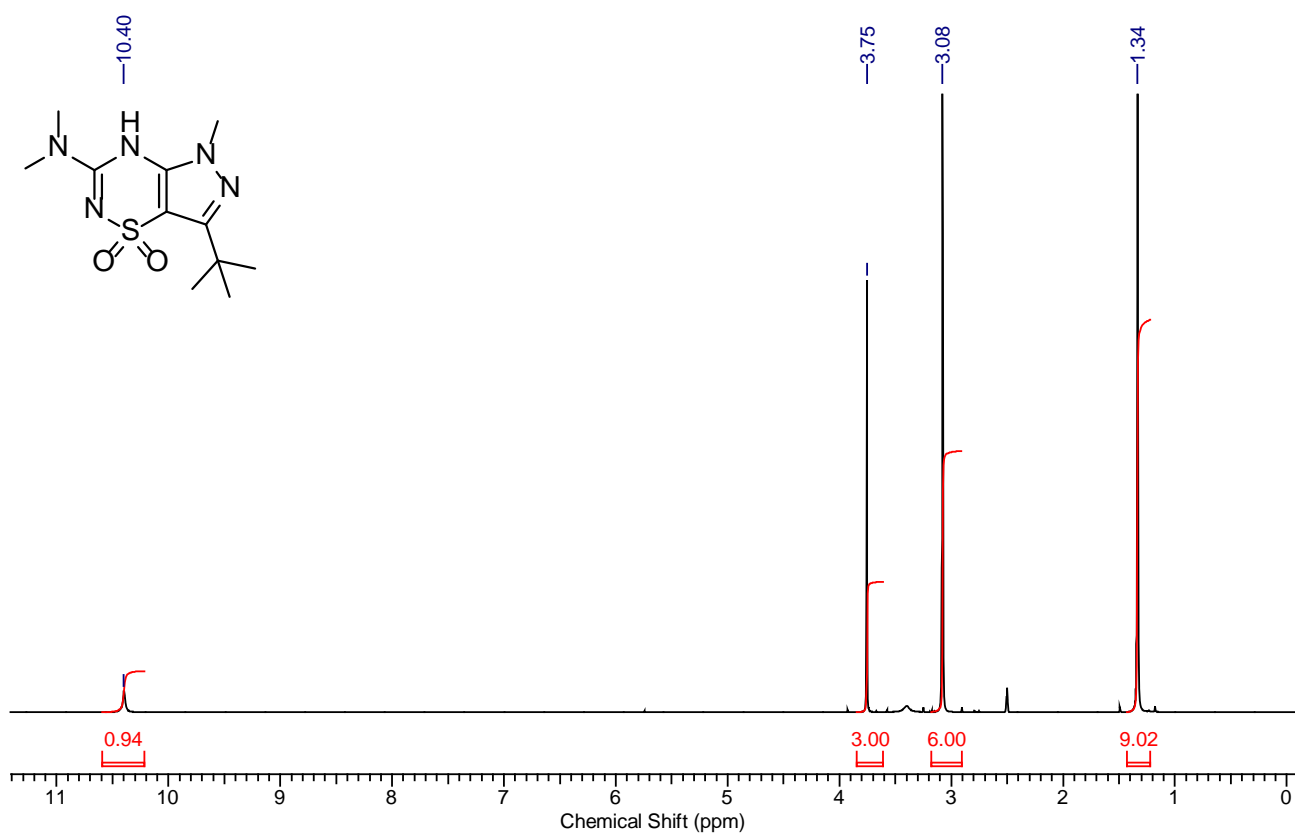
^1H NMR spectrum of **3i** 400MHz (DMSO- d_6) 36°C



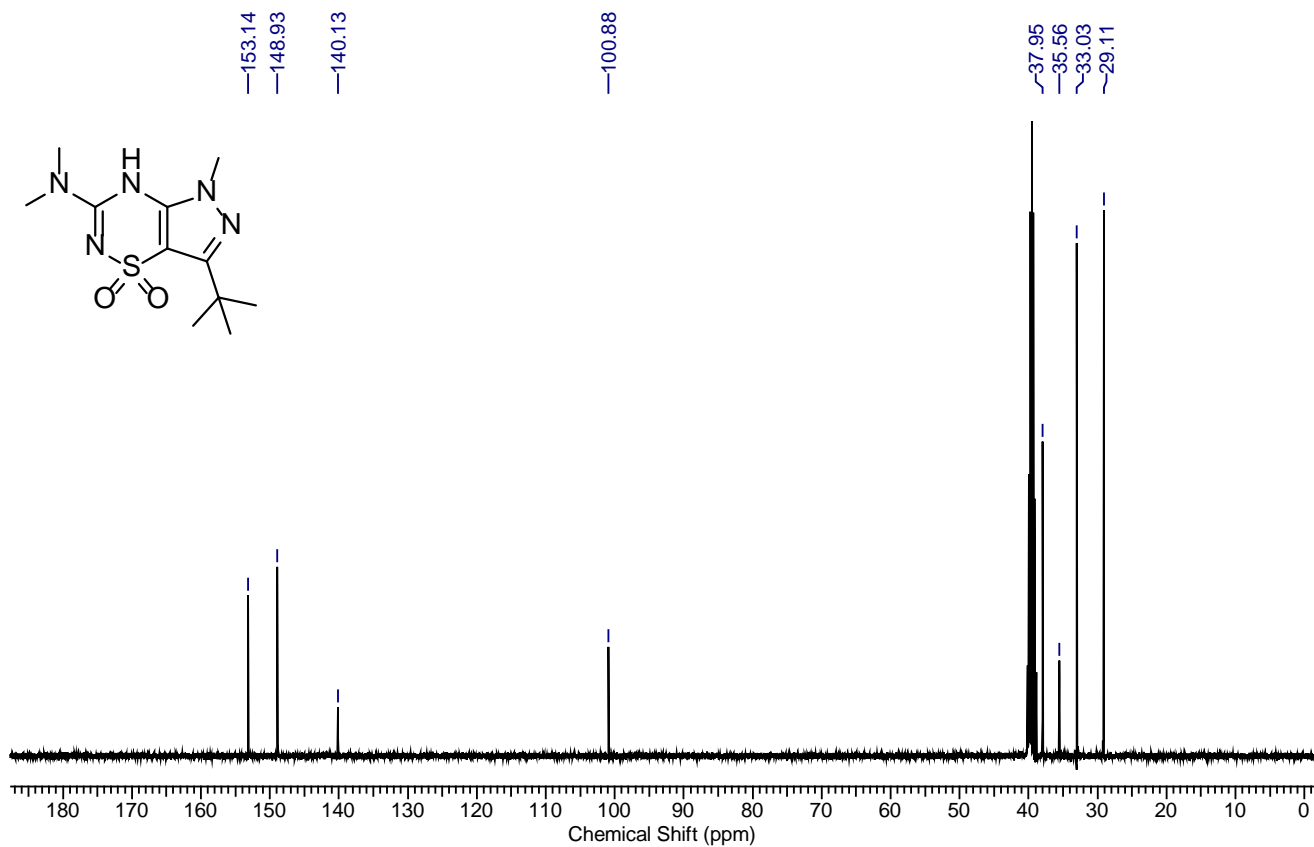
S9 ^{13}C NMR spectrum of **3i** 150MHz (DMSO- d_6) 56°C



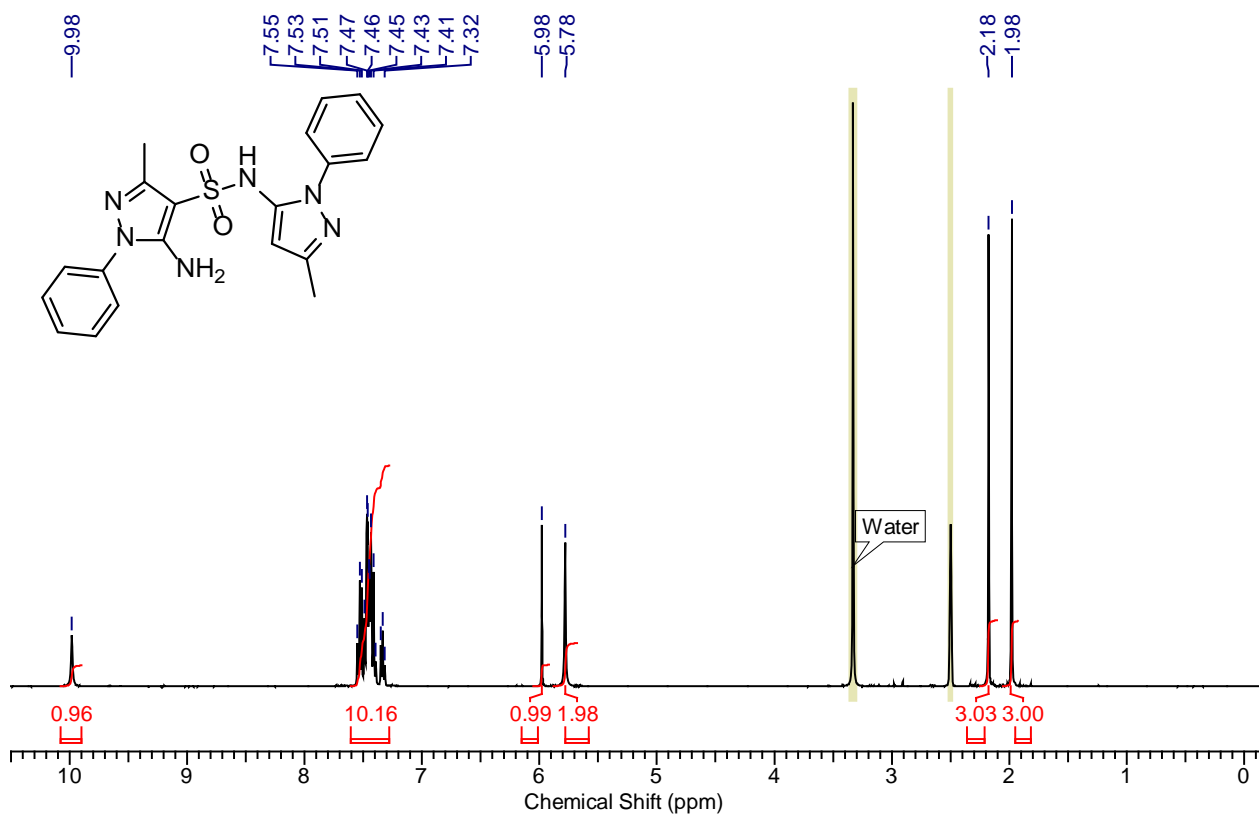
¹H NMR spectrum of **3j** 400MHz (DMSO-d⁶) 26°C



S10 ¹³C NMR spectrum of **3j** 100MHz (DMSO-d⁶) 26°C

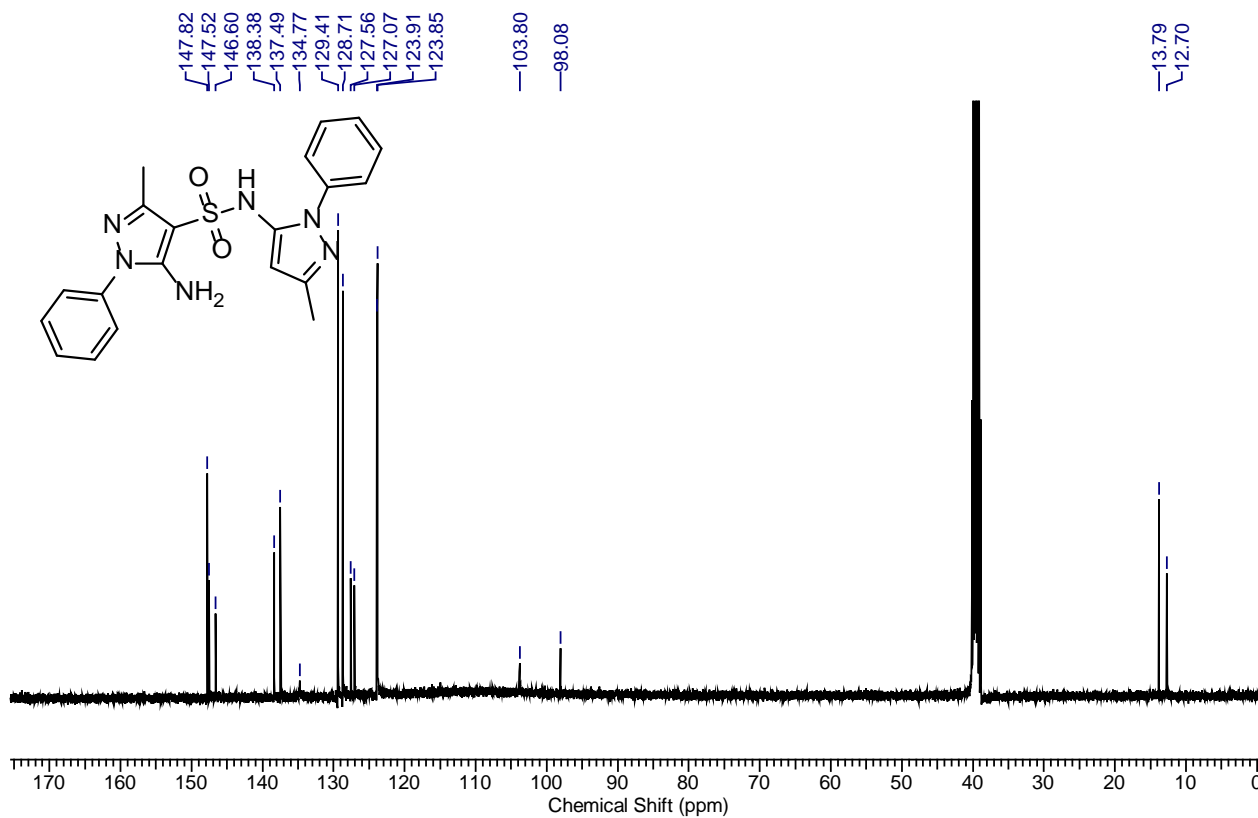


¹H NMR spectrum of **6** 400MHz (DMSO-d⁶) 26°C

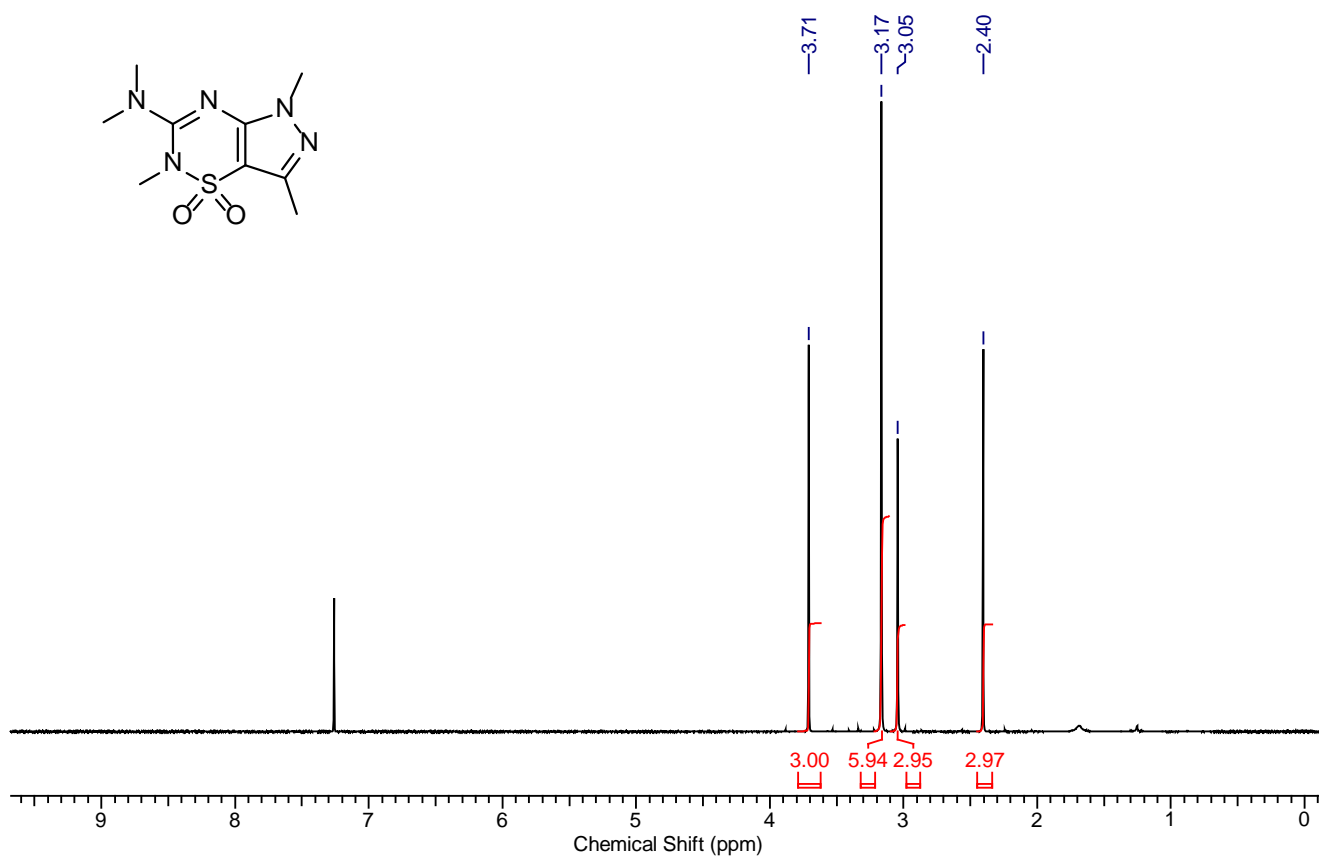


S11

¹³C NMR spectrum of **6** 100MHz (DMSO-d⁶) 26°C

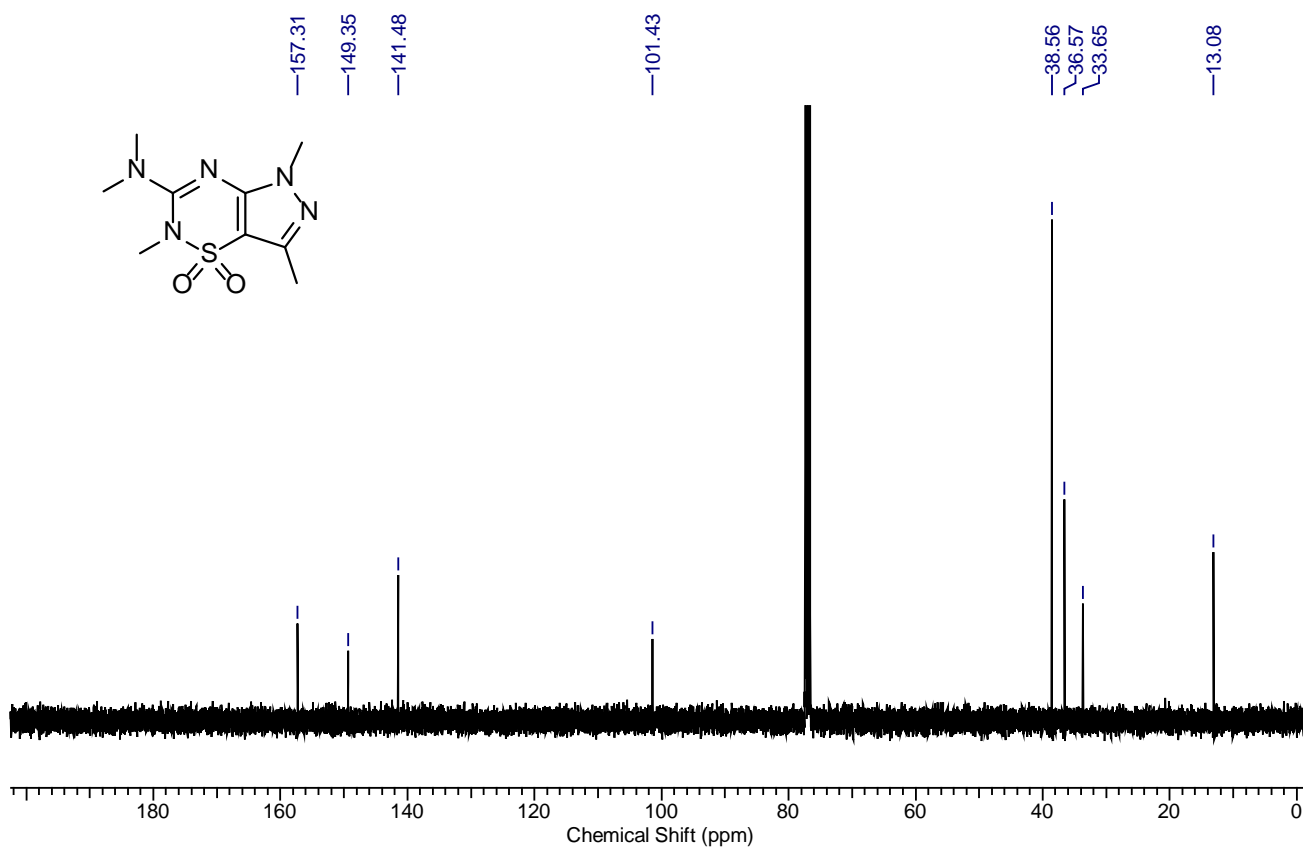


¹H NMR spectrum of **7a** 400MHz (CDCl₃)

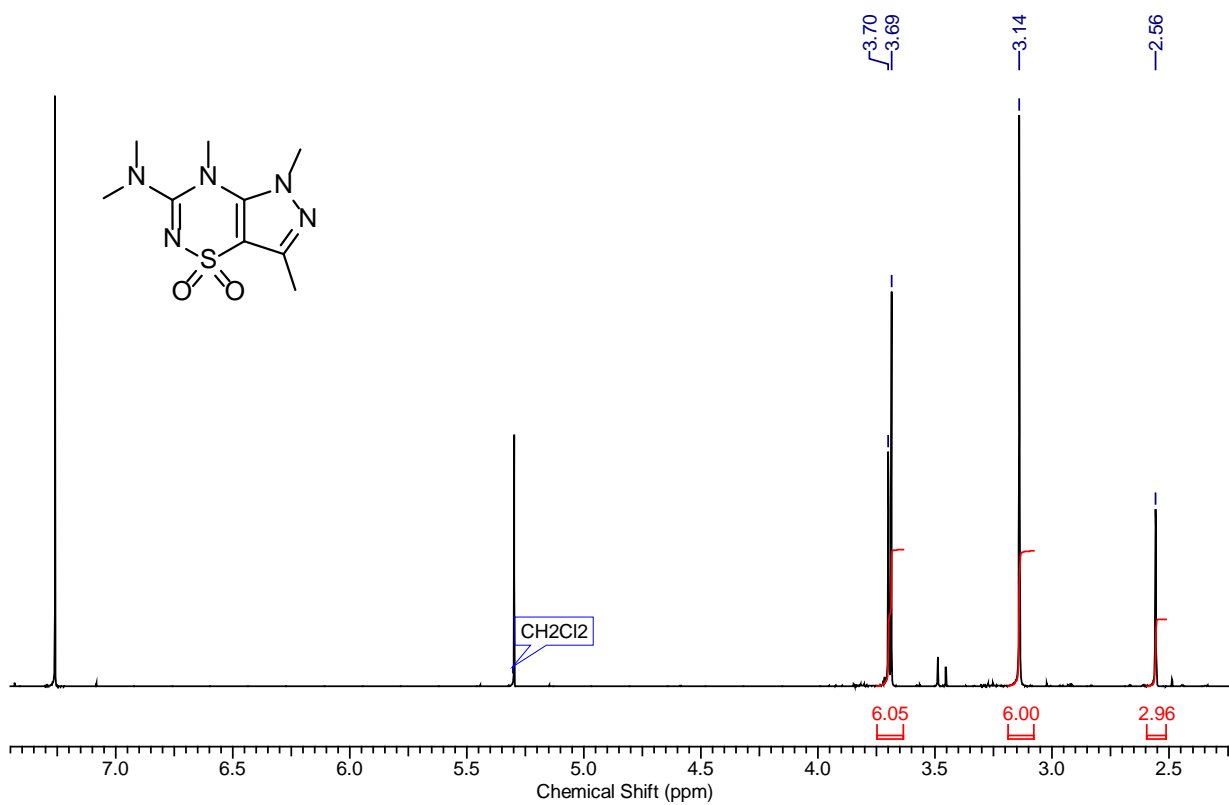


S12

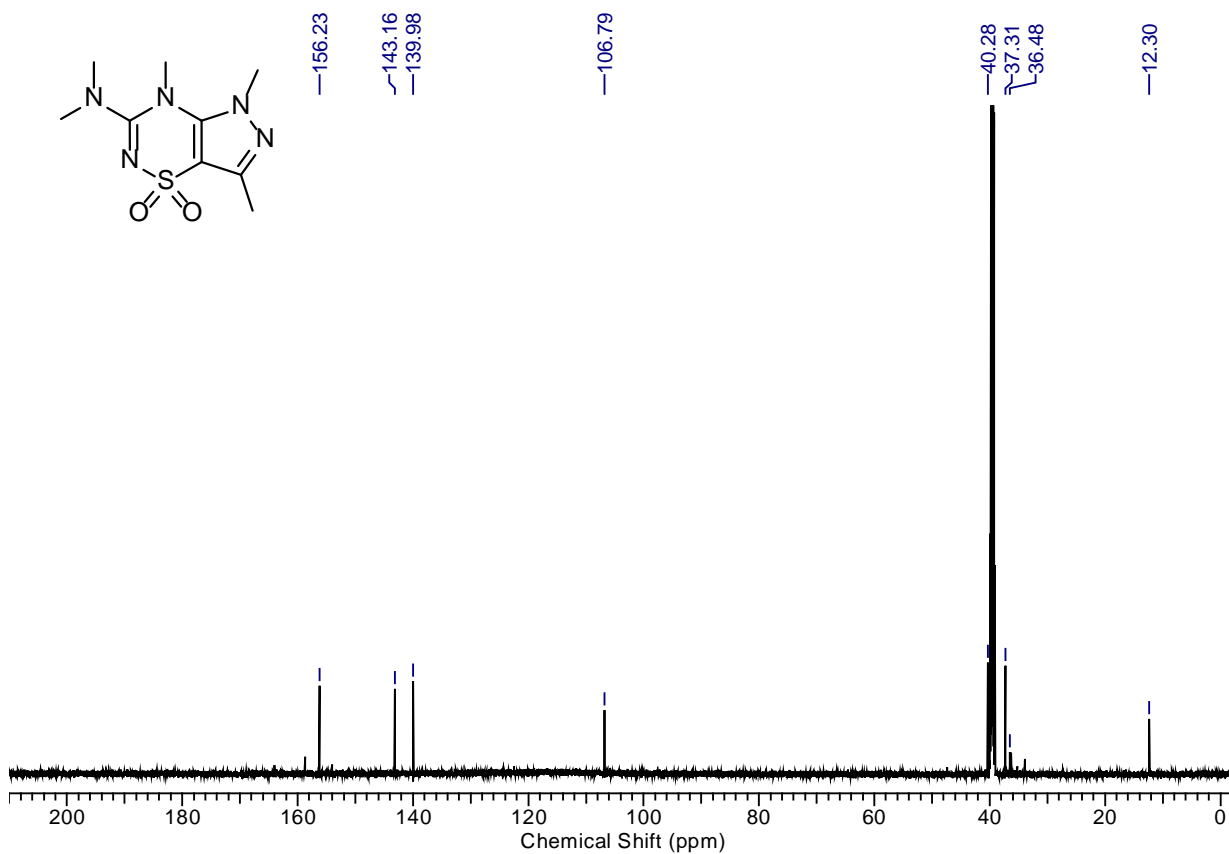
¹³C NMR spectrum of **7a** 100MHz (CDCl₃)



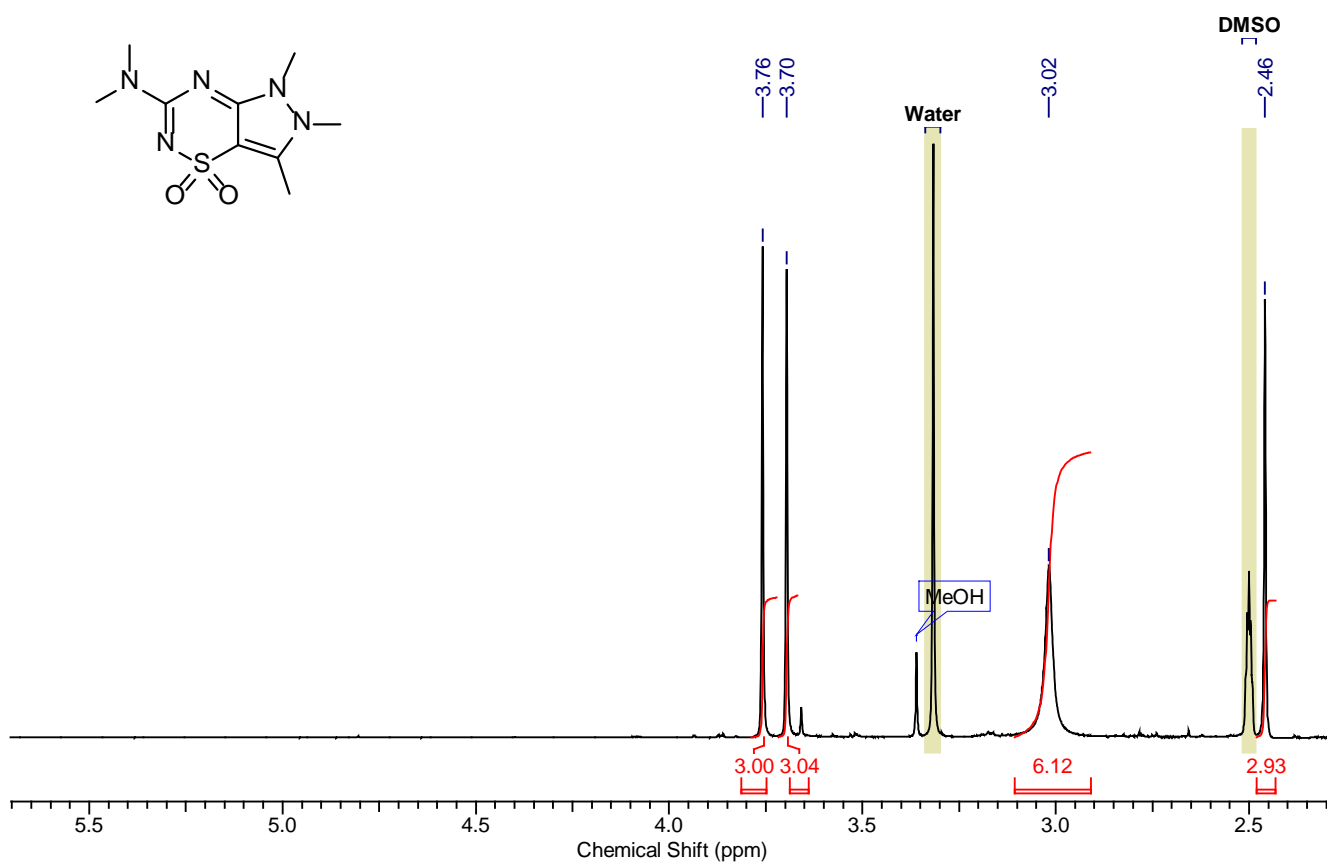
¹H NMR spectrum of **8a** 400MHz (CDCl₃)



S13 ¹³C NMR spectrum of **8a** 150MHz (DMSO-d₆)

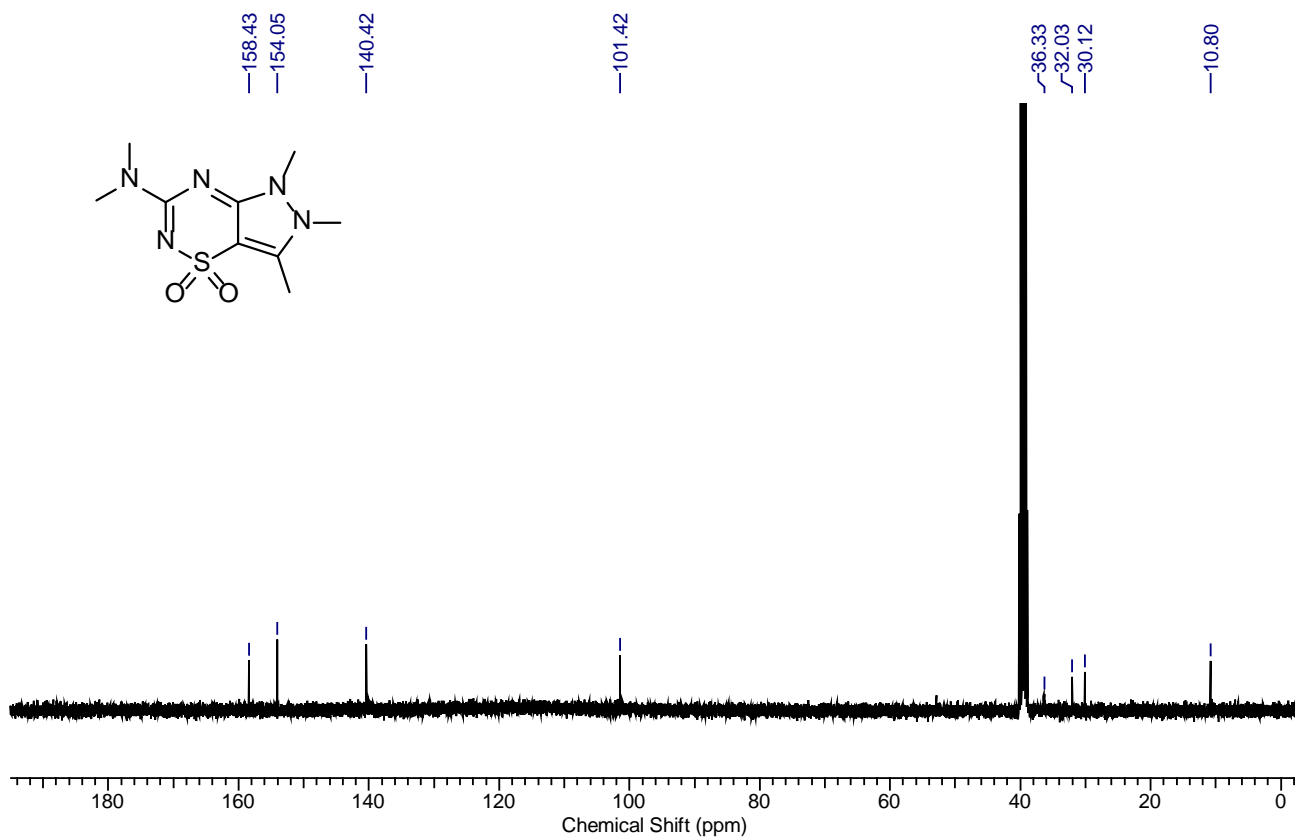


¹H NMR spectrum of **9a** 400MHz (DMSO-d⁶)

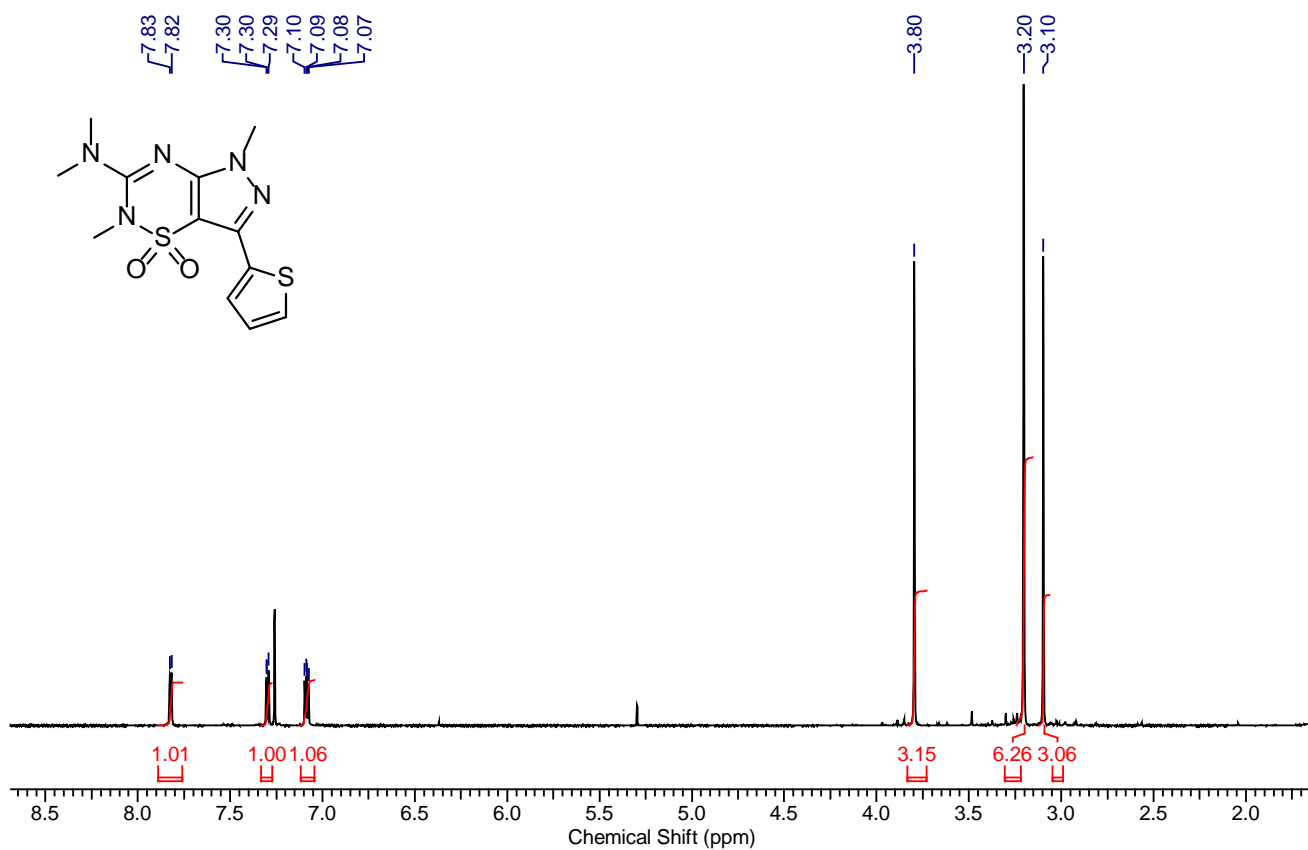


S14

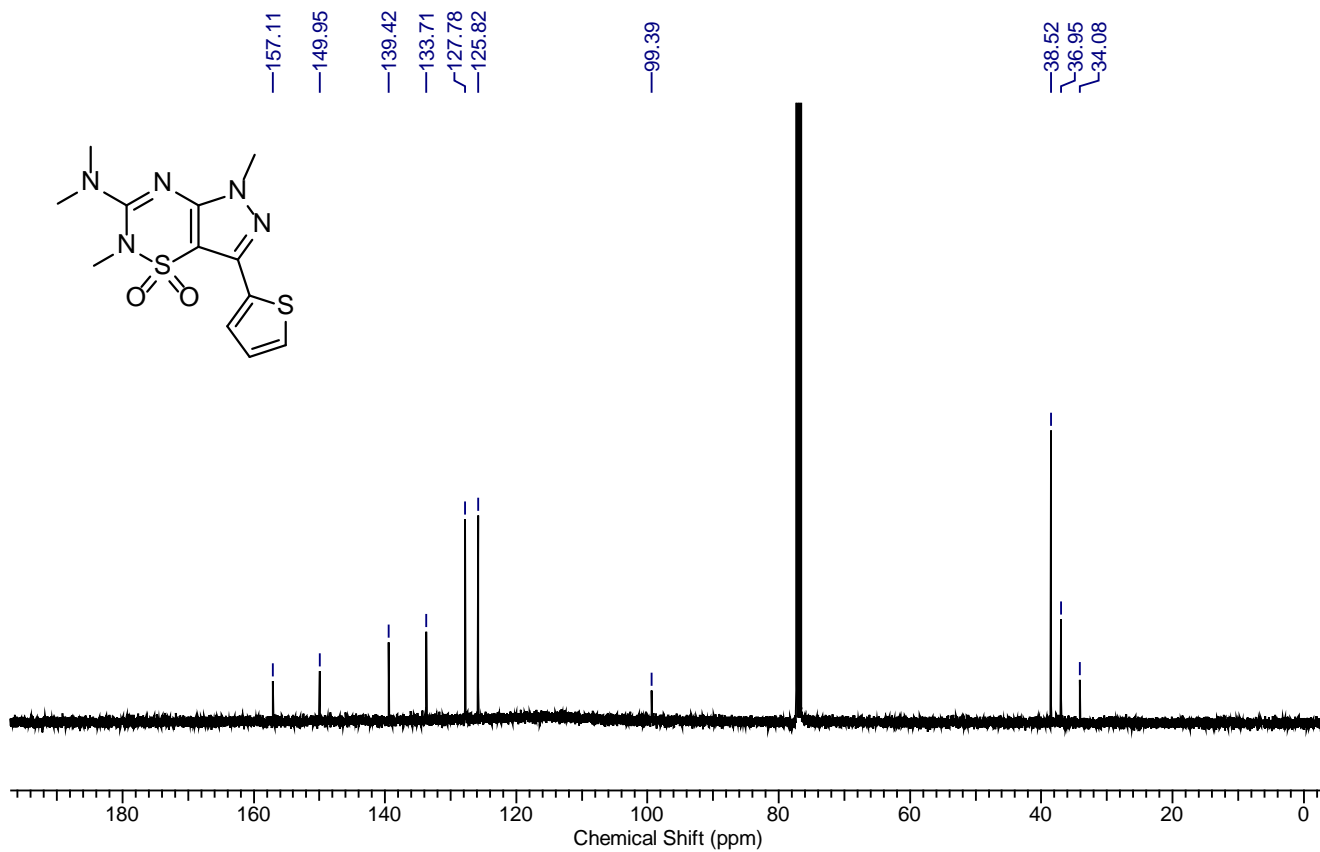
¹³C NMR spectrum of **9a** 100MHz (DMSO-d⁶)



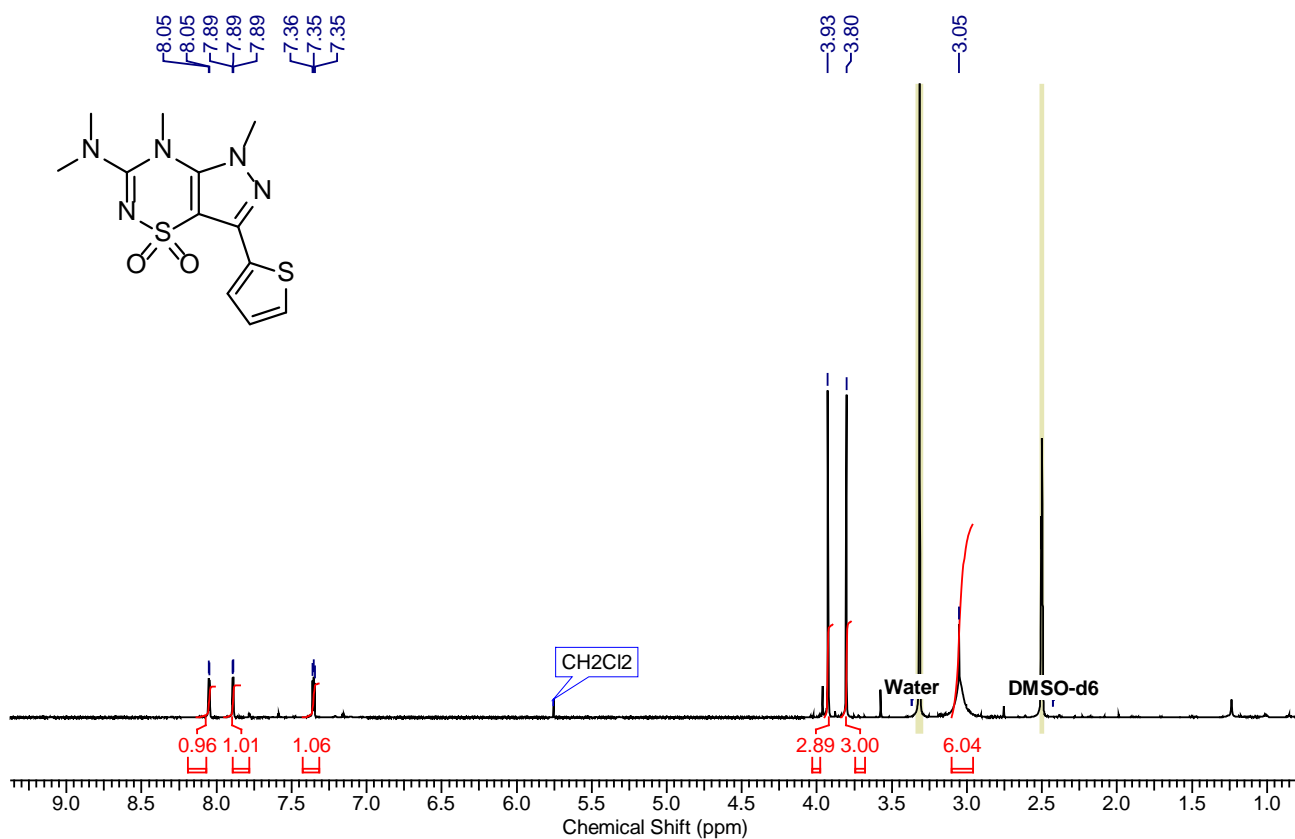
¹H NMR spectrum of **7b** 400MHz (CDCl₃)



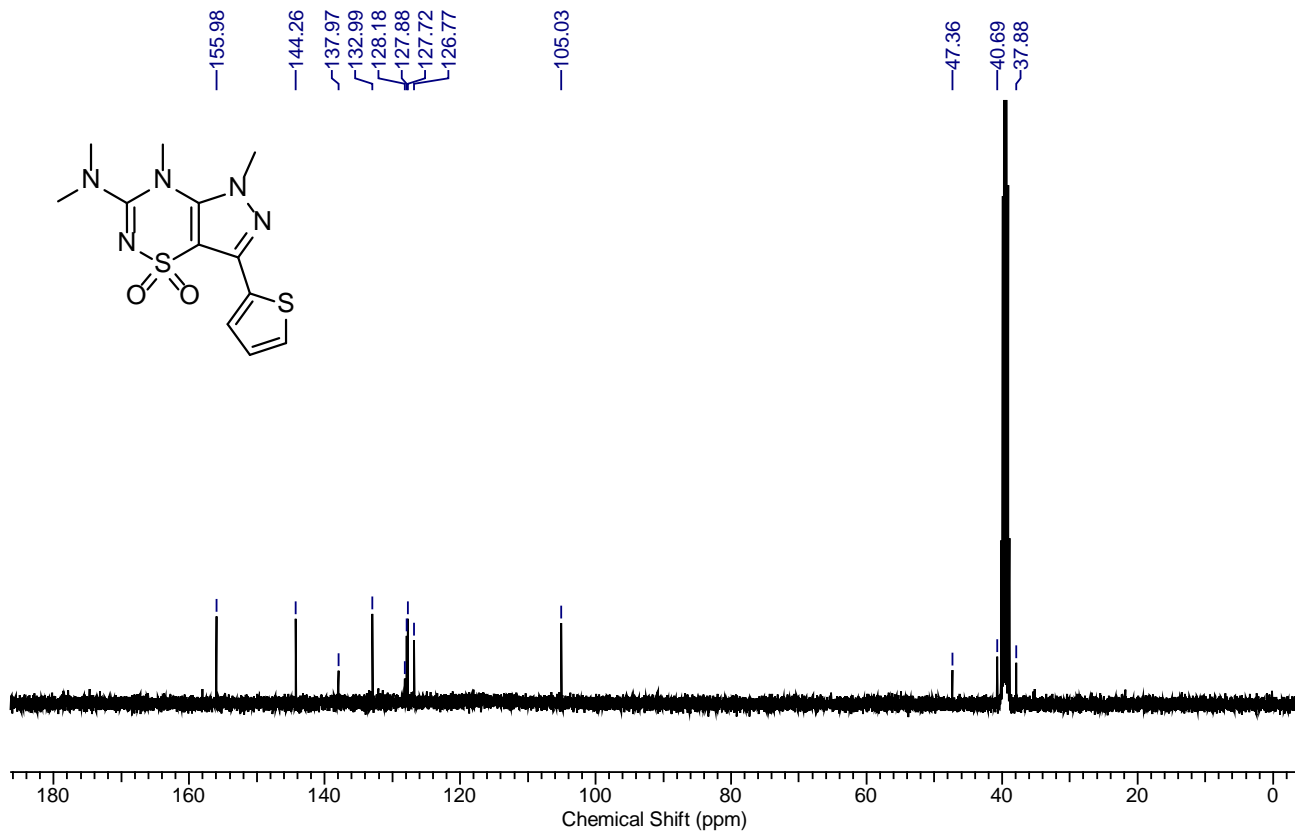
¹³C NMR spectrum of **7b** 100MHz (DMSO-d₆)



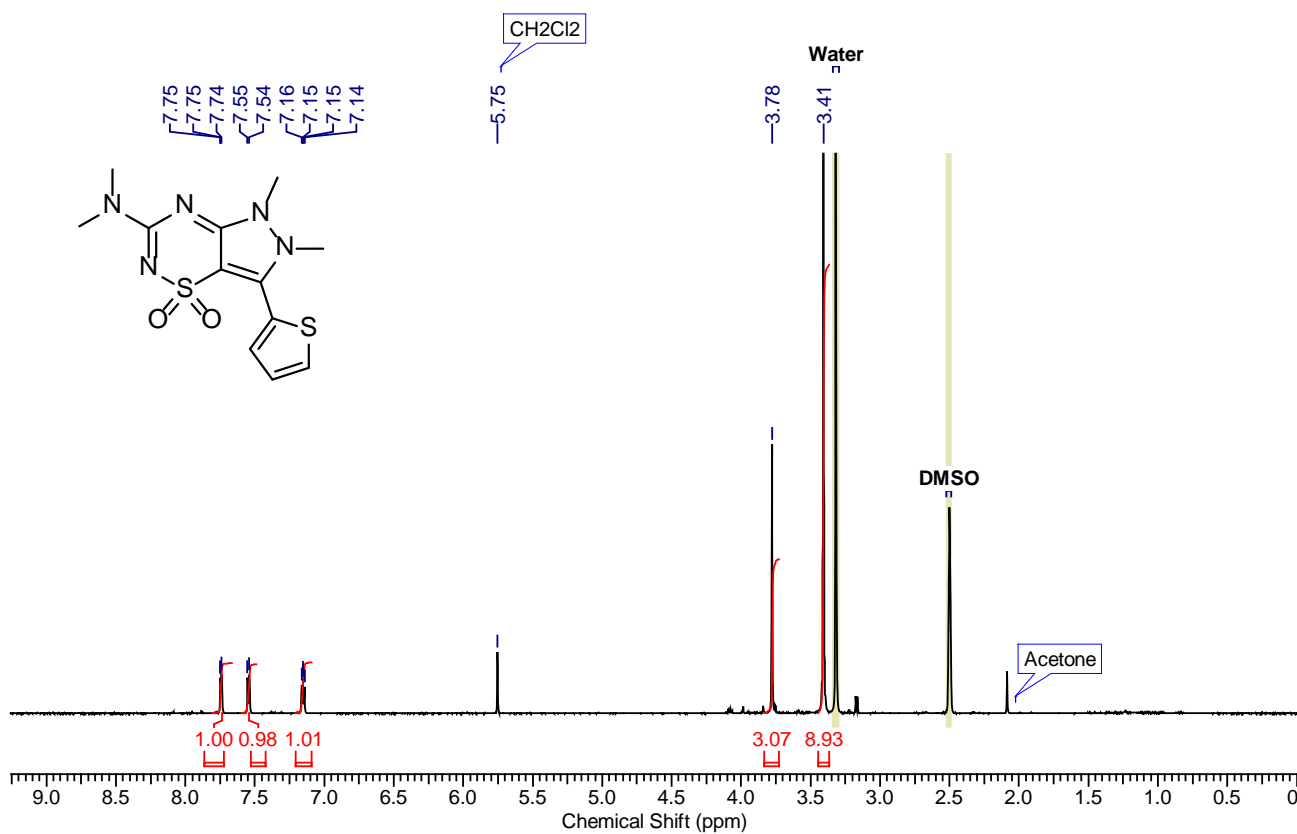
¹H NMR spectrum of **8b** 400MHz (DMSO-d⁶)



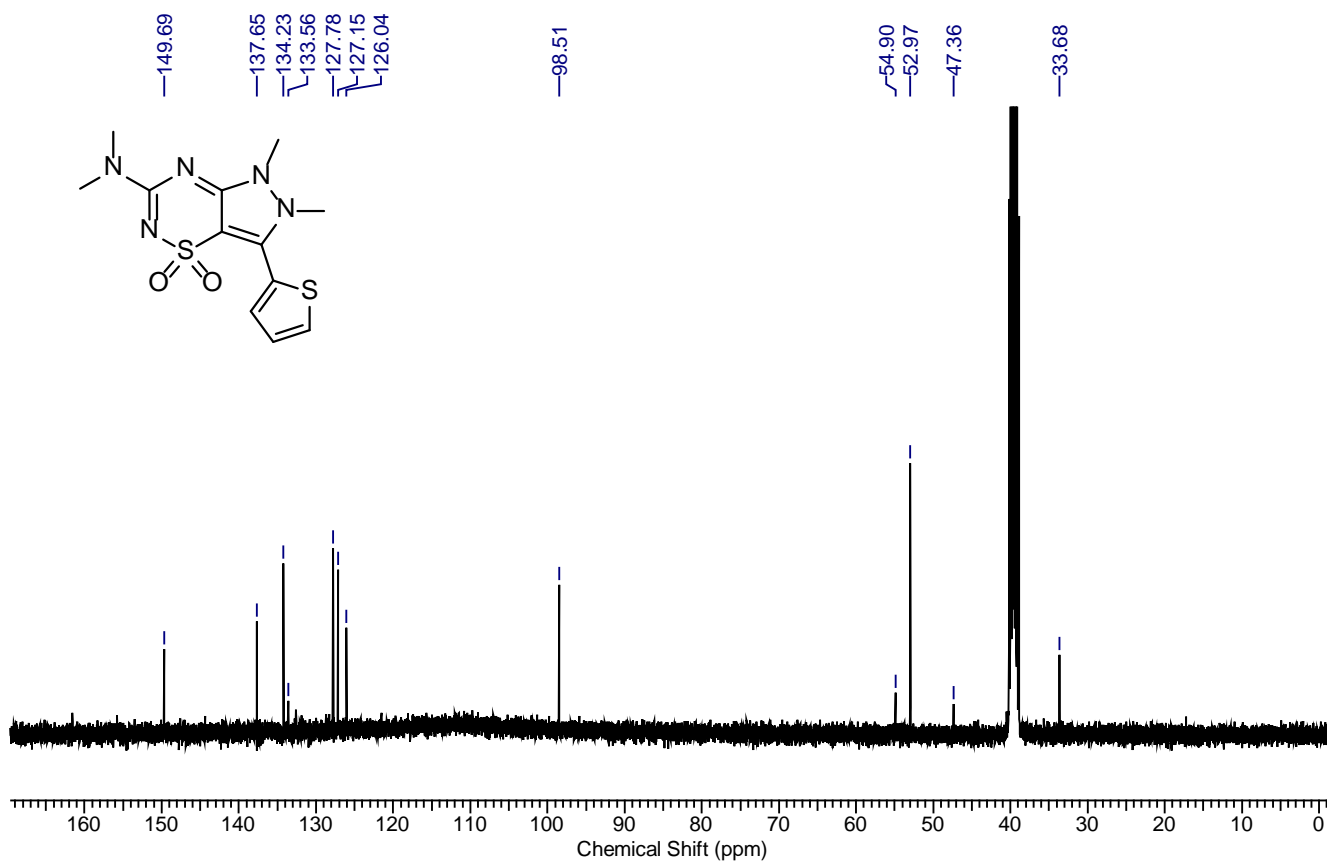
S16 ¹³C NMR spectrum of **8b** 100MHz (DMSO-d⁶)



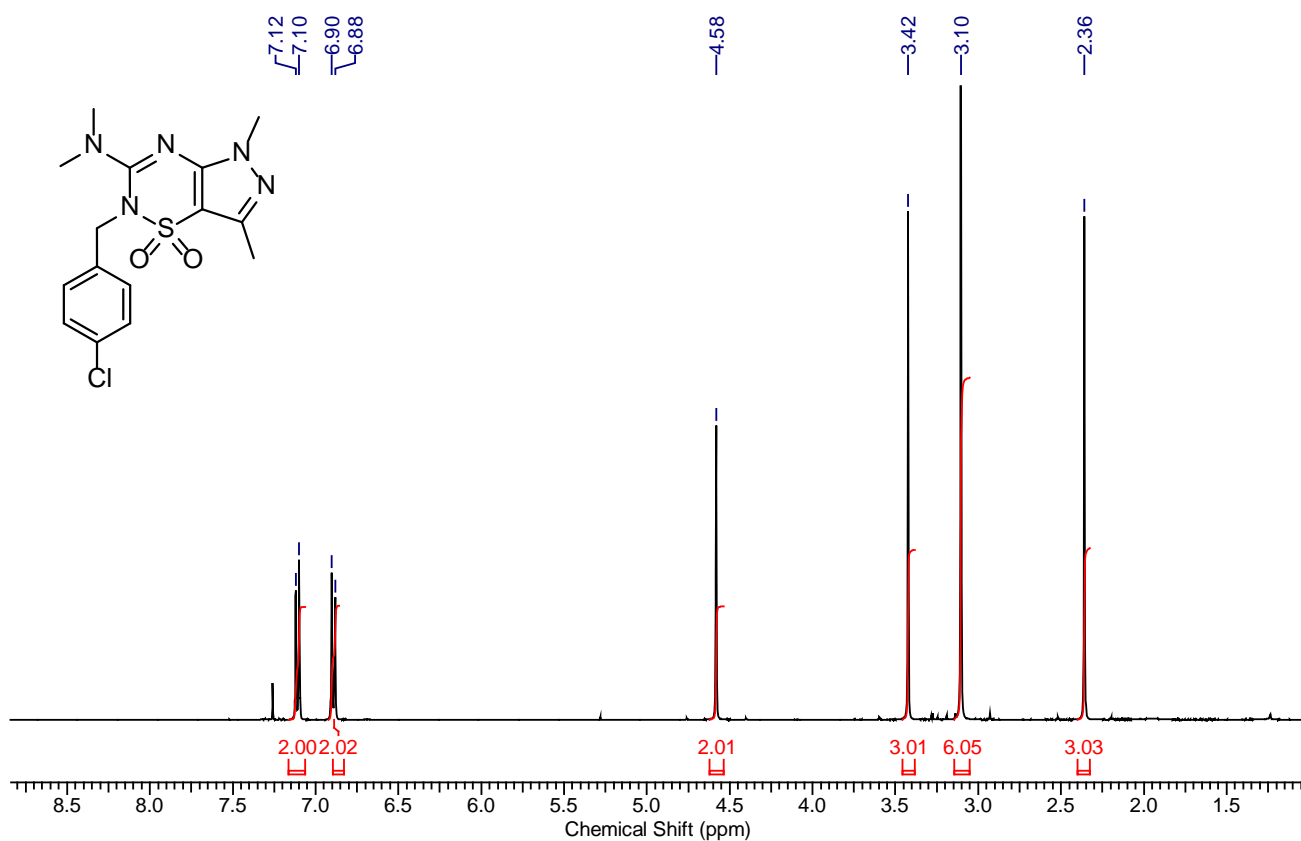
^1H NMR spectrum of **9b** 400MHz (DMSO- d_6)



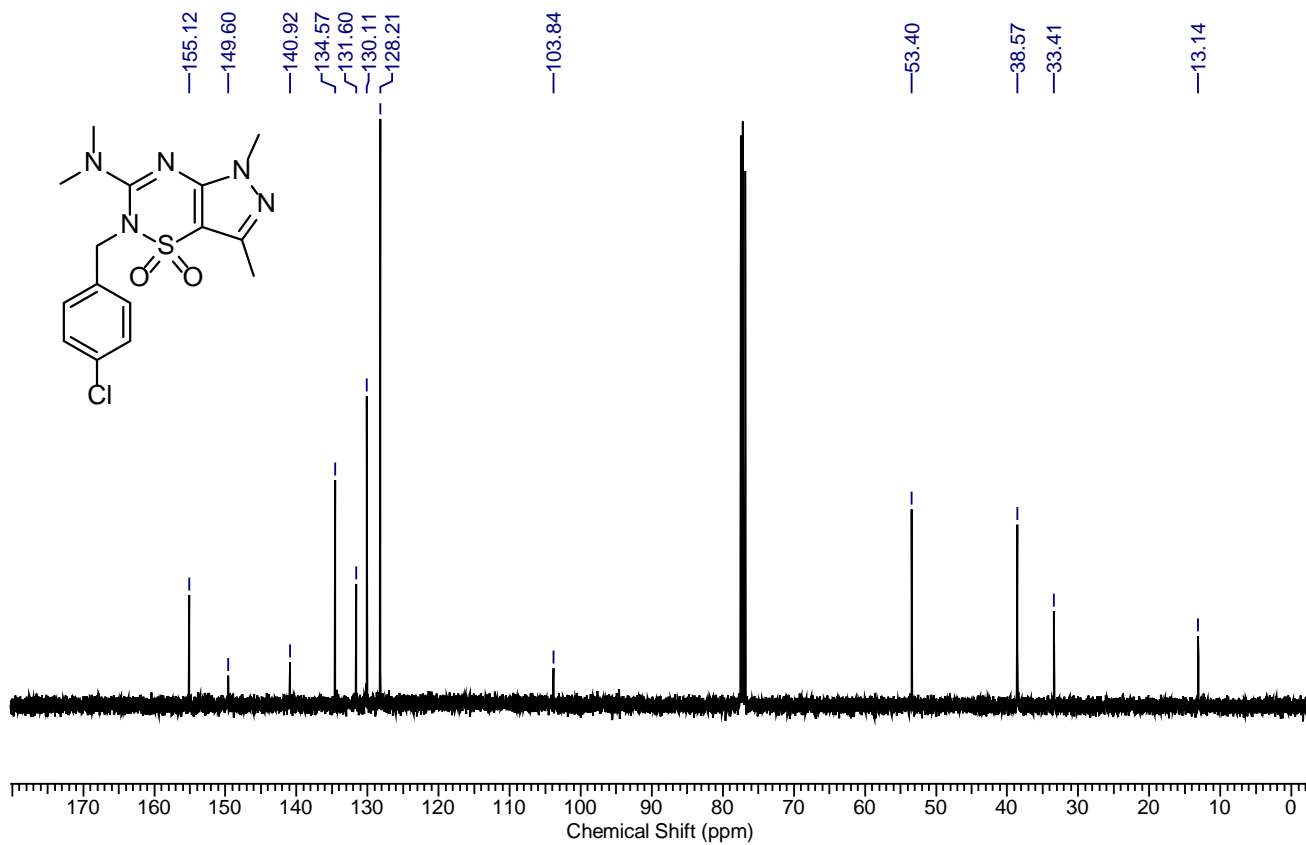
S17 ^{13}C NMR spectrum of **9b** 100MHz (DMSO- d_6)



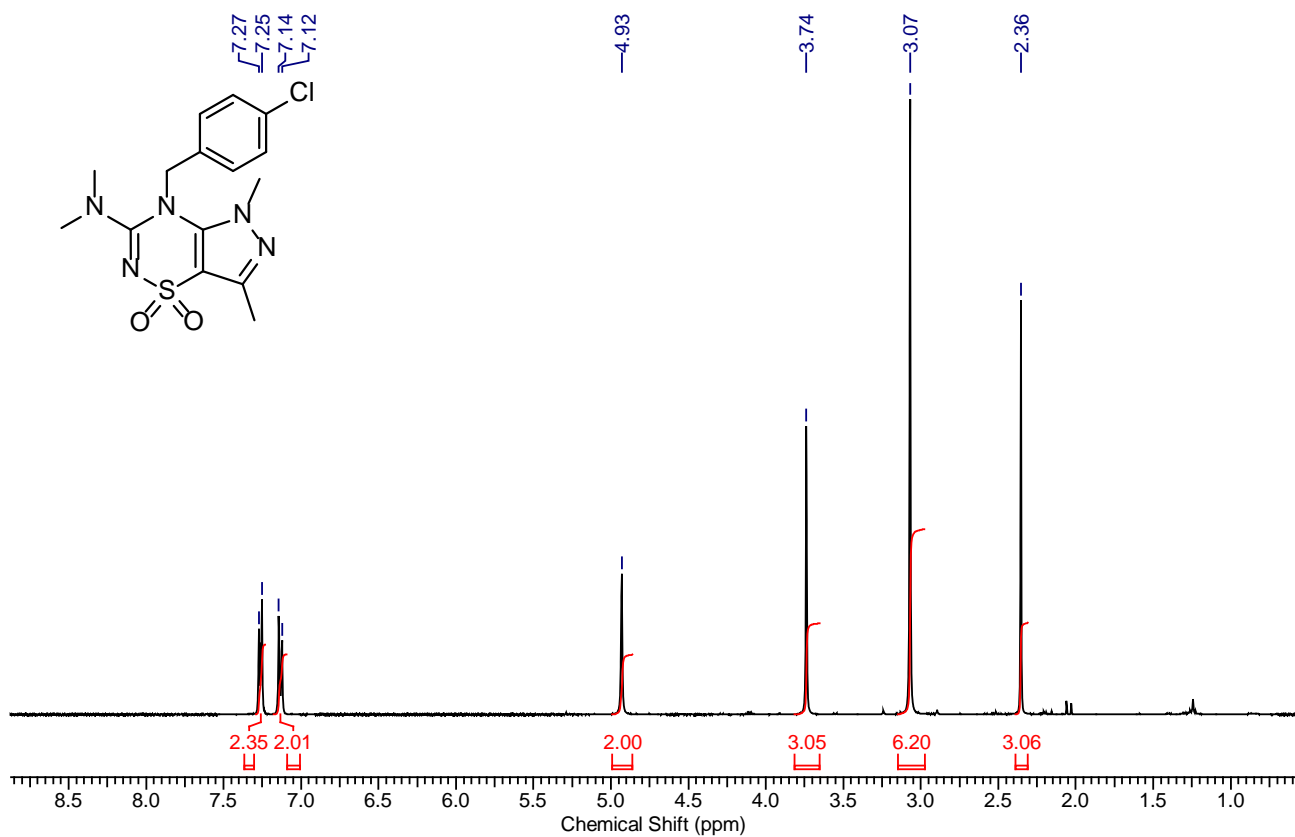
¹H NMR spectrum of **7c** 400MHz (CDCl₃)



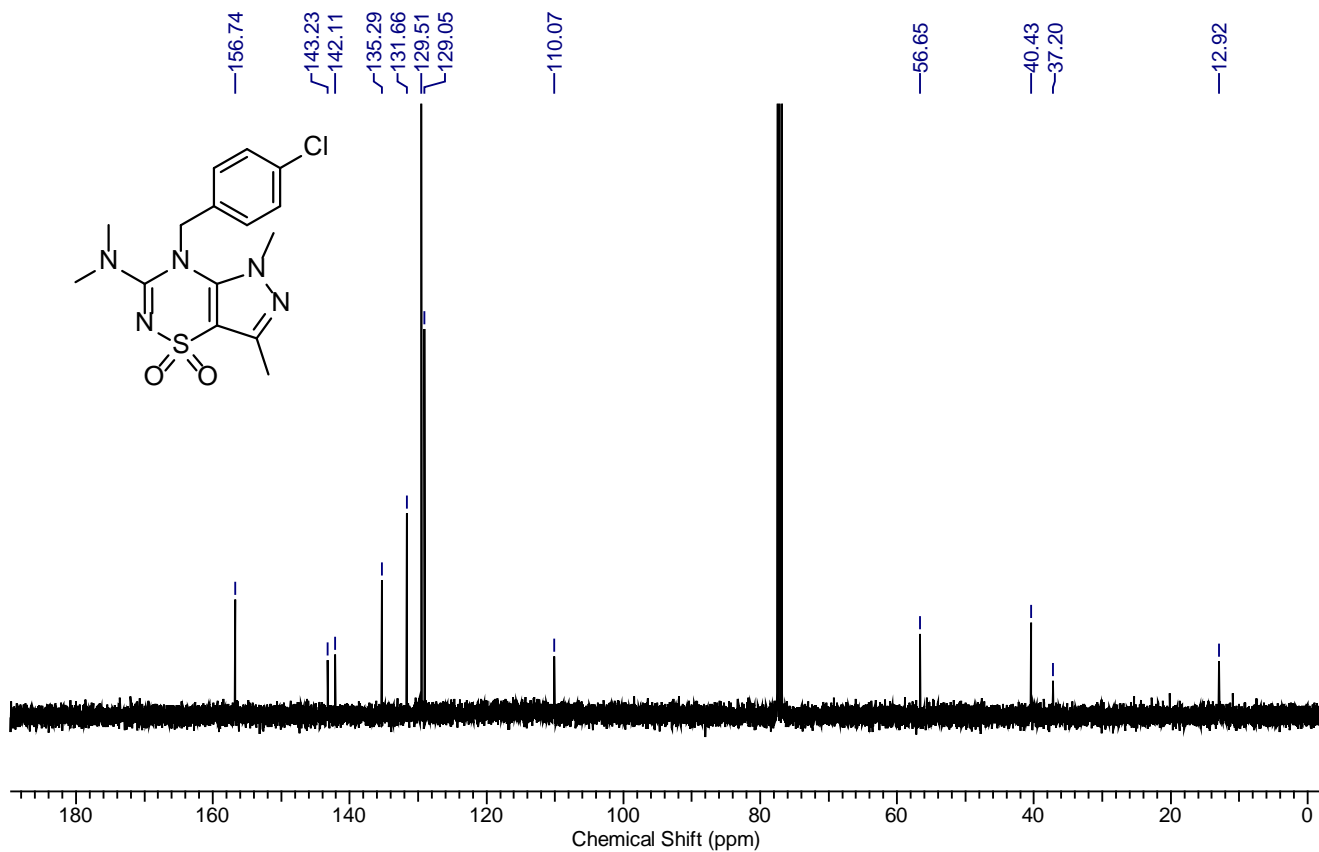
S18 ¹³C NMR spectrum of **7c** 100MHz (CDCl₃)



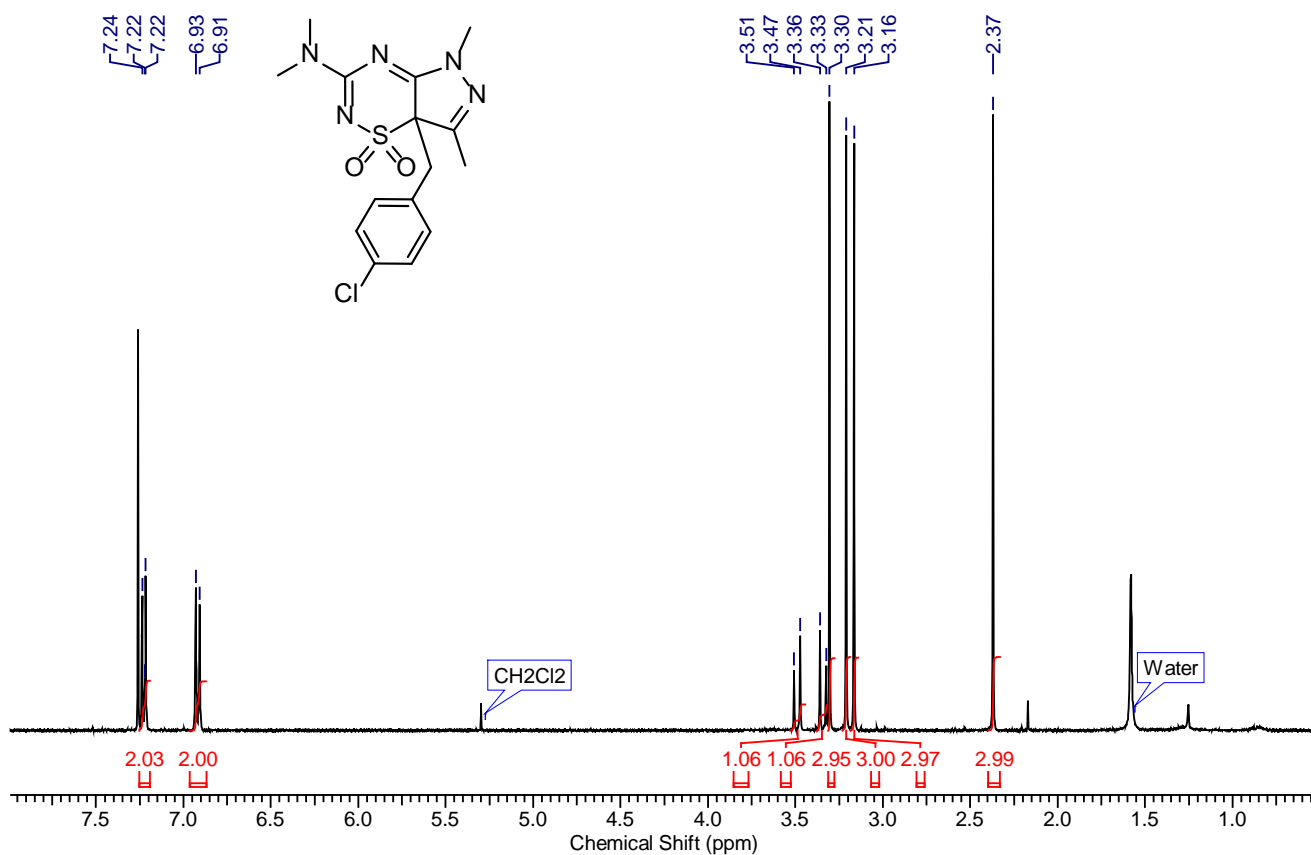
¹H NMR spectrum of **8c** 400MHz (CDCl₃)



S19 ¹³C NMR spectrum of **8c** 100MHz (CDCl₃)

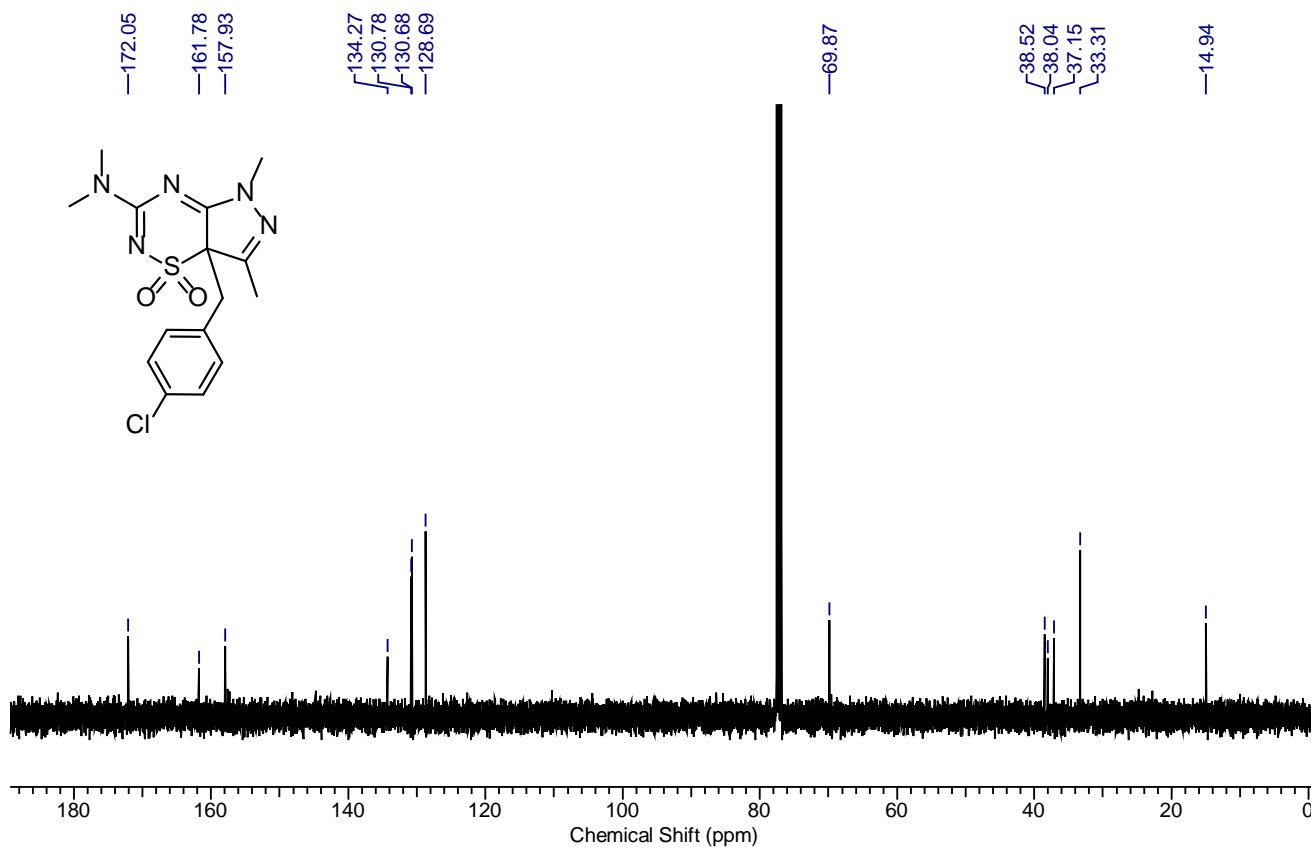


¹H NMR spectrum of **10c** 400MHz (CDCl₃)

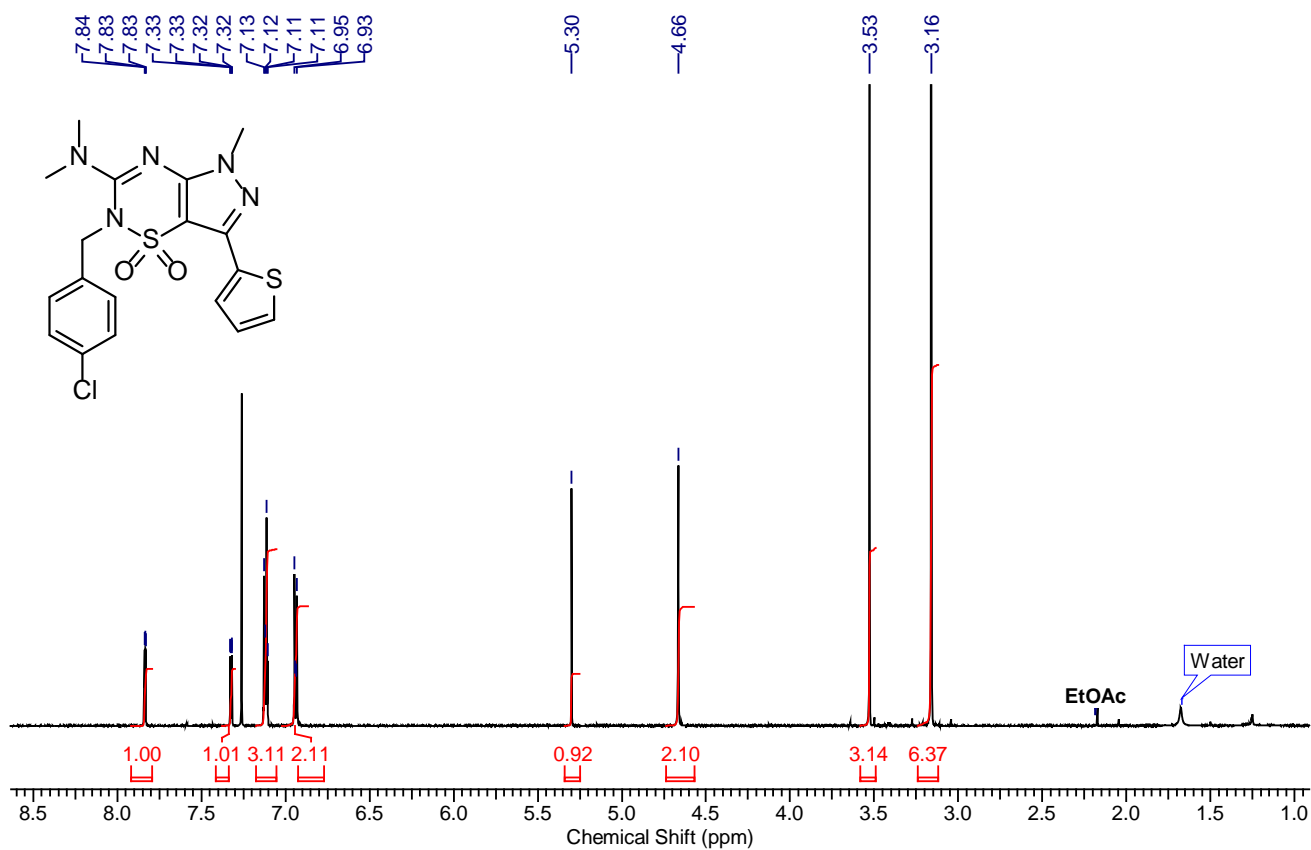


S20

¹³C NMR spectrum of **10c** 100MHz (CDCl₃)

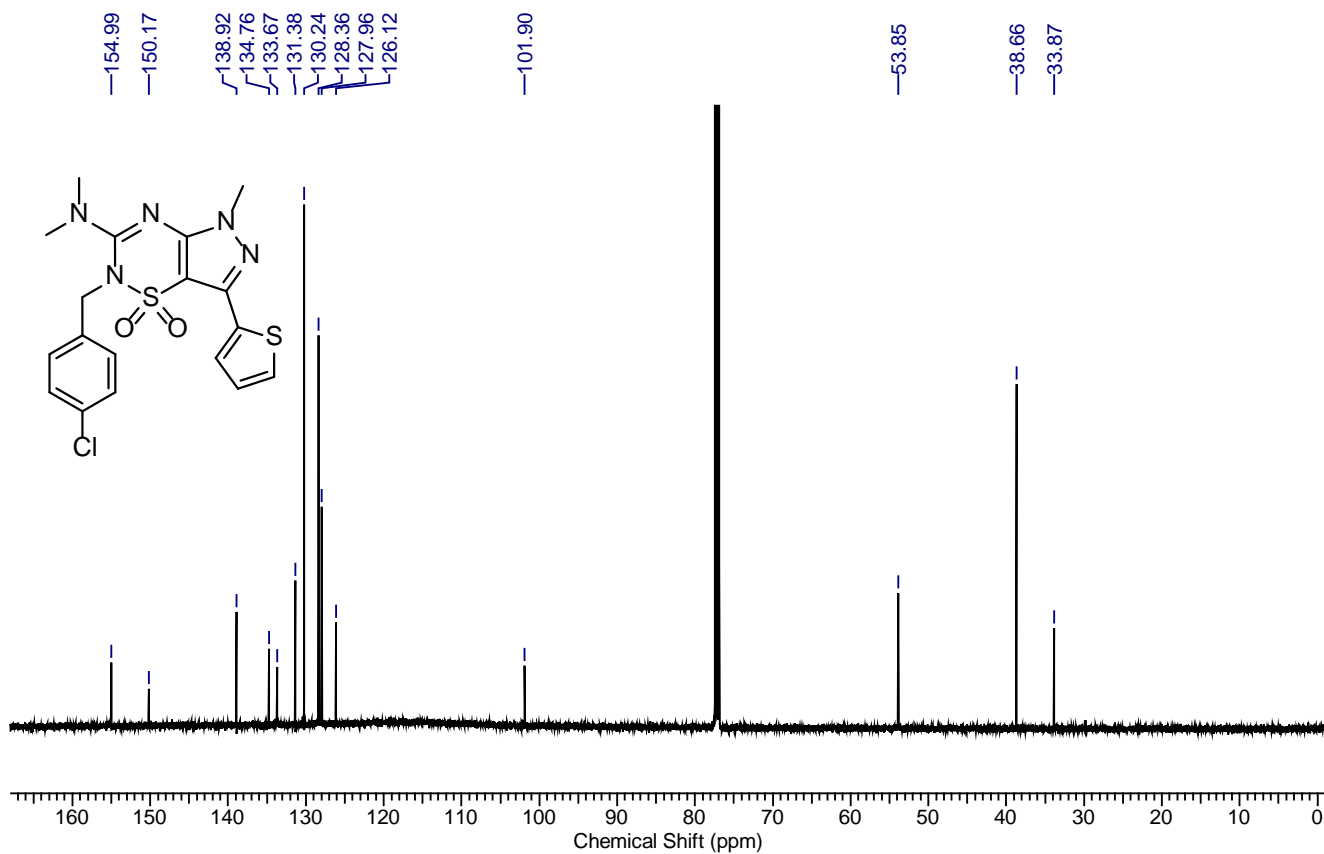


¹H NMR spectrum of **7d** 400MHz (CDCl₃)

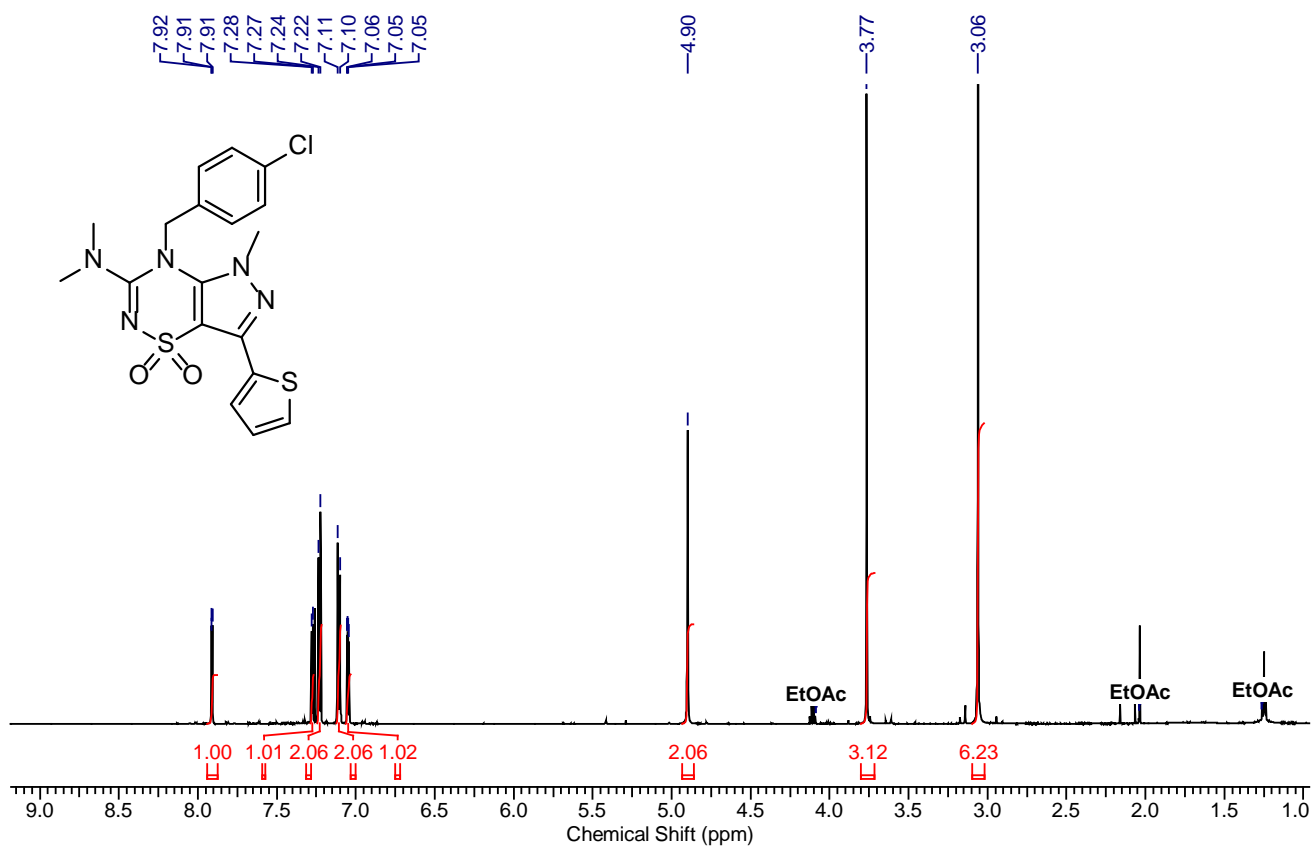


S21

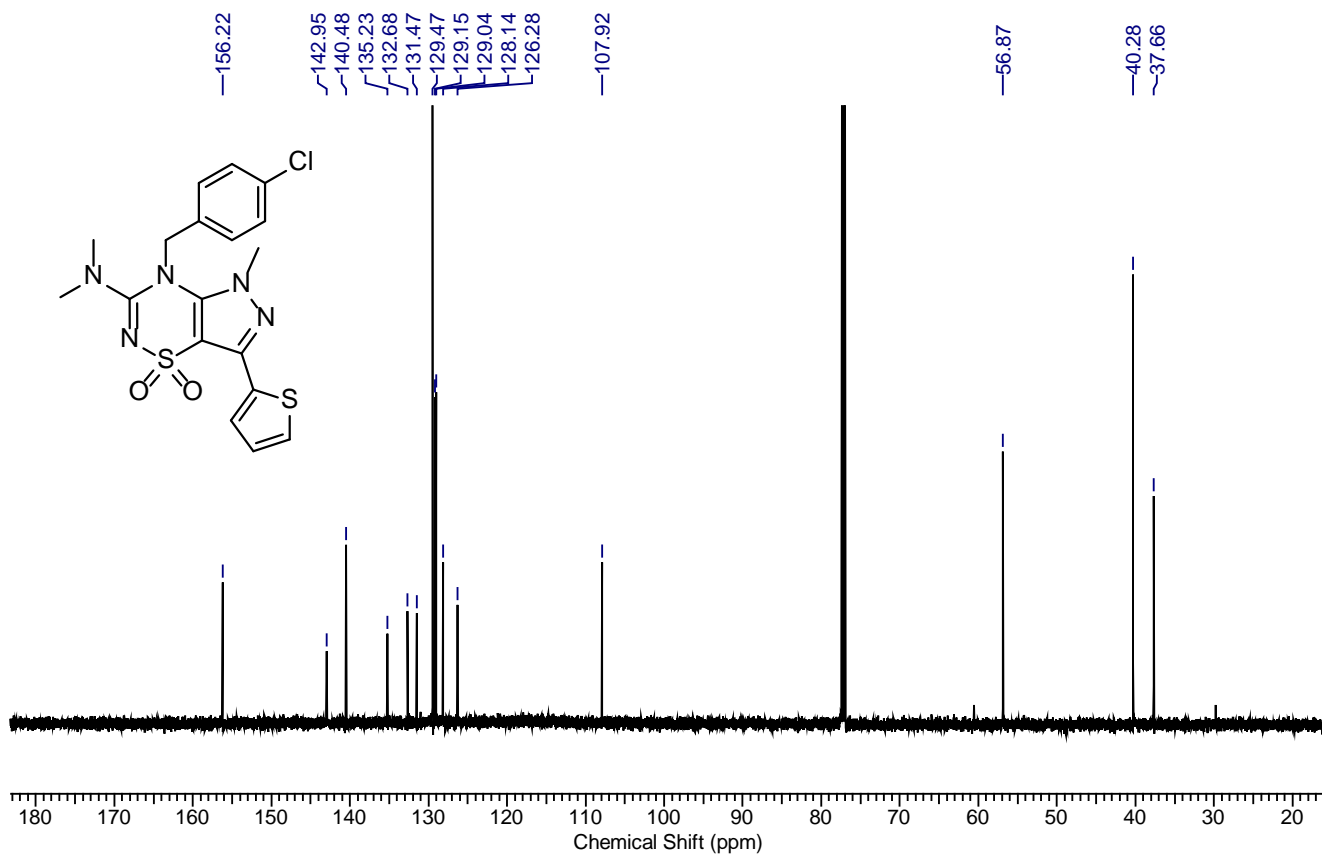
¹³C NMR spectrum of **7d** 100MHz (CDCl₃)



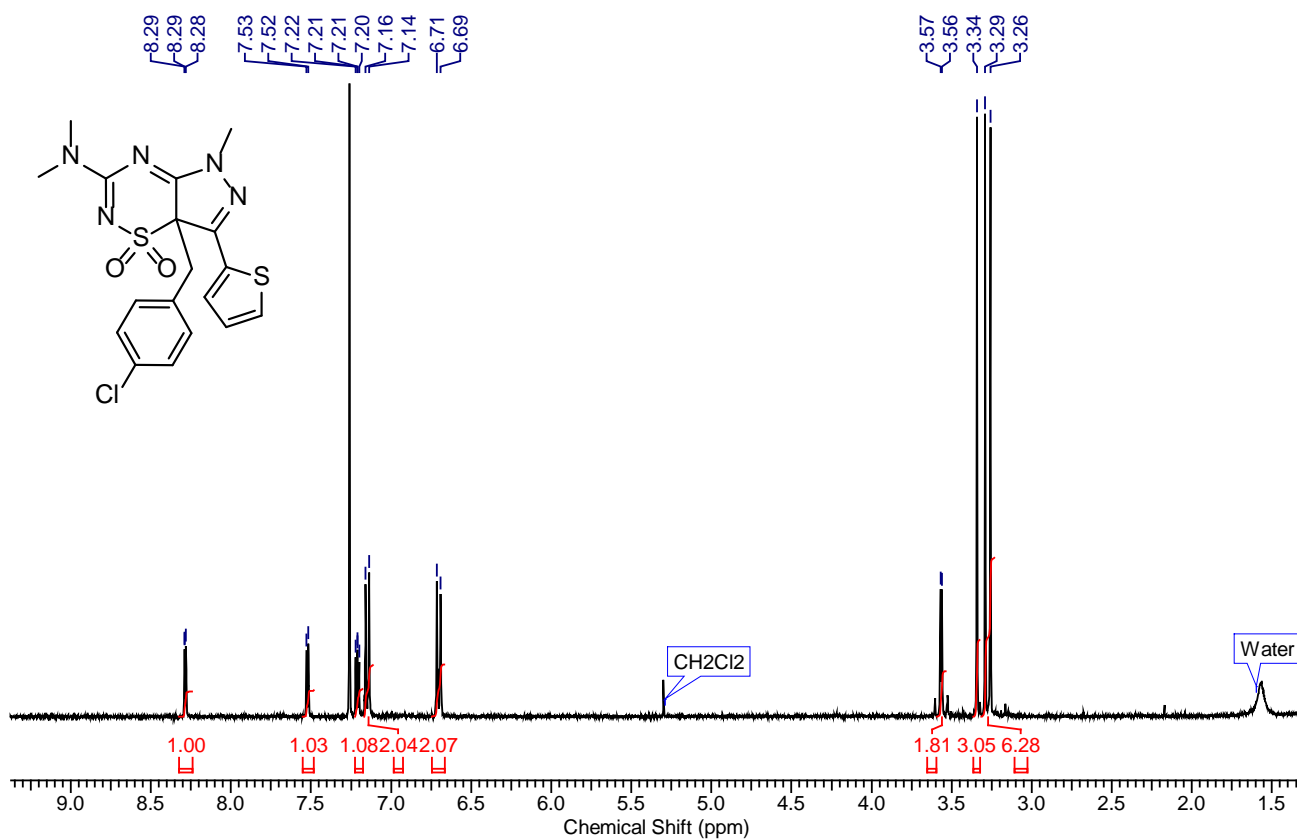
¹H NMR spectrum of **8d** 400MHz (CDCl₃)



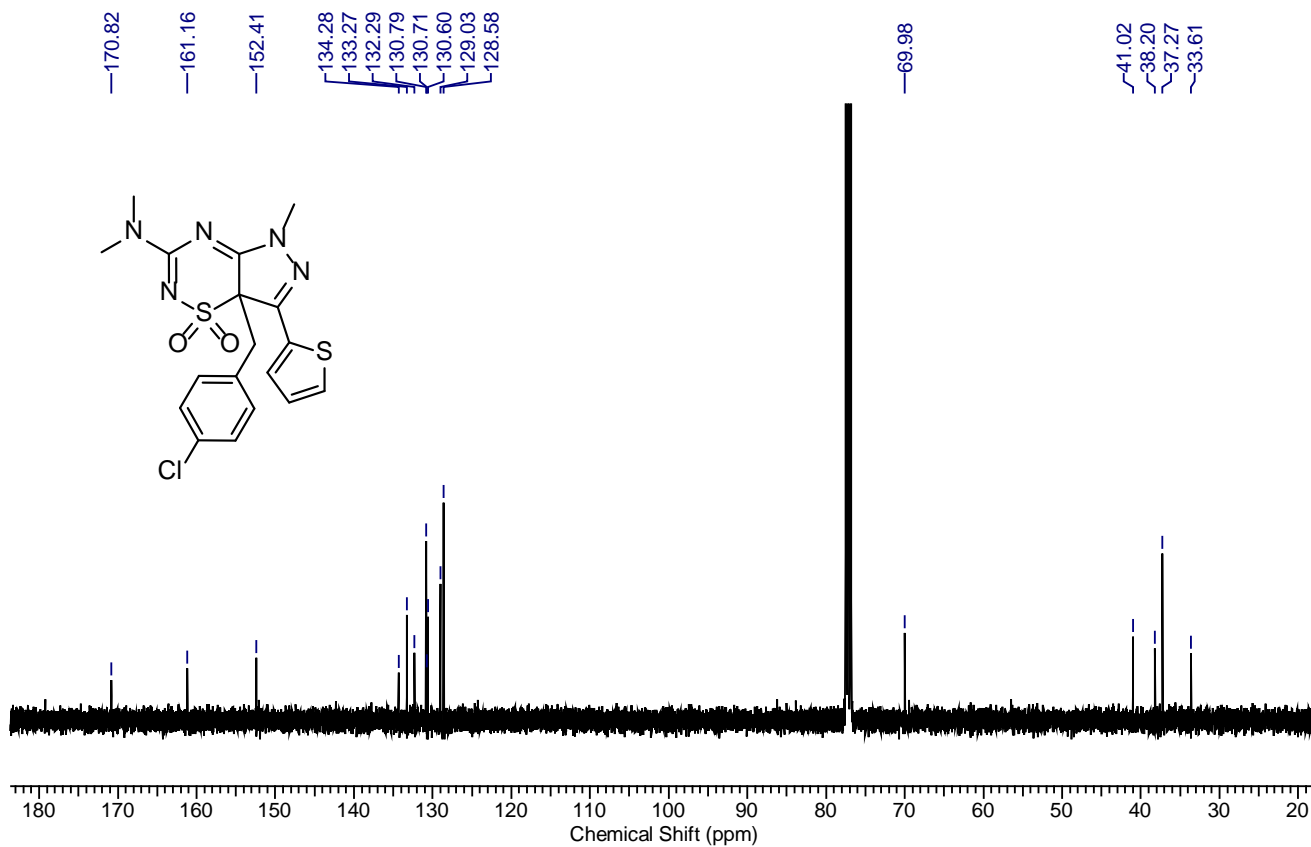
S22 ¹³C NMR spectrum of **8d** 100MHz (CDCl₃)



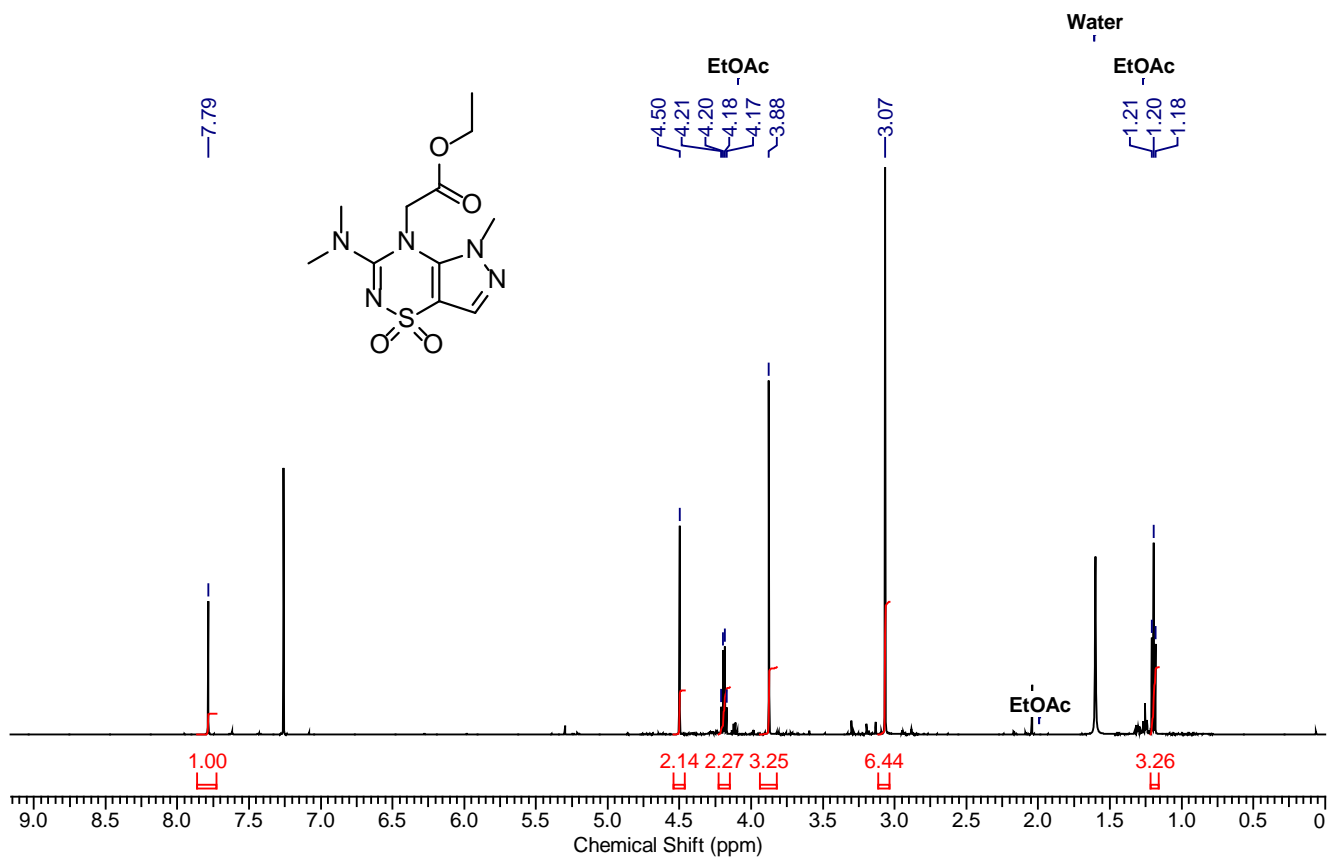
¹H NMR spectrum of **10d** 400MHz (CDCl₃)



S23 ¹³C NMR spectrum of **10d** 100MHz (CDCl₃)

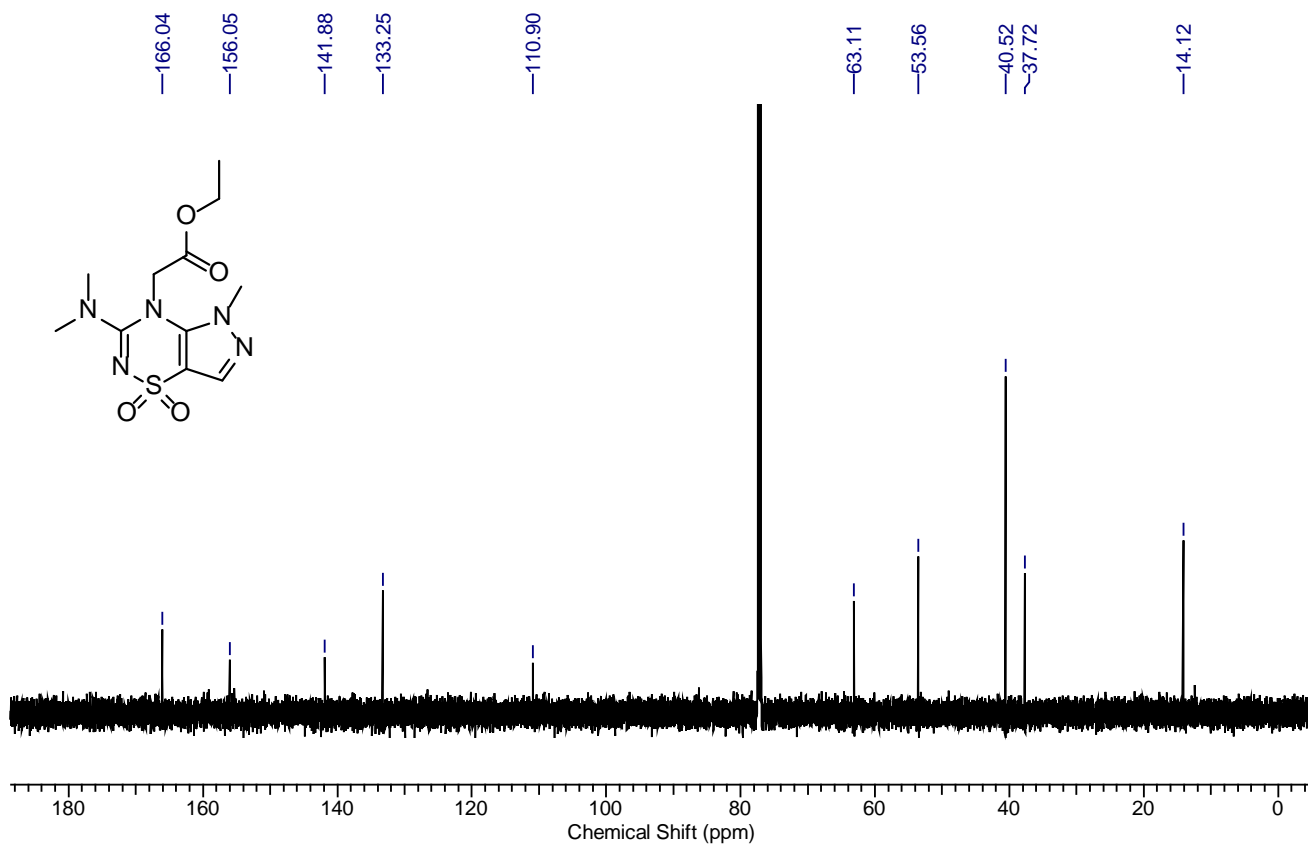


¹H NMR spectrum of **11a** 400MHz (CDCl₃)

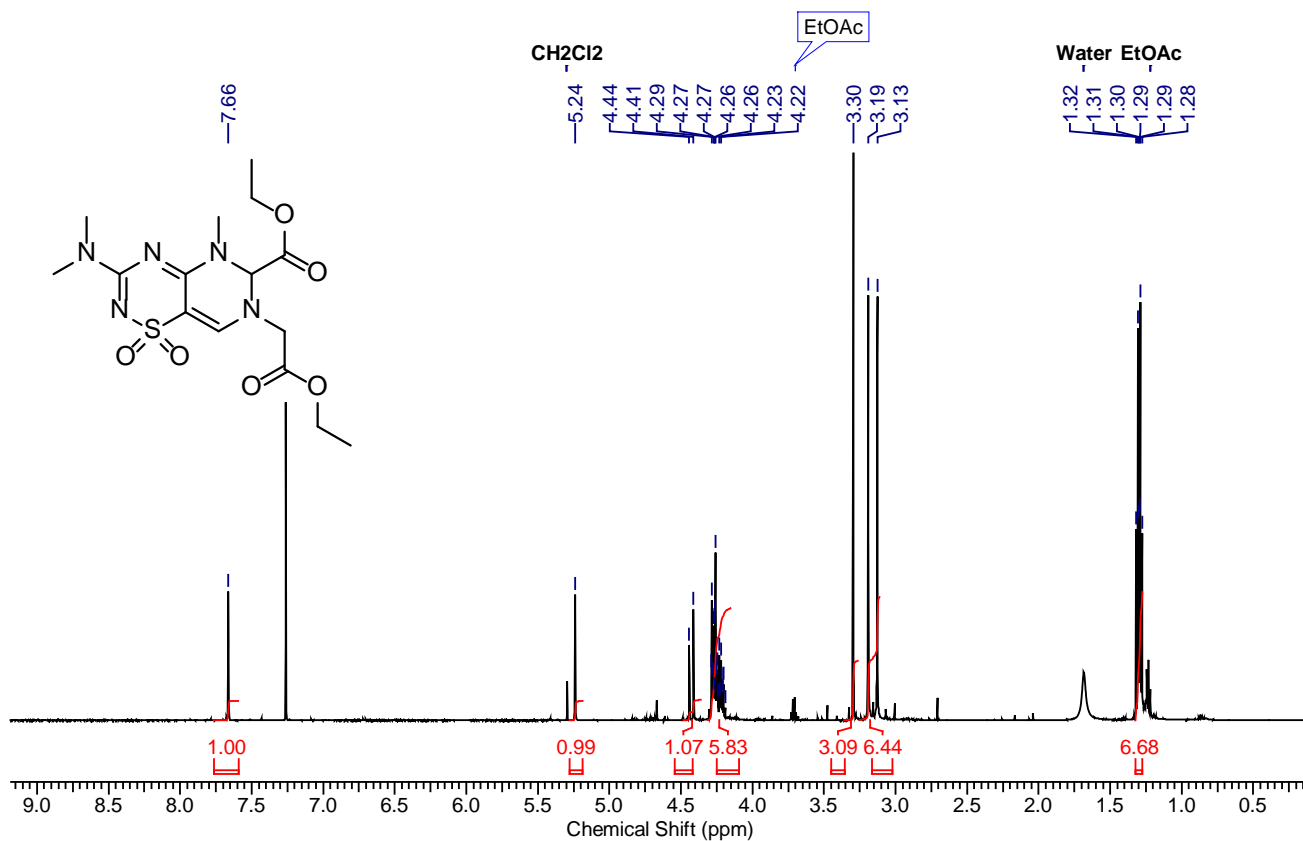


S24

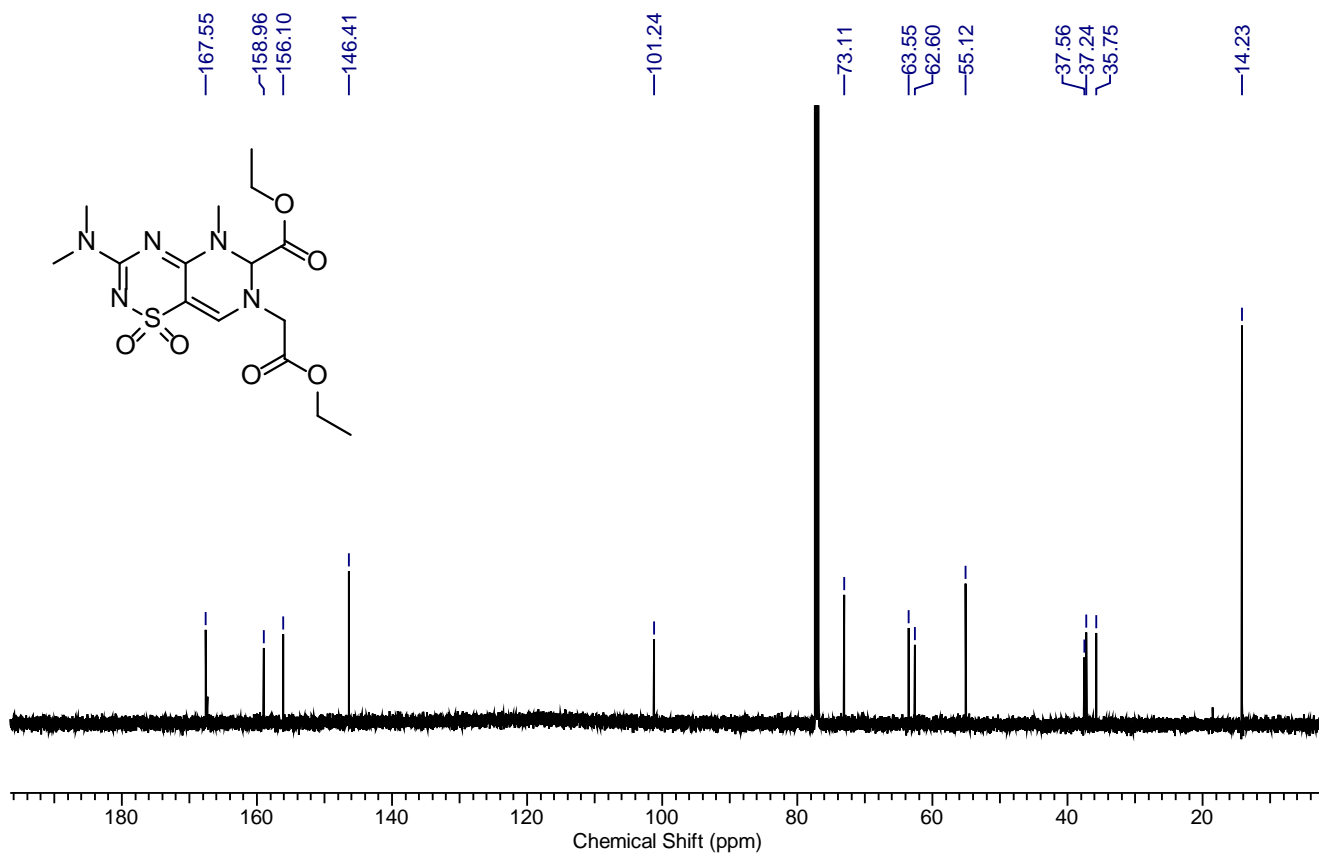
¹³C NMR spectrum of **11a** 100MHz (CDCl₃)



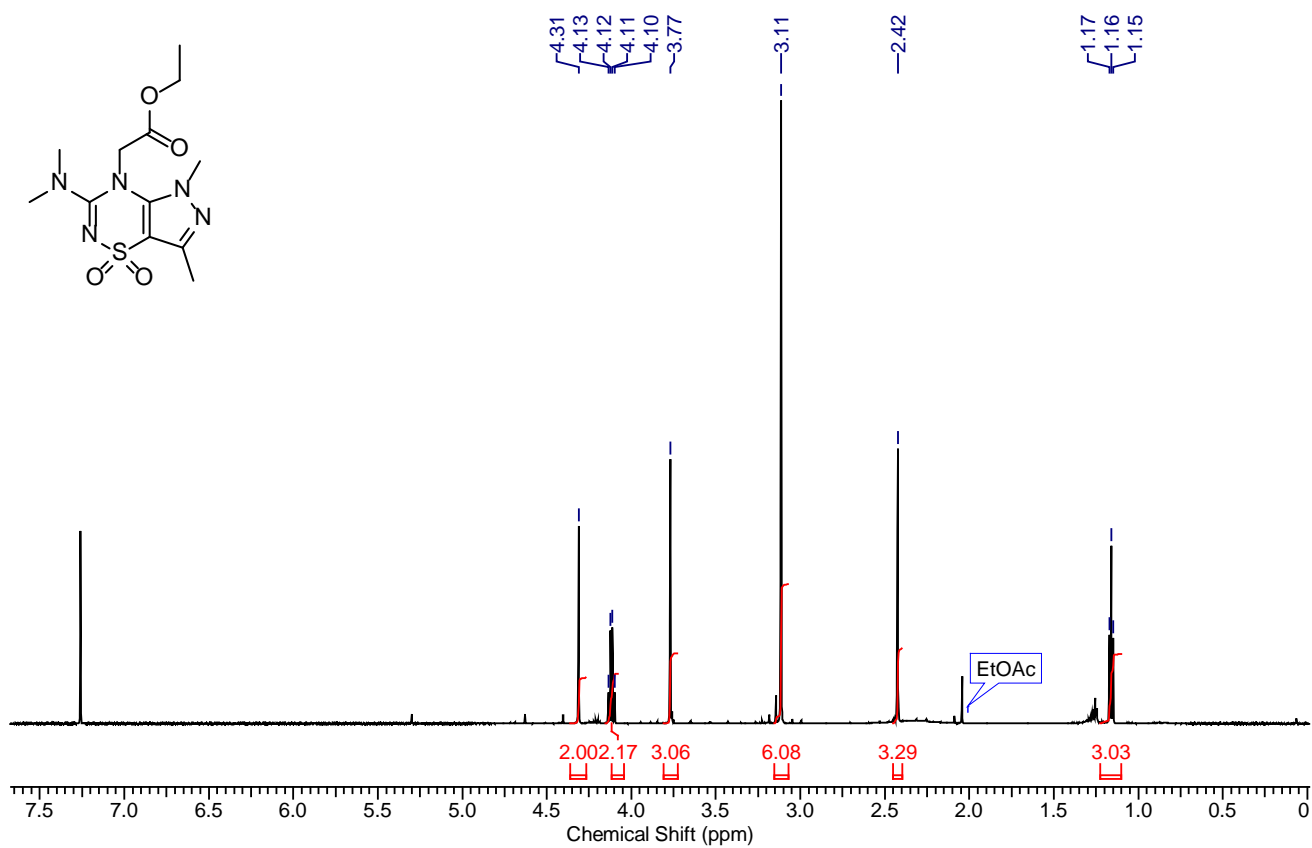
^1H NMR spectrum of **13a** 600MHz (CDCl_3)



S25 ^{13}C NMR spectrum of **13a** 150MHz (CDCl_3)

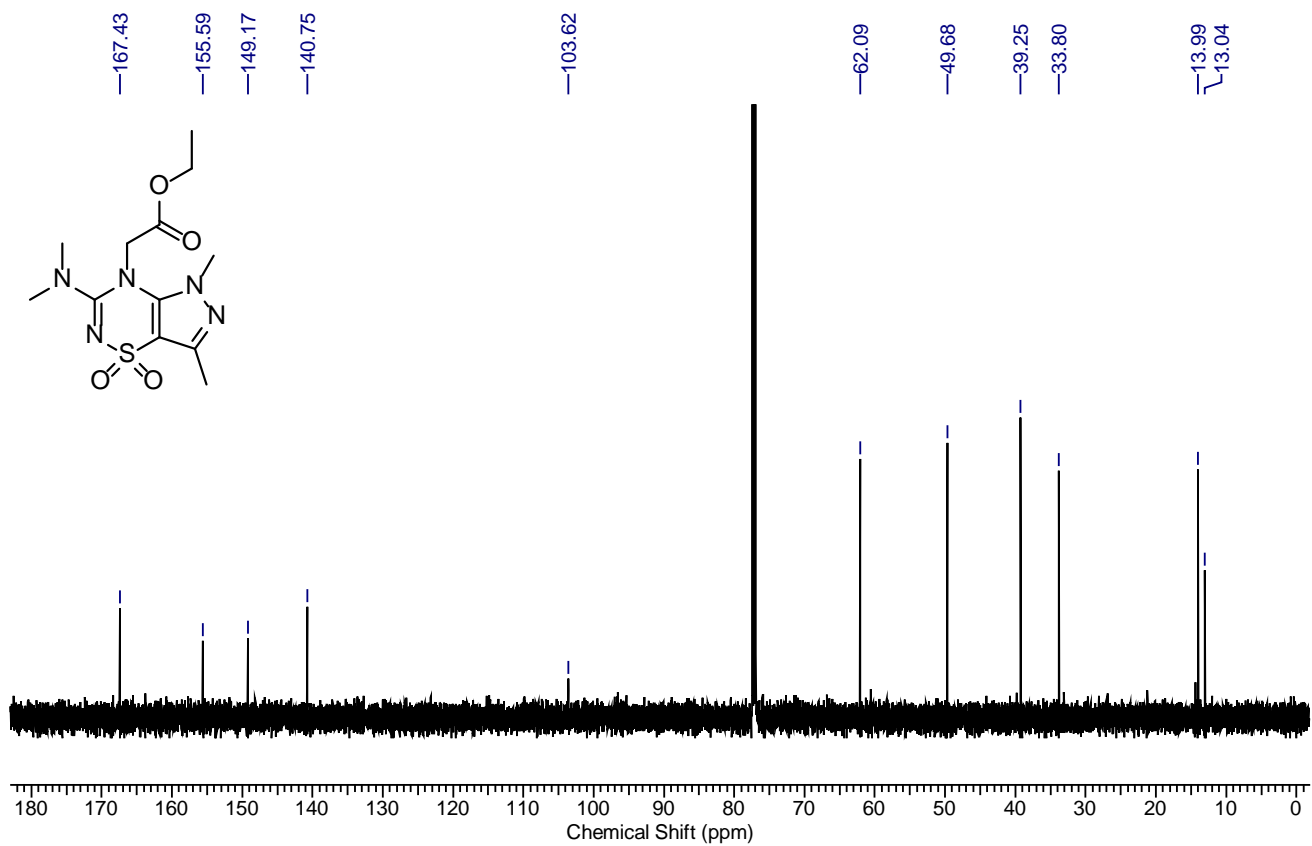


¹H NMR spectrum of **11b** 600MHz (CDCl₃)

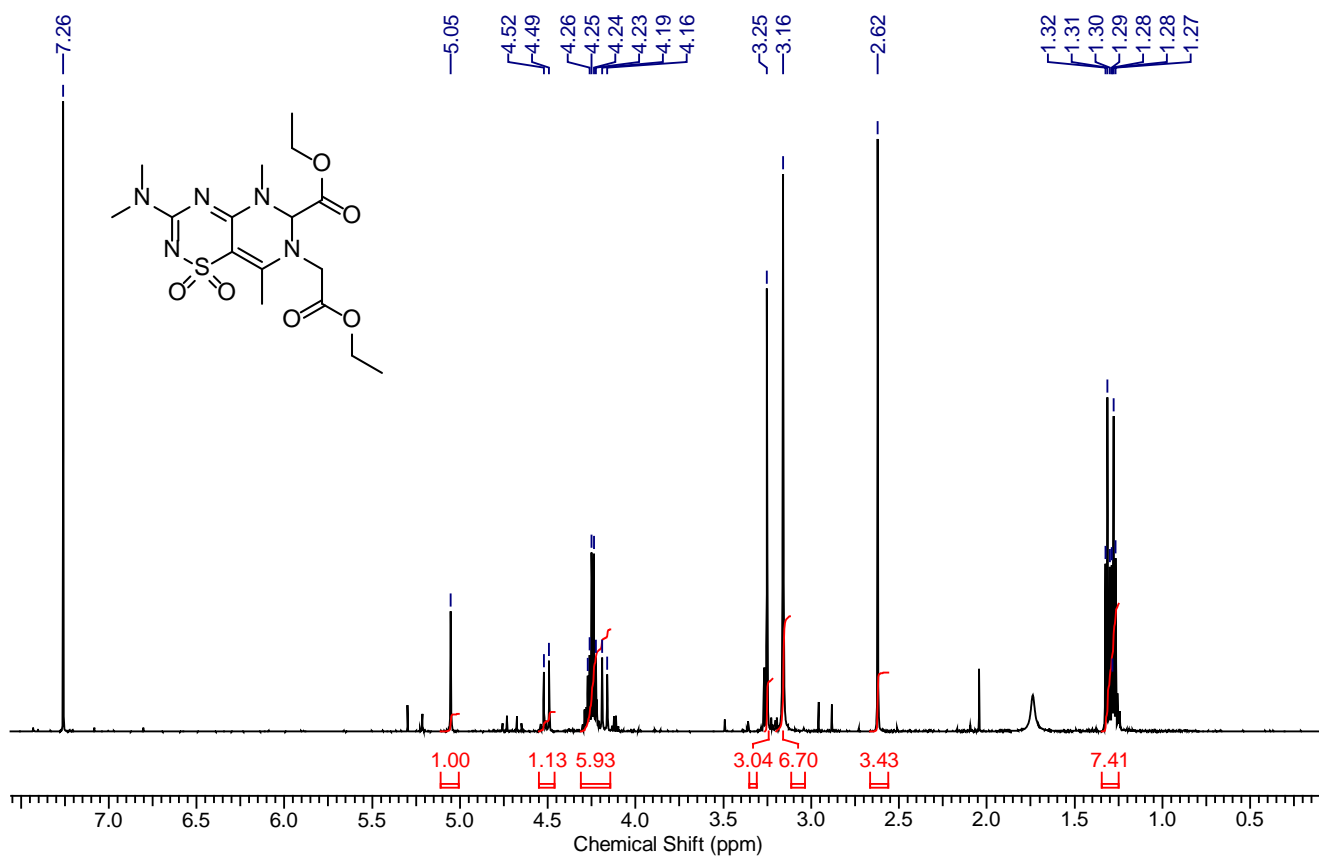


S26

¹³C NMR spectrum of **11b** 150MHz (CDCl₃)

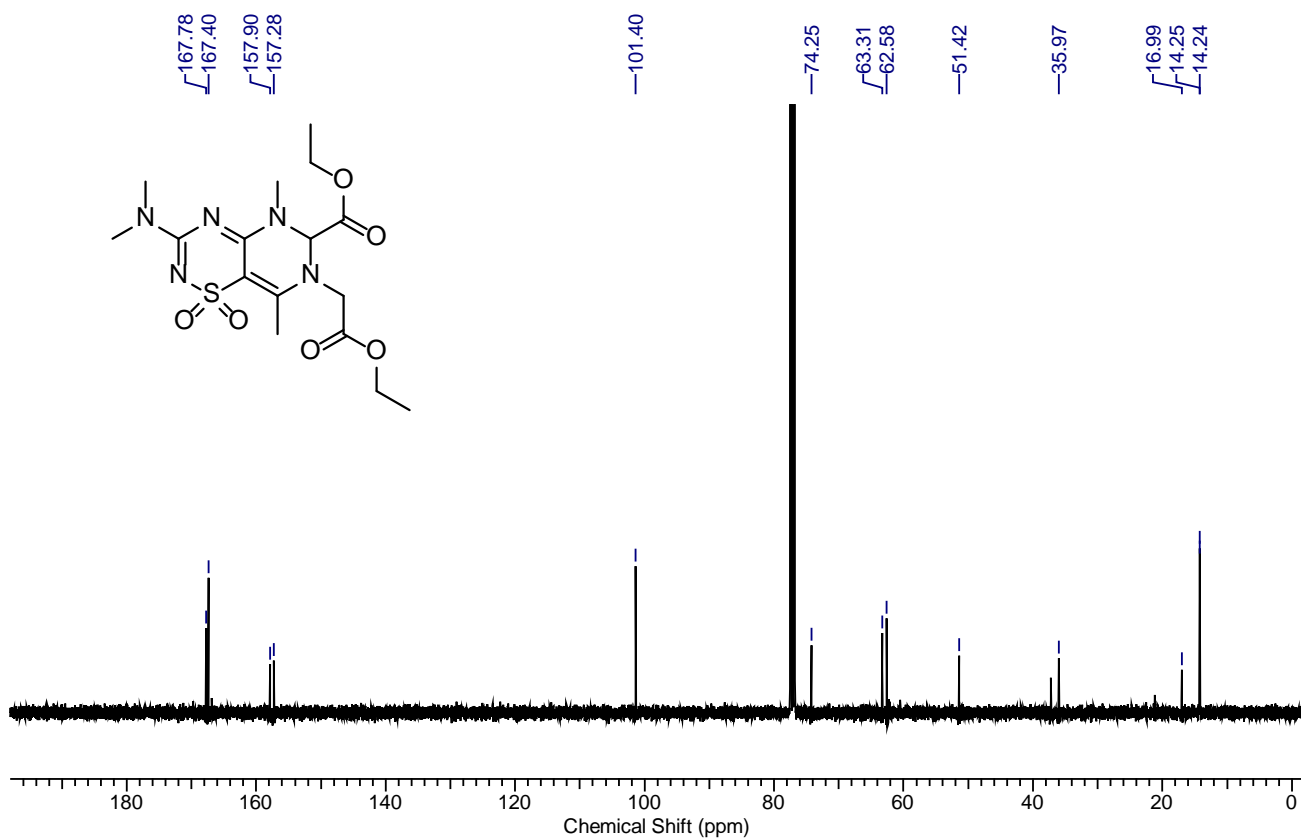


¹H NMR spectrum of **13b** 600MHz (CDCl₃)

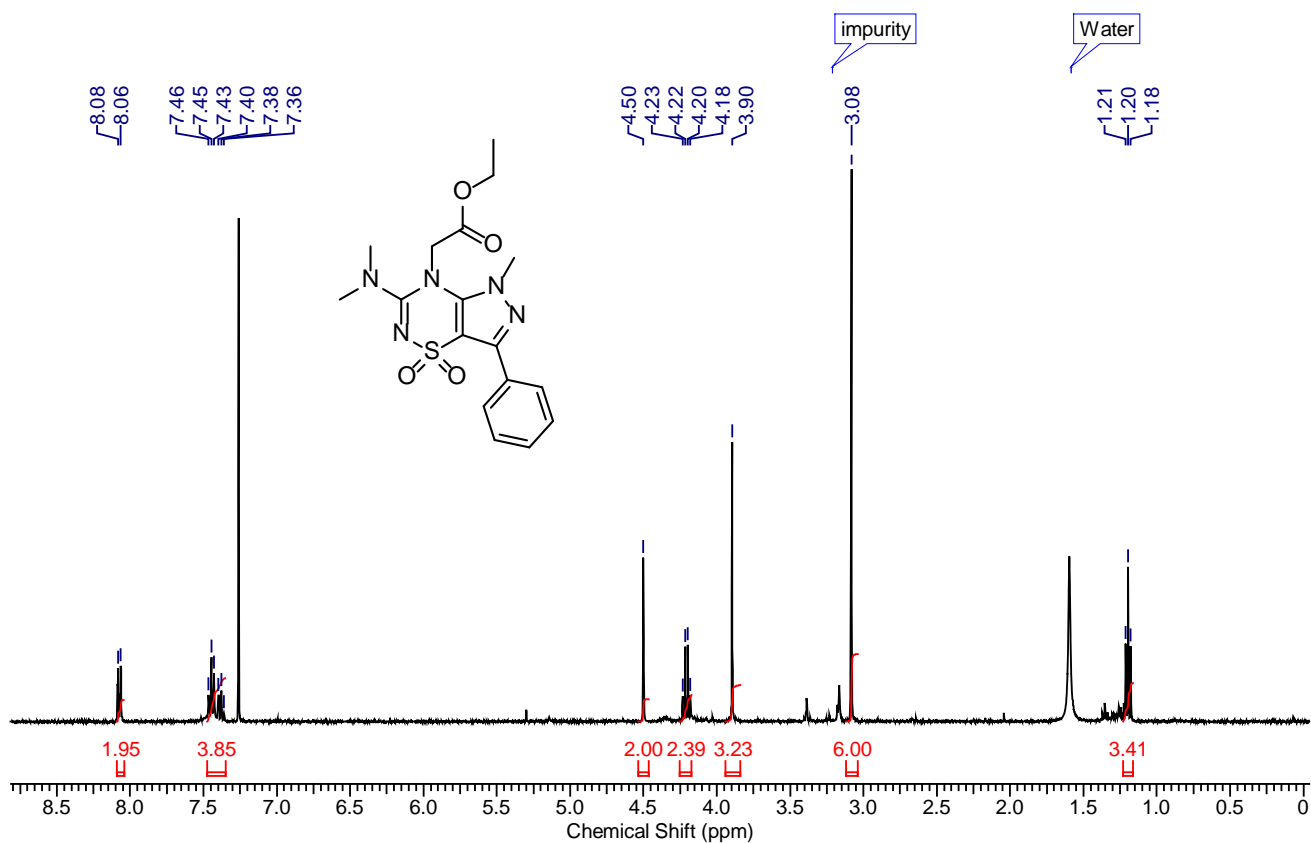


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¹³C NMR spectrum of **13b** 150MHz (CDCl₃)

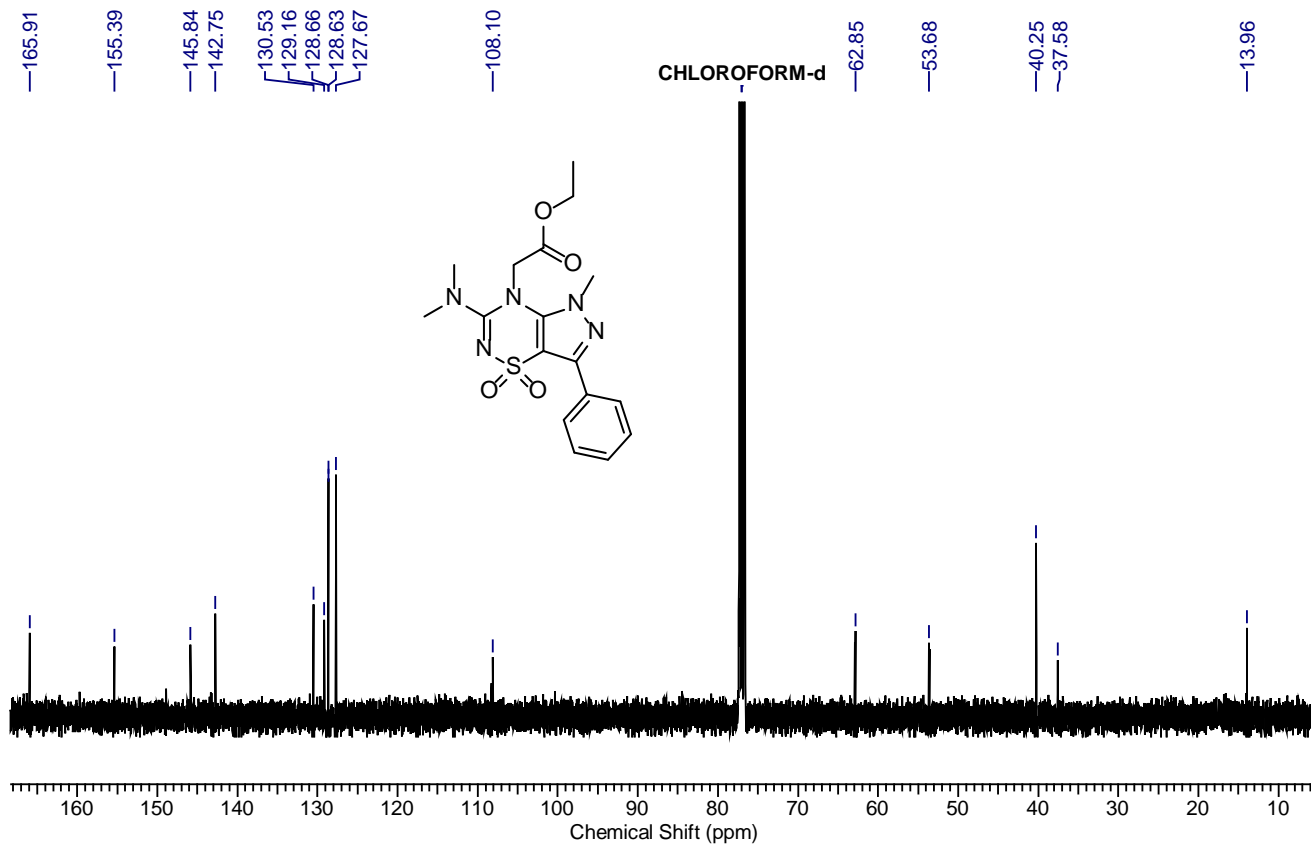


¹H NMR spectrum of **11c** 400MHz (CDCl₃)

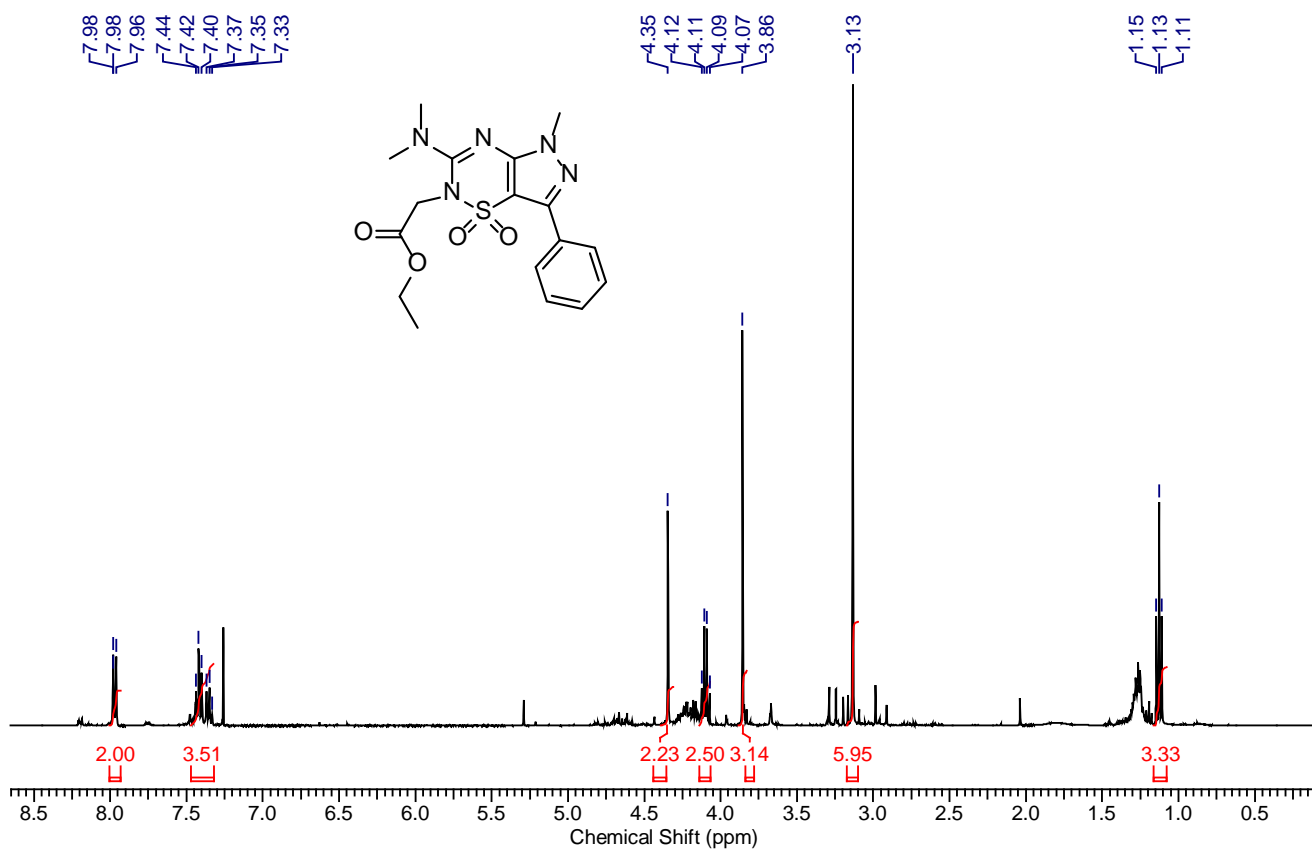


S28

¹³C NMR spectrum of **11c** 100MHz (CDCl₃)

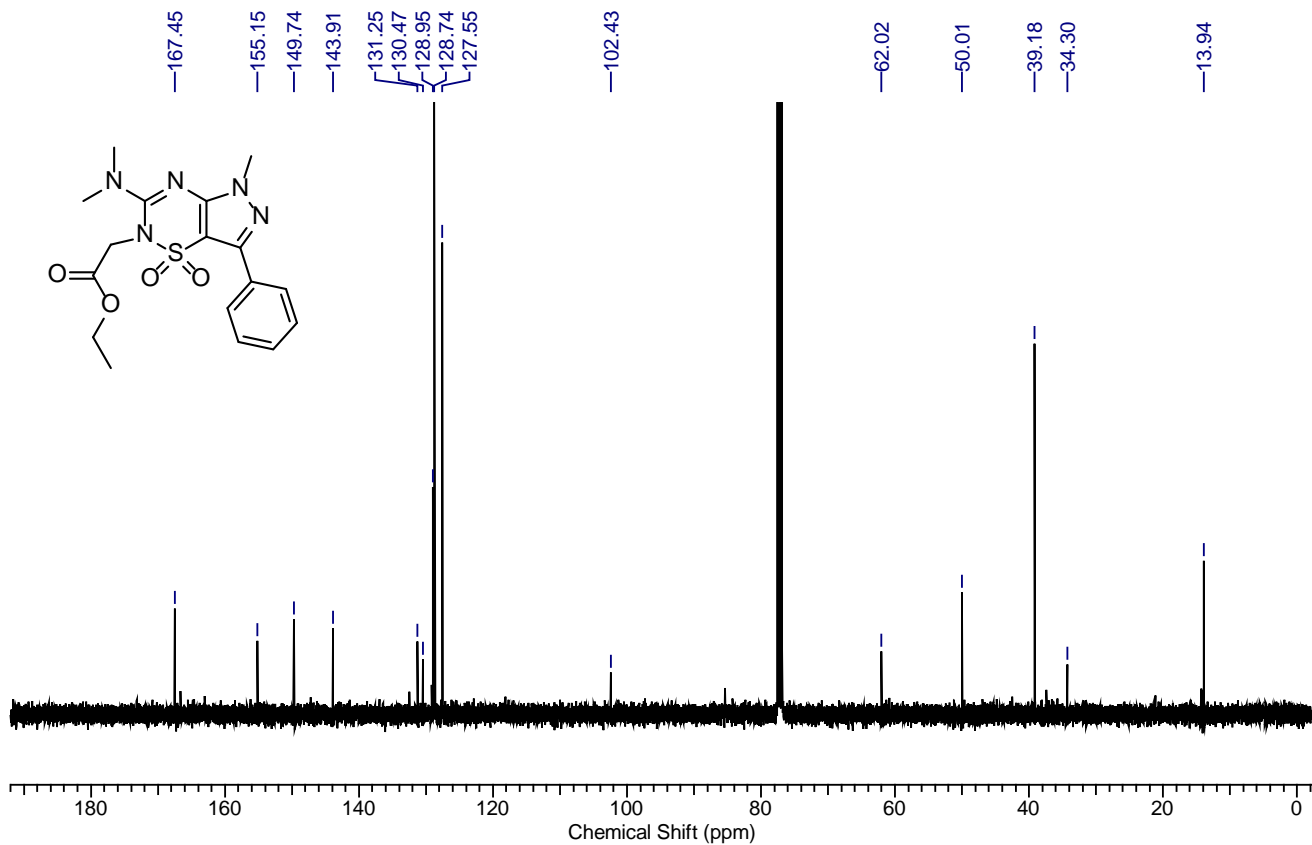


^1H NMR spectrum of **14c** 400MHz (CDCl_3)

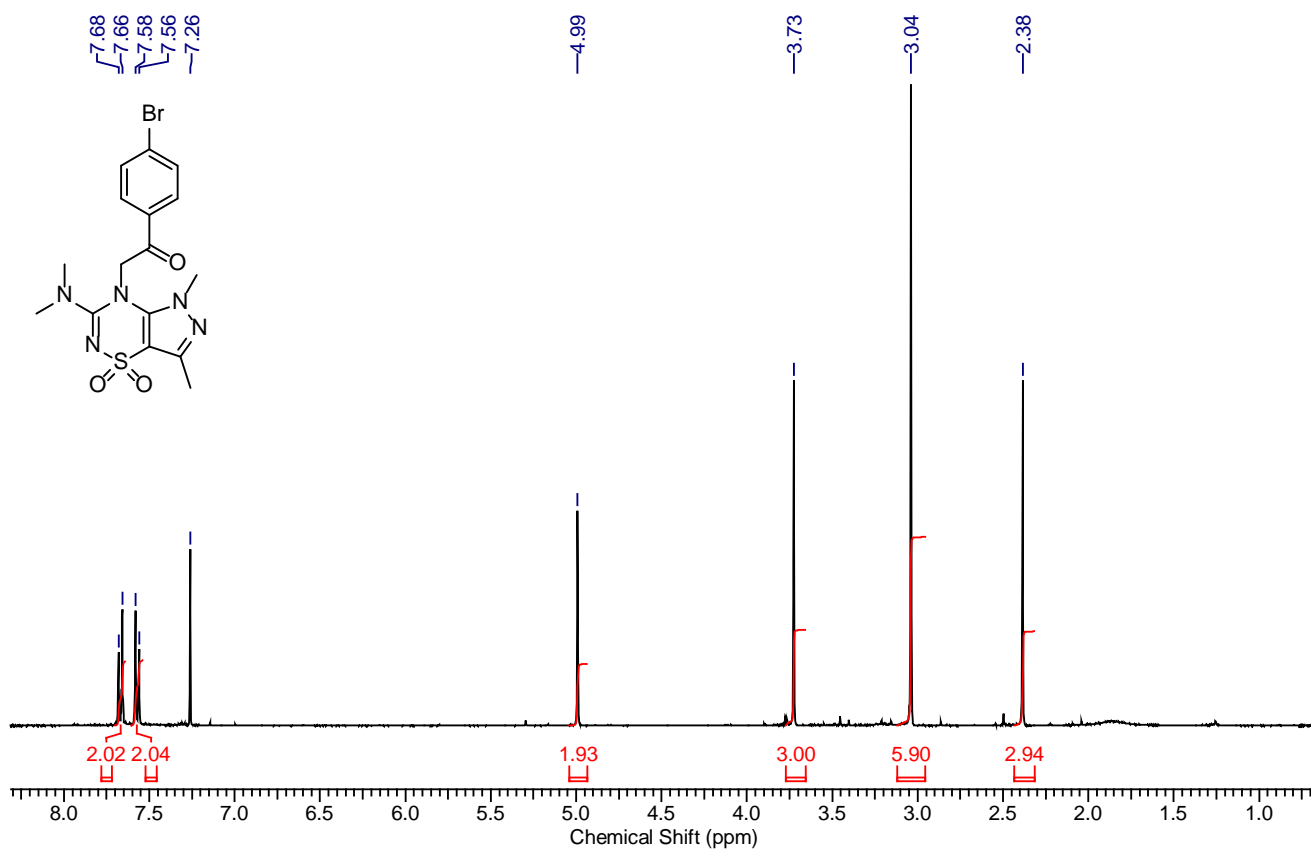


S29

^{13}C NMR spectrum of **14c** 100MHz (CDCl_3)

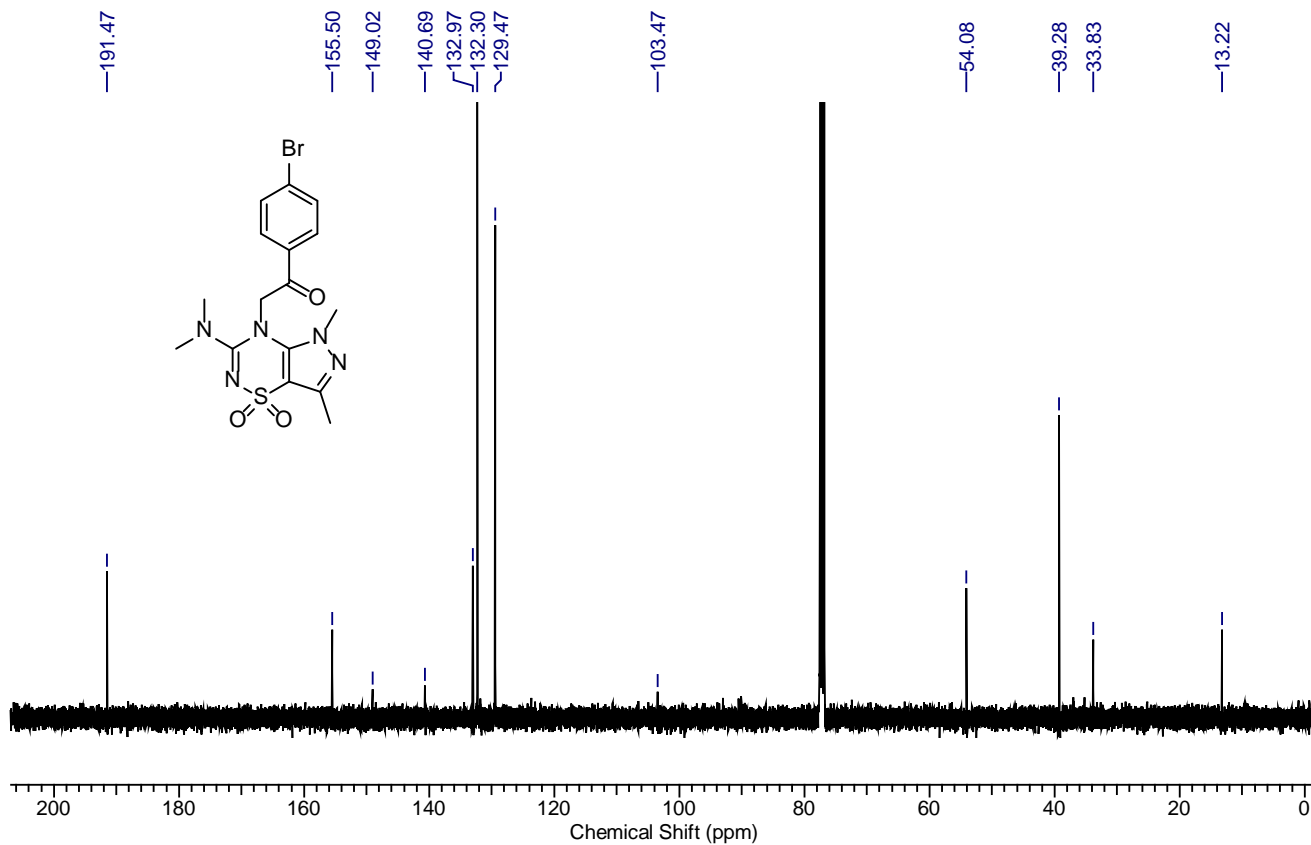


¹H NMR spectrum of **11d** 400MHz (CDCl₃)

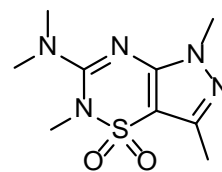
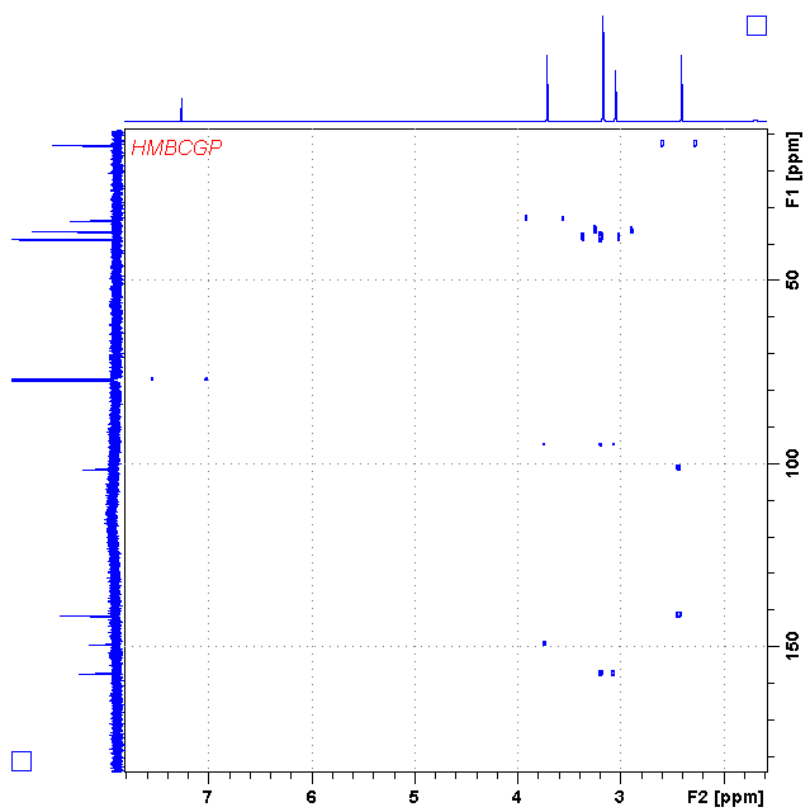


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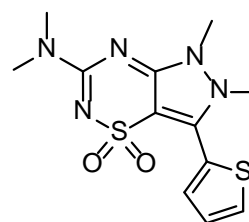
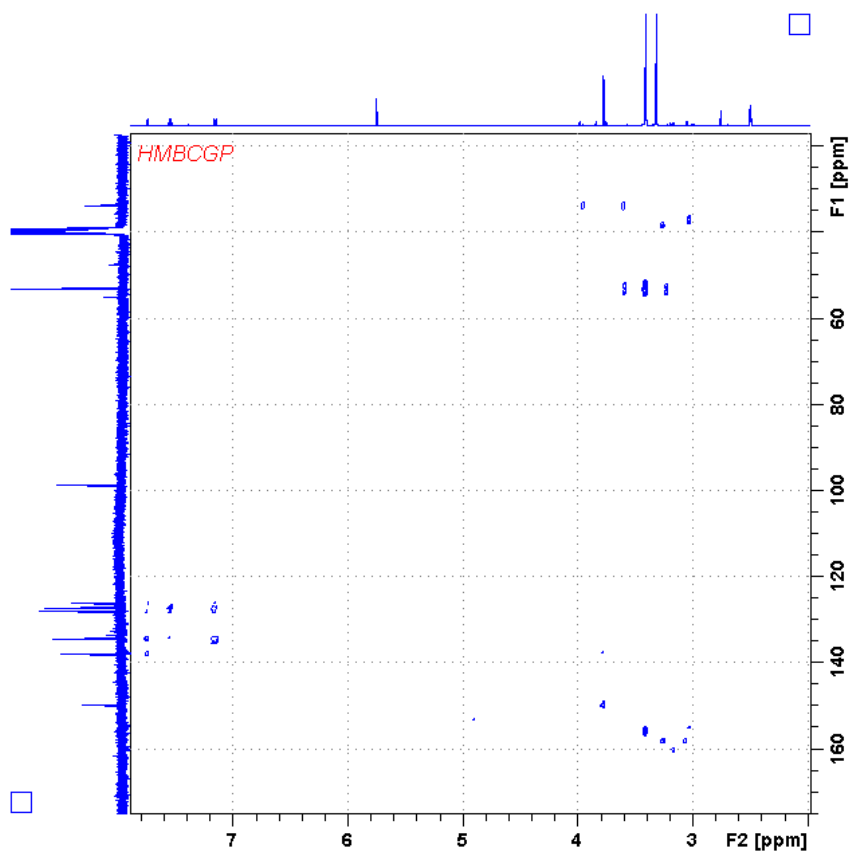
¹³C NMR spectrum of **11d** 100MHz (CDCl₃)



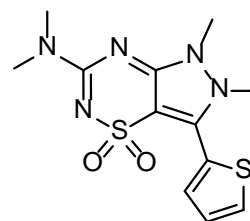
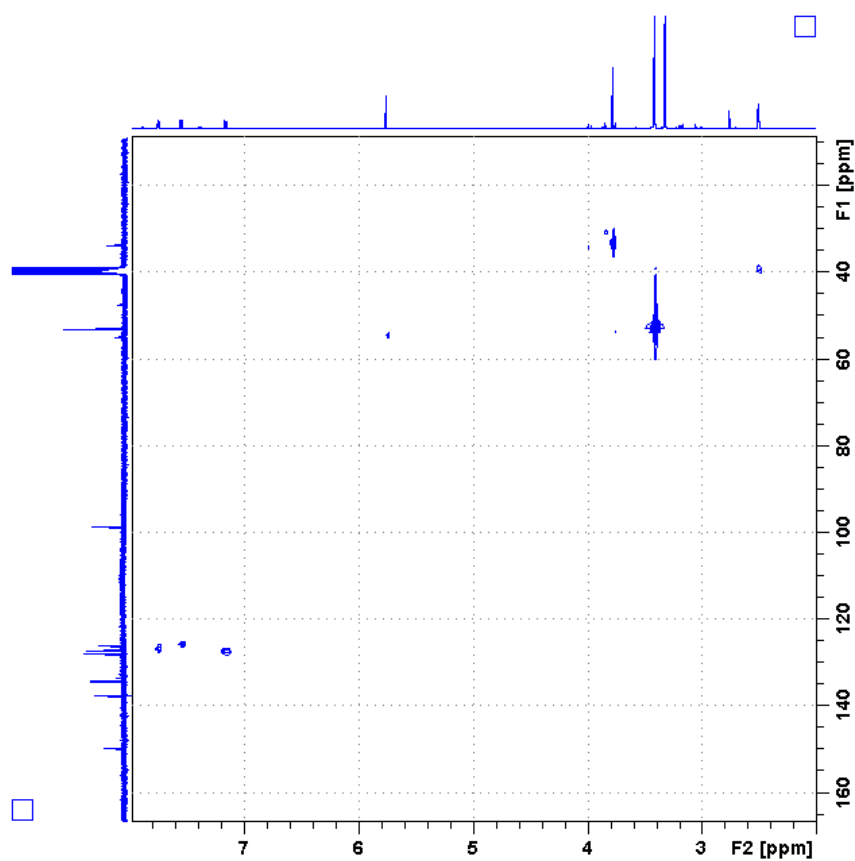
7a HMBC 400MHz



9b HMBC 400MHz

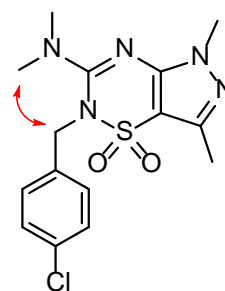
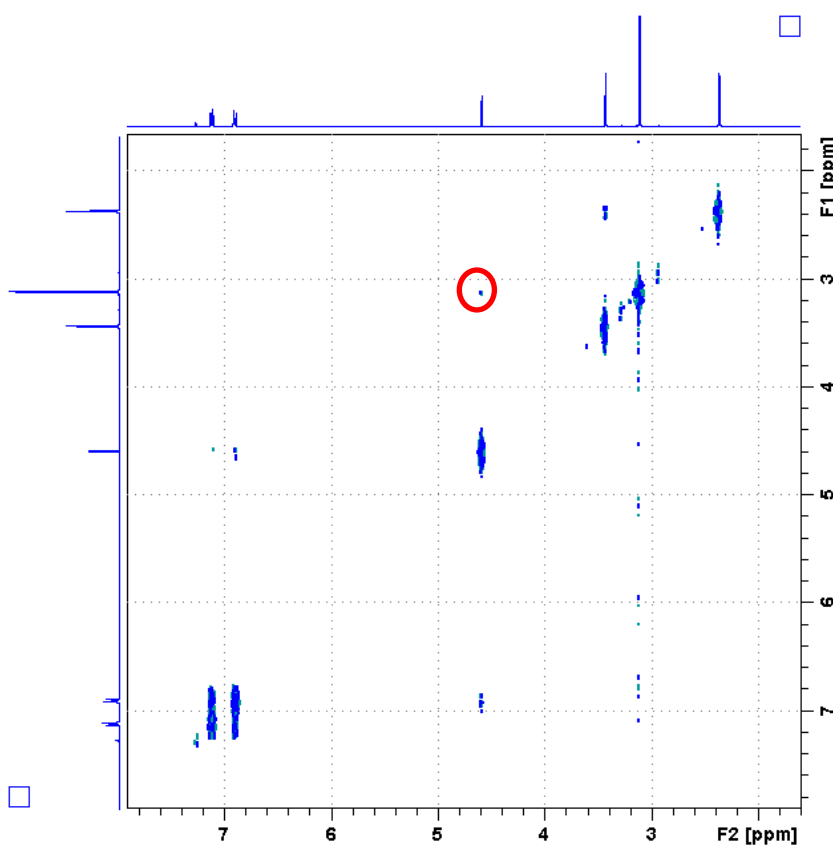


9b HMQC 400MHz

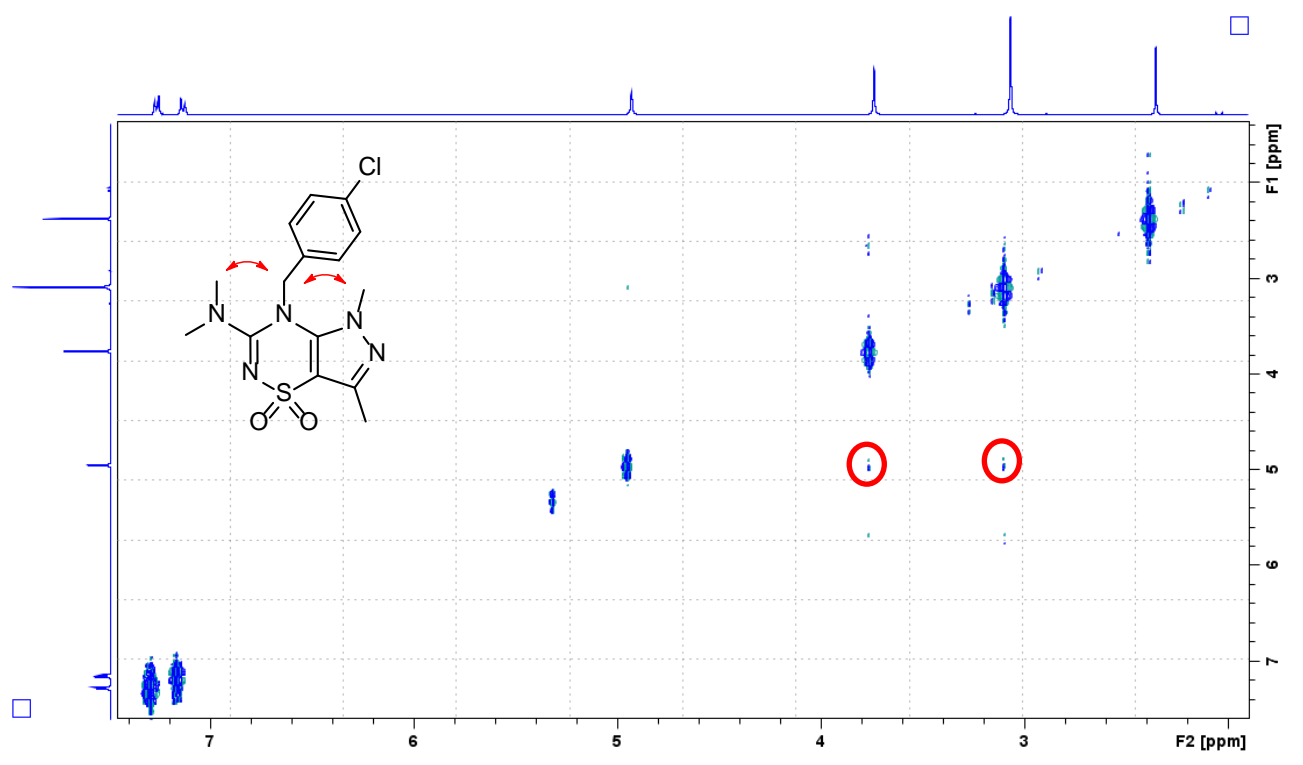


S32

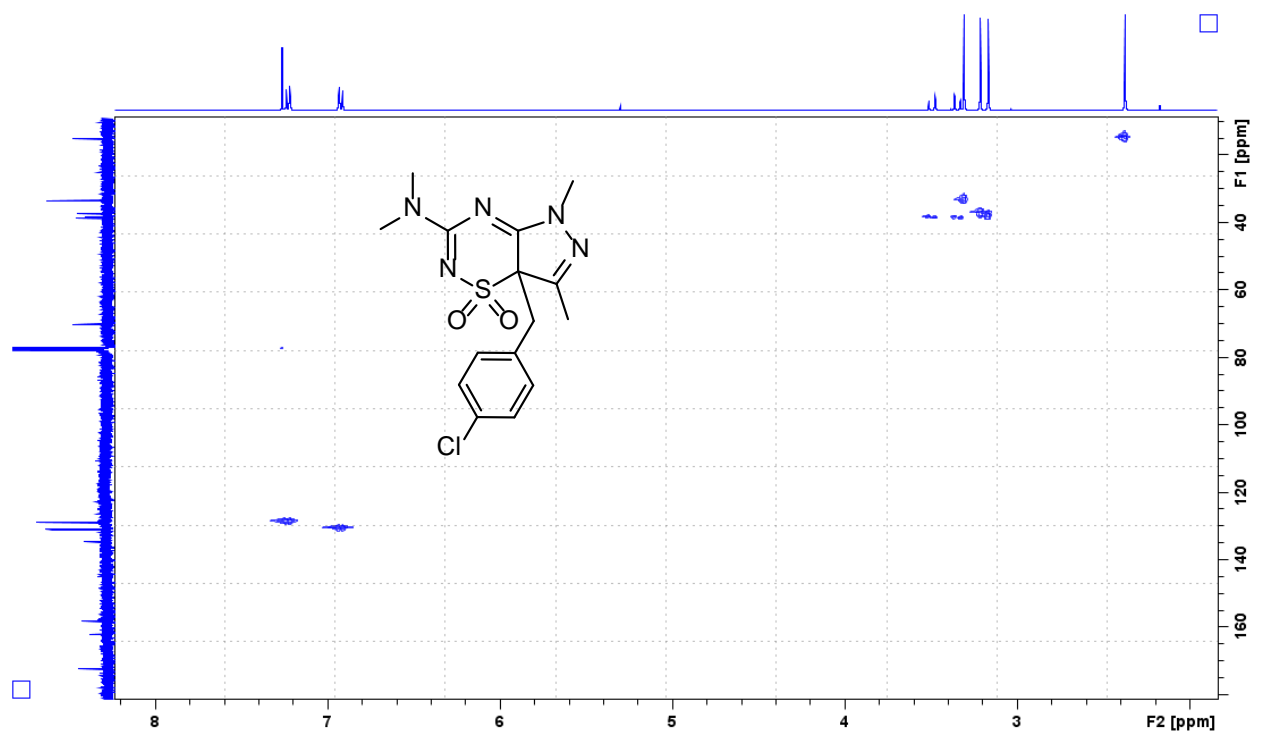
7c NOESY 400MHz



8c NOESY 400MHz

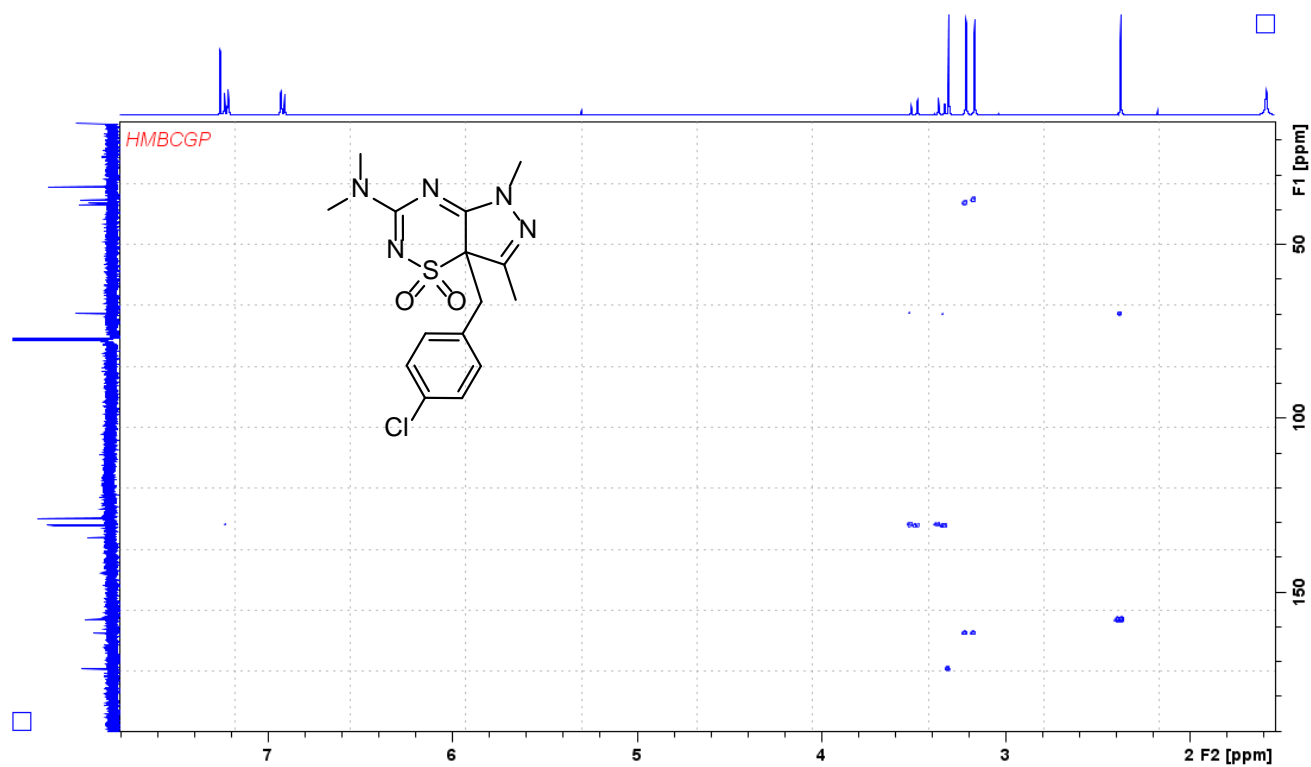


10c HMQC 400MHz



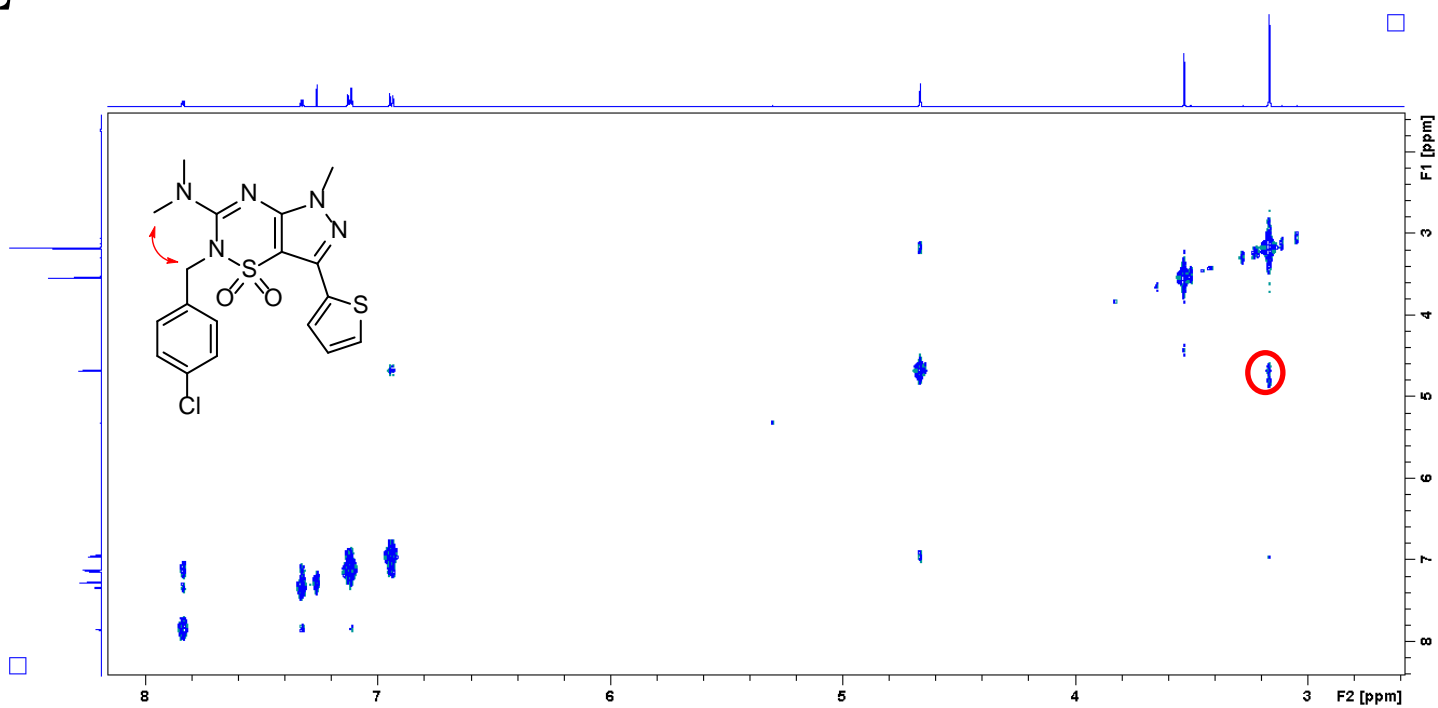
S33

10c HMBC 400MHz

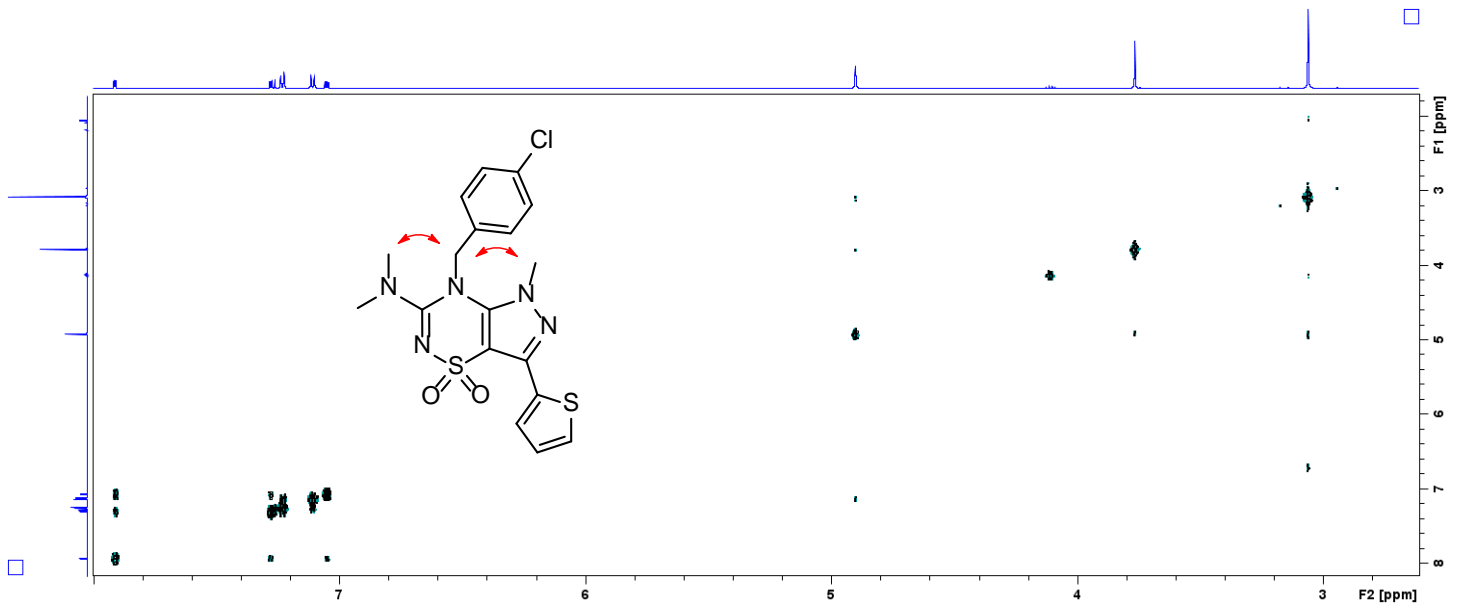


S34

7d NOESY 600MHz

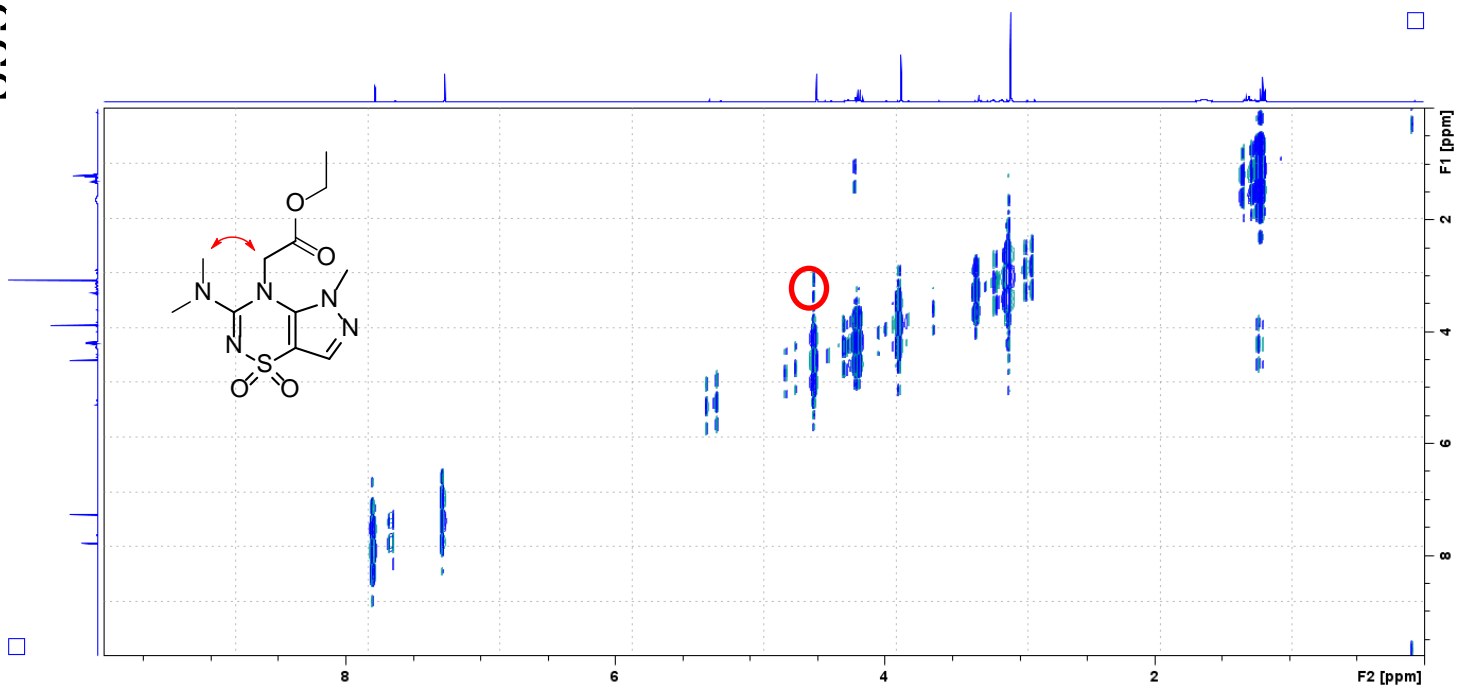


8d NOESY 600MHz

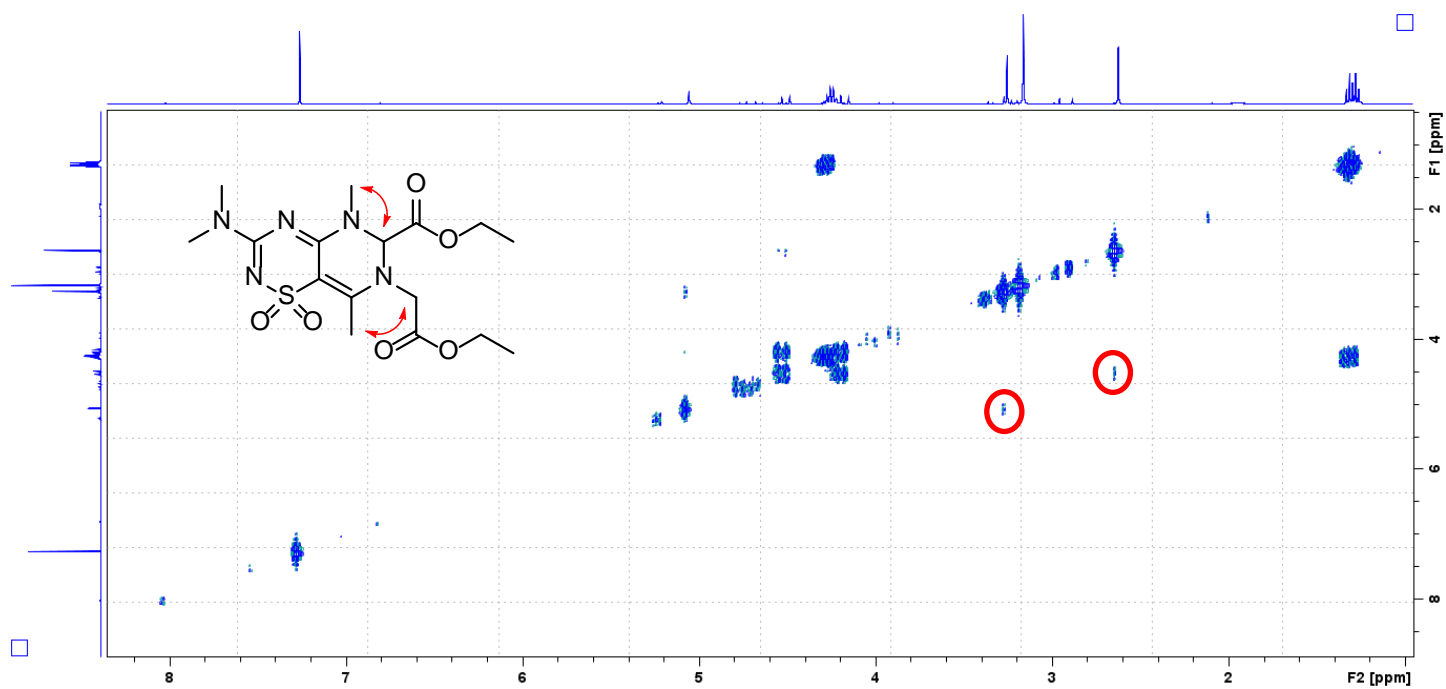


11a NOESY 400MHz

S35

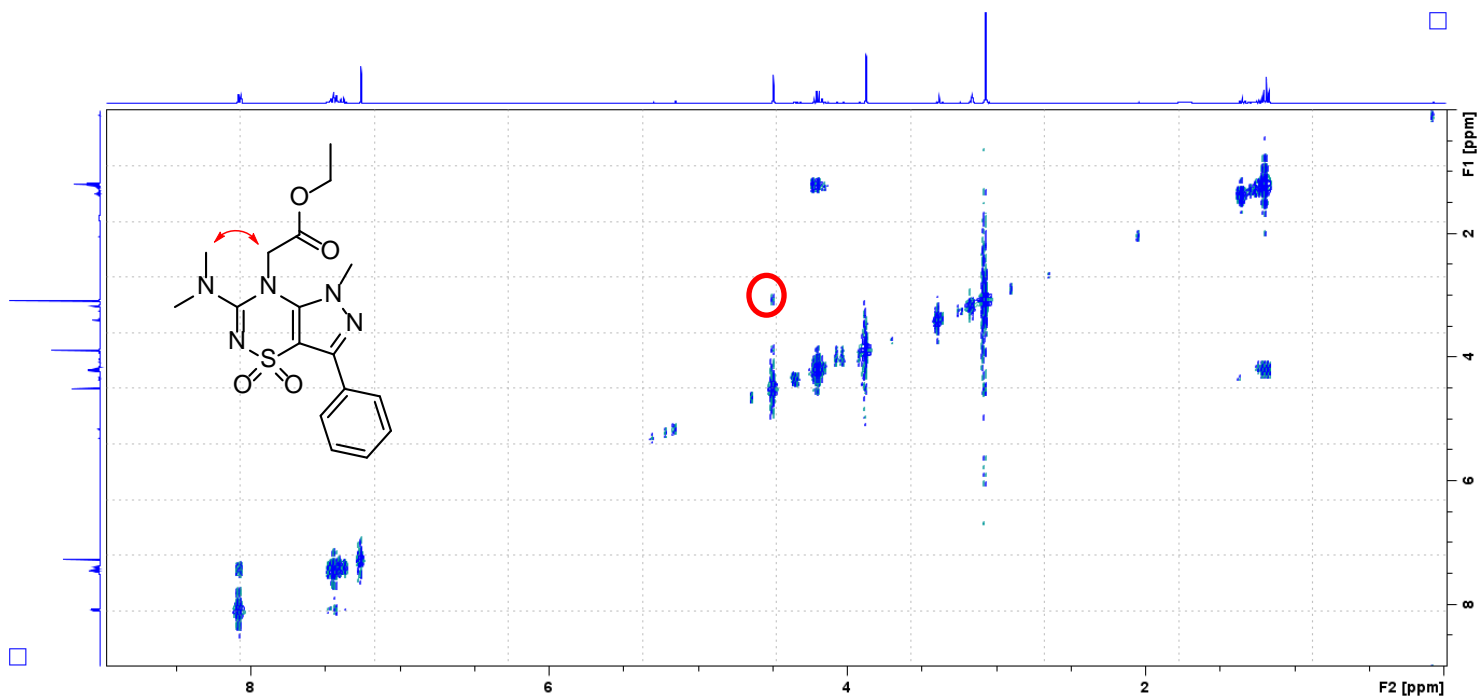


13b NOESY 400MHz

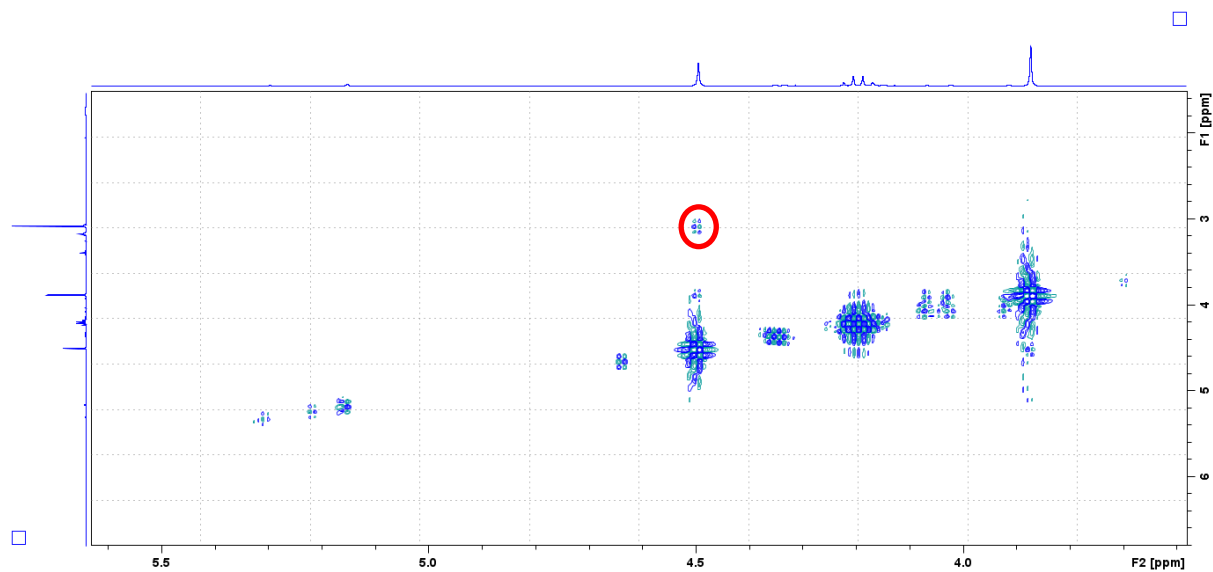


S36

11c NOESY 400MHz

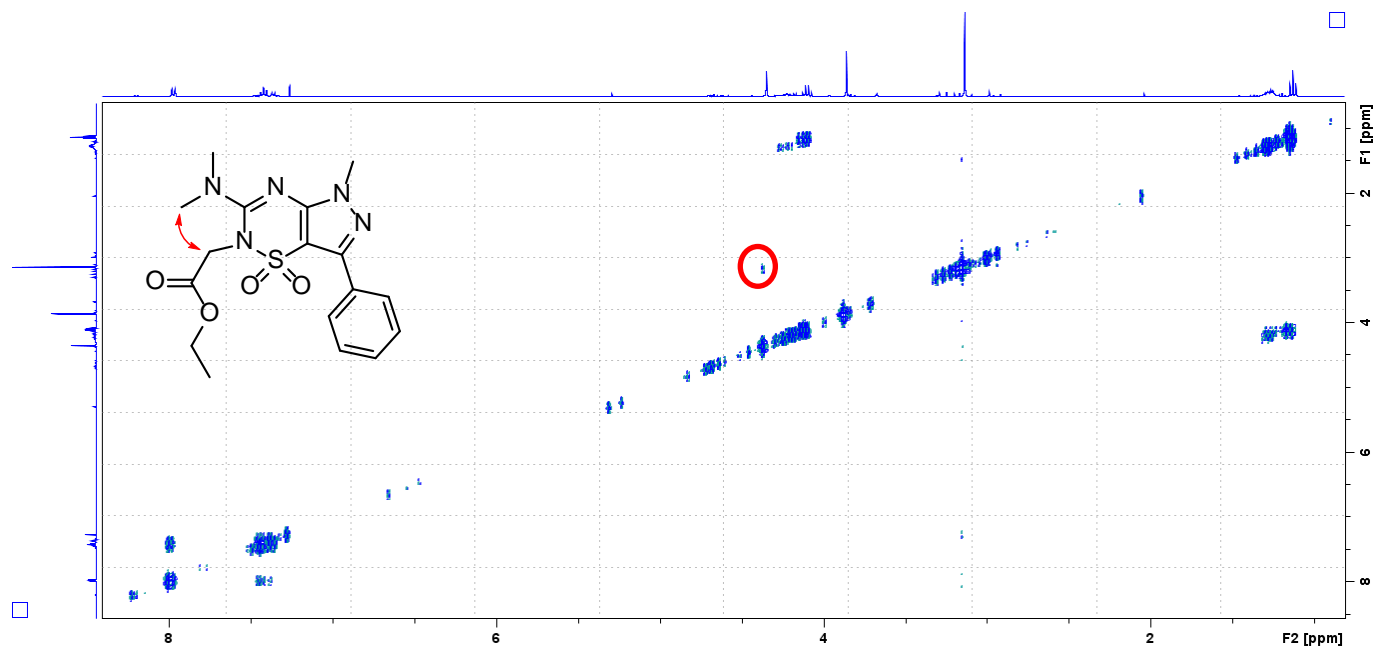


11c NOESY 400MHz expansion

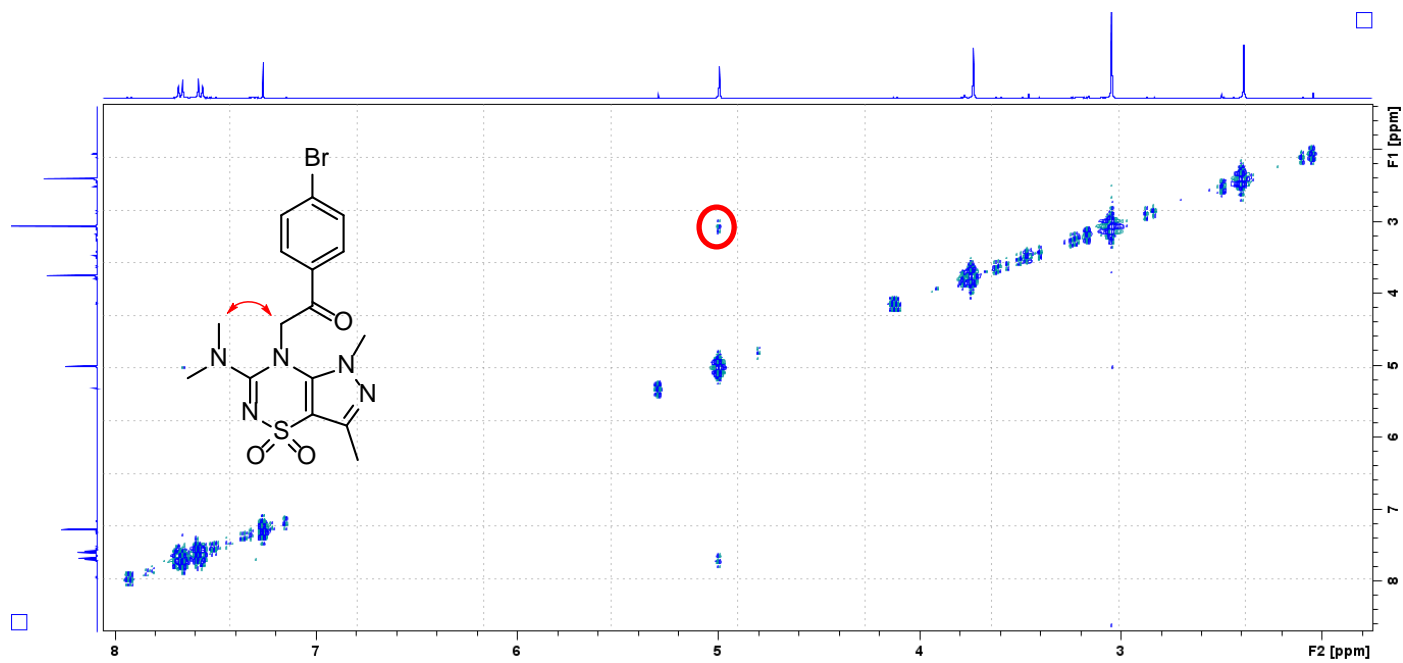


S37

14c NOESY 400MHz



11d NOESY 400MHz



S38