

Supplementary Information

for

The design, synthesis and biological evaluation of novel thiamin diphosphate analog inhibitors against pyruvate dehydrogenase multienzyme complex E1 from *Escherichia coli*

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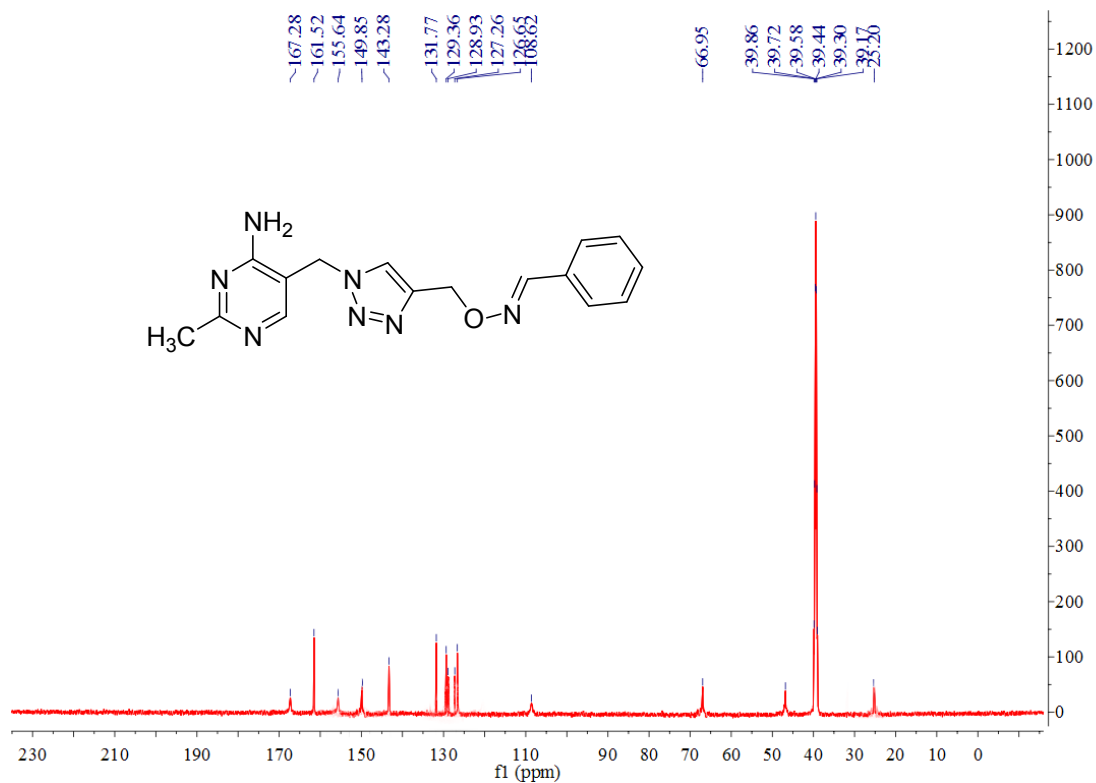
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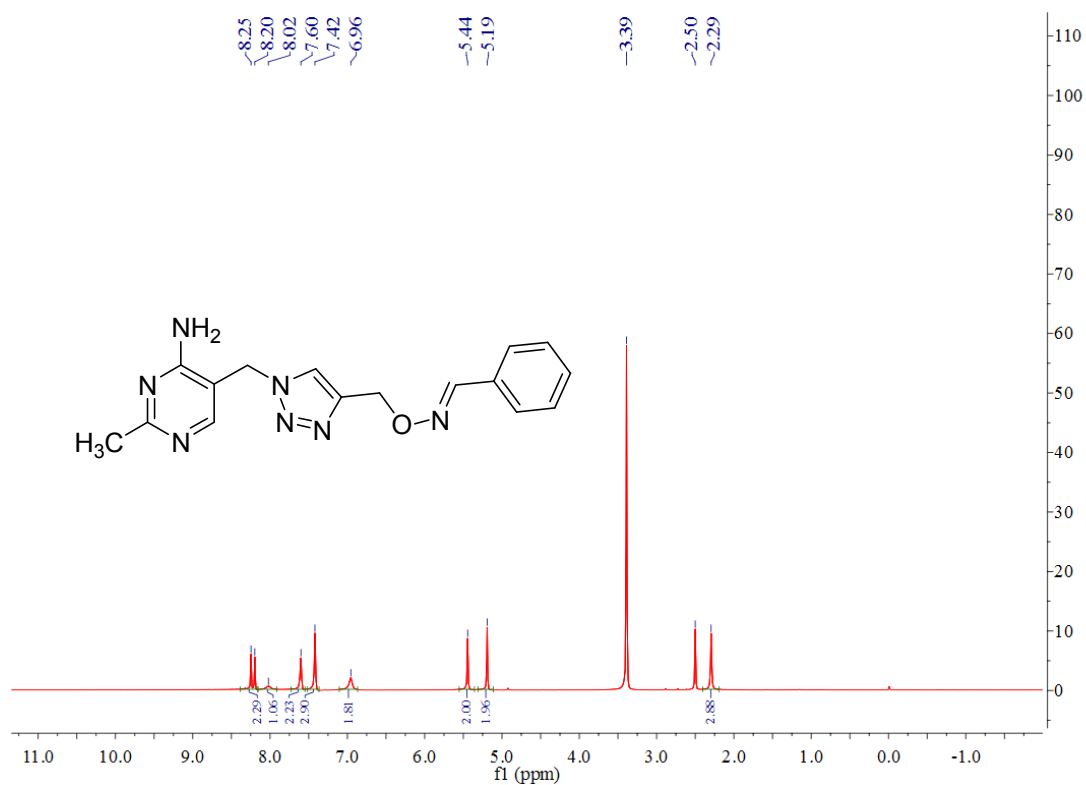
^cCollege of life science, Central China Normal University, Wuhan 430079, China.

1. The copies of all NMR spectra of the compounds

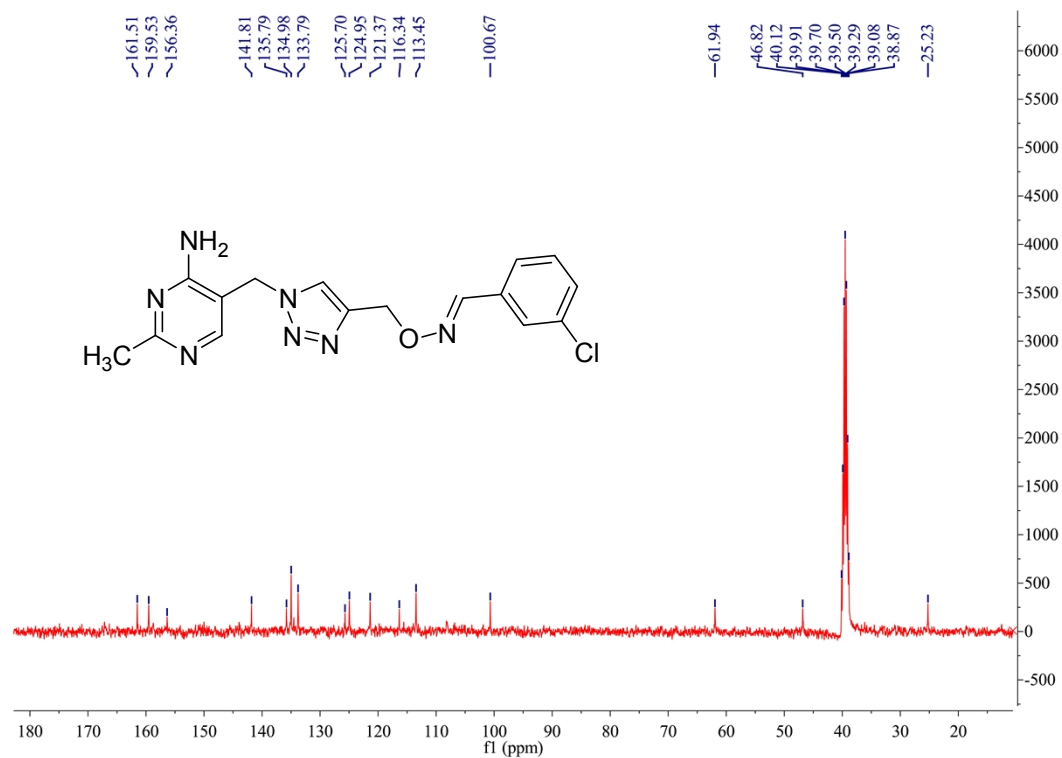
¹³C NMR of 4a in DMSO-d₆



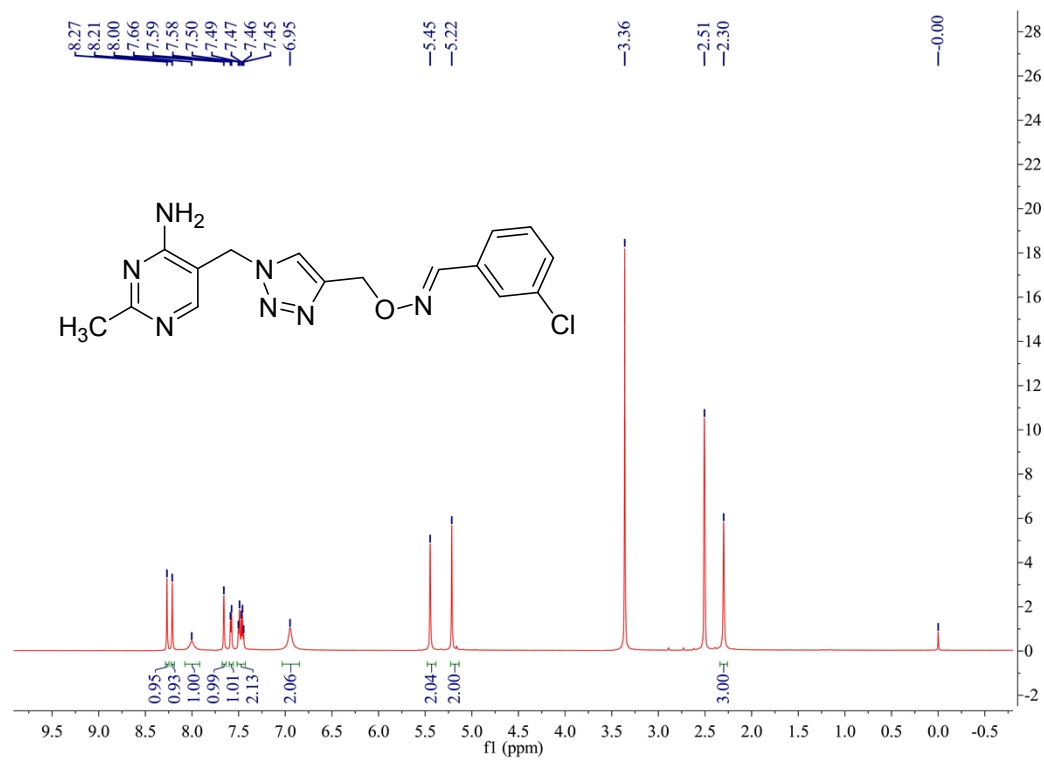
¹H NMR of 4a in DMSO-d₆



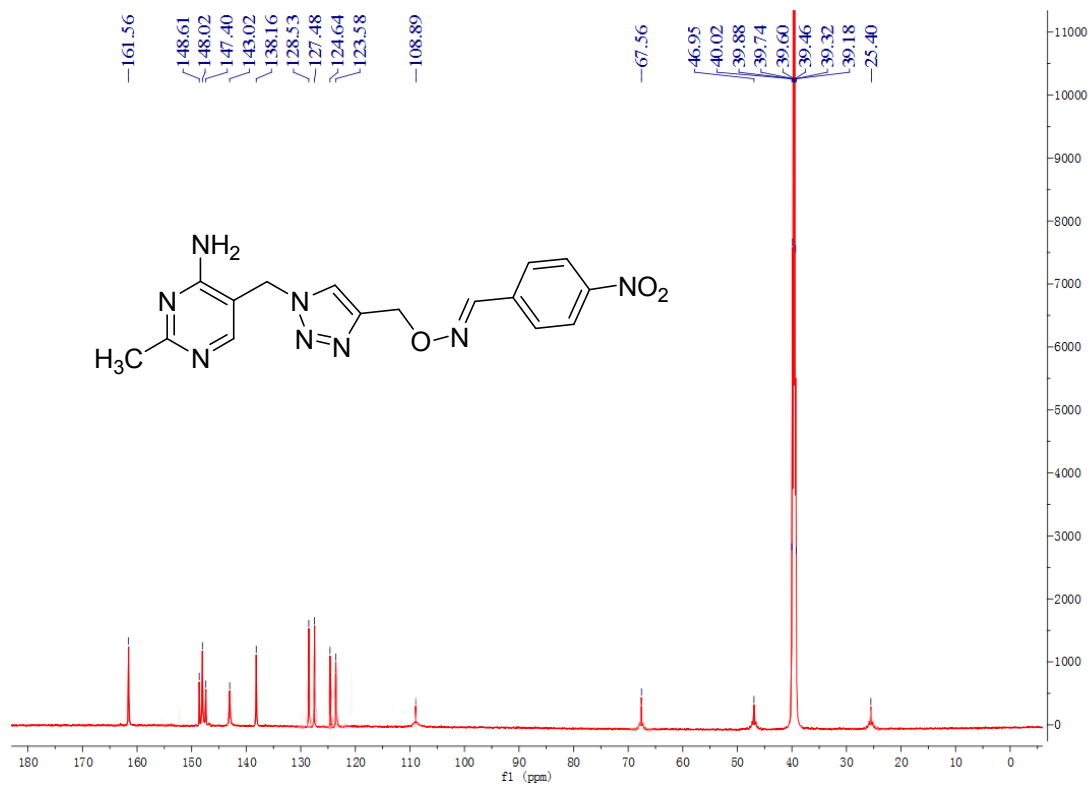
¹³C NMR of **4b** in DMSO-*d*₆



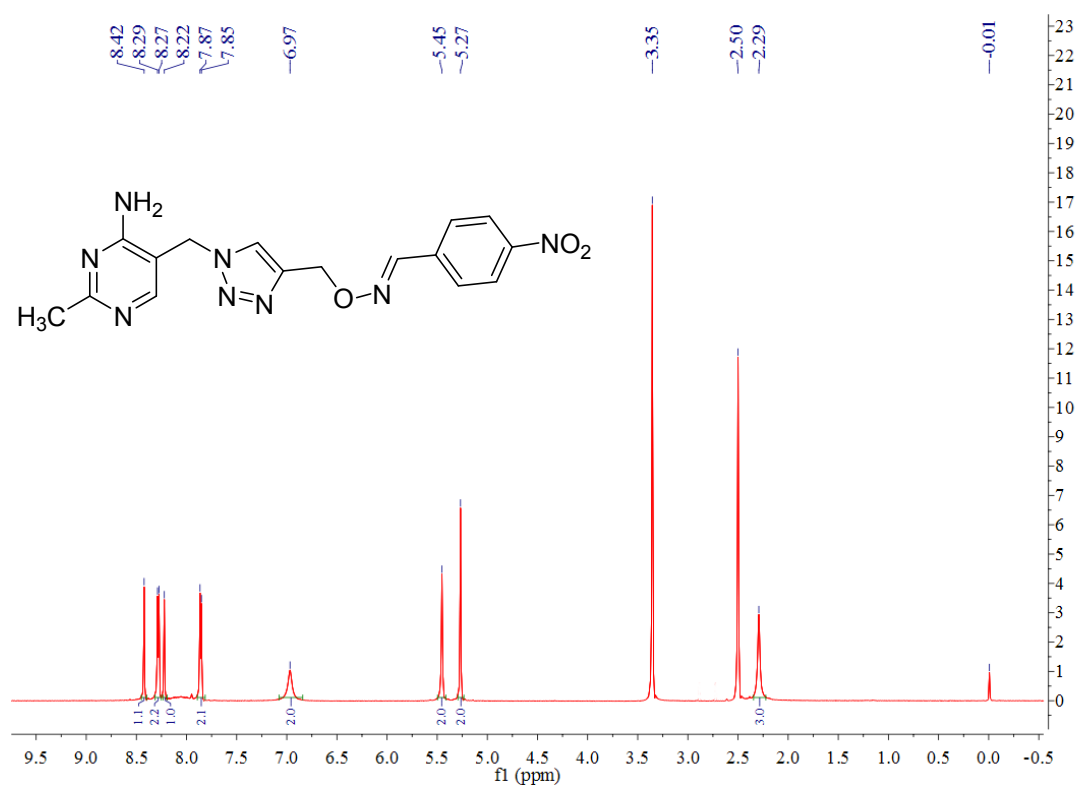
¹H NMR of **4b** in DMSO-*d*₆



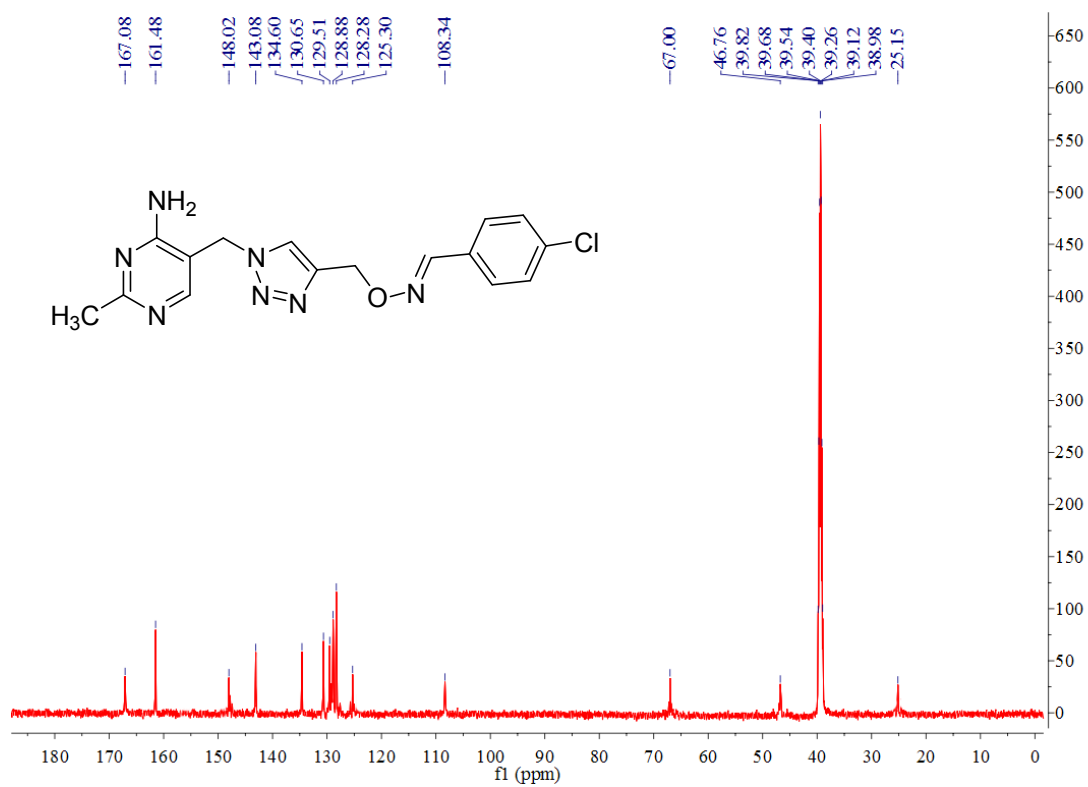
¹³C NMR of **4c** in DMSO-*d*₆



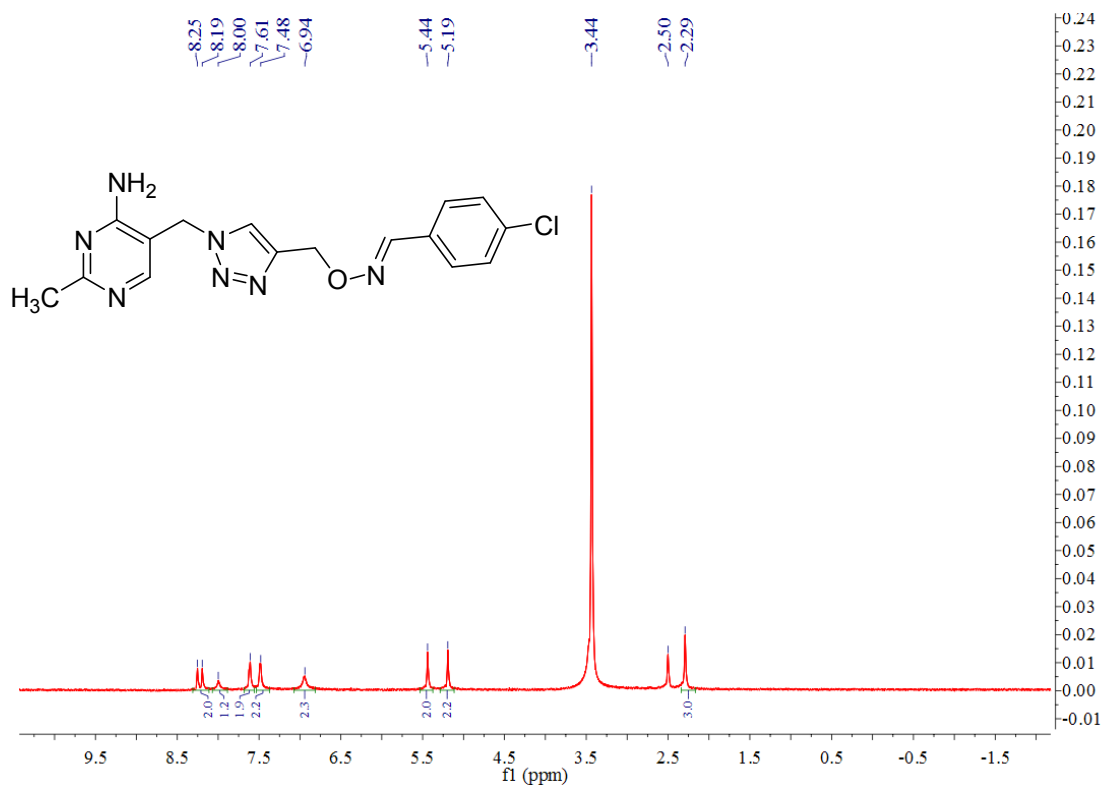
¹H NMR of **4c** in DMSO-*d*₆



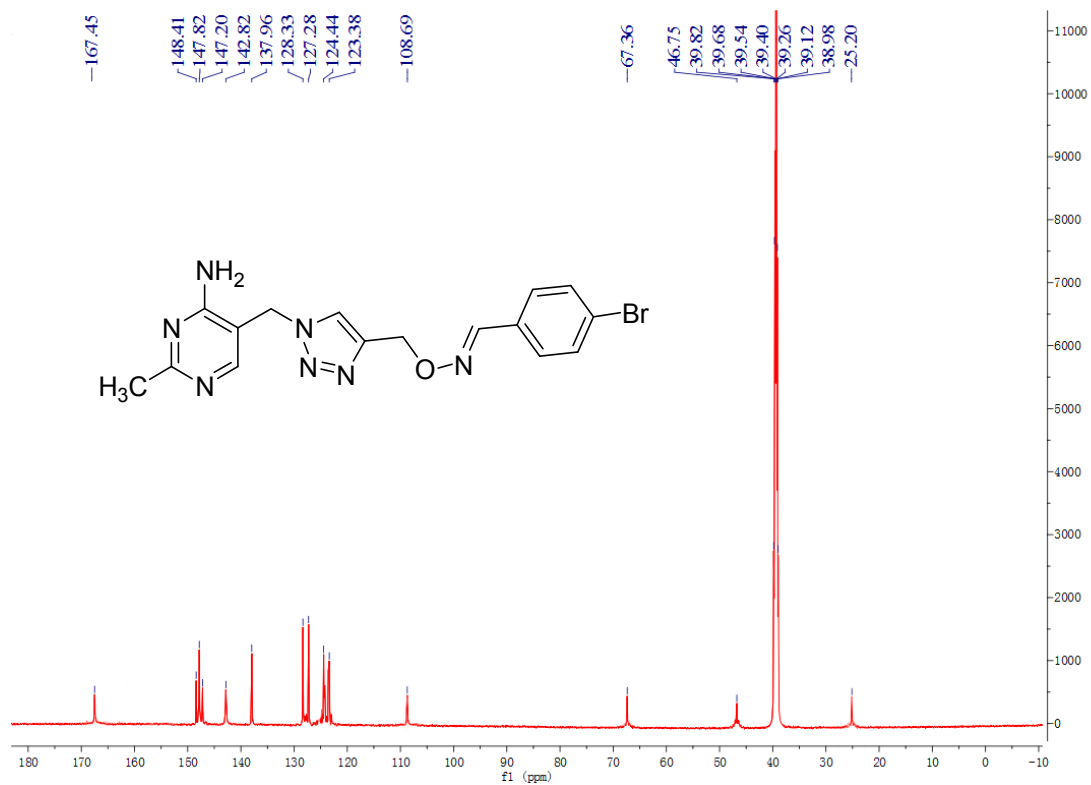
¹³C NMR of **4d** in DMSO-*d*₆



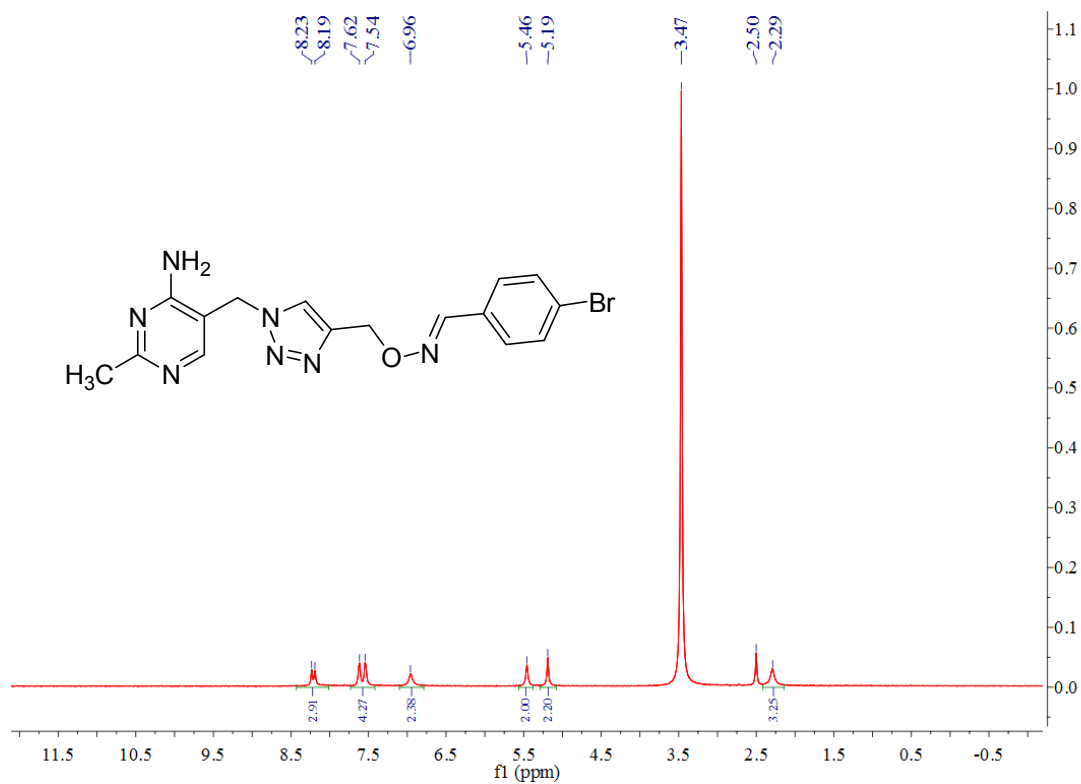
¹H NMR of **4d** in DMSO-*d*₆



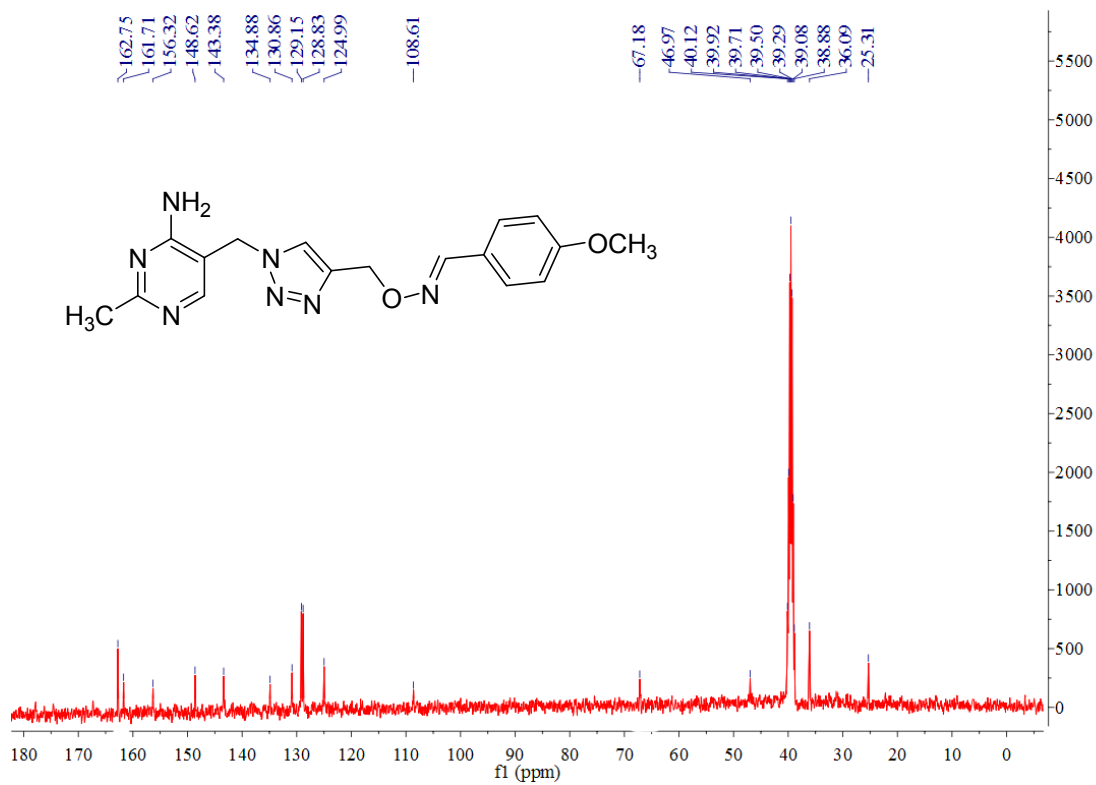
^{13}C NMR of **4e** in DMSO- d_6



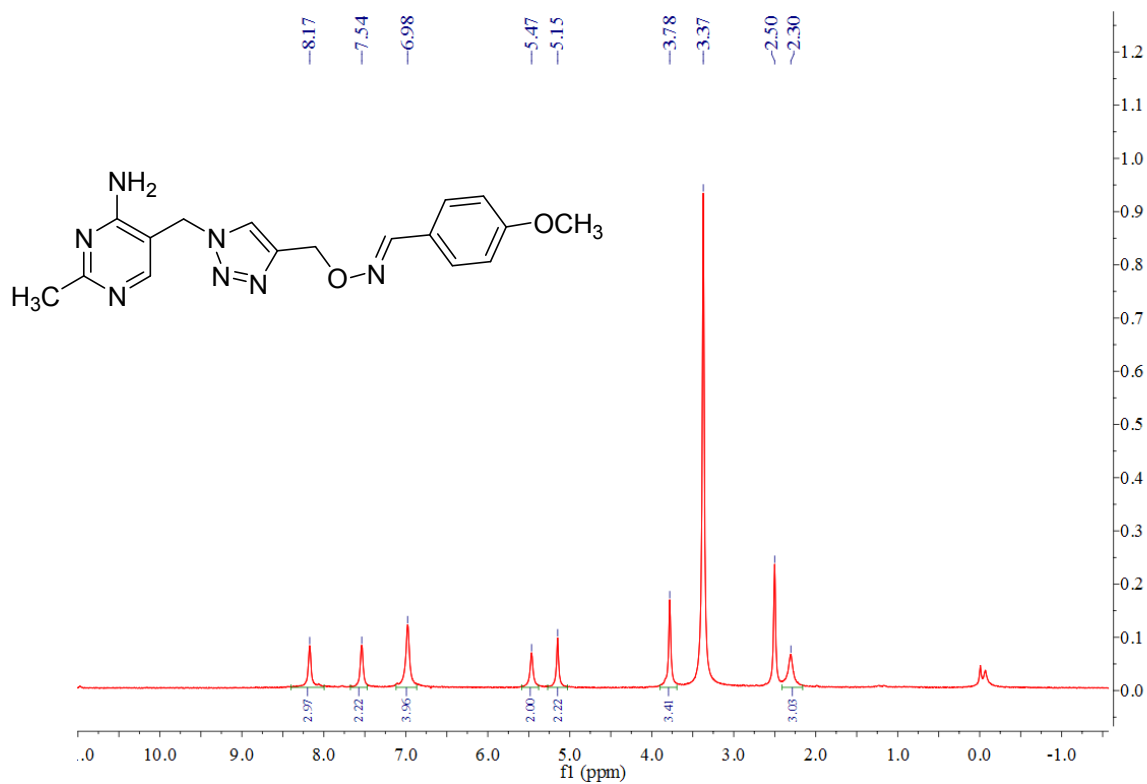
^1H NMR of **4e** in DMSO- d_6



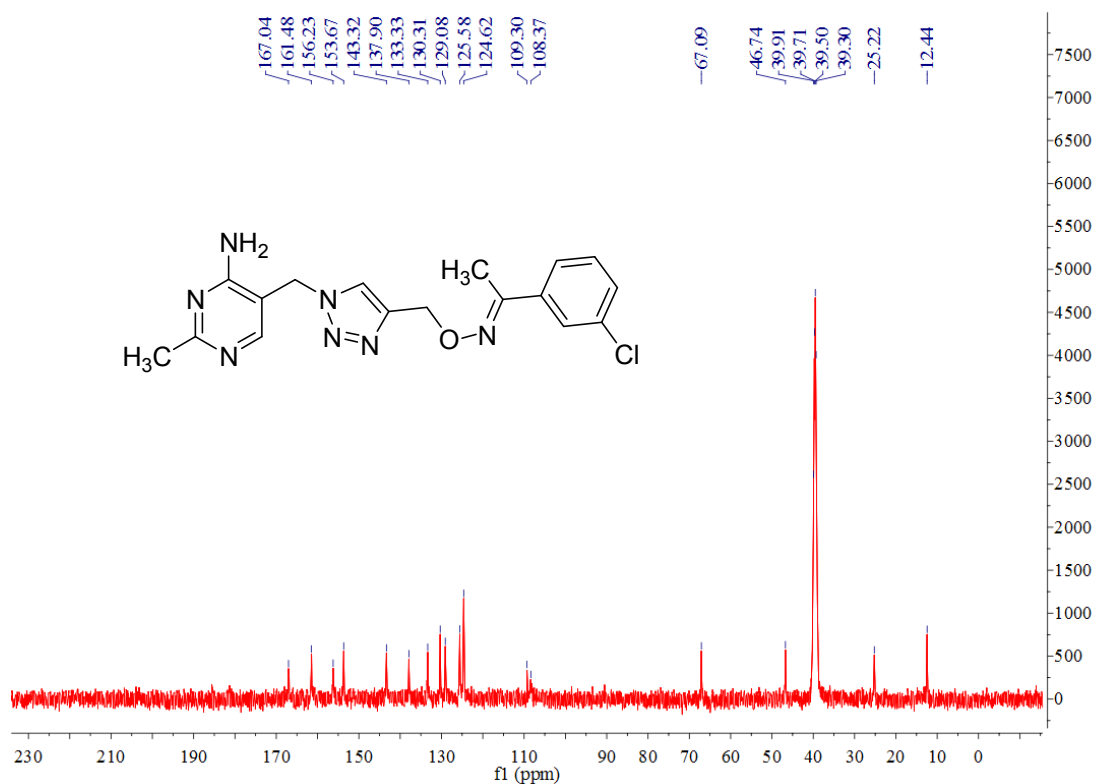
^{13}C NMR of **4f** in $\text{DMSO-}d_6$



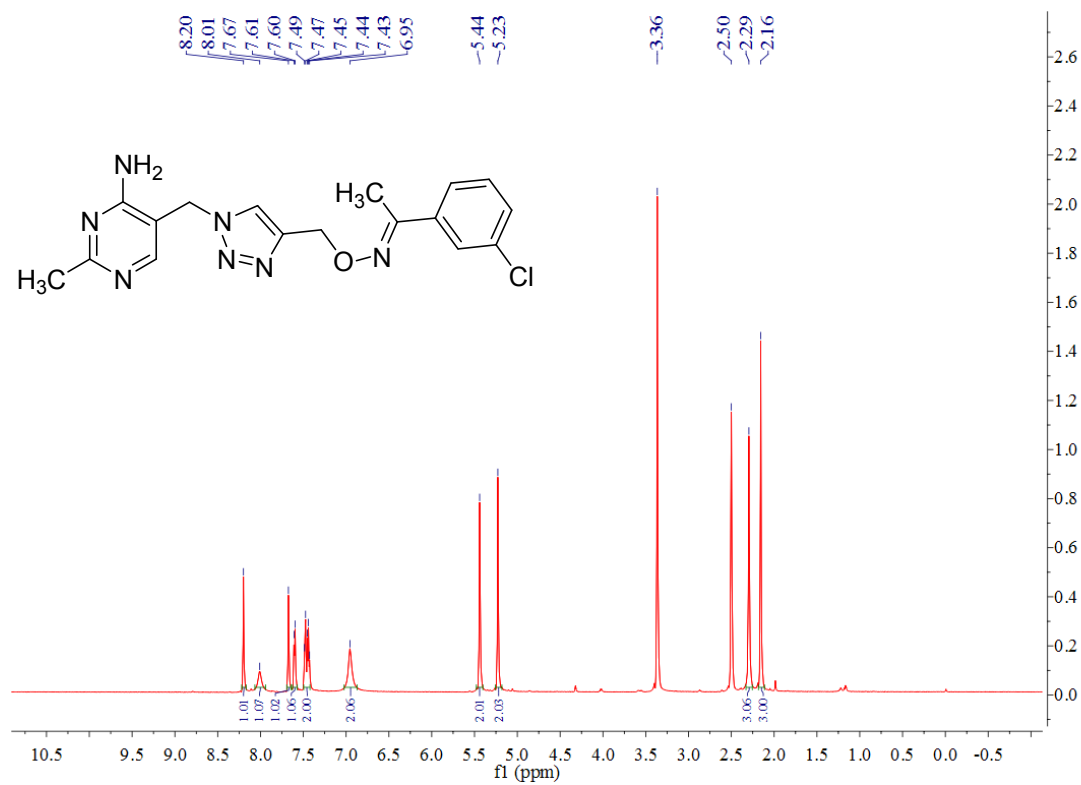
^1H NMR of **4f** in $\text{DMSO-}d_6$



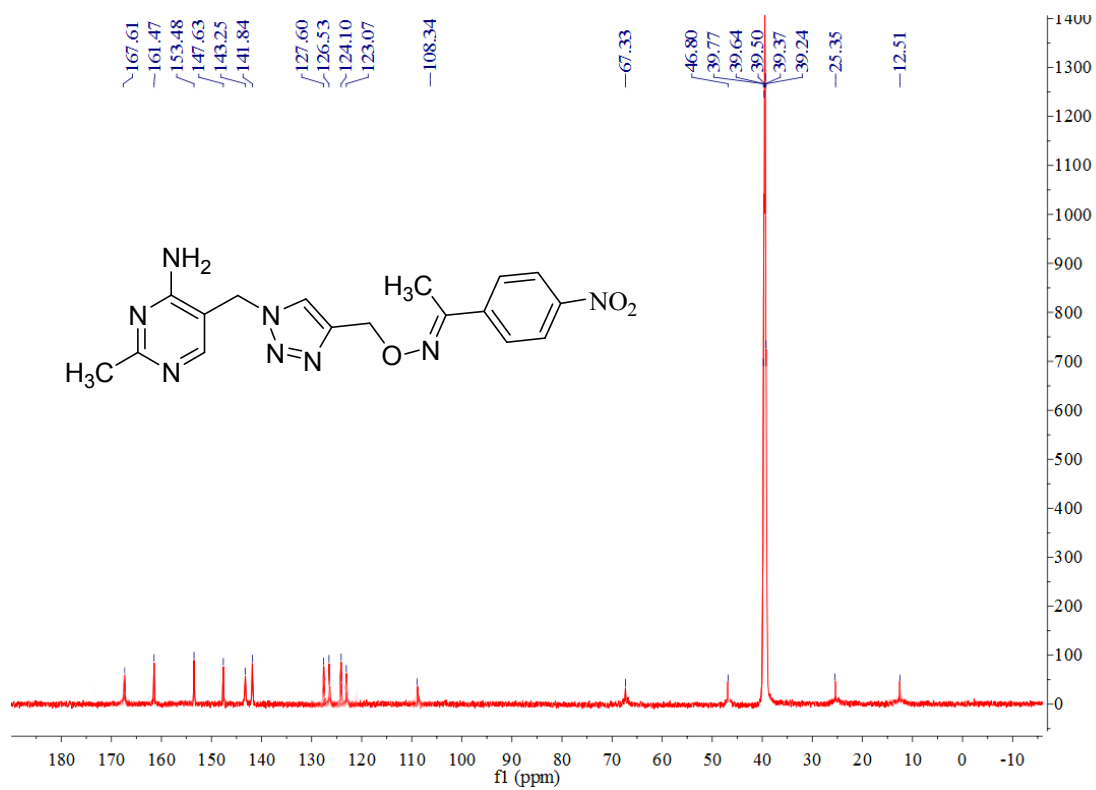
¹³C NMR of **4g** in DMSO-d₆



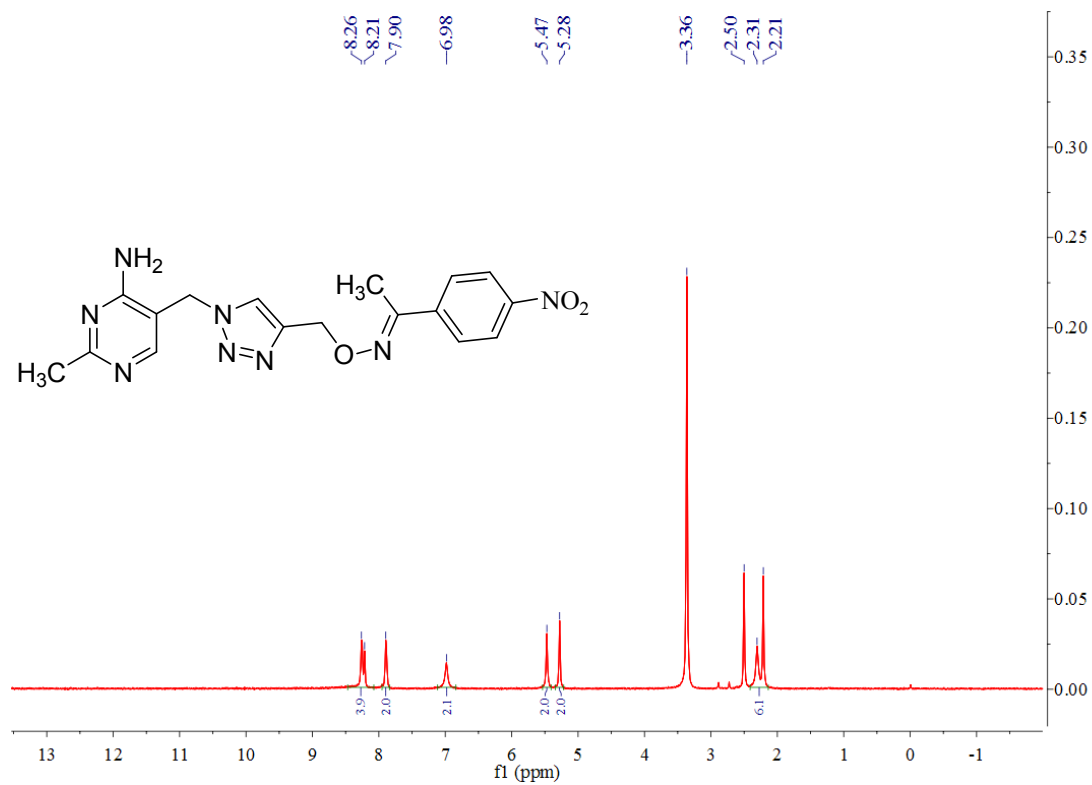
¹H NMR of **4g** in DMSO-d₆



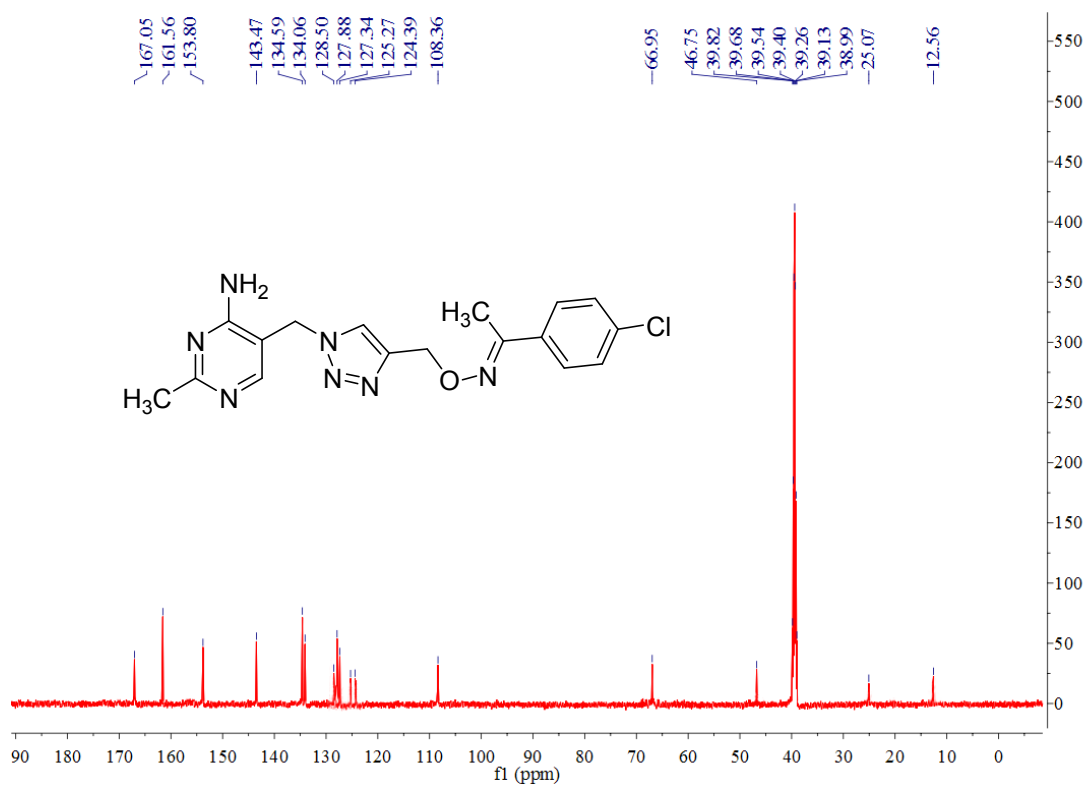
¹³C NMR of **4h** in DMSO-*d*₆



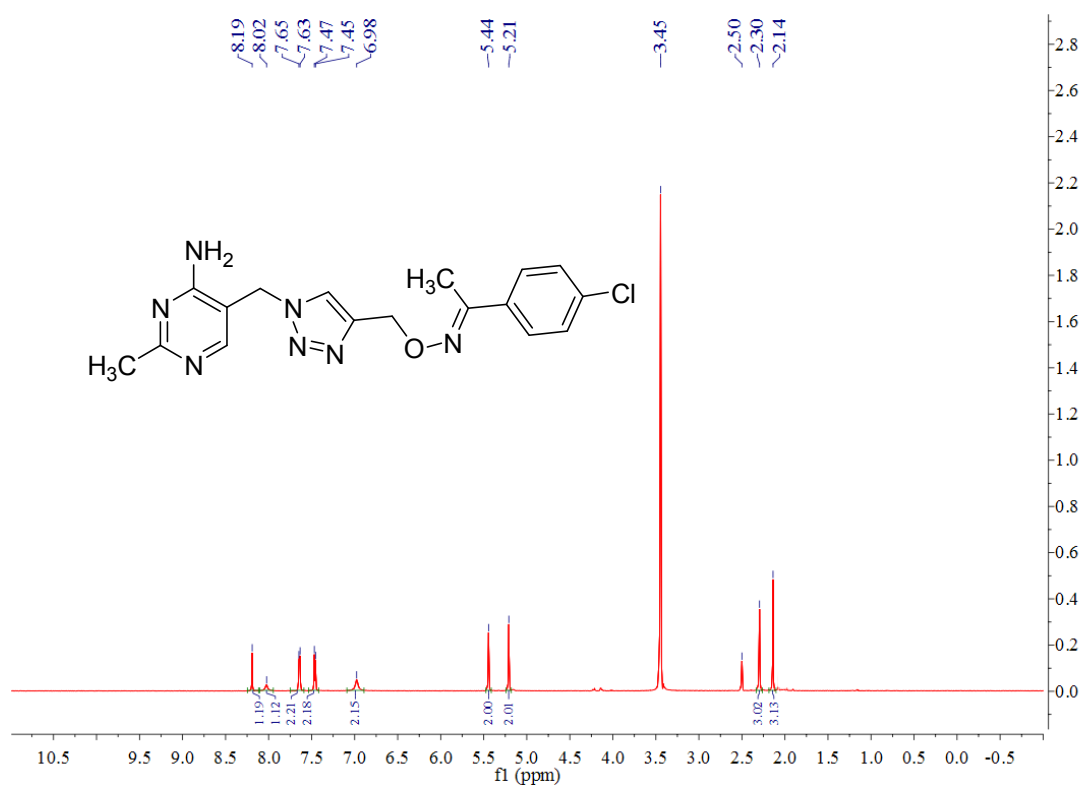
¹H NMR of **4h** in DMSO-*d*₆



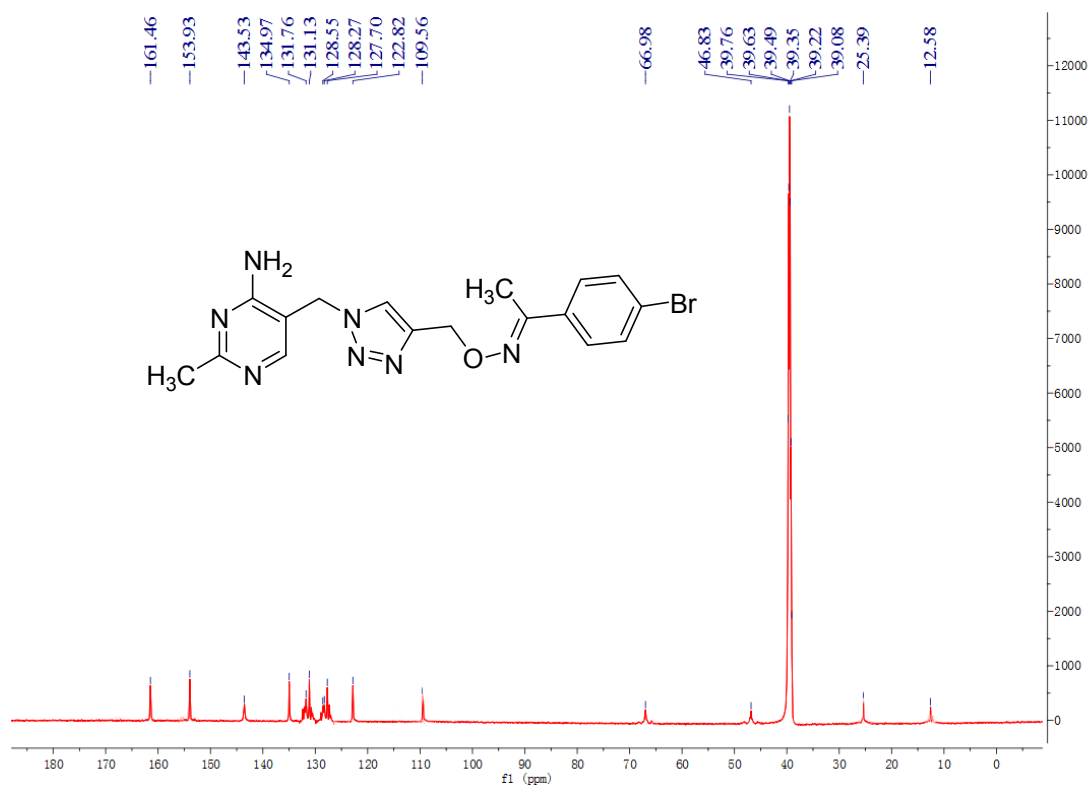
¹³C NMR of **4i** in DMSO-*d*₆



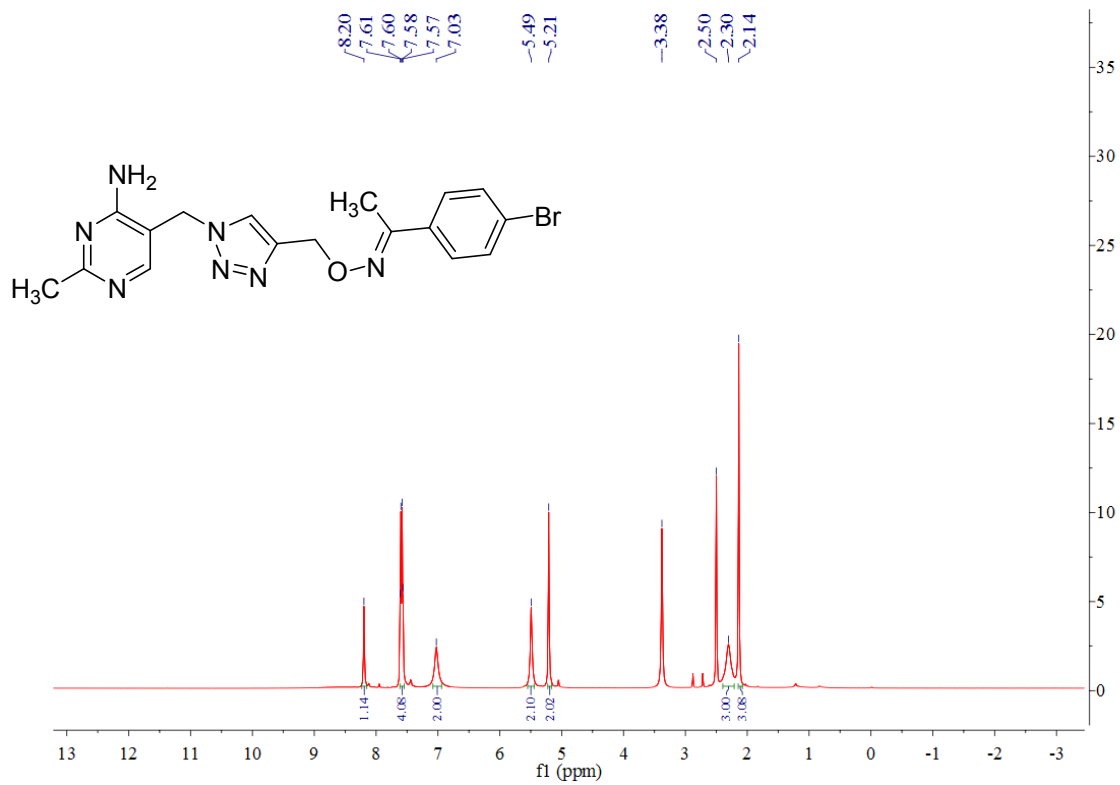
¹H NMR of **4i** in DMSO-*d*₆



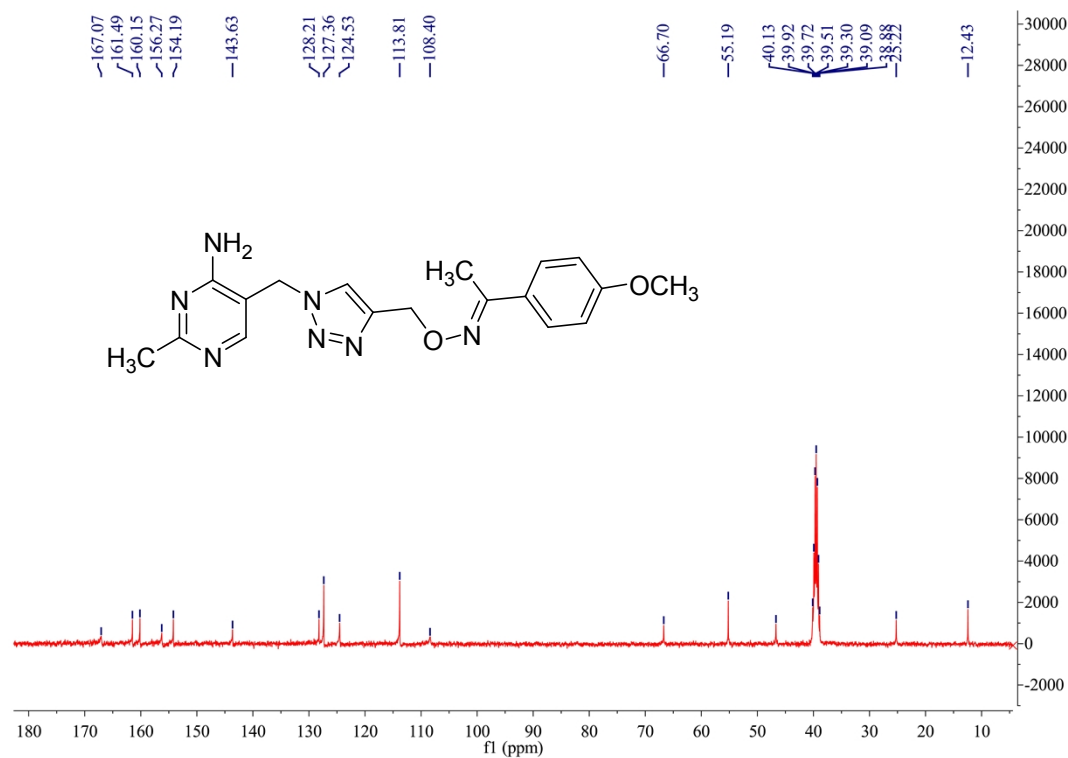
¹³C NMR of **4j** in DMSO-*d*₆



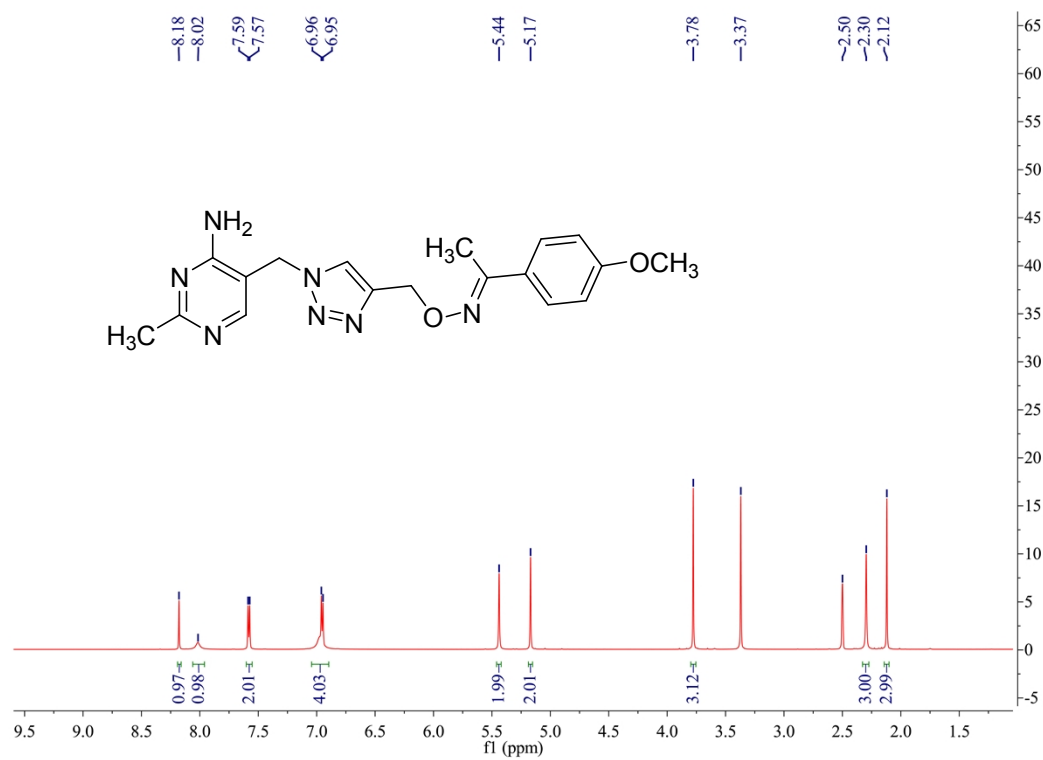
¹H NMR of **4j** in DMSO-*d*₆



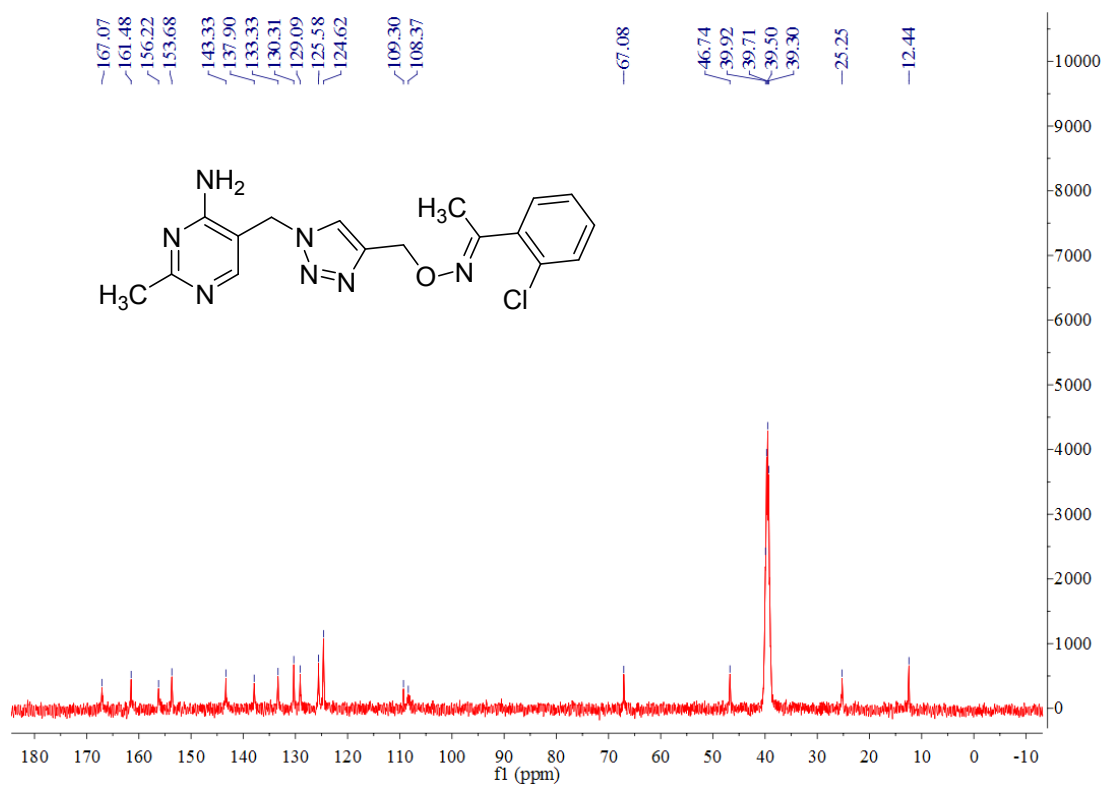
¹³C NMR of **4k** in DMSO-d₆



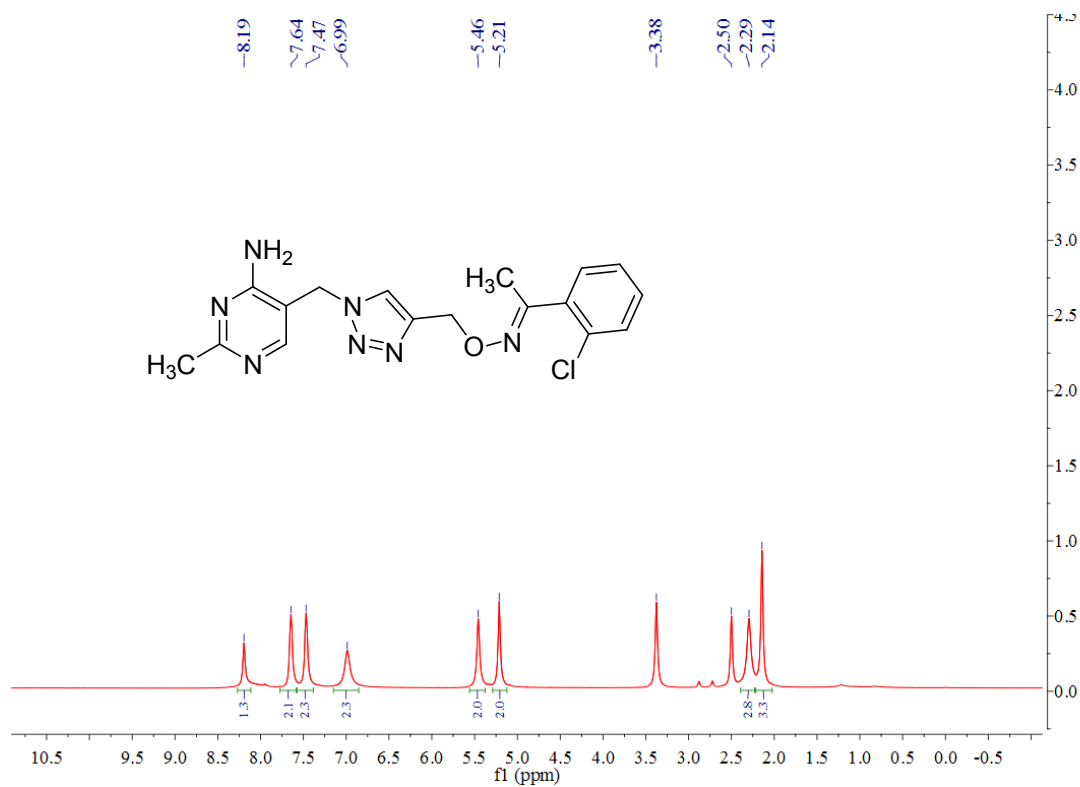
¹H NMR of **4k** in DMSO-d₆



¹³C NMR of **4I** in DMSO-*d*₆



¹H NMR of **4I** in DMSO-*d*₆



2. The representative figures for the dose-response effect of all applicable assays

