



Supporting Information

for

Cycloaddition reactions of heterocyclic azides with 2-cyanoacetamidines as a new route to C,N- diheteroarylcarbamidines

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Andrey N. Maslivets, Vladimir G. Ilkin, Wim Dehaen and Vasiliy A. Bakulev

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Copies of NMR spectra of all new compounds

Table of contents

NMR spectra of compounds 3a–u	S2
X-ray Single Crystal Data for 3g	S28

Fig. S1. ^1H NMR spectrum ($\text{DMSO-}d_6$) of **3a**

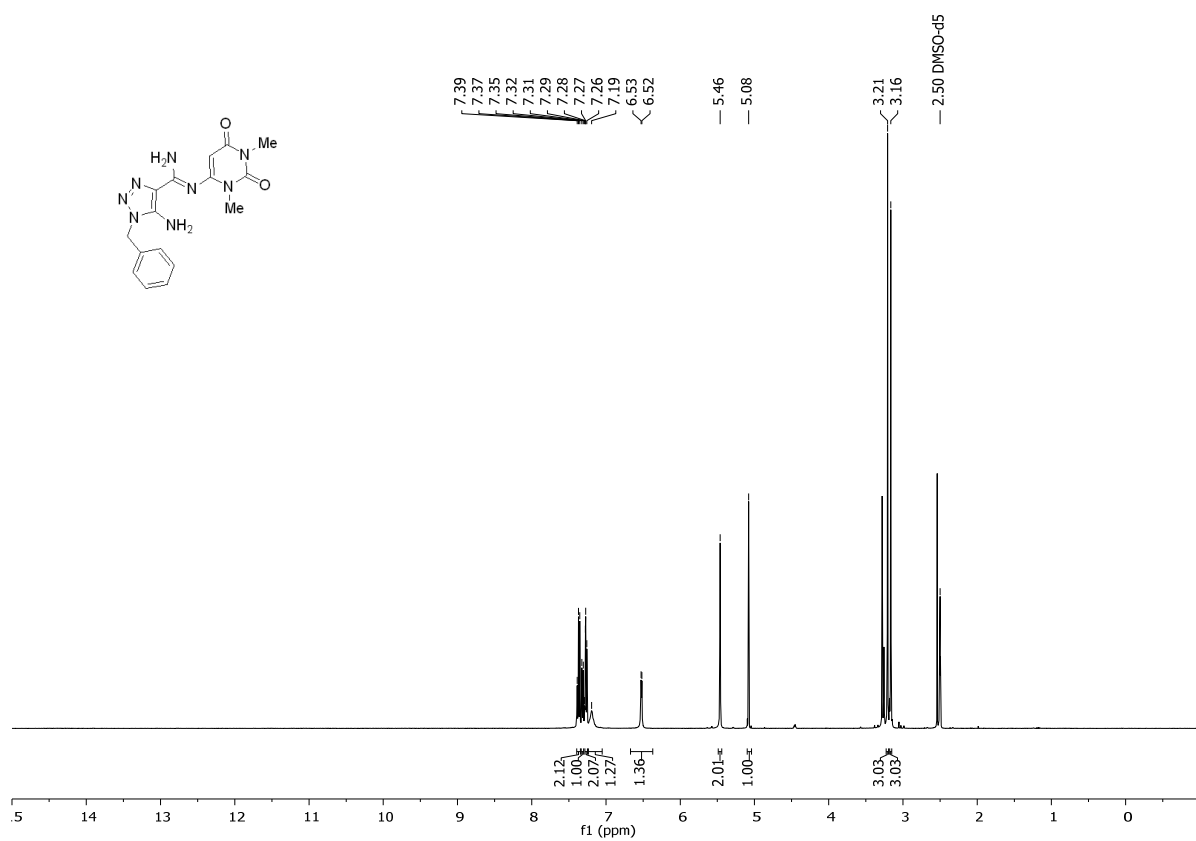


Fig. S2. ^{13}C NMR spectrum ($\text{DMSO-}d_6$) of **3a**

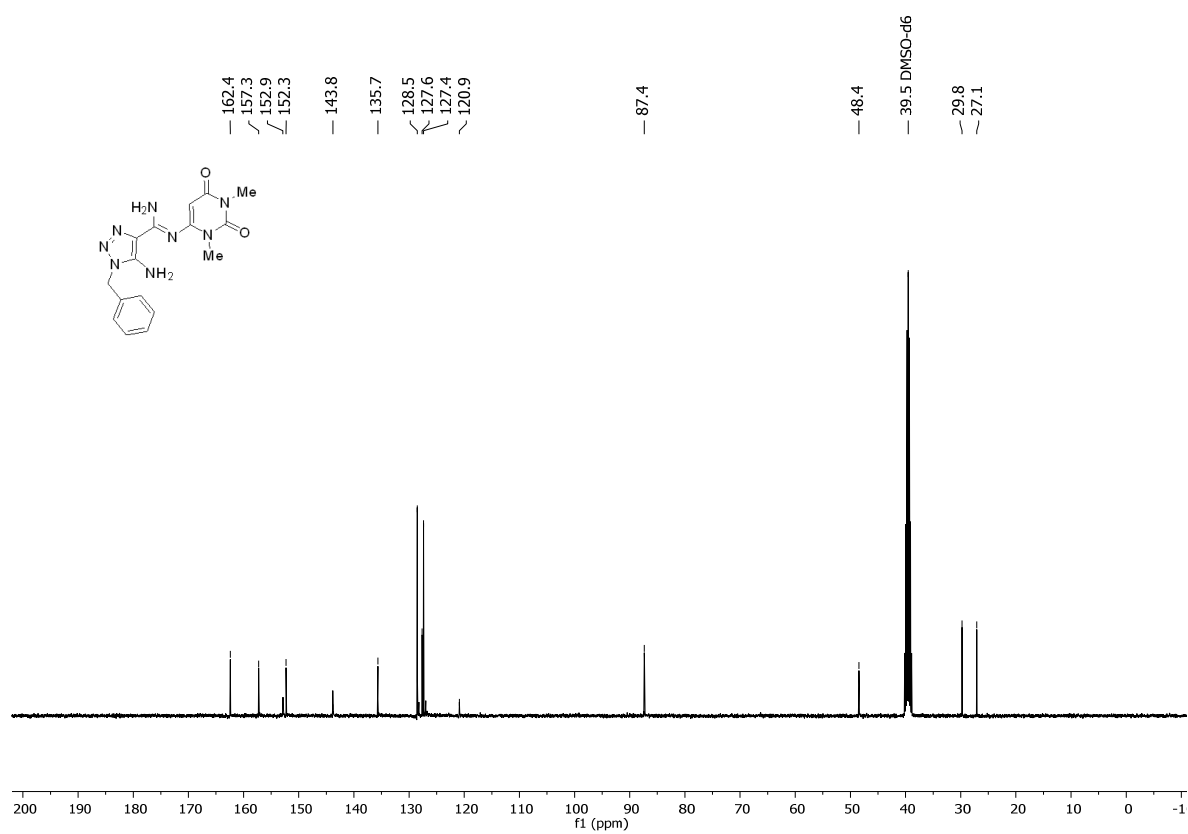


Fig. S3. ^1H NMR spectrum (DMSO- d_6) of **3b**

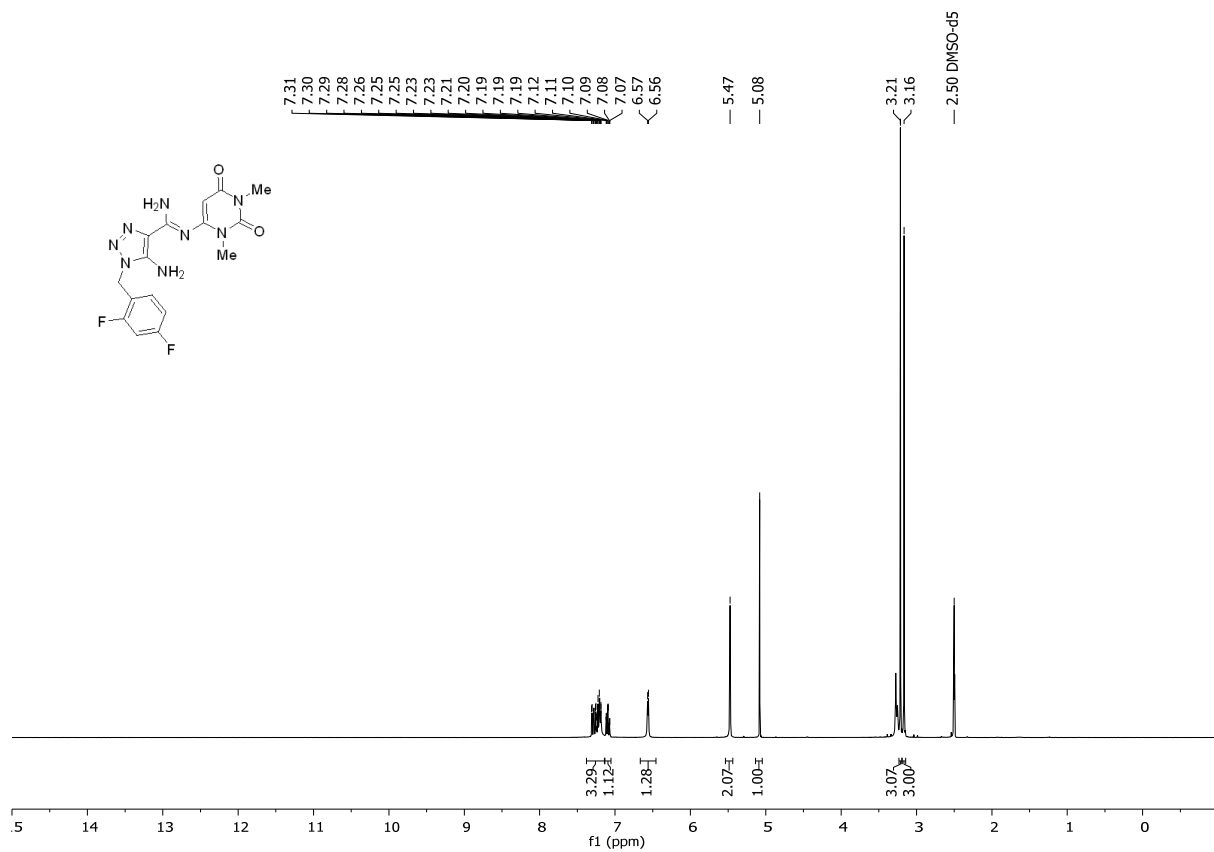


Fig. S4. ^{13}C NMR spectrum (DMSO- d_6) of **3b**

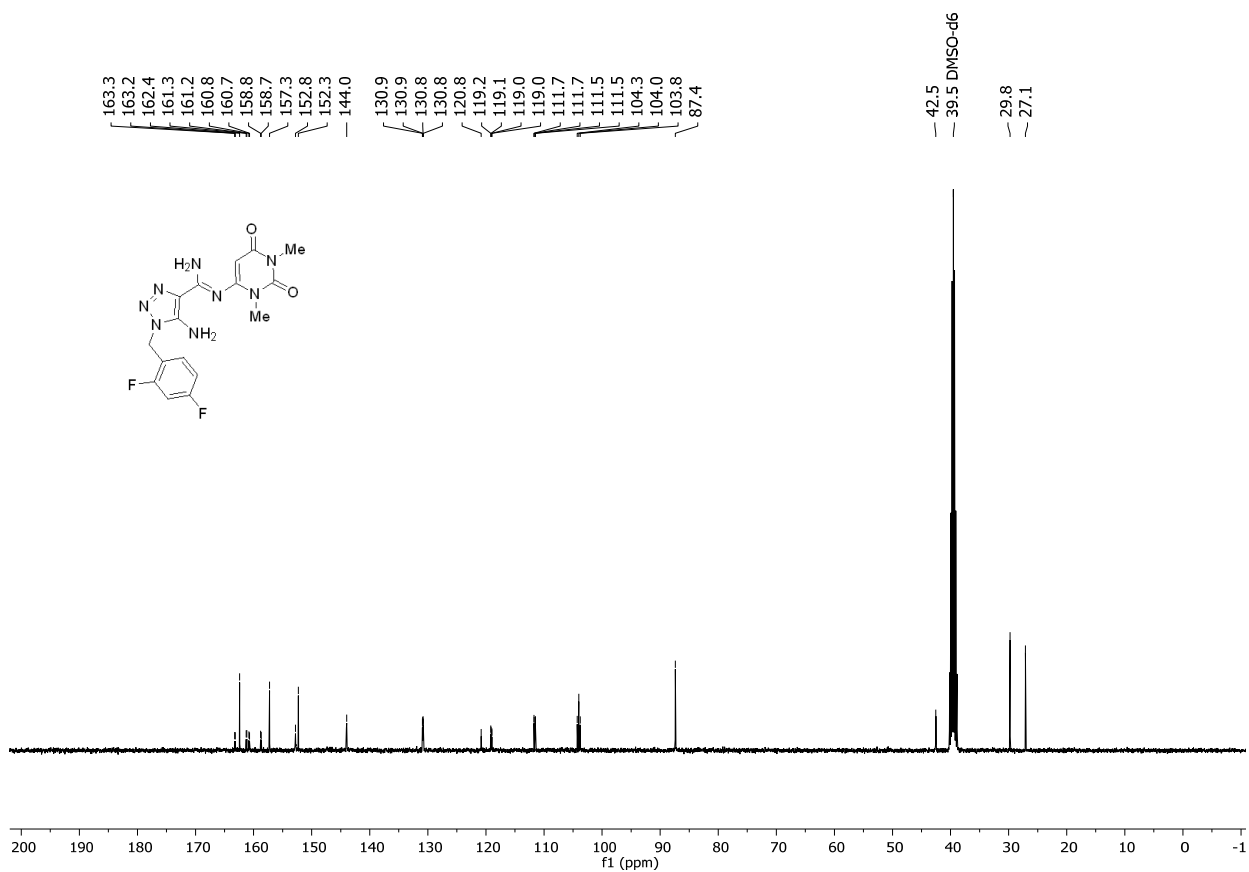


Fig. S5. ^{19}F NMR spectrum (DMSO- d_6) of **3b**

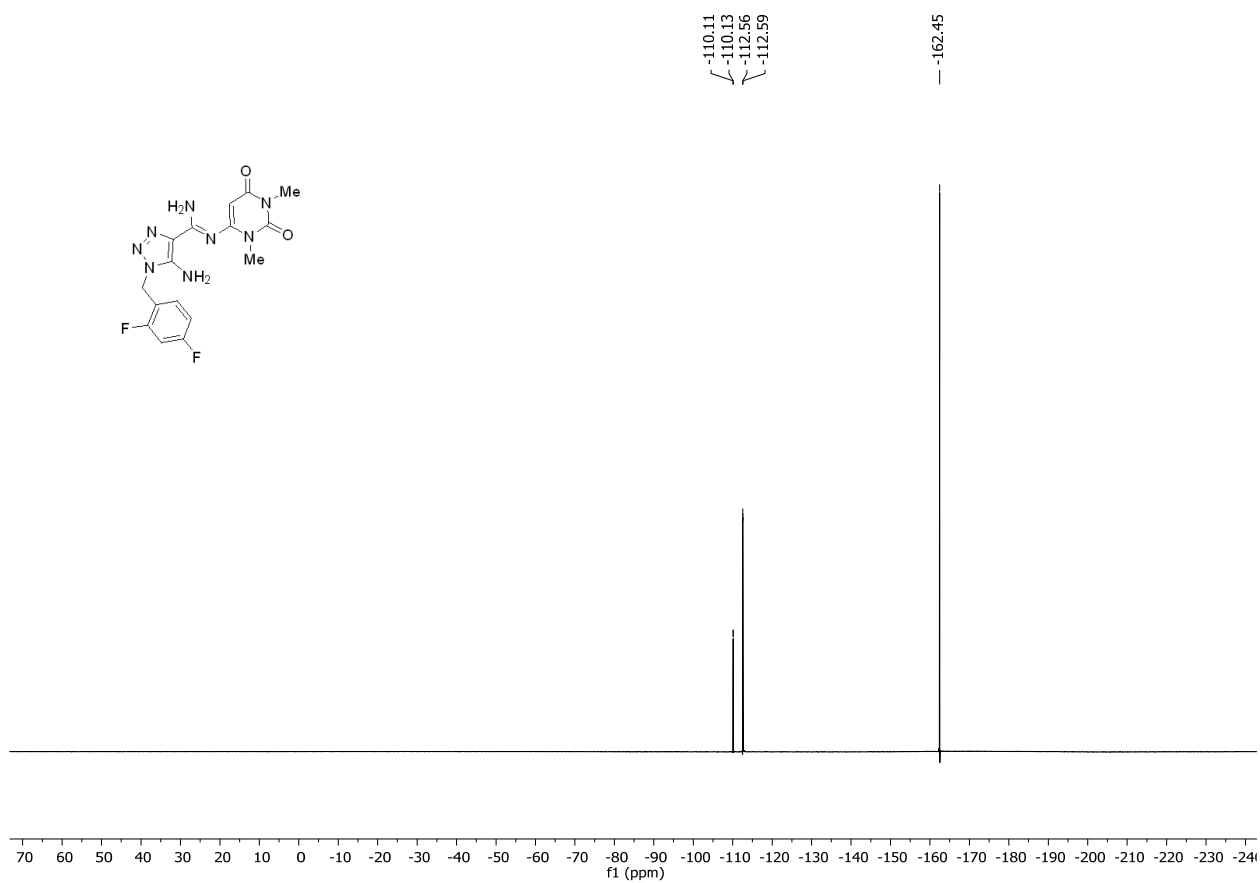


Fig. S6. ^1H NMR spectrum (DMSO- d_6) of **3c**

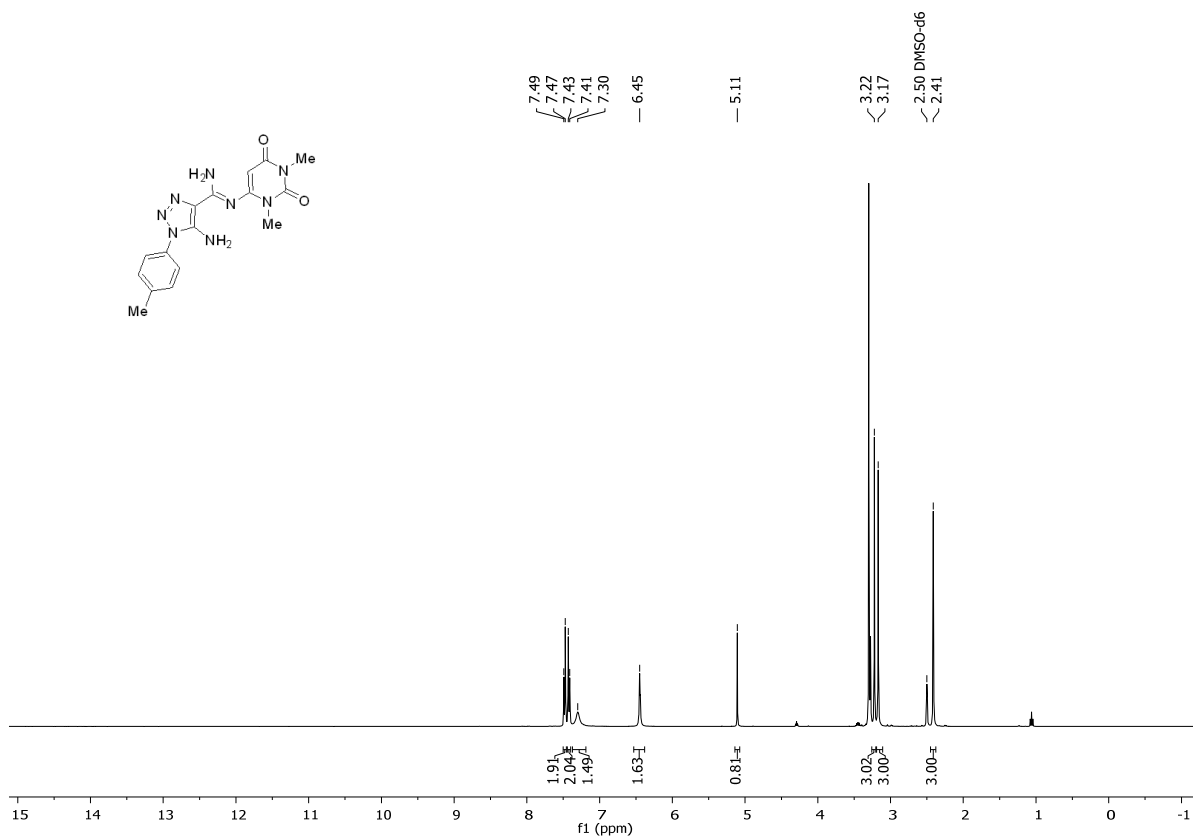


Fig. S7. ^{13}C NMR spectrum (DMSO- d_6) of **3c**

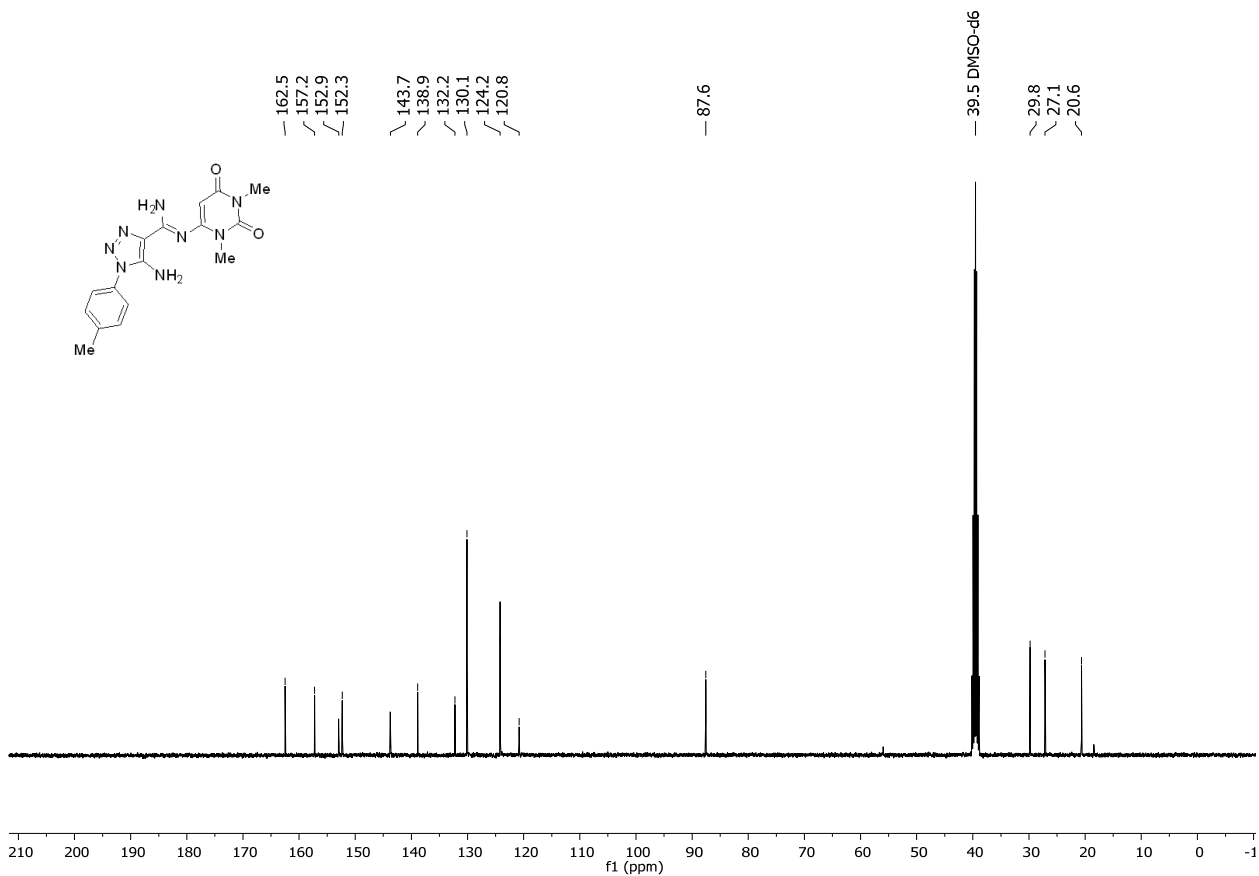


Fig. S8. ^1H NMR spectrum (DMSO- d_6) of **3d**

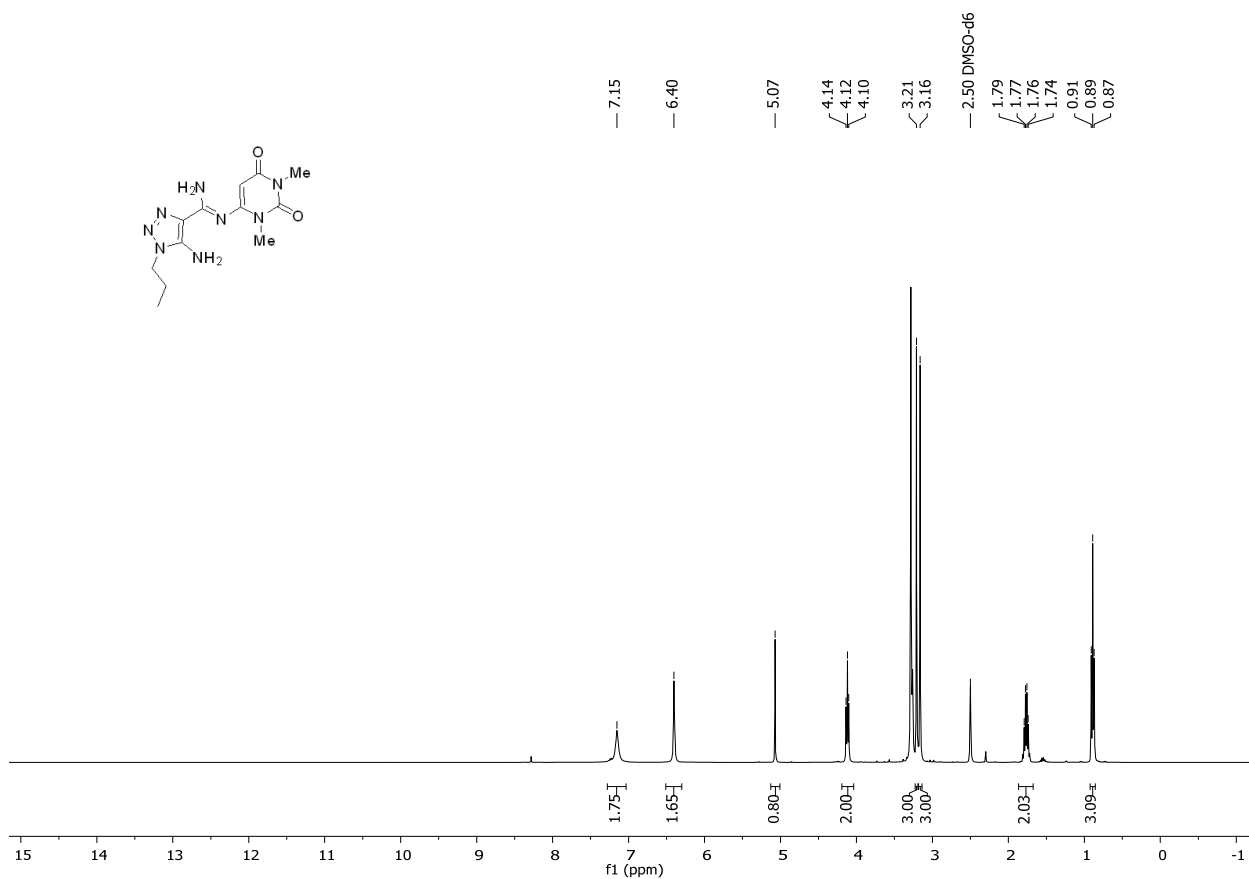


Fig. S9. ^{13}C NMR spectrum (DMSO- d_6) of **3d**

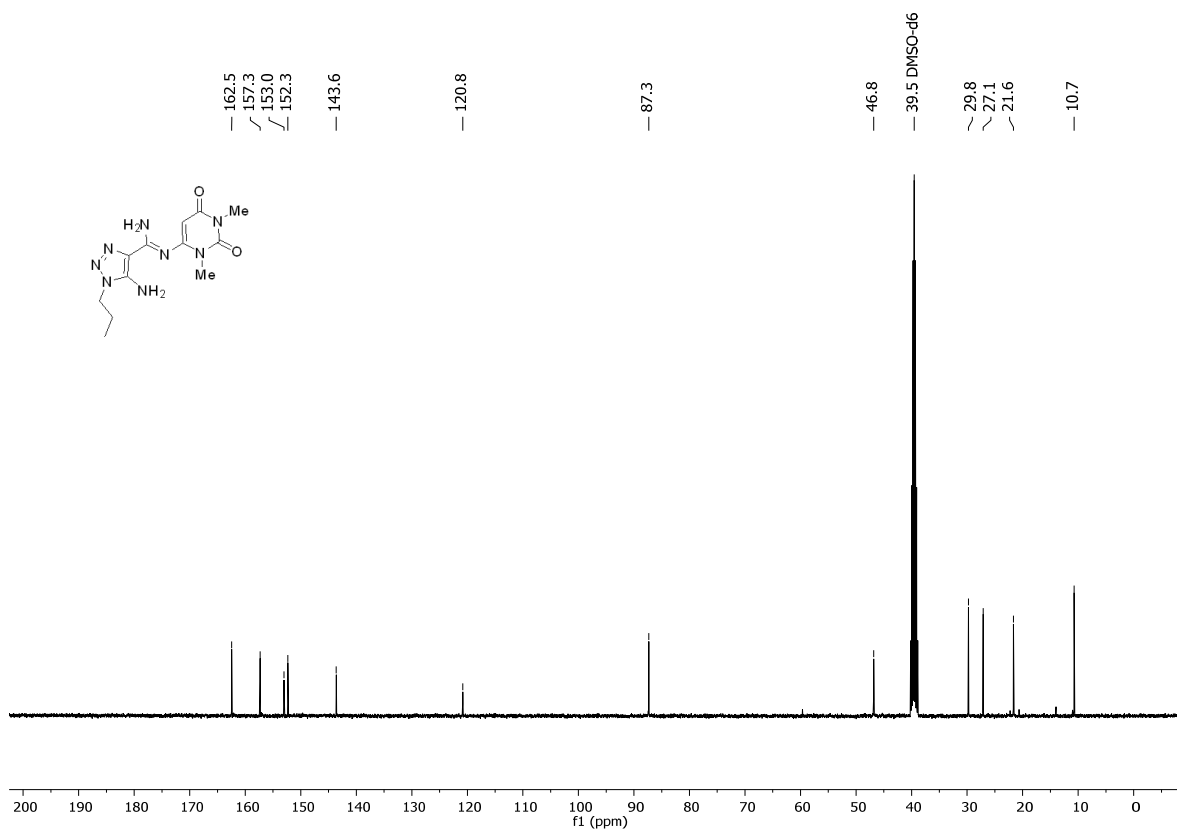


Fig. S10. ^1H NMR spectrum (DMSO- d_6) of **3e**

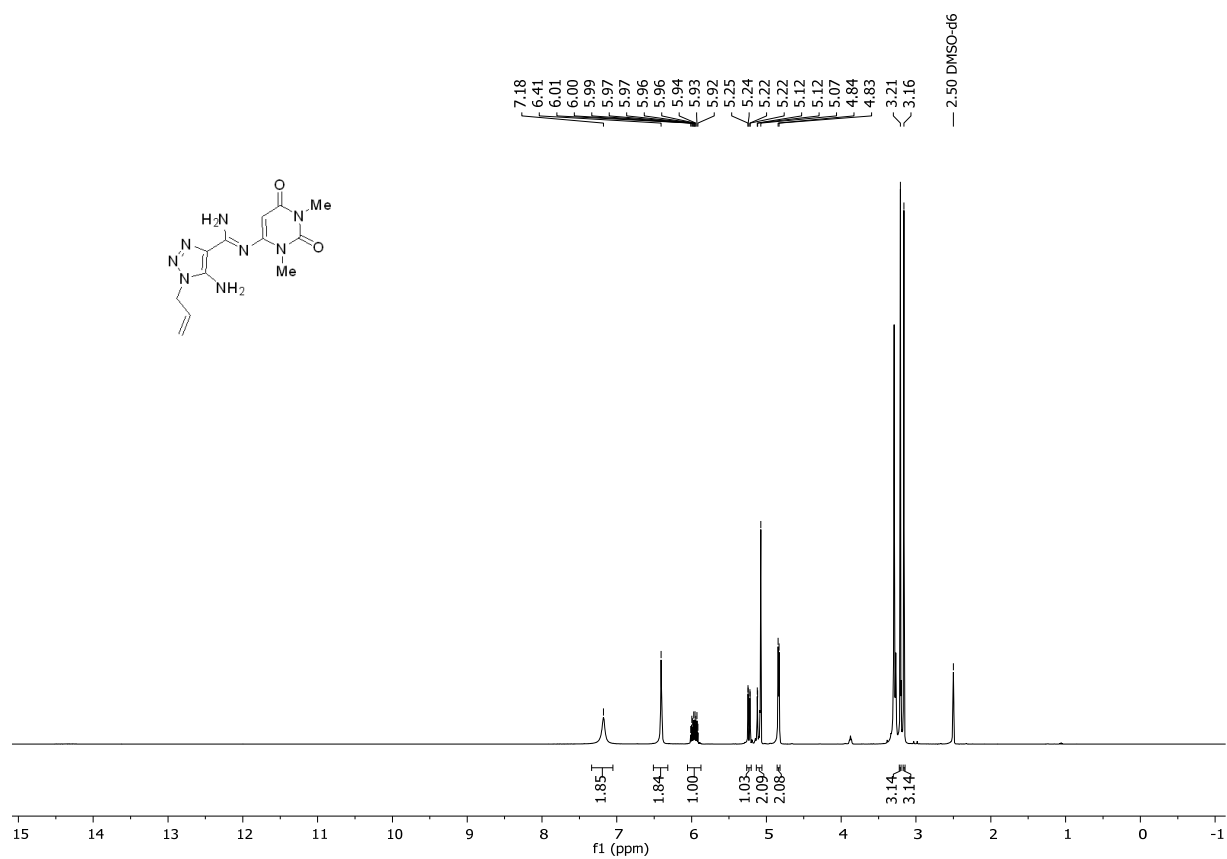


Fig. S11. ^{13}C NMR spectrum (DMSO- d_6) of **3e**

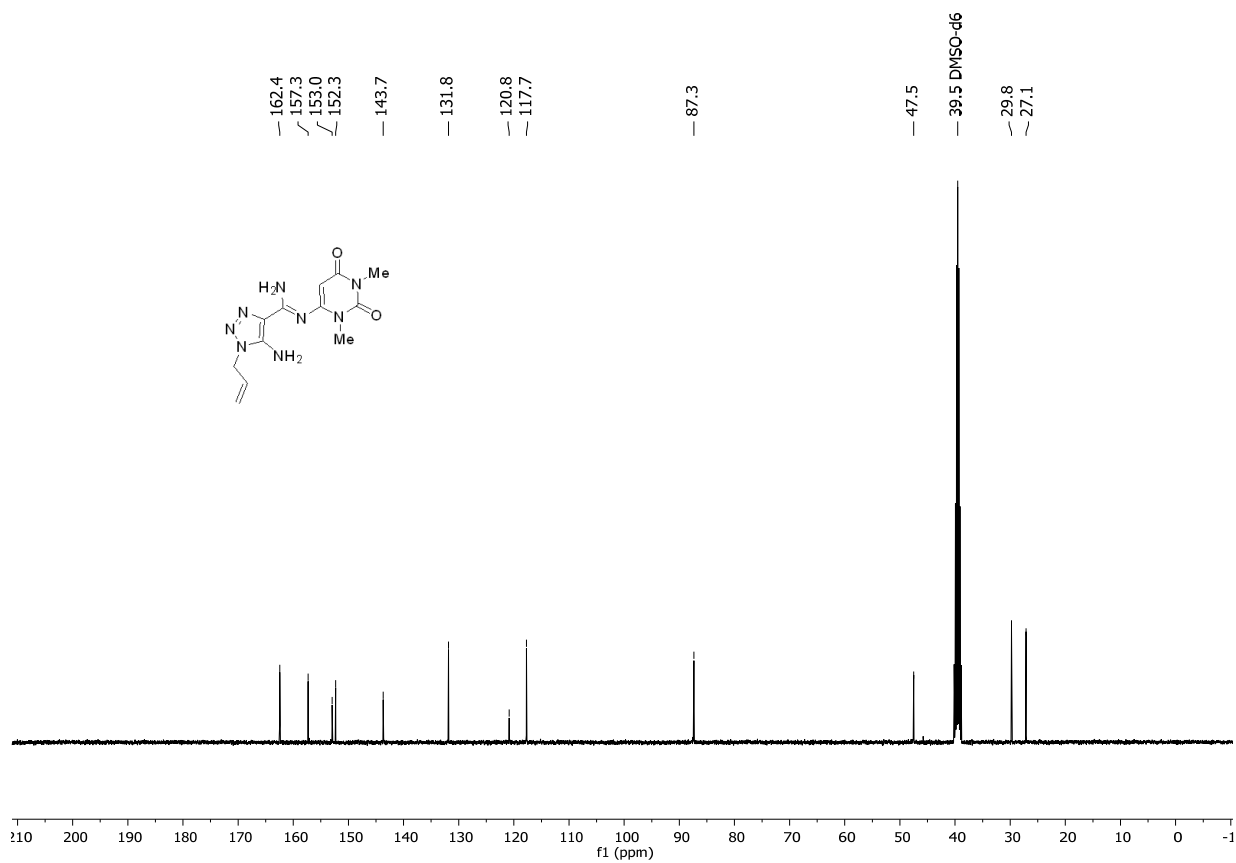


Fig. S12. ^1H NMR spectrum (DMSO- d_6) of 3f

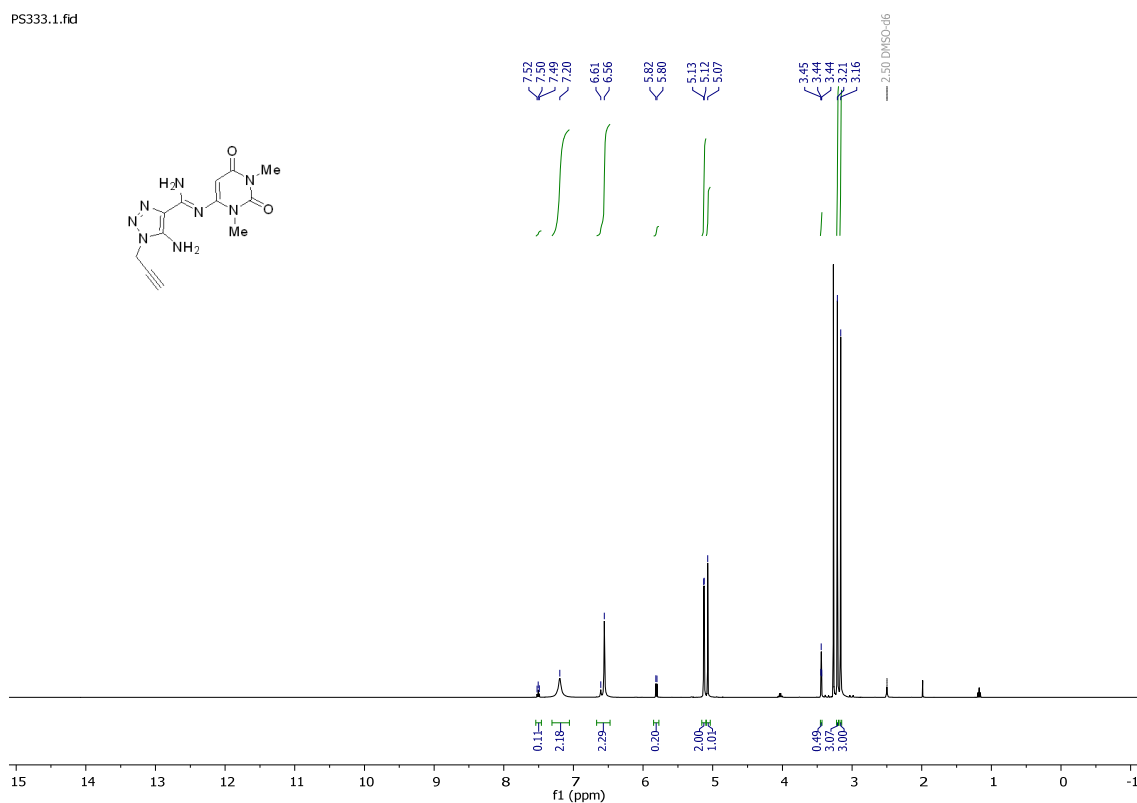


Fig. S13. ^{13}C NMR spectrum (DMSO- d_6) of 3f

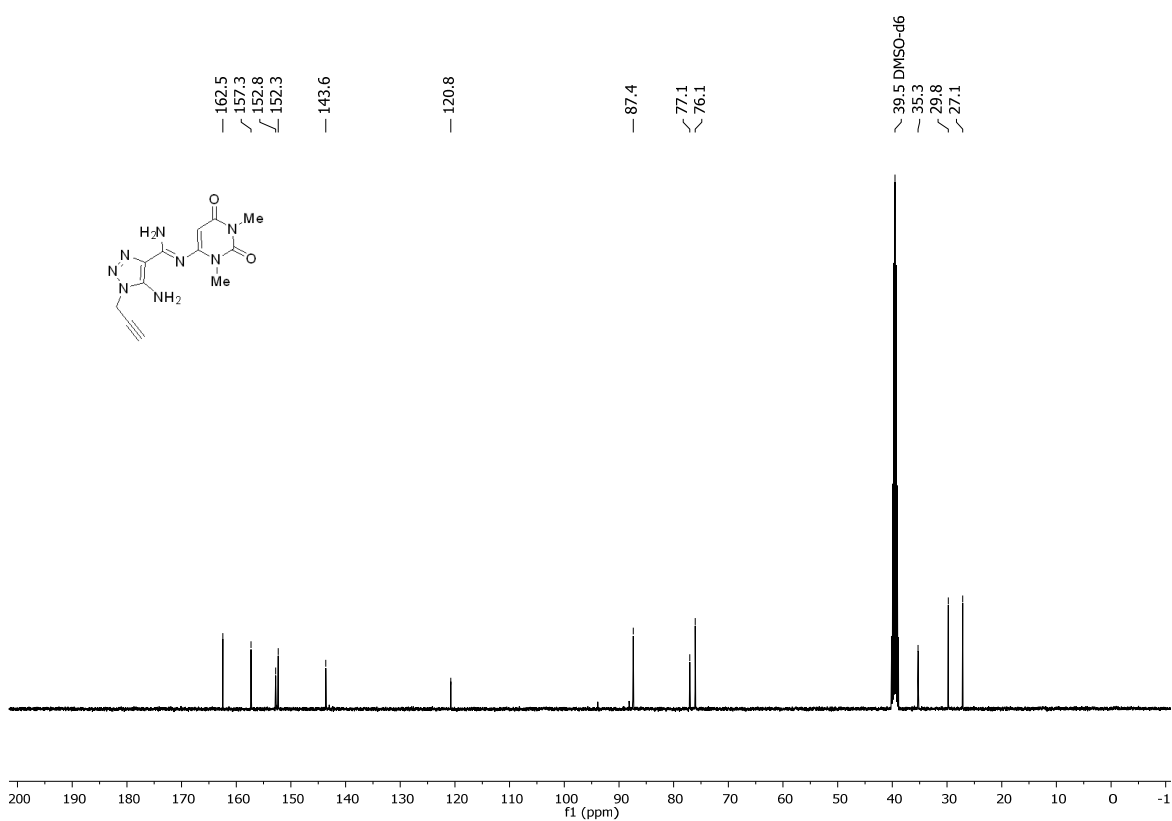


Fig. S14. ^1H NMR spectrum (DMSO- d_6) of **3g**

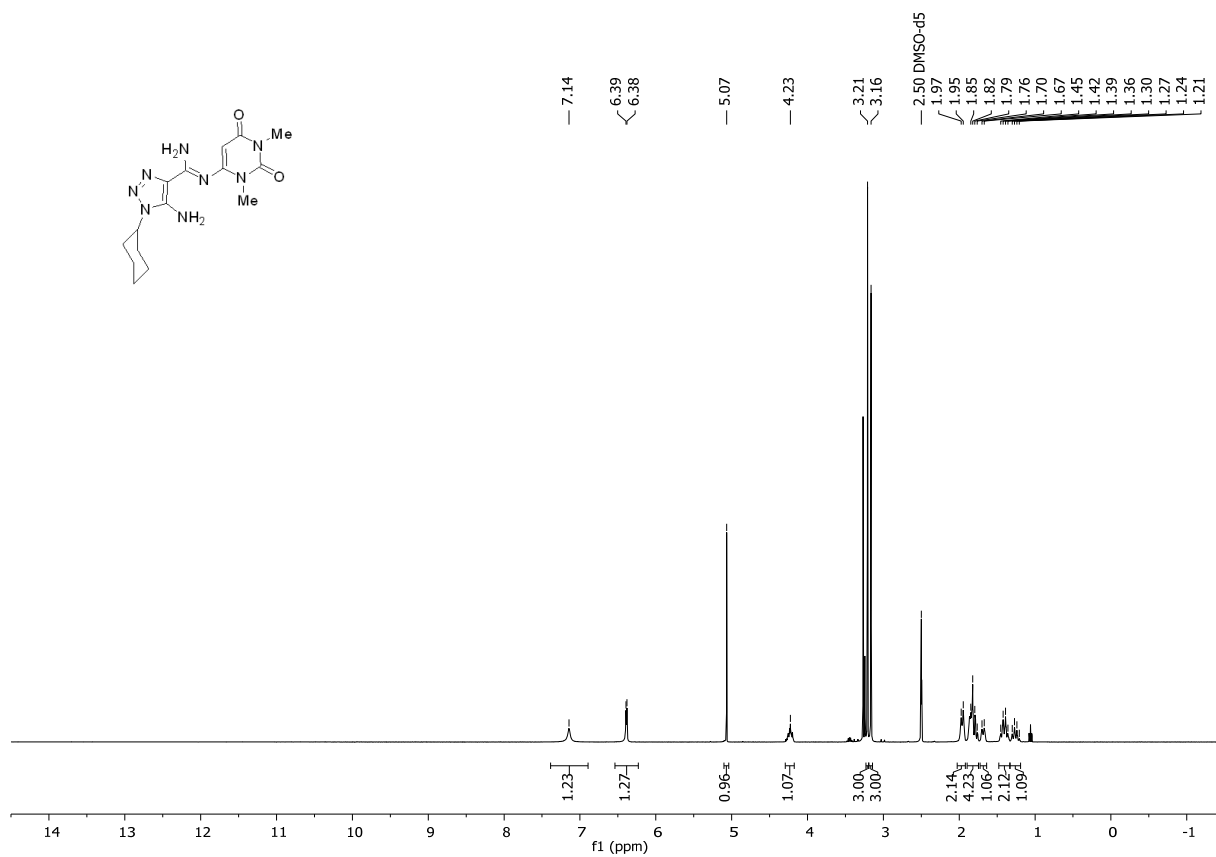


Fig. S15. ^{13}C NMR spectrum (DMSO- d_6) of **3g**

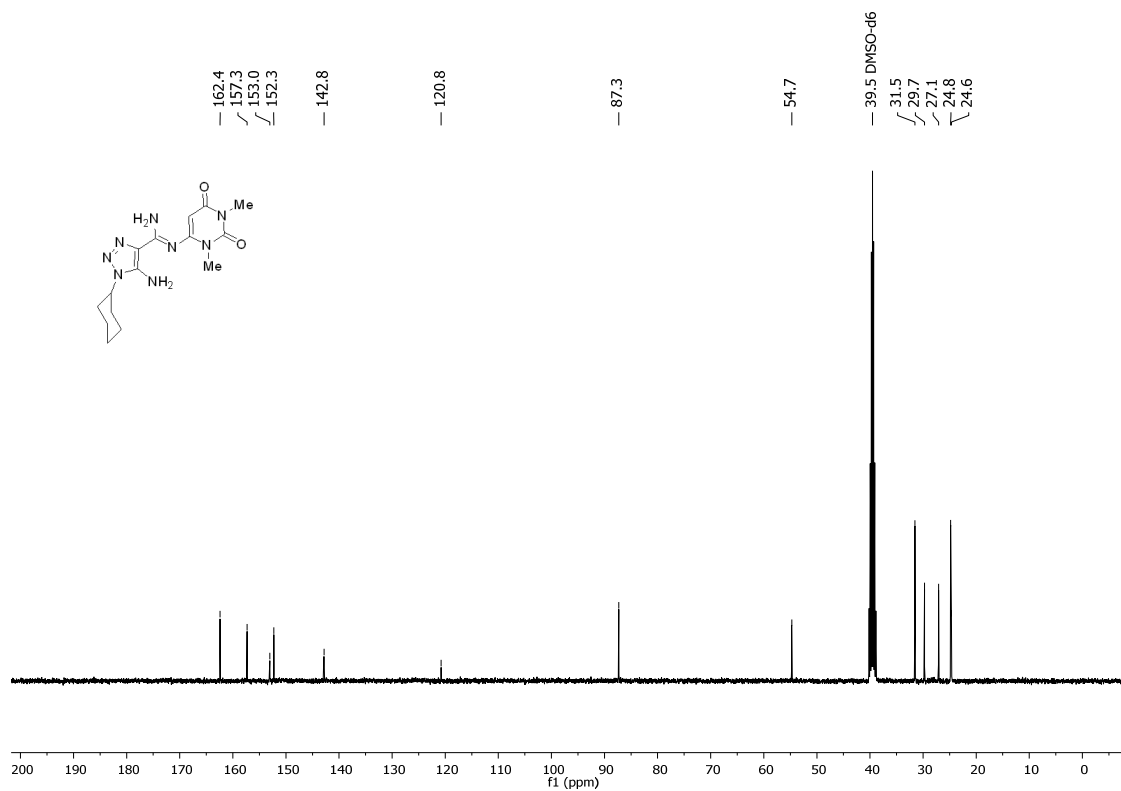


Fig. S16. ^1H NMR spectrum (DMSO- d_6) of **3h**

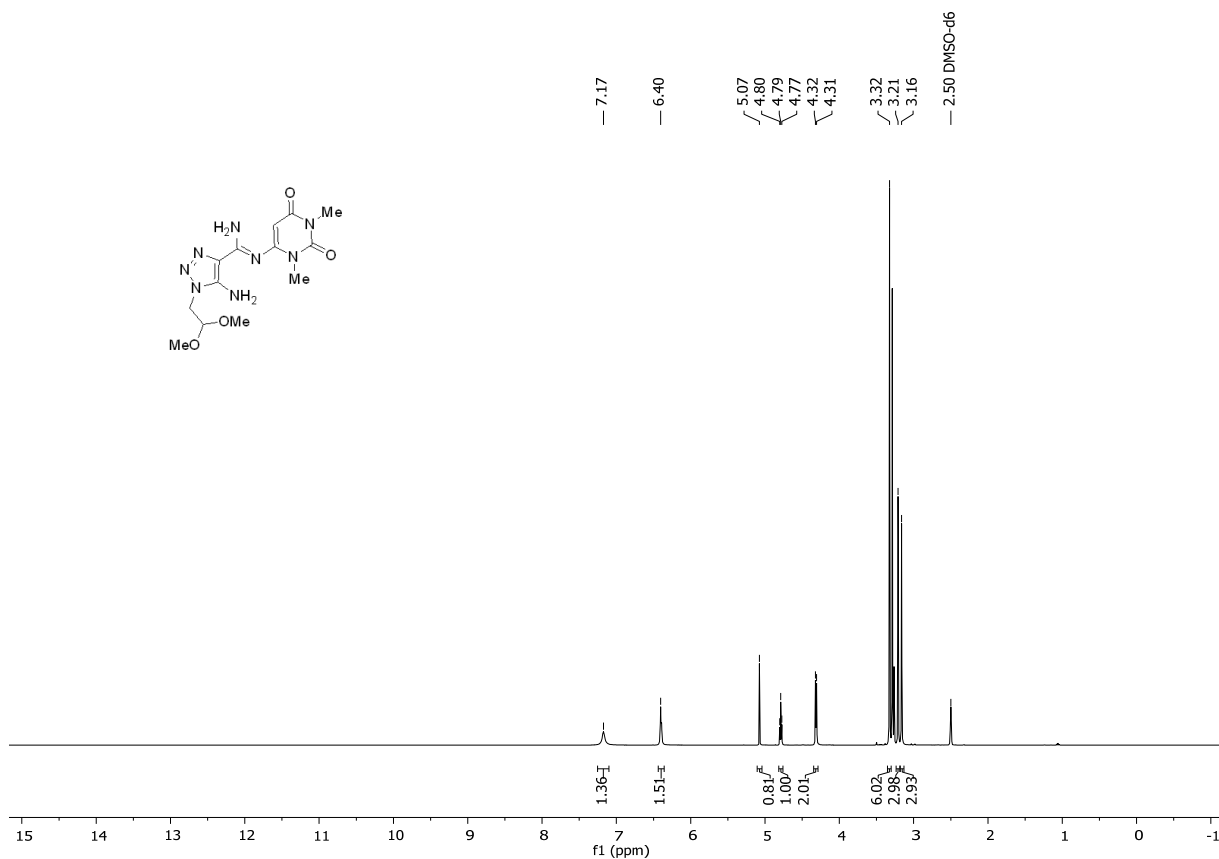


Fig. S17. ^{13}C NMR spectrum (DMSO- d_6) of **3h**

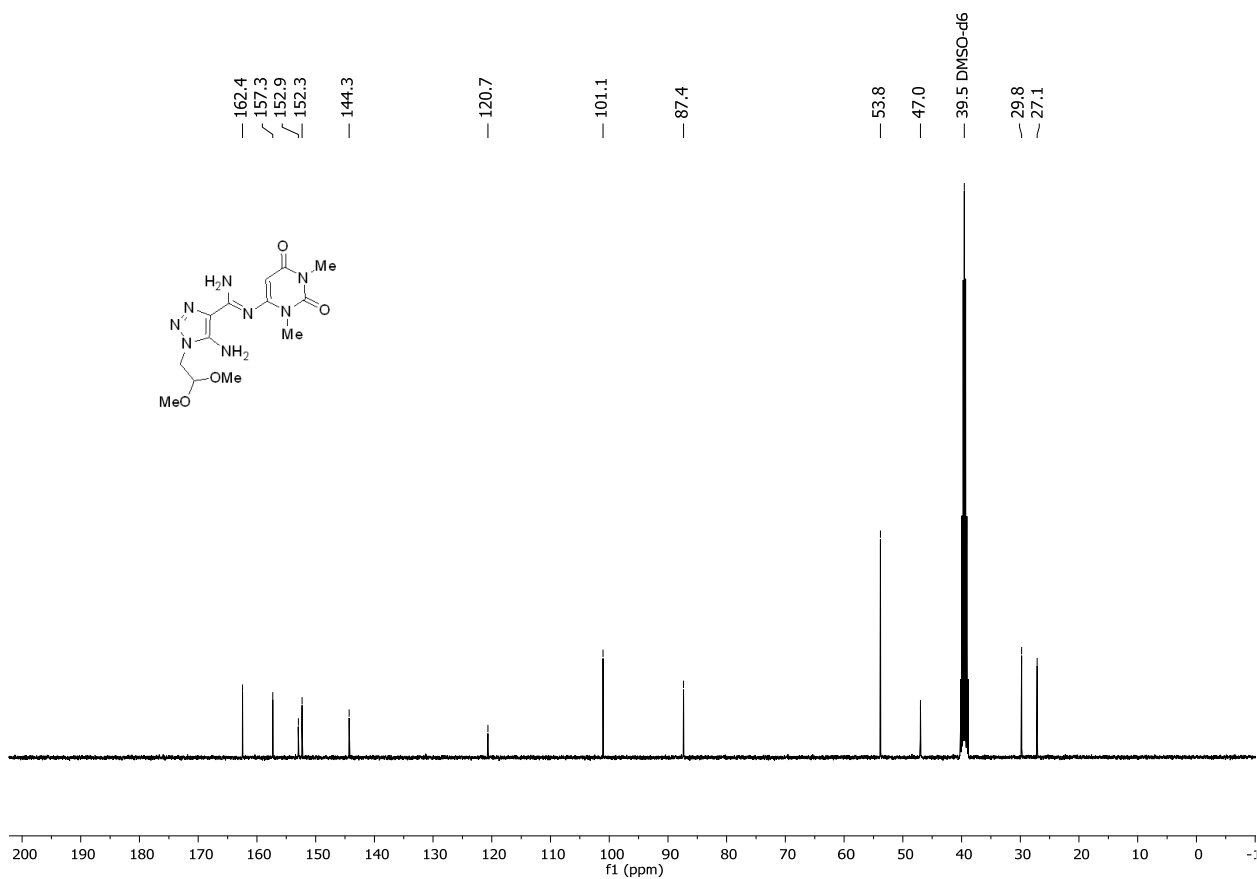


Fig. S18. ^1H NMR spectrum (DMSO- d_6) of 3i

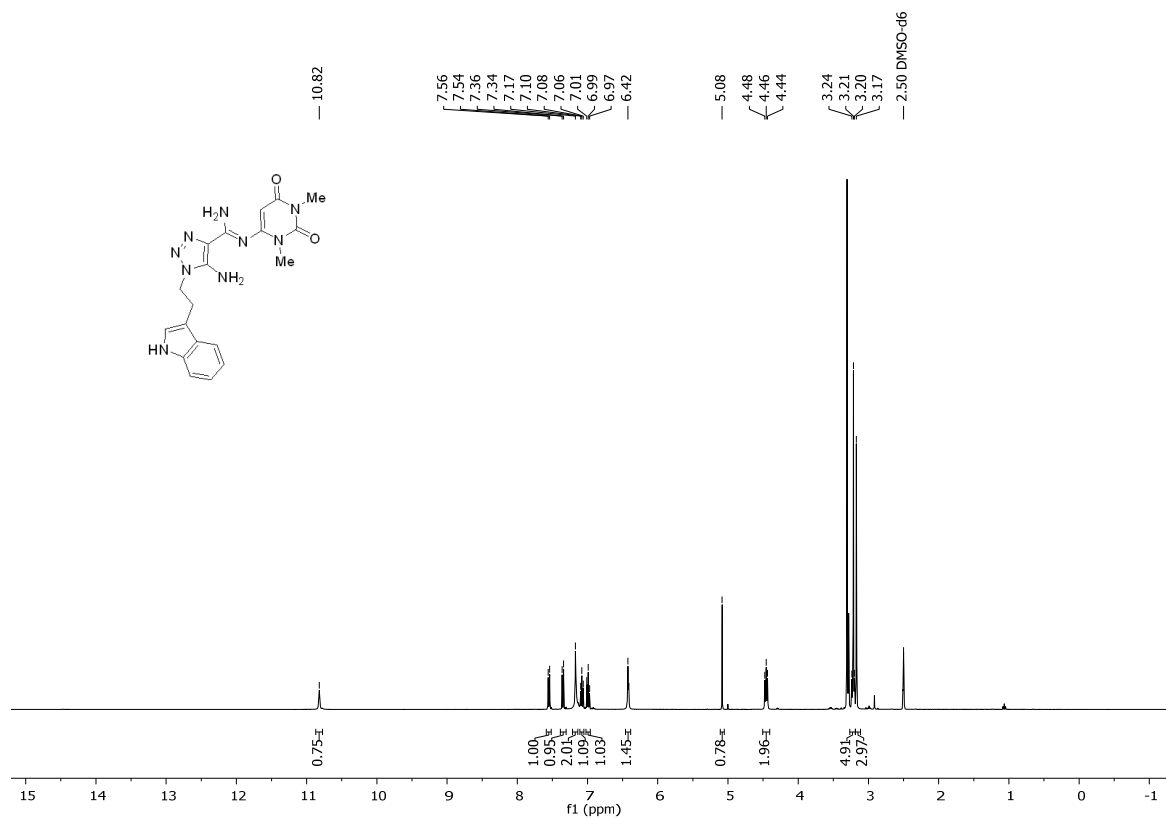


Fig. S19. ^{13}C NMR spectrum (DMSO- d_6) of 3i

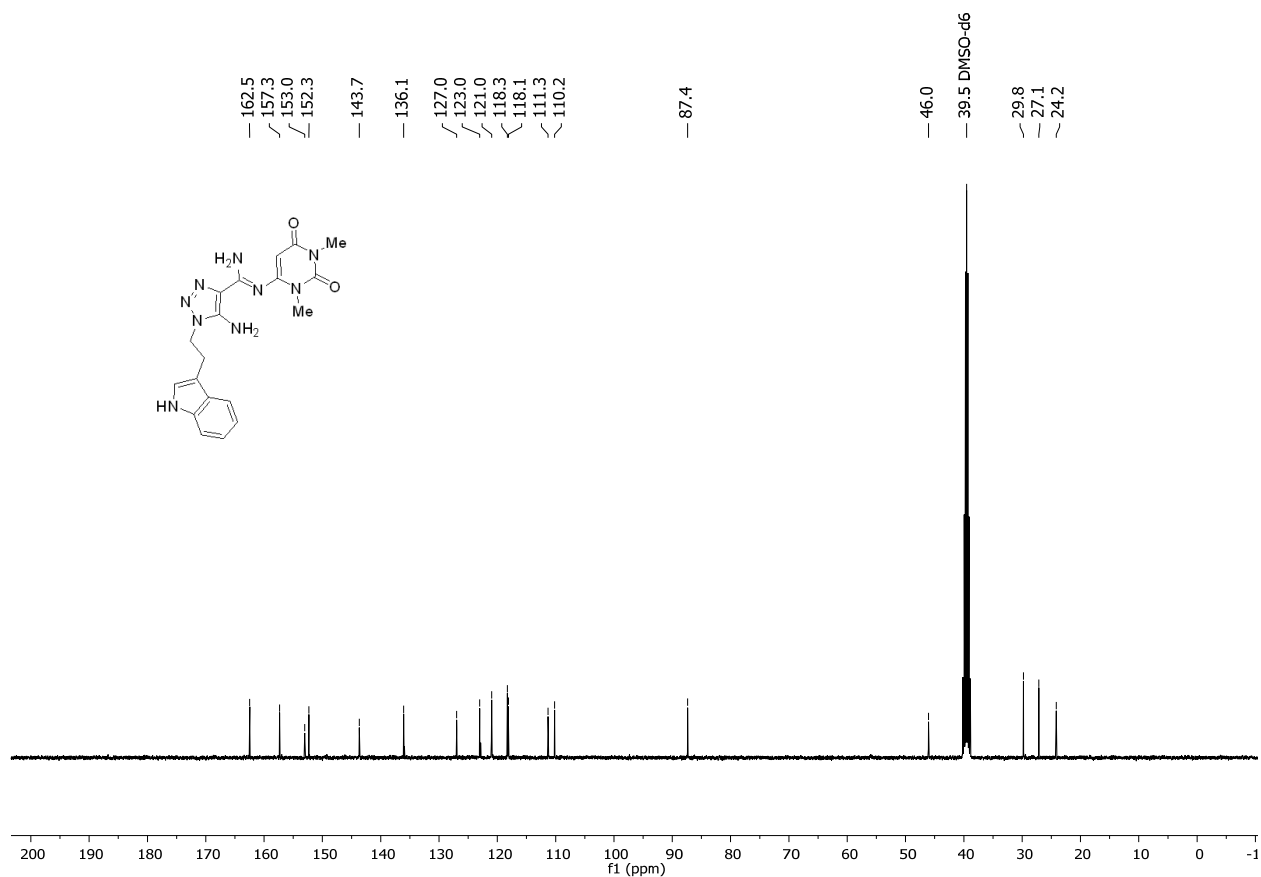


Fig. 19A. HMBC spectrum (DMSO-d₆) of **3r**

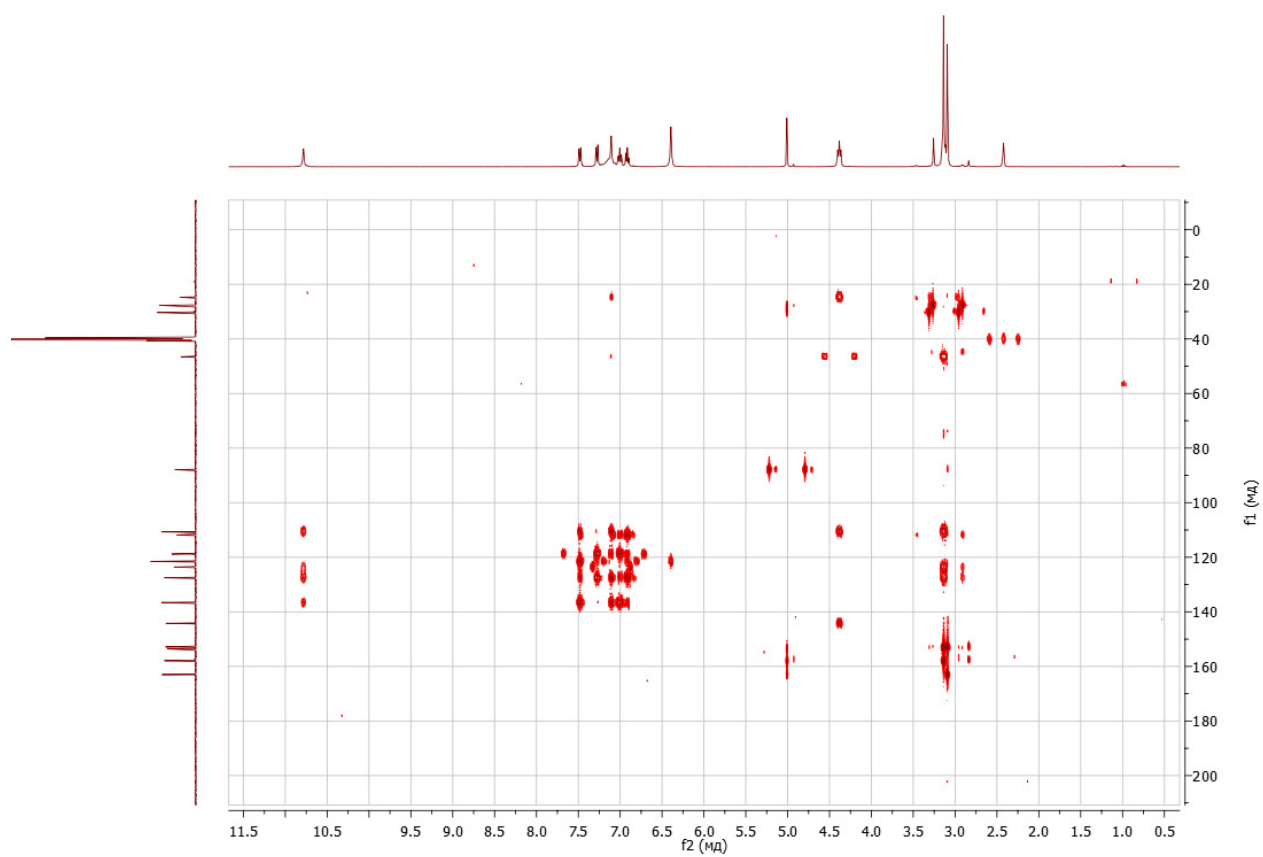


Fig. S20. ^1H NMR spectrum (DMSO- d_6) of **3j**

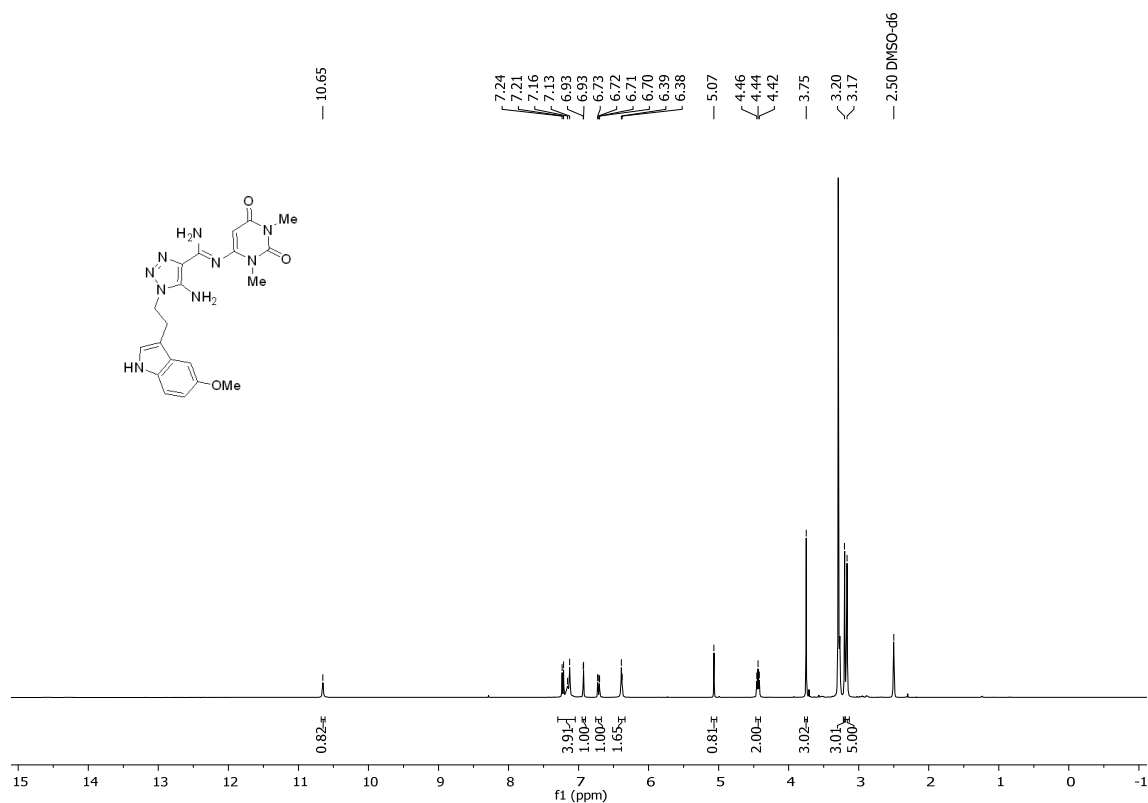


Fig. S21. ^{13}C NMR spectrum (DMSO- d_6) of **3j**

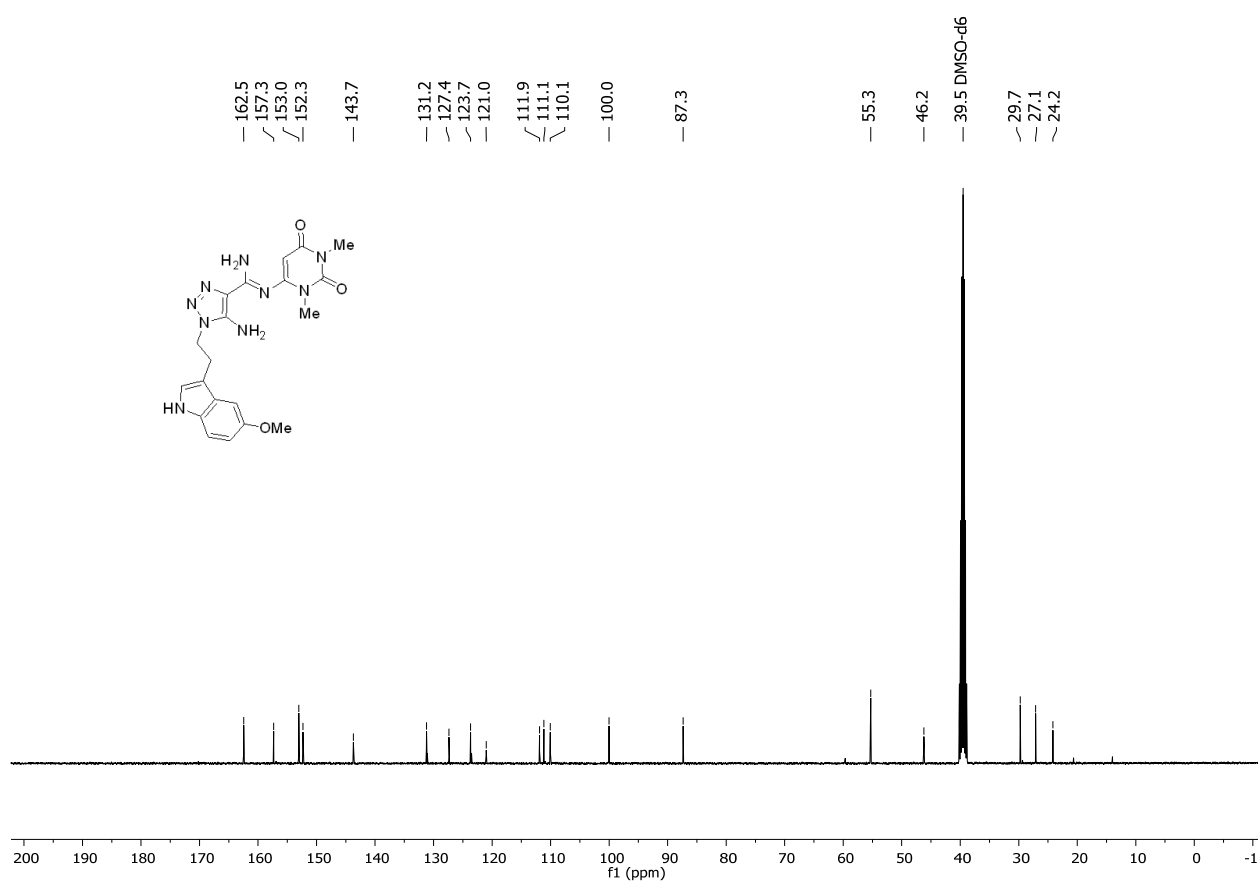


Fig. S22. ^1H NMR spectrum (DMSO- d_6) of 3k

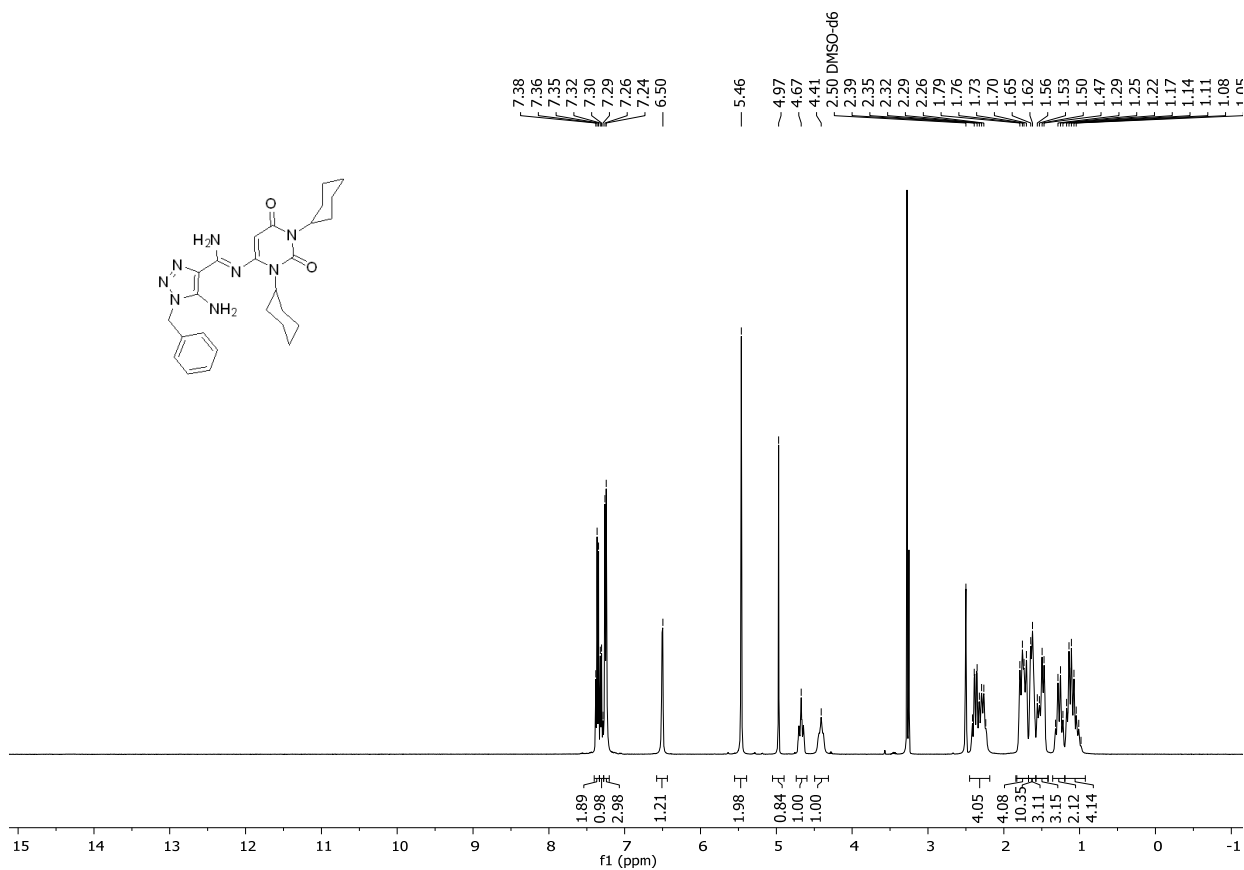


Fig. S23. ^{13}C NMR spectrum (DMSO- d_6) of 3k

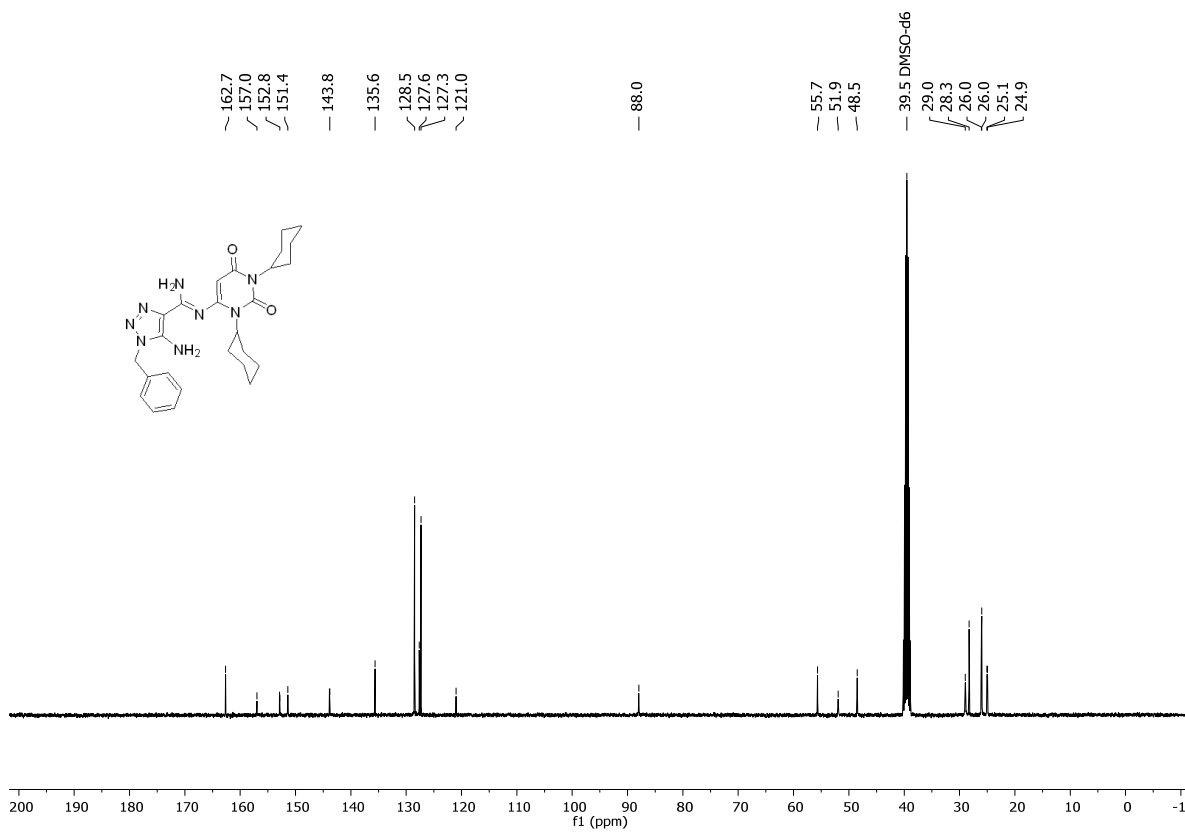


Fig. 23A. HMBC spectrum (DMSO-d₆) of **3k**

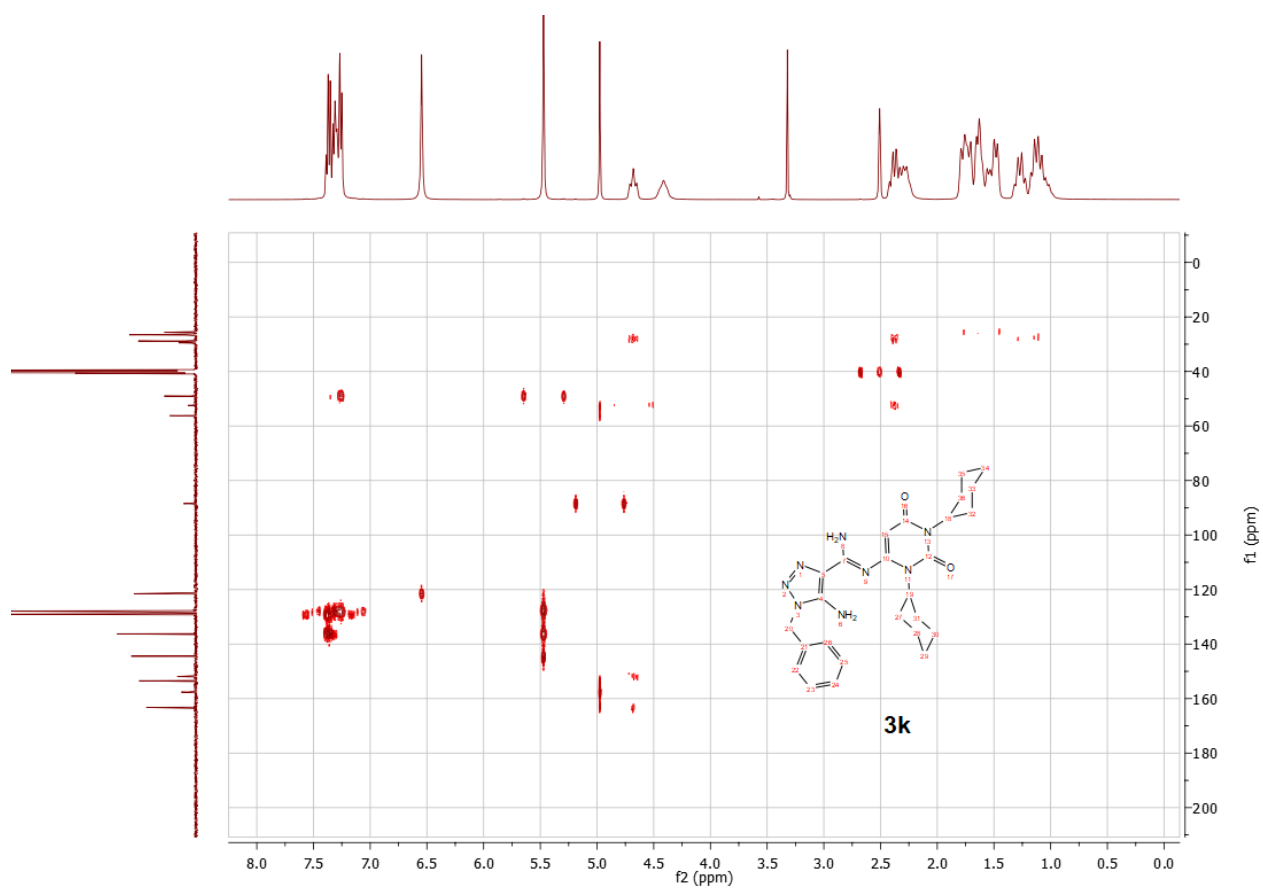


Fig. S24. ^1H NMR spectrum (DMSO- d_6) of 31

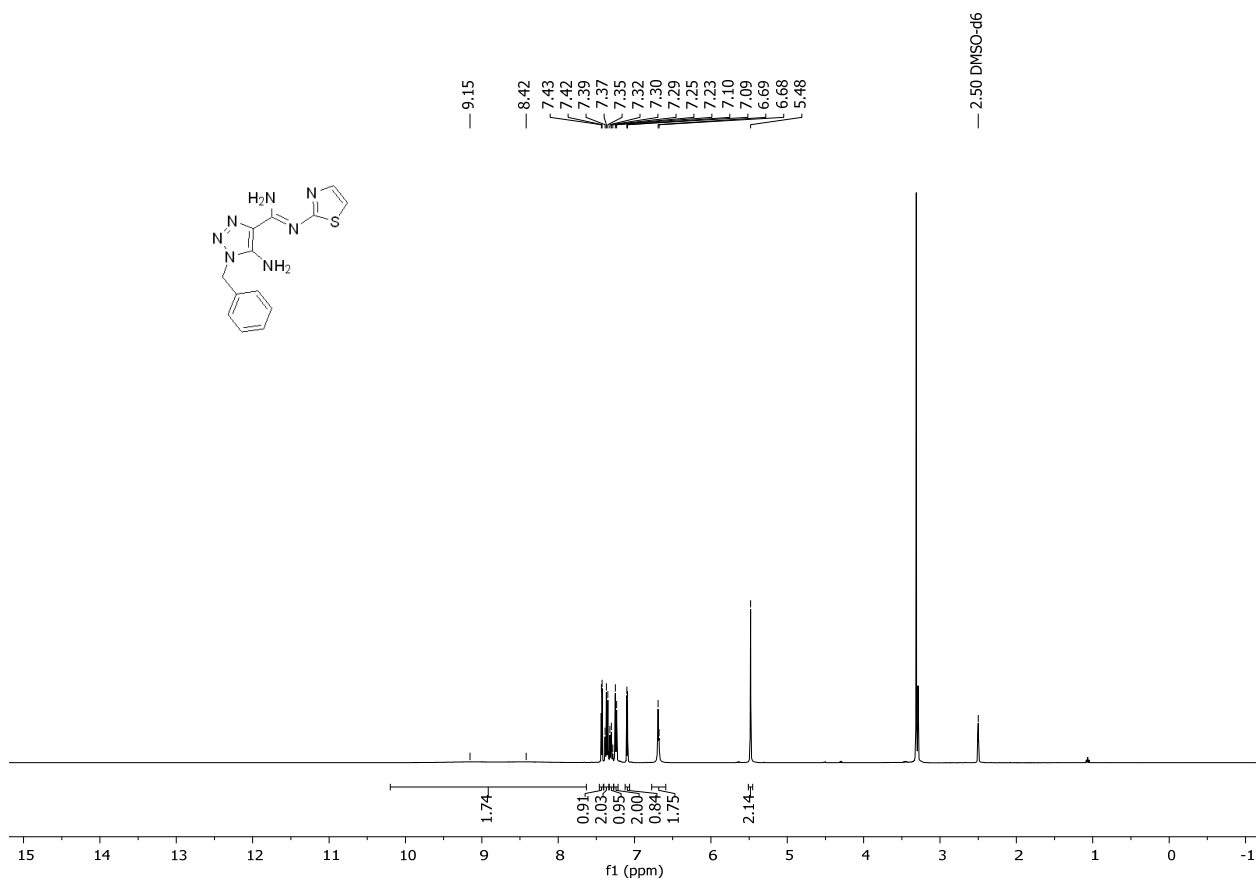


Fig. S25. ^{13}C NMR spectrum (DMSO- d_6) of 31

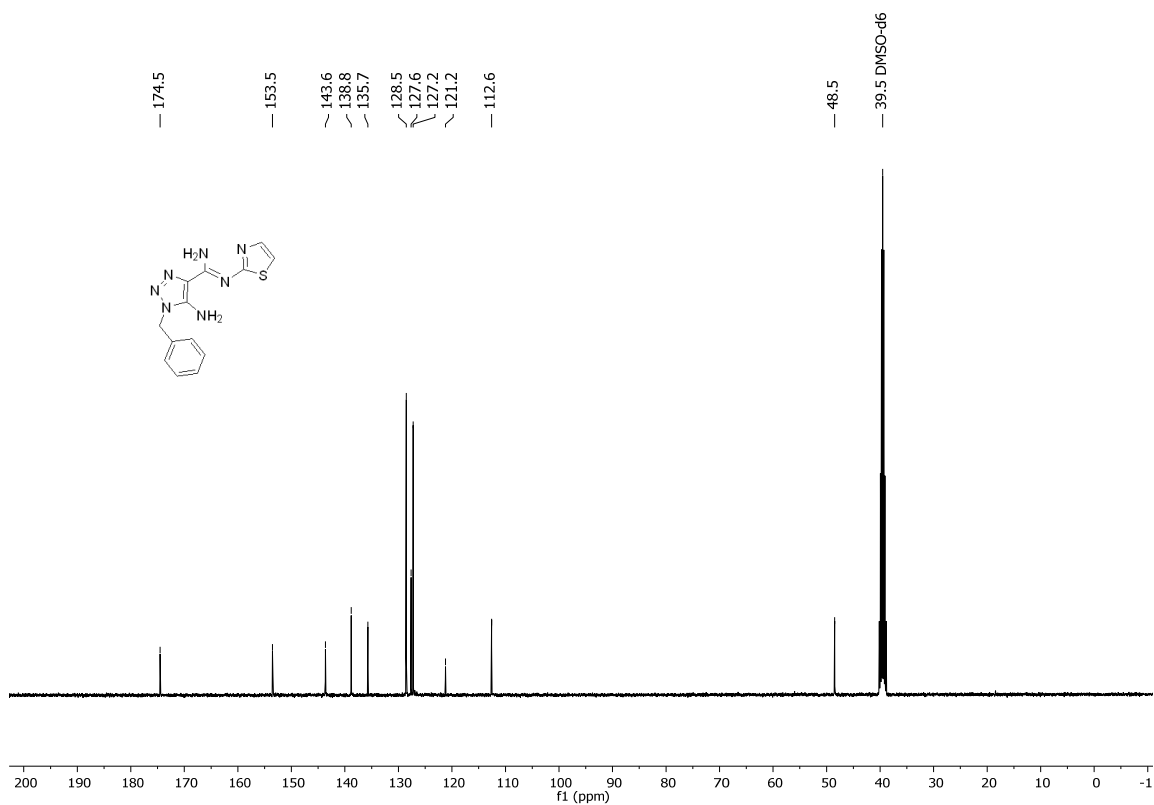


Fig. S26. ¹H NMR spectrum (DMSO-*d*₆) of **3m**

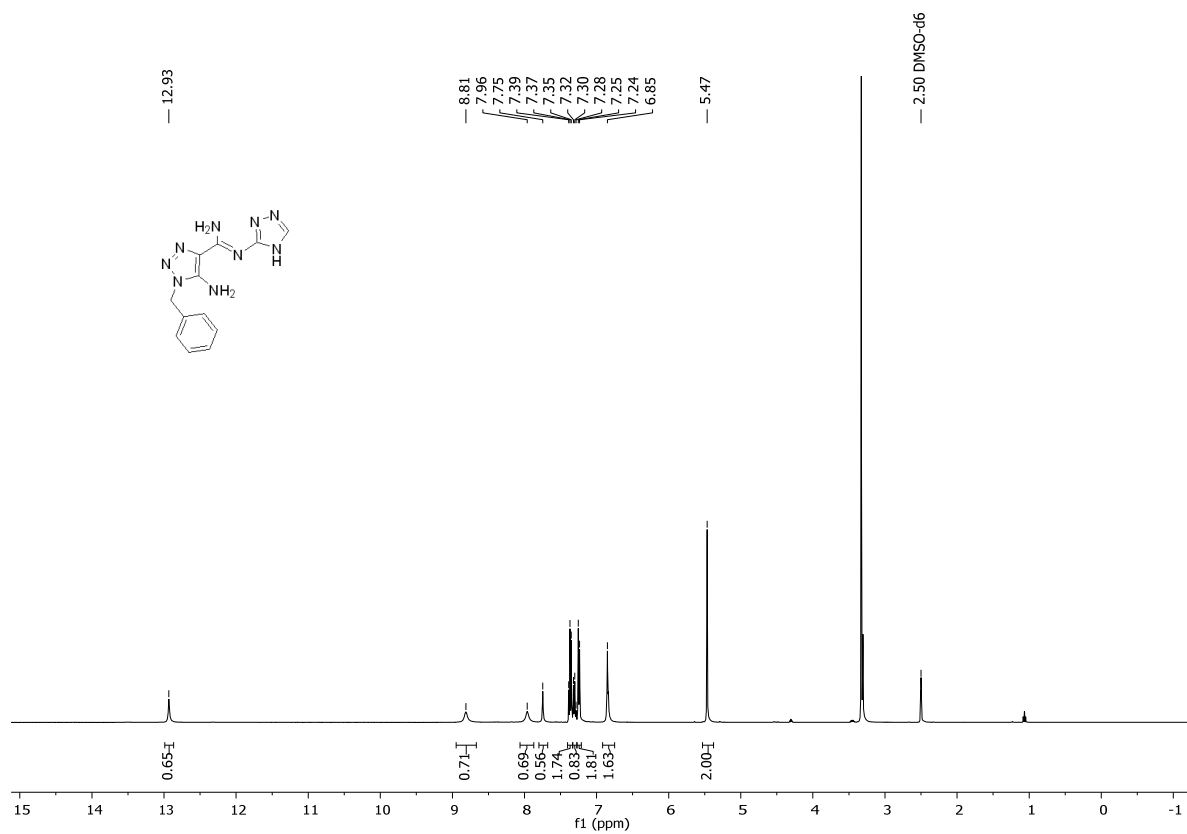


Fig. S27. ¹³C NMR spectrum (DMSO-*d*₆) of **3m**

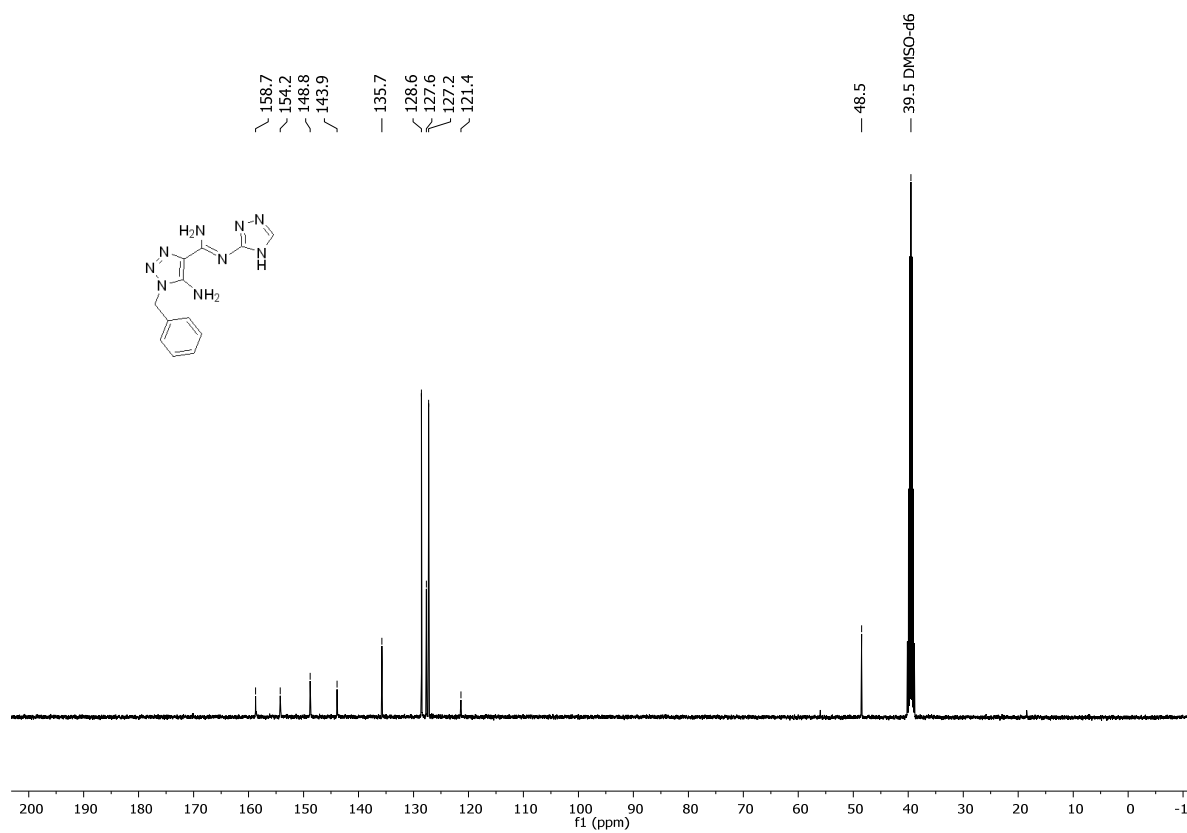


Fig. S28. ^1H NMR spectrum (DMSO- d_6) of **3n**

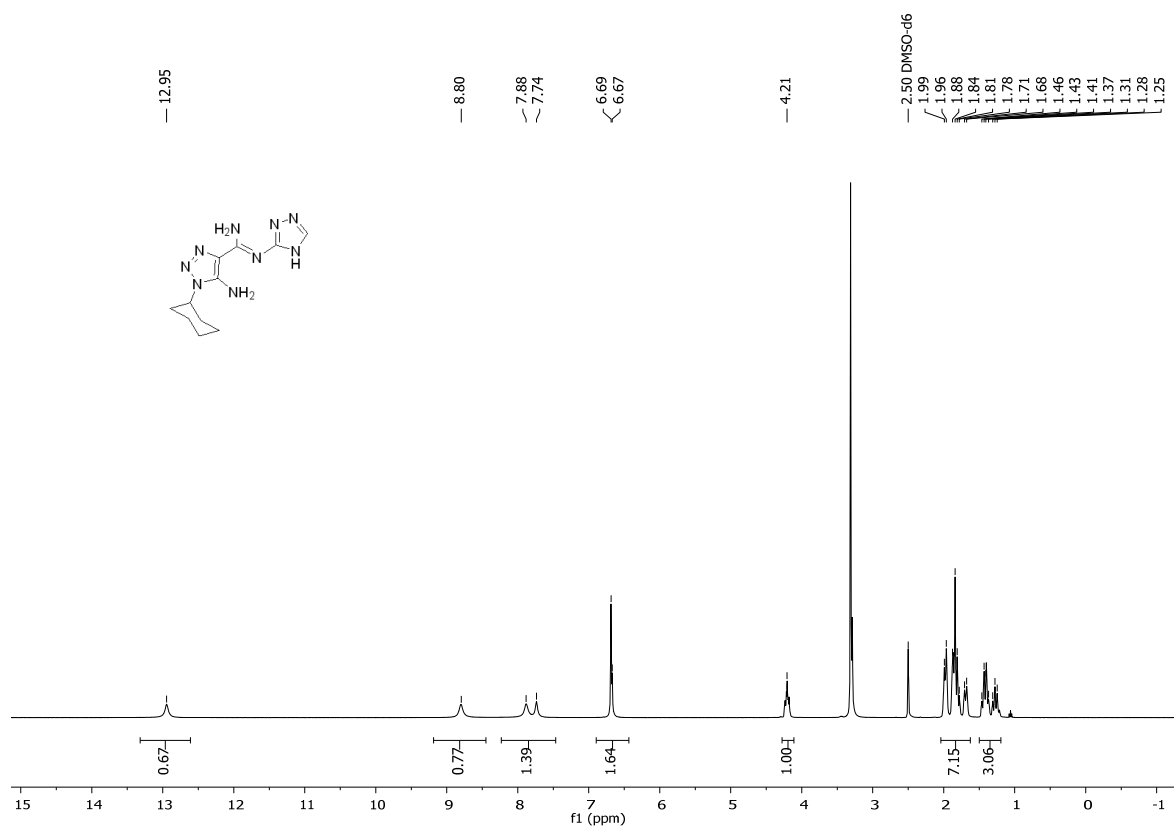


Fig. S29. ^{13}C NMR spectrum (DMSO- d_6) of **3n**

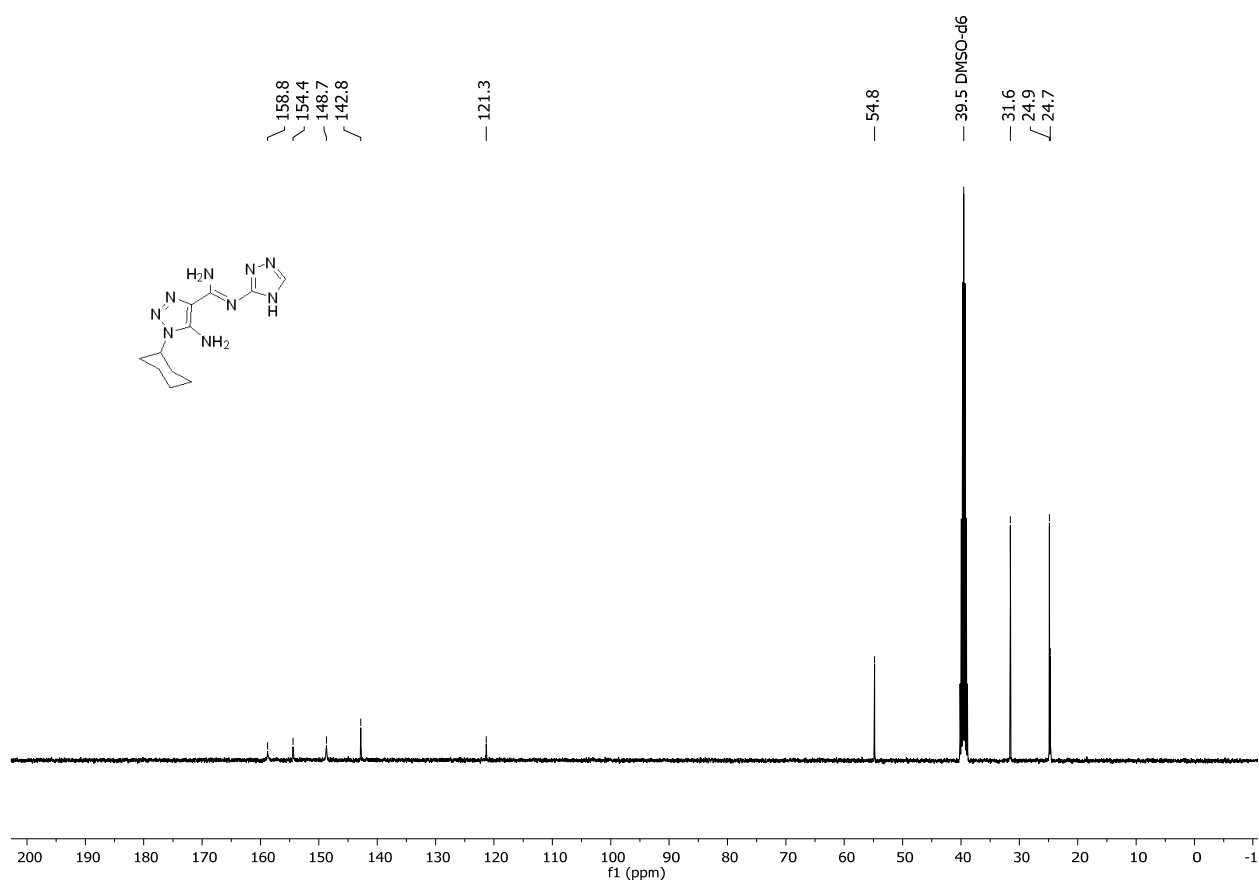


Fig. S30. ¹H NMR spectrum (DMSO-*d*₆) of **30**

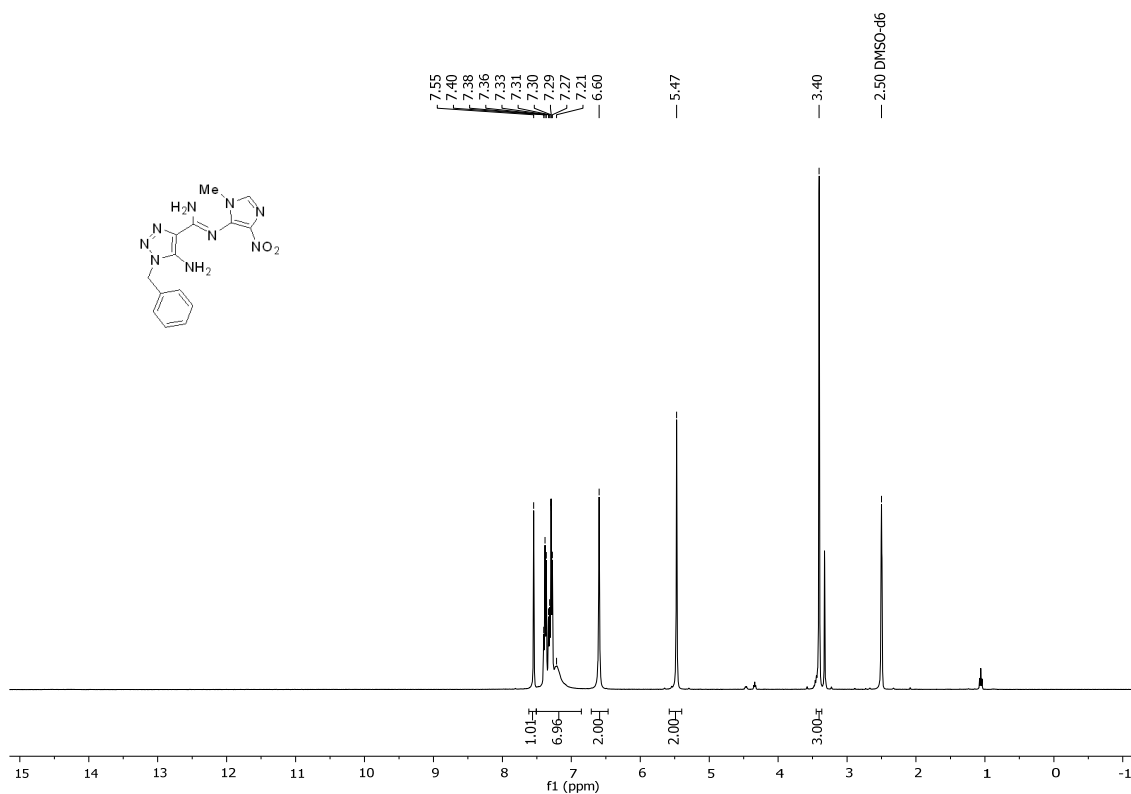


Fig. S31. ¹³C NMR spectrum (DMSO-*d*₆) of **30**

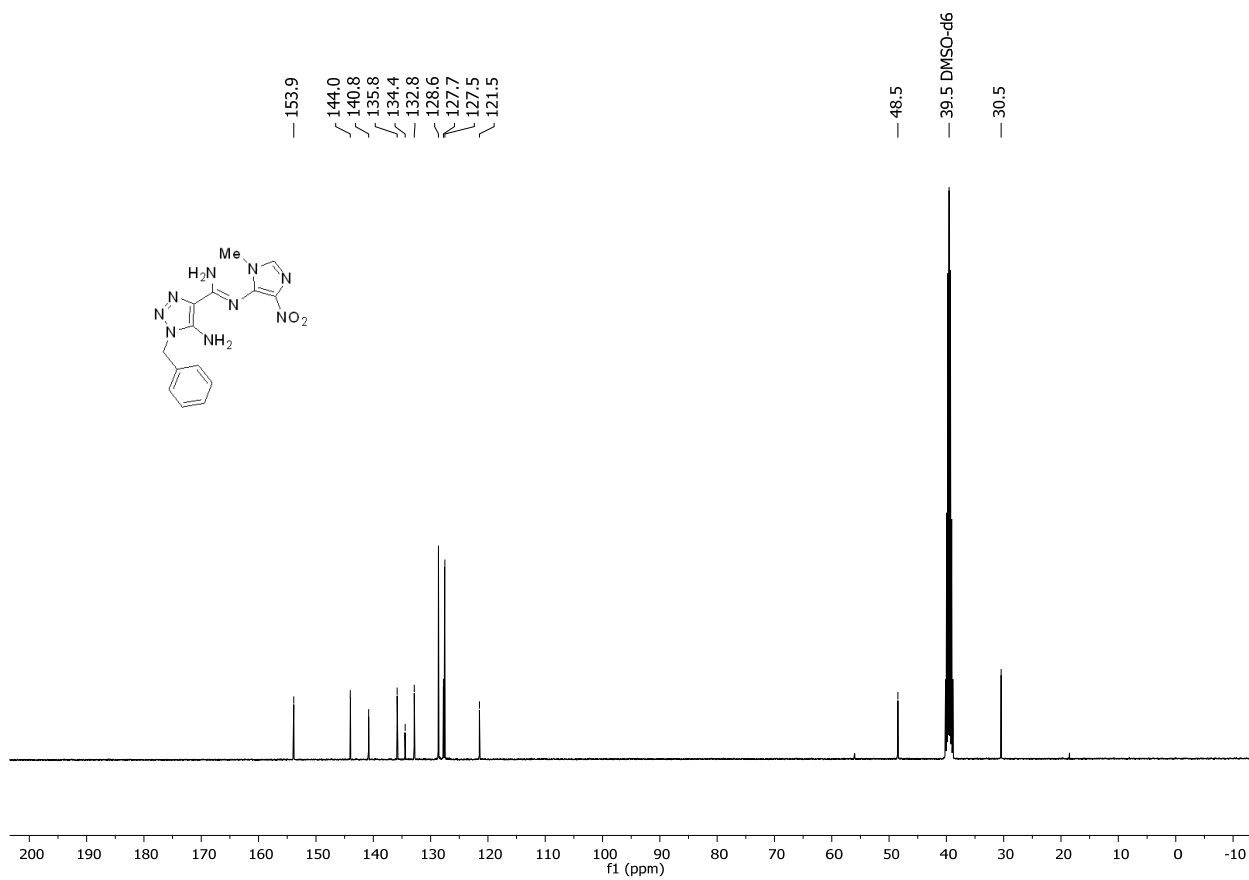


Fig. S32. ¹H NMR spectrum (DMSO-*d*₆) of 3p

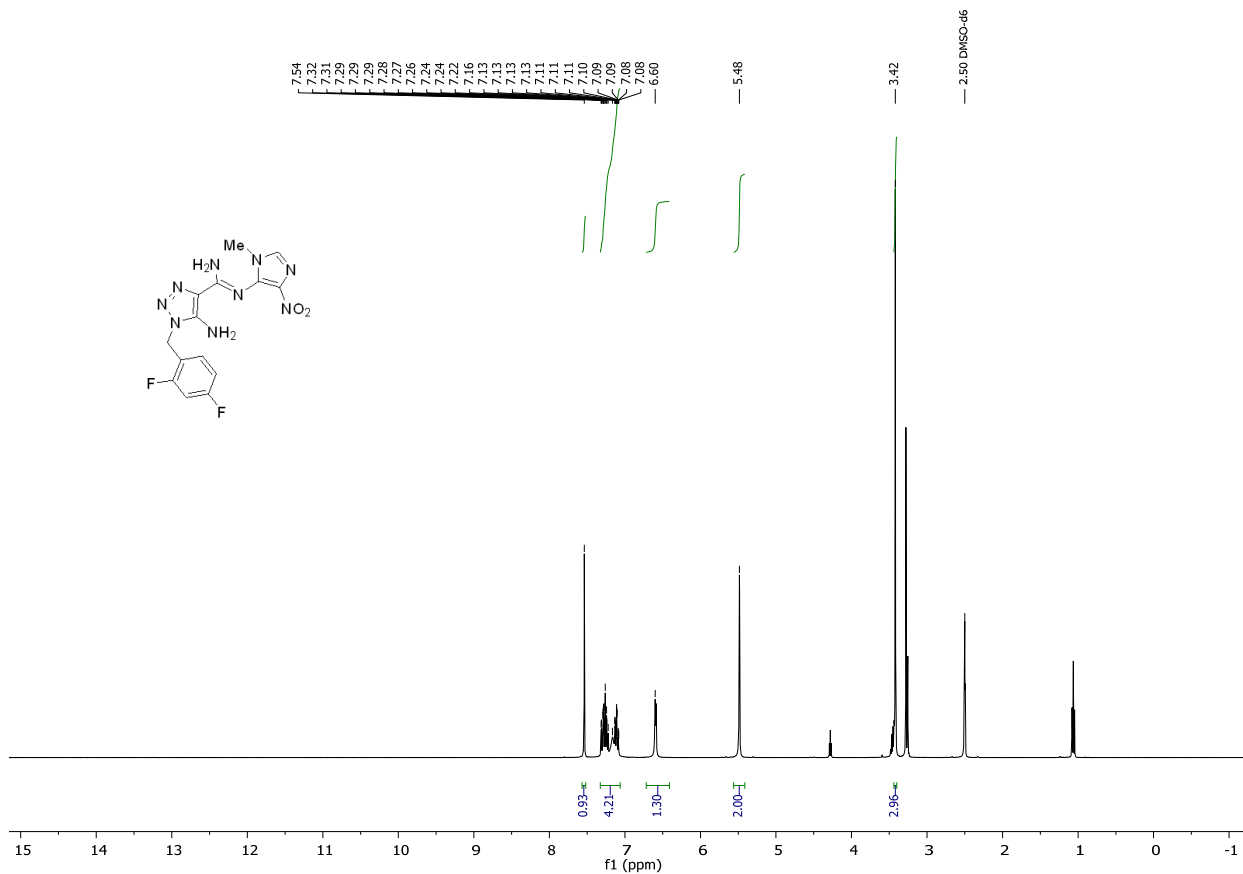


Fig. S33. ¹³C NMR spectrum (DMSO-*d*₆) of 3p

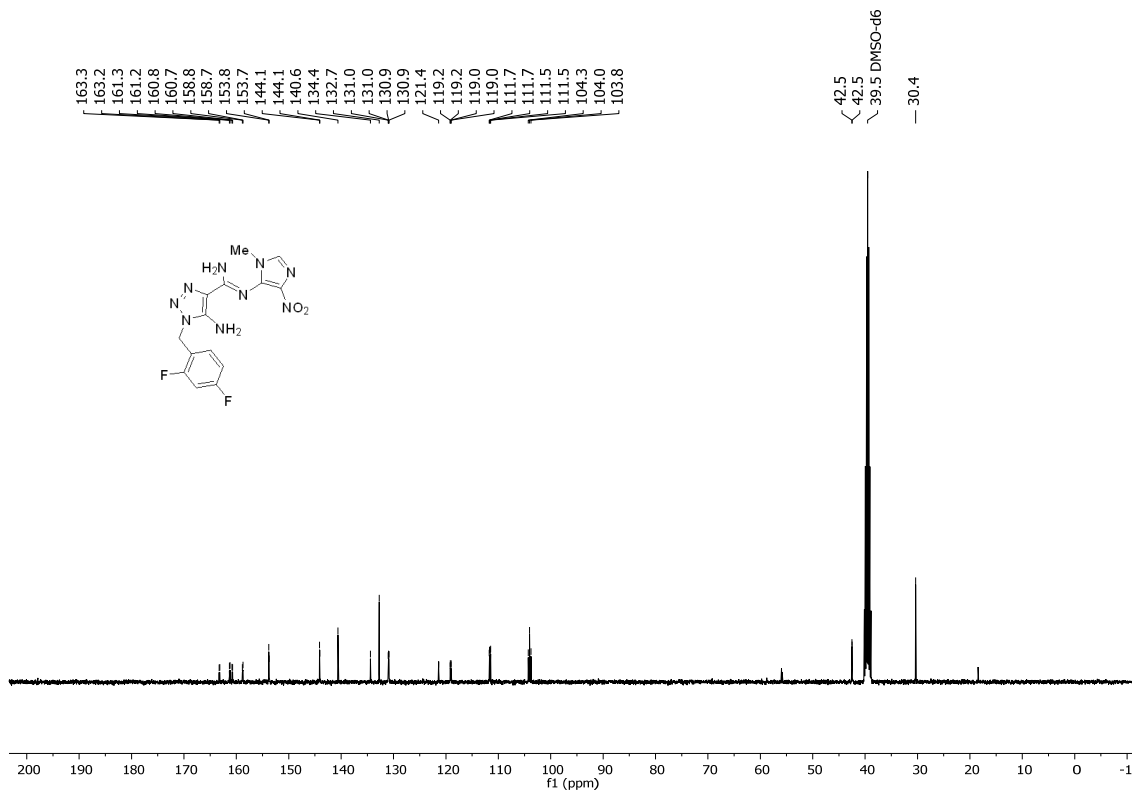


Fig. S34. ^{19}F NMR spectrum (DMSO- d_6) of **3p**

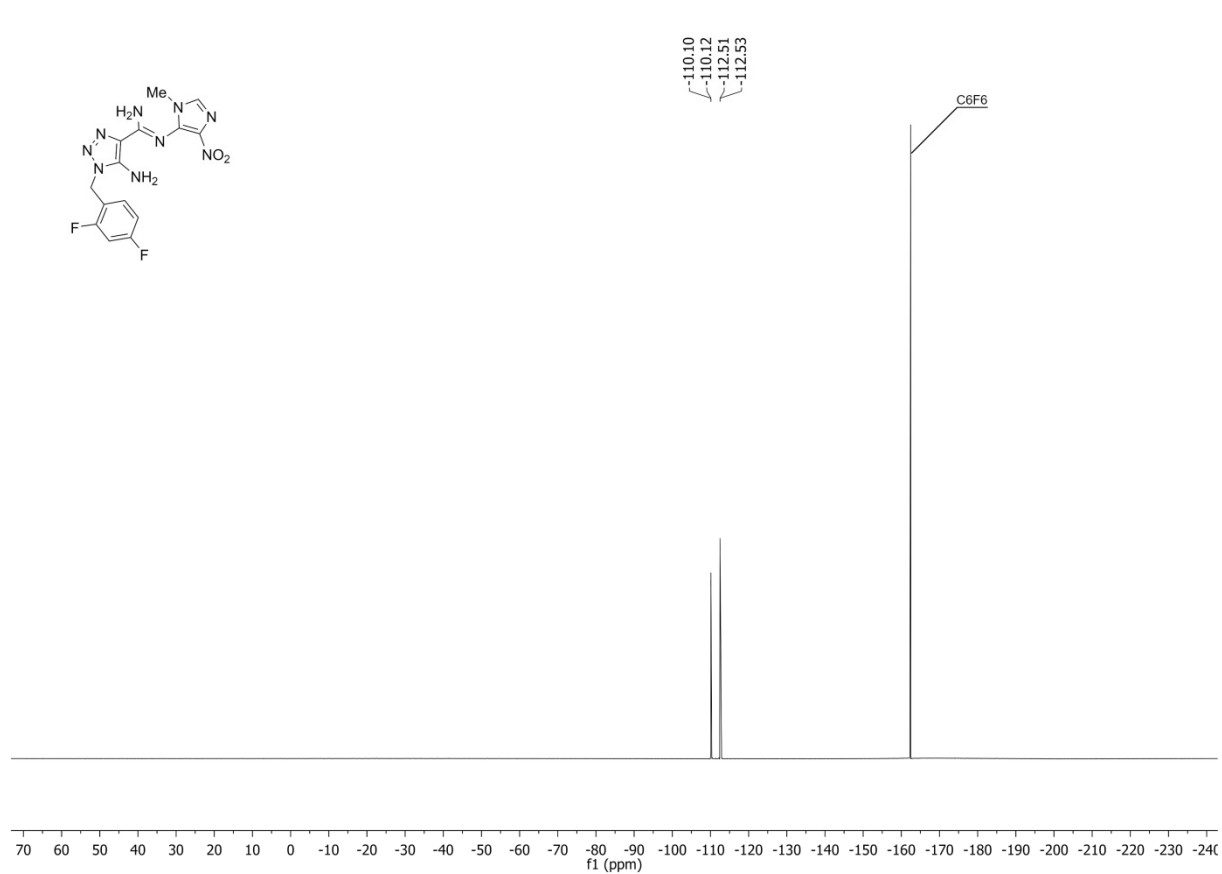


Fig. S35. ^1H NMR spectrum (DMSO- d_6) of **3q**

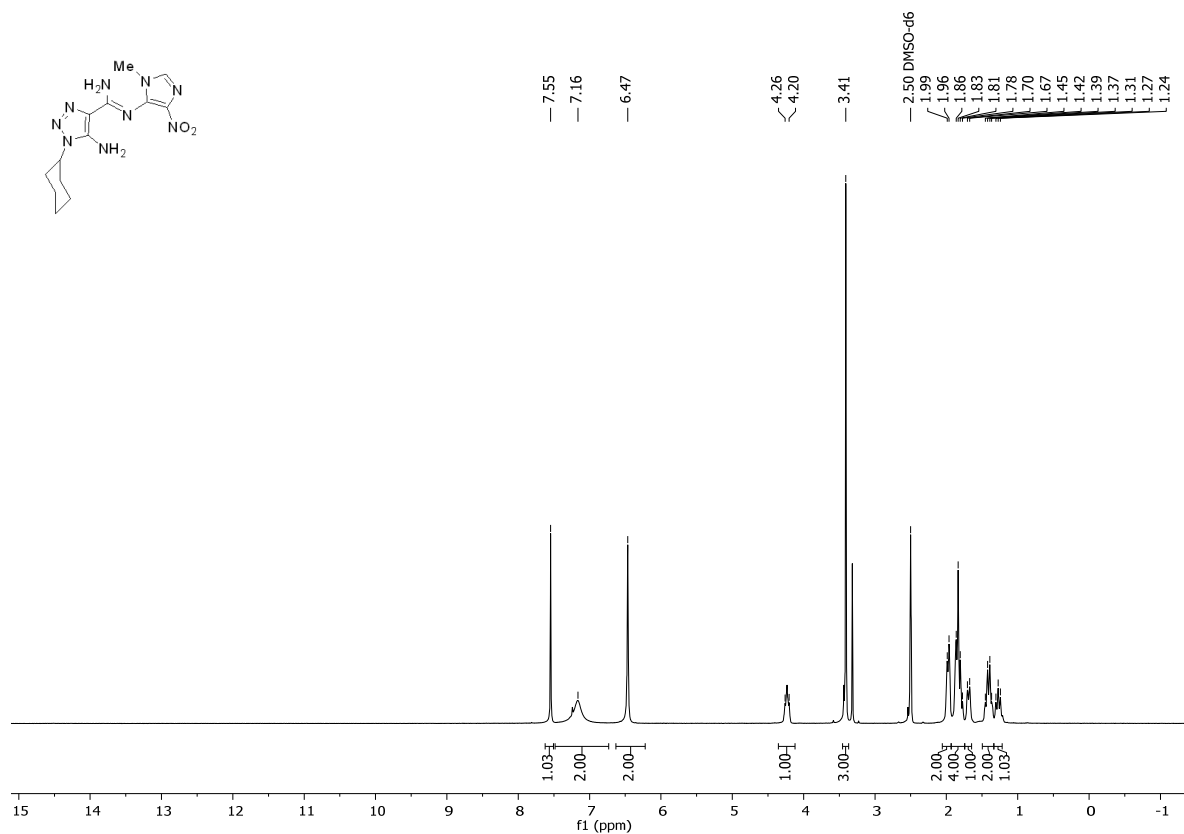


Fig. S36. ^{13}C NMR spectrum (DMSO- d_6) of **3q**

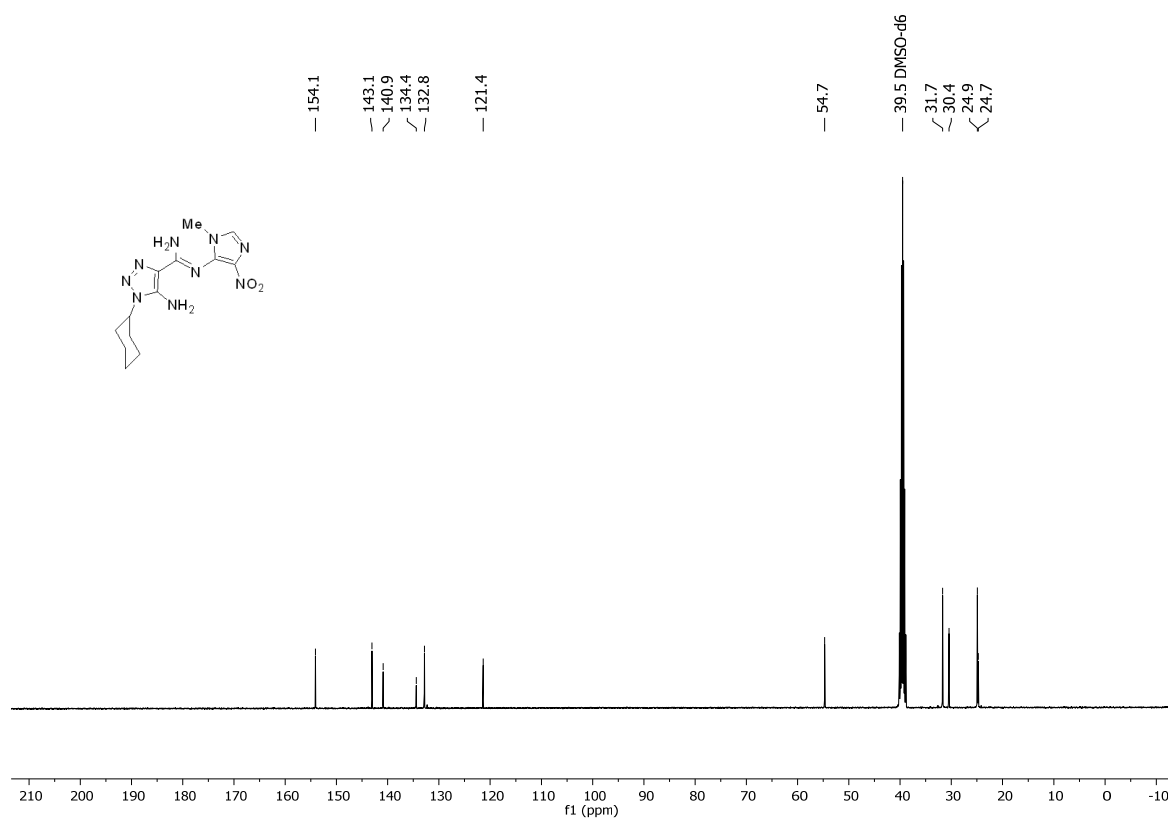


Fig. S37. ^1H NMR spectrum (DMSO- d_6) of **3r**

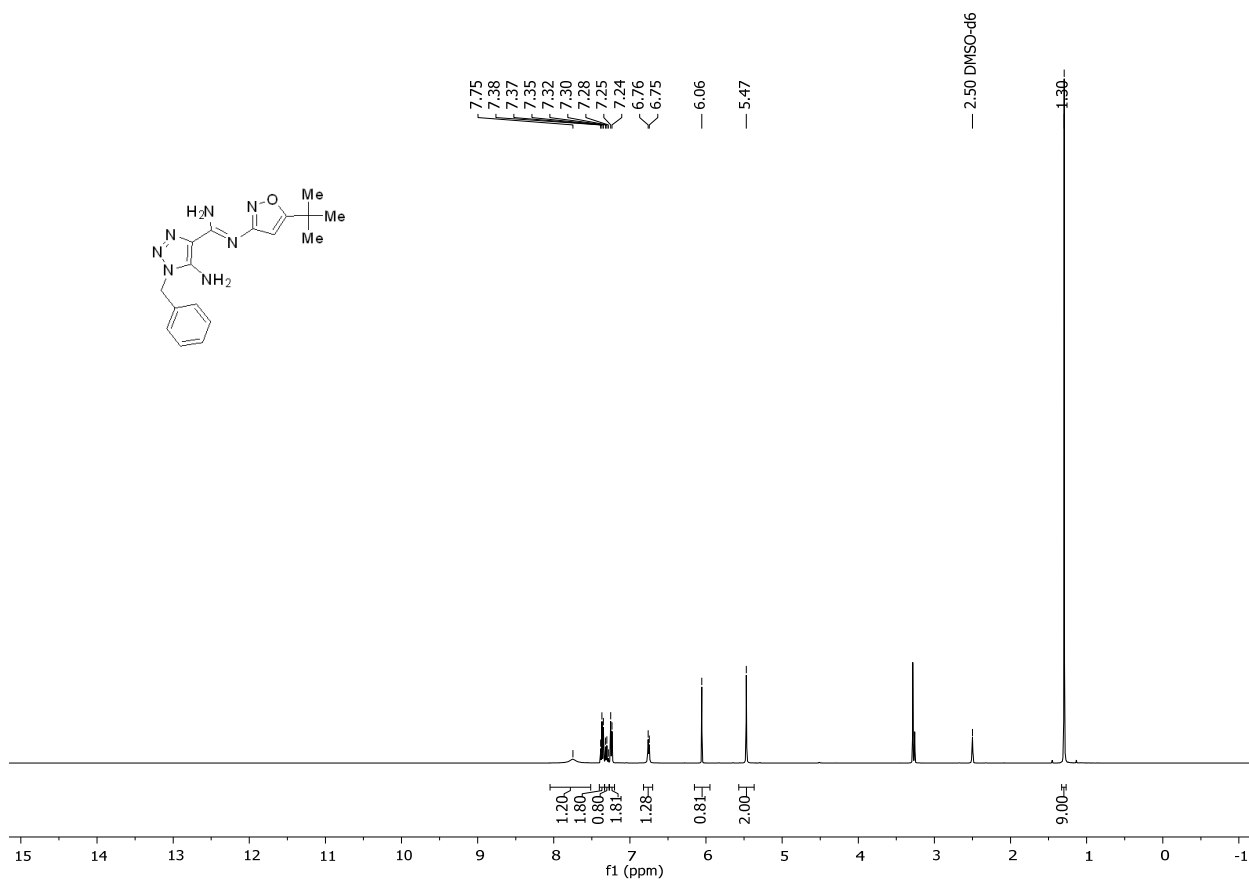


Fig. S38. ^{13}C NMR spectrum (DMSO- d_6) of **3r**

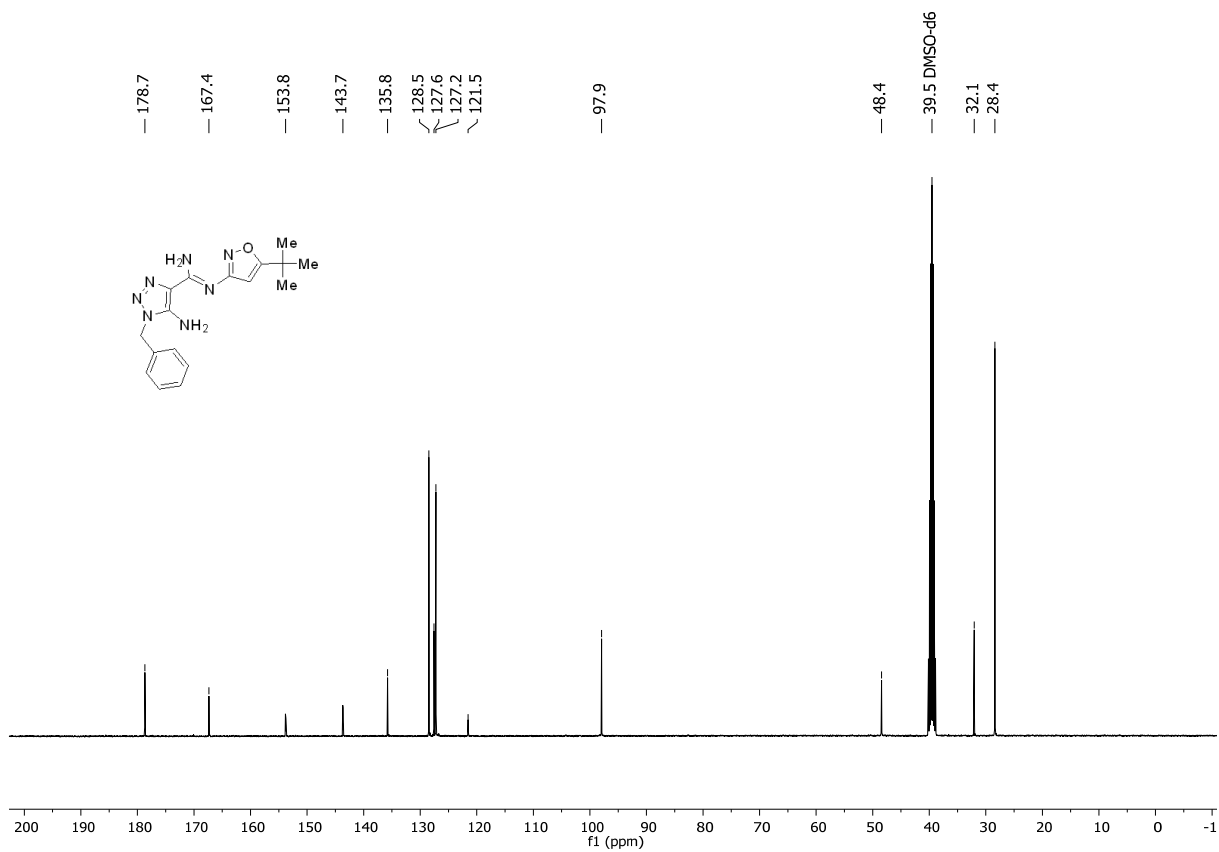


Fig. 38A. HMBC spectrum (DMSO-d₆) of **3r**

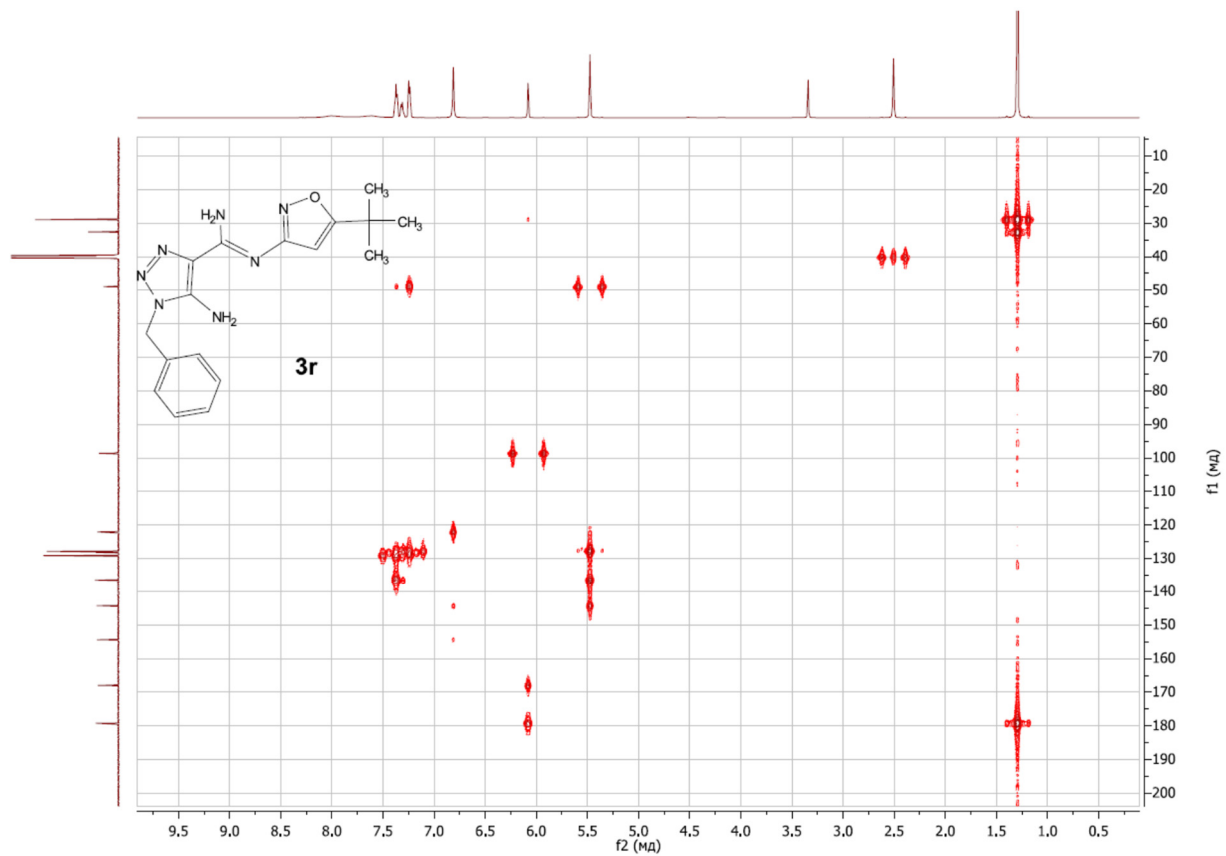


Fig. S39. ^1H NMR spectrum (DMSO- d_6) of **3s**

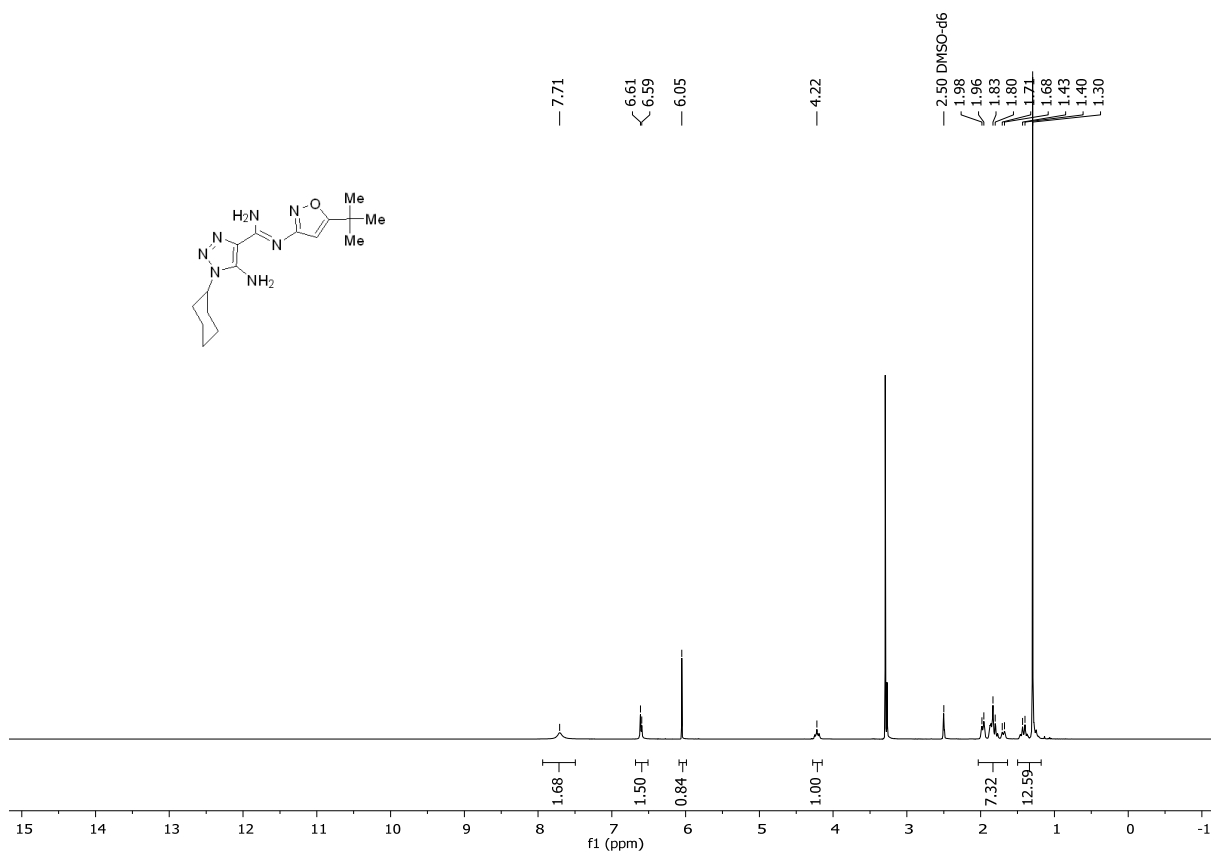


Fig. S40. ^{13}C NMR spectrum (DMSO- d_6) of **3s**

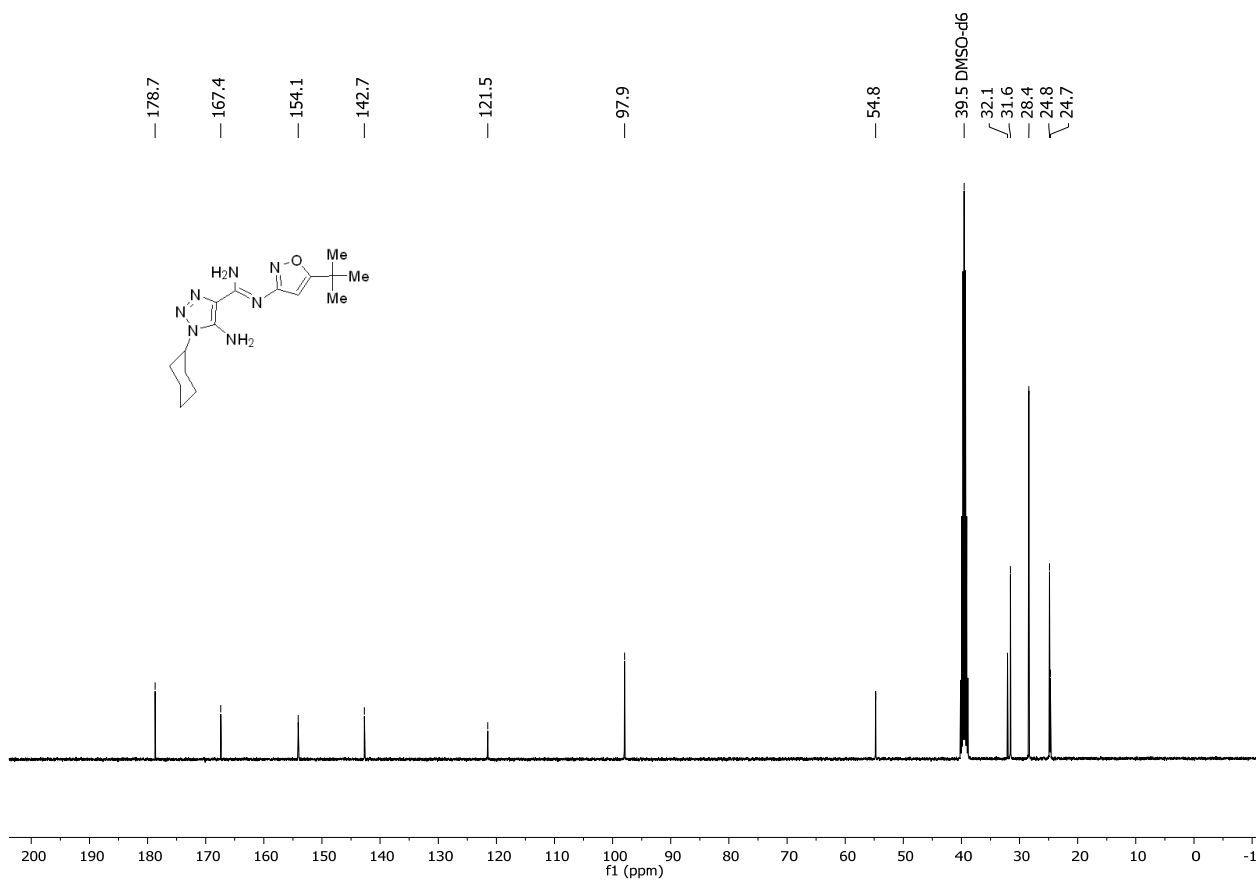


Fig. S41. ^1H NMR spectrum (DMSO- d_6) of 3t

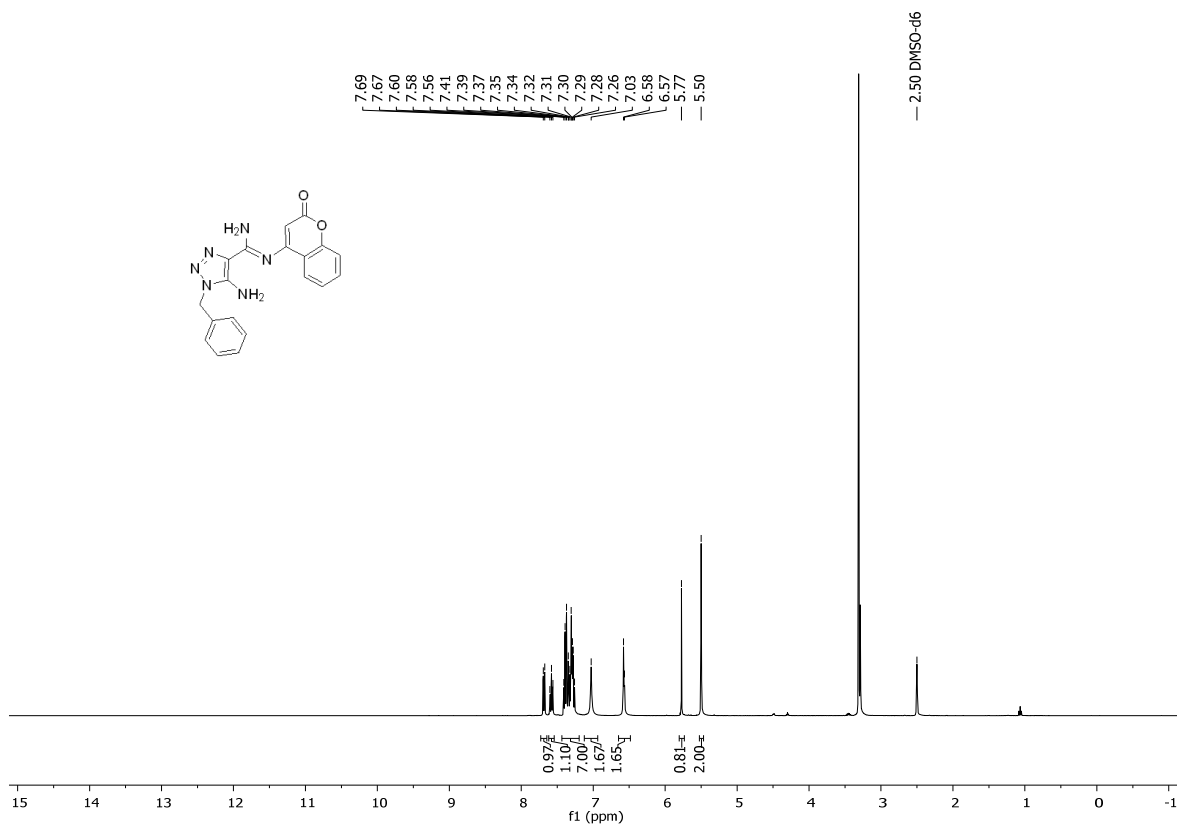


Fig. S42. ^{13}C NMR spectrum (DMSO- d_6) of 3t

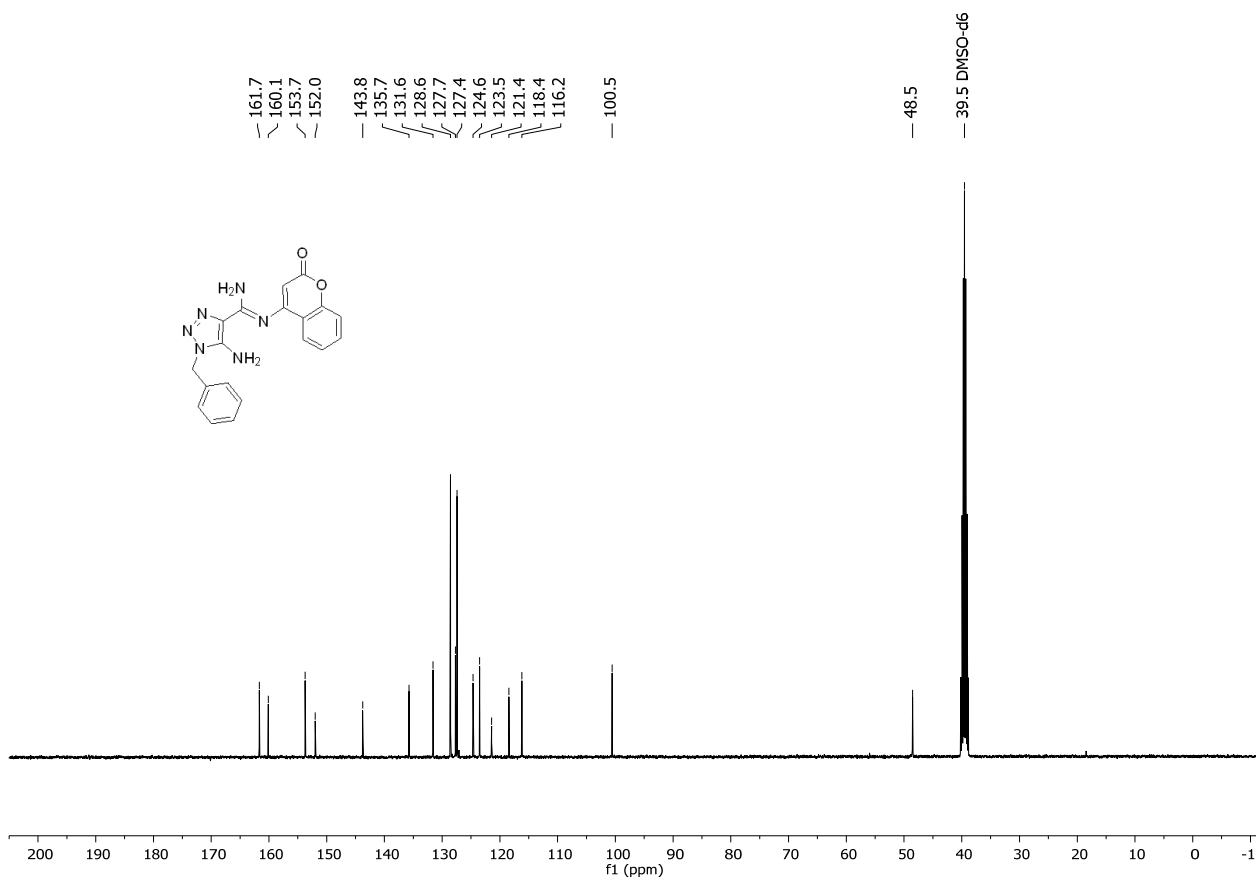


Fig. S43. ¹H NMR spectrum (DMSO-d₆) of **3u**

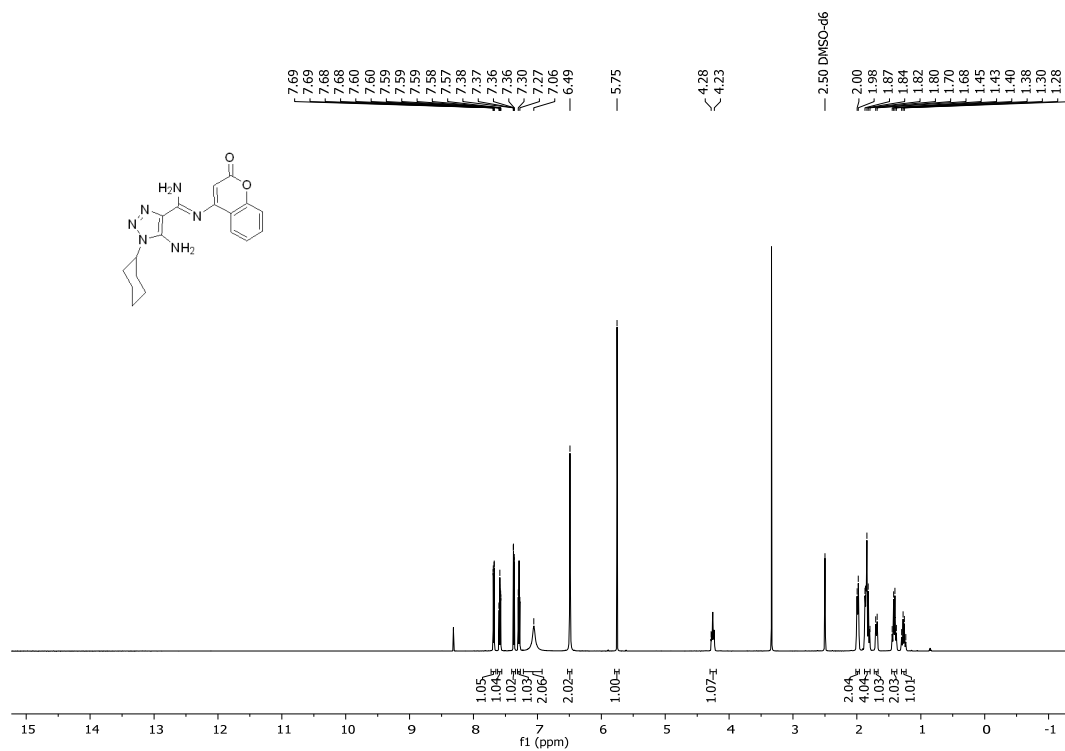
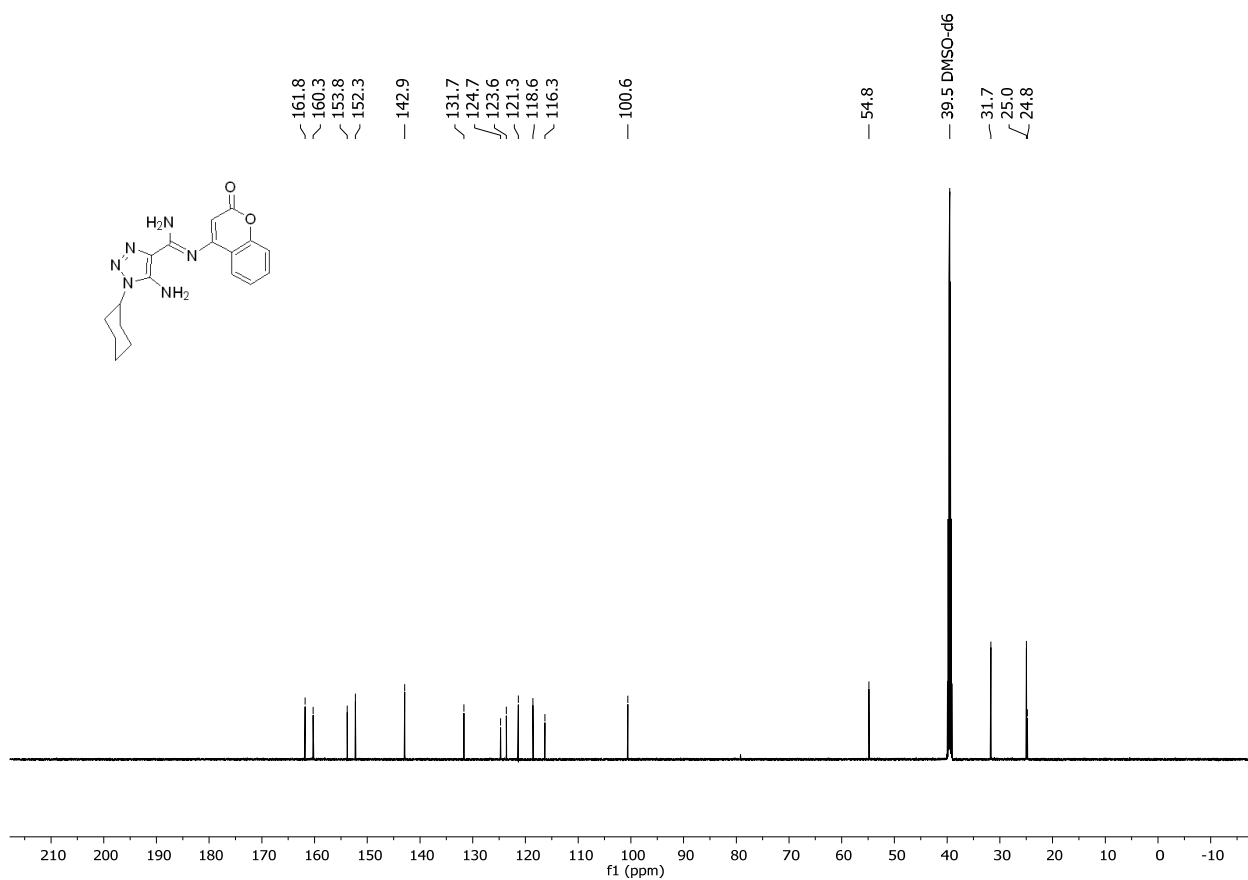


Fig. S44. ¹³C NMR spectrum (DMSO-d₆) of **3u**

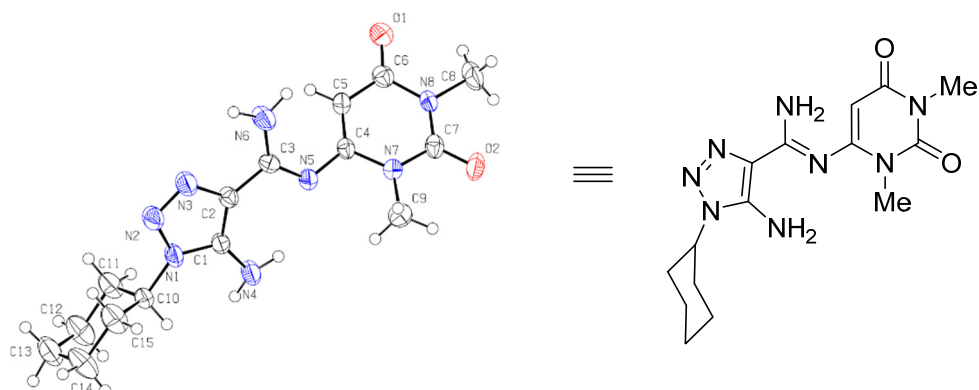


X-ray Single Crystal Data for 3g (CCDC: 2298850)

Procedure for the sample preparation: Compound 3g (20 mg) was dissolved in EtOH.

After slow evaporation at room temperature, the single crystals were afforded.

Fig. S45. Crystal Structure of 3g (50% probability level)



Chemical formula	C ₁₅ H ₂₂ N ₈ O ₂
Formula weight	346.40
Temperature/K	295
Crystal system	Monoclinic
Space group	<i>P</i> 2 ₁ / <i>c</i>
<i>a</i> /Å	14.734(3)
<i>b</i> /Å	9.000(2)
<i>c</i> /Å	13.125(4)
α /°	90
β /°	104.29
γ /°	90
Volume/Å ³	1686.6(8)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
<i>D</i> _x /Mg m ⁻³	1.364
μ /mm ⁻¹	0.10
<i>F</i> (000)	736
Crystal size/mm	0.45 × 0.3 × 0.04
θ_{\max} , θ_{\min} /°	29.5, 2.7
Index ranges	-20 ≤ <i>h</i> ≤ 20, -11 ≤ <i>k</i> ≤ 11, -17 ≤ <i>l</i> ≤ 17
Measured reflections	6415
Independent reflections	6415
Reflections with <i>I</i> > 2 σ (<i>I</i>)	3101
Reflections/parameters/restraints	6415/244/0
Goodness-of-fit	0.87
Final <i>R</i> indexes [<i>F</i> ² > 2 σ (<i>F</i> ²)]	<i>R</i> ₁ = 0.069, <i>wR</i> ₂ = 0.185
Final <i>R</i> indexes [all data]	<i>R</i> ₁ = 0.135, <i>wR</i> ₂ = 0.207
$\Delta\rho_{\max}$, $\Delta\rho_{\min}$ /e Å ⁻³	0.31, -0.35
