

Supporting Information

Uncatalyzed addition and cyclization of T_sN_3 to 1,1-enediamines: an effective green route to highly functionalized 1,2,3-triazole compounds

Chang-Long Yang¹, Yu-Hao Zhang¹, Quan-Xing Zi¹, Jun Lin^{1,*} and Sheng-Jiao Yan^{1,*}

¹ Key Laboratory of Medicinal Chemistry for Natural Resources (Yunnan University), Ministry of Education, School of Chemical Science and Technology, Yunnan University, Kunming, 650091, P. R. China.

Table of Contents

¹ H NMR and ¹³ C NMR Spectra for 1,2,3-Triazole Compounds 3–4 and 4'	3
Figure 1. ¹ H NMR (600 MHz, DMSO- <i>d</i> ₆) spectra of compound 3a	3
Figure 2. ¹³ C NMR (150 MHz, DMSO- <i>d</i> ₆) spectra of compound 3a	3
Figure 3. ¹ H NMR (600 MHz, DMSO- <i>d</i> ₆) spectra of compound 3b	4
Figure 4. ¹³ C NMR (150 MHz, DMSO- <i>d</i> ₆) spectra of compound 3b	4
Figure 5. ¹ H NMR (500 MHz, DMSO- <i>d</i> ₆) spectra of compound 3c	5
Figure 6. ¹³ C NMR (125 MHz, DMSO- <i>d</i> ₆) spectra of compound 3c	5
Figure 7. ¹ H NMR (600 MHz, DMSO- <i>d</i> ₆) spectra of compound 3d	6
Figure 8. ¹³ C NMR (150 MHz, DMSO- <i>d</i> ₆) spectra of compound 3d	6
Figure 9. ¹ H NMR (500 MHz, DMSO- <i>d</i> ₆) spectra of compound 3e	7
Figure 10. ¹³ C NMR (125 MHz, DMSO- <i>d</i> ₆) spectra of compound 3e	7
Figure 11. ¹ H NMR (600 MHz, DMSO- <i>d</i> ₆) spectra of compound 3f	8
Figure 12. ¹³ C NMR (150 MHz, DMSO- <i>d</i> ₆) spectra of compound 3f	8
Figure 13. ¹ H NMR (600 MHz, DMSO- <i>d</i> ₆) spectra of compound 3g	9
Figure 14. ¹³ C NMR (150 MHz, DMSO- <i>d</i> ₆) spectra of compound 3g	9
Figure 15. ¹ H NMR (500 MHz, DMSO- <i>d</i> ₆) spectra of compound 3h	10
Figure 16. ¹³ C NMR (125 MHz, DMSO- <i>d</i> ₆) spectra of compound 3h	10
Figure 17. ¹ H NMR (600 MHz, DMSO- <i>d</i> ₆) spectra of compound 3i	11
Figure 18. ¹³ C NMR (150 MHz, DMSO- <i>d</i> ₆) spectra of compound 3i	11
Figure 19. ¹ H NMR (600 MHz, CDCl ₃) spectra of compound 3j	12
Figure 20. ¹³ C NMR (150 MHz, CDCl ₃) spectra of compound 3j	12
Figure 21. ¹ H NMR (500 MHz, DMSO- <i>d</i> ₆) spectra of compound 3k	13
Figure 22. ¹³ C NMR (125 MHz, DMSO- <i>d</i> ₆) spectra of compound 3k	13
Figure 23. ¹ H NMR (600 MHz, DMSO- <i>d</i> ₆) spectra of compound 3l	14
Figure 24. ¹³ C NMR (150 MHz, DMSO- <i>d</i> ₆) spectra of compound 3l	14
Figure 25. ¹ H NMR (500 MHz, DMSO- <i>d</i> ₆) spectra of compound 3m	15
Figure 26. ¹³ C ¹ H NMR (125 MHz, DMSO- <i>d</i> ₆) spectra of compound 3m	15
Figure 27. ¹ H NMR (500 MHz, DMSO- <i>d</i> ₆) spectra of compound 3n	16
Figure 28. ¹³ C NMR (125 MHz, DMSO- <i>d</i> ₆) spectra of compound 3n	16

Figure 29.	^1H NMR (600 MHz, DMSO- d_6) spectra of compound 3o	17
Figure 30.	^{13}C NMR (150 MHz, DMSO- d_6) spectra of compound 3o	17
Figure 31.	^1H NMR (500 MHz, DMSO- d_6) spectra of compound 4a	18
Figure 32.	^{13}C NMR (125 MHz, DMSO- d_6) spectra of compound 4a	18
Figure 33.	^1H NMR (500 MHz, DMSO- d_6) spectra of compound 4a'	19
Figure 34.	^{13}C NMR (125 MHz, DMSO- d_6) spectra of compound 4a'	19
Figure 35.	^1H NMR (500 MHz, DMSO- d_6) spectra of compound 4b	20
Figure 36.	^{13}C NMR (125 MHz, DMSO- d_6) spectra of compound 4b	20
Figure 37.	^1H NMR (500 MHz, DMSO- d_6) spectra of compound 4c	21
Figure 38.	^{13}C NMR (125 MHz, DMSO- d_6) spectra of compound 4c	21
Figure 39.	^1H NMR (500 MHz, DMSO- d_6) spectra of compound 4d	22
Figure 40.	^{13}C NMR (125 MHz, DMSO- d_6) spectra of compound 4d	22
Figure 41.	^1H NMR (600 MHz, DMSO- d_6) spectra of compound 4d'	23
Figure 42.	^{13}C NMR (150 MHz, DMSO- d_6) spectra of compound 4d'	23
Figure 43.	^1H NMR (600 MHz, DMSO- d_6) spectra of compound 4e	24
Figure 44.	^{13}C NMR (150 MHz, DMSO- d_6) spectra of compound 4e	24
Figure 45.	^1H NMR (600 MHz, DMSO- d_6) spectra of compound 4f	25
Figure 46.	^{13}C NMR (150 MHz, DMSO- d_6) spectra of compound 4f	25
Figure 47.	^1H NMR (600 MHz, DMSO- d_6) spectra of compound 4g	26
Figure 48.	^{13}C NMR (150 MHz, DMSO- d_6) spectra of compound 4g	26
Figure 49.	^1H NMR (600 MHz, DMSO- d_6) spectra of compound 4g'	27
Figure 50.	^{13}C NMR (150 MHz, DMSO- d_6) spectra of compound 4g'	27

¹H NMR and ¹³C NMR Spectra for 1,2,3-Triazole Compounds 3

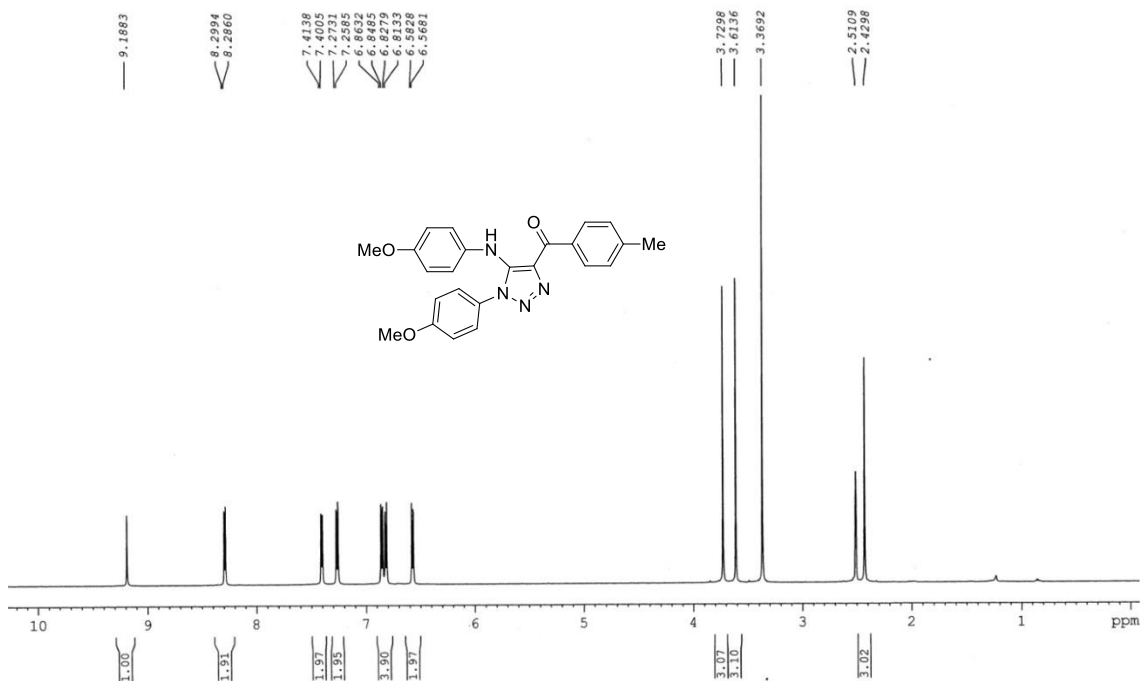


Figure 1. ¹H NMR (600 MHz, DMSO-*d*₆) spectra of compound 3a

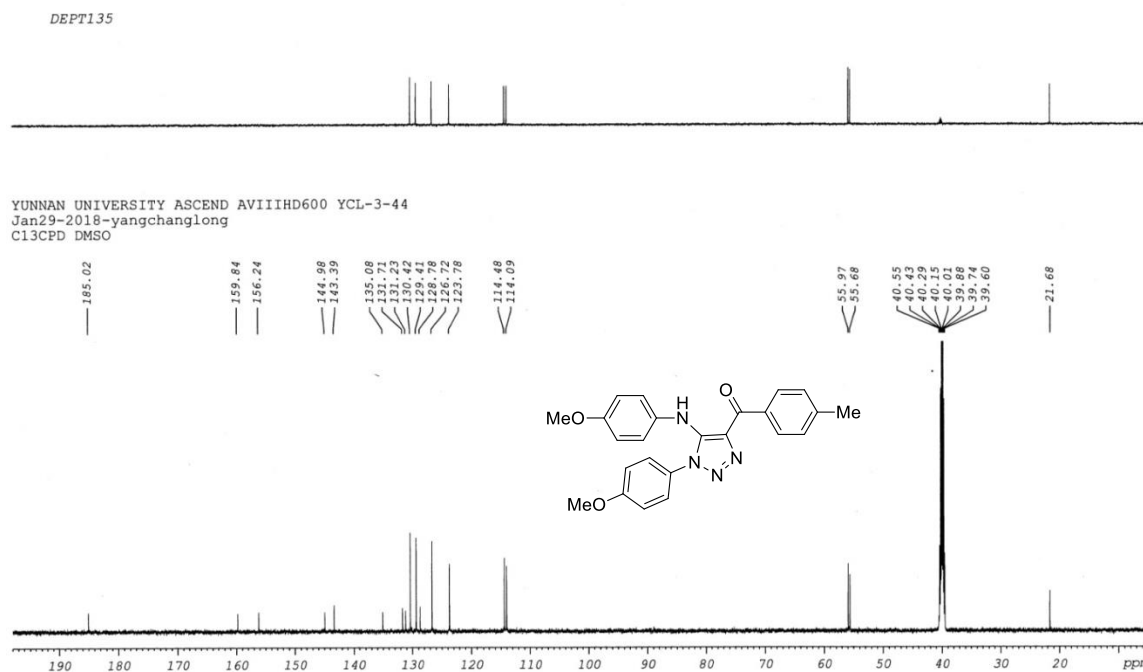


Figure 2. ¹³C NMR (150 MHz, DMSO-*d*₆) spectra of compound 3a

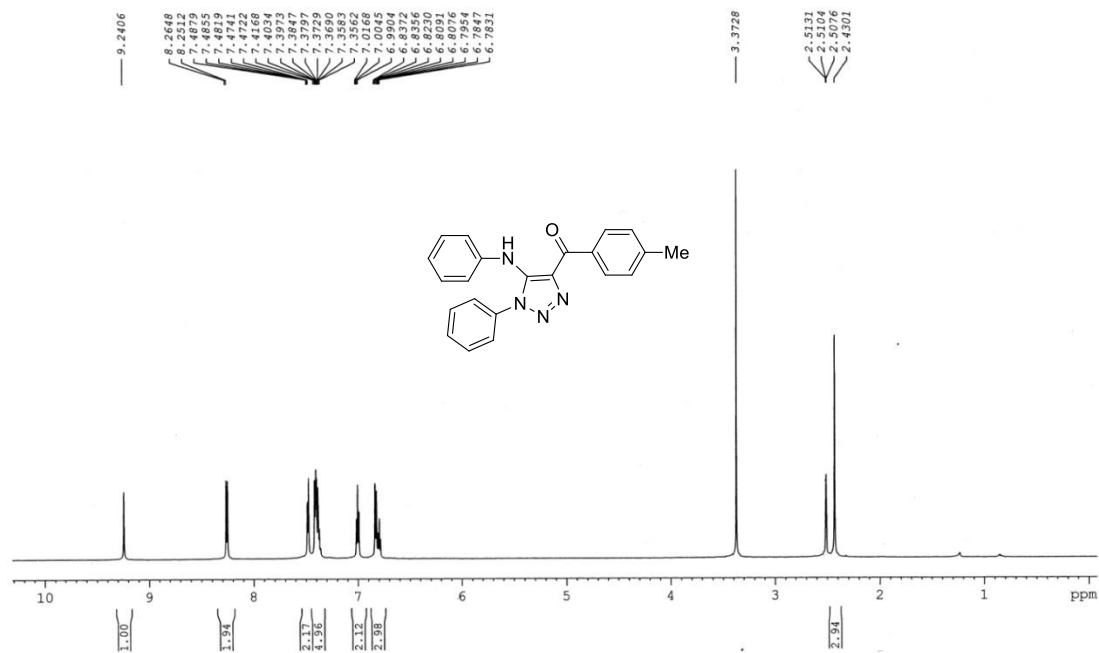


Figure 3. ¹H NMR (600 MHz, DMSO-*d*₆) spectra of compound **3b**

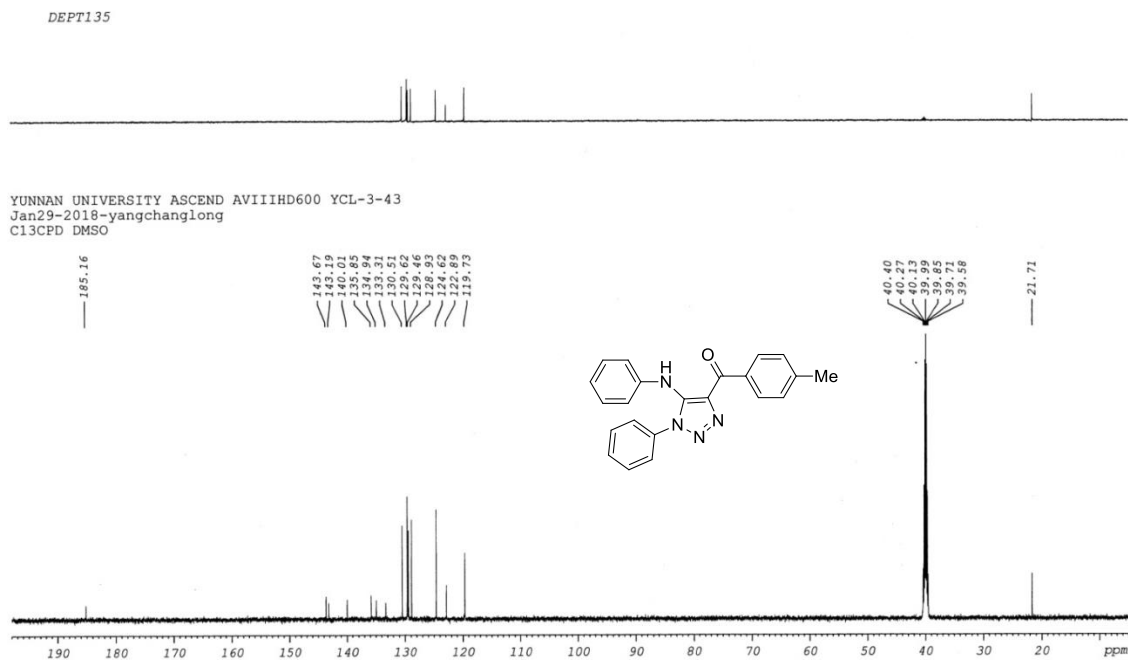


Figure 4. ¹³C NMR (150 MHz, DMSO-*d*₆) spectra of compound **3b**

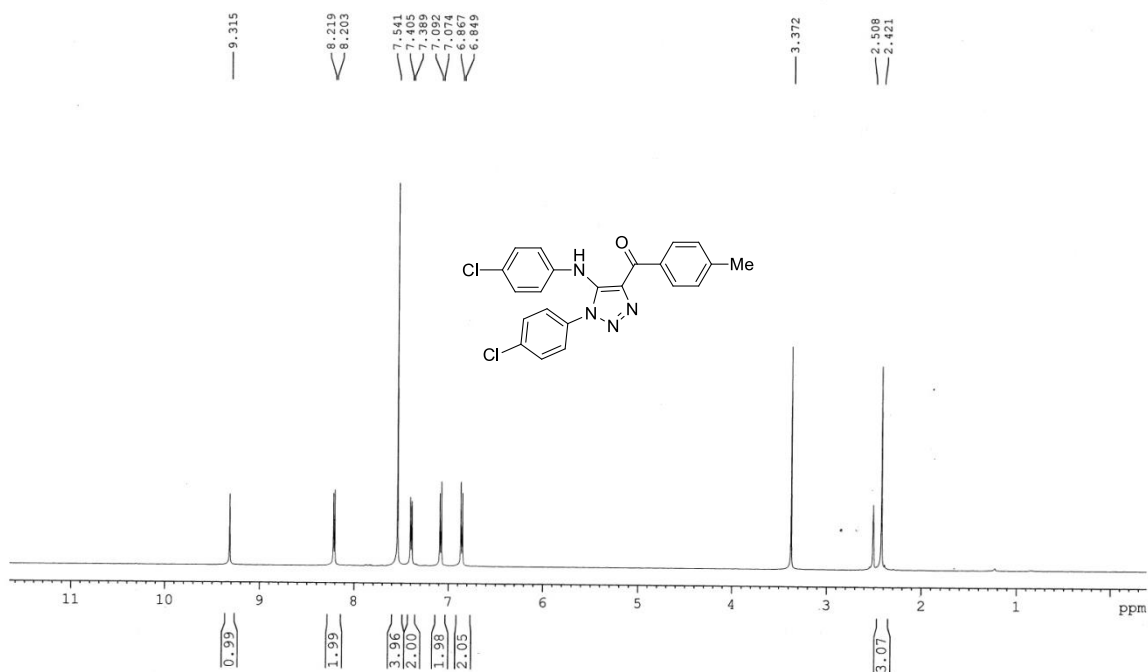


Figure 5. ¹H NMR (500 MHz, DMSO-*d*₆) spectra of compound **3c**

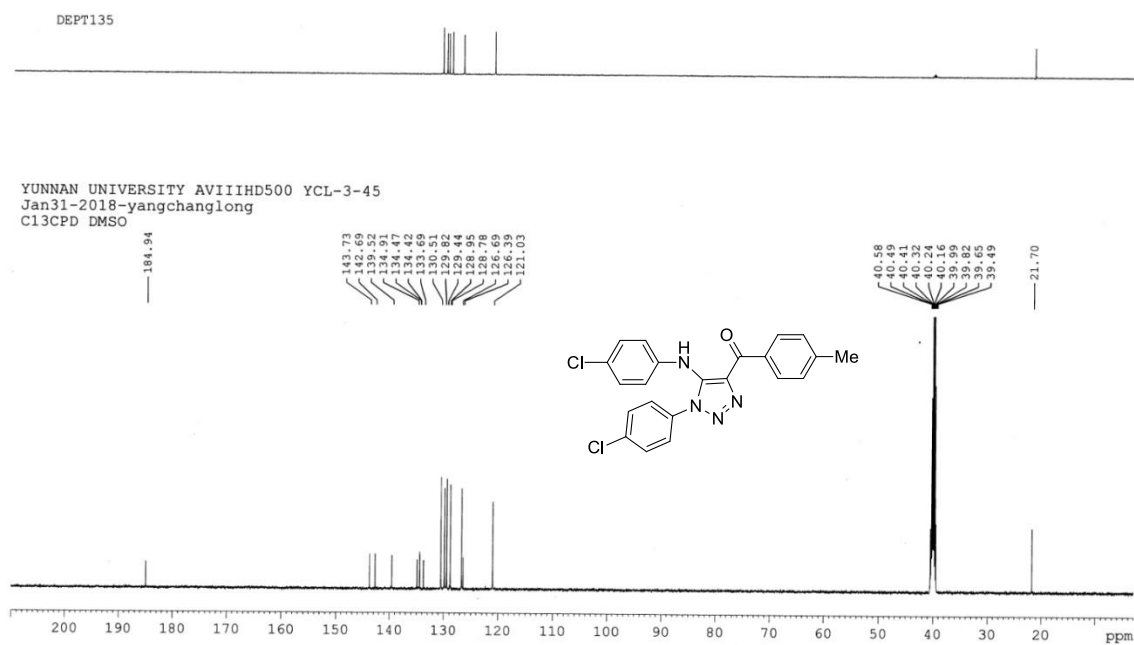


Figure 6. ¹³C NMR (125 MHz, DMSO-*d*₆) spectra of compound **3c**

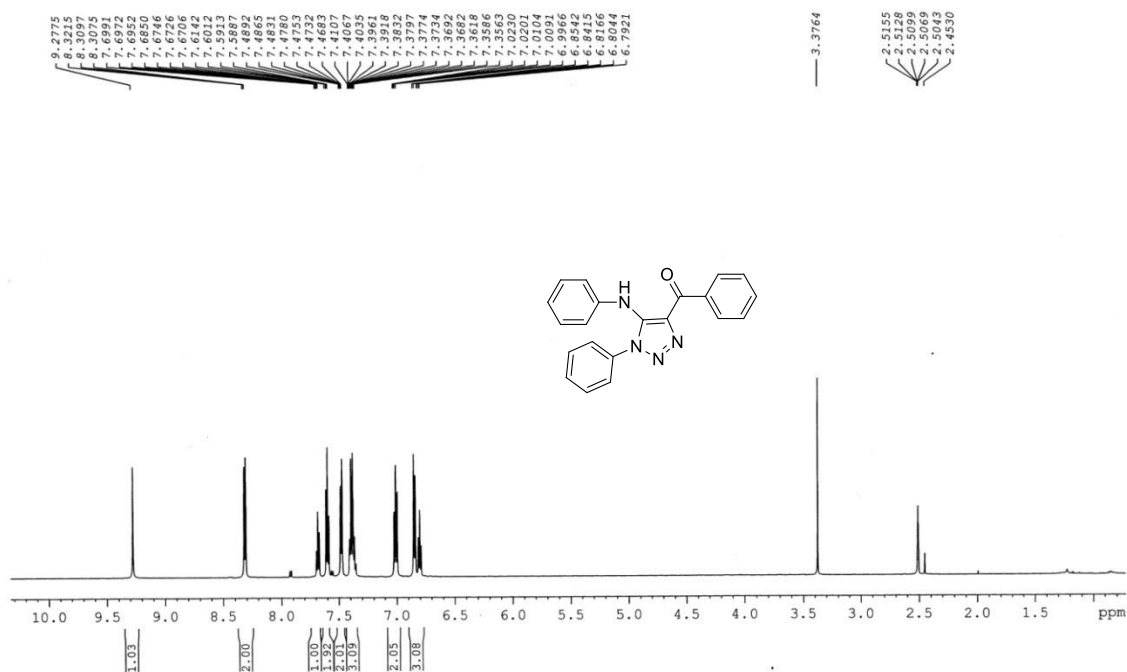


Figure 7. ¹H NMR (600 MHz, DMSO-*d*₆) spectra of compound 3d

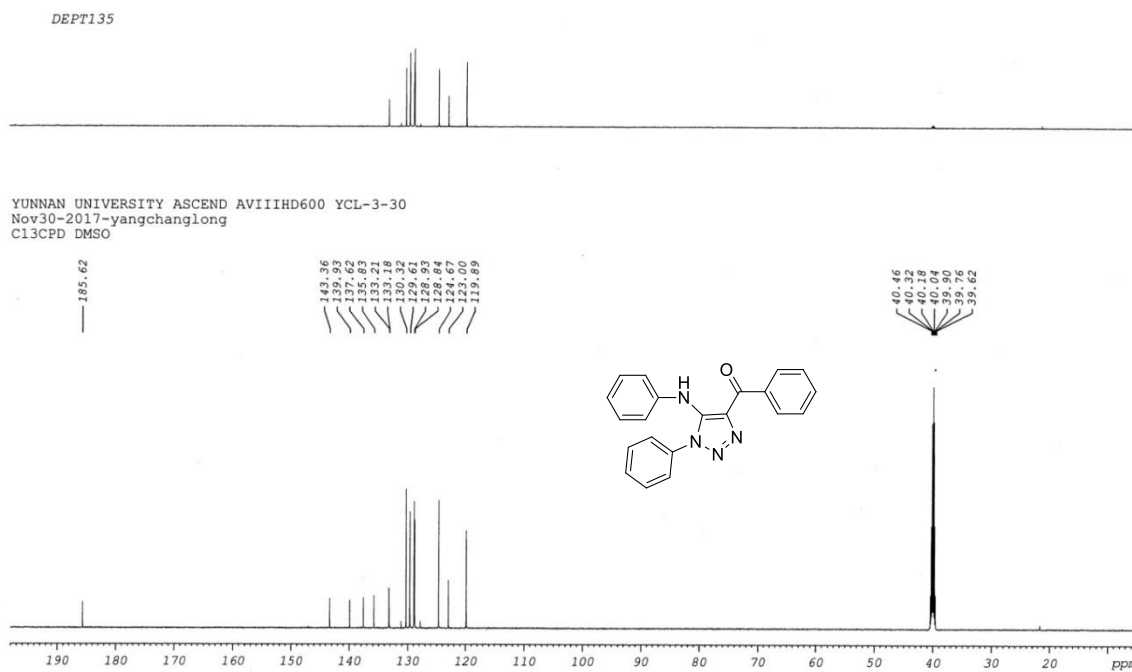


Figure 8. ¹³C NMR (150 MHz, DMSO-*d*₆) spectra of compound 3d

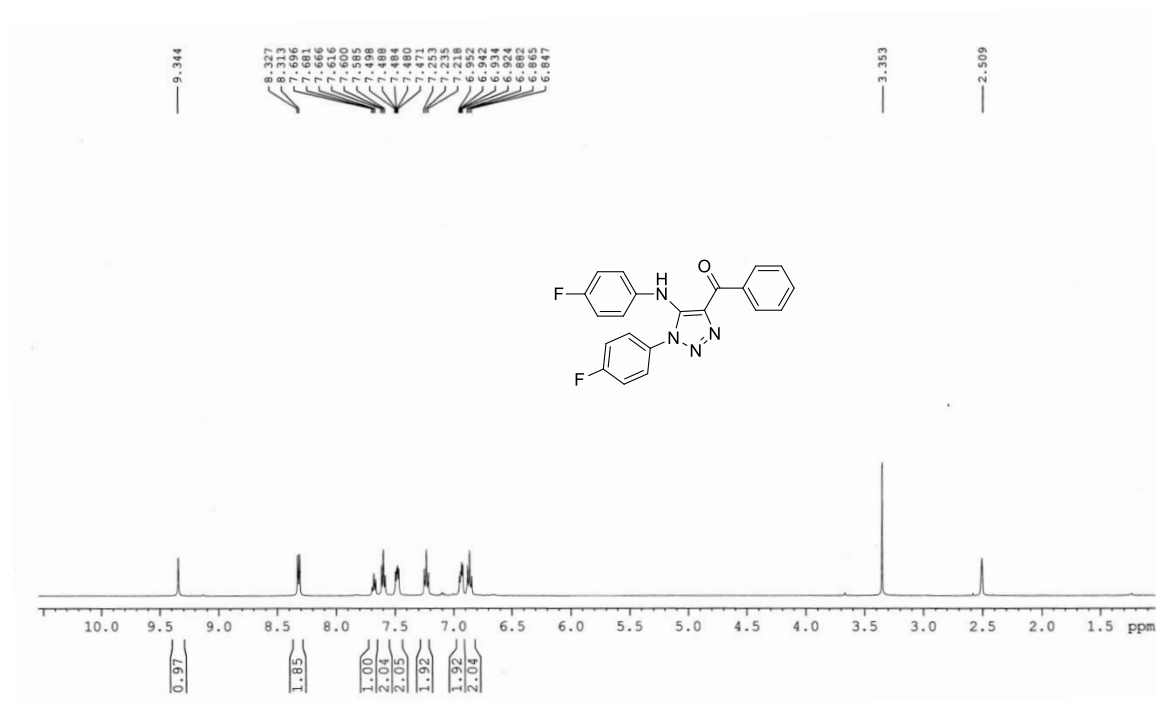


Figure 9. ¹H NMR (500 MHz, DMSO-*d*₆) spectra of compound 3e

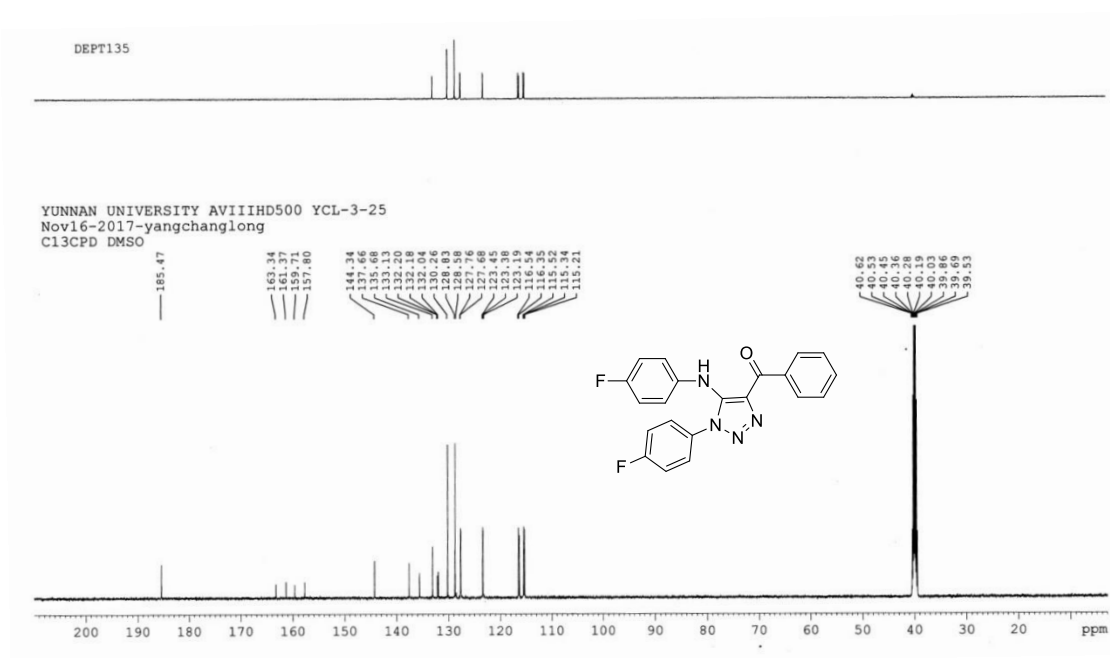


Figure 10. ¹³C NMR (125 MHz, DMSO-*d*₆) spectra of compound 3e

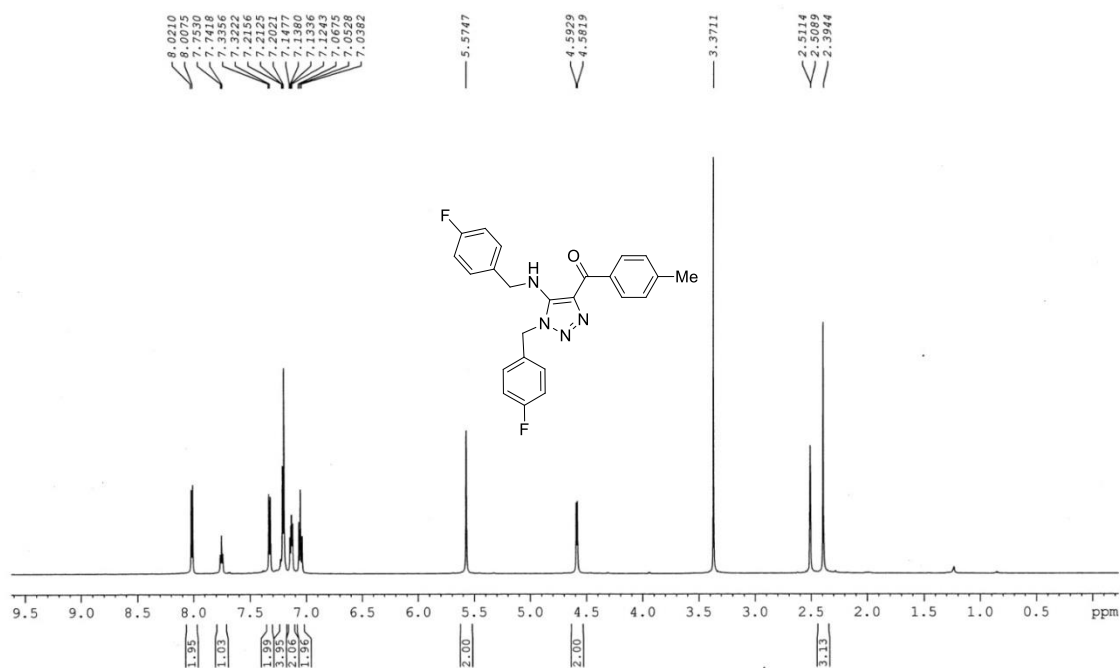


Figure 11. ¹H NMR (600 MHz, DMSO-*d*₆) spectra of compound **3f**

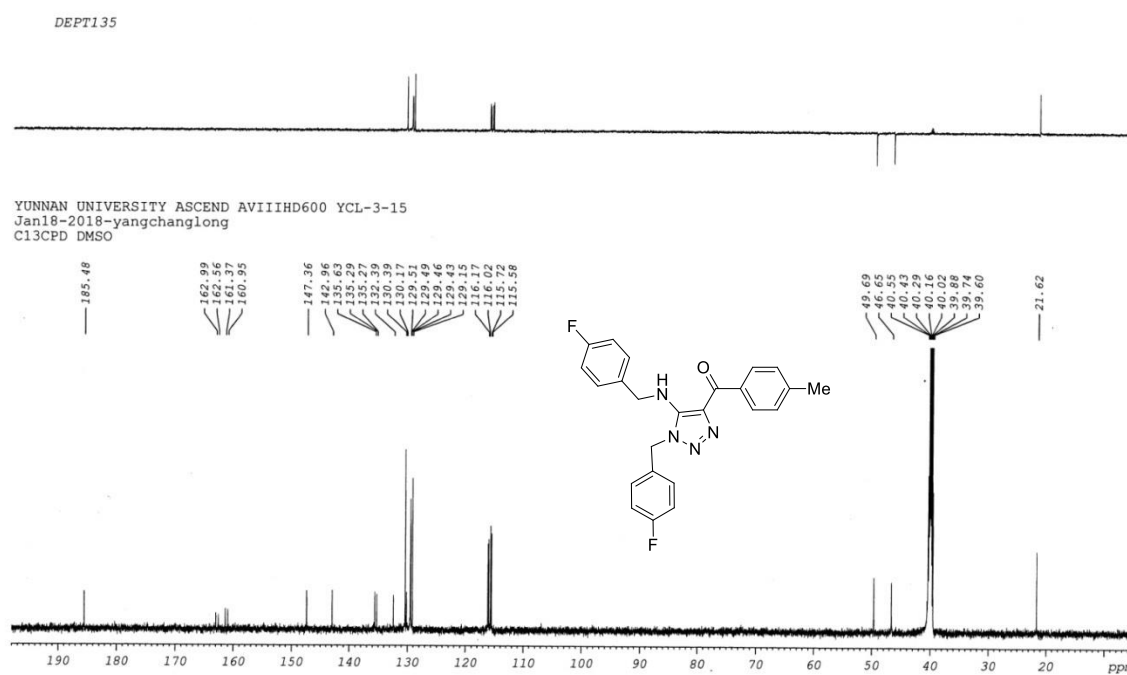


Figure 12. ¹³C NMR (150 MHz, DMSO-*d*₆) spectra of compound **3f**

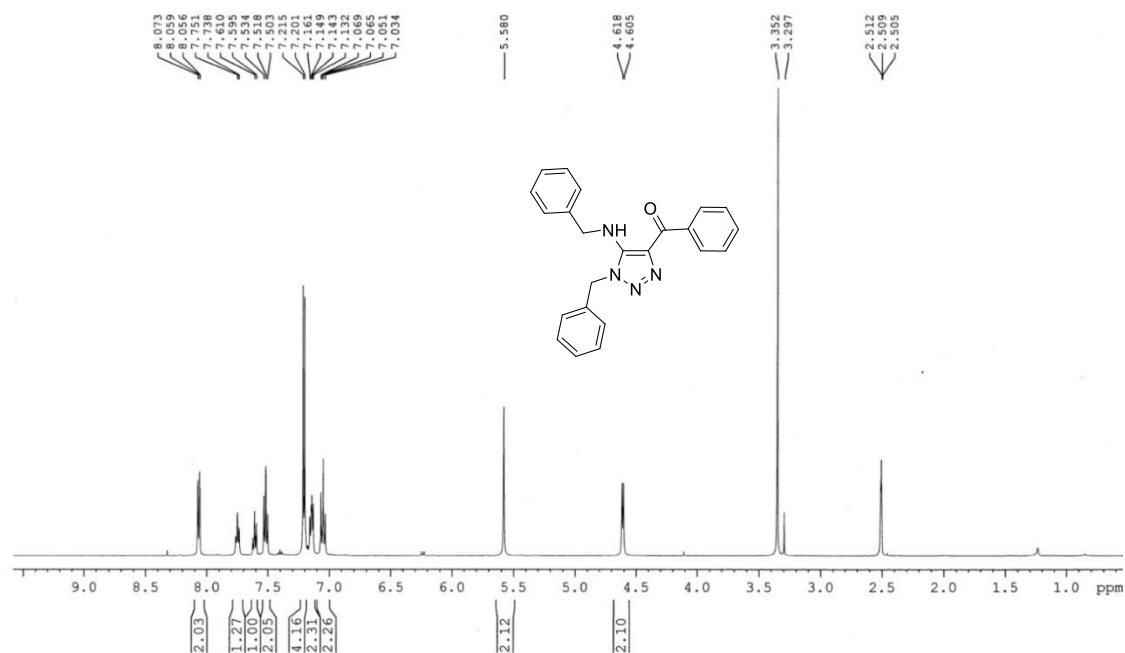


Figure 15. ¹H NMR (500 MHz, DMSO-*d*₆) spectra of compound **3h**

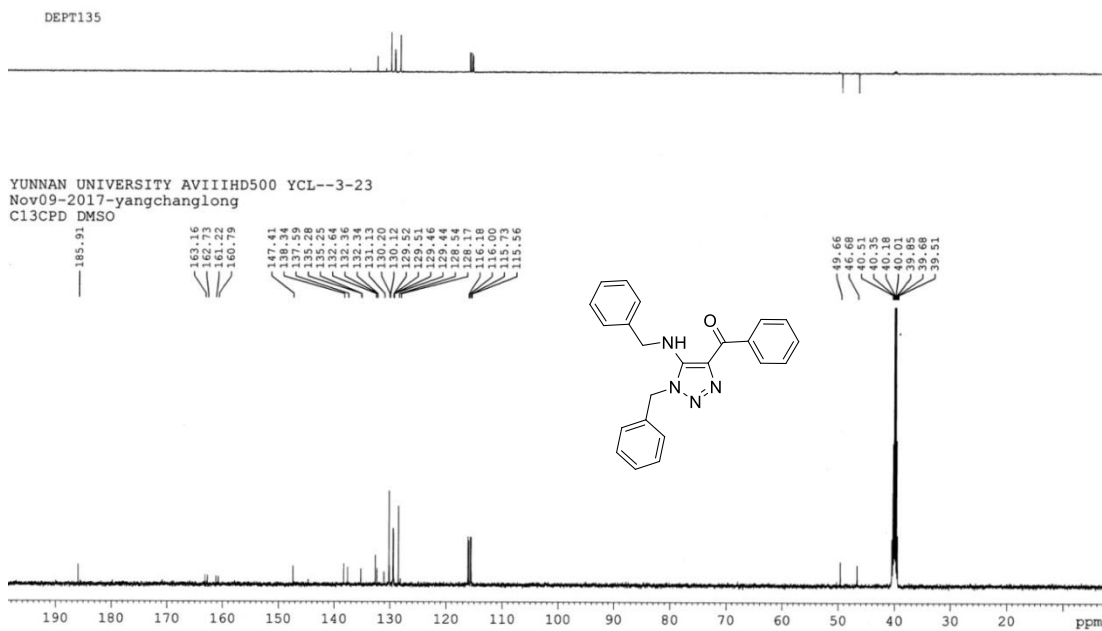


Figure 16. ¹³C NMR (125 MHz, DMSO-*d*₆) spectra of compound **3h**

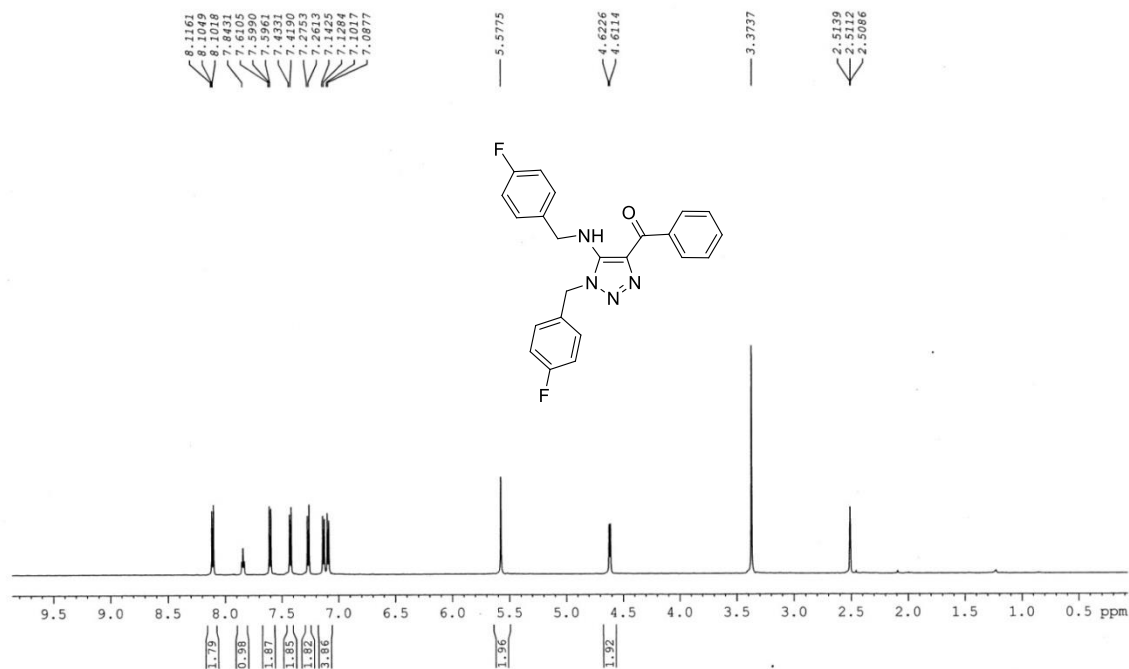


Figure 17. ¹H NMR (600 MHz, DMSO-*d*₆) spectra of compound **3i**

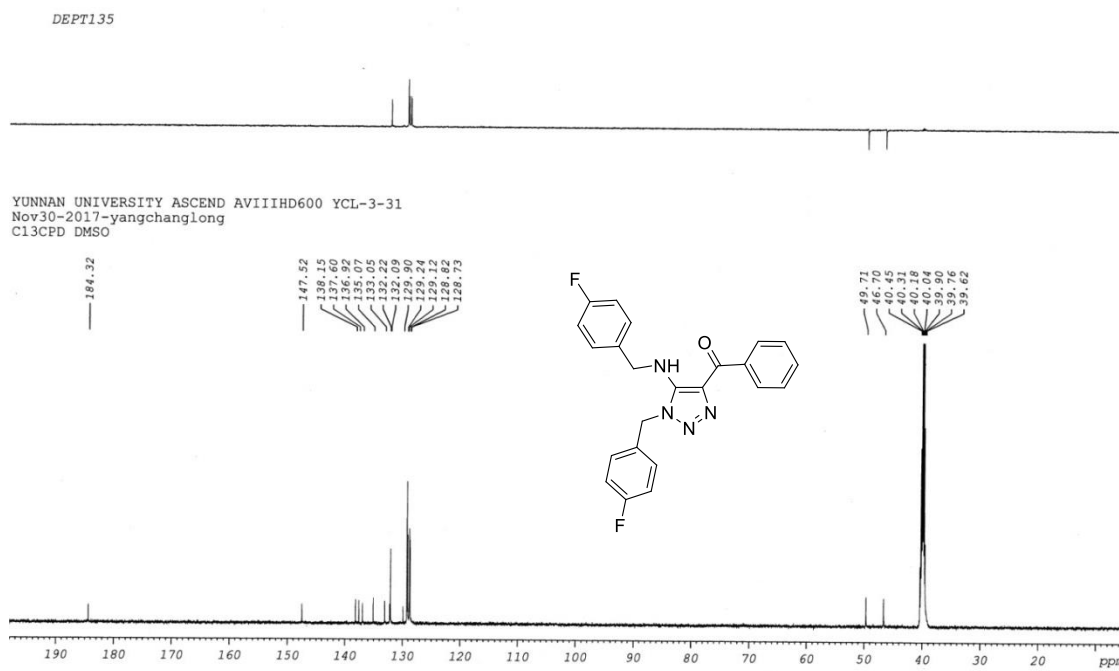


Figure 18. ¹³C NMR (150 MHz, DMSO-*d*₆) spectra of compound **3i**

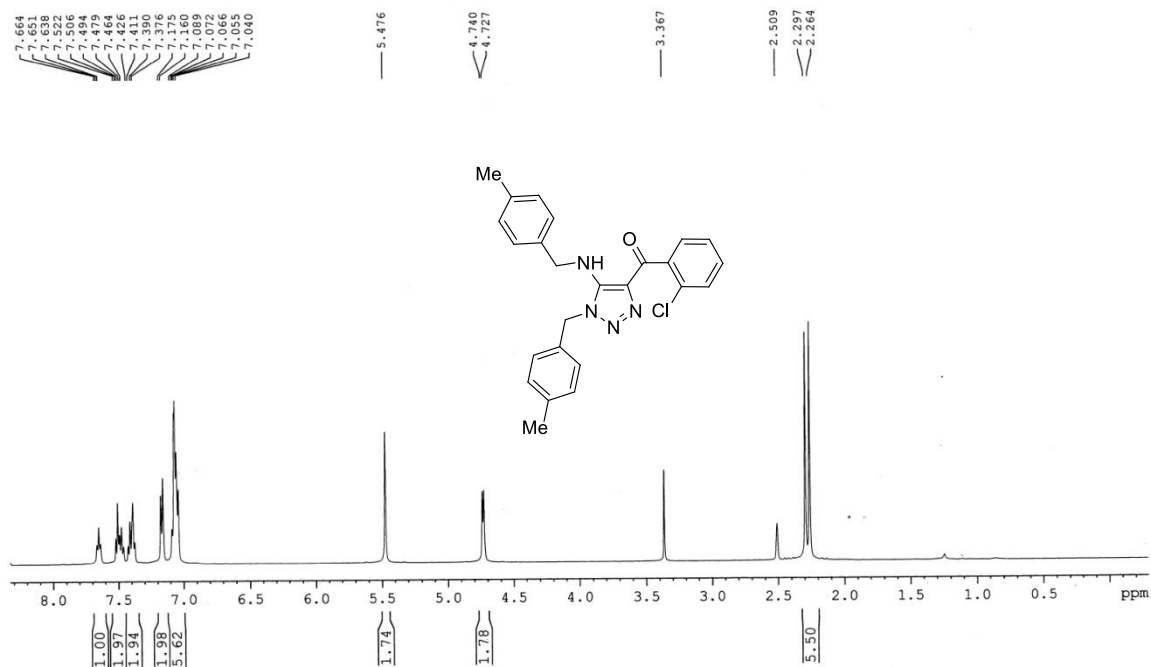


Figure 21. ¹H NMR (500 MHz, DMSO-*d*₆) spectra of compound 3k

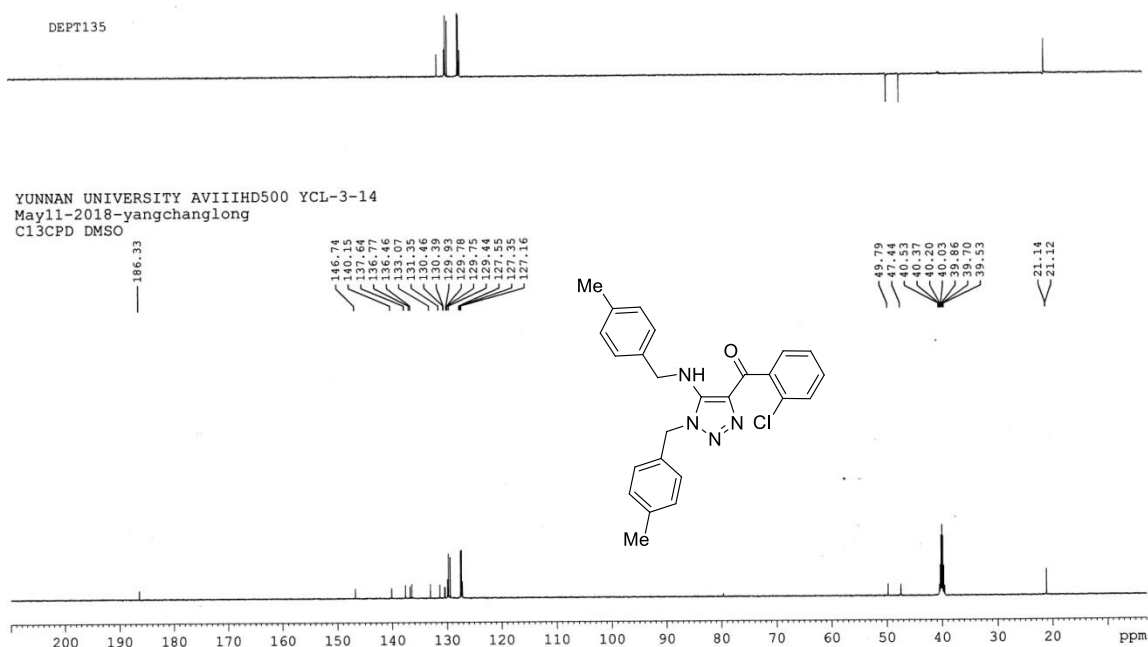


Figure 22. ¹³C NMR (125 MHz, DMSO-*d*₆) spectra of compound 3k

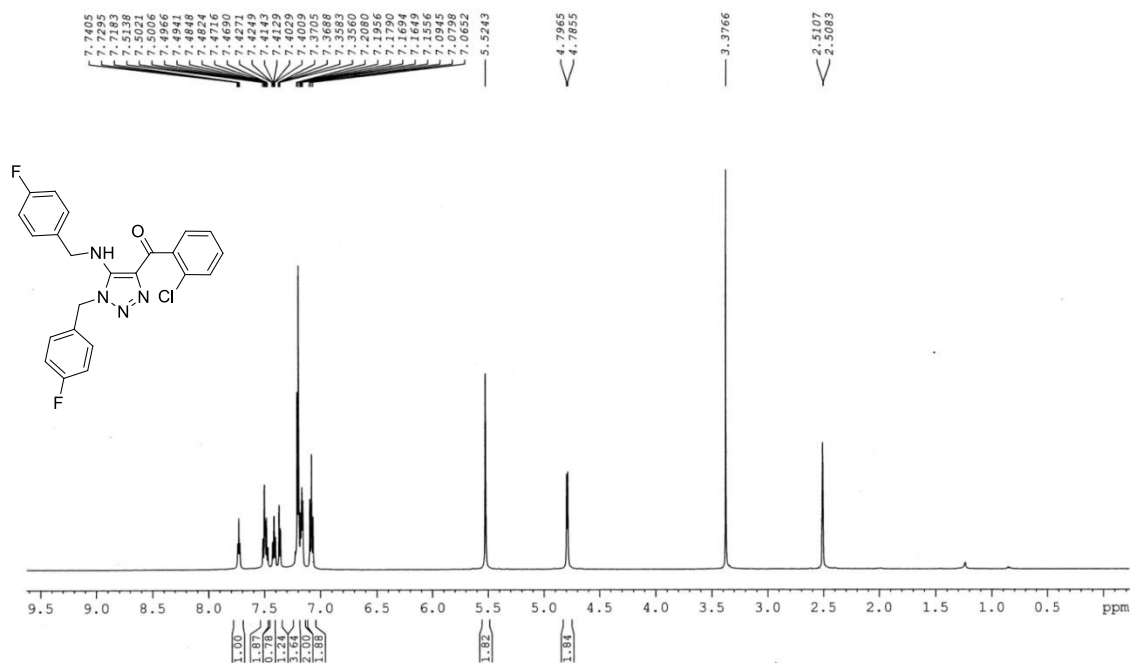


Figure 23. ¹H NMR (600 MHz, DMSO-*d*₆) spectra of compound **3l**

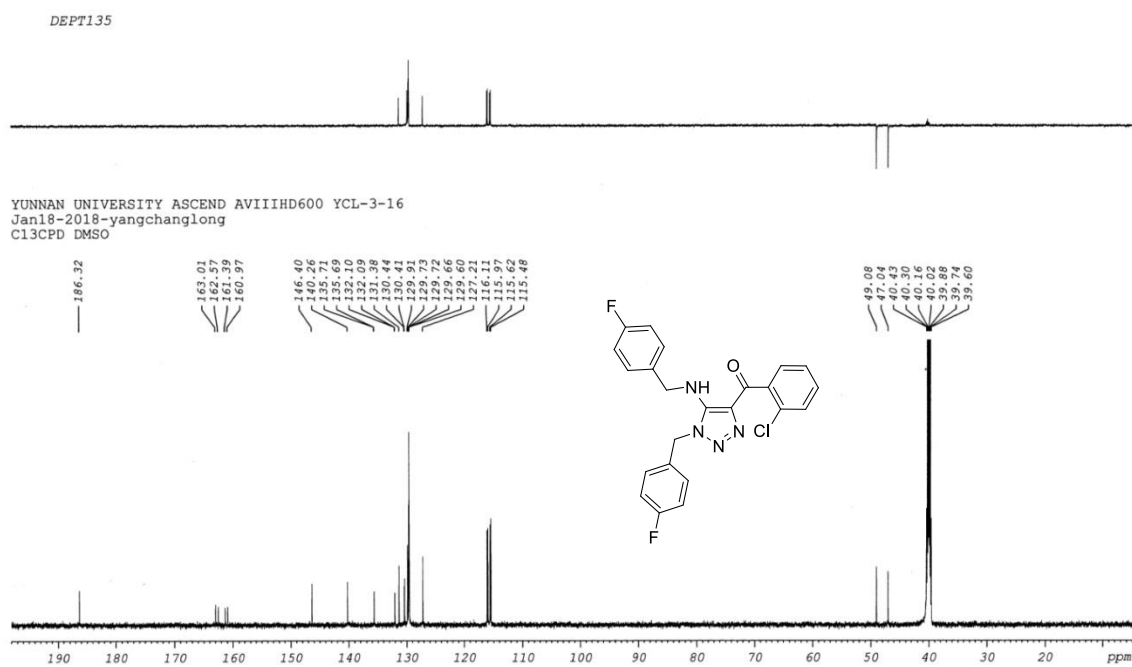


Figure 24. ¹³C NMR (150 MHz, DMSO-*d*₆) spectra of compound **3l**

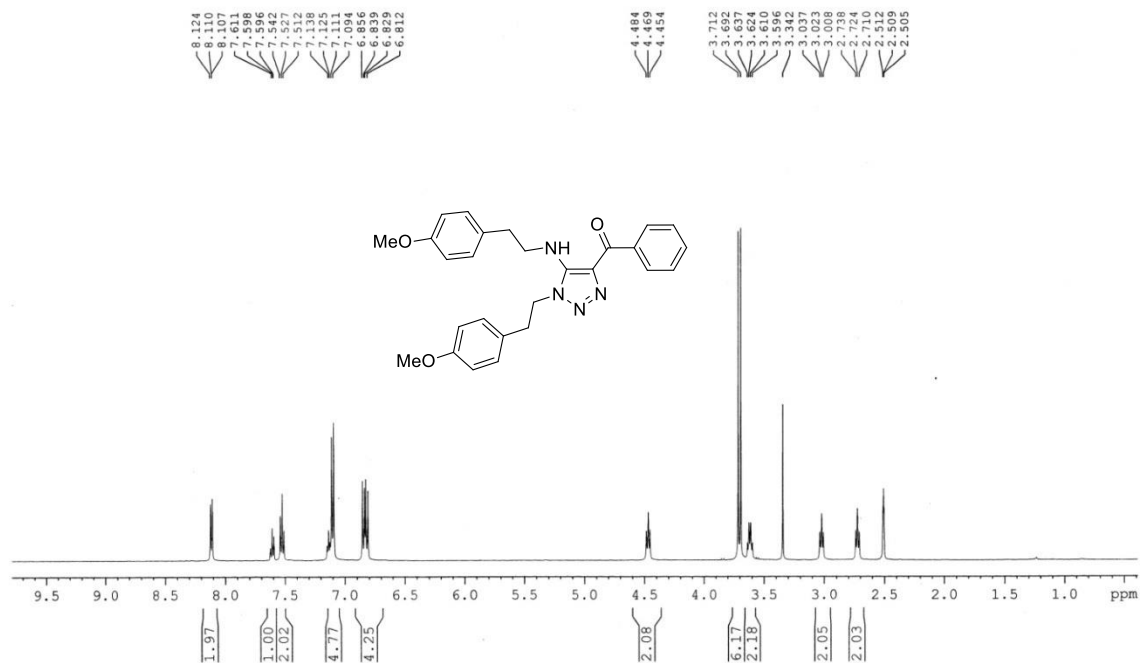


Figure 25. ¹H NMR (500 MHz, DMSO-*d*₆) spectra of compound 3m

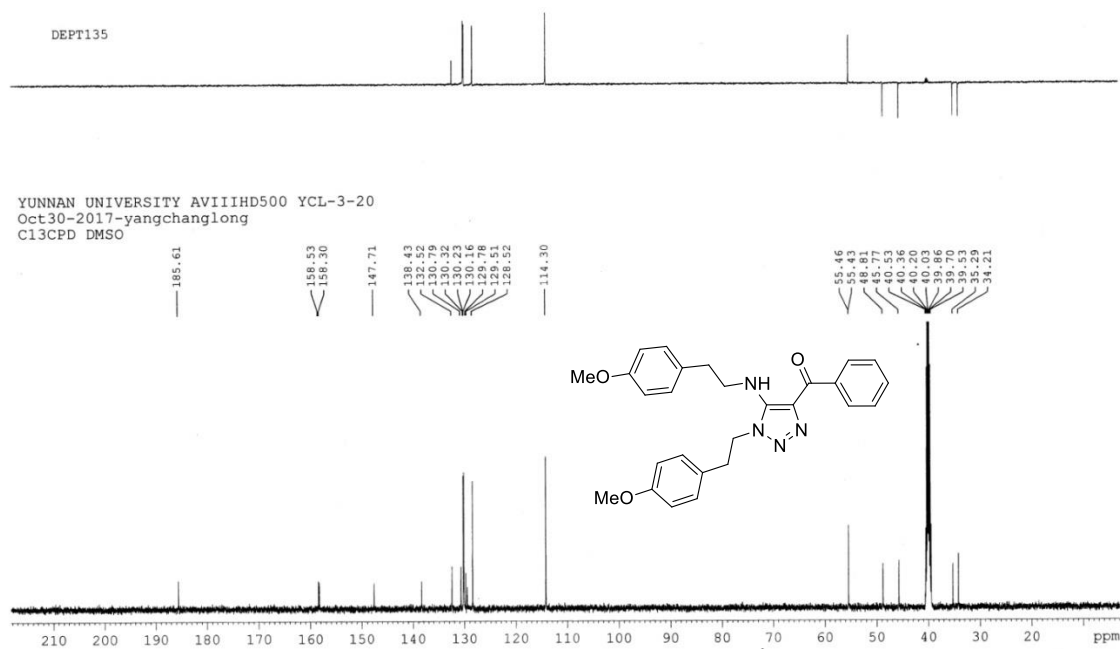


Figure 26. ¹³C ¹H NMR (125 MHz, DMSO-*d*₆) spectra of compound 3m

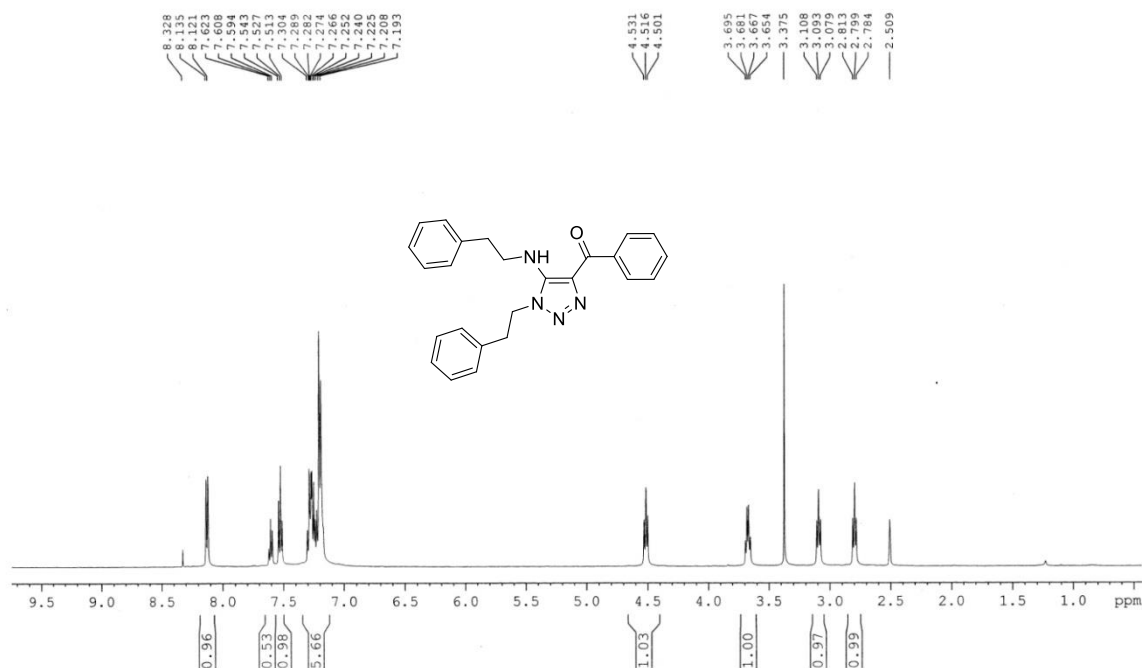


Figure 27. ¹H NMR (500 MHz, DMSO-*d*₆) spectra of compound **3n**

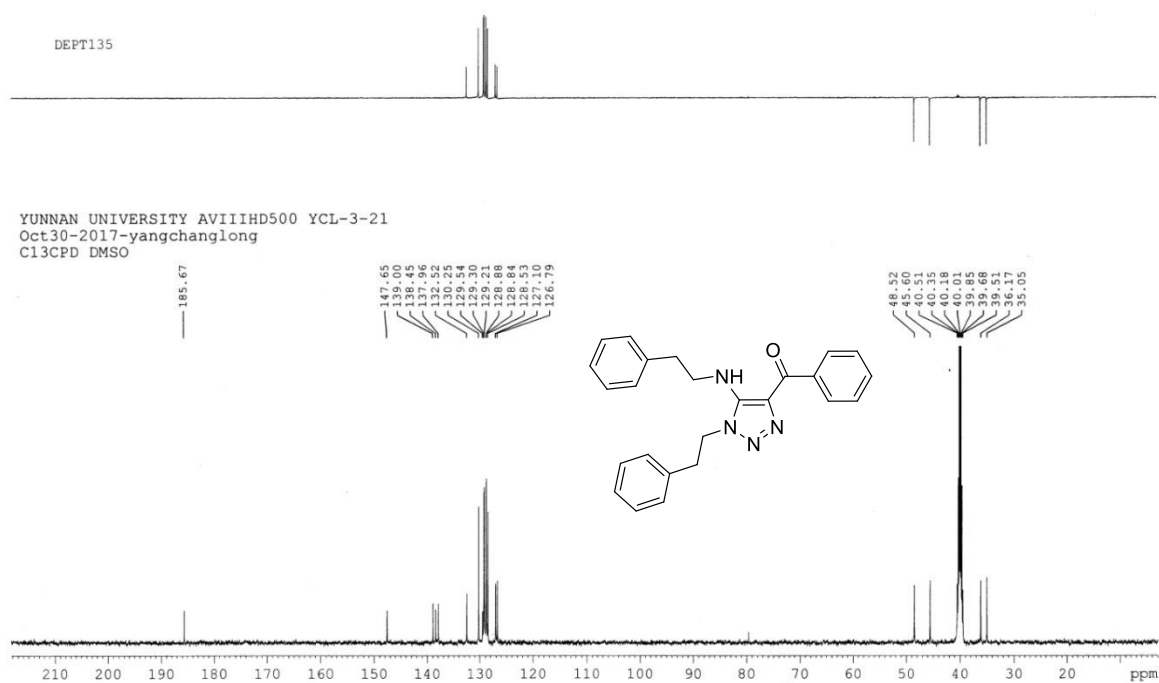


Figure 28. ¹³C NMR (125 MHz, DMSO-*d*₆) spectra of compound **3n**

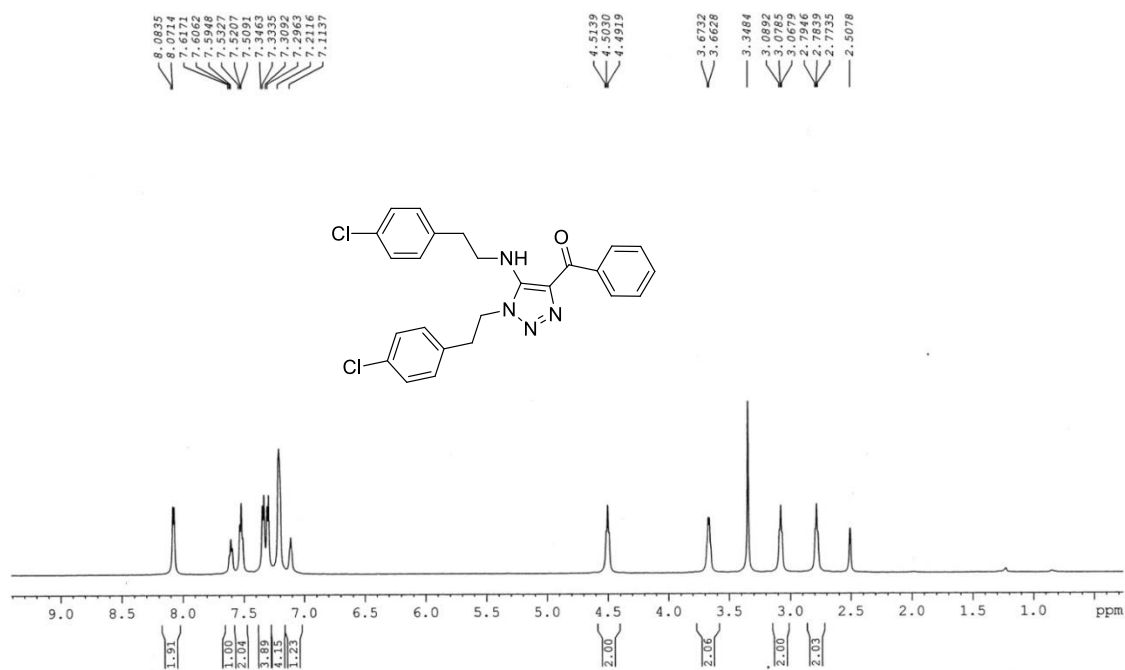


Figure 29. ¹H NMR (600 MHz, DMSO-*d*₆) spectra of compound **3o**

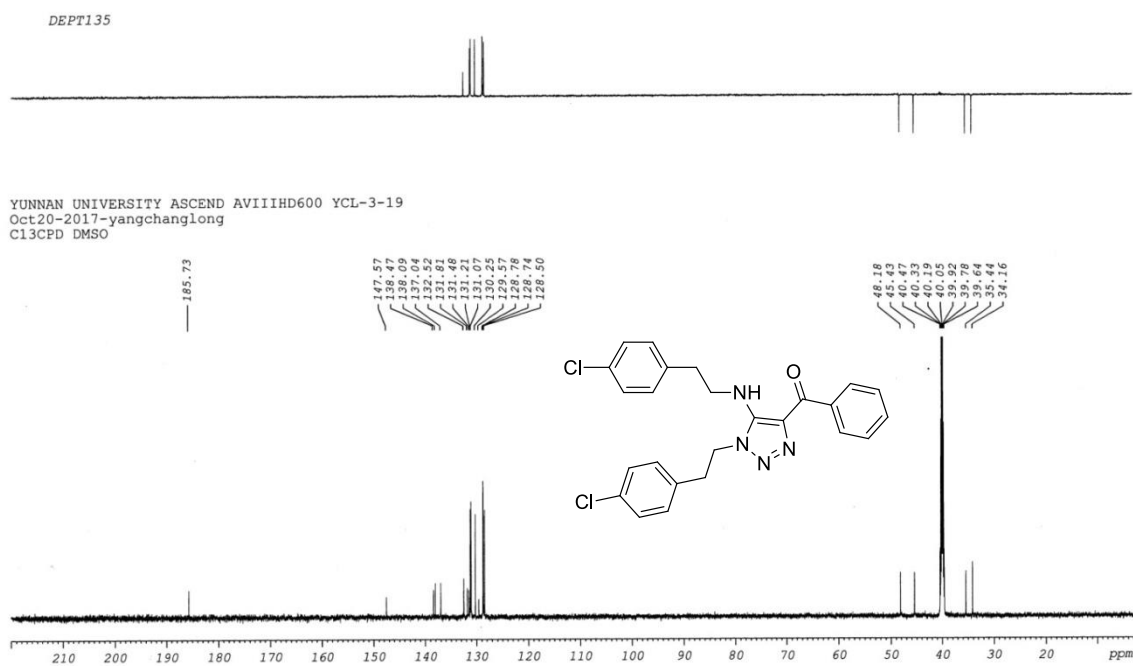


Figure 30. ¹³C NMR (150 MHz, DMSO-*d*₆) spectra of compound **3o**

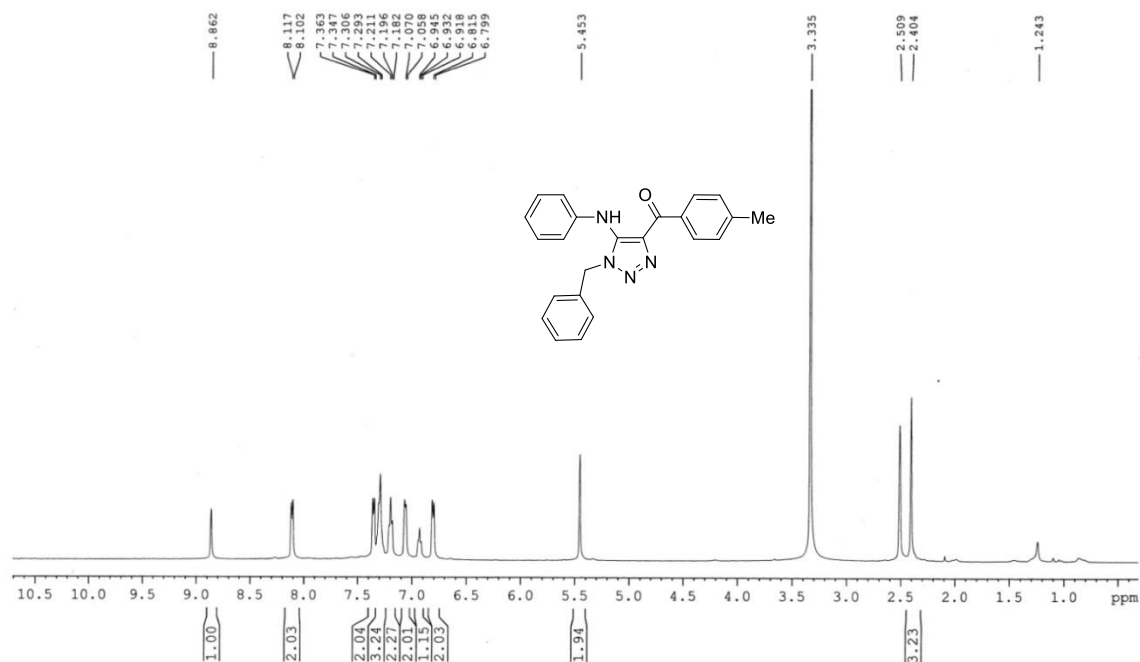


Figure 31. ¹H NMR (500 MHz, DMSO-*d*₆) spectra of compound 4a

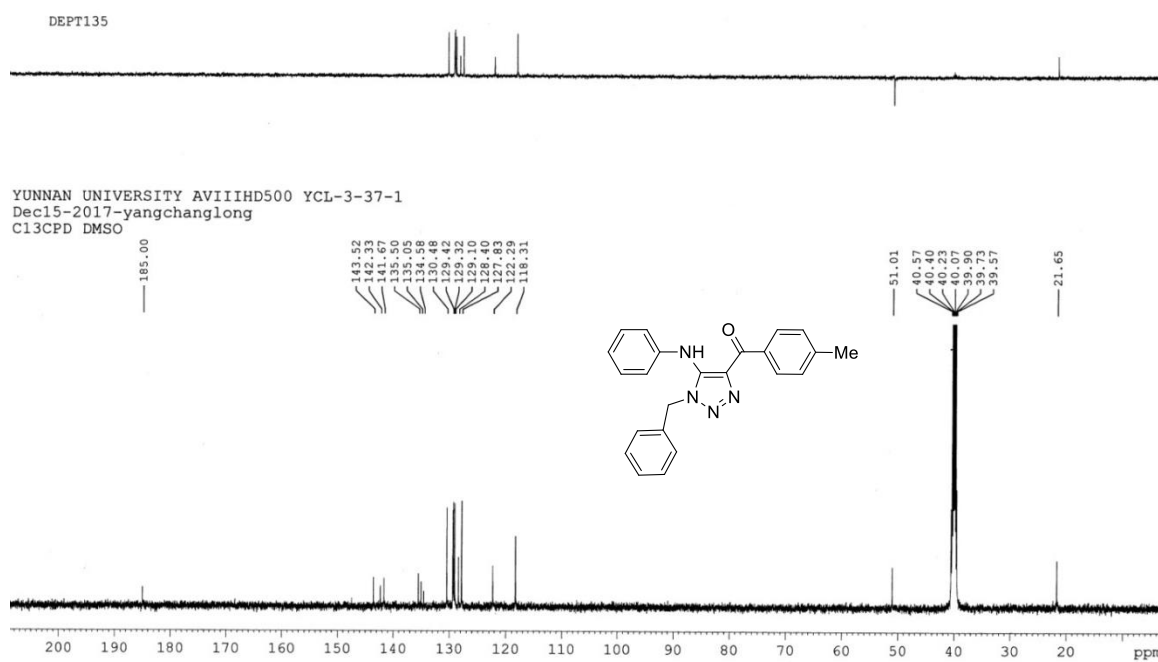


Figure 32. ¹³C NMR (125 MHz, DMSO-*d*₆) spectra of compound 4a

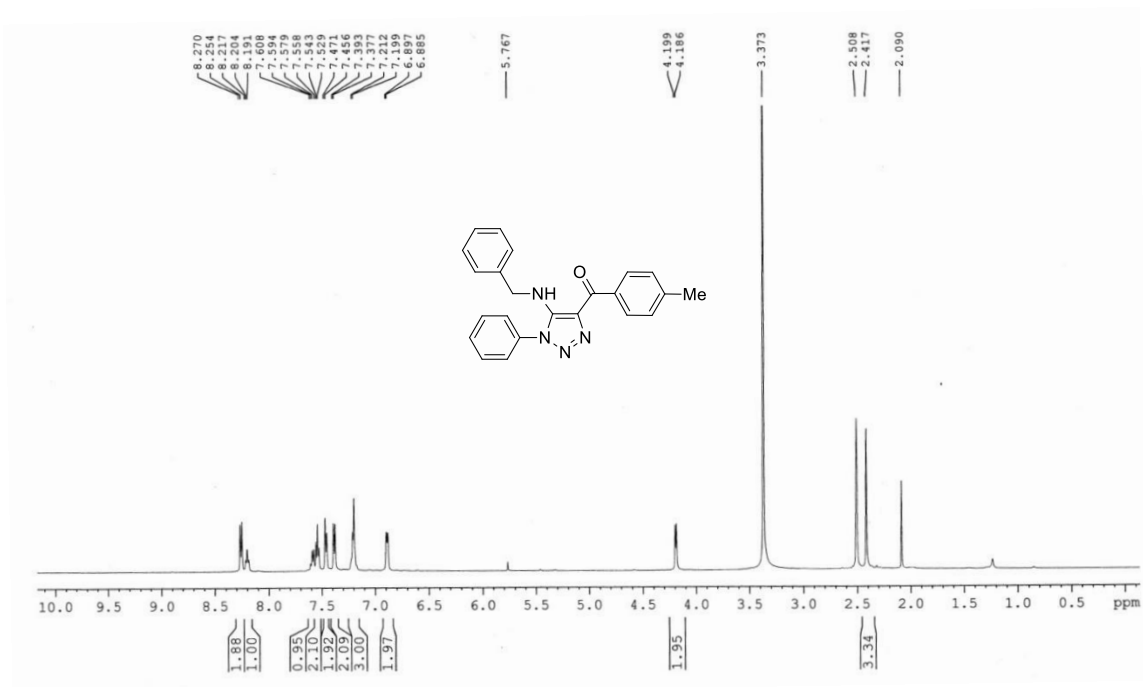


Figure 33. ¹H NMR (500 MHz, DMSO-*d*₆) spectra of compound 4a'

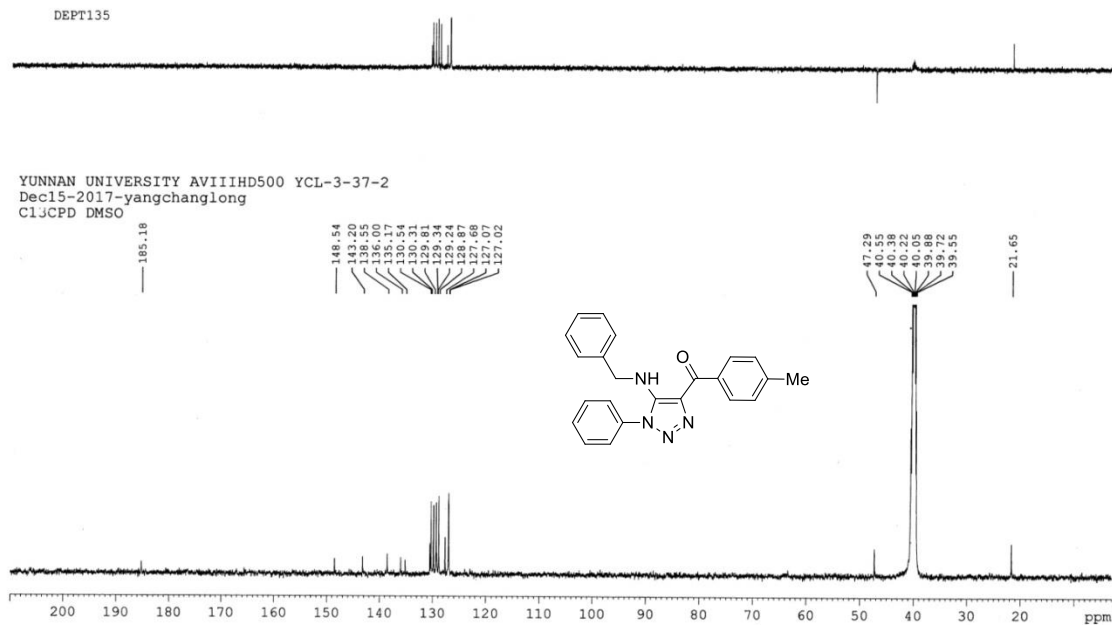


Figure 34. ¹³C NMR (125 MHz, DMSO-*d*₆) spectra of compound 4a'

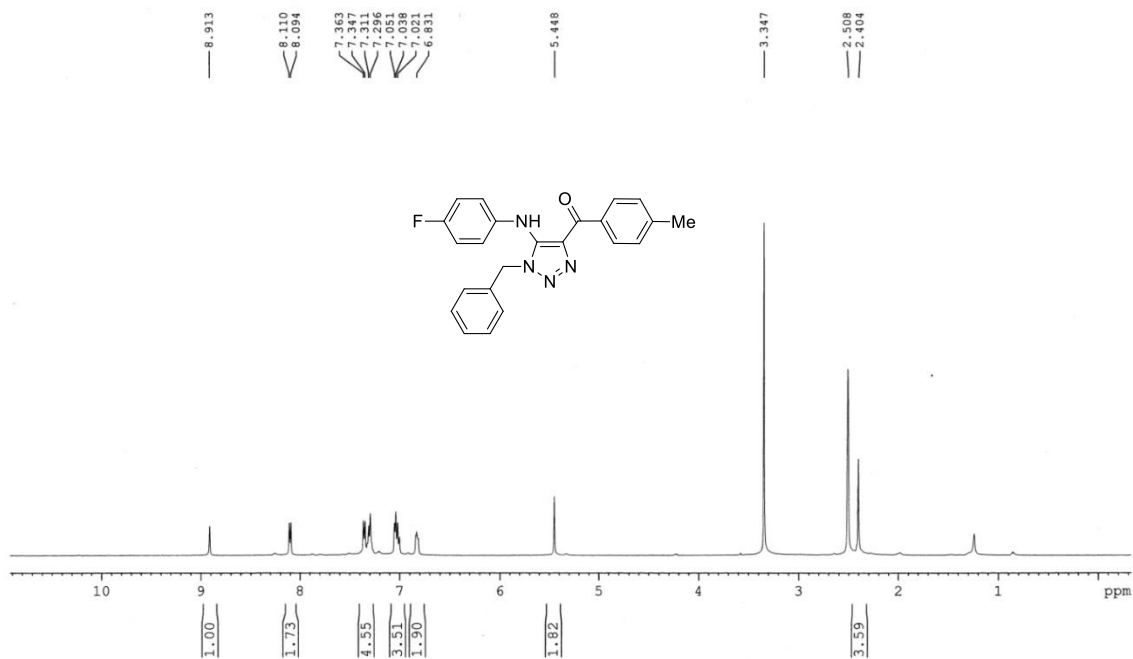


Figure 35. ¹H NMR (500 MHz, DMSO-*d*₆) spectra of compound 4b

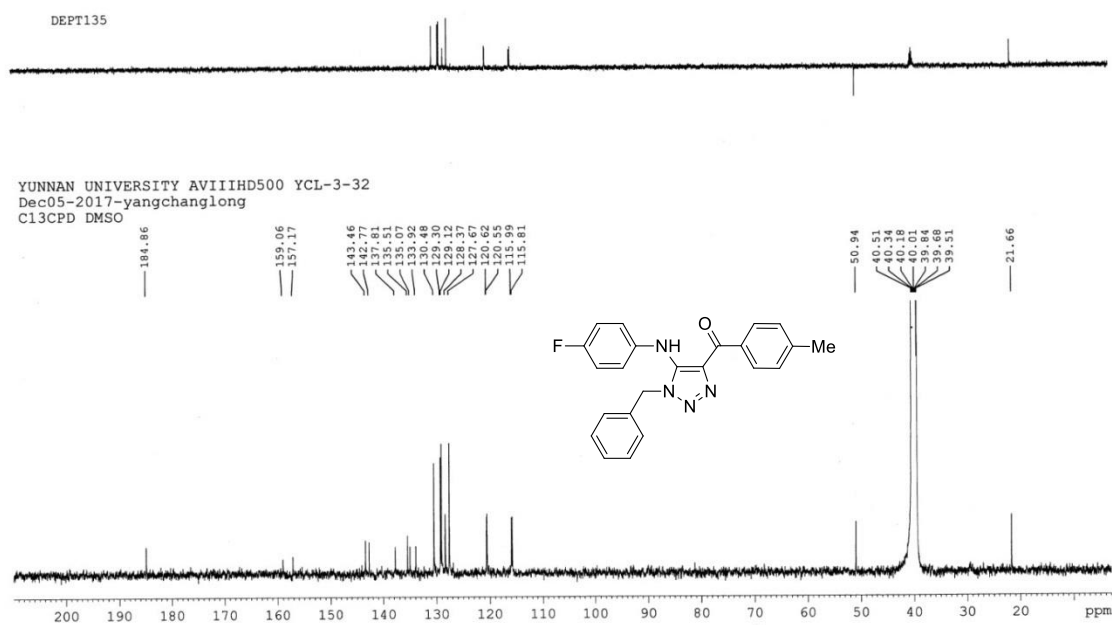


Figure 36. ¹³C NMR (125 MHz, DMSO-*d*₆) spectra of compound 4b

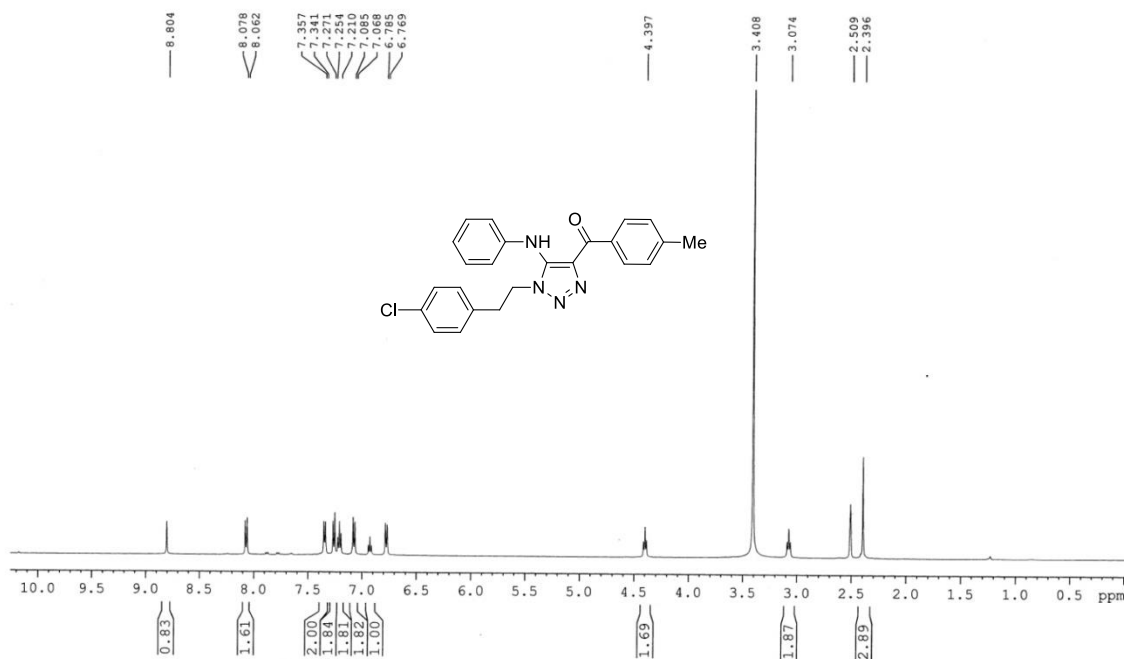


Figure 37. ¹H NMR (500 MHz, DMSO-*d*₆) spectra of compound 4c

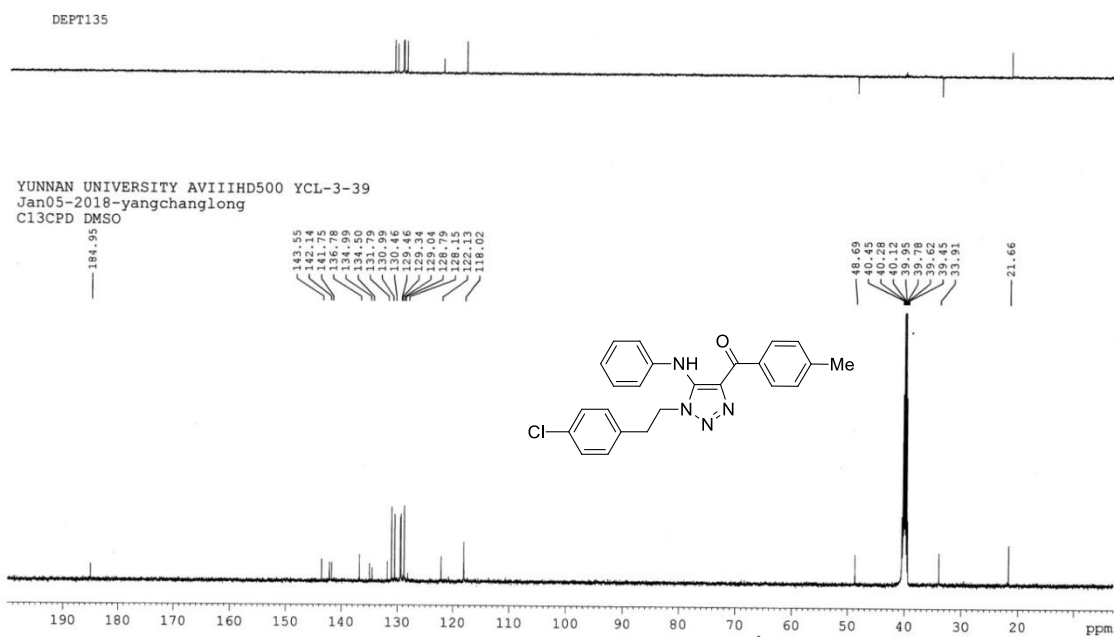


Figure 38. ¹³C NMR (125 MHz, DMSO-*d*₆) spectra of compound 4c

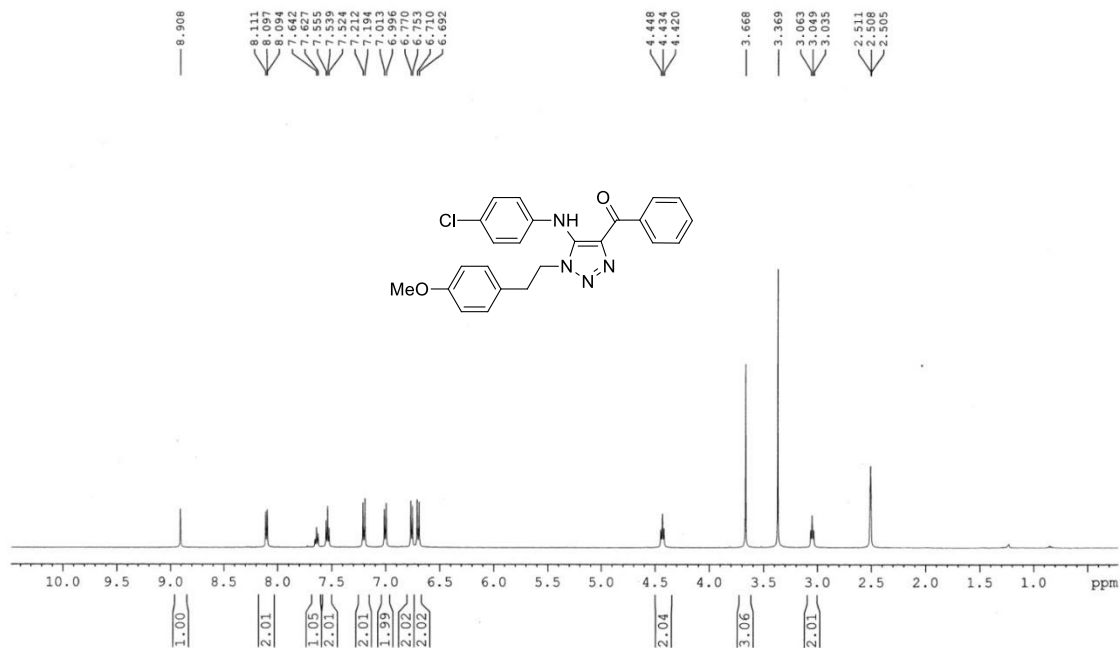


Figure 39. ¹H NMR (500 MHz, DMSO-*d*₆) spectra of compound 4d

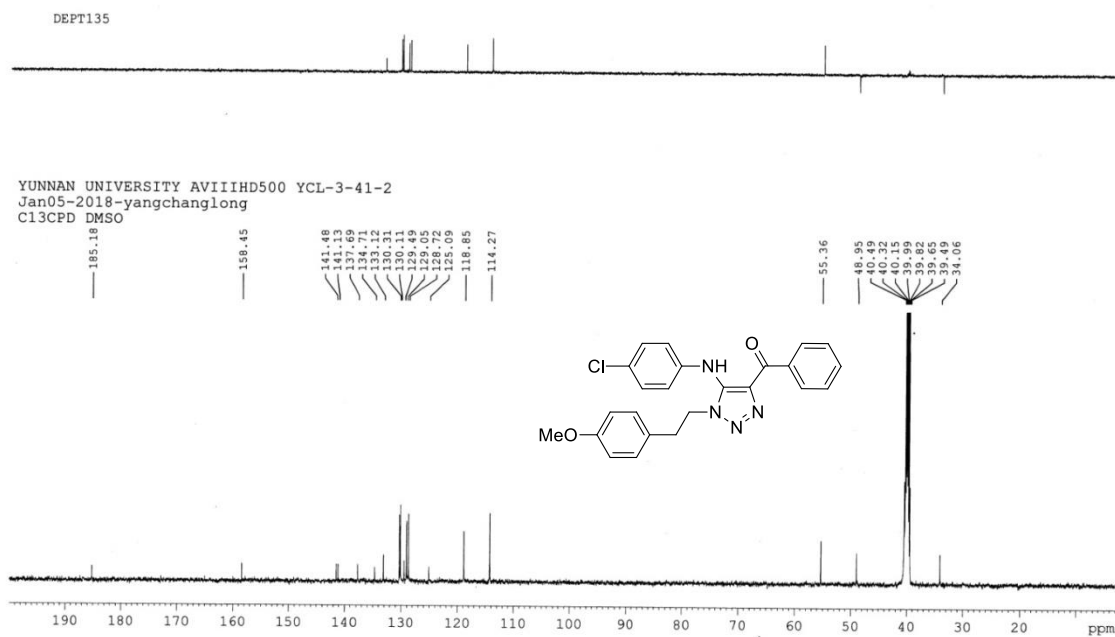


Figure 40. ¹³C NMR (125 MHz, DMSO-*d*₆) spectra of compound 4d

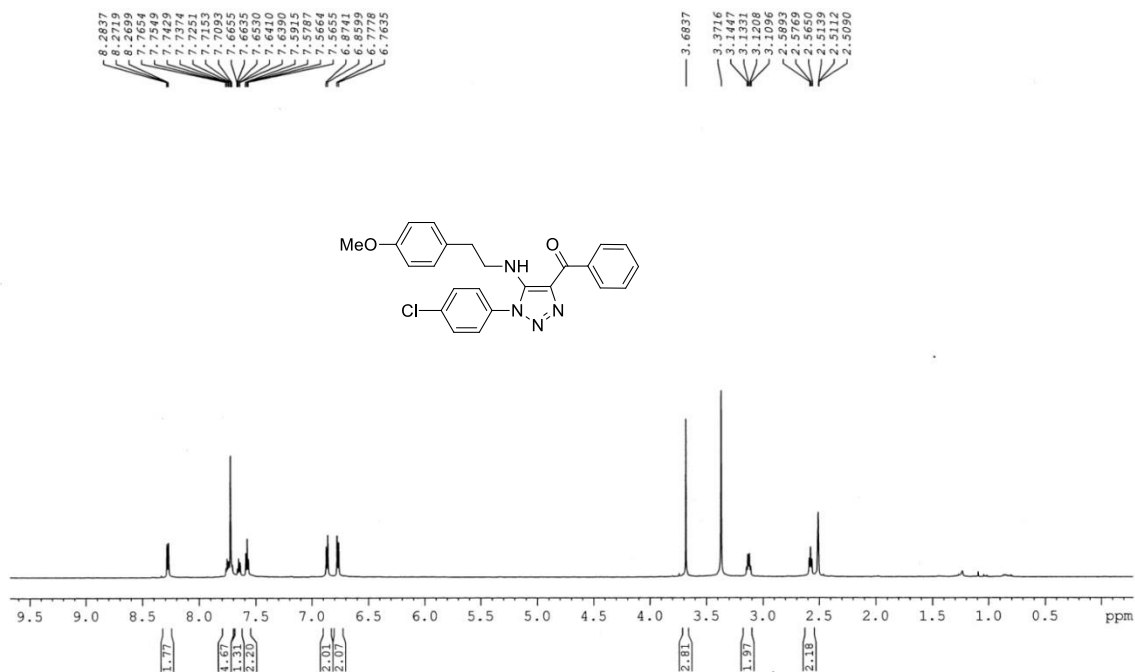


Figure 41. ¹H NMR (600 MHz, DMSO-*d*₆) spectra of compound 4d'

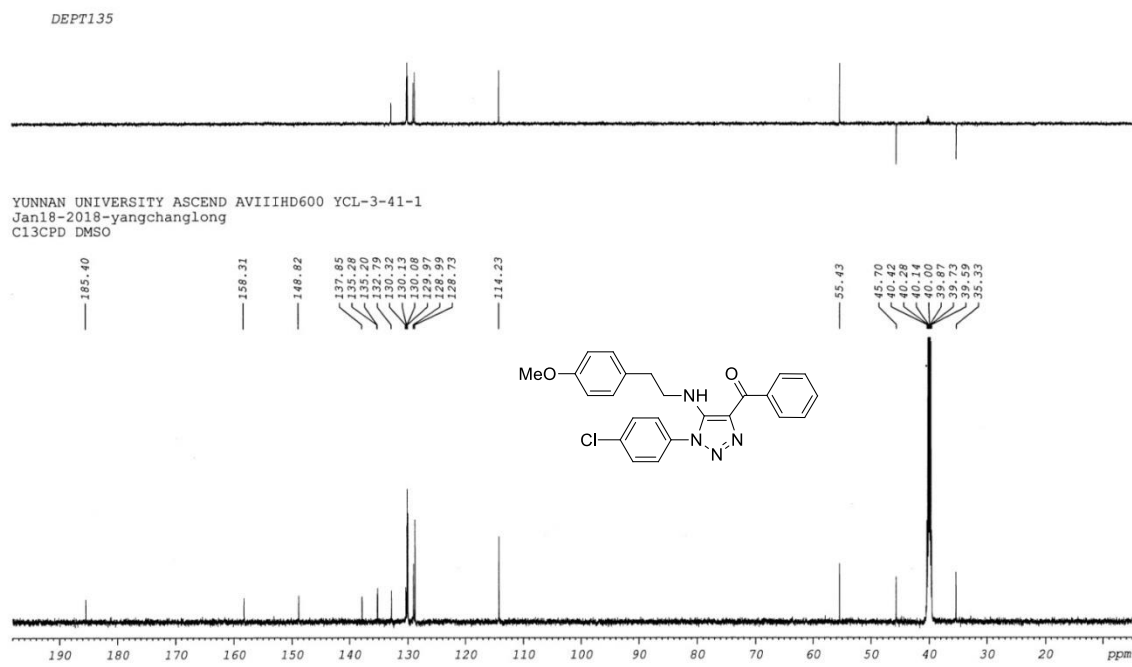


Figure 42. ¹³C NMR (150 MHz, DMSO-*d*₆) spectra of compound 4d'

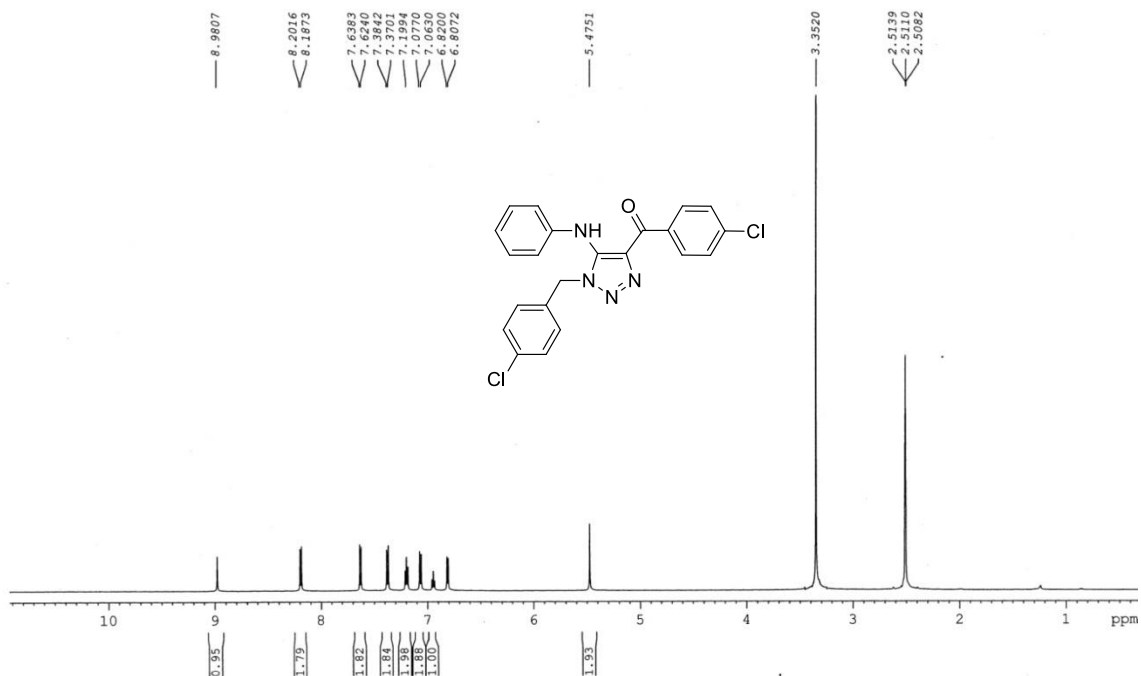


Figure 43. ¹H NMR (600 MHz, DMSO-*d*₆) spectra of compound 4e

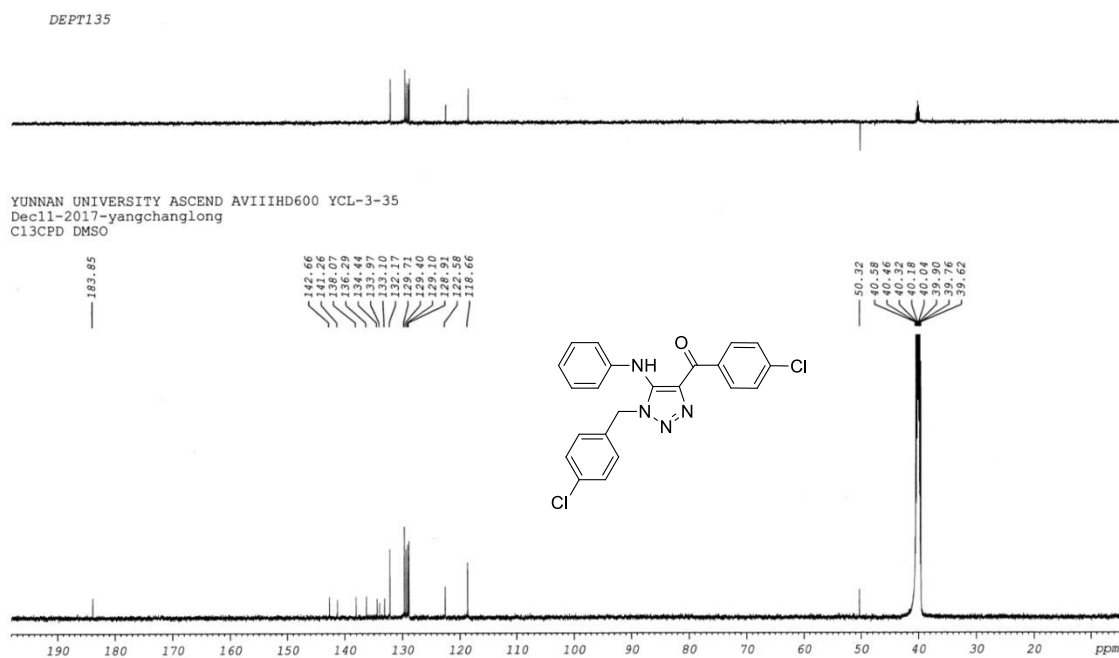


Figure 44. ¹³C NMR (150 MHz, DMSO-*d*₆) spectra of compound 4e

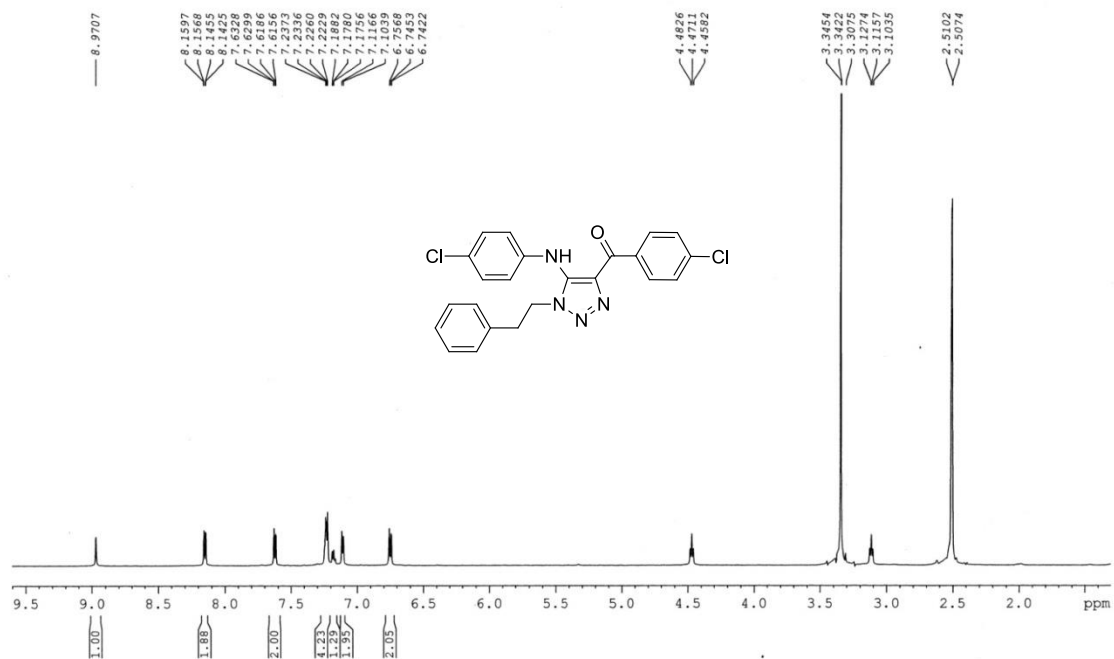


Figure 45. ¹H NMR (600 MHz, DMSO-*d*₆) spectra of compound 4f

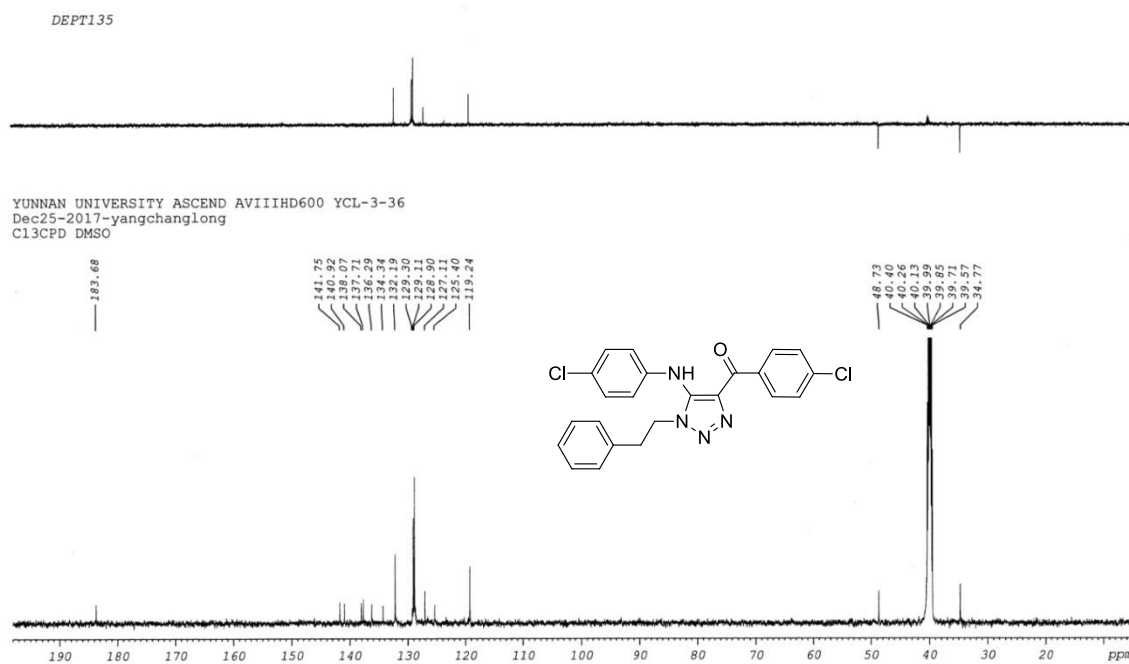


Figure 46. ¹³C NMR (150 MHz, DMSO-*d*₆) spectra of compound 4f

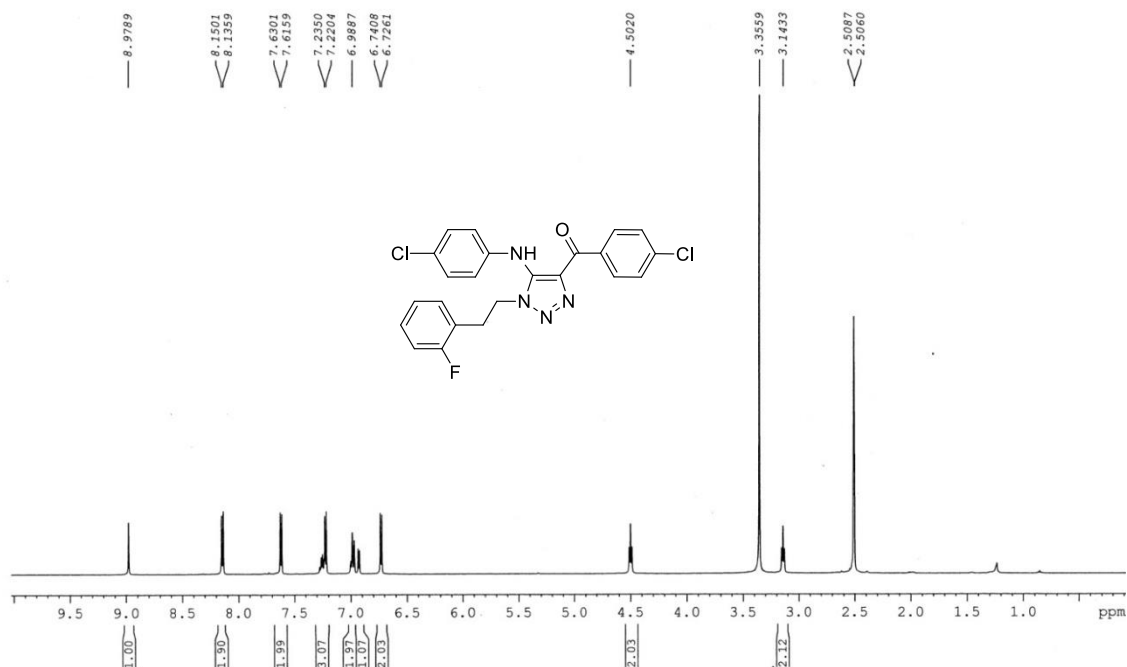


Figure 47. ¹H NMR (600 MHz, DMSO-*d*₆) spectra of compound **4g**

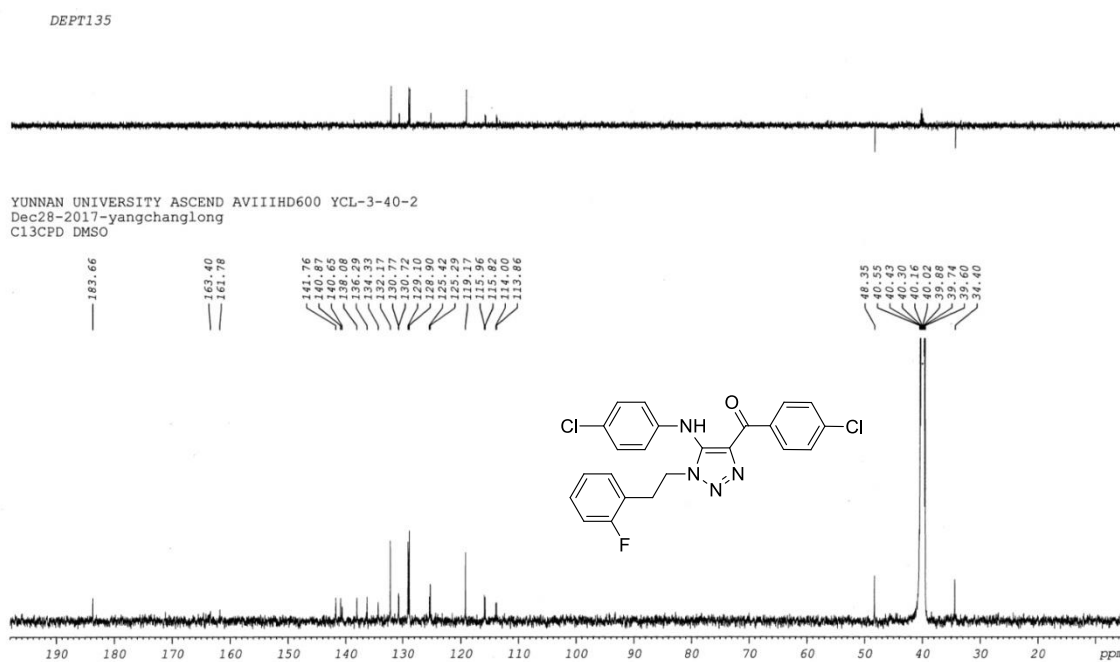


Figure 48. ¹³C NMR (150 MHz, DMSO-*d*₆) spectra of compound **4g**

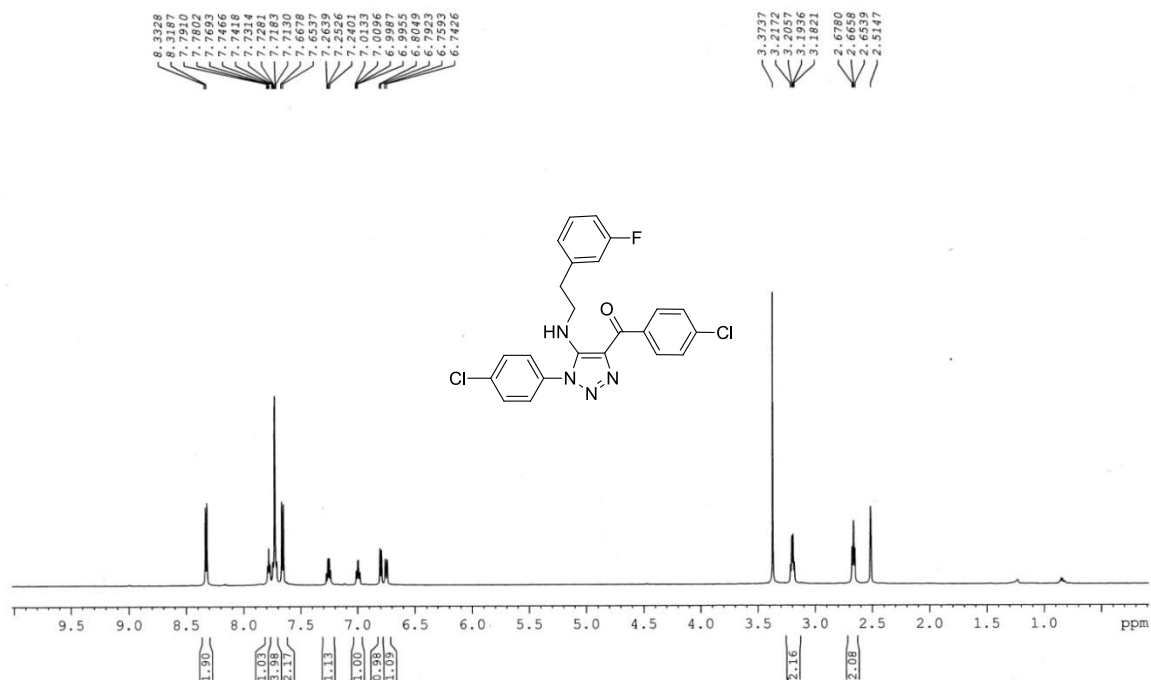


Figure 49. ¹H NMR (600 MHz, DMSO-*d*₆) spectra of compound 4g'

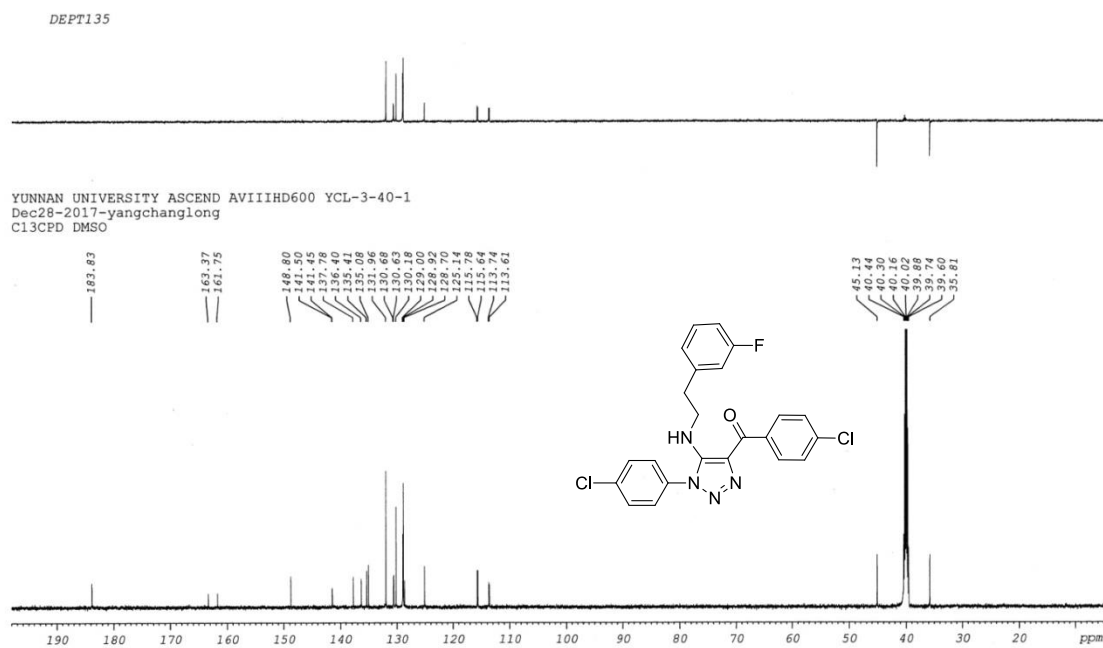


Figure 50. ¹³C NMR (150 MHz, DMSO-*d*₆) spectra of compound 4g'