Supplementary Information

Synthesis and antibacterial activity of furo[3,2-b]pyrrole derivatives

Ivana Zemanová^a, Renata Gašparová^a*, Andrej Boháč^b, Tibor Maliar^c, Filip Kraic^d and Gabriela Addová^e

^aDepartment of Chemistry and ^cDepartment of Biotechnology, Faculty of Natural Sciences, University of Ss. Cyril and Methodius, Námestie J. Herdu 2, 917 01 Trnava, Slovak Republic ^bDepartment of Organic Chemistry and ^eInstitute of Chemistry, Faculty of Natural Sciences, Comenius University, Ilkovičova 6, 842 15 Bratislava, Slovak Republic ^dSaneca Pharmaceuticals, Nitrianska 100, 920 01 Hlohovec, Slovak Republic E-mail: renata.gasparova@ucm.sk

Table of Contents

Figure S1. ¹H NMR spectrum (300 MHz, DMSO-*d*₆) of compound 1d Figure S2. ¹³C NMR spectrum (75 MHz, DMSO- d_6) of compound 1d **Figure S3.** ¹H NMR spectrum (300 MHz, DMSO- d_6) of compound **4 Figure S4**. ¹³C NMR spectrum (75 MHz, DMSO- d_6) of compound **4 Figure S5.** ¹H NMR spectrum (300 MHz, DMSO- d_6) of compound **5a** Figure S6. ¹³C NMR spectrum (75 MHz, DMSO- d_6) of compound 5a Figure S7. FTIR (ATR) spectrum of compound 5a Figure S8. ¹H NMR spectrum (300 MHz, DMSO-*d*₆) of compound **5b Figure S9**. ¹³C NMR spectrum (75 MHz, DMSO- d_6) of compound **5b** Figure S10. FTIR (ATR) spectrum of compound 5b **Figure S11.** ¹H NMR spectrum (300 MHz, DMSO- d_6) of compound **5c Figure S12**. ¹³C NMR spectrum (75 MHz, DMSO- d_6) of compound **5**c Figure S13. FTIR (ATR) spectrum of compound 5c **Figure S14.** ¹H NMR spectrum (300 MHz, DMSO- d_6) of compound **6a Figure S15**. ¹³C NMR spectrum (75 MHz, DMSO- d_6) of compound **6a** Figure S16. FTIR (ATR) spectrum of compound 6a **Figure S17.** ¹H NMR spectrum (300 MHz, DMSO- d_6) of compound **6b Figure S18**. ¹³C NMR spectrum (75 MHz, DMSO- d_6) of compound **6b** Figure S19. FTIR (ATR) spectrum of compound 6b **Figure S20.** ¹H NMR spectrum (300 MHz, DMSO- d_6) of compound **7a** Figure S21. ¹³C NMR spectrum (75 MHz, DMSO- d_6) of compound **7a Figure S22.** ¹H NMR spectrum (300 MHz, DMSO- d_6) of compound **7b Figure S23**. ¹³C NMR spectrum (75 MHz, DMSO- d_6) of compound **7b** Figure S24. FTIR (ATR) spectrum of compound 7b **Figure S25.** ¹H NMR spectrum (300 MHz, DMSO- d_6) of compound **7c Figure S26**. ¹³C NMR spectrum (75 MHz, DMSO- d_6) of compound **7**c Figure S27. FTIR (ATR) spectrum of compound 7c Figure S28. ¹H NMR spectrum (300 MHz, DMSO- d_6) of compound 8a Figure S29. ¹³C NMR spectrum (75 MHz, DMSO- d_6) of compound 8a **Figure S30.** ¹H NMR spectrum (300 MHz, DMSO- d_6) of compound **8b Figure S31**. ¹³C NMR spectrum (75 MHz, DMSO- d_6) of compound **8b** Figure S32. FTIR (ATR) spectrum of compound 8b Figure S33. ¹H NMR spectrum (300 MHz, DMSO- d_6) of compound 8c **Figure S34**. ¹³C NMR spectrum (75 MHz, DMSO- d_6) of compound **8**c Figure S35. MS (ESI-) spectrum of compound 8c Figure S36. FTIR (ATR) spectrum of compound 8c Figure S37. ¹H NMR (300 MHz, DMSO- d_6) of compound 9 Figure S38. ¹³C NMR spectrum (75 MHz, DMSO- d_6) of compound 9 Figure S39. FTIR (ATR) spectrum of compound 9 **Figure S40.** ¹H NMR spectrum (300 MHz, DMSO- d_6) of compound **10a** Figure S41. ¹³C NMR spectrum (75 MHz, DMSO-*d*₆) of compound **10a** Figure S42. FTIR (ATR) spectrum of compound 10a Figure S43. ¹H NMR (300 MHz, DMSO- d_6) of compound **10b** Figure S44. ¹³C NMR spectrum (75 MHz, DMSO-*d*₆) of compound **10b** Figure S45. FTIR (ATR) spectrum of compound 10b Figure S46. HSQC spectrum (DMSO- d_6) of compound 10b Figure S47. HMBC spectrum (DMSO- d_6) of compound 10b **Figure S48.** HMBC spectrum (DMSO- d_6) of compound **10b** Figure S49. NOESY1D spectrum (DMSO-*d*₆) of compound 10b

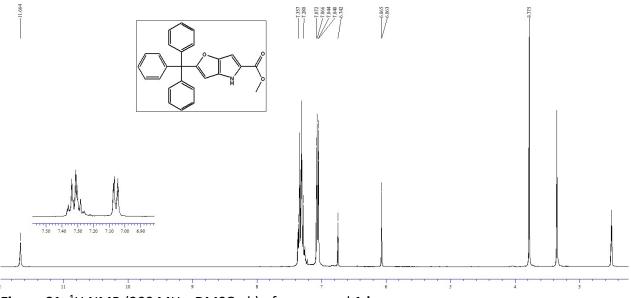


Figure S1. ¹H NMR (300 MHz, DMSO-d₆) of compound 1d

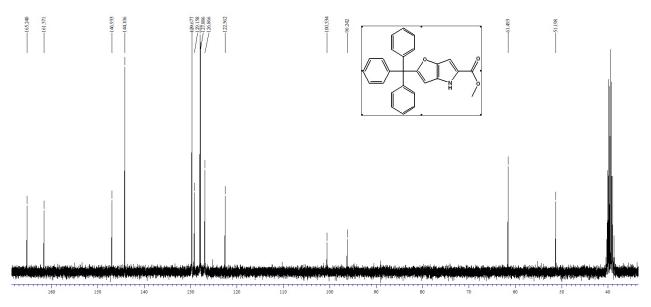


Figure S2. ¹³C NMR spectrum (75 MHz, DMSO- d_6) of compound 1d

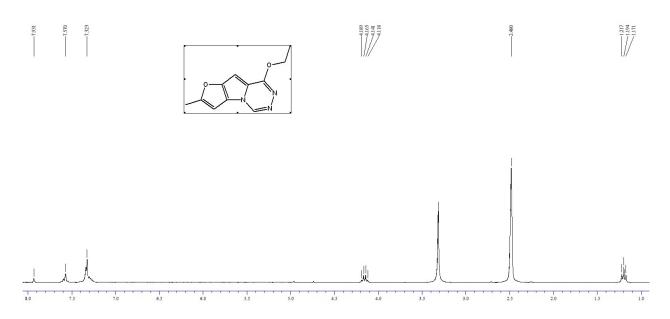


Figure S3. ¹H NMR (300 MHz, DMSO- d_6) of compound 4

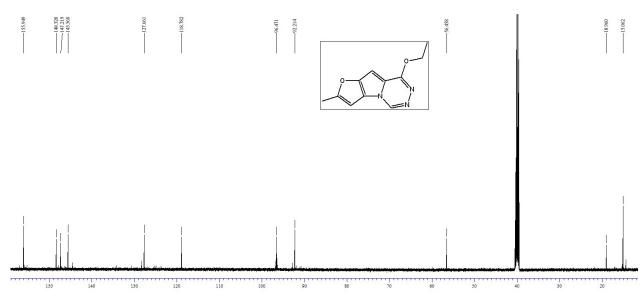


Figure S4. ¹³C NMR spectrum (75 MHz, DMSO-*d*₆) of compound 4

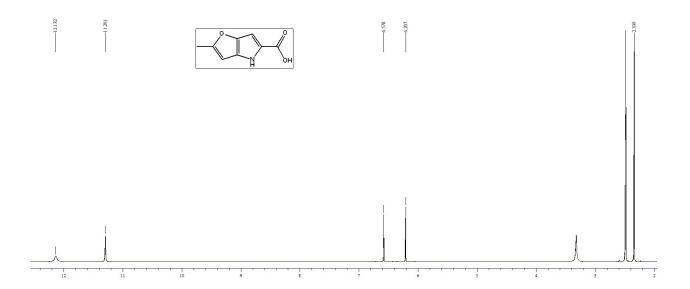


Figure S5. ¹H NMR (300 MHz, DMSO-*d*₆) of compound 5a

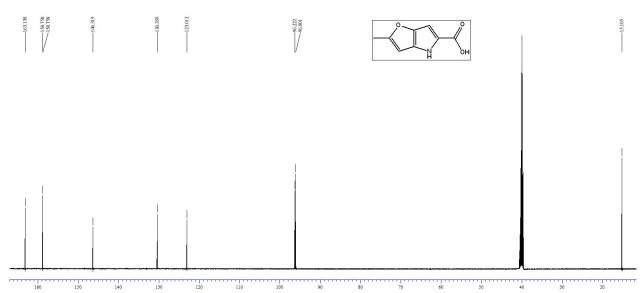


Figure S6. ¹³C NMR spectrum (75 MHz, DMSO- d_6) of compound 5a

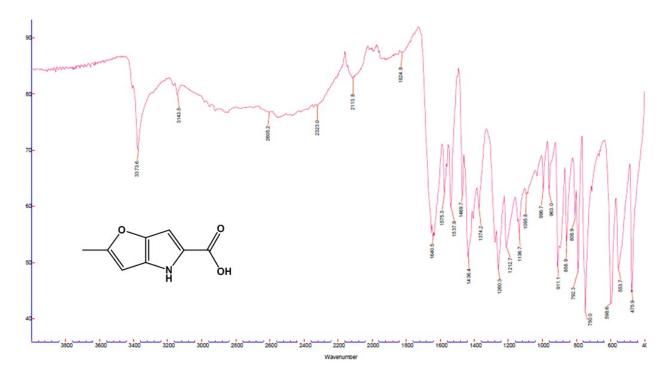


Figure S7. FTIR (ATR) spectrum of compound 5a

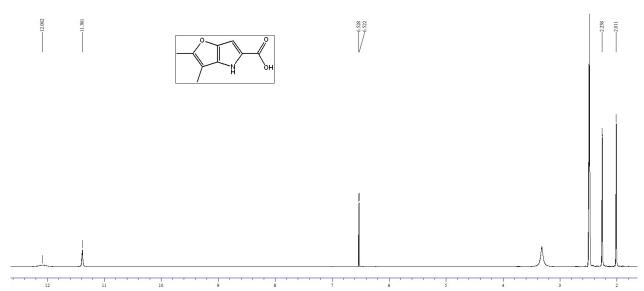


Figure S8. ¹H NMR (300 MHz, DMSO-*d*₆) of compound **5b**

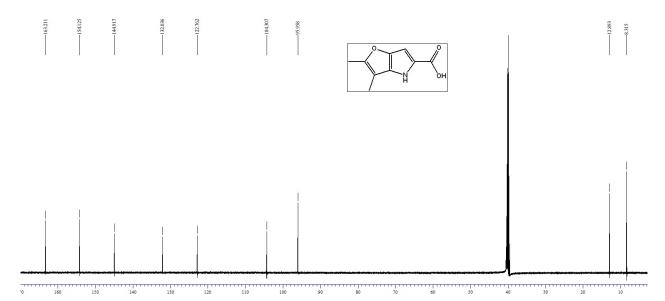


Figure S9. ¹³C NMR spectrum (75 MHz, DMSO-*d*₆) of compound **5b**

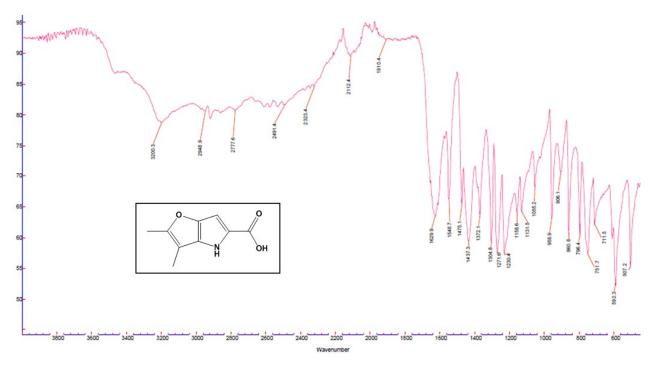
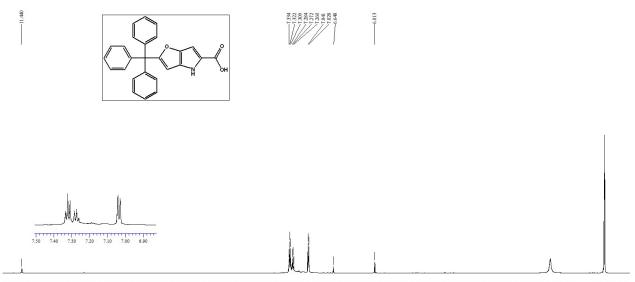


Figure S10. FTIR (ATR) spectrum of compound 5b



11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5

Figure S11. ¹H NMR (300 MHz, DMSO- d_6) of compound **5**c

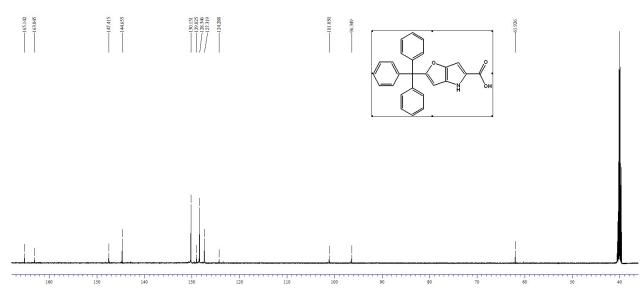


Figure S12. ¹³C NMR spectrum (75 MHz, DMSO- d_6) of compound 5c

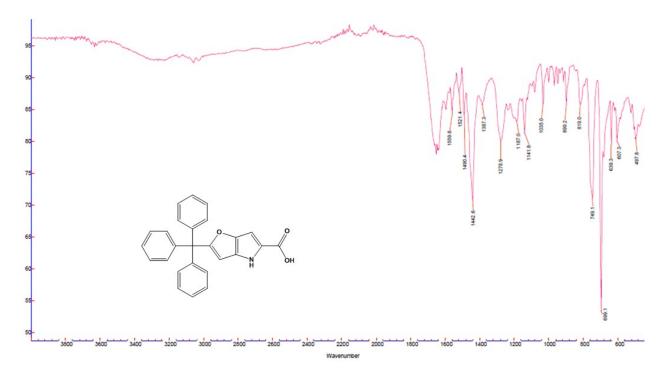


Figure S13. FTIR (ATR) spectrum of compound 5c

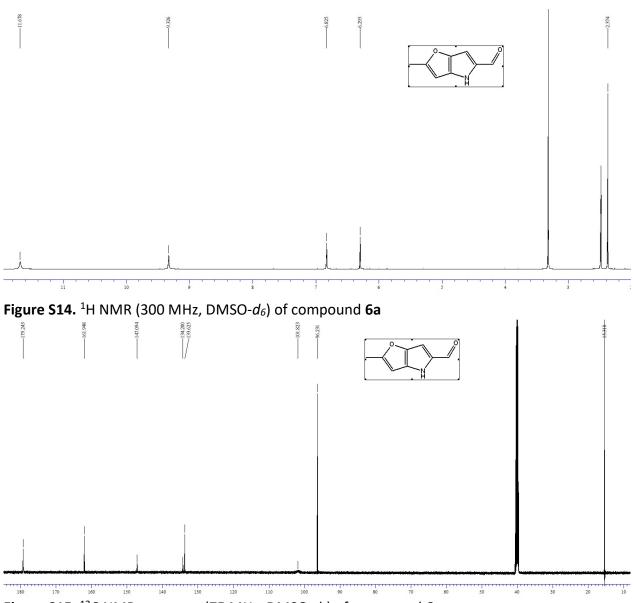


Figure S15. ¹³C NMR spectrum (75 MHz, DMSO-*d*₆) of compound 6a

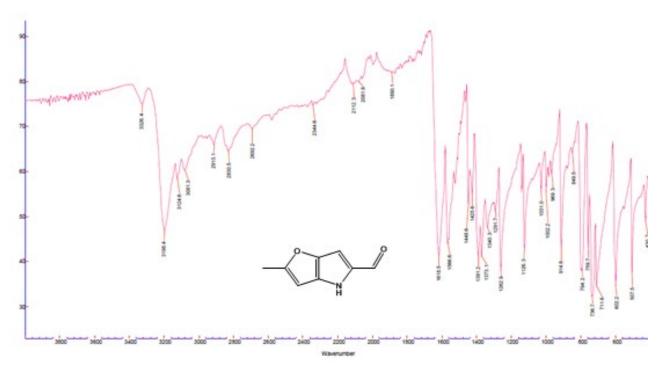


Figure S16. FTIR (ATR) spectrum of compound 6a

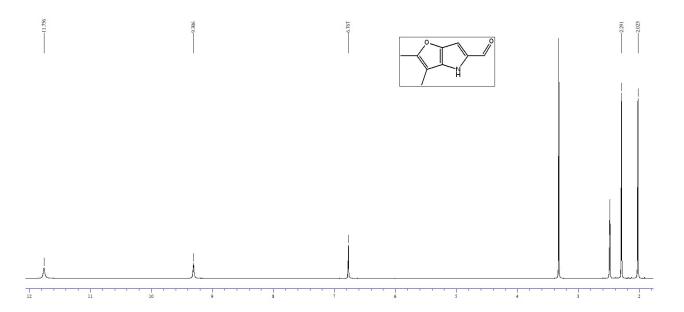


Figure S17. ¹H NMR (300 MHz, DMSO- d_6) of compound **6b**



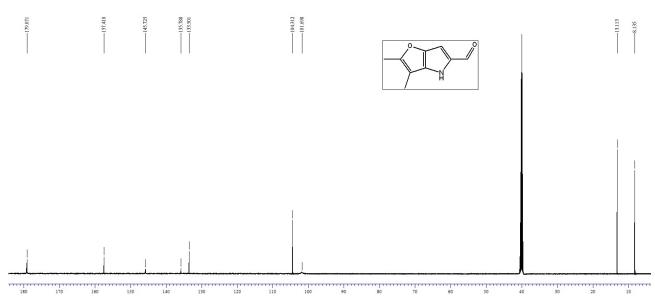


Figure S18. ¹³C NMR spectrum (75 MHz, DMSO-*d*₆) of compound 6b

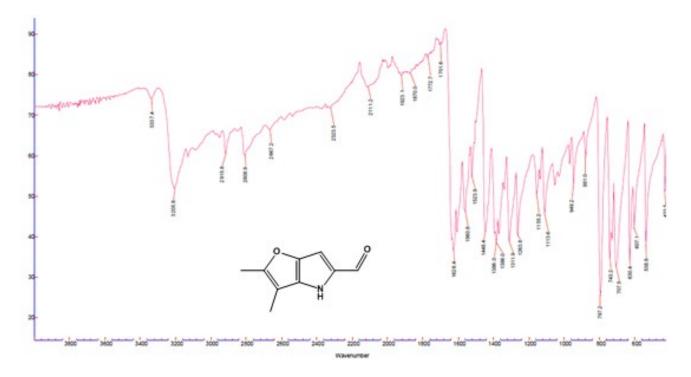


Figure S19. FTIR (ATR) spectrum of compound 6b

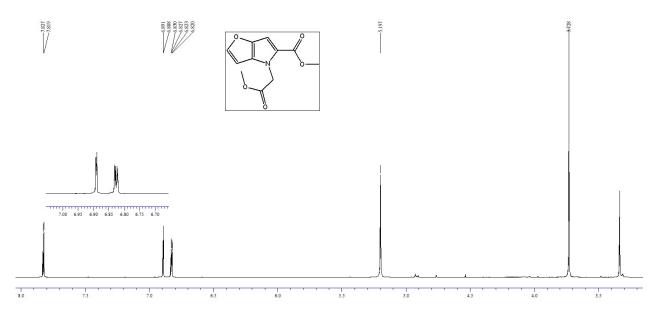


Figure S20. ¹H NMR (300 MHz, DMSO-*d*₆) of compound 7a

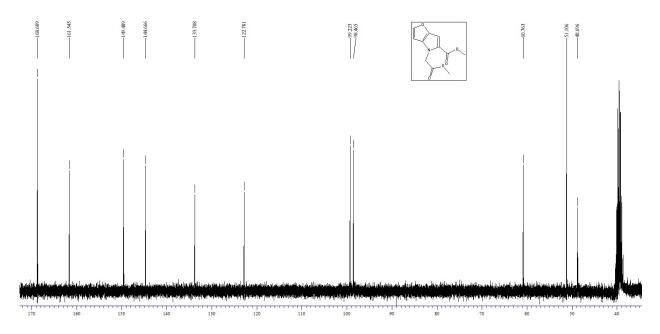


Figure S21. ¹³C NMR spectrum (75 MHz, DMSO-*d*₆) of compound 7a

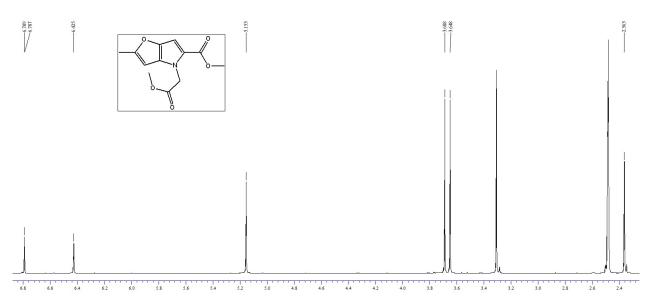


Figure S22. ¹H NMR (300 MHz, DMSO-*d*₆) of compound **7b**

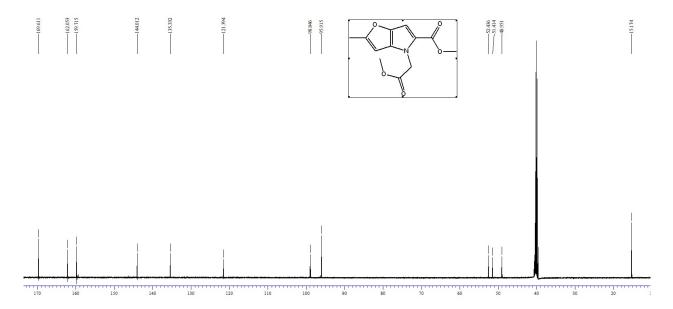


Figure S23. ¹³C NMR spectrum (75 MHz, DMSO-*d*₆) of compound 7b

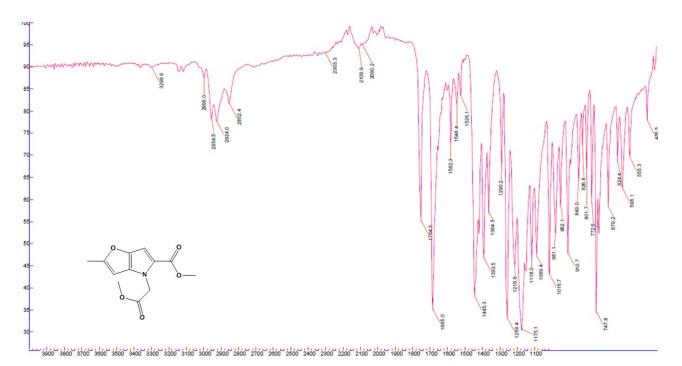


Figure S24. FTIR (ATR) spectrum of compound 7b

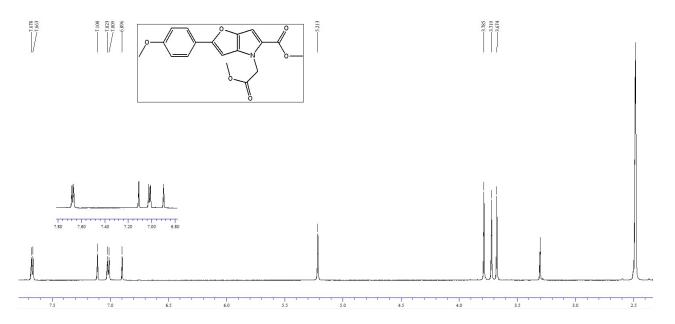


Figure S25. ¹H NMR (300 MHz, DMSO- d_6) of compound 7c

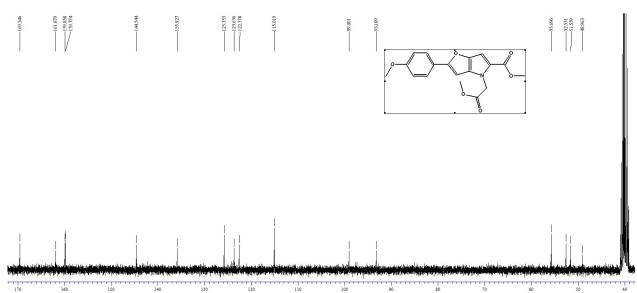
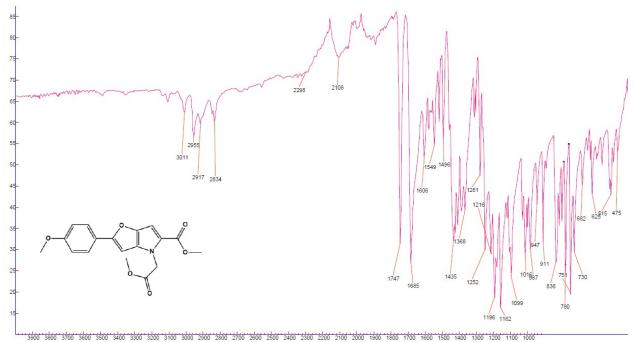
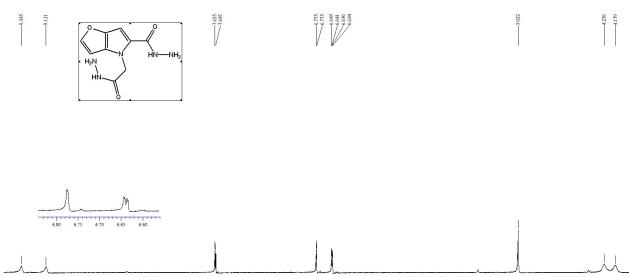


Figure S26. ¹³C NMR spectrum (75 MHz, DMSO-*d*₆) of compound 7c



Wavenumber

Figure S27. FTIR (ATR) spectrum of compound 7c



5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5

Figure S28. ¹H NMR (300 MHz, DMSO-*d*₆) of compound 8a

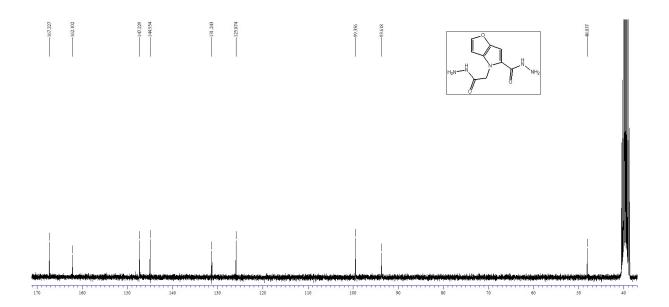


Figure S29. ¹³C NMR spectrum (75 MHz, DMSO-*d*₆) of compound 8a

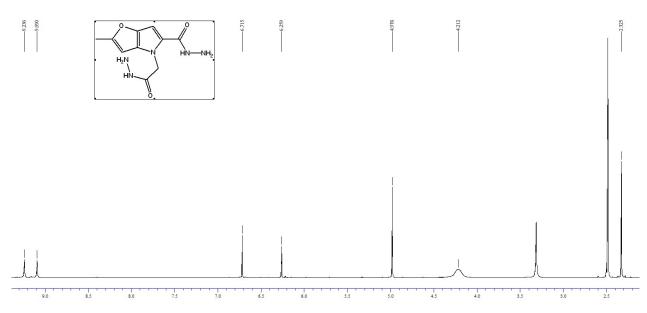


Figure S30. ¹H NMR (300 MHz, DMSO-*d*₆) of compound **8b**

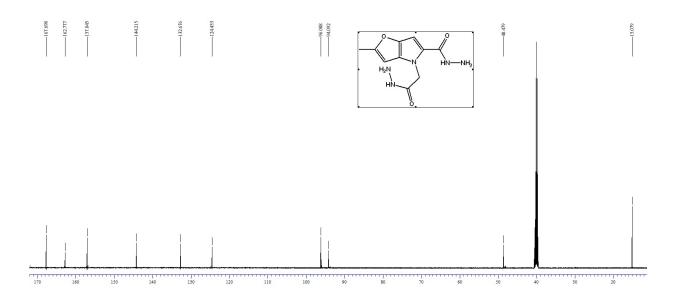


Figure S31. ¹³C NMR spectrum (75 MHz, DMSO-*d*₆) of compound 8b

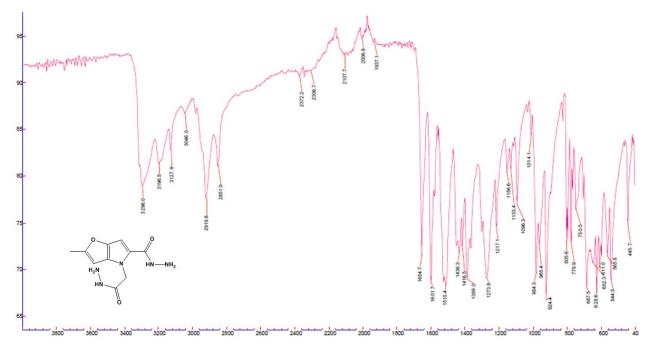


Figure S32. FTIR (ATR) spectrum of compound 8b

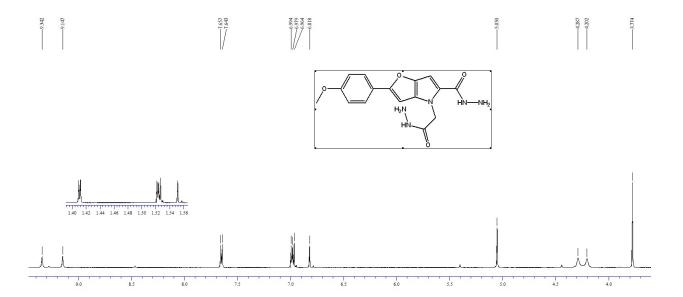


Figure S33. ¹H NMR (300 MHz, DMSO- d_6) of compound 8c

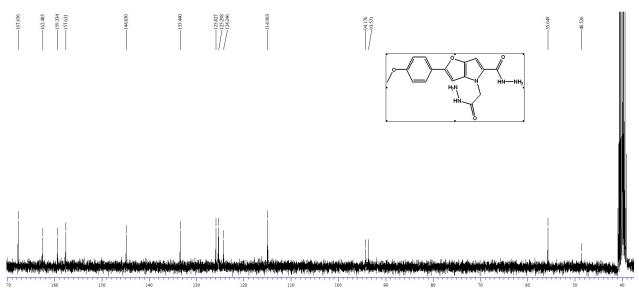


Figure S34. ¹³C NMR spectrum (75 MHz, DMSO- d_6) of compound 8c

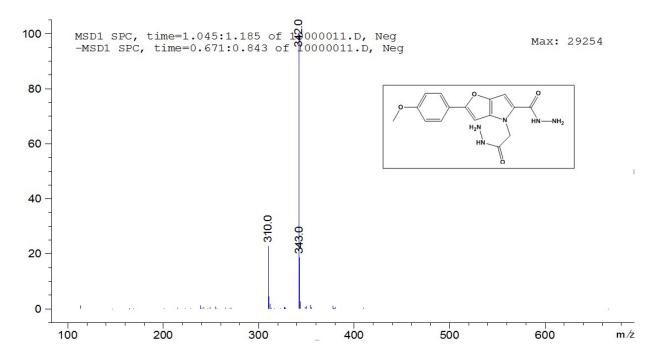


Figure S35. MS (ESI-) spectrum of compound 8c

General Papers

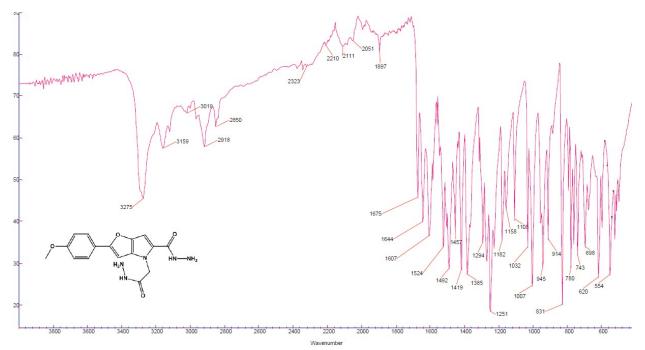


Figure S36. FTIR (ATR) spectrum of compound 8c

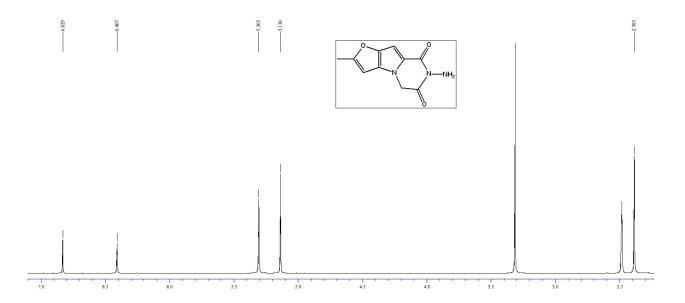


Figure S37. ¹H NMR (300 MHz, DMSO- d_6) of compound 9

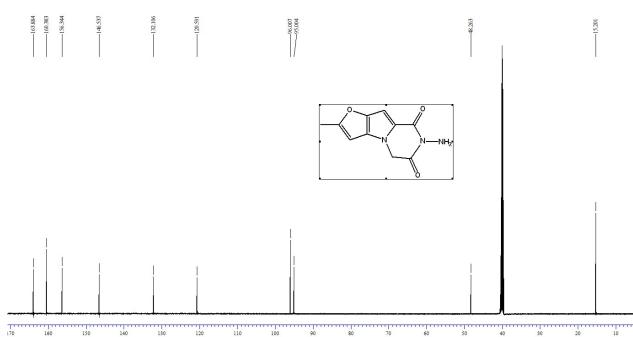


Figure S38. ¹³C NMR spectrum (75 MHz, DMSO-*d*₆) of compound 9

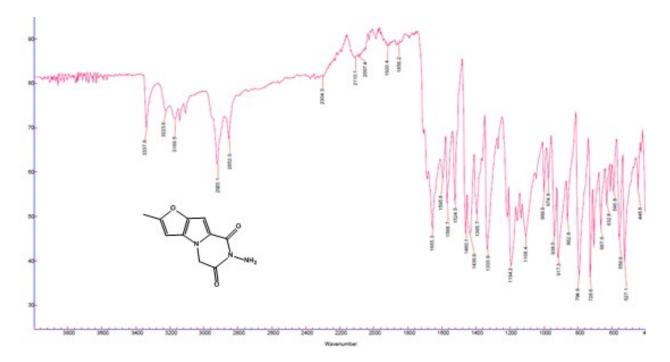
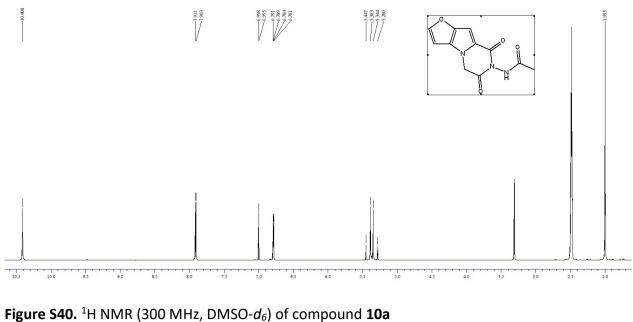
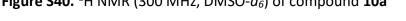


Figure S39. FTIR (ATR) spectrum of compound 9





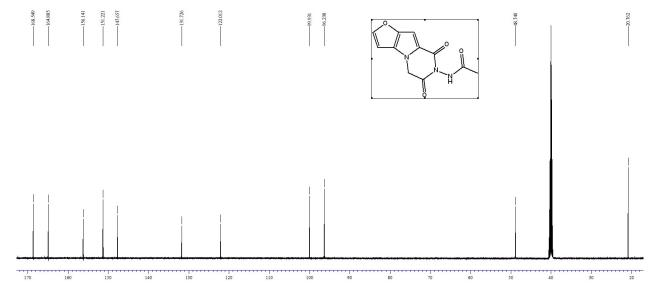


Figure S41. ¹³C NMR spectrum (75 MHz, DMSO-*d*₆) of compound **10a**

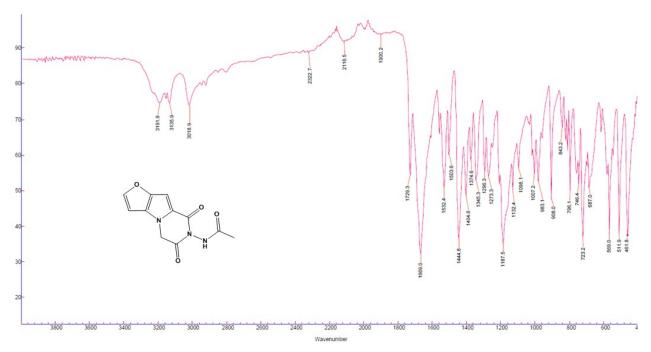


Figure S42. FTIR (ATR) spectrum of compound 10a

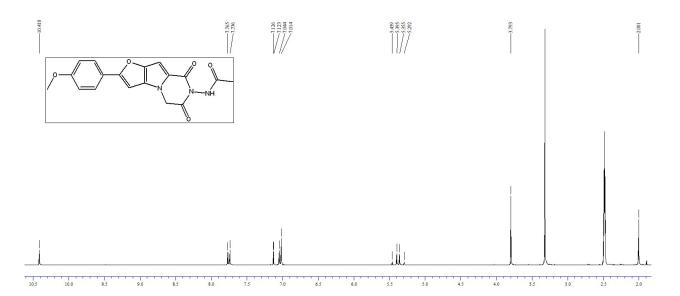


Figure S43. ¹H NMR (300 MHz, DMSO-*d*₆) of compound **10b**

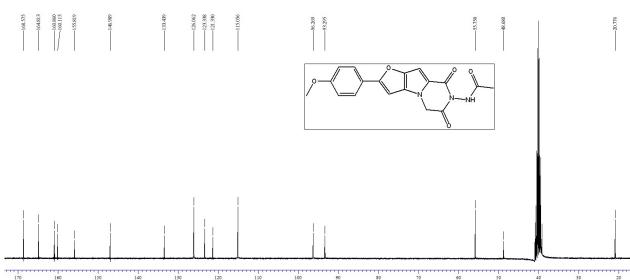


Figure S44. ¹³C NMR spectrum (75 MHz, DMSO-*d*₆) of compound **10b**

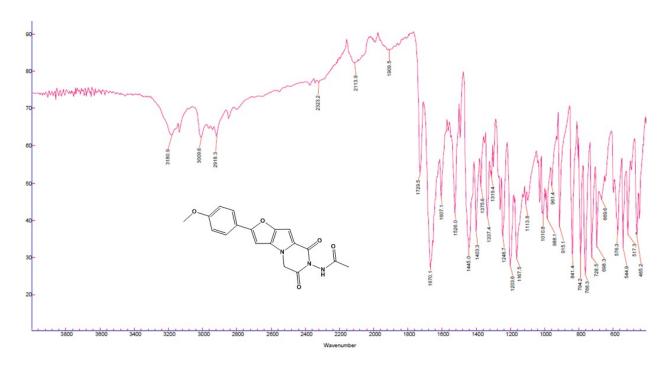


Figure S45. FTIR (ATR) spectrum of compound 10b

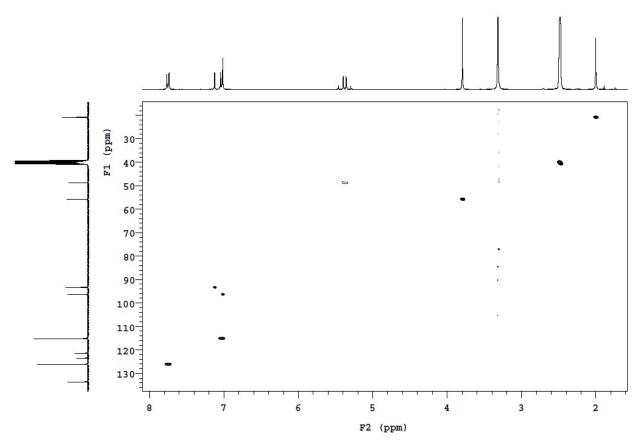


Figure S46. HSQC spectrum (DMSO-d6) of compound 10b

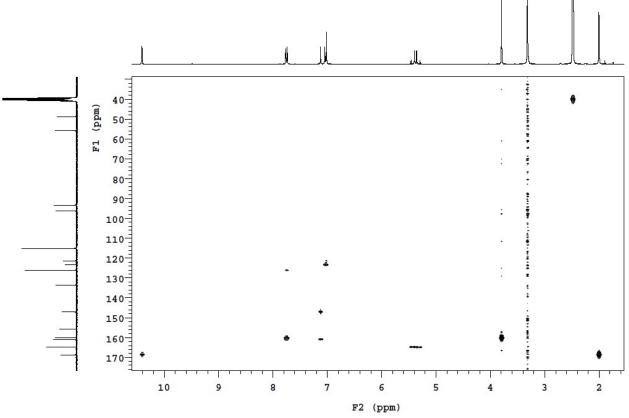


Figure S47. HMBC spectrum (DMSO-d6) of compound 10b

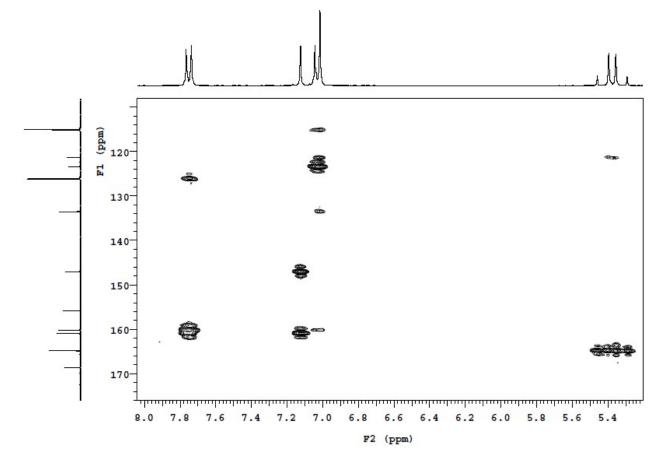


Figure S48. HMBC spectrum (DMSO-d₆) of compound **10b**

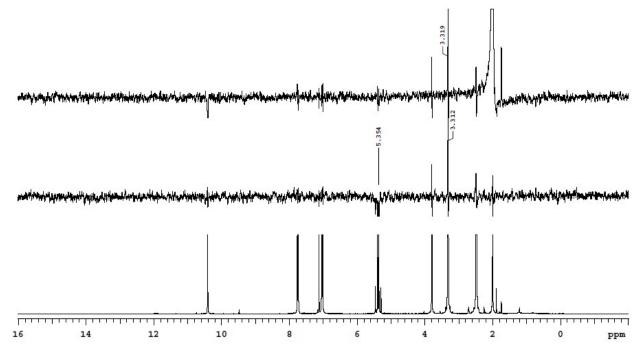


Figure S49. NOESY1D spectrum (DMSO-d₆) of compound 10b