

Supplementary Materials

Synthesis and Biological Evaluation of New Pyridothienopyrimidine Derivatives as Antibacterial Agents and *Escherichia coli* Topoisomerase II Inhibitors

Eman M. Mohi El-Deen ^{1,*}, Eman A. Abd El-Meguid ², Eman A. Karam ³, Eman S. Nossier ⁴ and Marwa F. Ahmed ^{5,6}

¹ Department of Therapeutic Chemistry, National Research Centre, Dokki, Cairo, 12622 Egypt.

² Department of Chemistry of Natural and Microbial Products, National Research Centre, Dokki, Cairo, 12622 Egypt.

³ Microbial Chemistry Department, National Research Centre, Dokki, Cairo, 12622 Egypt.

⁴ Department of Pharmaceutical Medicinal Chemistry, Faculty of Pharmacy (Girls), Al-Azhar University, Cairo 11754, Egypt.

⁵ Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Taif University, Taif 21974, Kingdom of Saudi Arabia.

⁶ Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Helwan University, Cairo, 11795, Egypt.

* Correspondence: e.mohi.2010@live.com; Tel.: +20-0106-385-3338.

Table of contents

	Page
Figure S1. ¹ H-NMR (400 MHz, DMSO-d ₆) spectrum of 2a .	S3
Figure S2. ¹³ C-NMR (100 MHz, DMSO- d ₆) spectrum of 2a .	S3
Figure S3. ¹ H-NMR (400 MHz, DMSO-d ₆) spectrum of 2b .	S4
Figure S4. ¹³ C-NMR (100 MHz, DMSO- d ₆) spectrum of 2b .	S4
Figure S5. ¹ H-NMR (400 MHz, DMSO- d ₆) spectrum of 3a .	S5
Figure S6. ¹³ C-NMR (100 MHz, DMSO- d ₆) spectrum of 3a .	S5
Figure S7. ¹ H-NMR (400 MHz, DMSO- d ₆) spectrum of 3b .	S6
Figure S8. ¹³ C-NMR (100 MHz, DMSO- d ₆) spectrum of 3b .	S6
Figure S9. ¹ H-NMR (400 MHz, DMSO- d ₆) spectrum of 4a .	S7
Figure S10. ¹³ C-NMR (100 MHz, DMSO- d ₆) spectrum of 4a .	S7
Figure S11. ¹ H-NMR (400 MHz, DMSO- d ₆) spectrum of 4b .	S8

Figure S12. ^{13}C -NMR (100 MHz, DMSO- d_6) spectrum of 4b .	S8
Figure S13. ^1H -NMR (400 MHz, DMSO- d_6) spectrum of 4c .	S9
Figure S14. ^{13}C -NMR (100 MHz, DMSO- d_6) spectrum of 4c .	S9
Figure S15. ^1H -NMR (400 MHz, DMSO- d_6) spectrum of 4d .	S10
Figure S16. ^{13}C -NMR (100 MHz, DMSO- d_6) spectrum of 4d .	S10
Figure S17. ^1H -NMR (400 MHz, DMSO- d_6) spectrum of 4e .	S11
Figure S18. ^1H -NMR (400 MHz, DMSO- d_6) spectrum of 5a .	S11
Figure S19. ^{13}C -NMR (100 MHz, DMSO- d_6) spectrum of 5a .	S12
Figure S20. ^1H -NMR (400 MHz, DMSO- d_6) spectrum of 5b .	S12
Figure S21. ^{13}C -NMR (100 MHz, DMSO- d_6) spectrum of 5b .	S13
Figure S22. ^1H -NMR (400 MHz, DMSO- d_6) spectrum of 6a .	S13
Figure S23. ^1H -NMR (400 MHz, DMSO- d_6) spectrum of 6b .	S14
Figure S24. ^{13}C -NMR (100 MHz, DMSO- d_6) spectrum of 6b .	S14
Figure S25. ^1H -NMR (400 MHz, DMSO- d_6) spectrum of 7a .	S15
Figure S26. ^1H -NMR (400 MHz, DMSO- d_6) spectrum of 8a .	S15
Figure S27. ^{13}C -NMR (100 MHz, DMSO- d_6) spectrum of 8a .	S16
Figure S28. ^1H -NMR (400 MHz, DMSO- d_6) spectrum of 8b .	S16

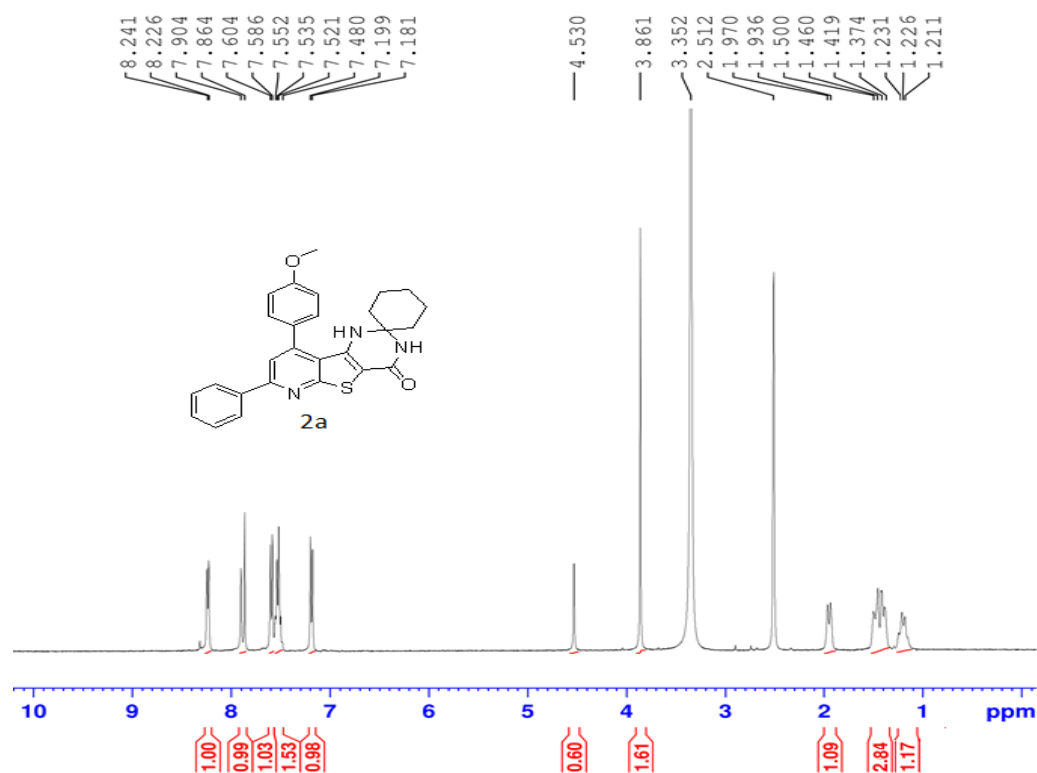


Fig. S1 ^1H NMR (400 MHz) in $\text{DMSO-}d_6$ of compound **2a**

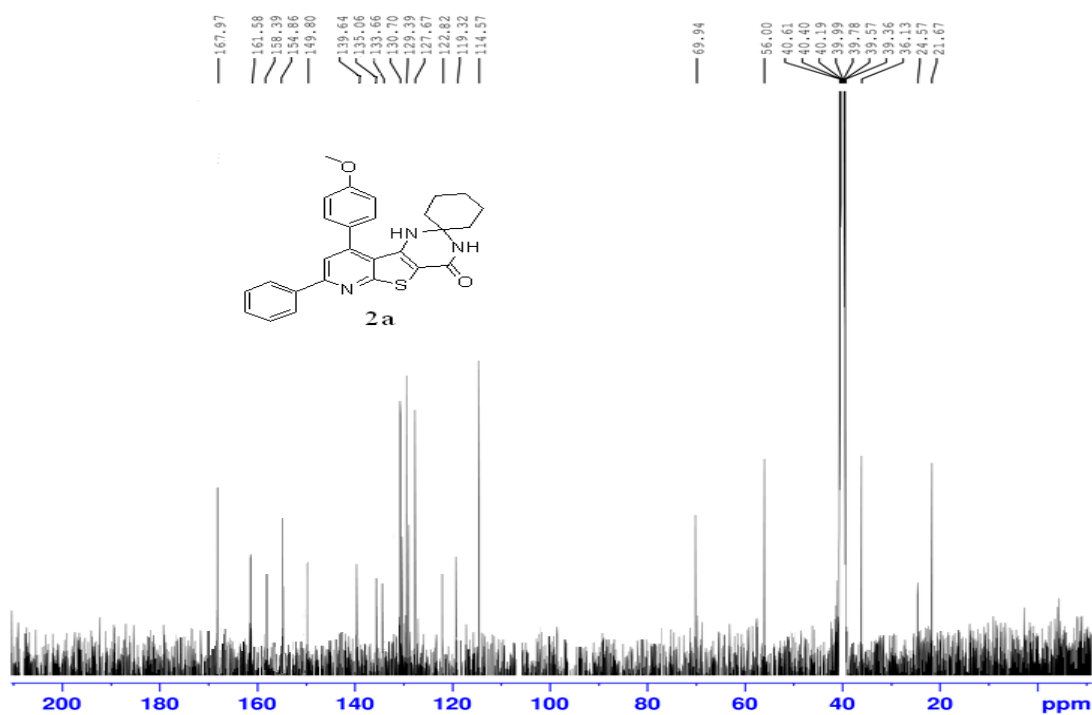


Fig. S2 ^{13}C NMR (100 MHz) in $\text{DMSO-}d_6$ of compound **2a**

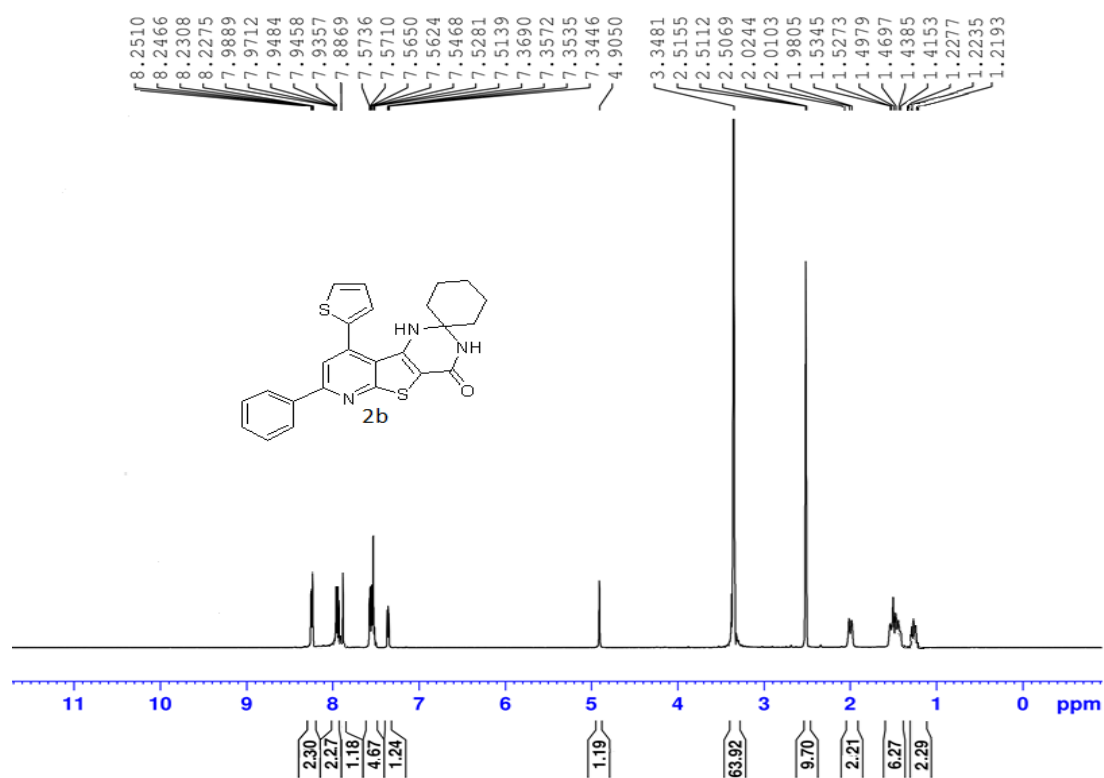


Fig. S3 ¹H NMR (400 MHz) in DMSO-d₆ of compound **2b**

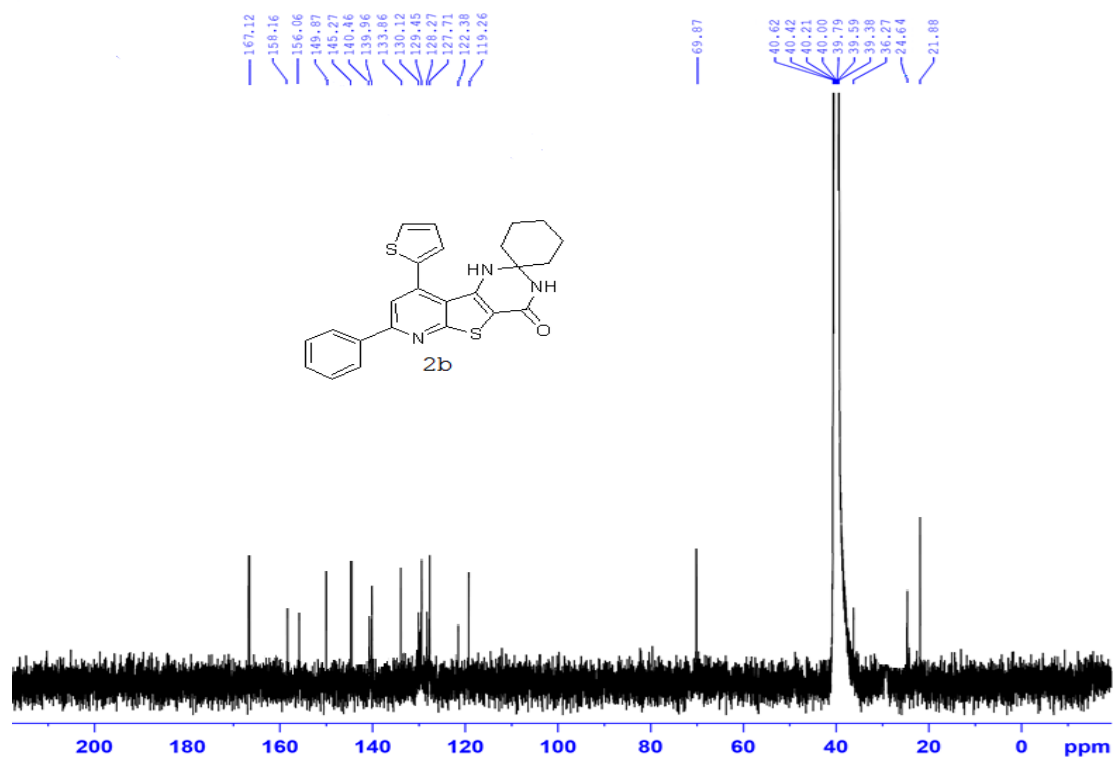


Fig. S4 ¹³C NMR (100 MHz) in DMSO-d₆ of compound **2b**

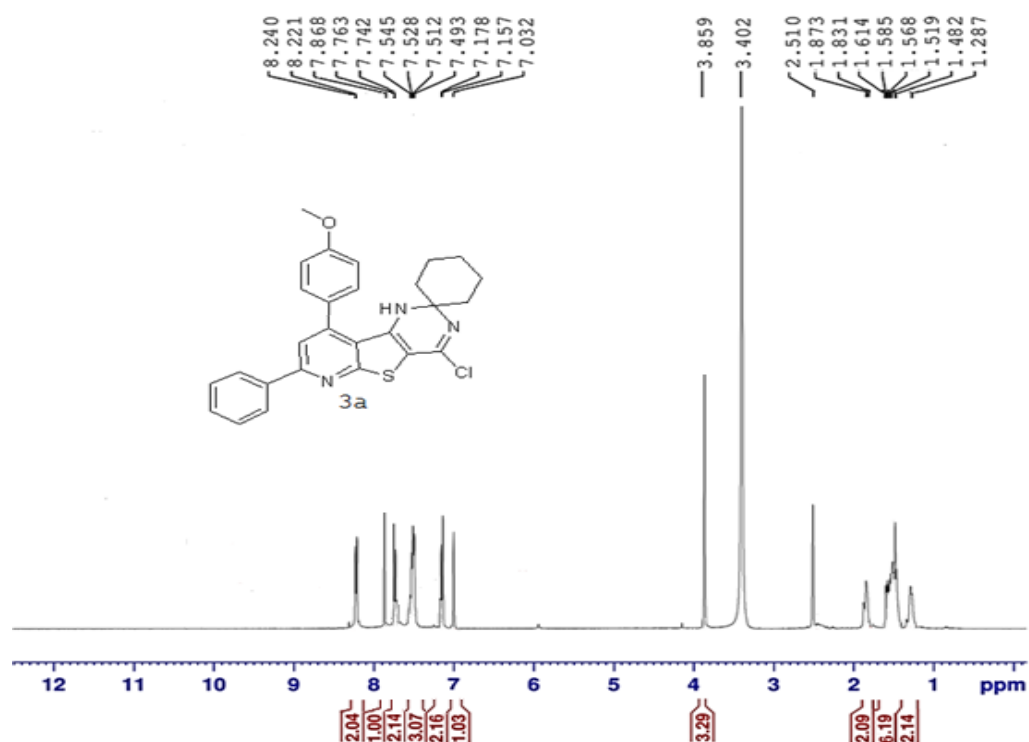


Fig. S5 ^1H NMR (400 MHz) in $\text{DMSO}-d_6$ of compound 3a

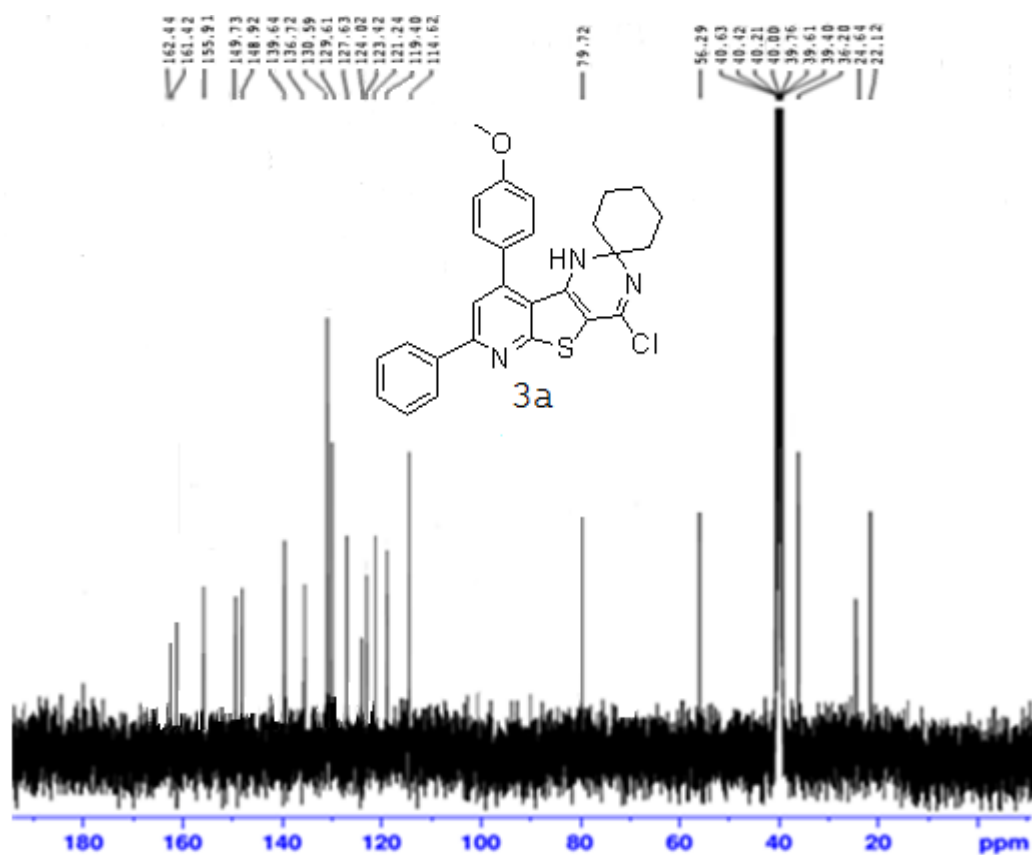


Fig. S6 ^{13}C NMR (100 MHz) in $\text{DMSO}-d_6$ of compound 3a

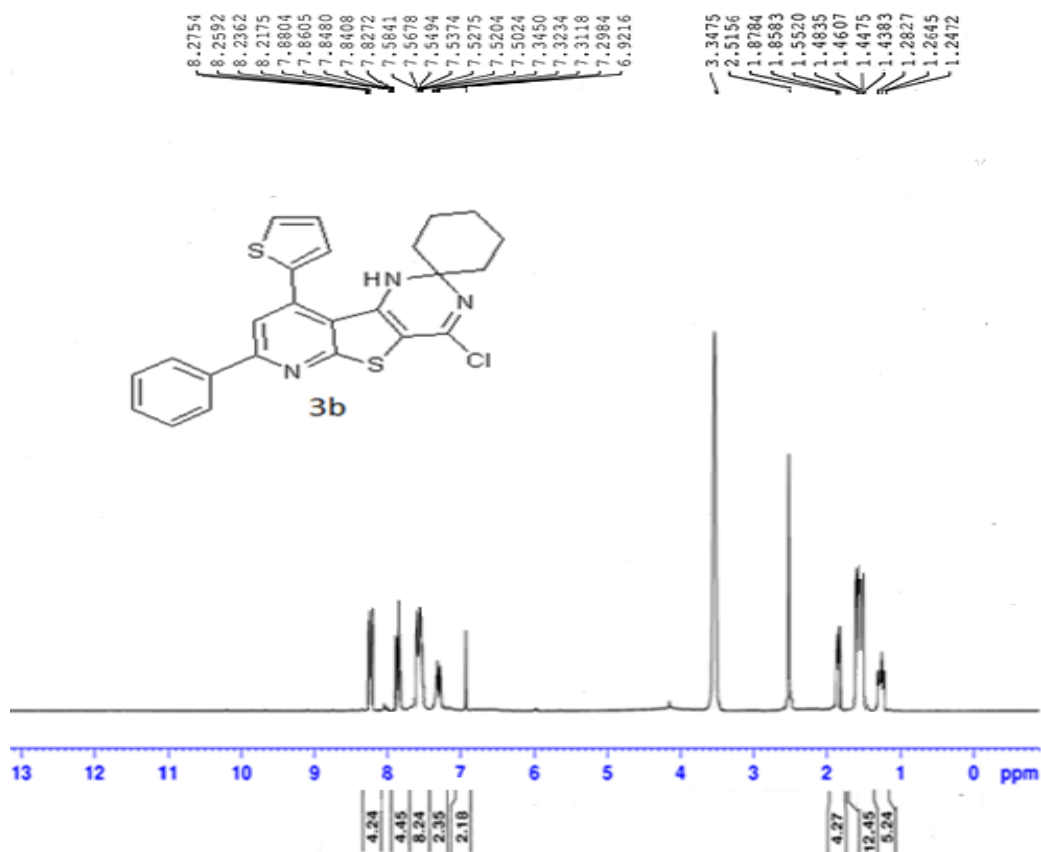


Fig. S7 ^1H NMR (400 MHz) in $\text{DMSO}-d_6$ of compound **3b**

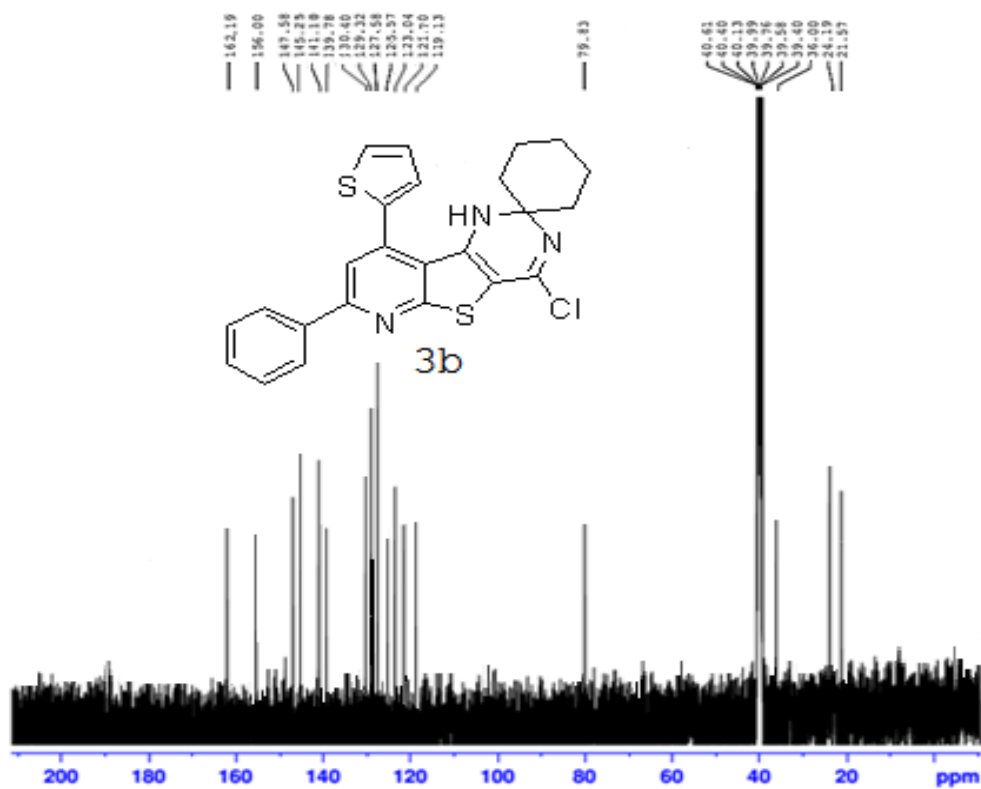


Fig. S8 ^{13}C NMR (100 MHz) in $\text{DMSO}-d_6$ of compound **3b**

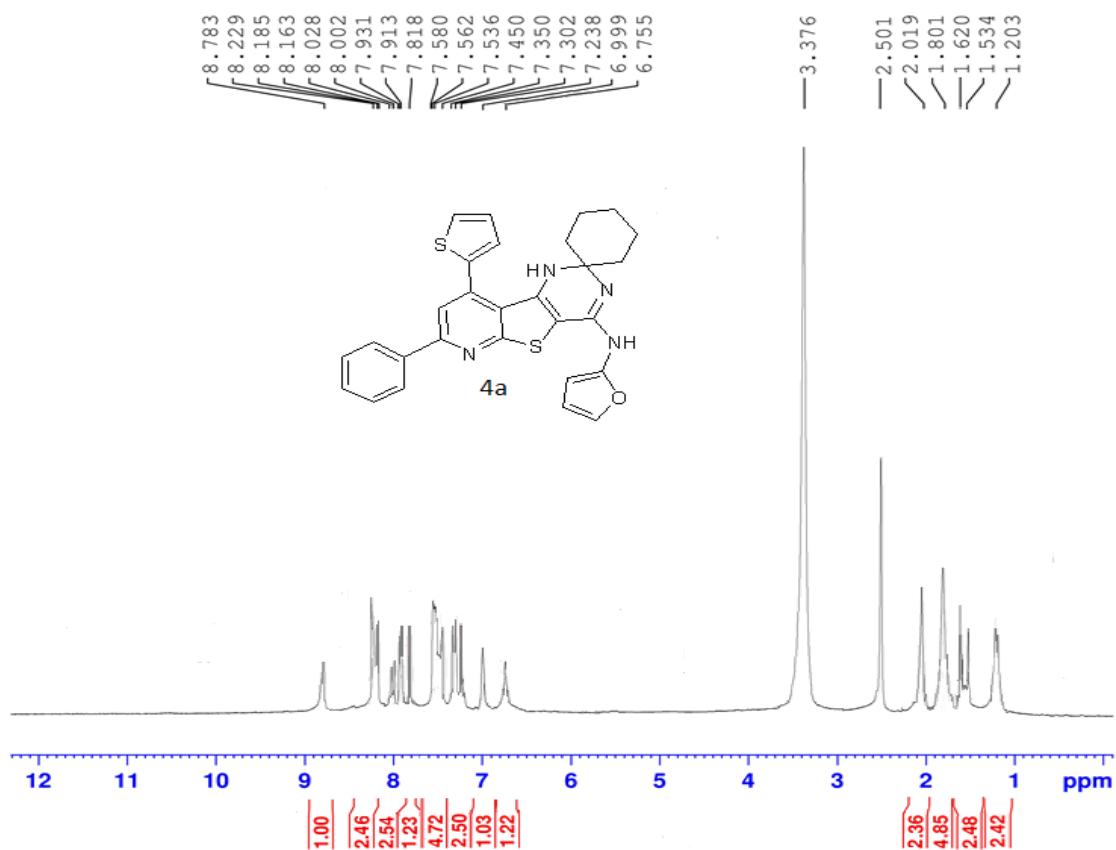


Fig. S9 ¹H NMR (400 MHz) in DMSO-*d*₆ of compound **4a**

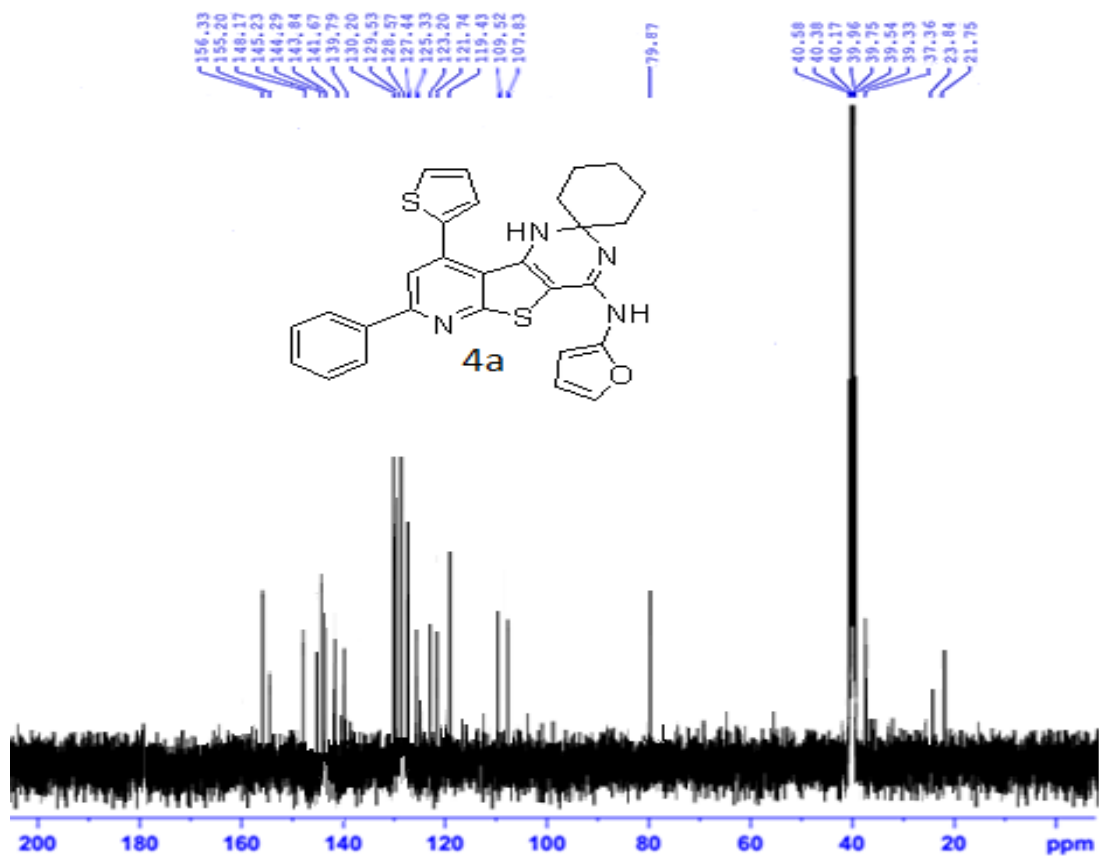


Fig. S10 ¹³C NMR (100 MHz) in DMSO-*d*₆ of compound **4a**

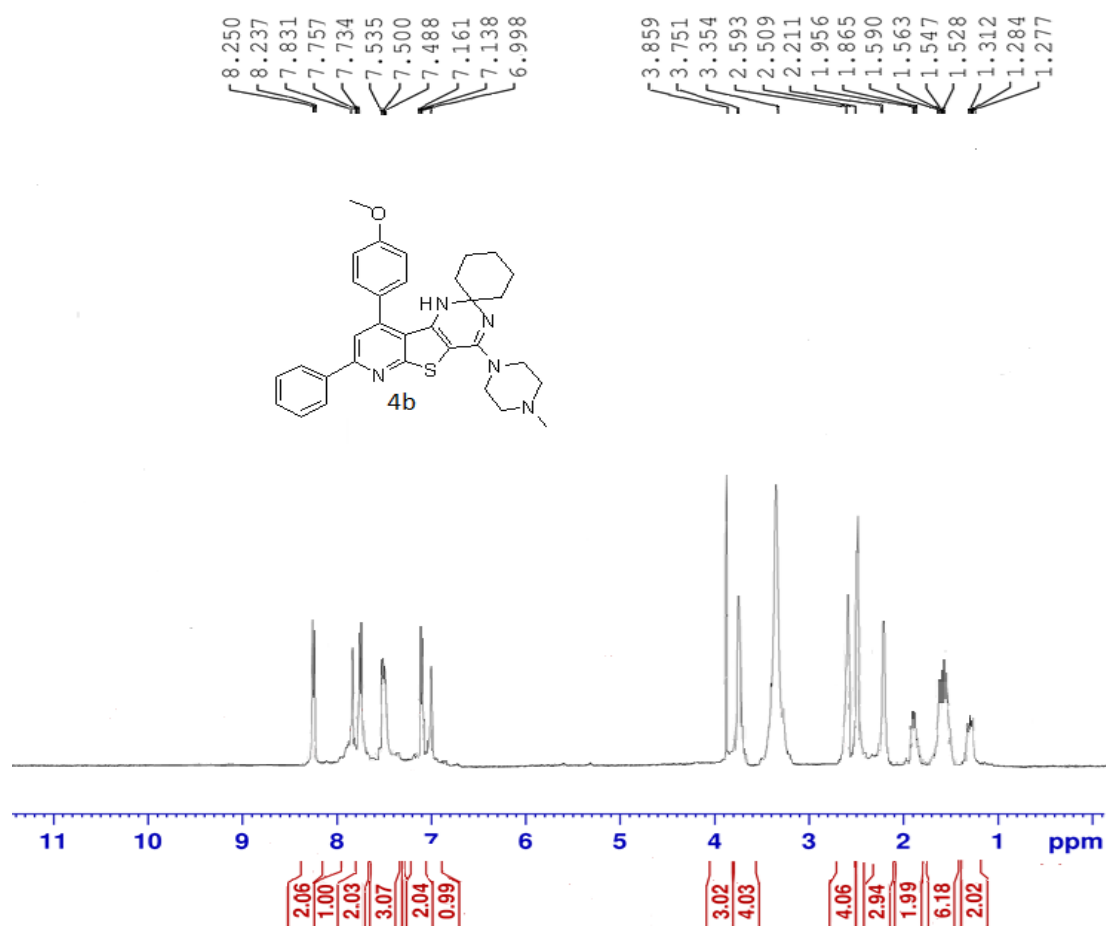


Fig. S11 ^1H NMR (400 MHz) in $\text{DMSO}-d_6$ of compound **4b**

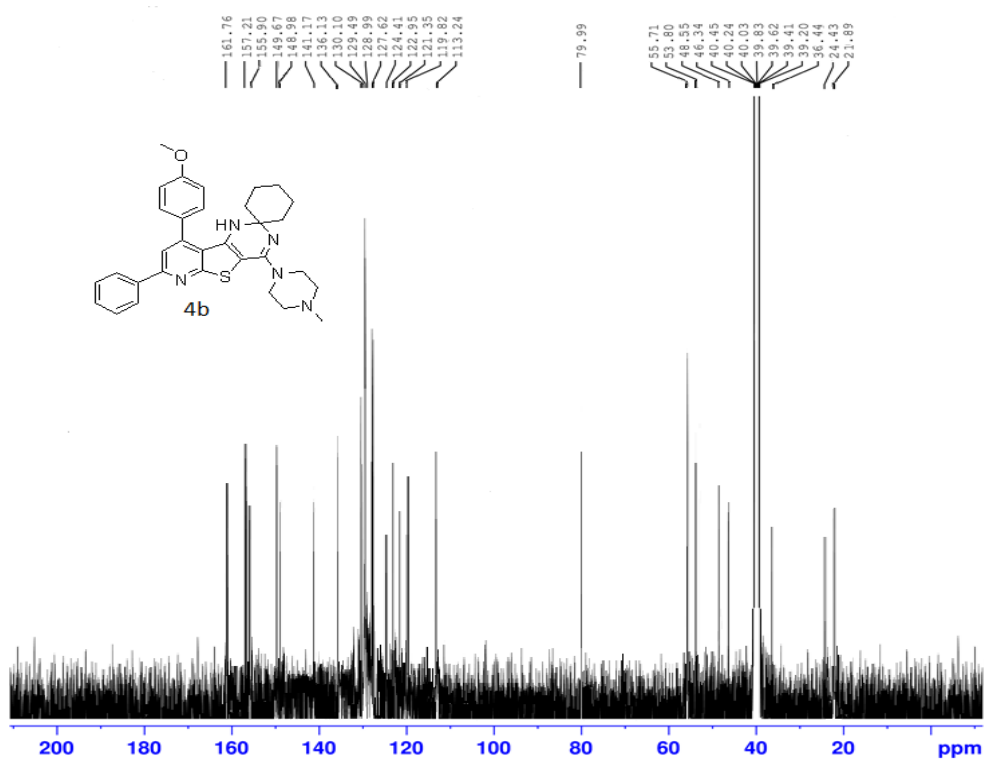


Fig. S12 ^{13}C NMR (100 MHz) in $\text{DMSO}-d_6$ of compound **4b**

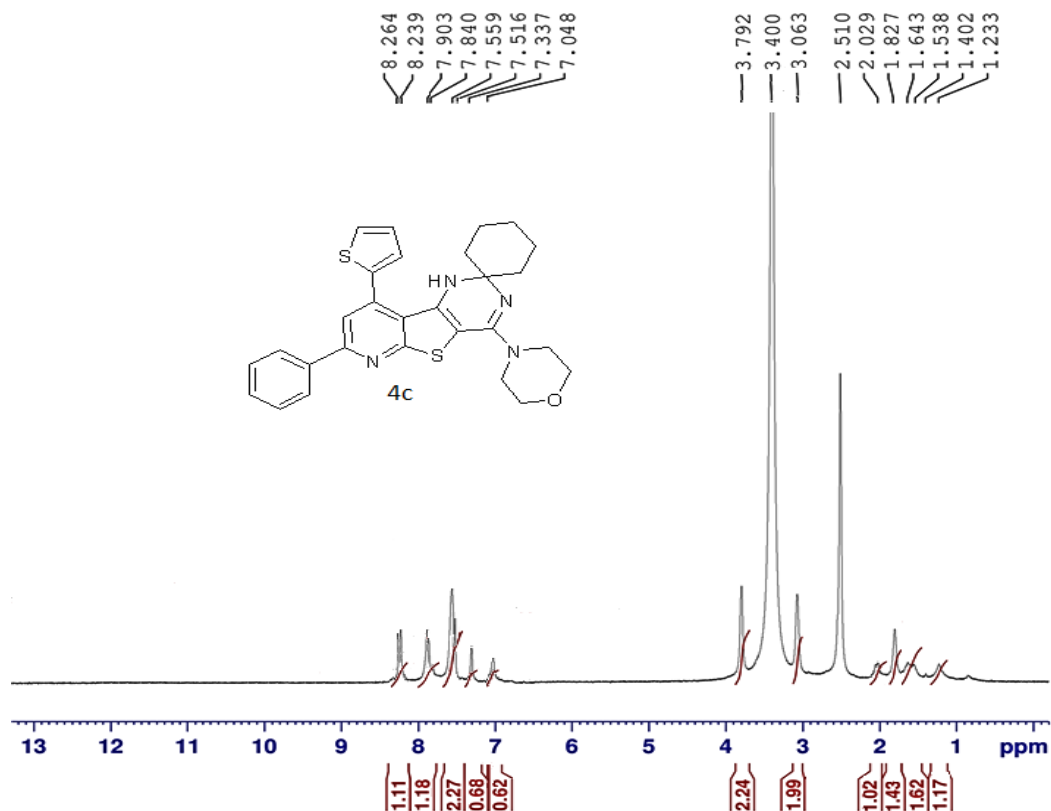


Fig. S13 ^1H NMR (400 MHz) in $\text{DMSO}-d_6$ of compound **4c**

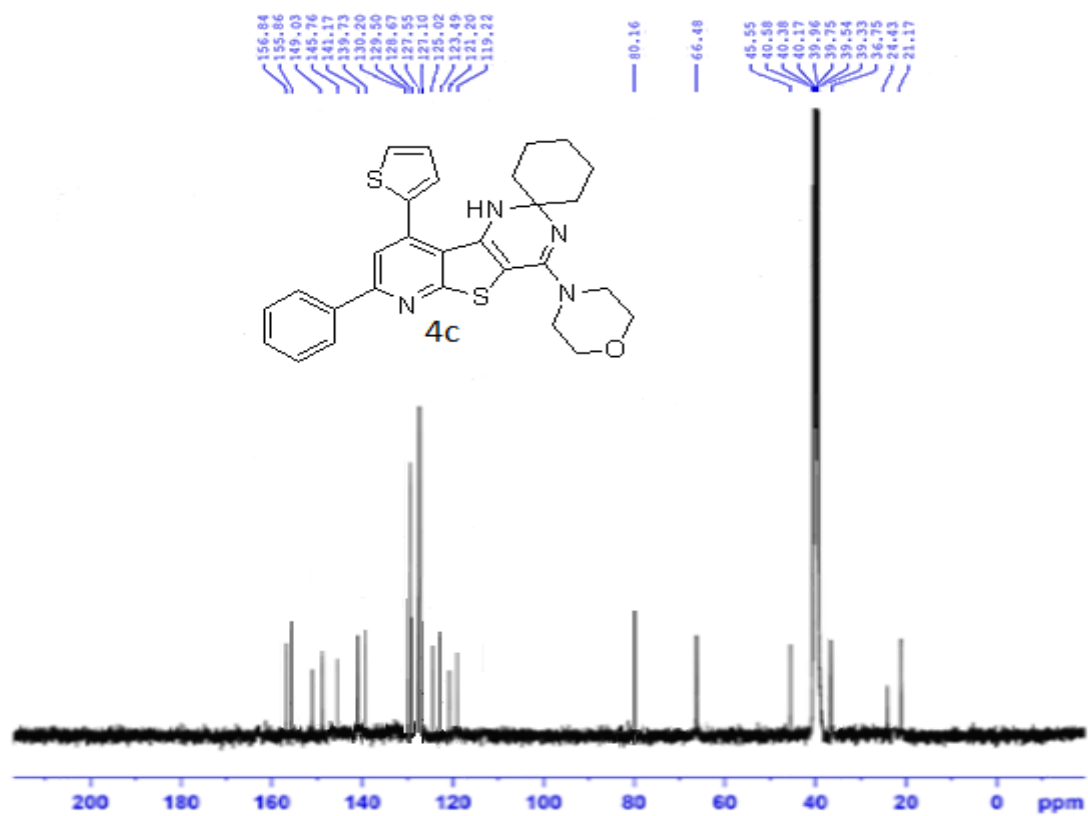


Fig. S14 ^{13}C NMR (100 MHz) in $\text{DMSO}-d_6$ of compound **4c**

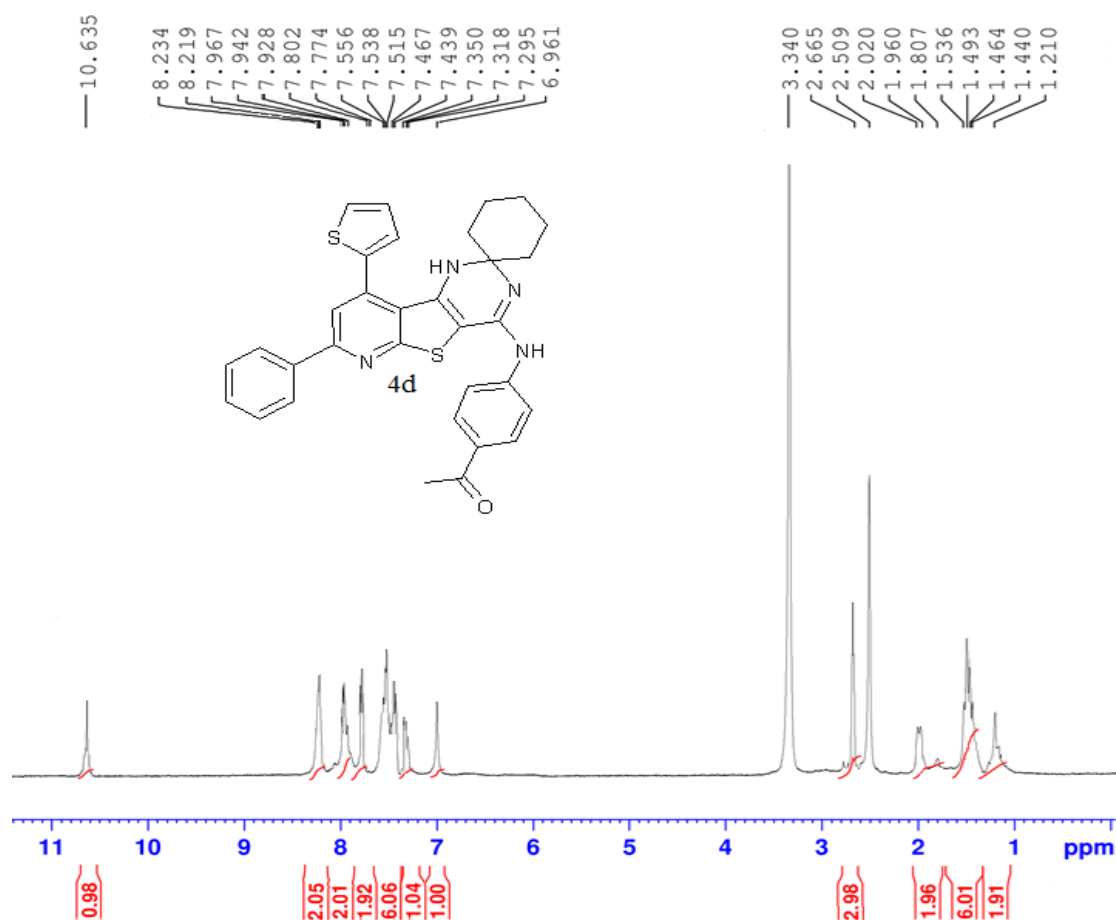


Fig. S15 ¹H NMR (400 MHz) in DMSO-*d*₆ of compound **4d**

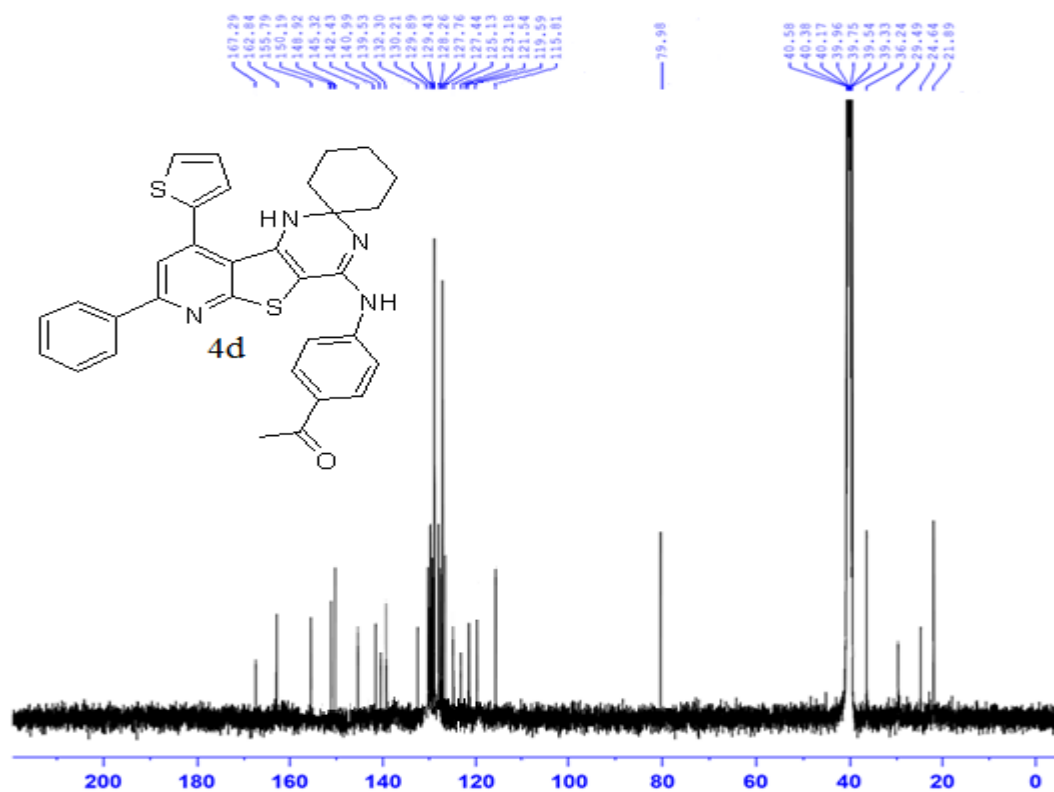


Fig. S16 ¹³C NMR (100 MHz) in DMSO-*d*₆ of compound **4d**

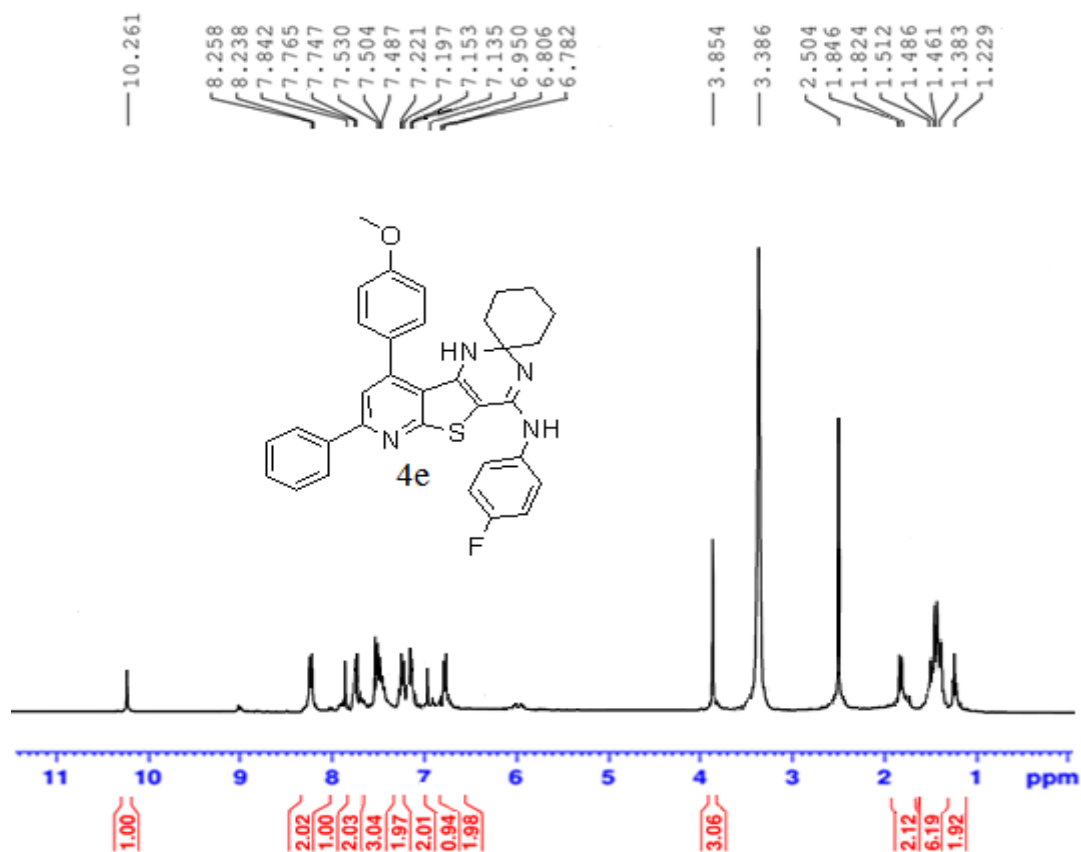


Fig. S17 ^1H NMR (400 MHz) in $\text{DMSO}-d_6$ of compound **4e**

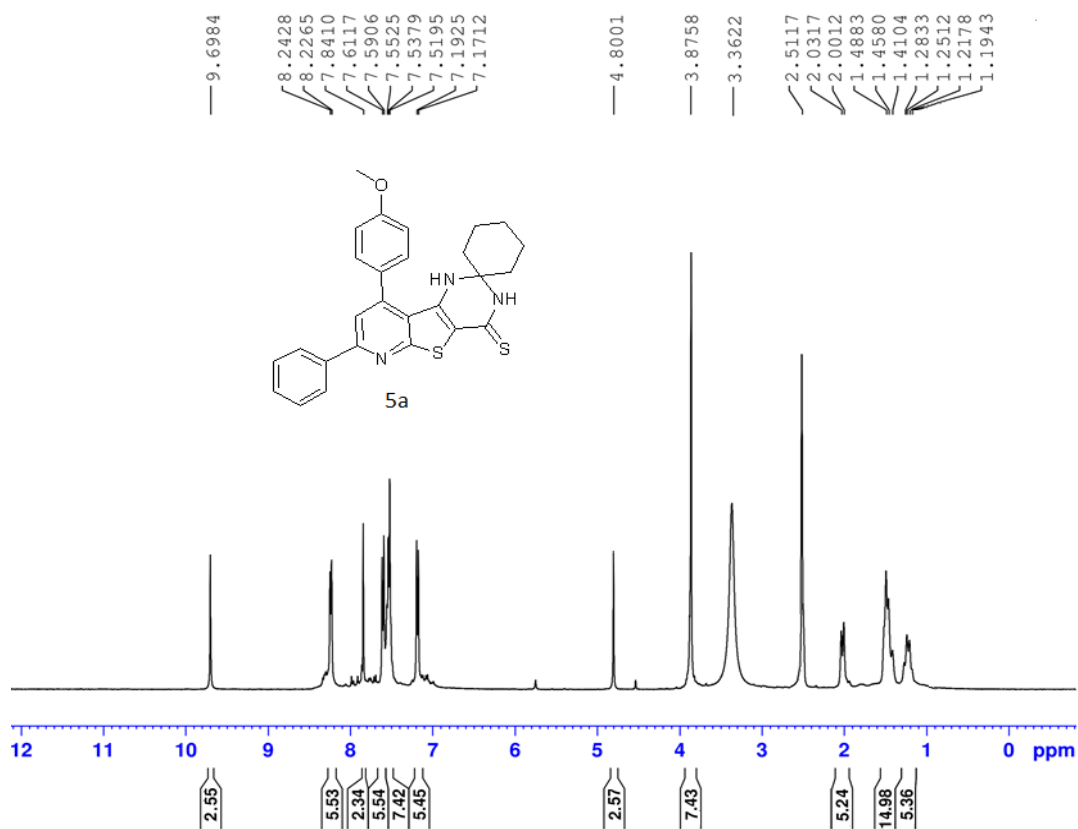


Fig. S18 ^1H NMR (400 MHz) in $\text{DMSO}-d_6$ of compound **5a**

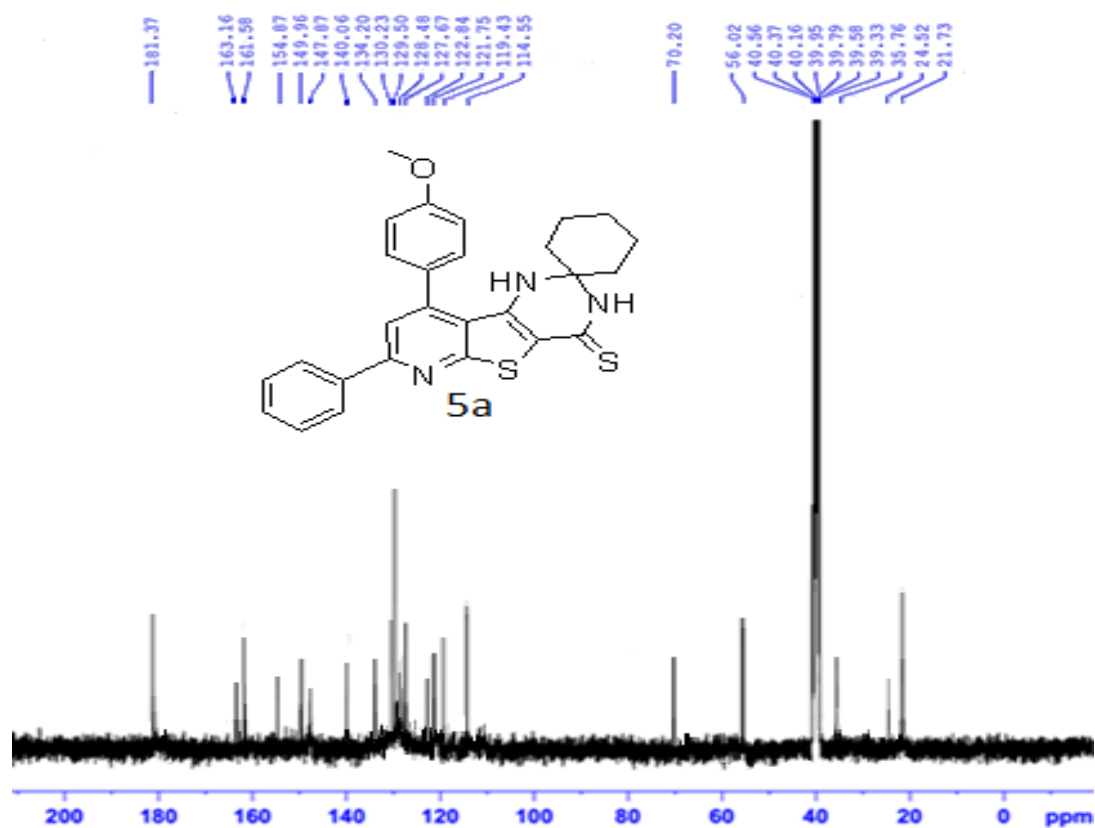


Fig. S19 ¹³C NMR (100 MHz) in DMSO-*d*₆ of compound **5a**

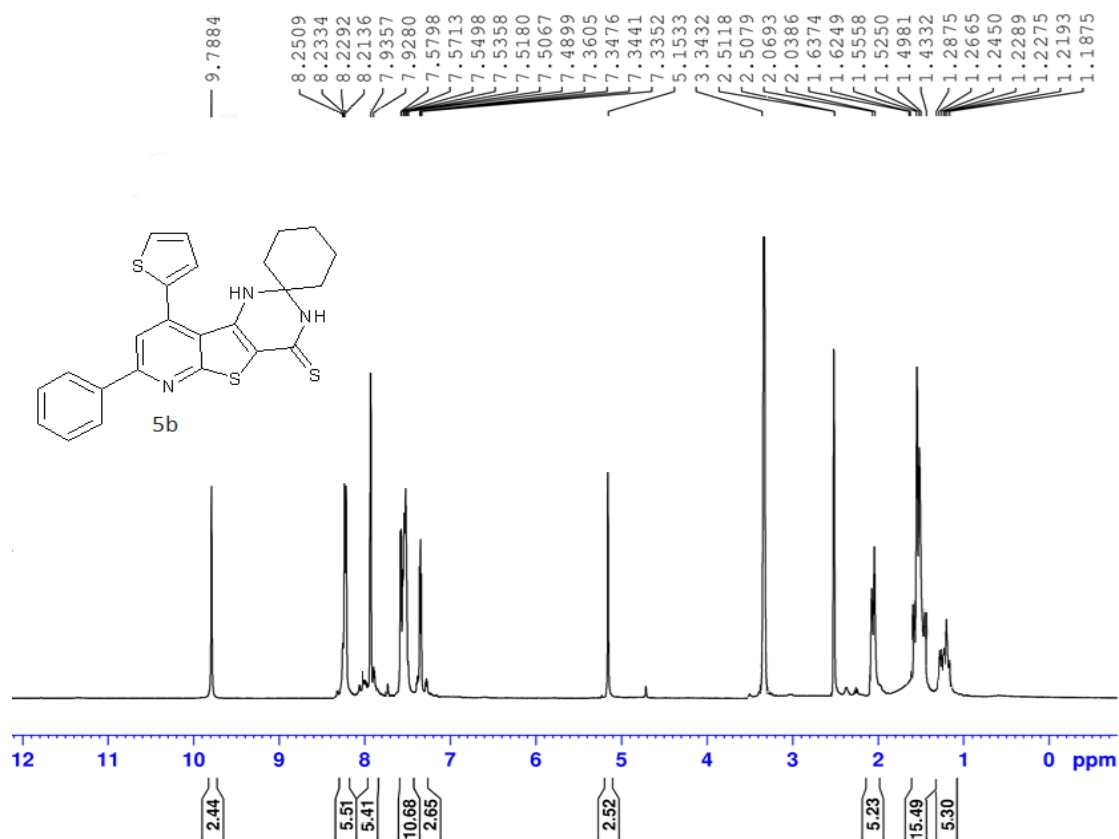


Fig. S20 ¹H NMR (400 MHz) in DMSO-*d*₆ of compound **5b**

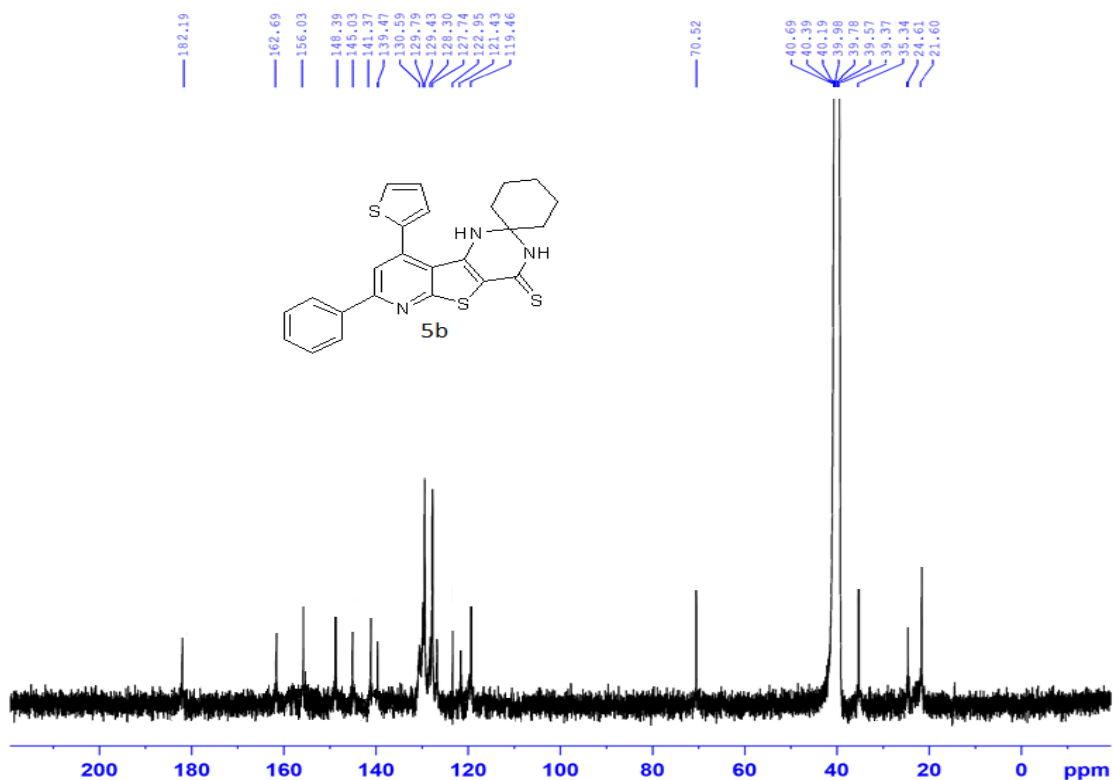


Fig. S21 ¹³C NMR (100 MHz) in DMSO-*d*₆ of compound **5b**

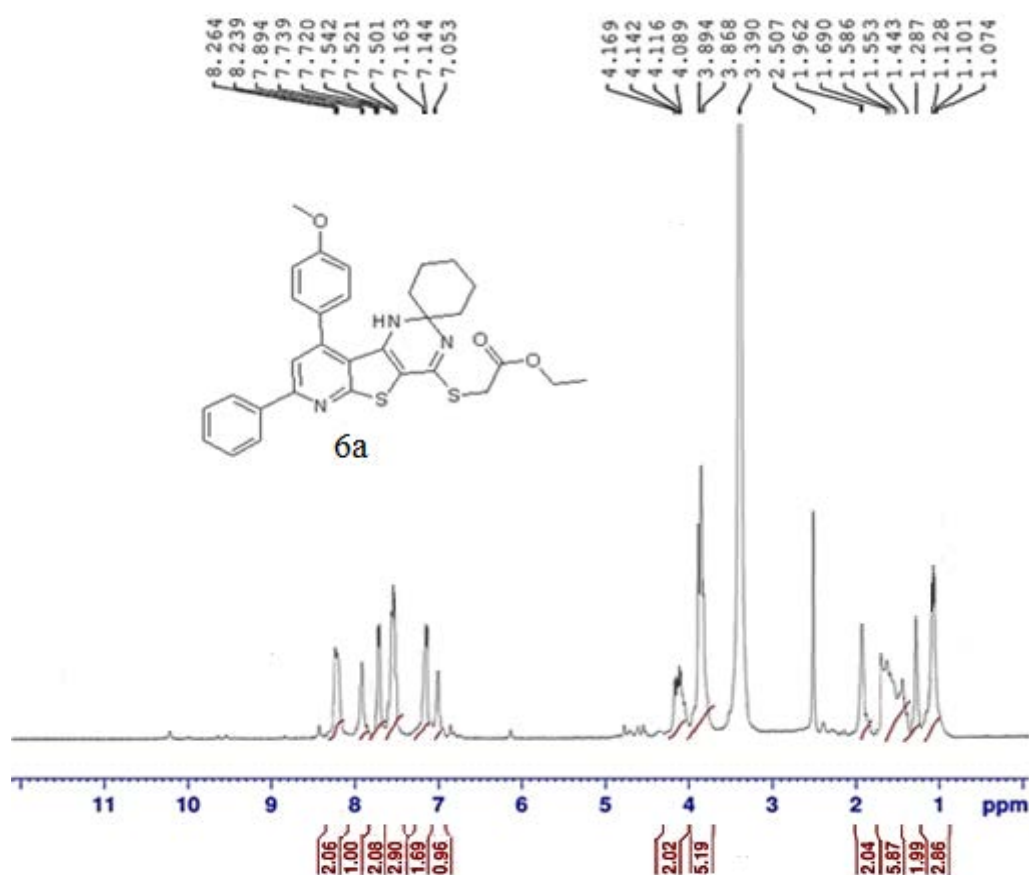


Fig. S22 ¹H NMR (400 MHz) in DMSO-*d*₆ of compound **6a**

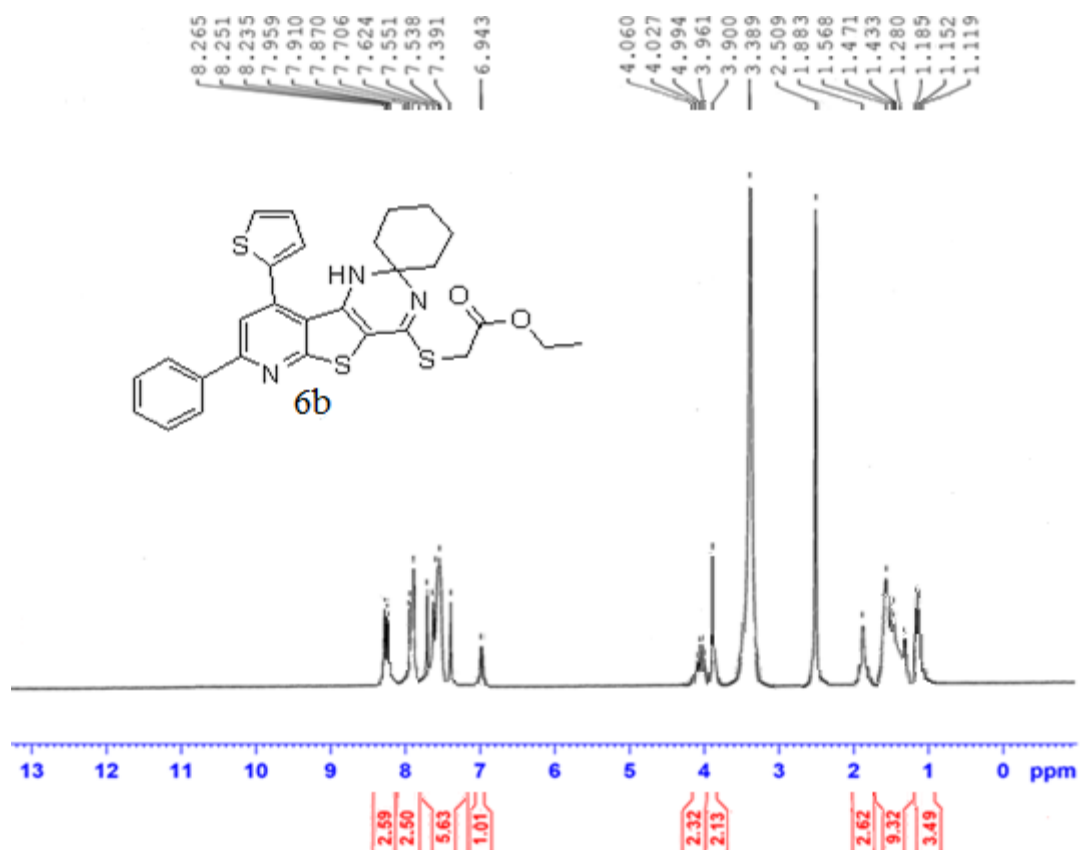


Fig. S23 ¹H NMR (400 MHz) in DMSO-*d*₆ of compound **6b**

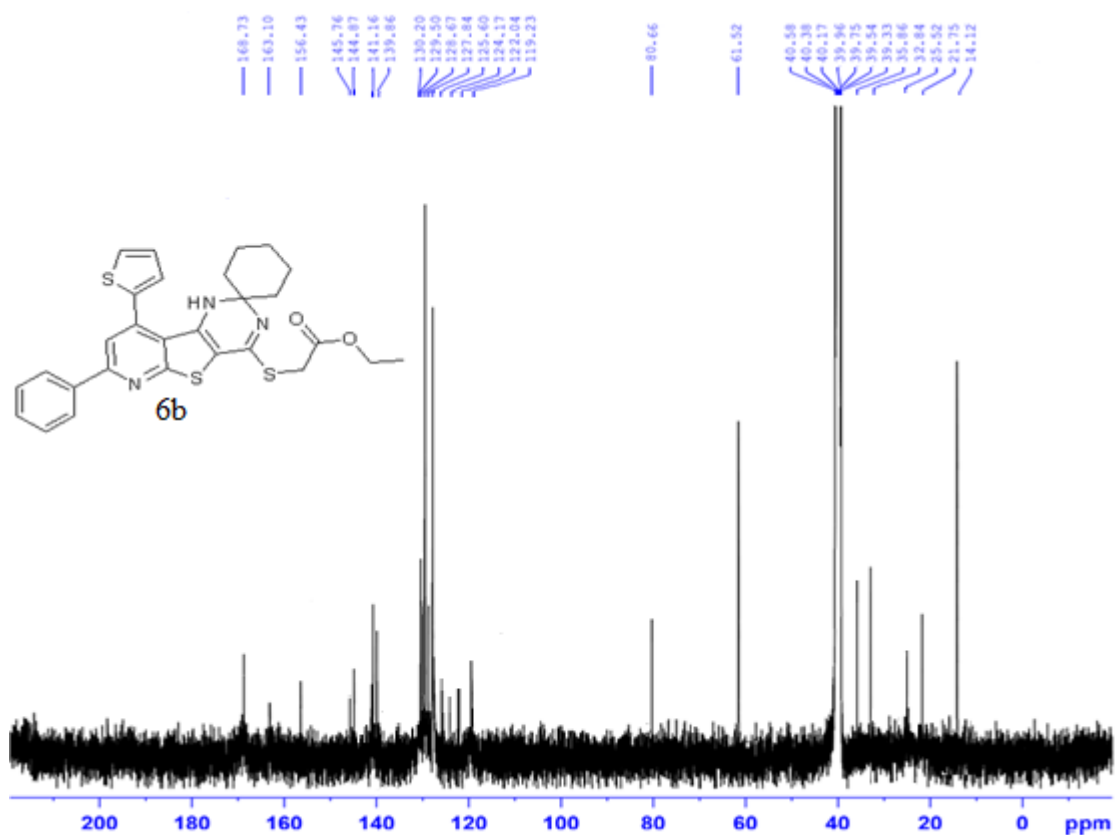


Fig. S24 ¹³C NMR (100 MHz) in DMSO-*d*₆ of compound **6b**

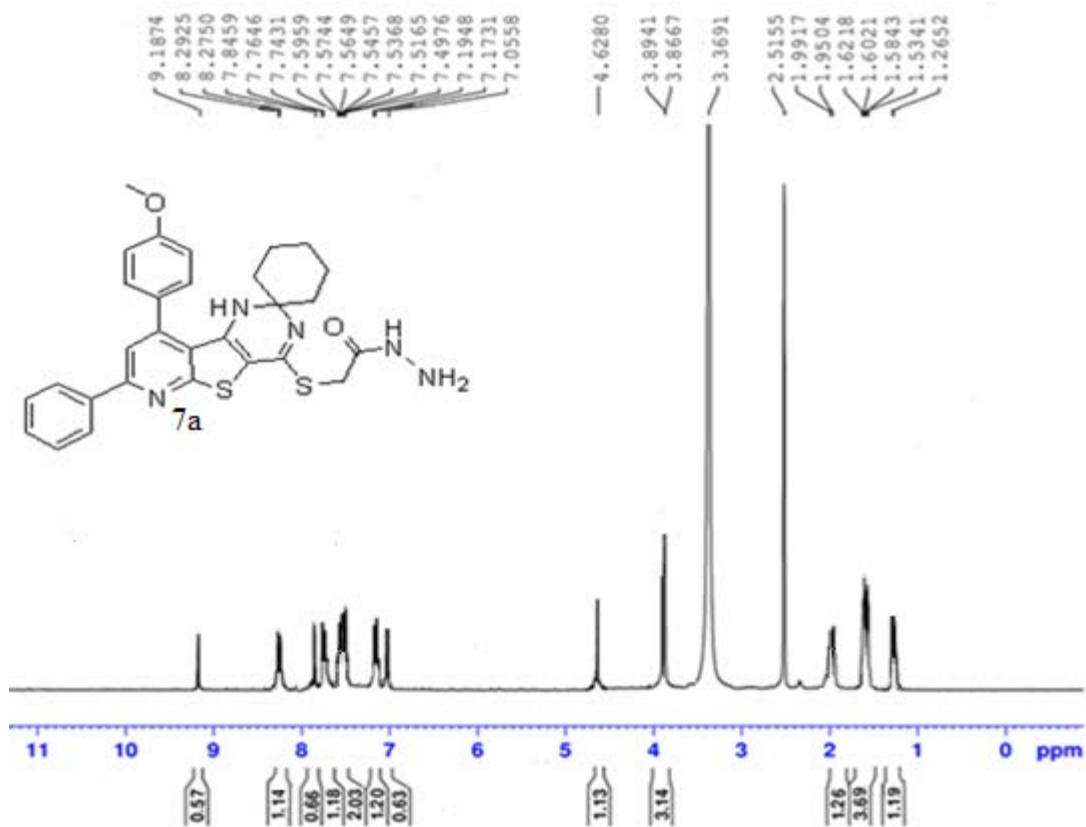


Fig. S25 ^1H NMR (400 MHz) in $\text{DMSO}-d_6$ of compound 7a.

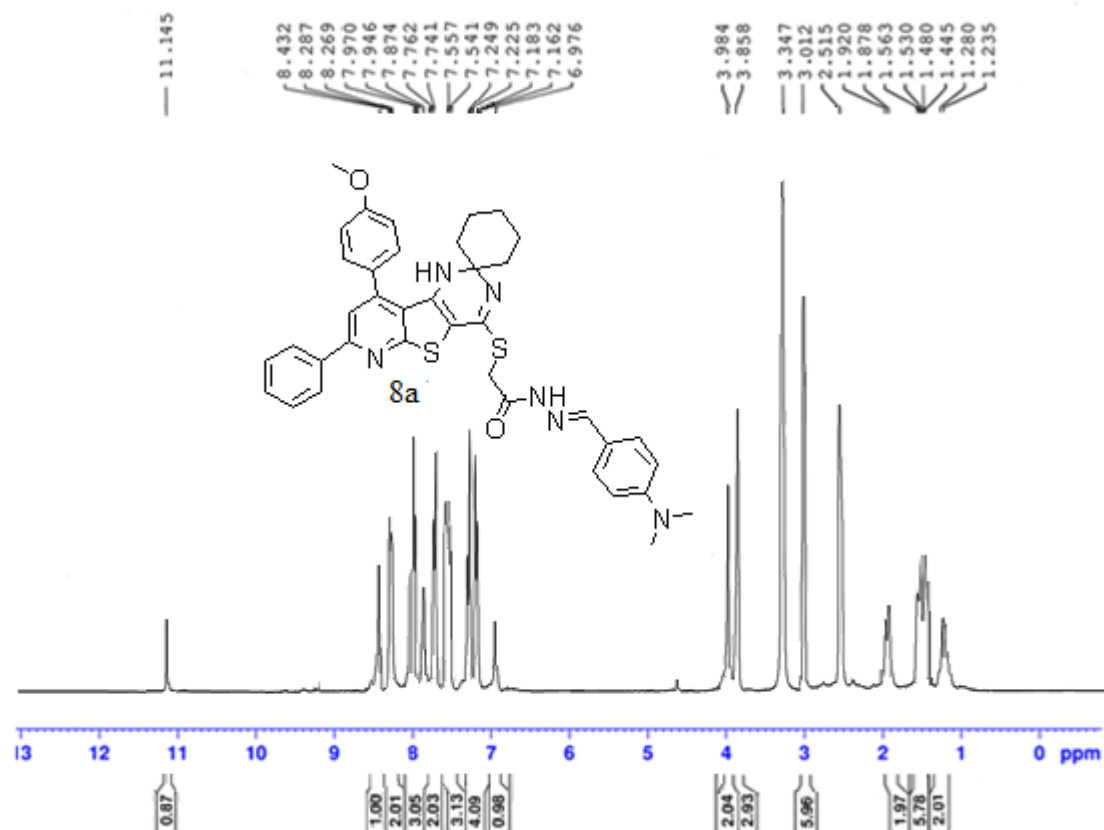


Fig. S26 ^1H NMR (400 MHz) in $\text{DMSO}-d_6$ of compound 8a

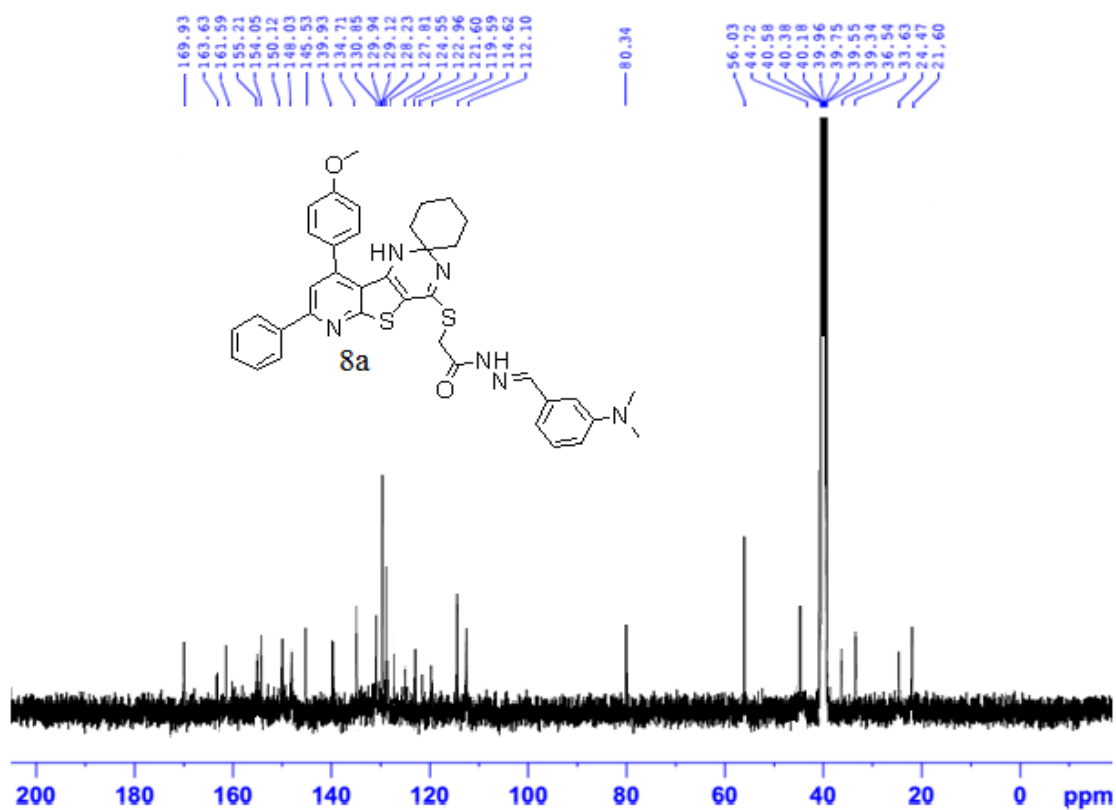


Fig. S27 ¹³C NMR (100 MHz) in DMSO-*d*₆ of compound **8a**

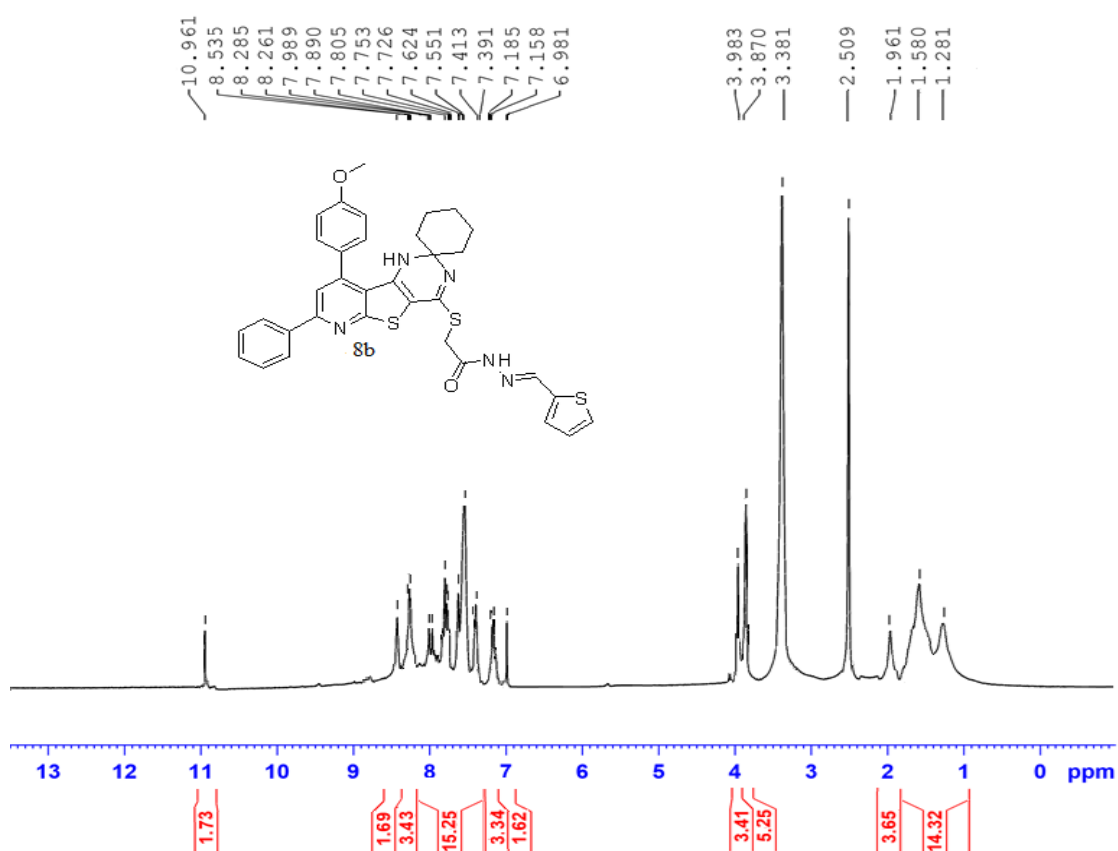


Fig. S28 ¹H NMR (400 MHz) in DMSO-*d*₆ of compound **8b**