

Supplementary Materials

Synthesis, Docking Studies and *In Vitro* Evaluation of Some Novel Thienopyridines and Fused Thienopyridine-Quinolines as Antibacterial Agents and DNA Gyrase Inhibitors

Eman M. Mohi El-Deen^{1*}, Eman A. Abd El-Meguid², Sherifa Hasabelnaby³, Eman A. Karam⁴, and Eman S. Nossier⁵,

¹Department of Therapeutic Chemistry, National Research Centre, Dokki, Cairo, 12622 Egypt;
e.mohi.2010@live.com

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

³Pharmaceutical chemistry department, Faculty of Pharmacy, Helwan University, Ein Helwan, Cairo, 11795 Egypt.

⁴Microbiology chemistry department, National Research Centre, Dokki, Cairo, 12622 Egypt.

⁵Department of Pharmaceutical Medicinal Chemistry, Faculty of Pharmacy (Girls), Al-Azhar University, Cairo 11754, Egypt.

Table of contents

	Page
Figure S1. ¹ H-NMR (400 MHz, DMSO-d ₆) spectrum of 2a .	S3
Figure S2. Mass spectrum of 2a .	S3
Figure S3. ¹ H-NMR (400 MHz, DMSO-d ₆) spectrum of 2b .	S4
Figure S4. Mass 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 .	S6
Figure S7. Mass spectrum of 3a .	S6
Figure S8. ¹ H-NMR (400 MHz, DMSO- d ₆) spectrum of 3b .	S7
Figure S9. ¹³ C-NMR (100 MHz, DMSO- d ₆) spectrum of 3b .	S8
Figure S10. Mass spectrum of 3b .	S8
Figure S11. ¹ H-NMR (400 MHz, DMSO- d ₆) spectrum of 4a .	S9
Figure S12. ¹³ C-NMR (100 MHz, DMSO- d ₆) spectrum of 4a .	S10
Figure S13. Mass spectrum of 4a .	S10
Figure S14. ¹ H-NMR (400 MHz, DMSO- d ₆) spectrum of 4b .	S11
Figure S15. Mass spectrum of 4b .	S12
Figure S16. ¹ H-NMR (400 MHz, CDCl ₃) spectrum of 5a .	S13
Figure S17. ¹³ C-NMR (100 MHz, DMSO- d ₆) spectrum of 5a .	S14
Figure S18. Mass spectrum of 5a .	S14
Figure S19. ¹ H-NMR (400 MHz, DMSO- d ₆) spectrum of 5b .	S15
Figure S20. ¹³ C-NMR (100 MHz, DMSO- d ₆) spectrum of 5b .	S15
Figure S21. Mass spectrum of 5b .	S16

Figure S22. ^1H -NMR (400 MHz, DMSO- d ₆) spectrum of 6a .	S16
Figure S23. Mass spectrum of 6a .	S17
Figure S24. ^1H -NMR (400 MHz, DMSO- d ₆) spectrum of 6b .	S17
Figure S25. ^{13}C -NMR (100 MHz, DMSO- d ₆) spectrum of 6b .	S18
Figure S26. Mass spectrum of 6b .	S18
Figure S27. ^1H -NMR (400 MHz, DMSO- d ₆) spectrum of 7a .	S19
Figure S28. Mass spectrum of 7a .	S19
Figure S29. ^1H -NMR (400 MHz, DMSO- d ₆) spectrum of 7b .	S20
Figure S30. Mass spectrum of 7b .	S20
Figure S31. ^1H -NMR (400 MHz, DMSO- d ₆) spectrum of 8a .	S21
Figure S32. ^{13}C -NMR (100 MHz, DMSO- d ₆) spectrum of 8a .	S22
Figure S33. Mass spectrum of 8a .	S22
Figure S34. ^1H -NMR (400 MHz, DMSO- d ₆) spectrum of 8b .	S23
Figure S35. Mass spectrum of 8b .	S23
Figure S36. ^1H -NMR (400 MHz, CDCl ₃) spectrum of 9a .	S24
Figure S37. ^{13}C -NMR (100 MHz, CDCl ₃) spectrum of 9a .	S24
Figure S38. Mass spectrum of 9a .	S25
Figure S39. ^1H -NMR (400 MHz, DMSO- d ₆) spectrum of 9b .	S25
Figure S40. Mass spectrum of 9b .	S26
Figure S41. ^1H -NMR (400 MHz, DMSO- d ₆) spectrum of 10 .	S26
Figure S42. Mass spectrum of 10 .	S27
Figure S43. ^1H -NMR (400 MHz, DMSO- d ₆) spectrum of 11 .	S27
Figure S44. Mass spectrum of 11 .	S28
Figure S45. ^1H -NMR (400 MHz, DMSO- d ₆) spectrum of 12a .	S28
Figure S46. ^{13}C -NMR (100 MHz, DMSO- d ₆) spectrum of 12a .	S29
Figure S47. Mass spectrum of 12a .	S29
Figure S48. ^1H -NMR (400 MHz, DMSO- d ₆) spectrum of 12b .	S30
Figure S49. Mass spectrum of 12b	S30
Figure S50. ^1H -NMR (400 MHz, CDCl ₃) spectrum of 13 .	S31
Figure S51. Mass spectrum of 13 .	S32
Figure S52. ^1H -NMR (400 MHz, DMSO- d ₆) spectrum of 14	S32
Figure S53. Mass spectrum of 14 .	S33

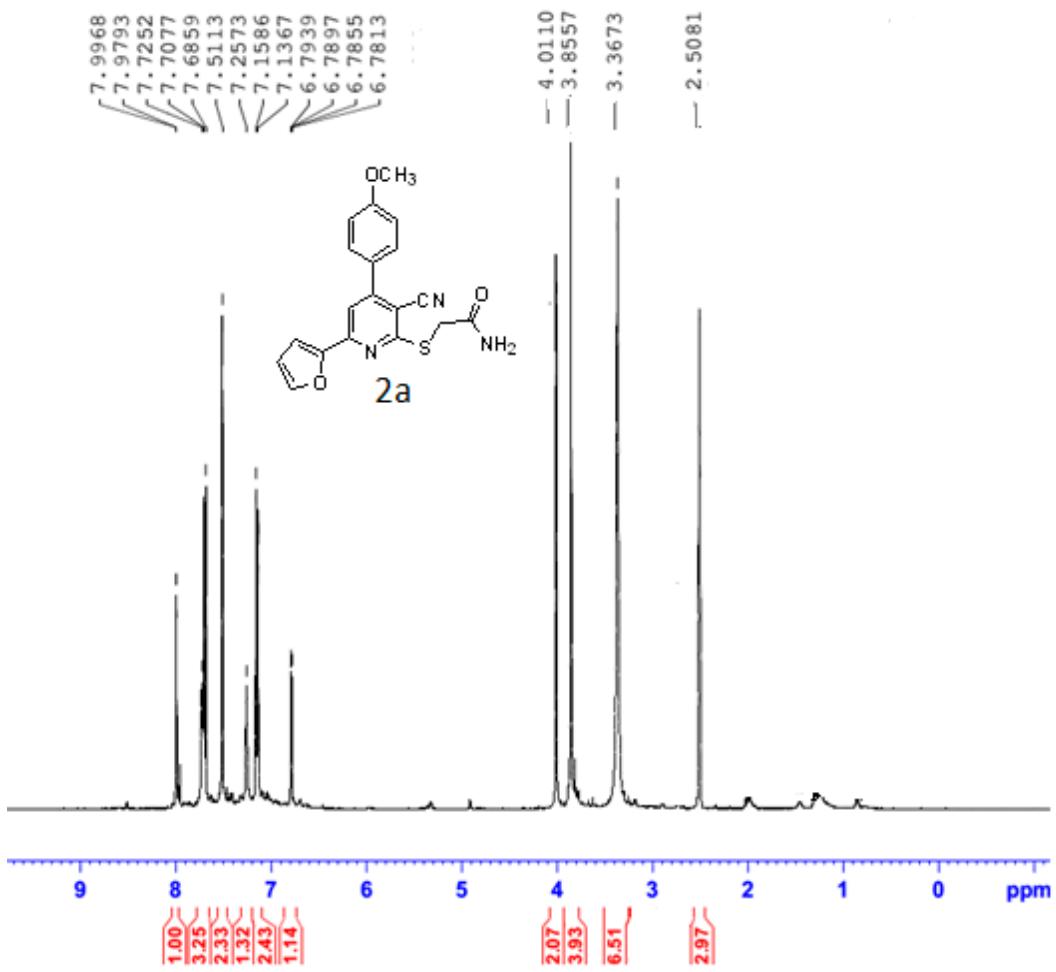


Fig. S1 ^1H NMR (400 MHz) in $\text{DMSO}-d_6$ of compound **2a**

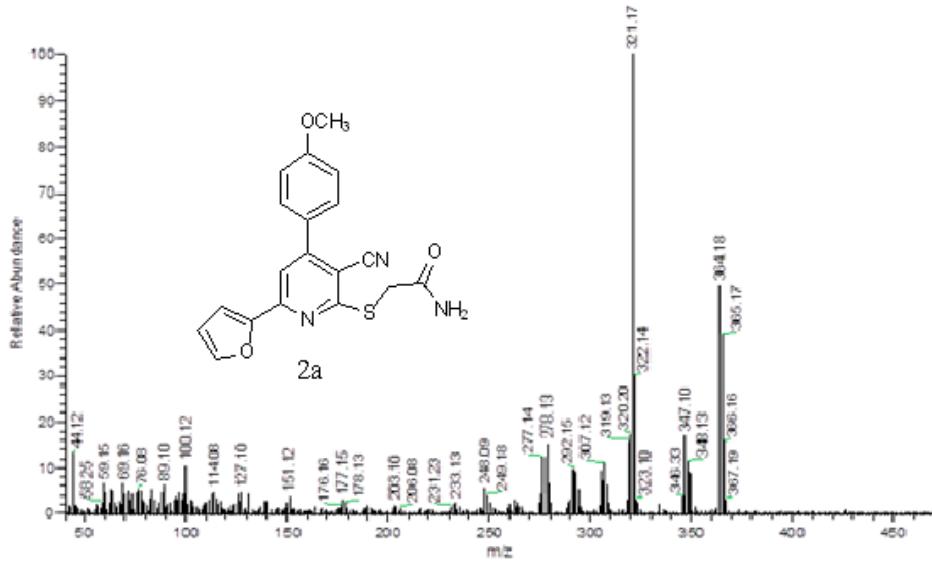


Fig. S2 Mass spectrum of compound **2a**

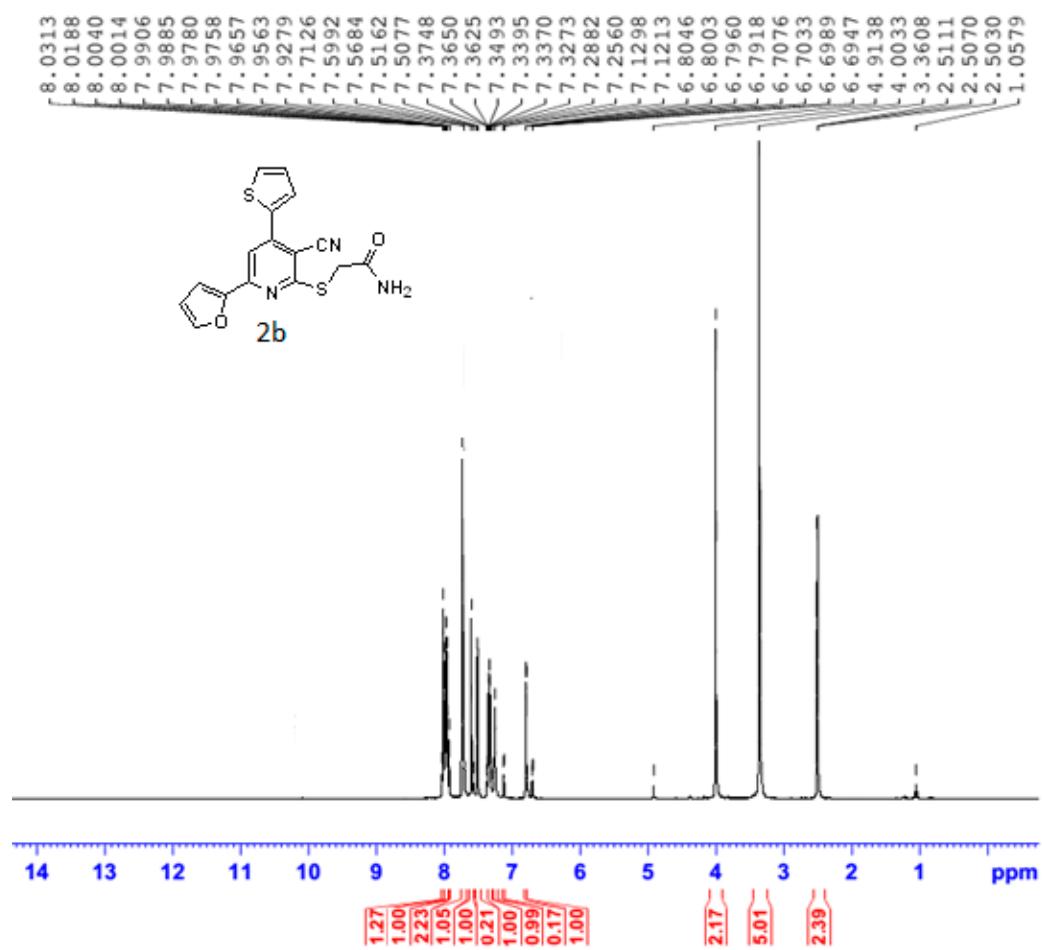


Fig. S3 ^1H NMR (400 MHz) in $\text{DMSO}-d_6$ of compound **2b**

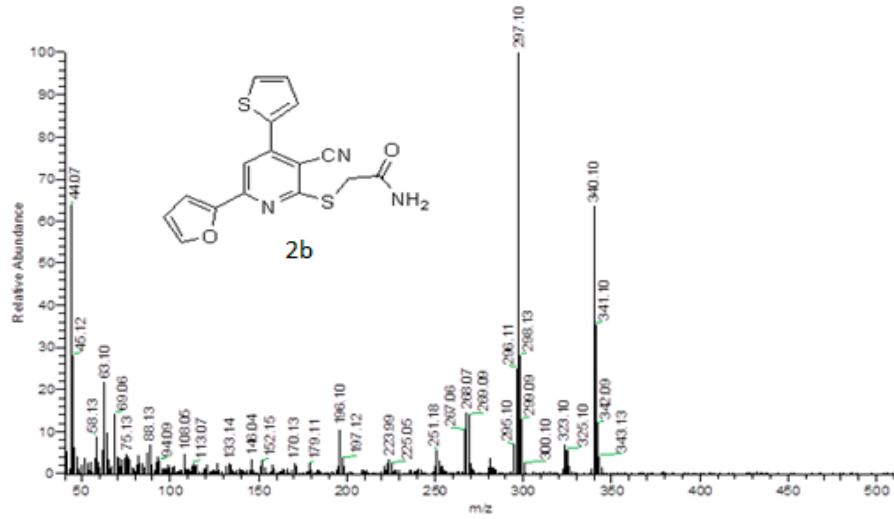


Fig. S4 Mass spectrum of compound **2b**

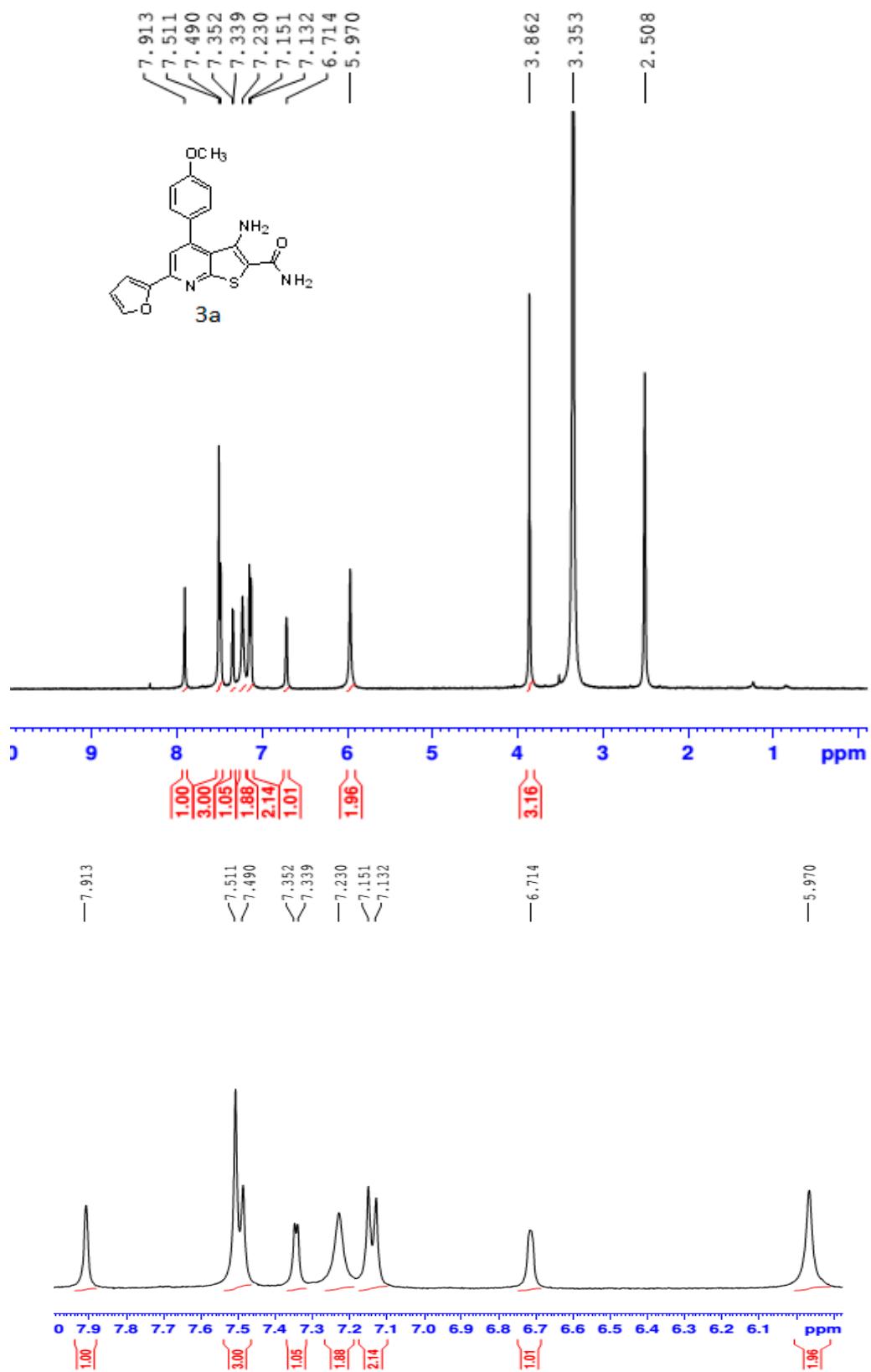


Fig. S5 ^1H NMR (400 MHz) in DMSO-*d*₆ of compound **3a**

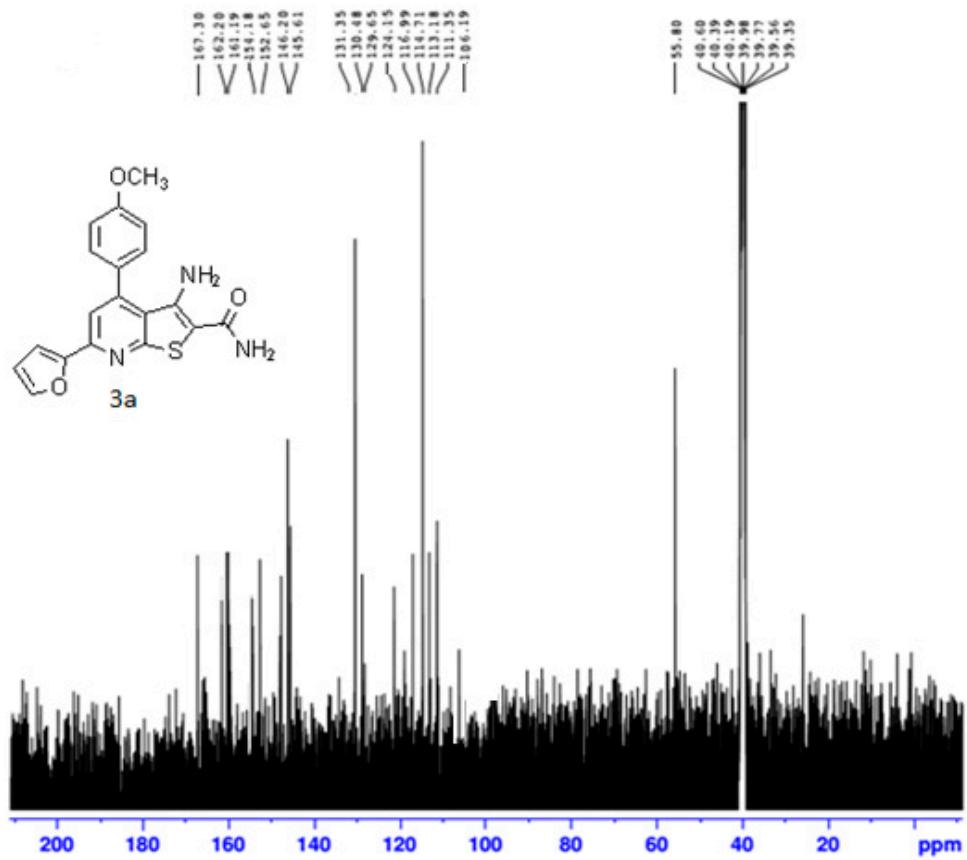


Fig. S6 ^{13}C NMR (100 MHz) in $\text{DMSO}-d_6$ of compound **3a**

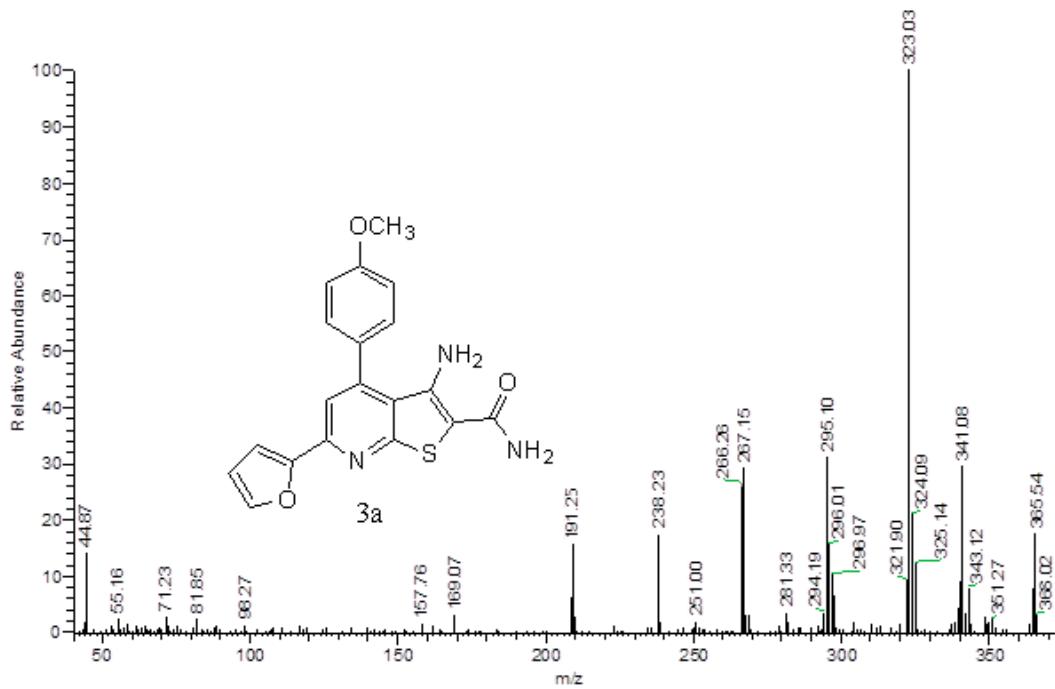


Fig. S7 Mass spectrum of compound **3a**

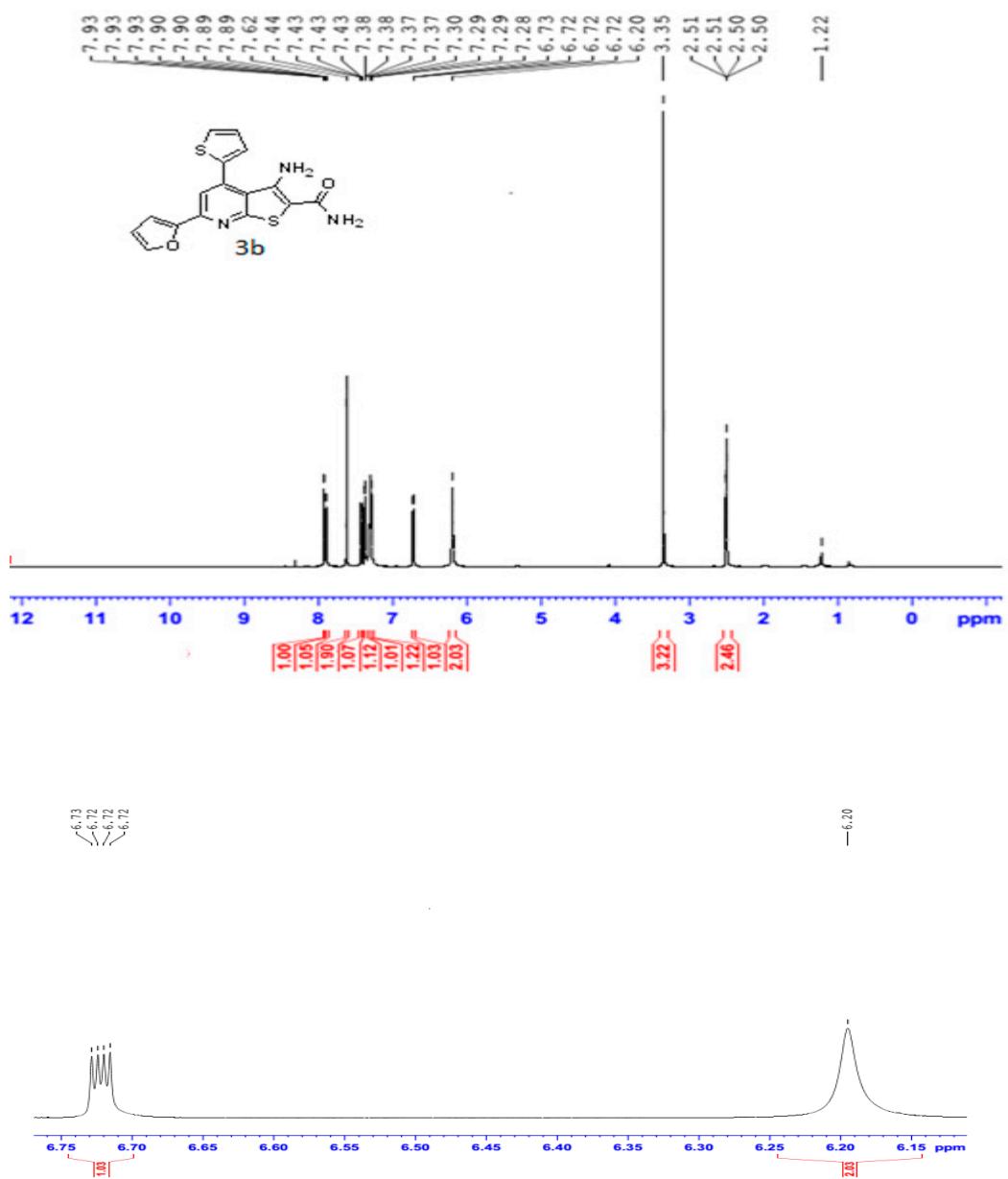


Fig. S8 ^1H NMR (400 MHz) in $\text{DMSO}-d_6$ of compound **3b**

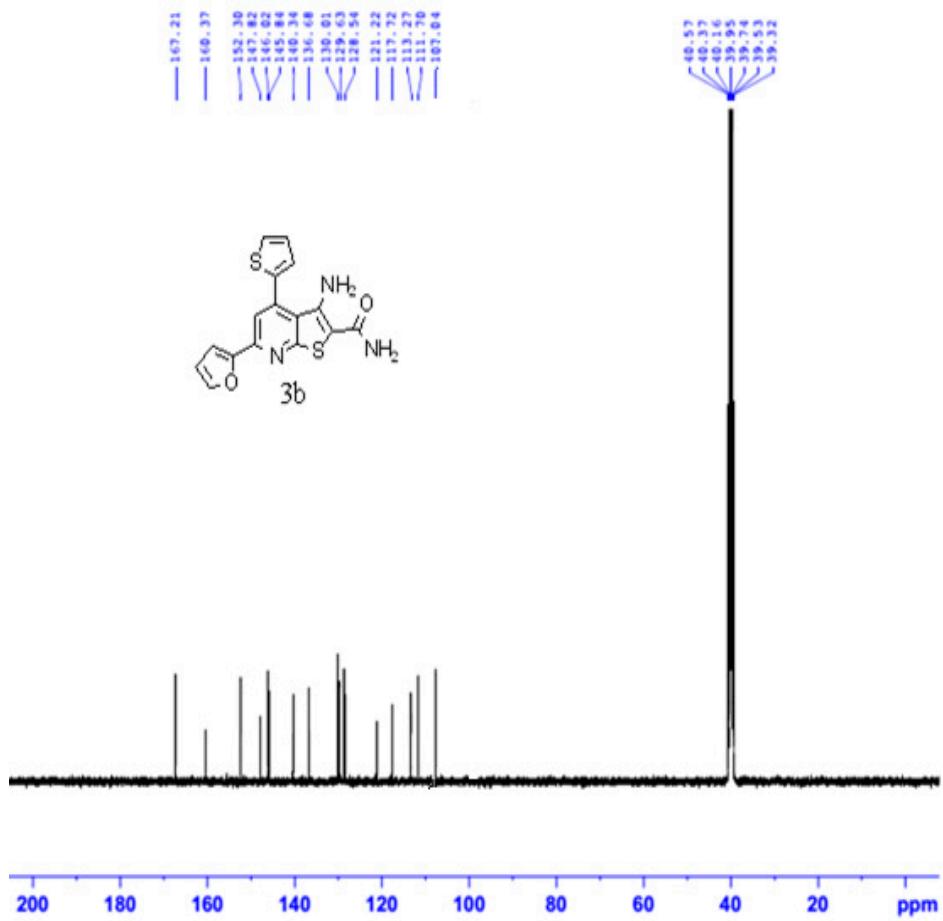


Fig. S9 ^{13}C NMR (100 MHz) in $\text{DMSO}-d_6$ of compound **3b**

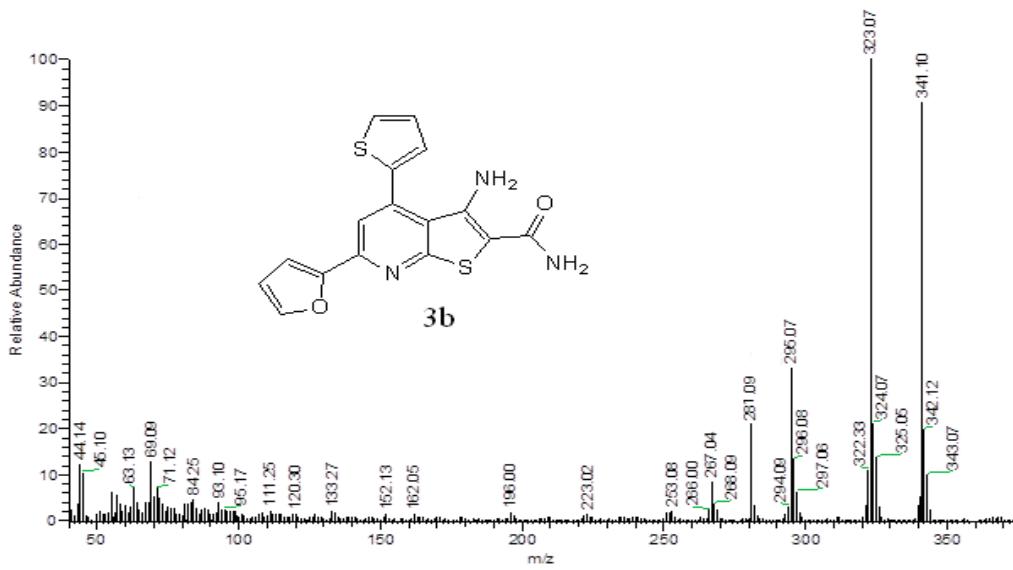


Fig. S10 Mass spectrum of compound **3b**

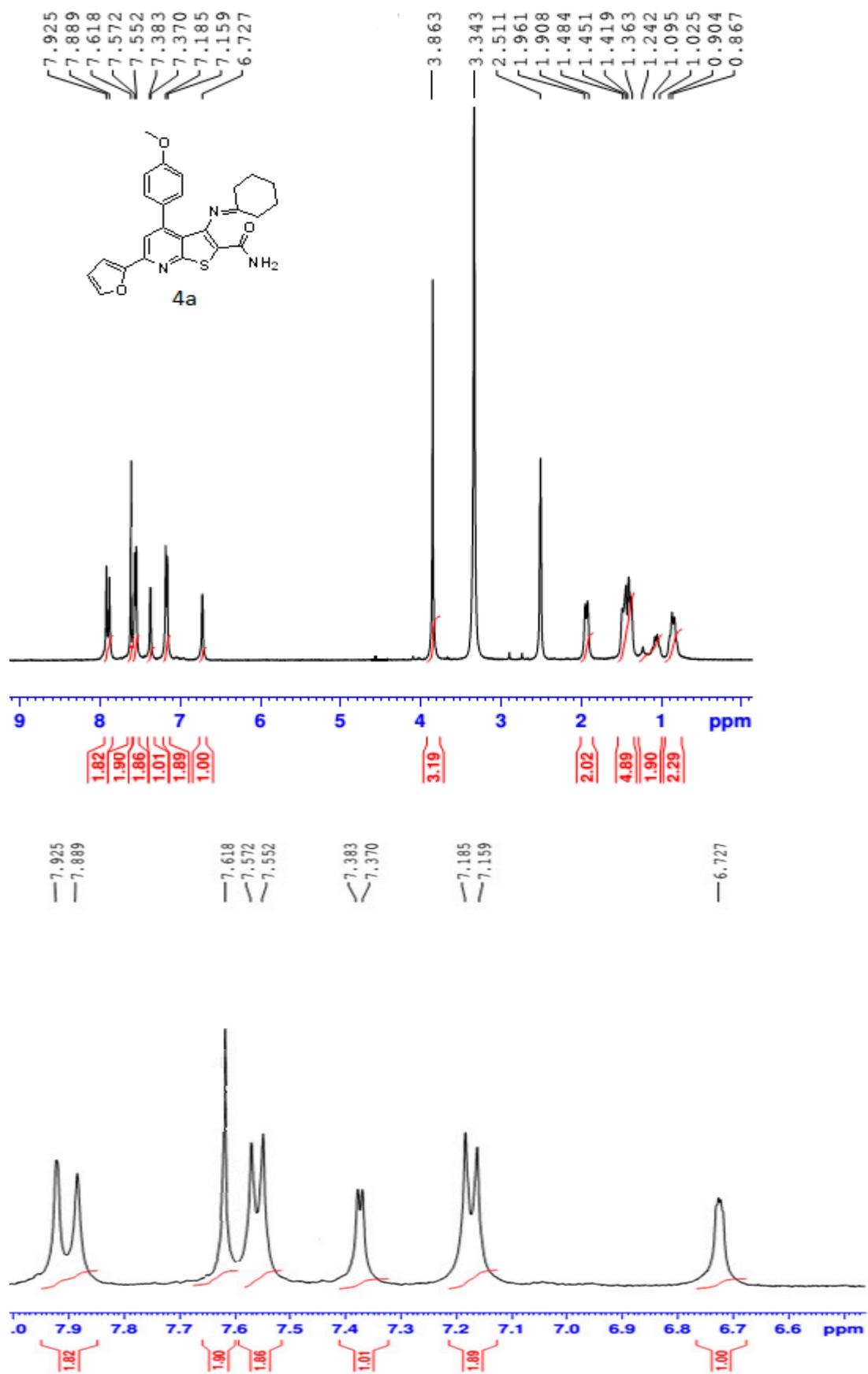


Fig. S11 ¹H NMR (400 MHz) in DMSO-*d*₆ of compound **4a**

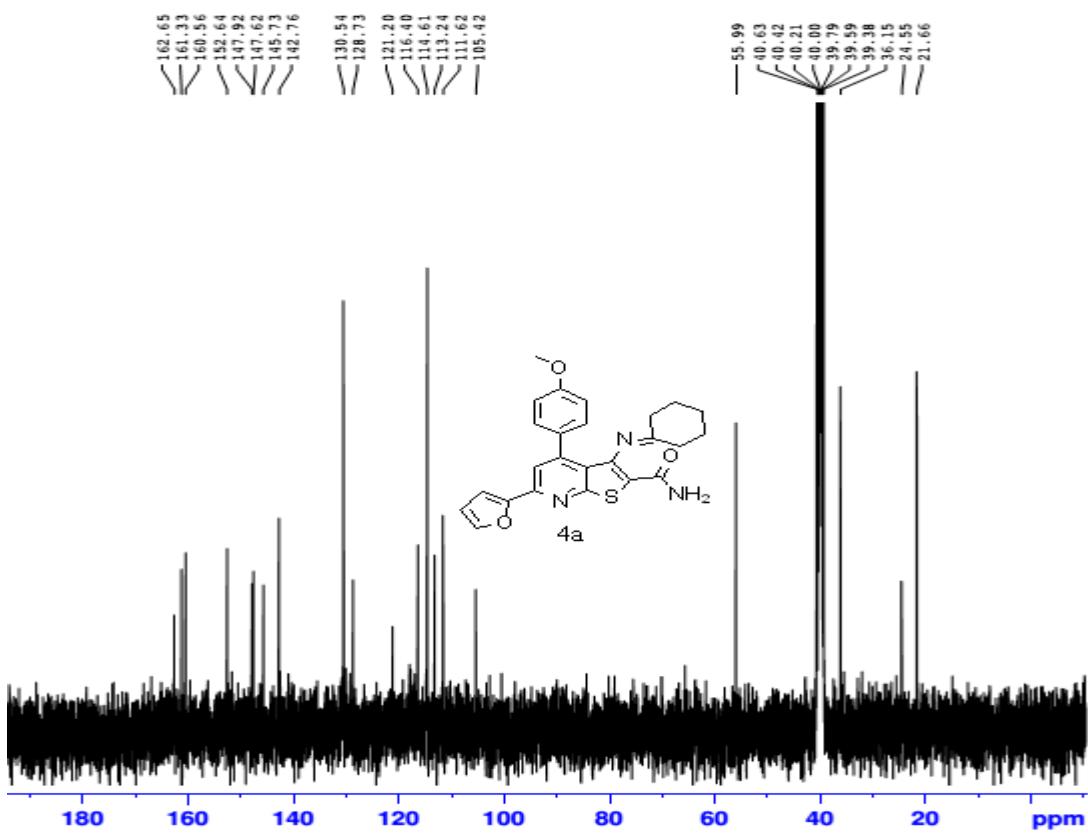


Fig. S12 ^{13}C NMR (100 MHz) in $\text{DMSO}-d_6$ of compound **4a**

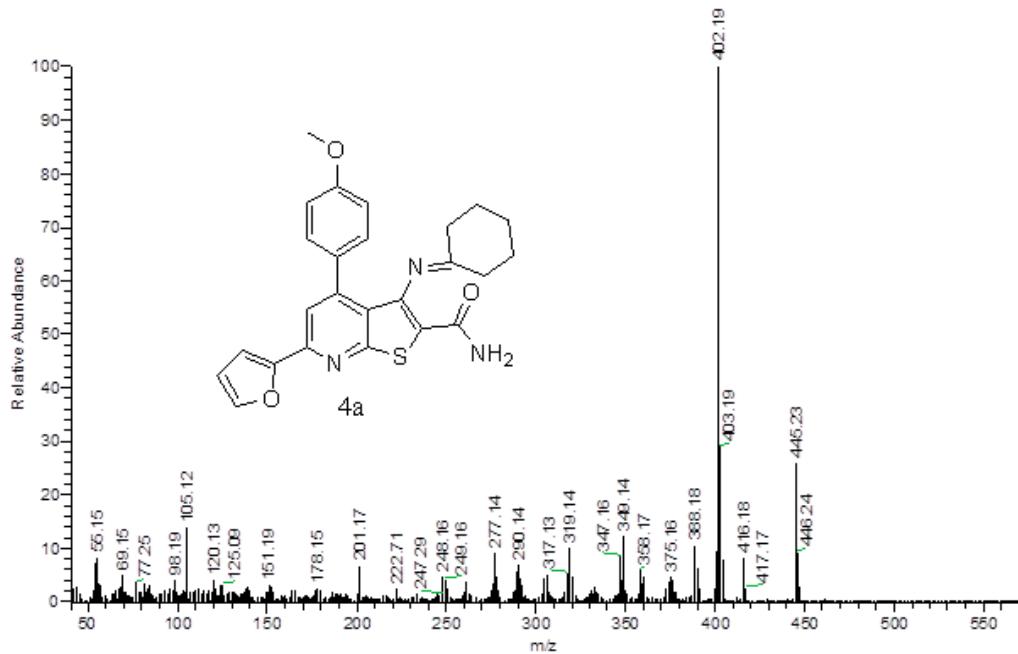


Fig. S13 Mass spectrum of compound **4a**

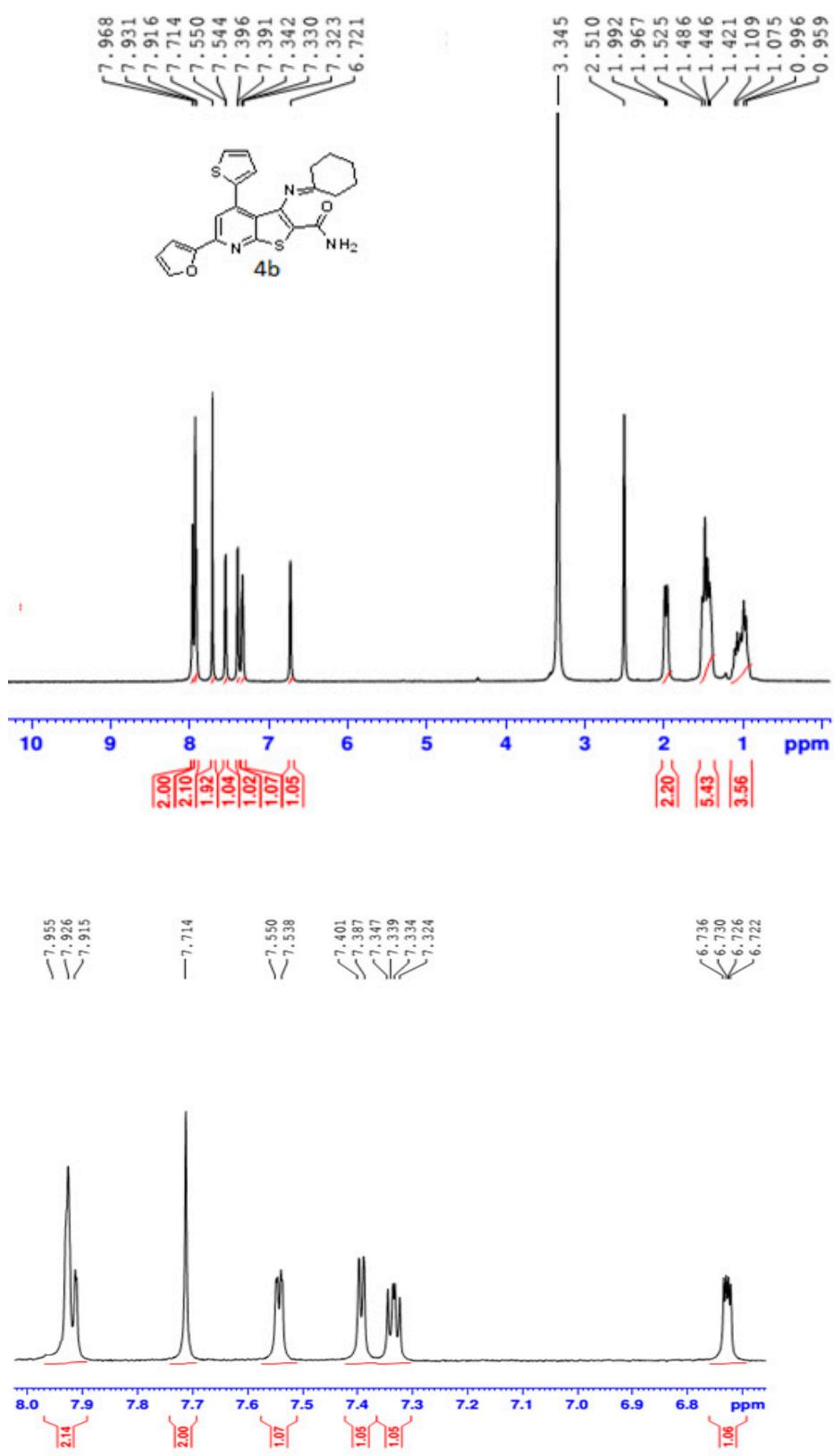


Fig. S14 ¹H NMR (400 MHz) in DMSO-*d*₆ of compound **4b**

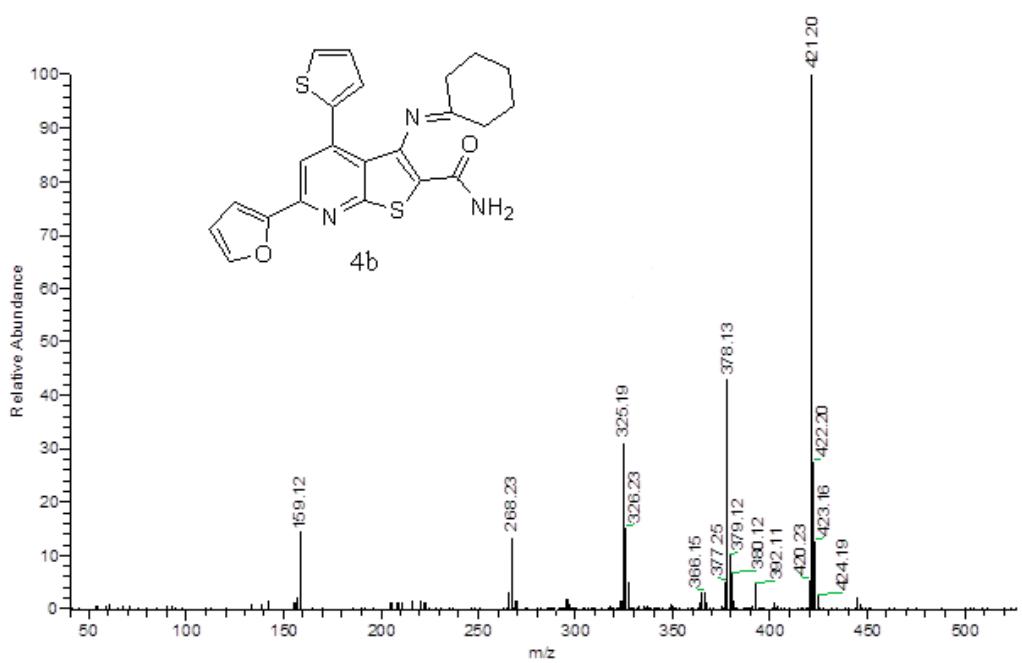


Fig. S15 Mass spectrum of compound **4b**

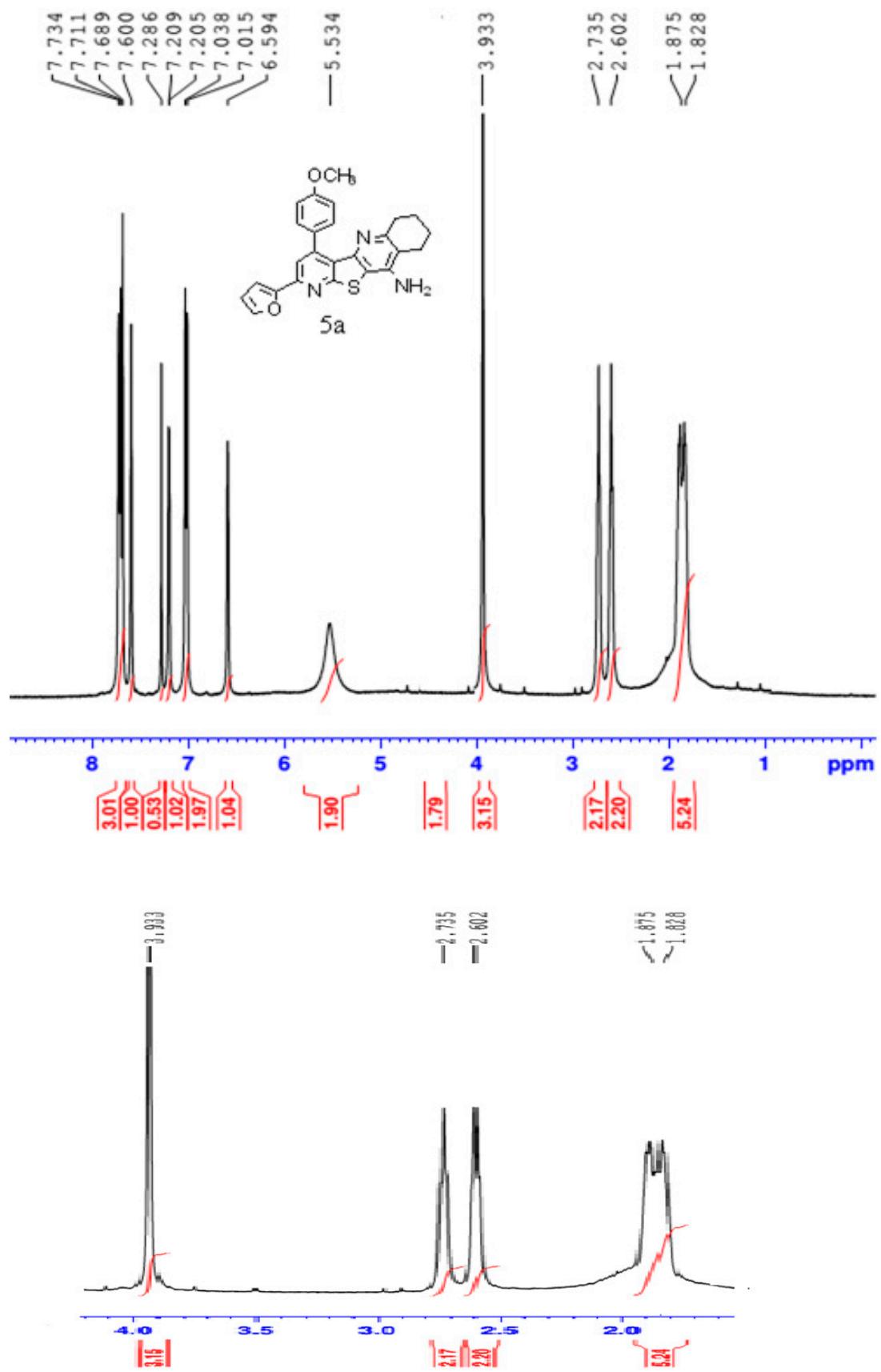


Fig. S16 ^1H NMR (400 MHz) spectrum in CDCl_3 of compound **5a**

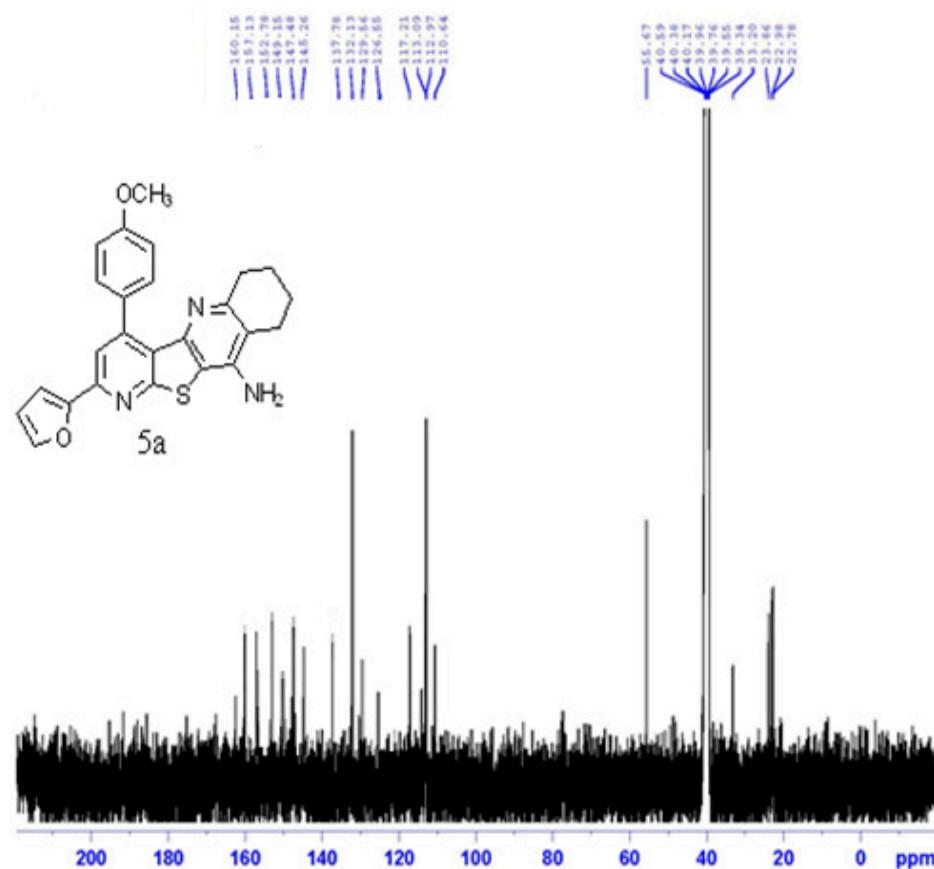


Fig. S17 ^{13}C NMR (100 MHz) in $\text{DMSO}-d_6$ of compound **5a**

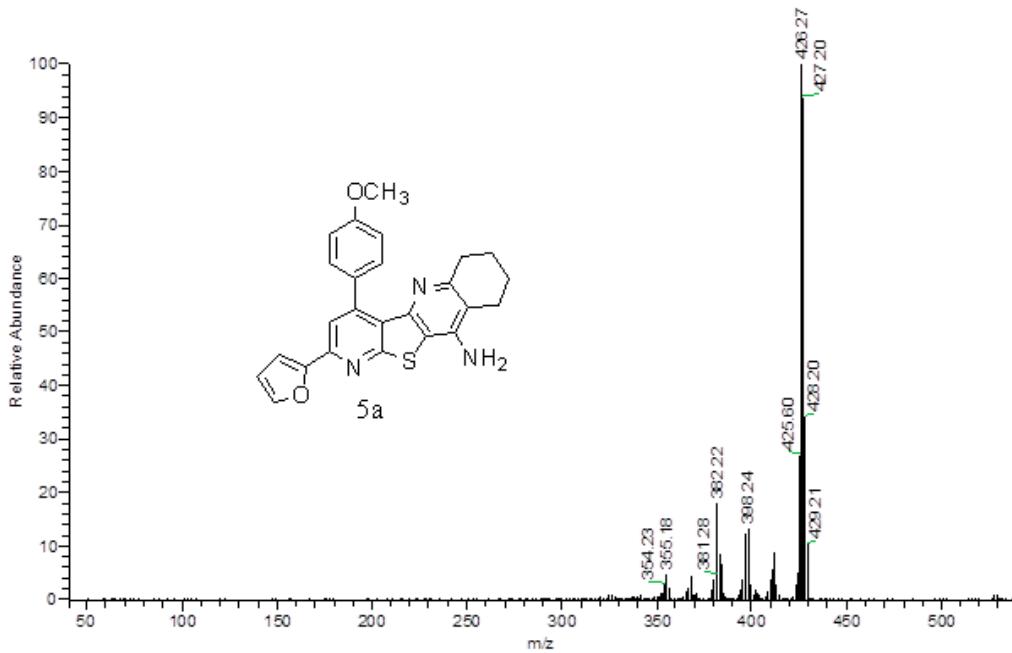


Fig. S18 Mass spectrum of compound **5a**

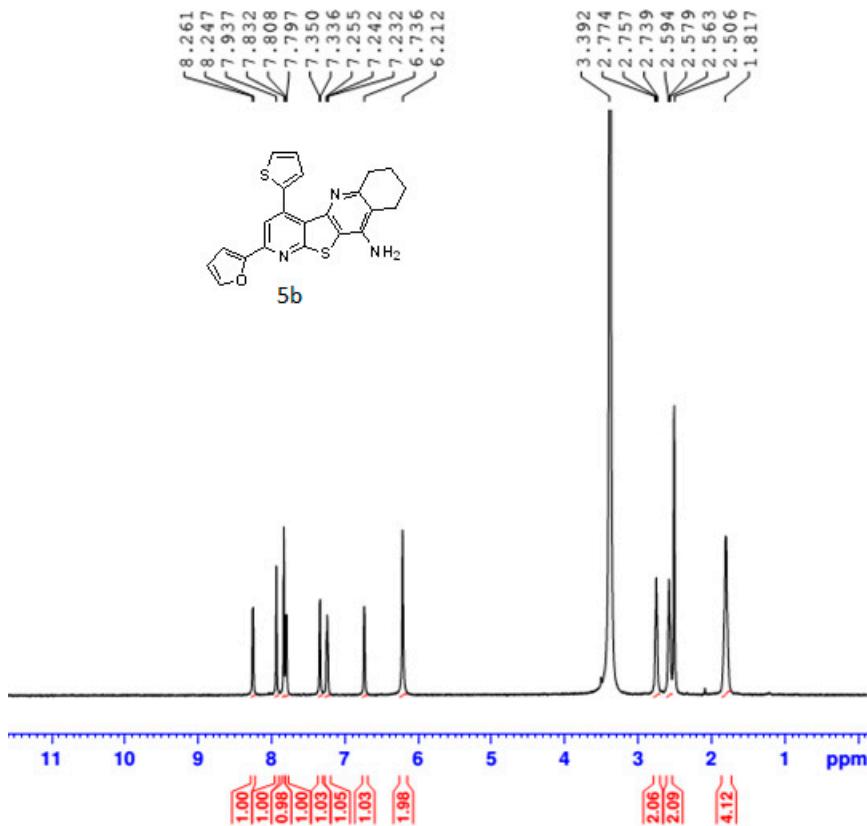


Fig. S19 ^1H NMR (400 MHz) in DMSO- d_6 of compound **5b**

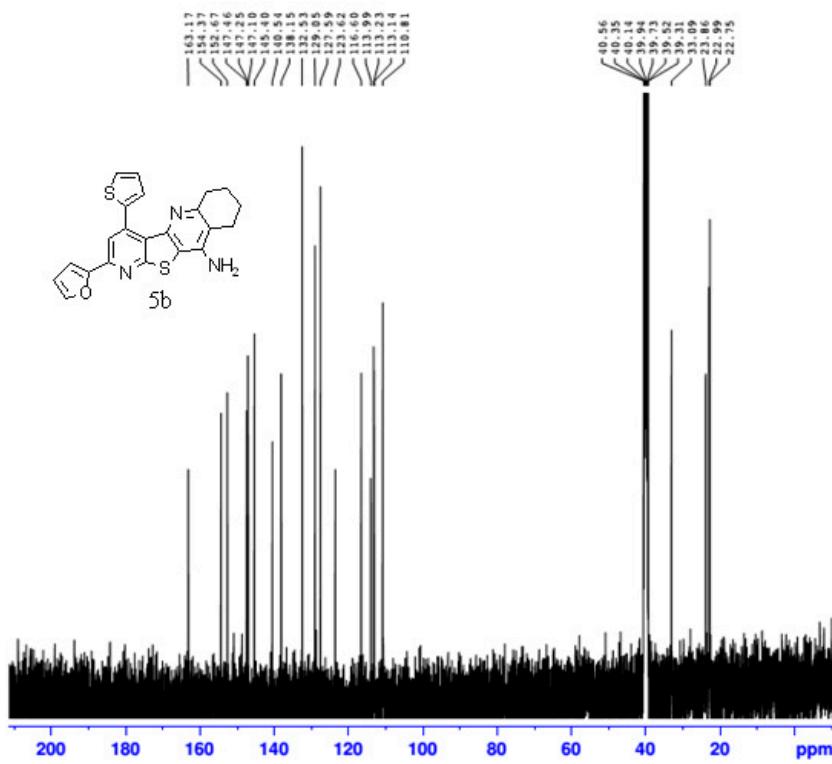


Fig. S20 ^{13}C NMR (100 MHz) in DMSO- d_6 of compound **5b**

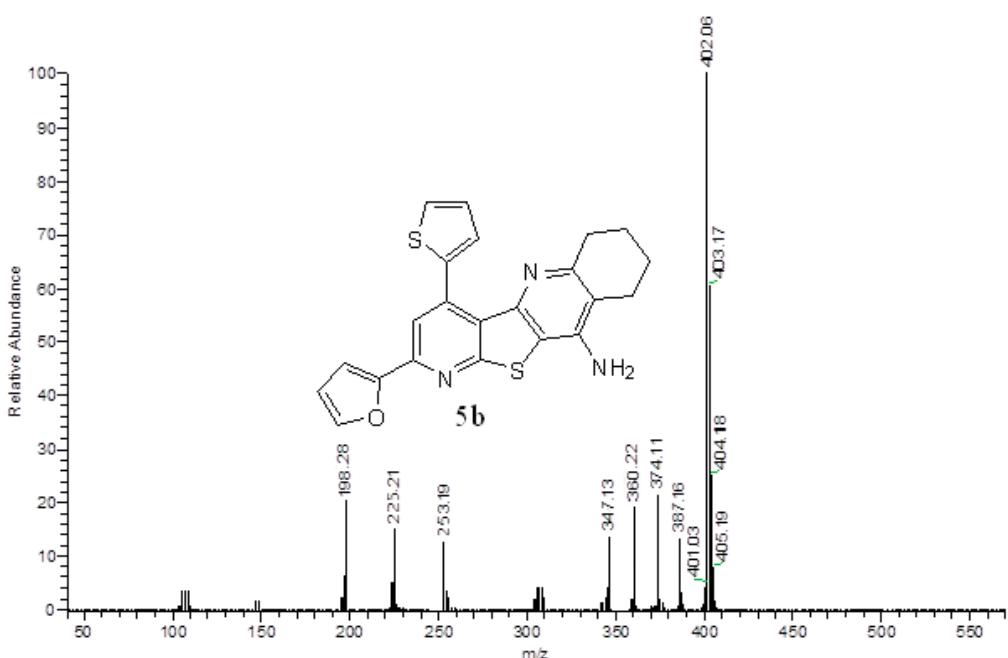


Fig. S21 Mass spectrum of compound **5b**

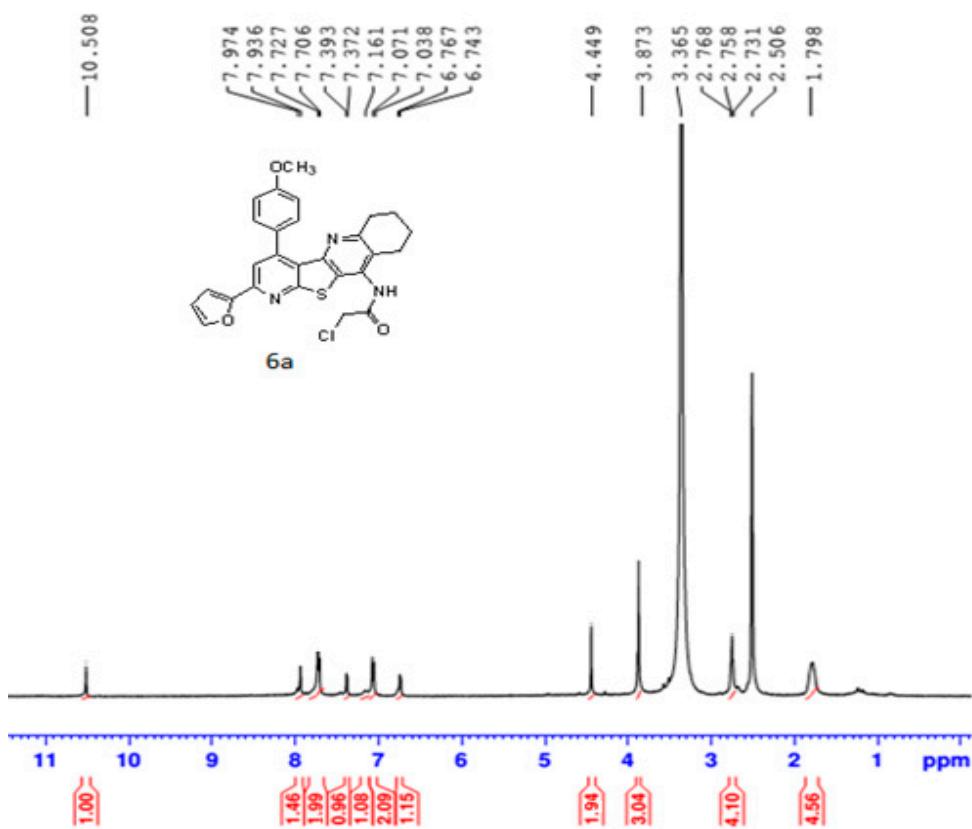


Fig. S22 ^1H NMR (400 MHz) in $\text{DMSO}-d_6$ of compound **6a**

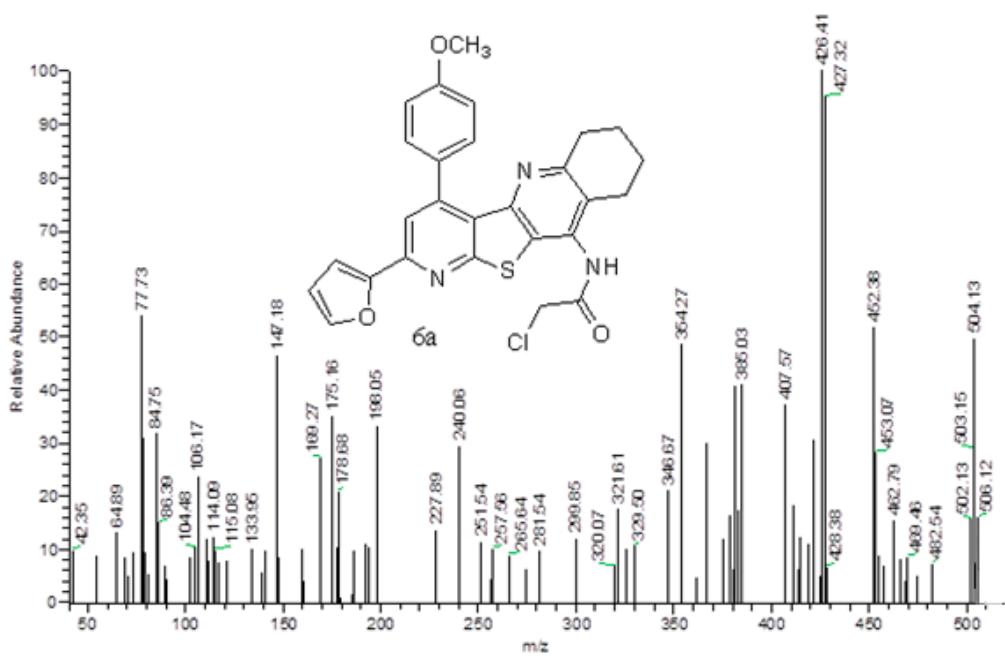


Fig. S23 Mass spectrum of compound 6a

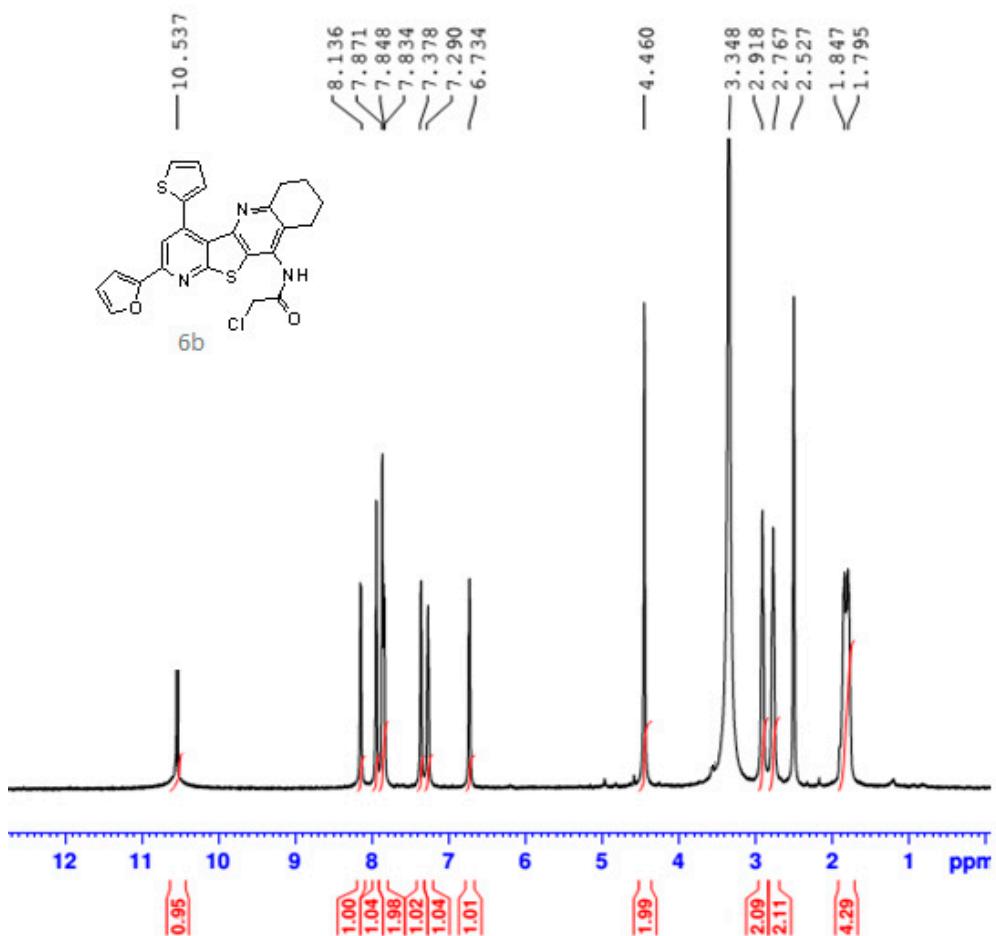


Fig. S24 ^1H NMR (400 MHz) in $\text{DMSO}-d_6$ of compound 6b

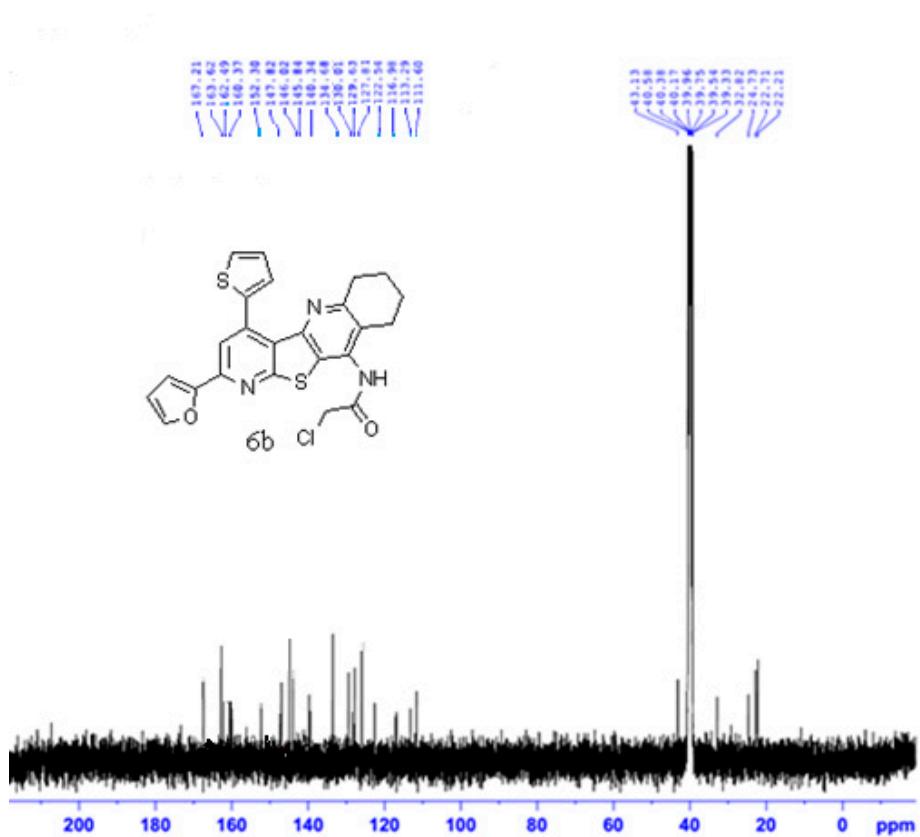


Fig. S25 ^{13}C NMR (100 MHz) in $\text{DMSO}-d_6$ of compound **6b**

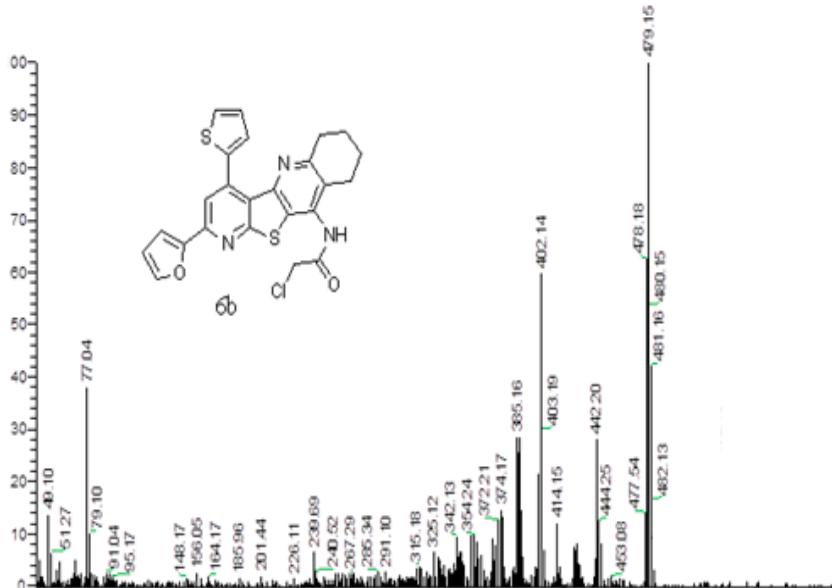


Fig. S26 Mass spectrum of compound **6b**

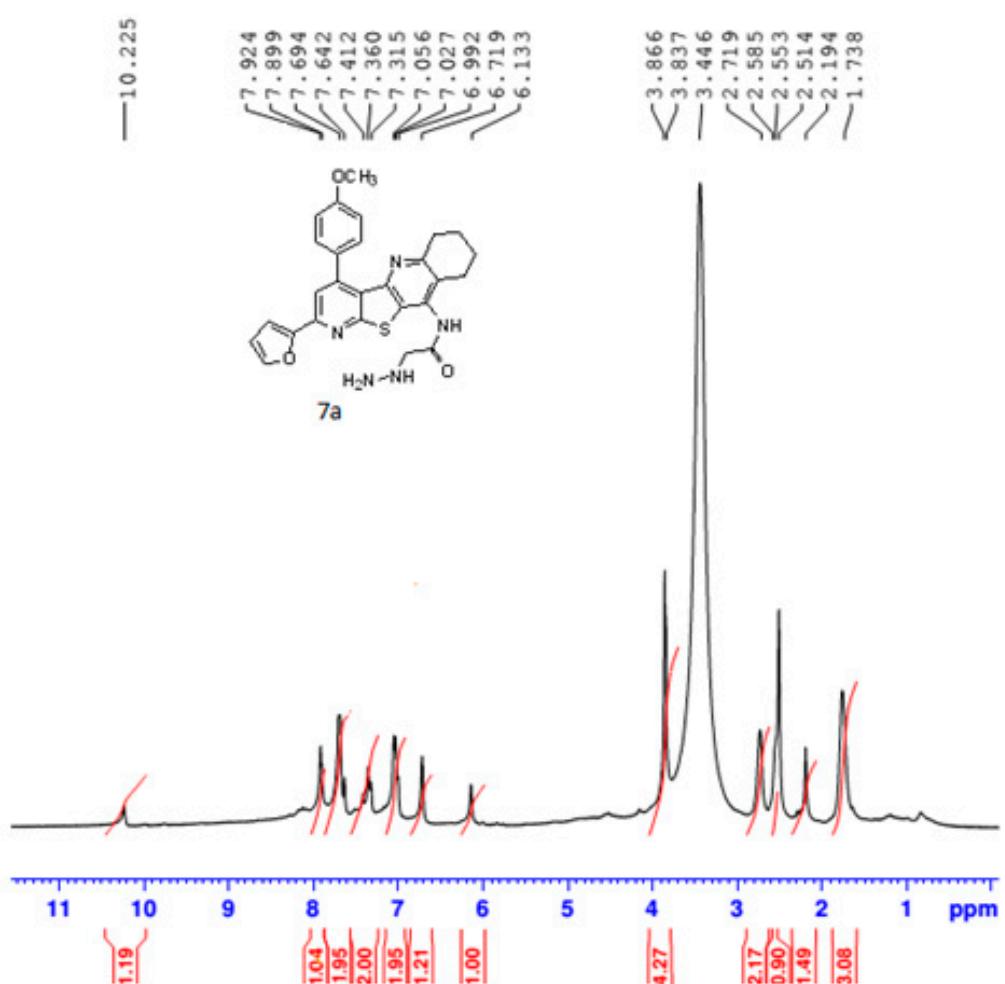


Fig. S27 ^1H NMR (400 MHz) in $\text{DMSO}-d_6$ of compound **7a**

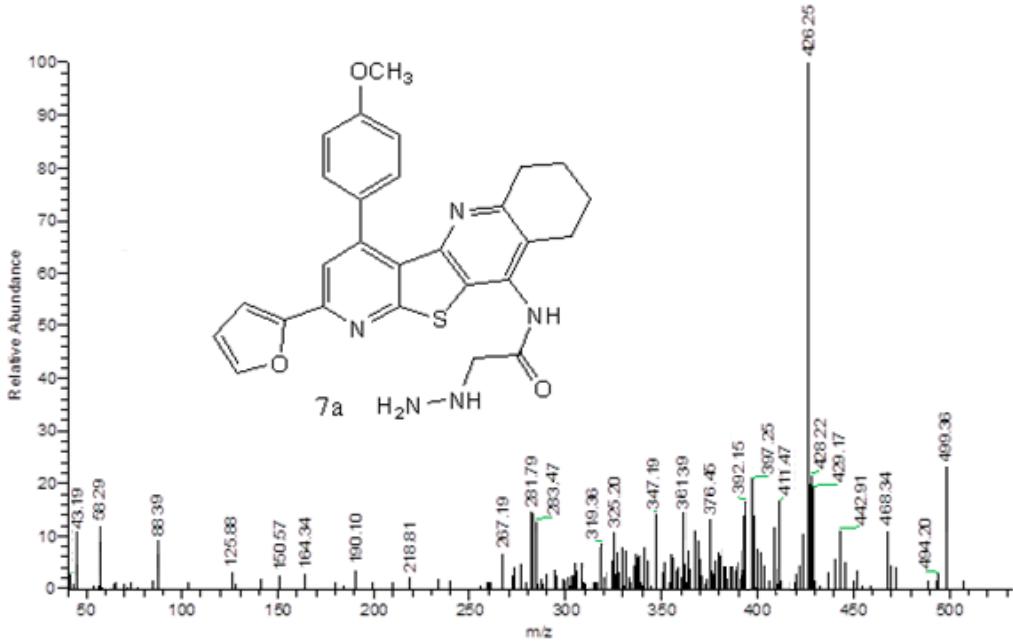


Fig. S28 Mass spectrum of compound **7a**

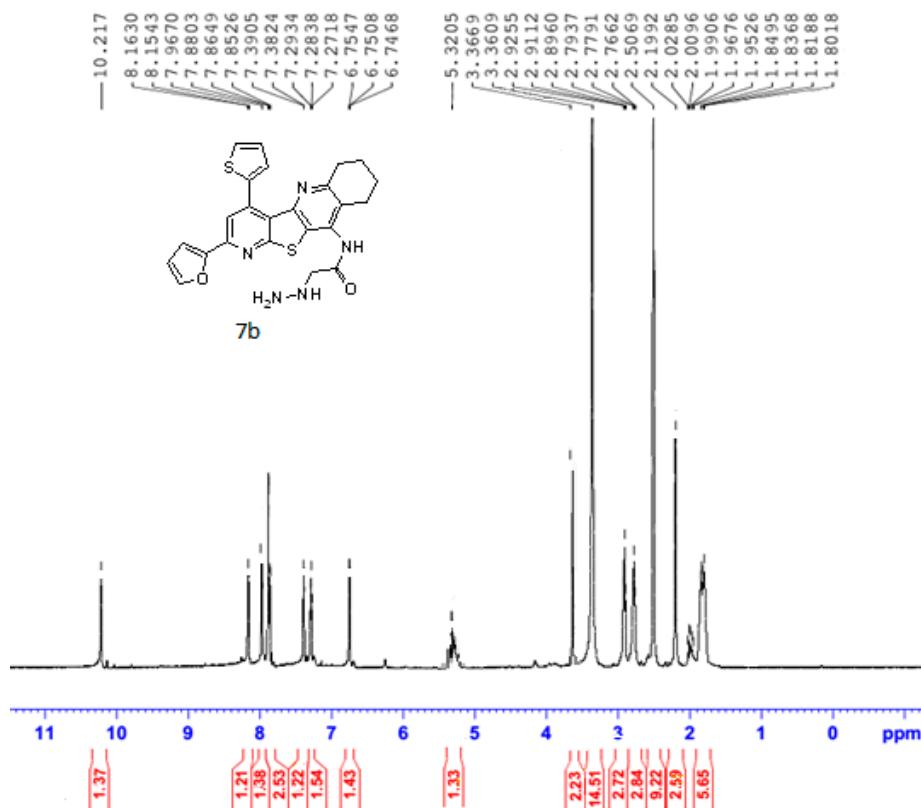


Fig. S29 ^1H NMR (400 MHz) in DMSO- d_6 of compound **7b**

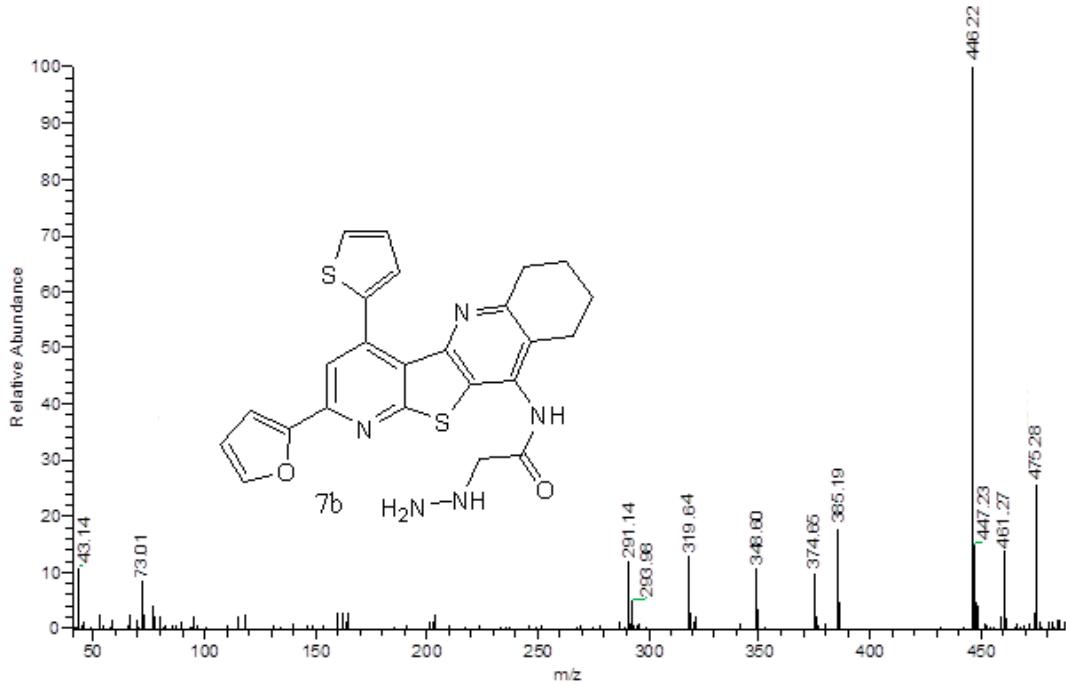


Fig. S30 Mass spectrum of compound **7b**

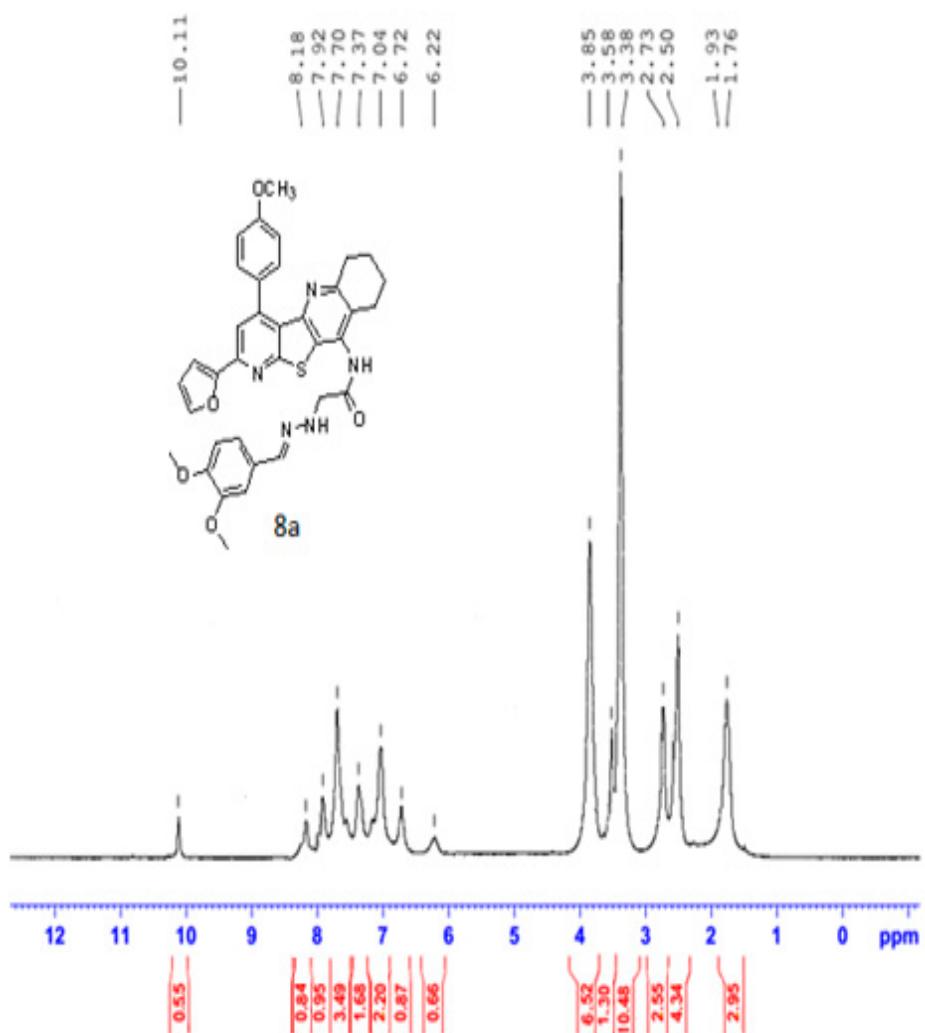


Fig. S31 ^1H NMR (400 MHz) in $\text{DMSO}-d_6$ of compound **8a**

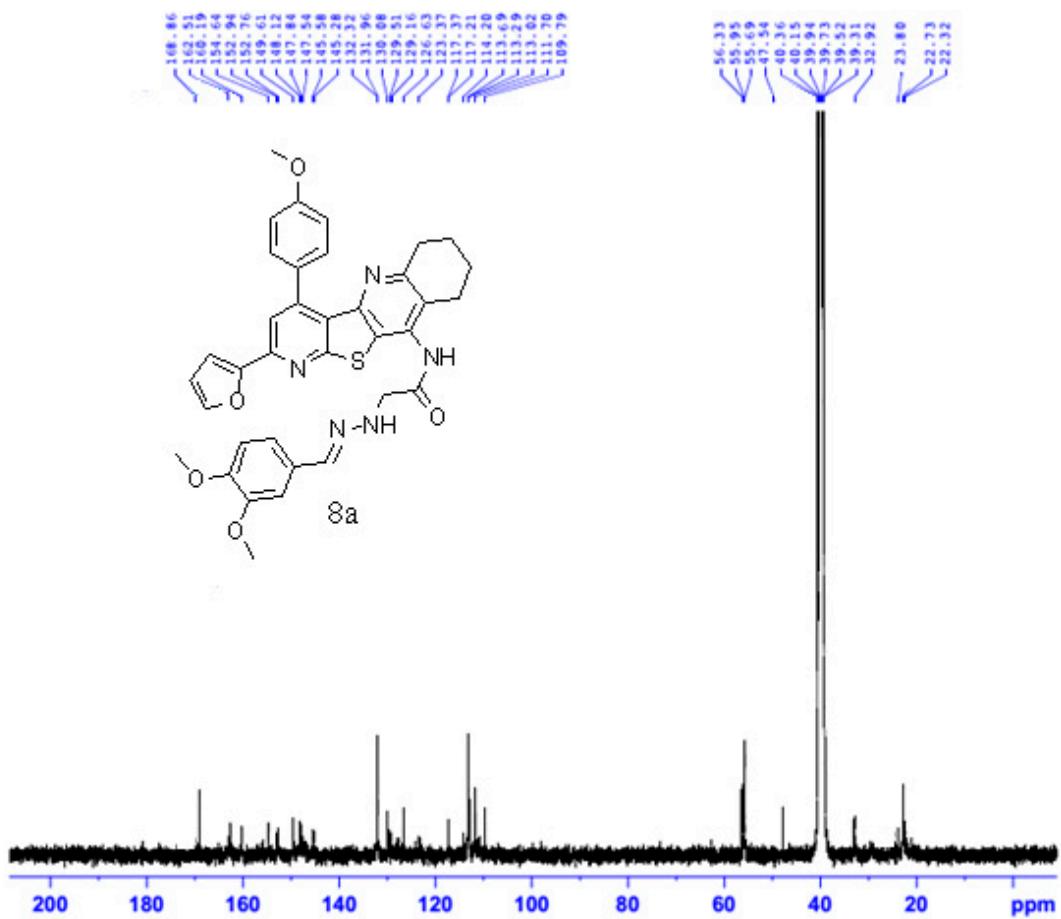


Fig. S32 ^{13}C NMR (100 MHz) in $\text{DMSO}-d_6$ of compound **8a**

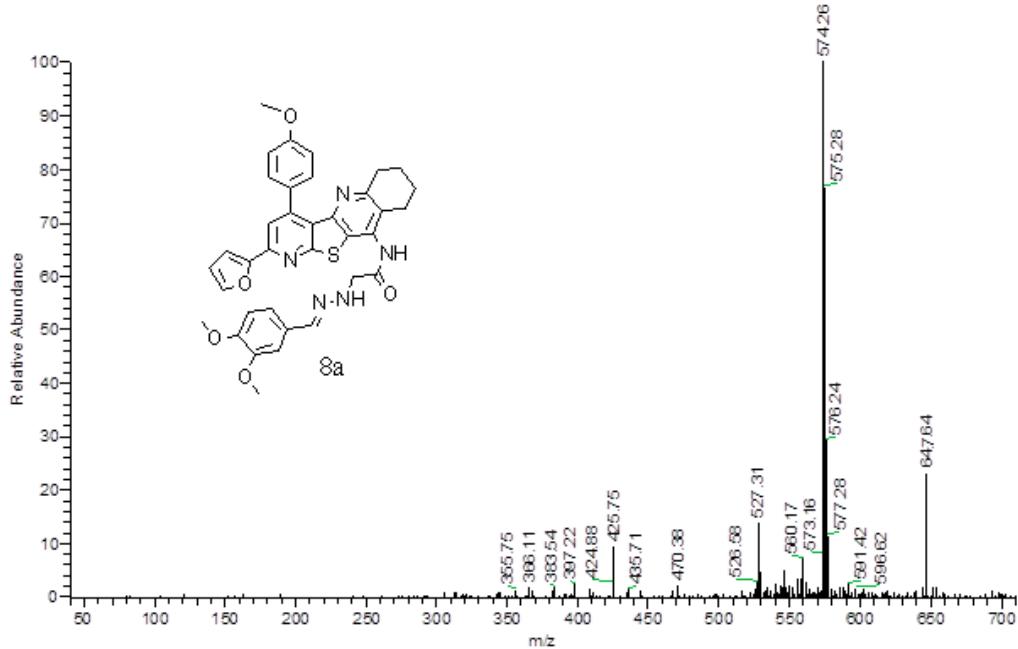


Fig. S33 Mass spectrum of compound **8a**

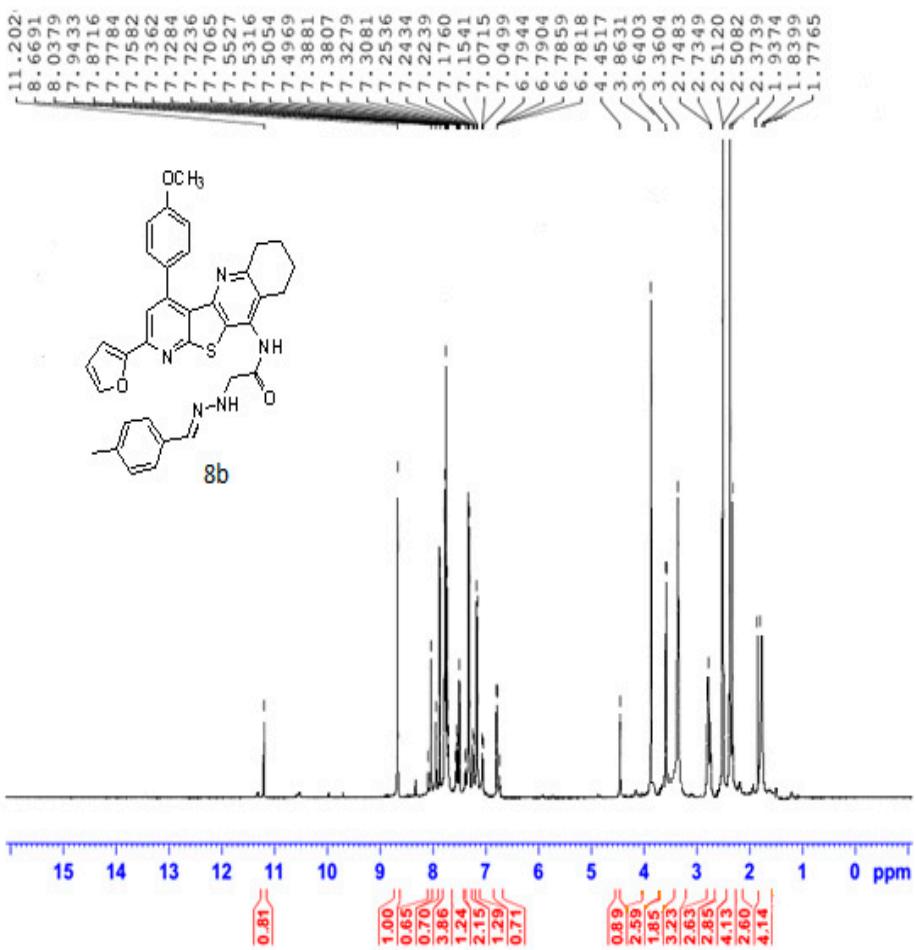


Fig. S34 ¹H NMR (400 MHz) in DMSO-*d*₆ of compound **8b**

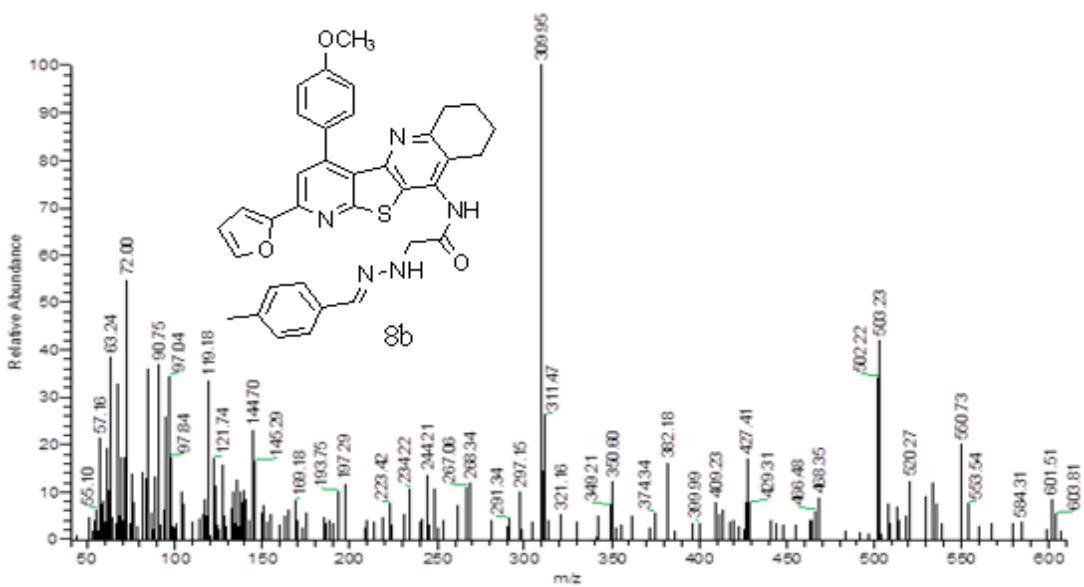


Fig. S35 Mass spectrum of compound **8b**

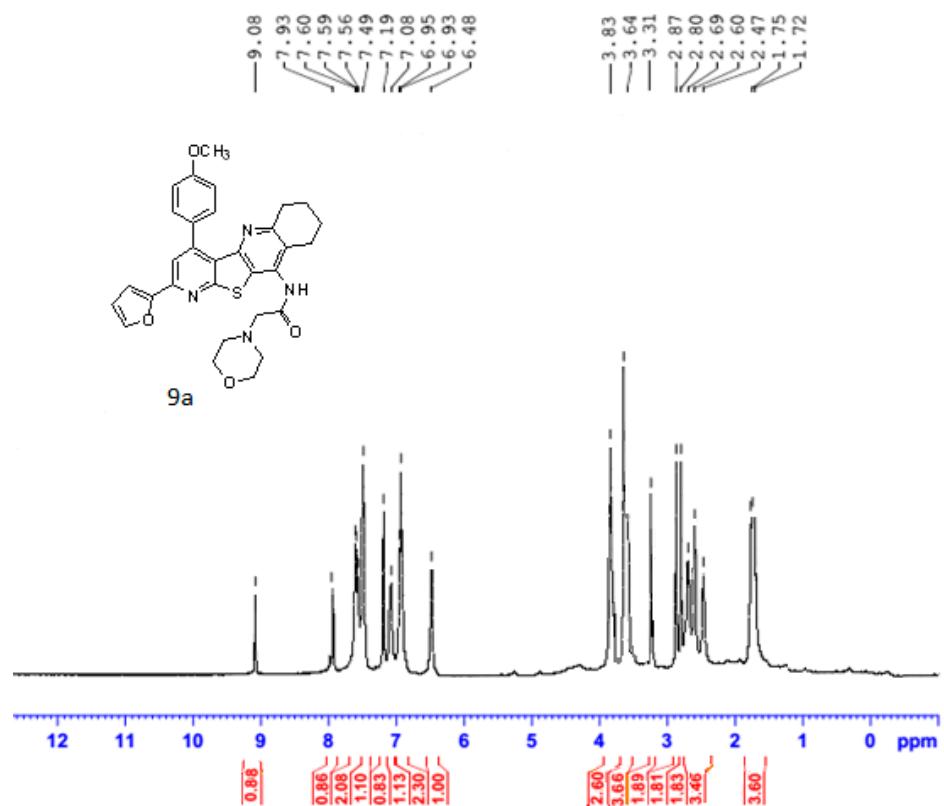


Fig. S36 ¹H NMR (400 MHz) in CDCl₃ of compound 9a

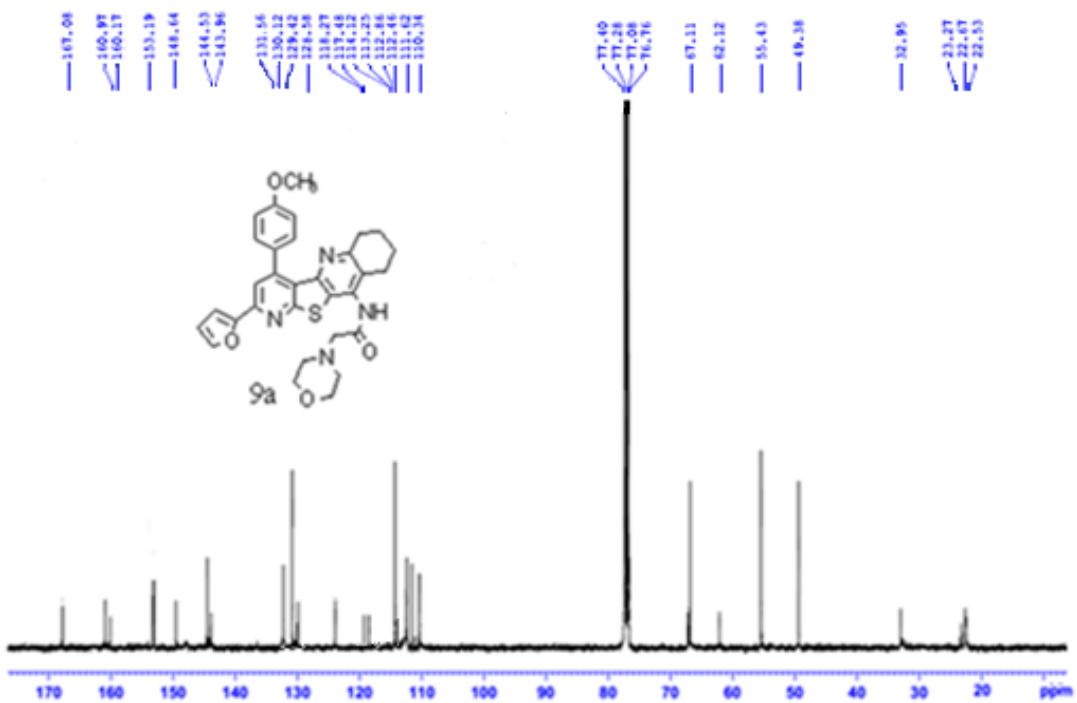


Fig. S37 ¹³C NMR (100 MHz) in CDCl₃ of compound 9a

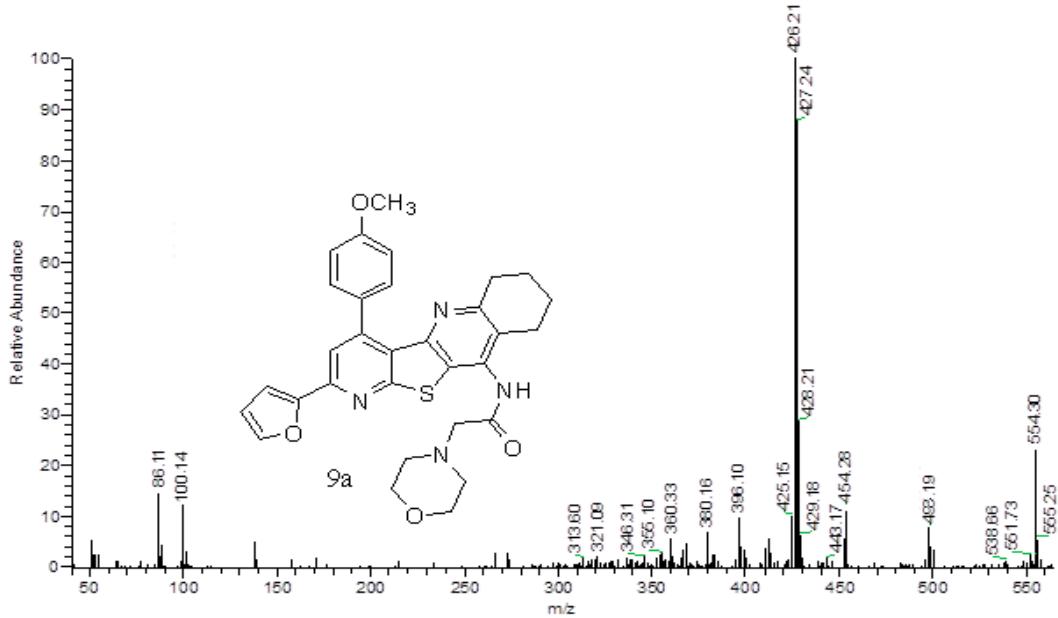
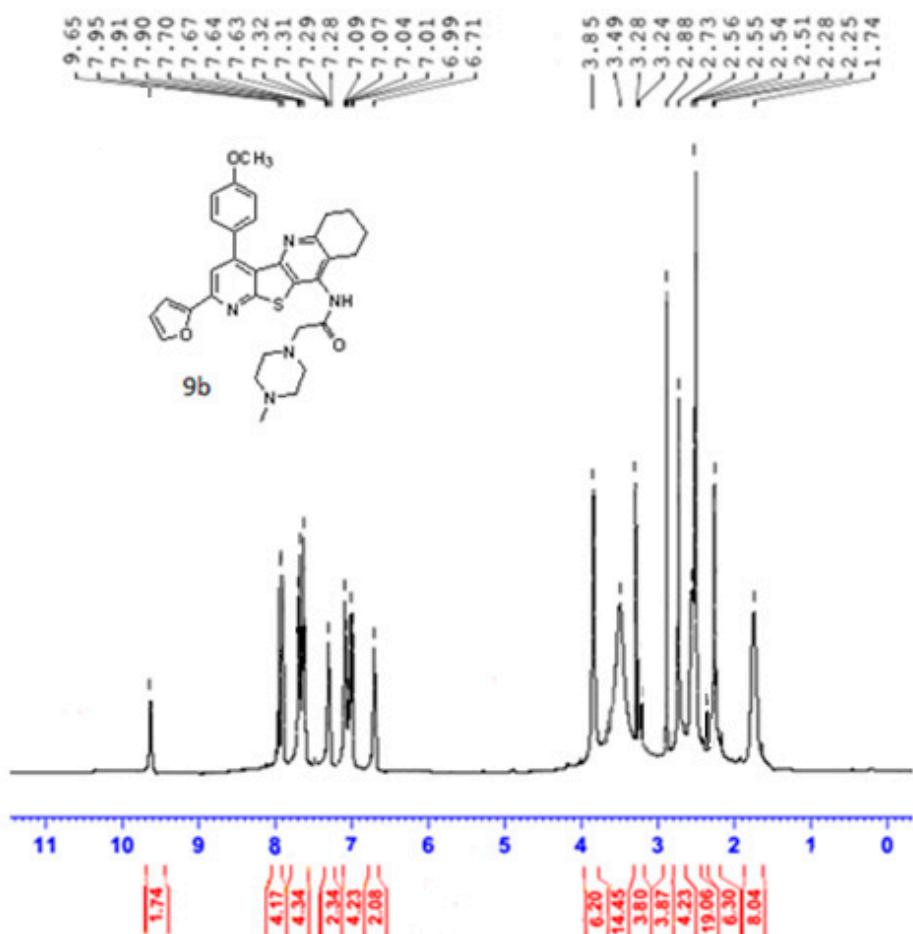


Fig. S38 Mass spectrum of compound 9a



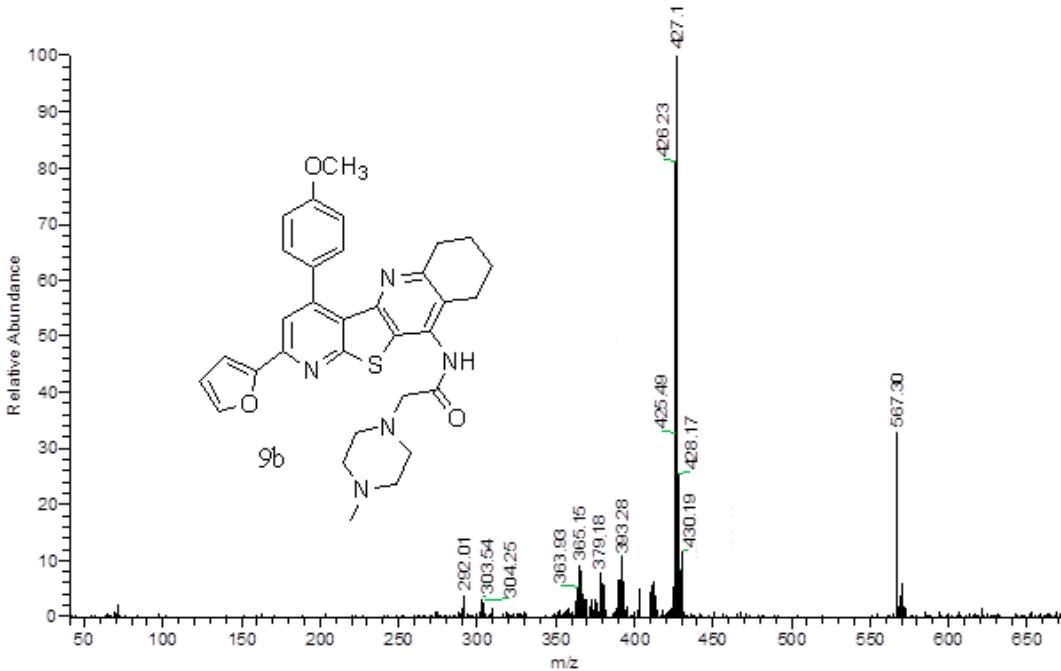


Fig. S40 Mass spectrum of compound **9b**

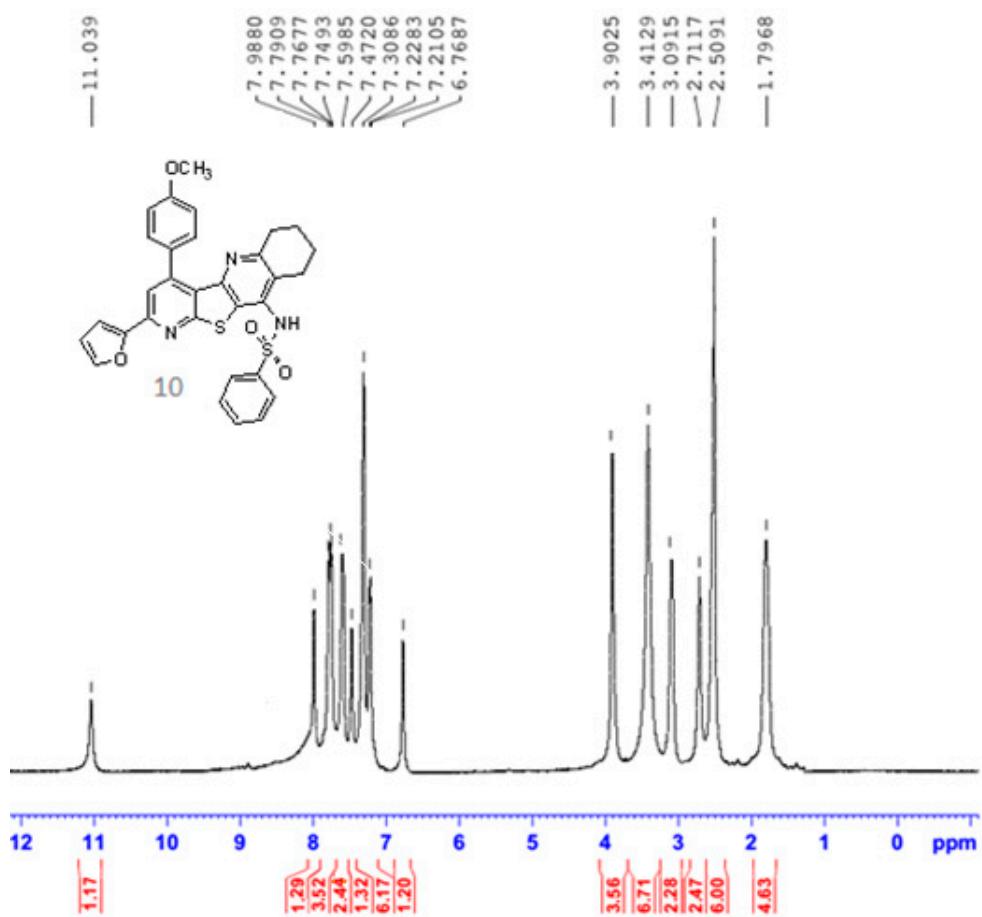


Fig. S41 ^1H NMR (400 MHz) in $\text{DMSO}-d_6$ of compound **10**

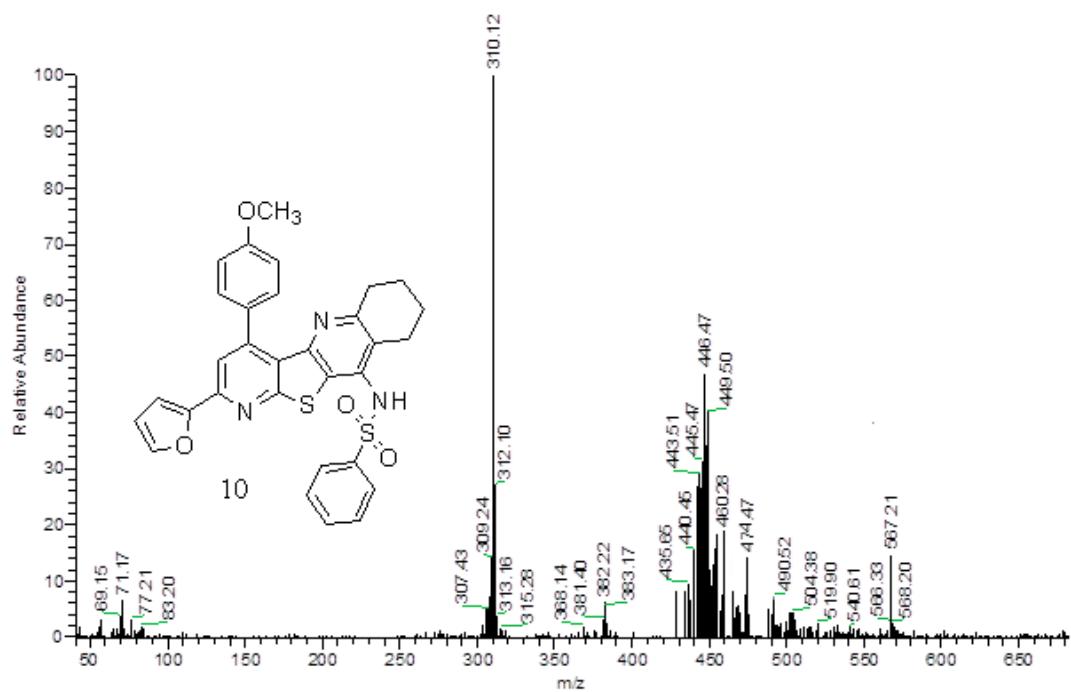


Fig. S42 Mass spectrum of compound **10**

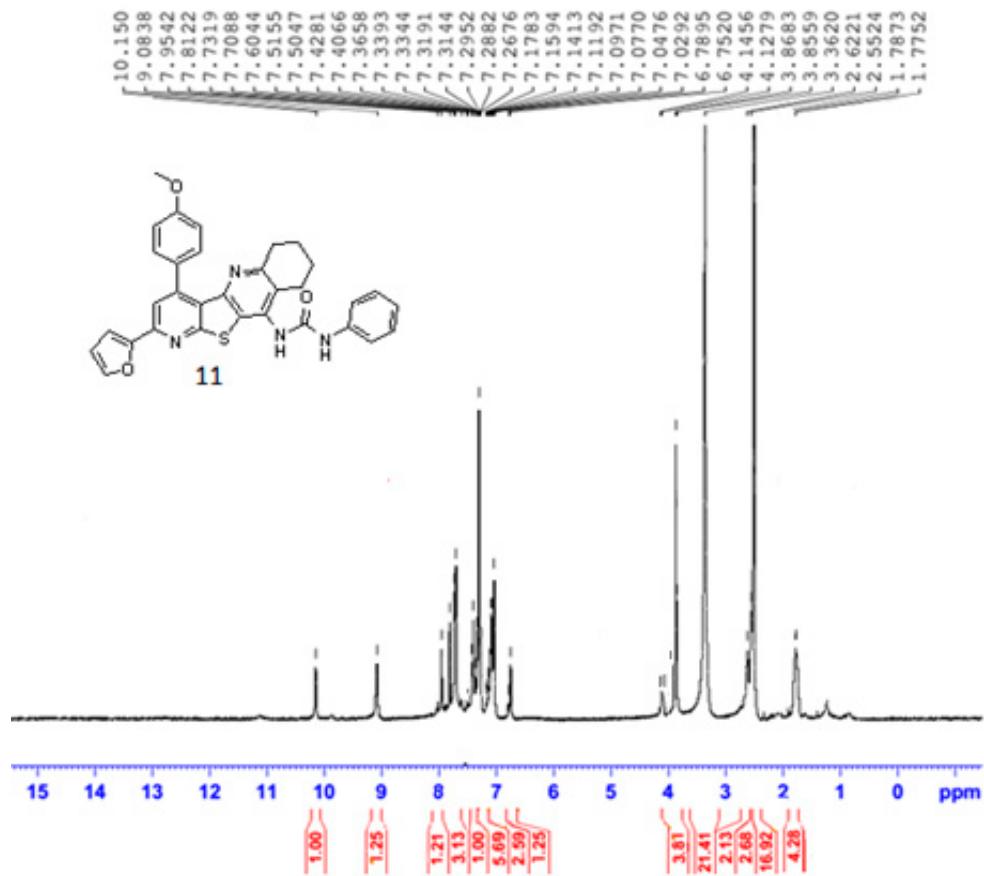


Fig. S43 ^1H NMR (400 MHz) in $\text{DMSO}-d_6$ of compound **11**

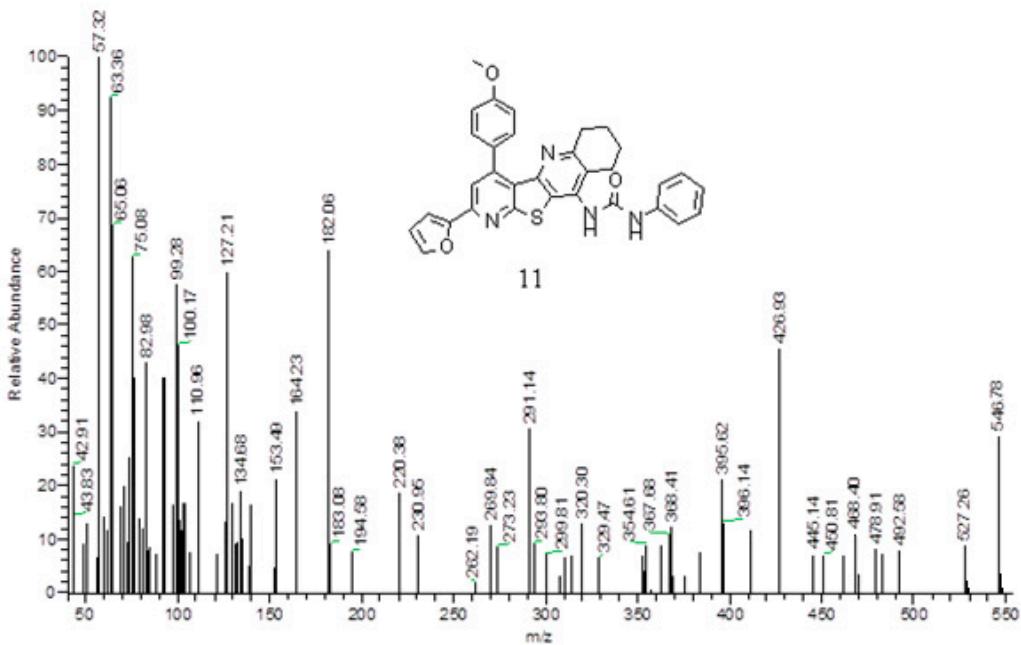


Fig. S44 Mass spectrum of compound **11**

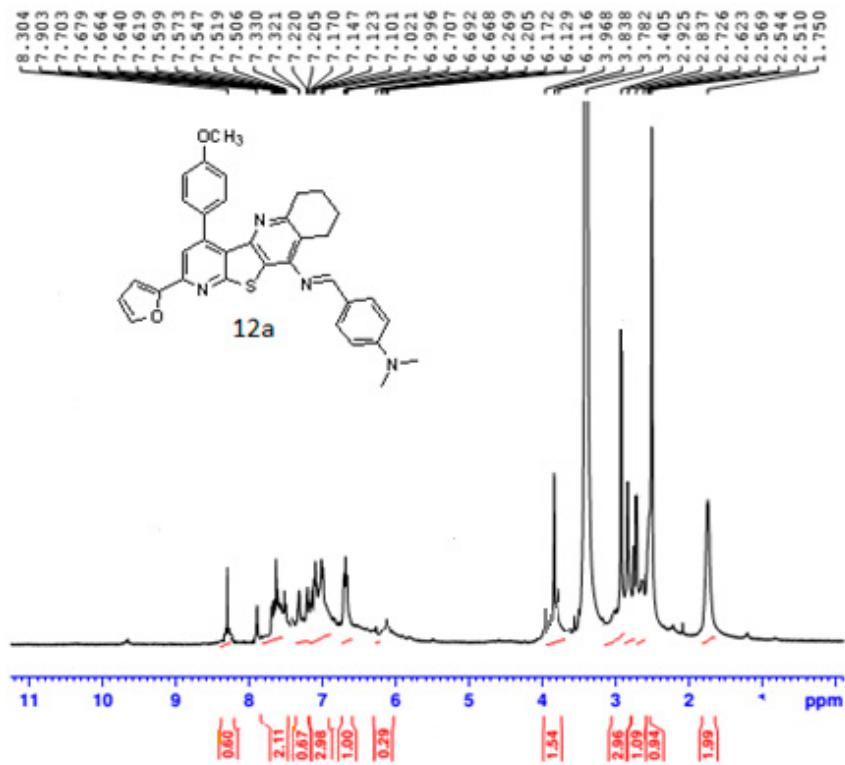


Fig. S45 ¹H NMR (400 MHz) in DMSO-*d*₆ of compound **12a**

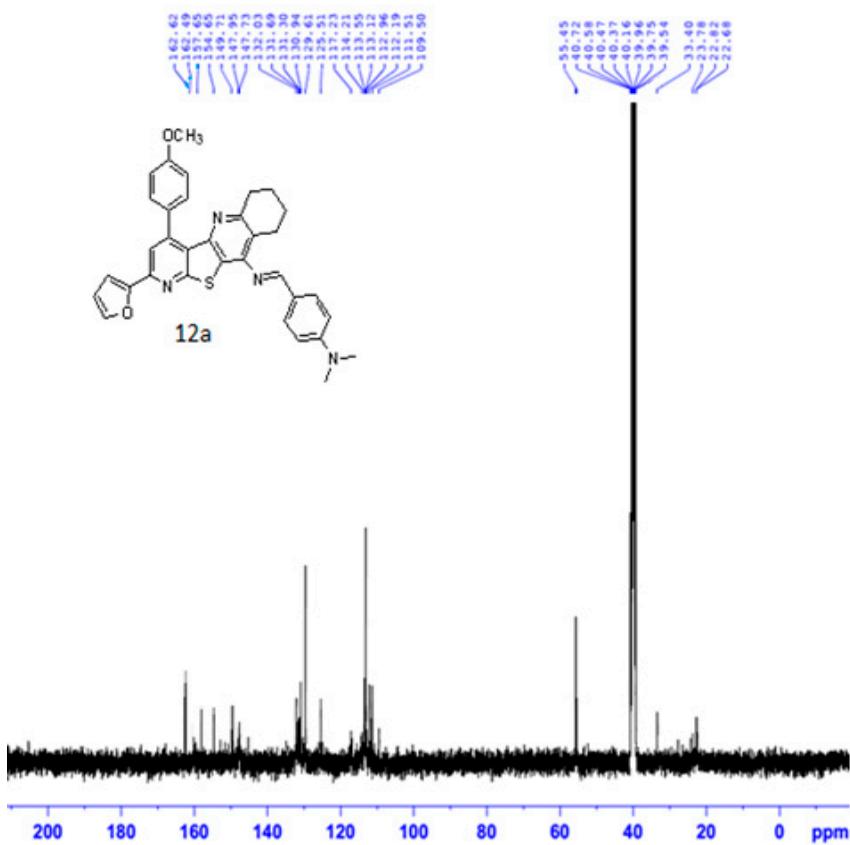


Fig. S46 ^{13}C NMR (100 MHz) in $\text{DMSO}-d_6$ of compound **12a**

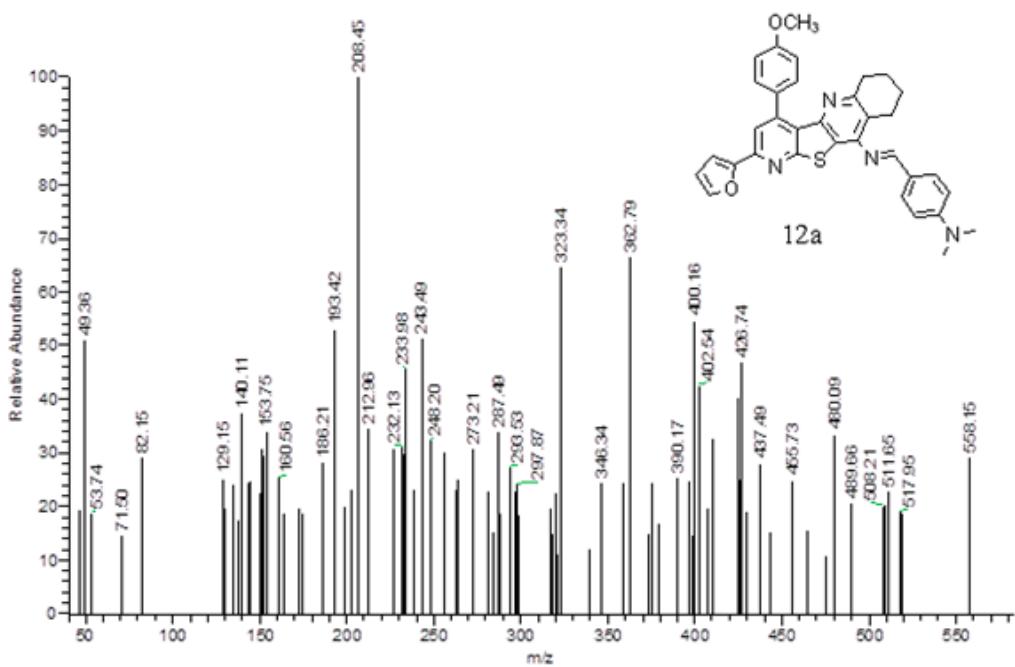


Fig. S47 Mass spectrum of compound **12a**

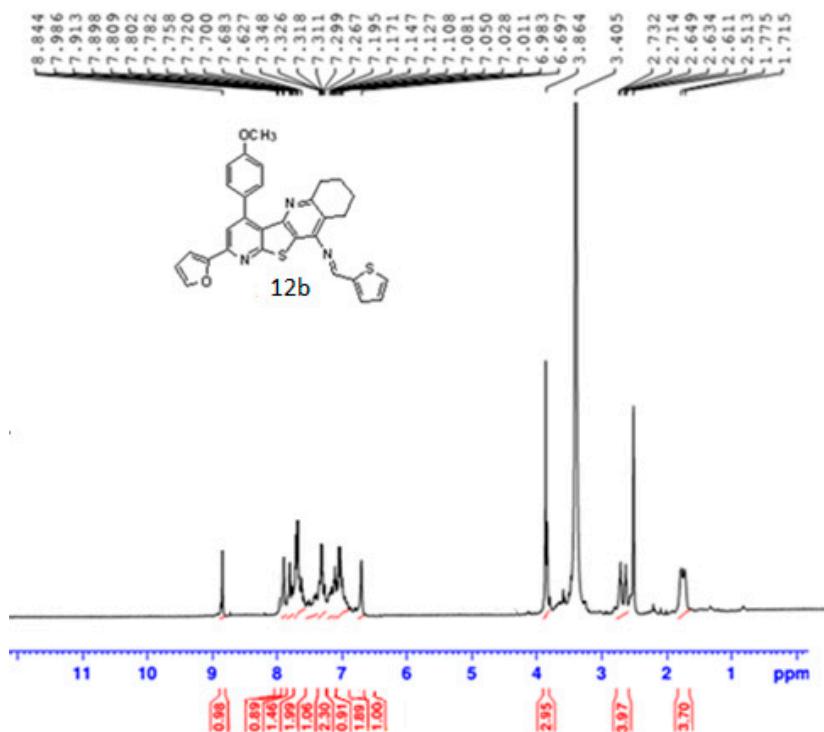


Fig. S48 ^1H NMR (400 MHz) in $\text{DMSO}-d_6$ of compound **12b**

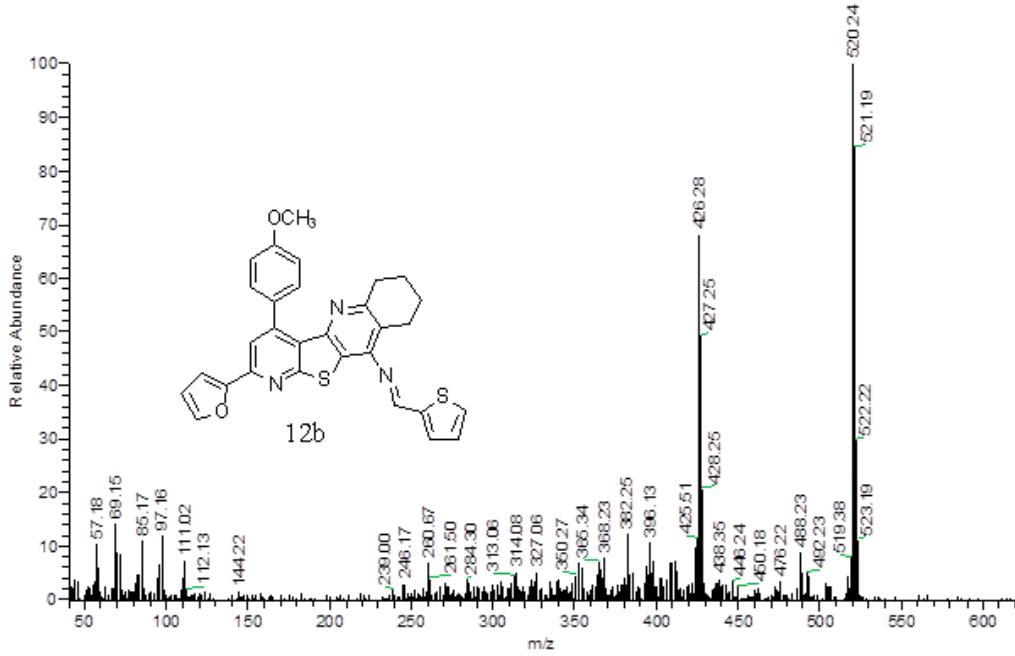


Fig. S49 Mass spectrum of compound **12b**

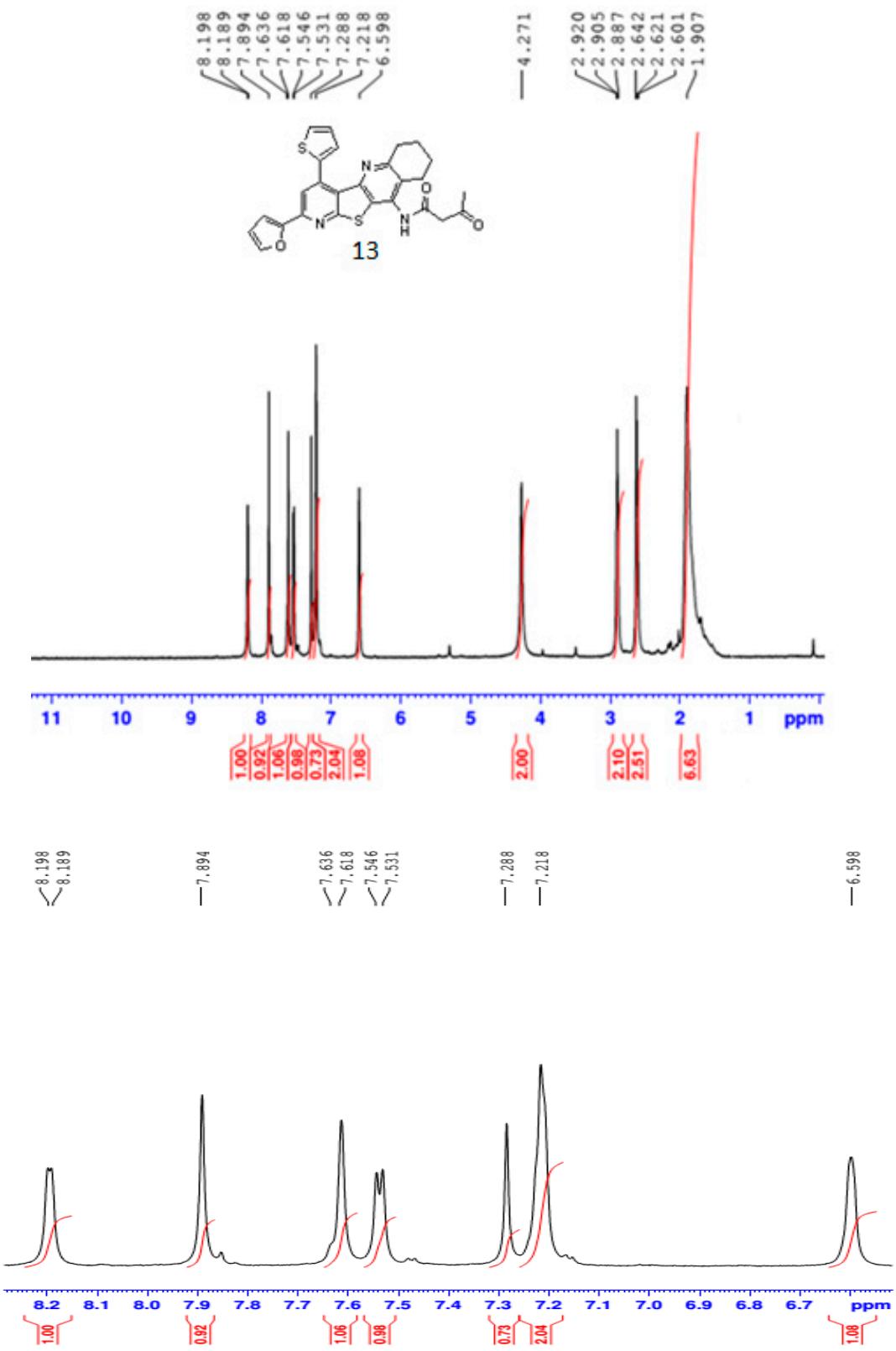


Fig. S50 ^1H NMR (400 MHz) in CDCl_3 of compound **13**

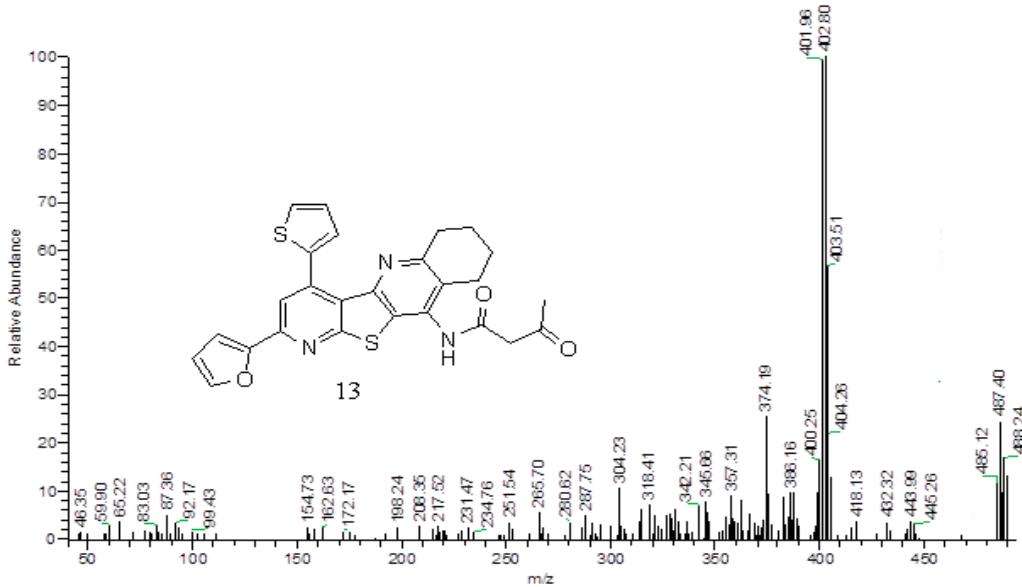


Fig. S51 Mass spectrum of compound **13**

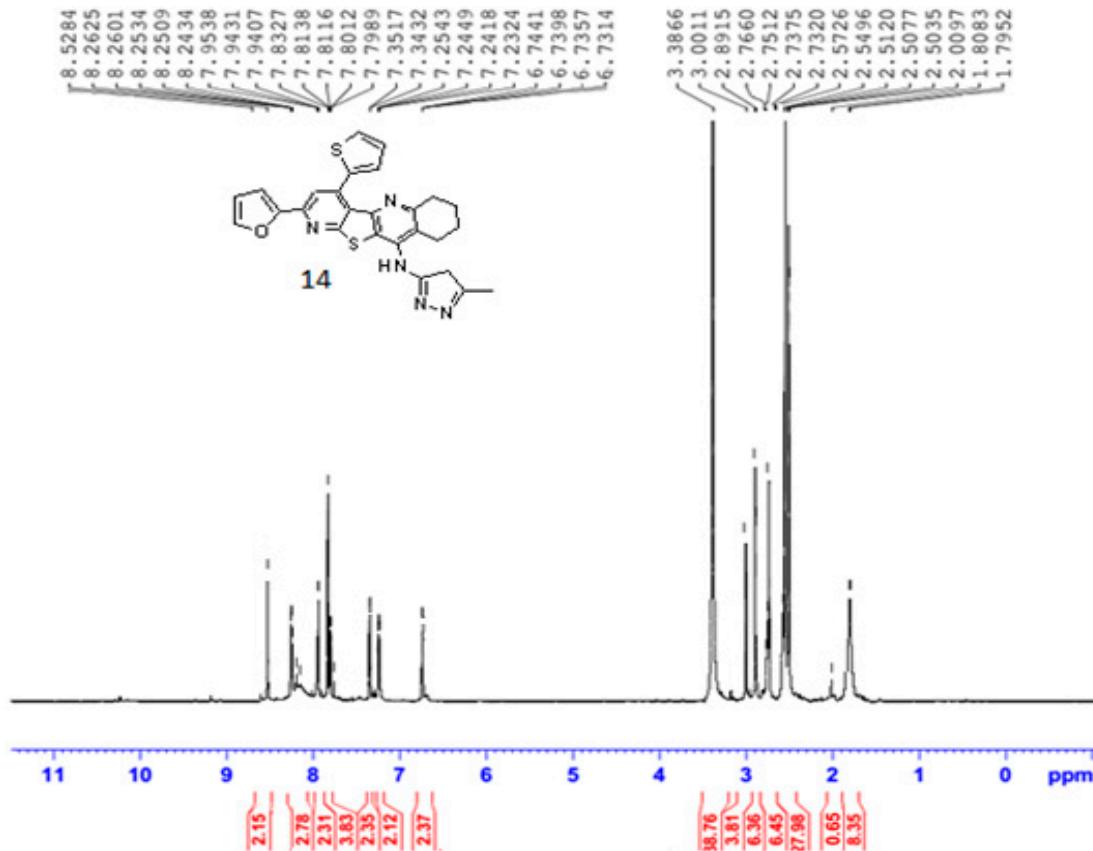


Fig. S52 ^1H NMR (400 MHz) in $\text{DMSO}-d_6$ of compound **14**.

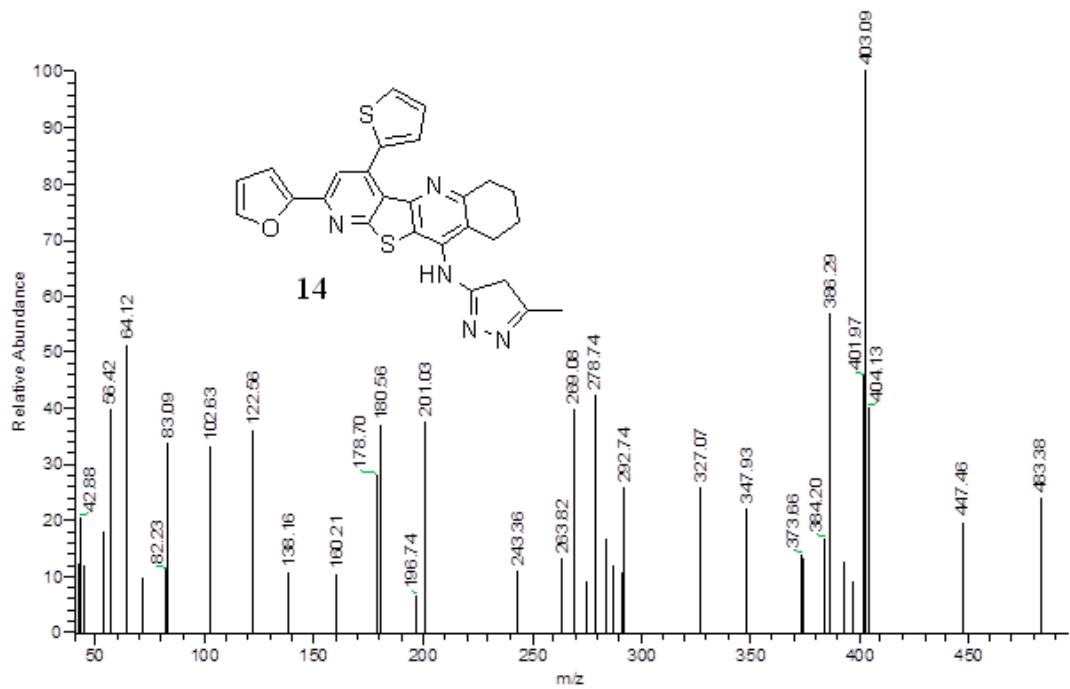


Fig. S53 Mass spectrum of compound 14