

Supplementary material

Figure Captions

Table S1. Molecular descriptor values of the BMLR-QSAR model for the vasodilatory active agents.

Figure S1. Effect of synthesized compounds and the standard reference (Amiodarone hydrochloride) on contracture induced by norepinephrine hydrochloride (NE.HCl) in rat thoracic aortic rings.

Figure S2. Potency (IC₅₀, mM) of the tested compounds on contracture induced by norepinephrine hydrochloride in rat thoracic aortic rings compared with (Amiodarone hydrochloride) used as a reference standard.

Figure S3. ¹H NMR spectrum of **4a**.

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Figure S37. ^1H NMR spectrum of **4u**.

Figure S38. ^1H NMR spectrum of **4v**.

Figure S39. ^{13}C NMR spectrum of **4v**.

Figure S40. ^1H NMR spectrum of **4w**.

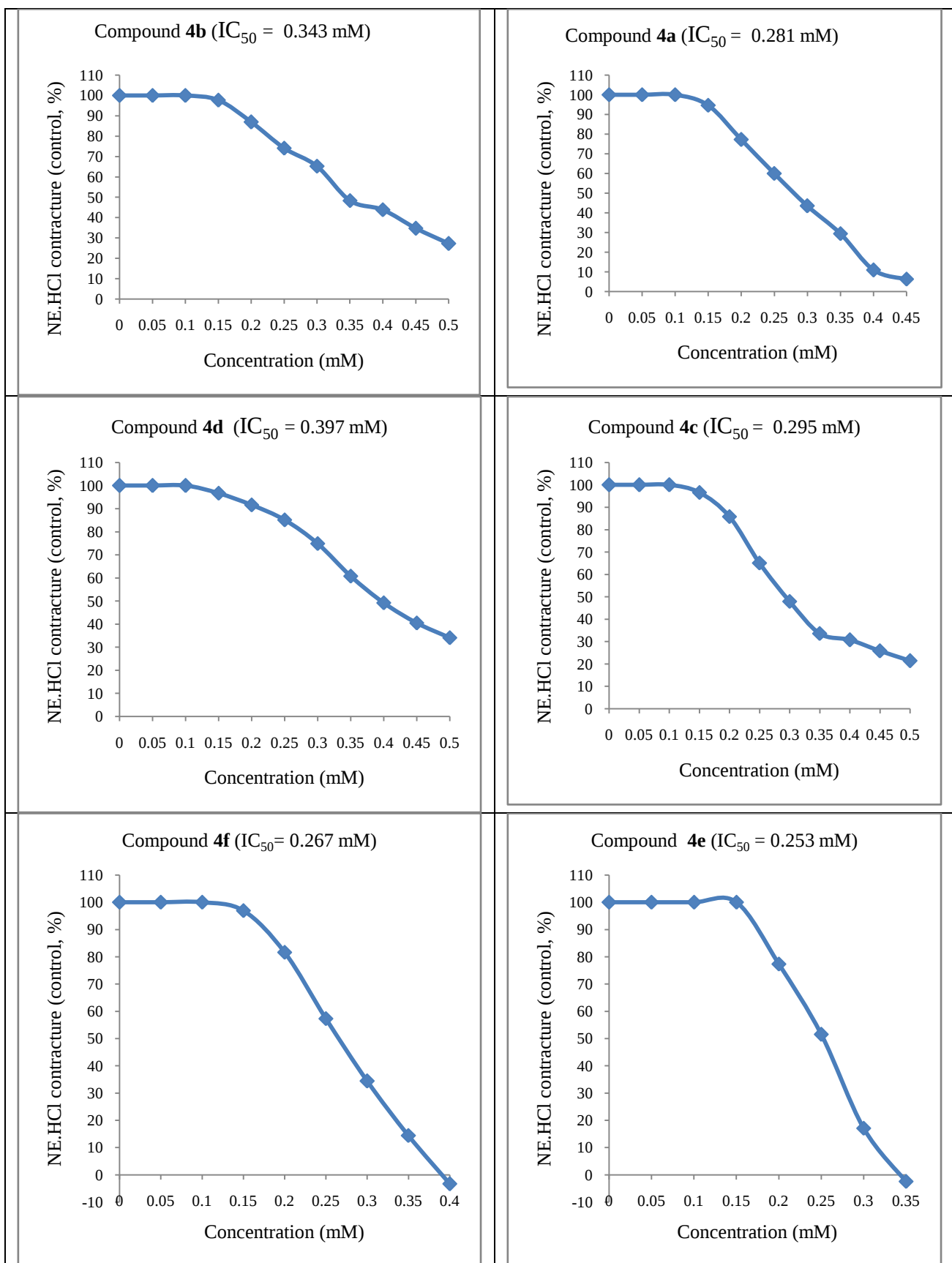
Figure S41. ^1H NMR spectrum of **4x**.

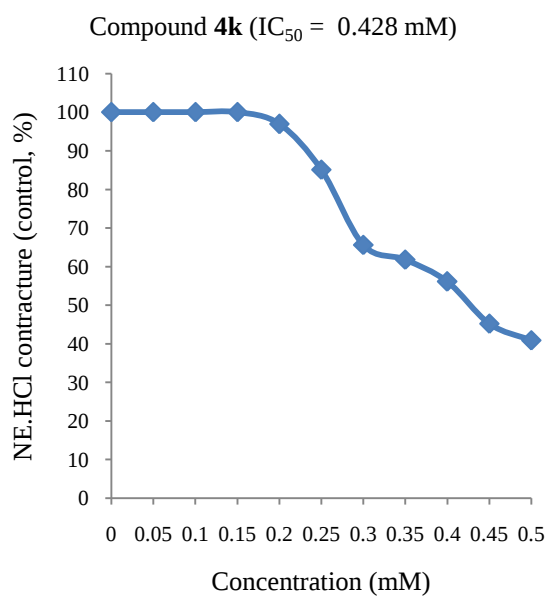
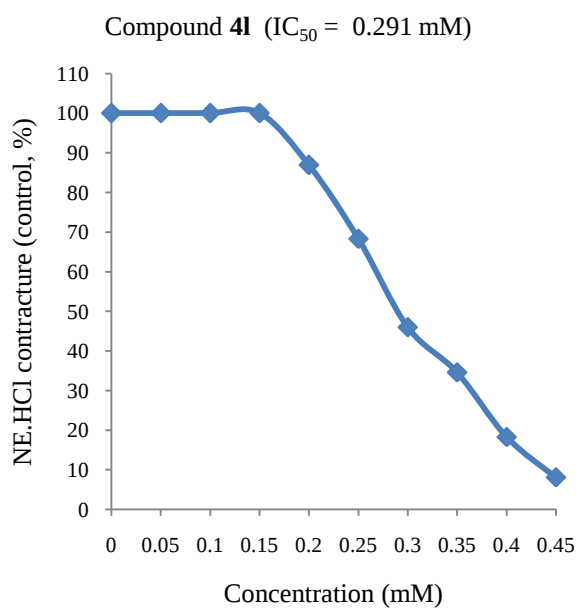
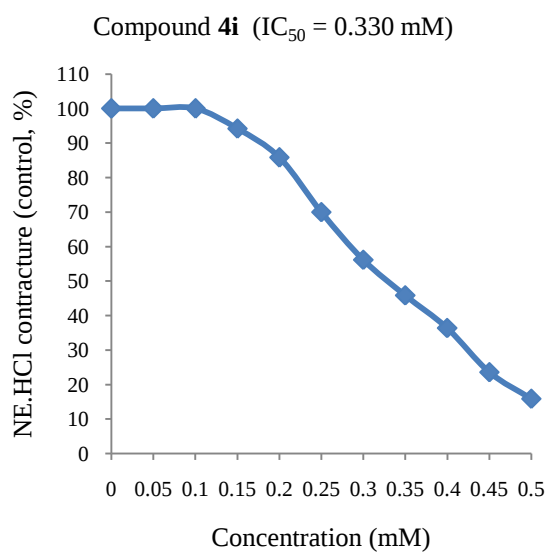
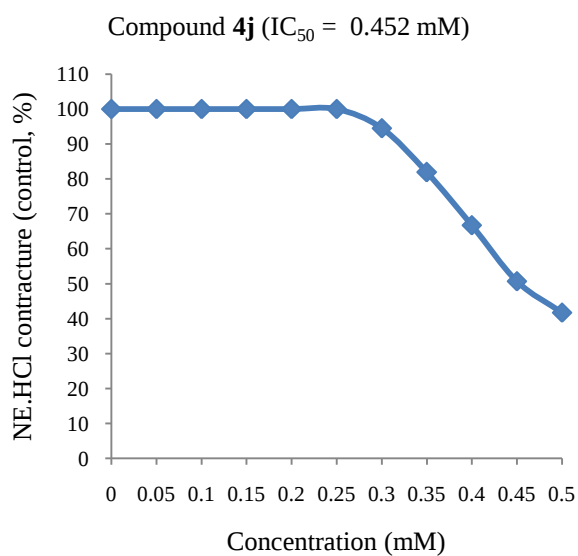
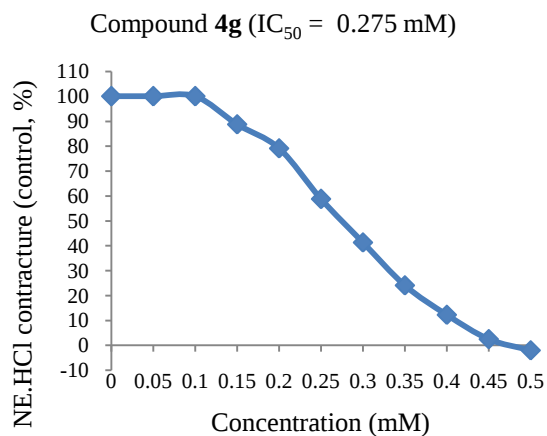
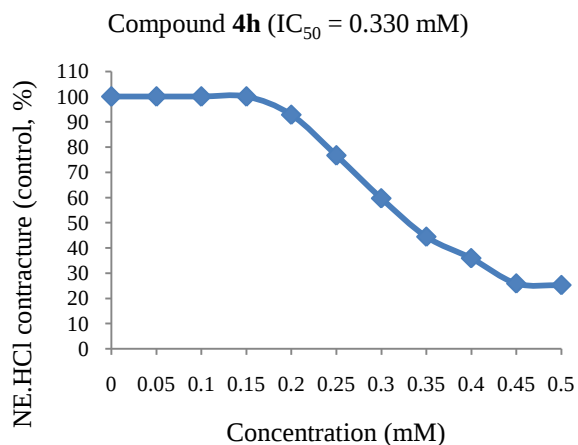
Figure S42. ^{13}C NMR spectrum of **4x**.

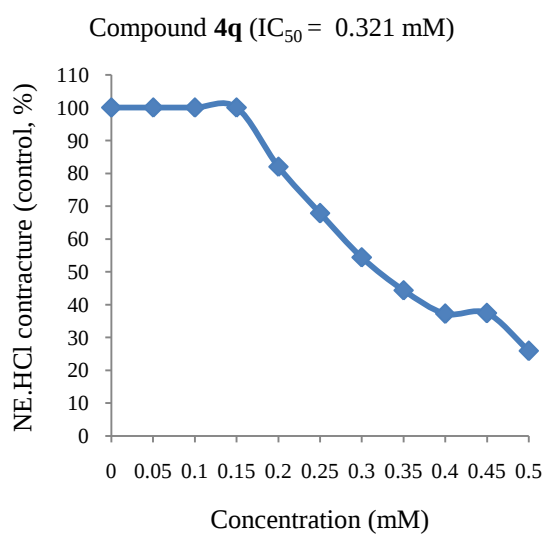
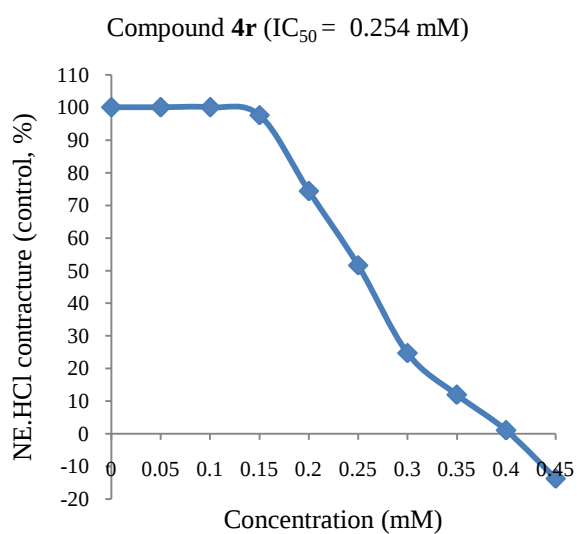
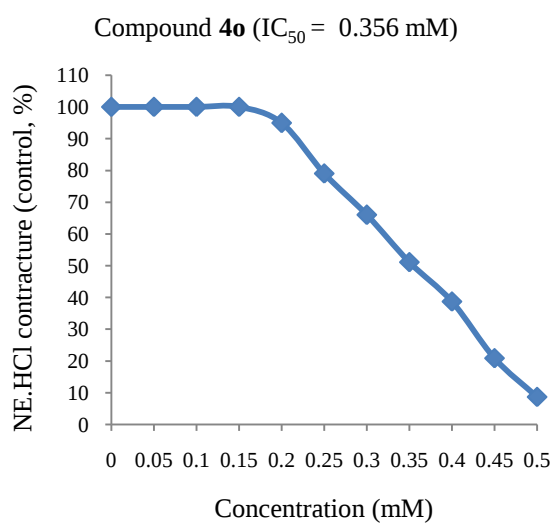
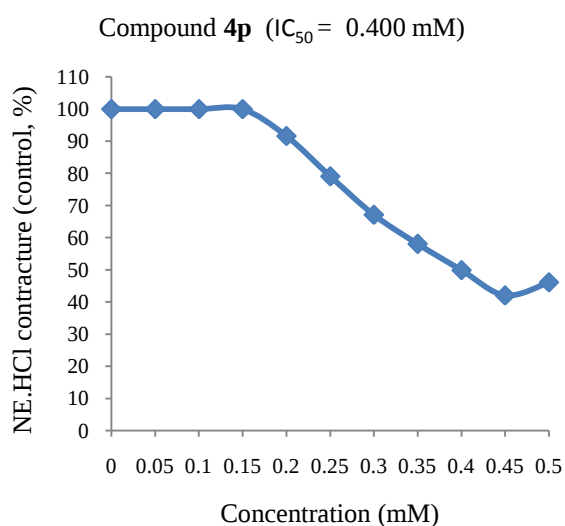
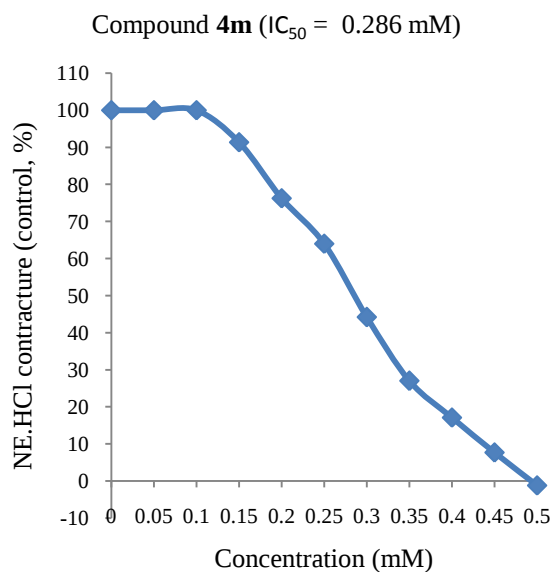
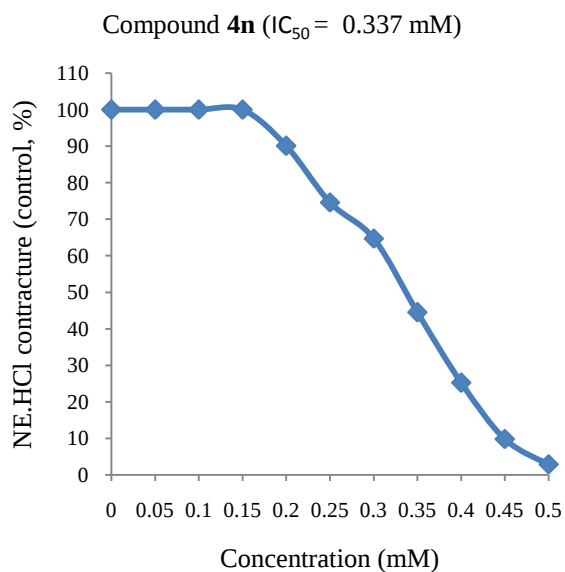
Table S1. Molecular descriptor values of the BMLR-QSAR model for the vasodilatory active agents.

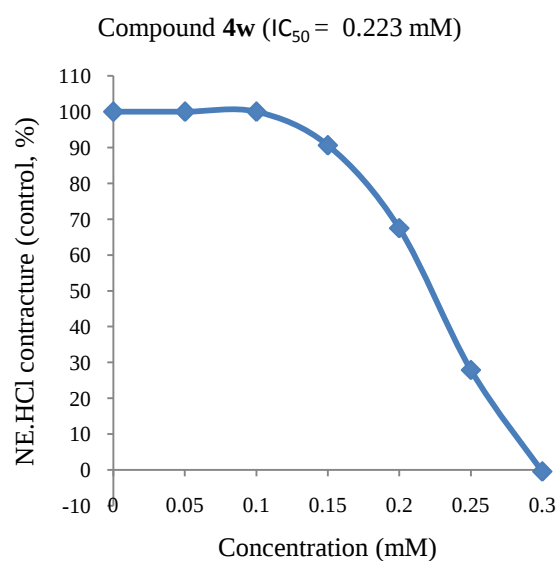
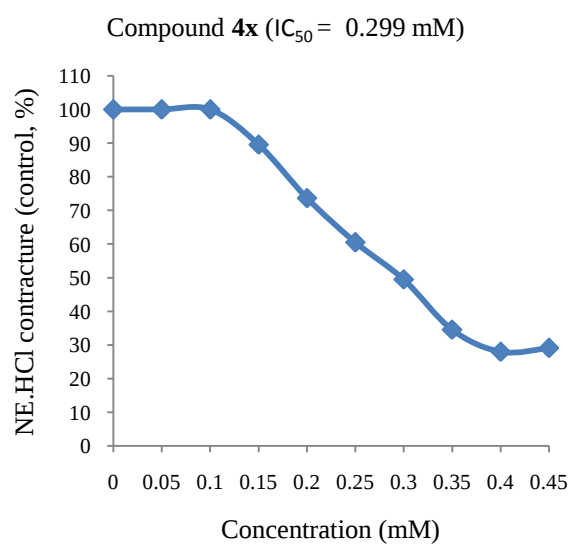
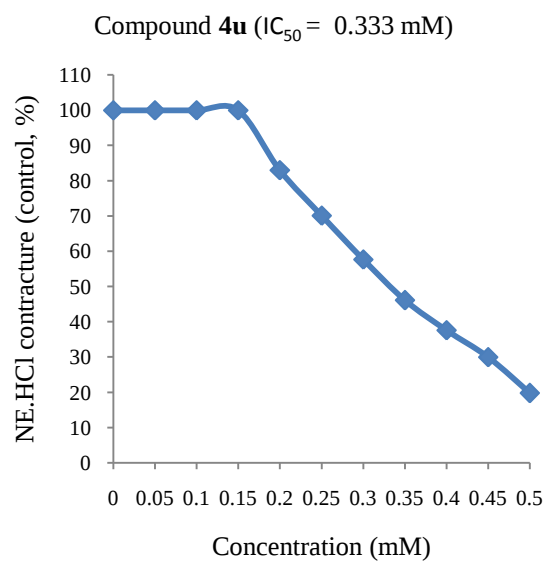
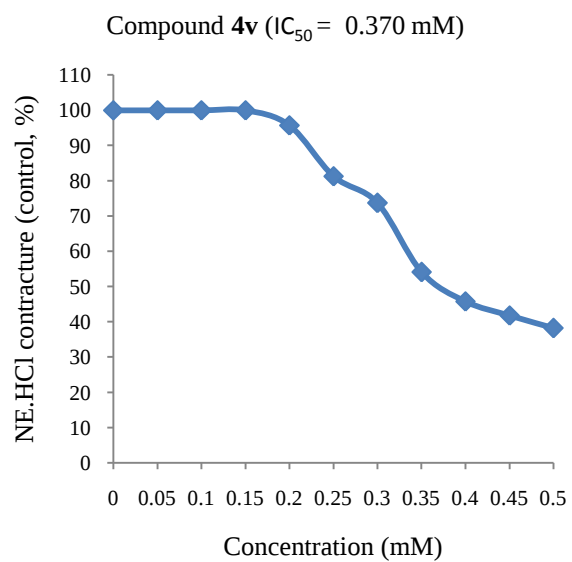
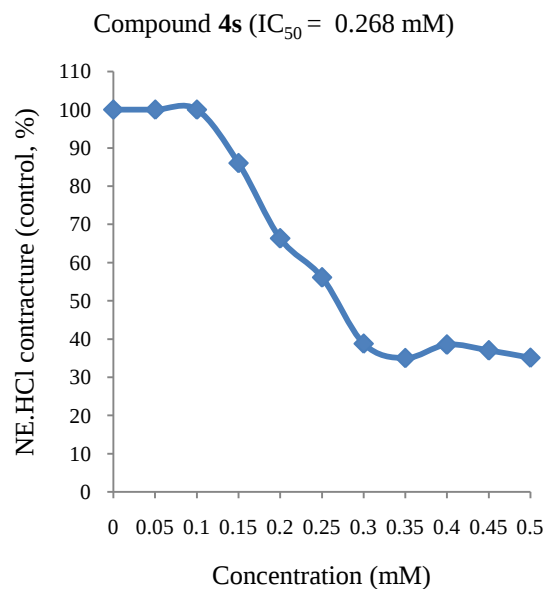
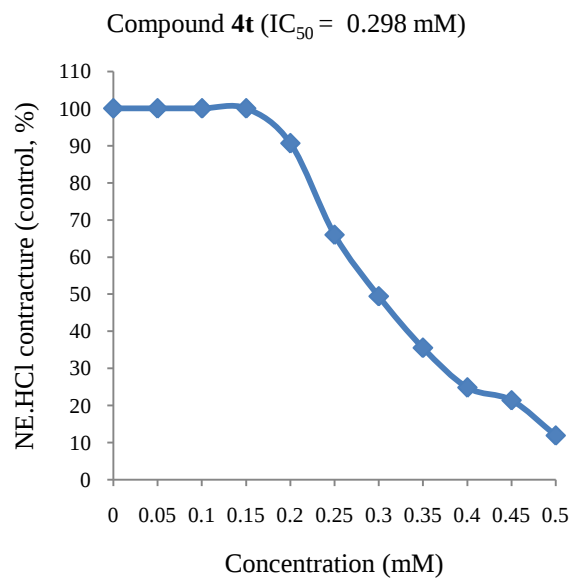
Entry	Compd.	Descriptors*			
		D_1	D_2	D_3	D_4
1	4a	196.7354	294.6783	0.00796	350.9802
2	4b	193.9982	266.2766	0.00769	351.0109
3	4c	196.7631	318.9088	0.00693	350.993
4	4d	193.9671	364.9057	0.00634	350.9712
5	4e	196.7521	283.3206	0.00708	350.9765
6	4f	193.9576	280.1435	0.00621	350.9558
7	4g	196.7126	331.4414	0.00822	350.9776
8	4h	193.5552	303.7959	0.00584	351.0034
9	4i	196.7445	309.5561	0.00817	351.0101
10	4j	193.5273	284.8733	0.00679	351.0018
11	4k	198.4084	301.8383	0.01218	351.0151
12	4l	198.3929	315.658	0.01065	351.0124
13	4m	196.8043	256.5694	0.00756	351.0373
14	4n	194.0101	302.4001	0.00608	351.0104
15	4o	196.8059	261.9922	0.01086	351.0023
16	4p	194.0591	256.2957	0.00759	351.0759
17	4q	196.6616	274.1543	0.01027	350.9653
18	4r	196.5003	255.6172	0.00738	350.9988
19	4s	196.7666	255.4456	0.00916	351.0069
20	4t	194.0979	236.8933	0.00633	351.0407
21	4u	196.6594	296.6829	0.01042	350.9755
22	4v	194.0351	271.8696	0.00829	350.979
23	4w	196.657	361.9157	0.00842	350.6562
24	4x	193.4009	352.4049	0.00726	350.6691

* D_1 = Max. e-e repulsion for bond C-O, D_2 = WNSA-1 Weighted PNSA (PNSA1*TMSA/1000) (MOPAC PC), D_3 = FHACA Fractional HACA (HACA/TMSA) (MOPAC PC), D_4 = Max. e-n attraction for bond C-N.









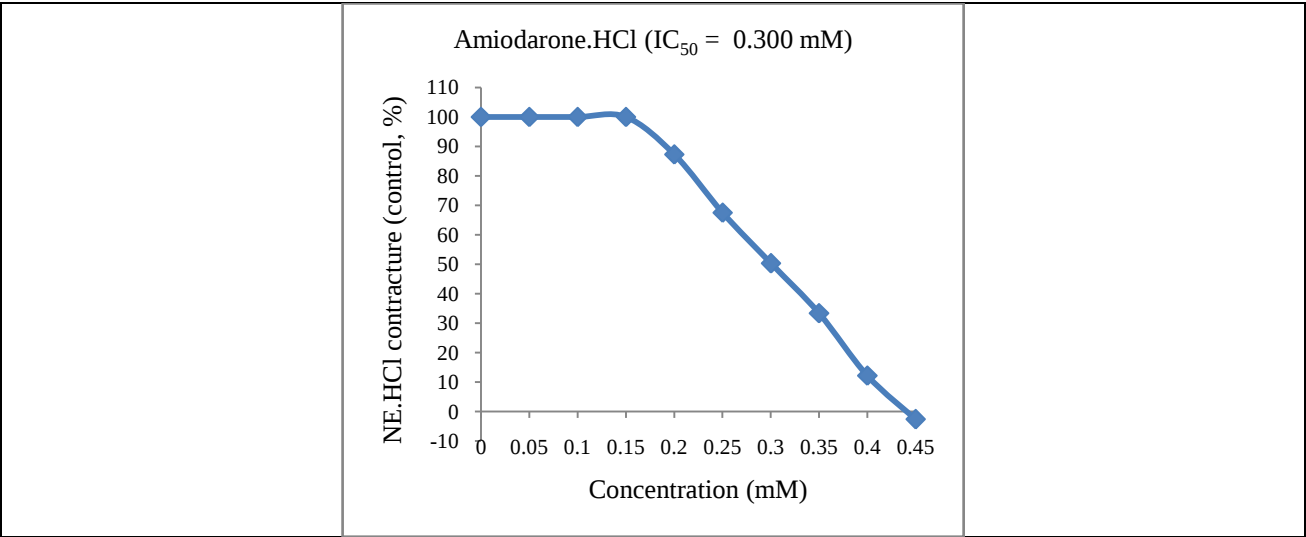


Figure S1: Effect of new chemical entities and the reference standard (Amiodarone hydrochloride) on contracture induced by norepinephrine hydrochloride (NE.HCl) in rat thoracic aortic rings.

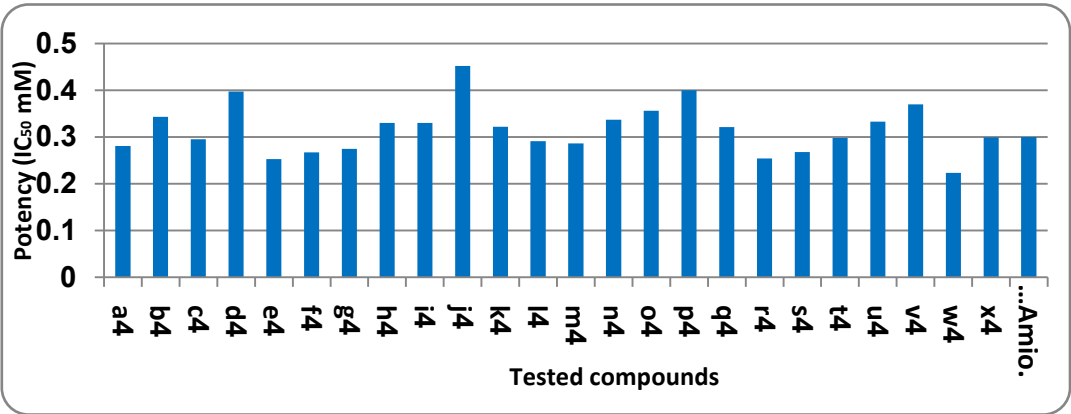


Figure S2. Potency (IC_{50} , mM) of the tested compounds on contracture induced by norepinephrine hydrochloride in rat thoracic aortic rings compared with (Amiodarone hydrochloride) used as a reference standard.

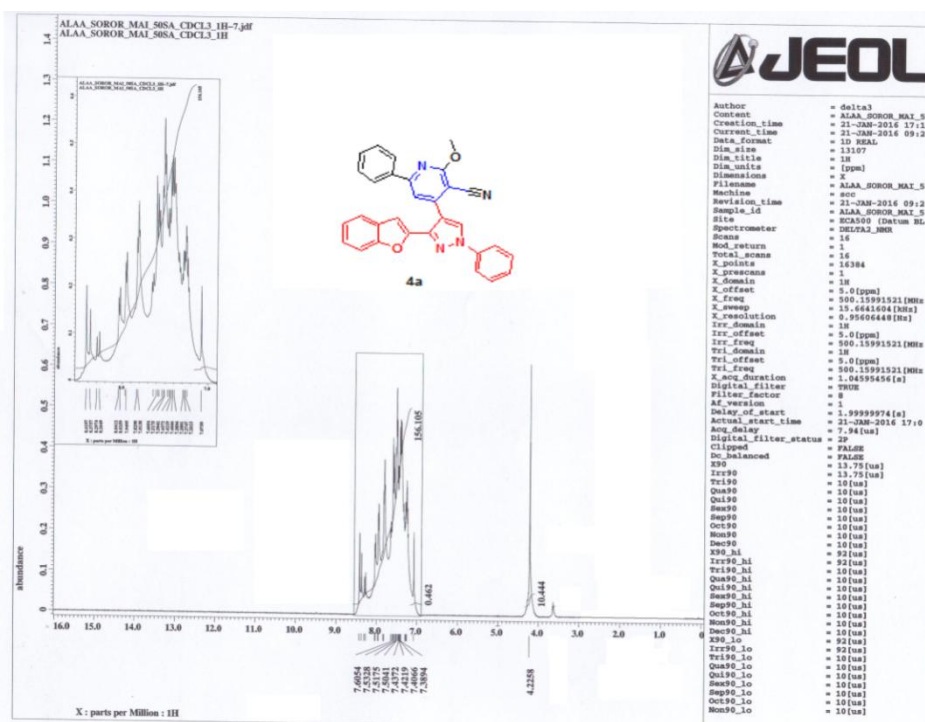


Figure S3. ^1H NMR spectrum of **4a**.

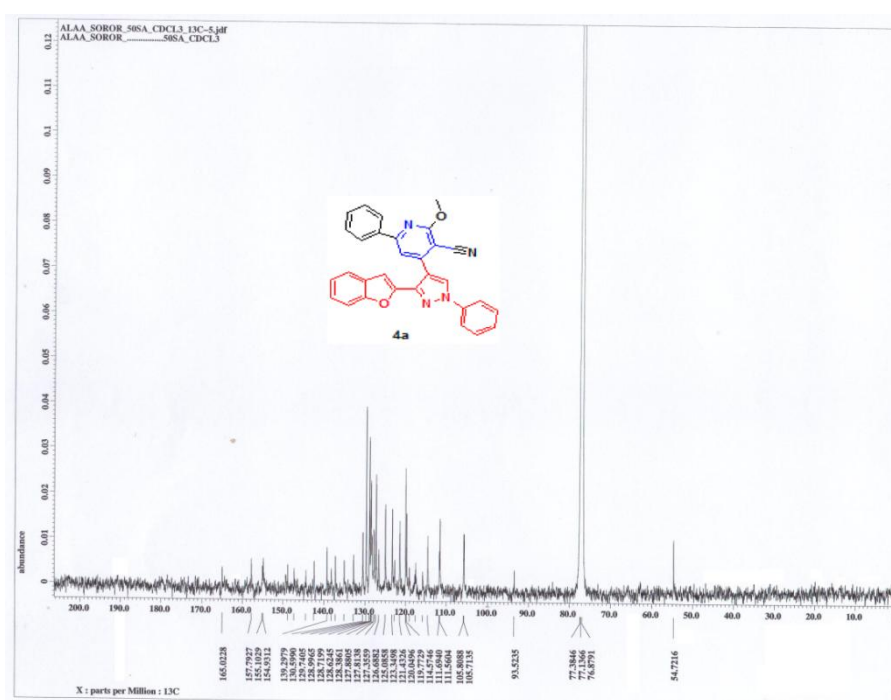
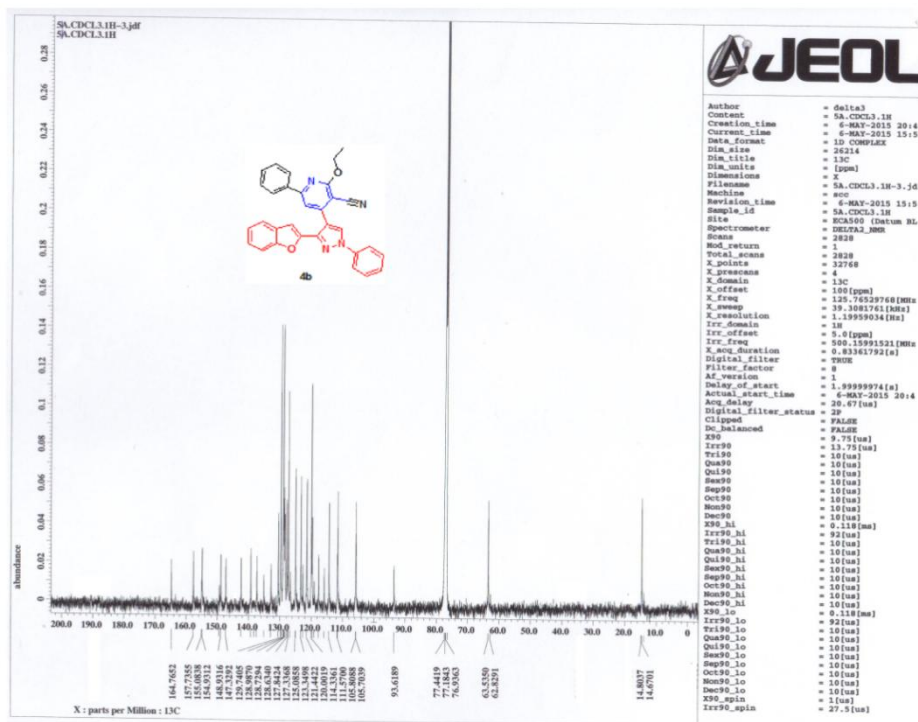
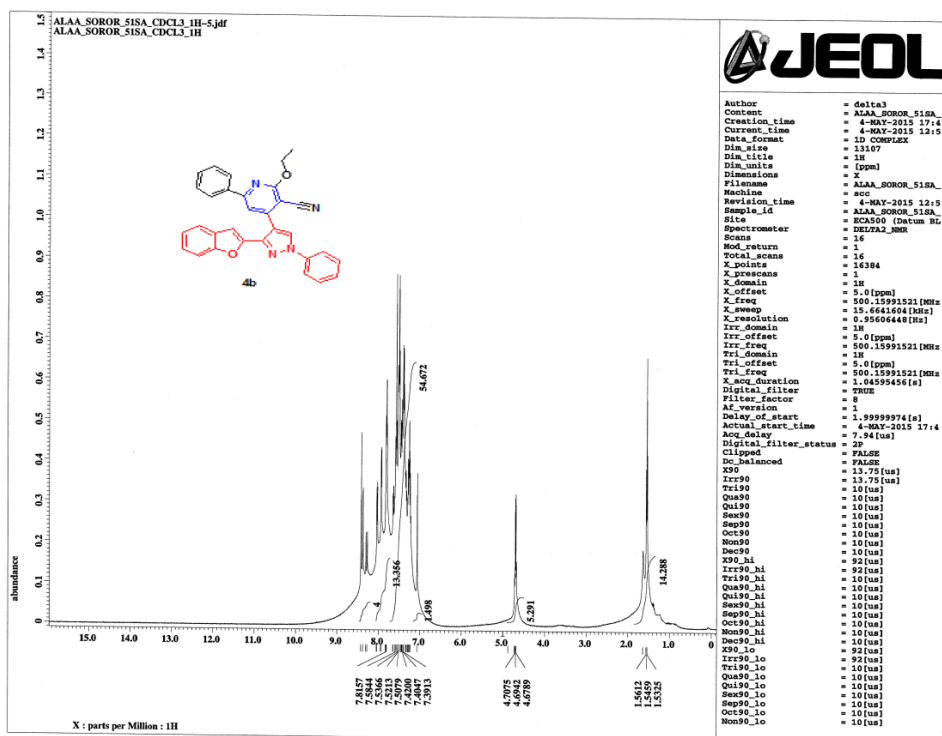


Figure S4. ^{13}C NMR spectrum of **4a**.



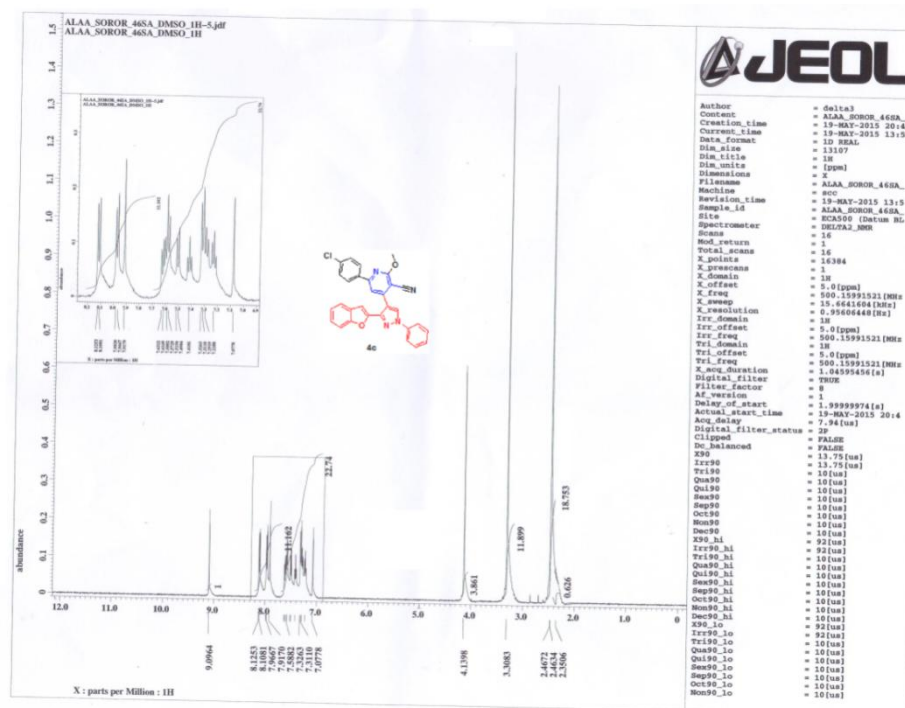


Figure S7. ^1H NMR spectrum of **4c**.

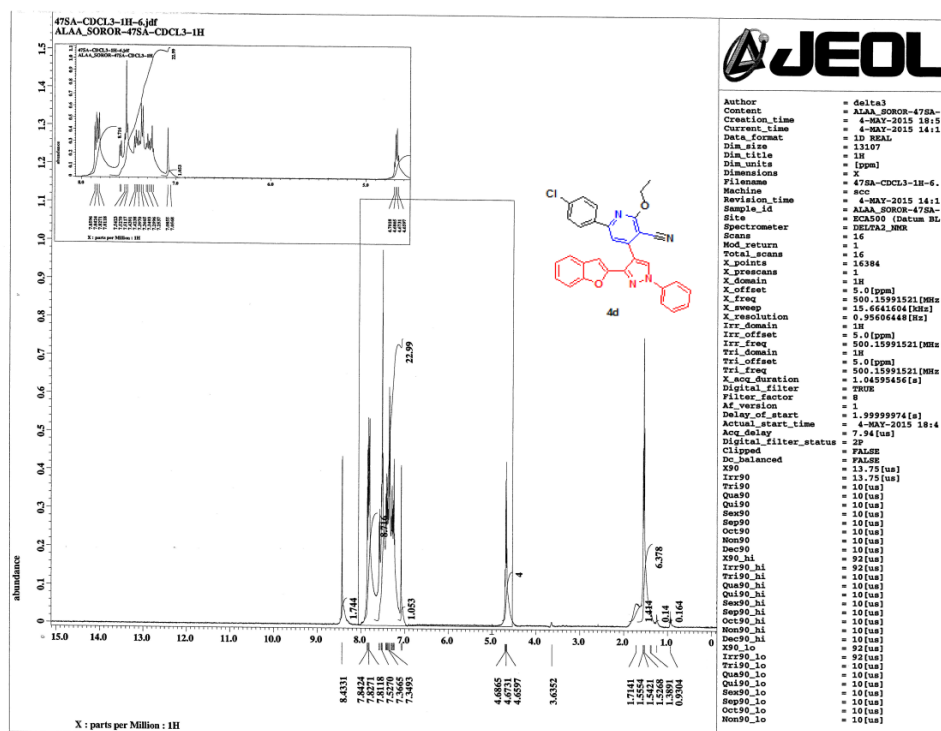


Figure S8. ^1H NMR spectrum of **4d**.

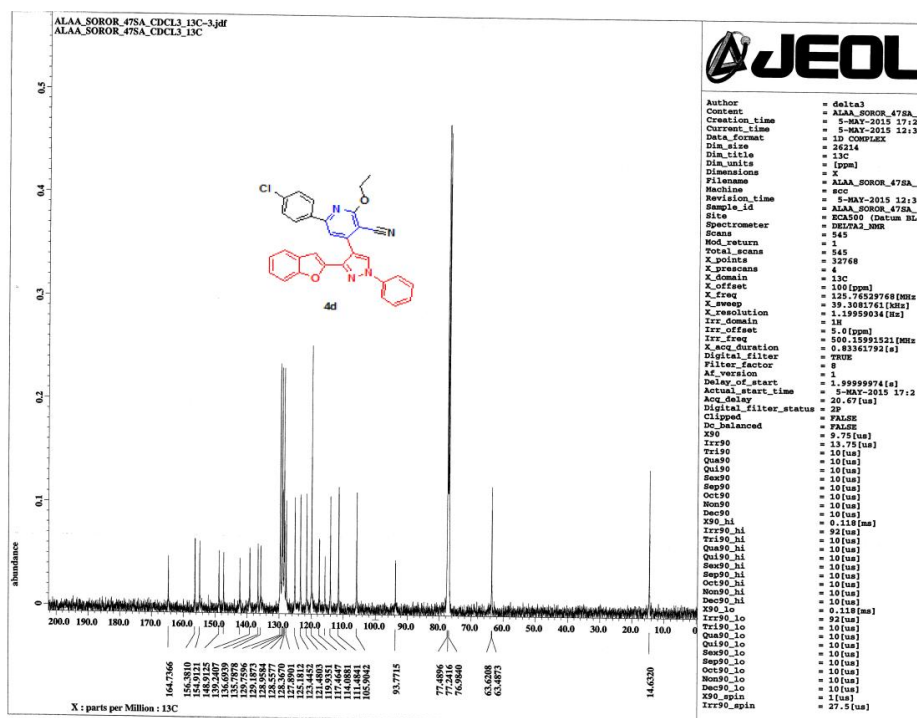


Figure S9. ^{13}C NMR spectrum of 4d.

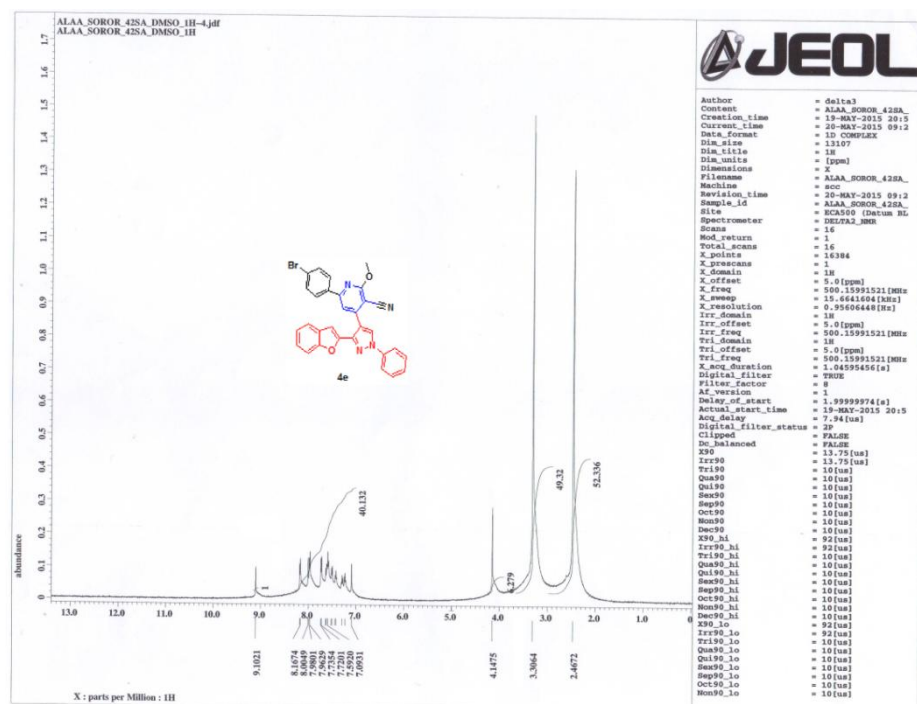


Figure S10. ^1H NMR spectrum of 4e.

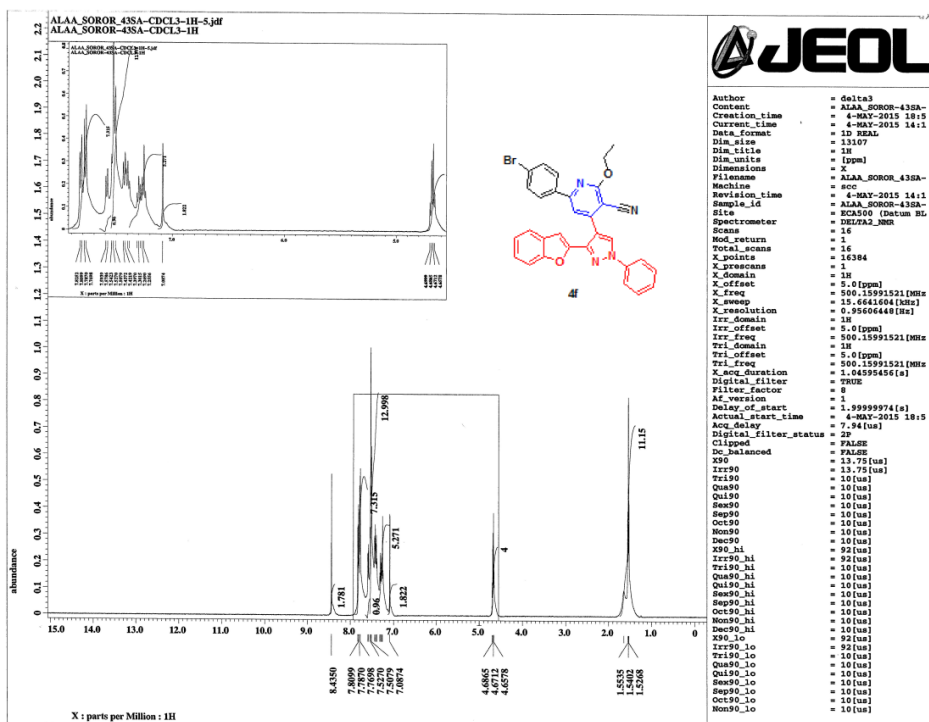


Figure S11. ¹H NMR spectrum of 4f.

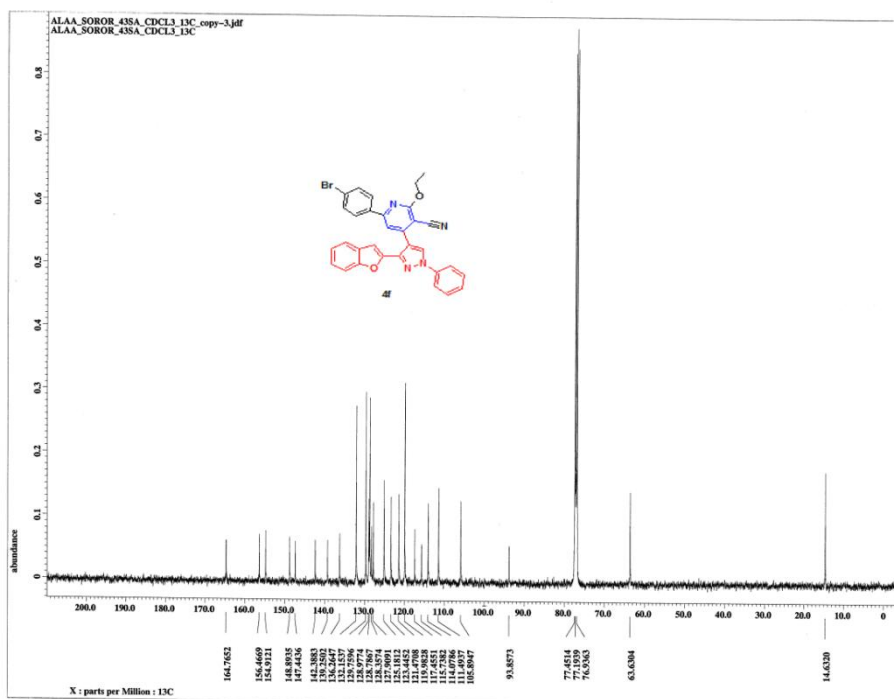


Figure S12. ¹³C NMR spectrum of 4f.

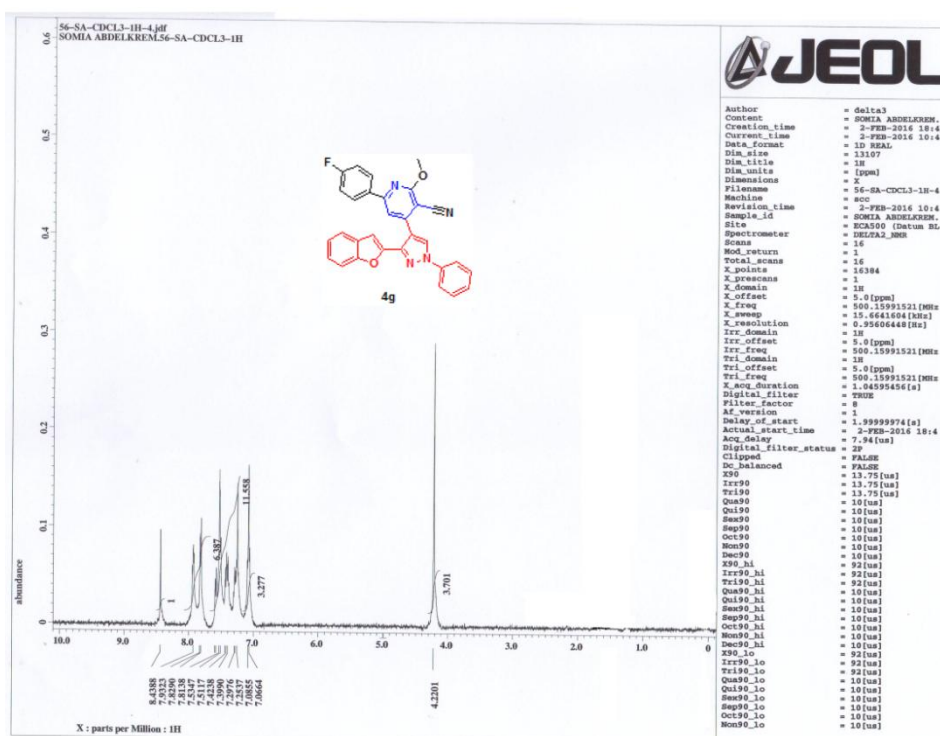


Figure S13. ¹H NMR spectrum of 4g.

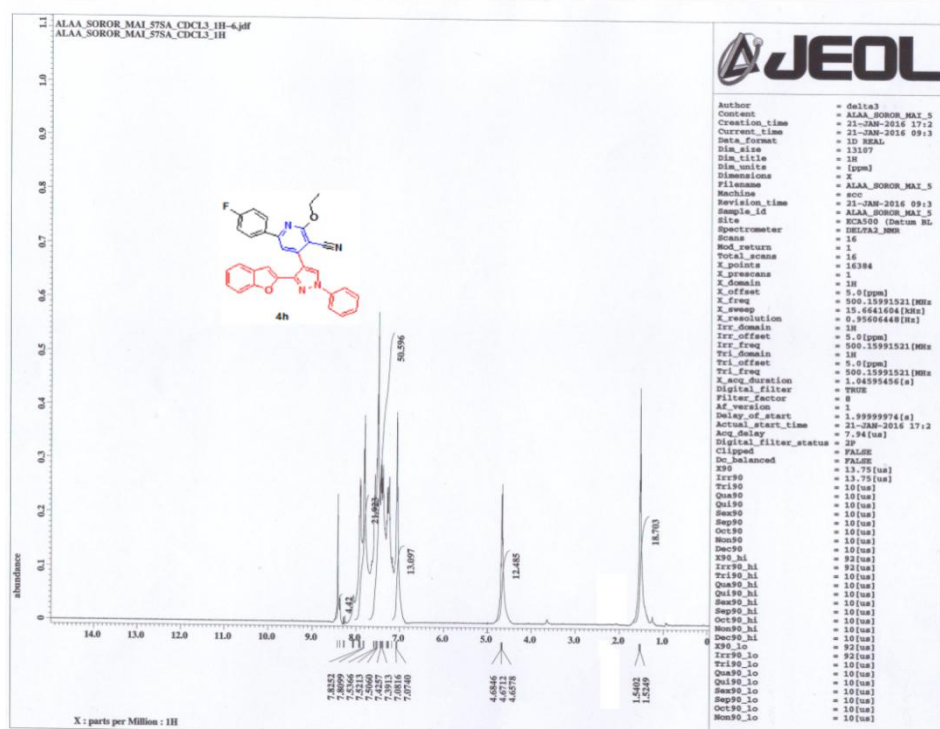


Figure S14. ¹H NMR spectrum of 4h.

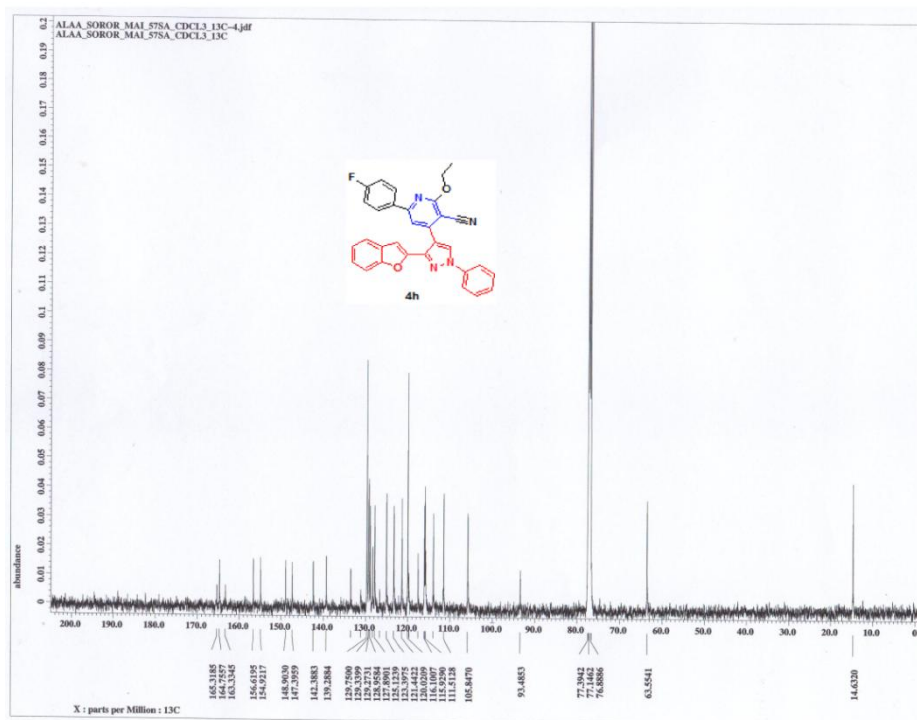


Figure S15. ^{13}C NMR spectrum of 4h.

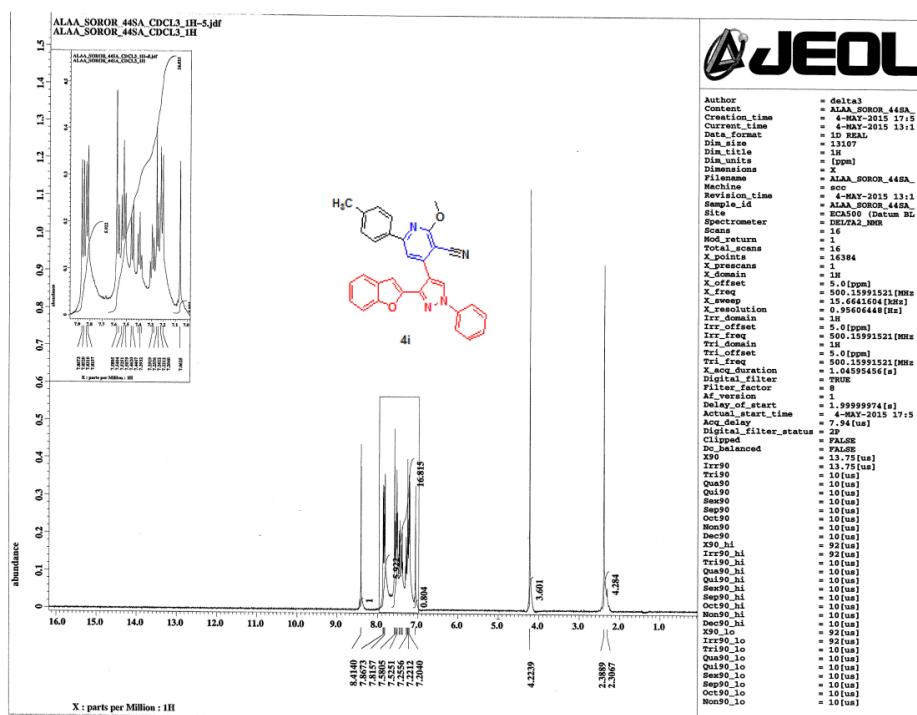


Figure S16. ^1H NMR spectrum of 4i.

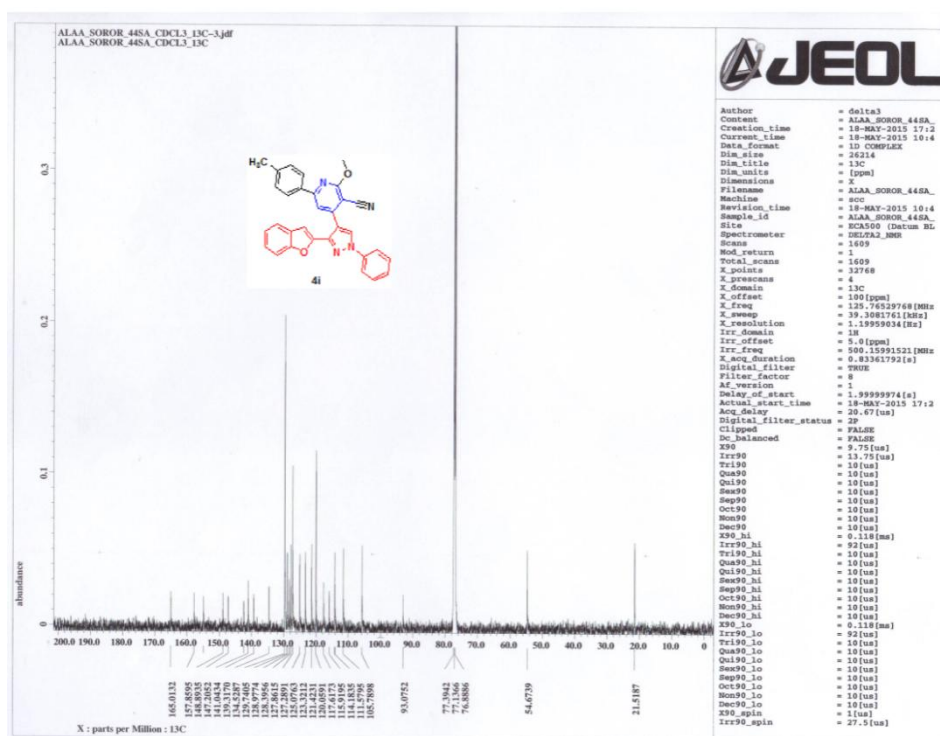


Figure S17. ^{13}C NMR spectrum of 4i.

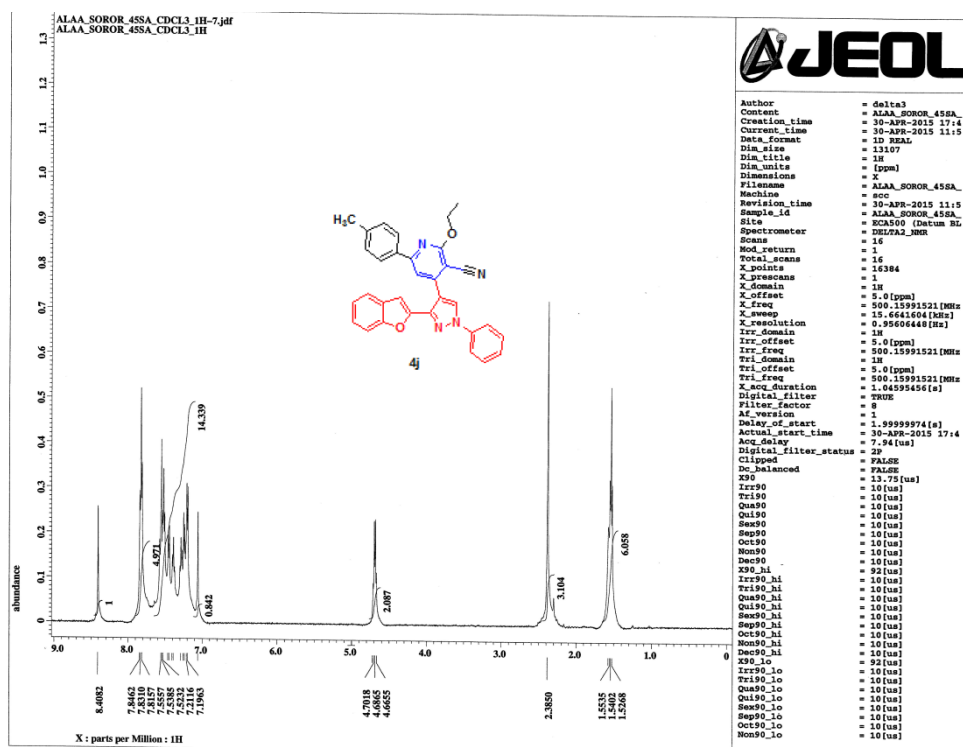


Figure S18. ^1H NMR spectrum of 4j.

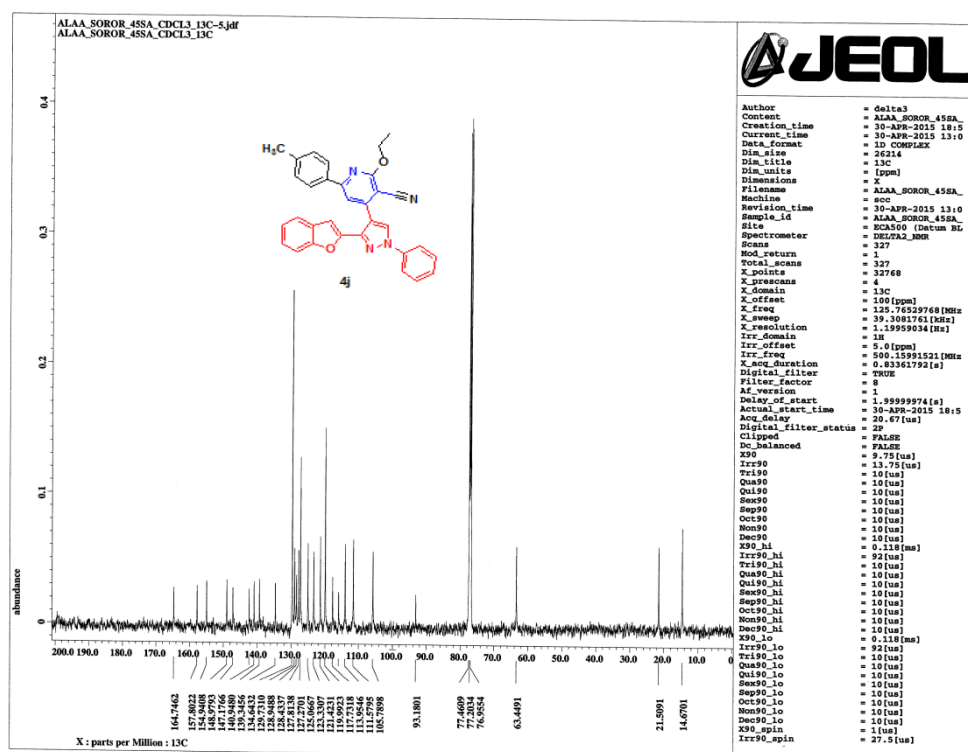


Figure S19. ^{13}C NMR spectrum of 4j.

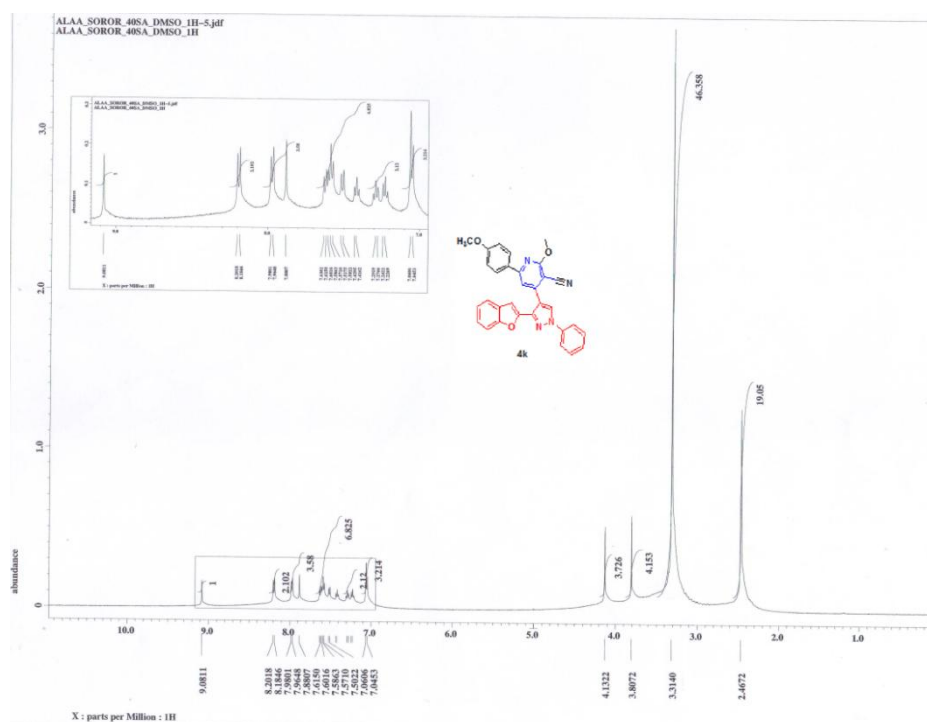


Figure S20. ^1H NMR spectrum of 4k.

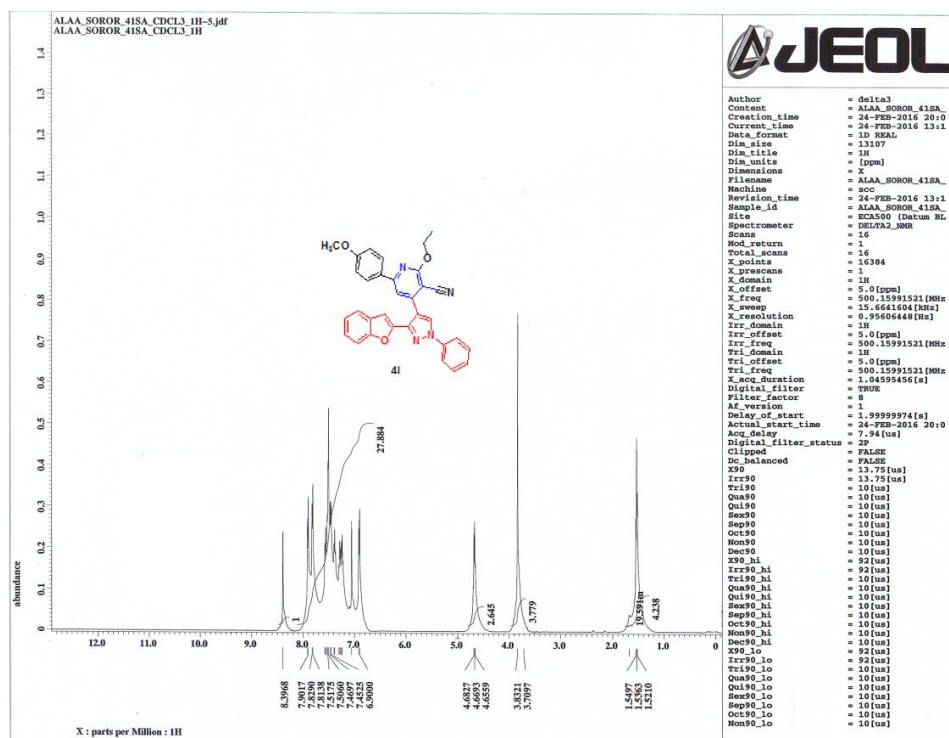


Figure S21. ^1H NMR spectrum of 4l.

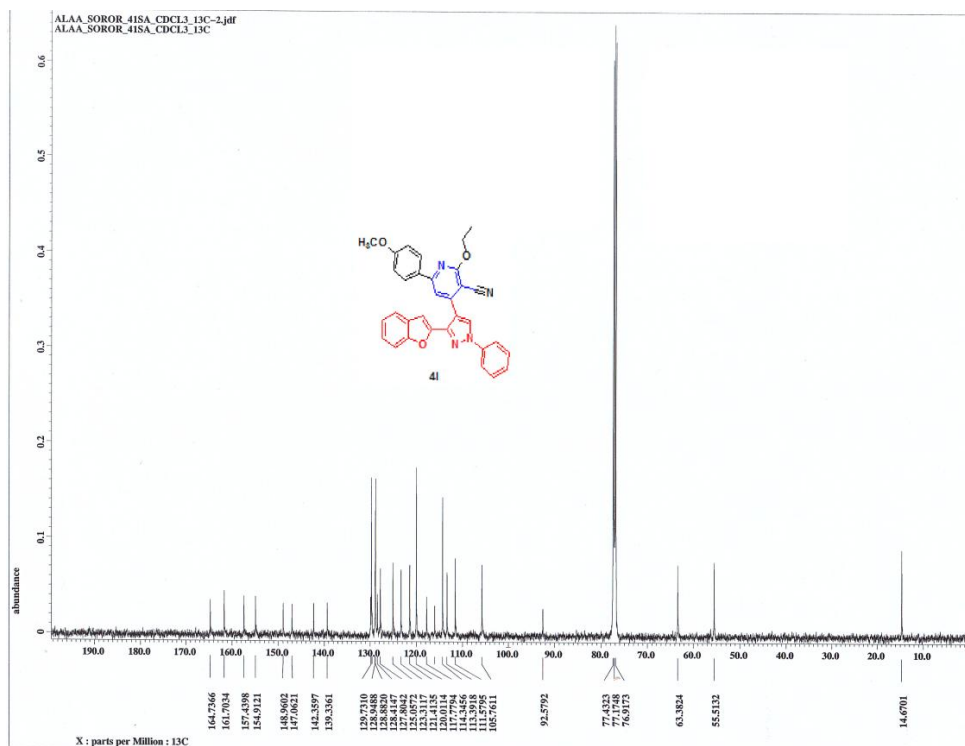


Figure S22. ^{13}C NMR spectrum of 4l.

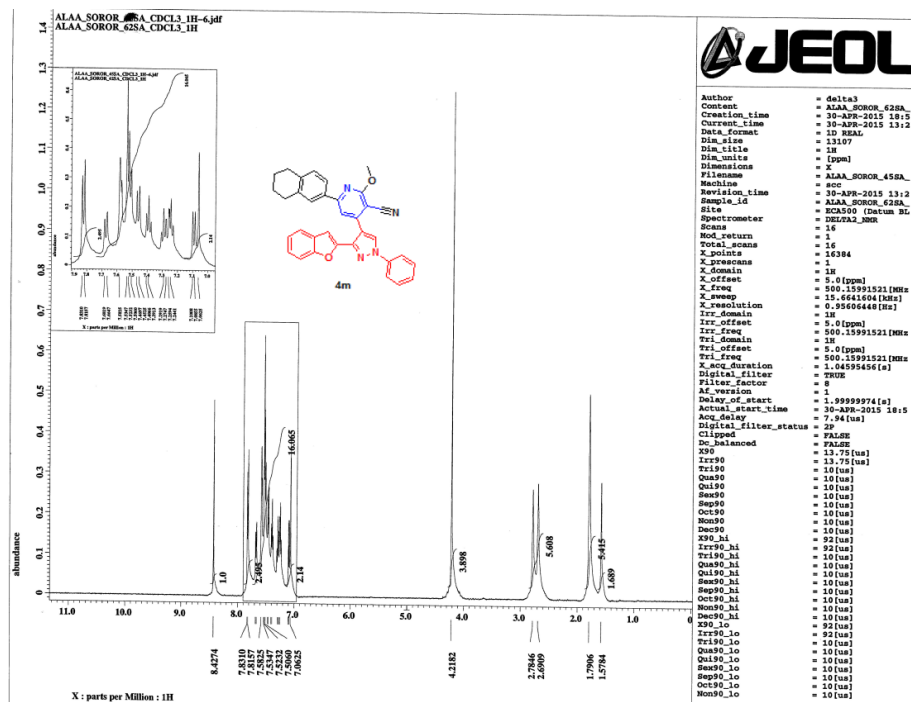


Figure S23. ^1H NMR spectrum of 4m.

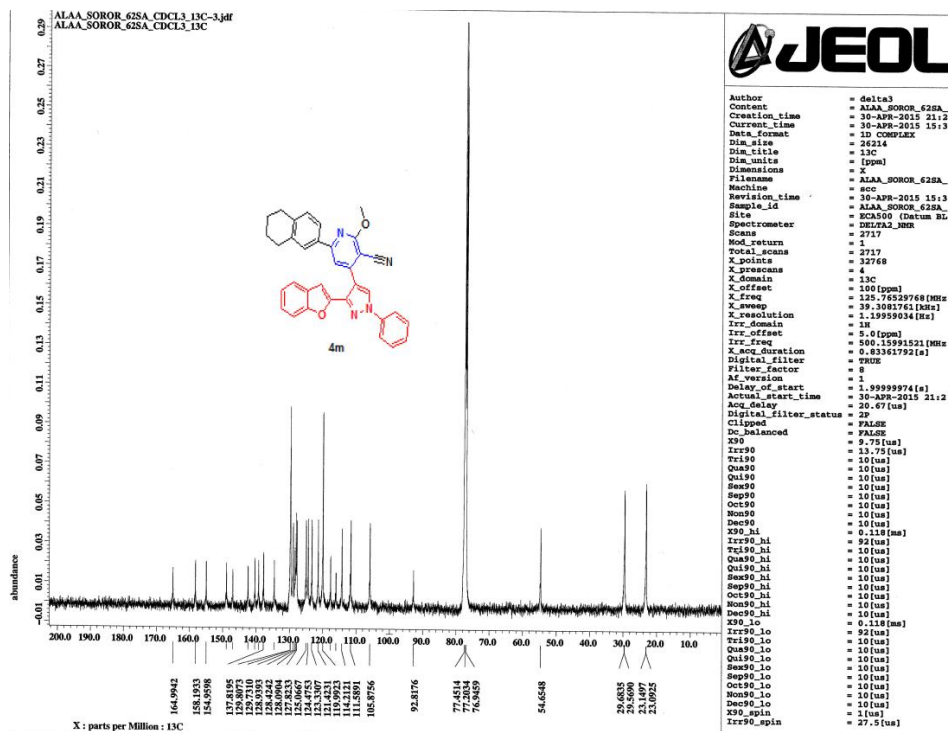


Figure S24. ^{13}C NMR spectrum of 4m.

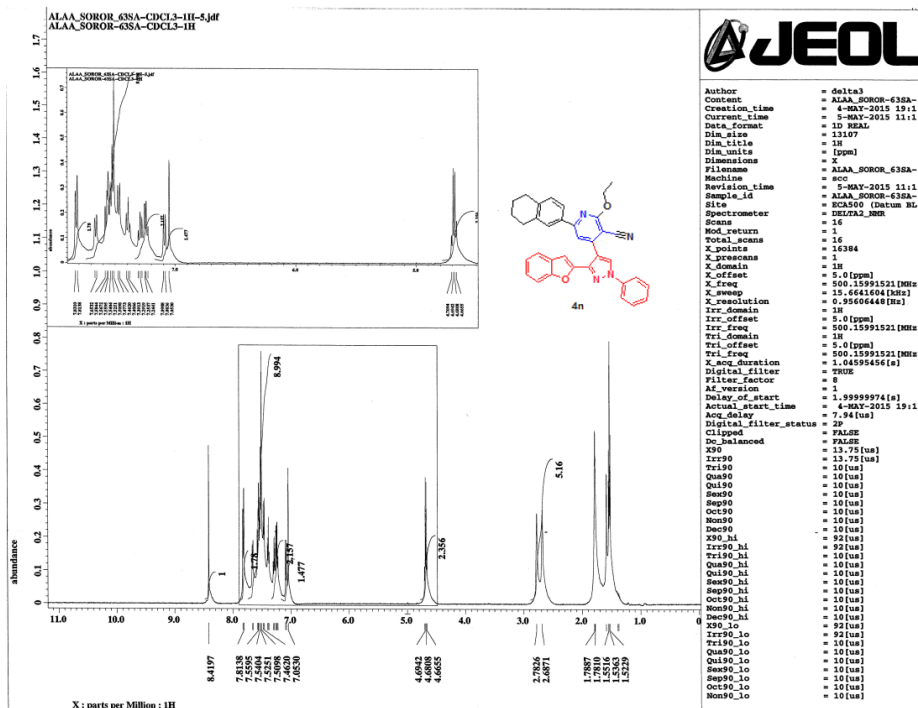


Figure S25. ^1H NMR spectrum of 4n.

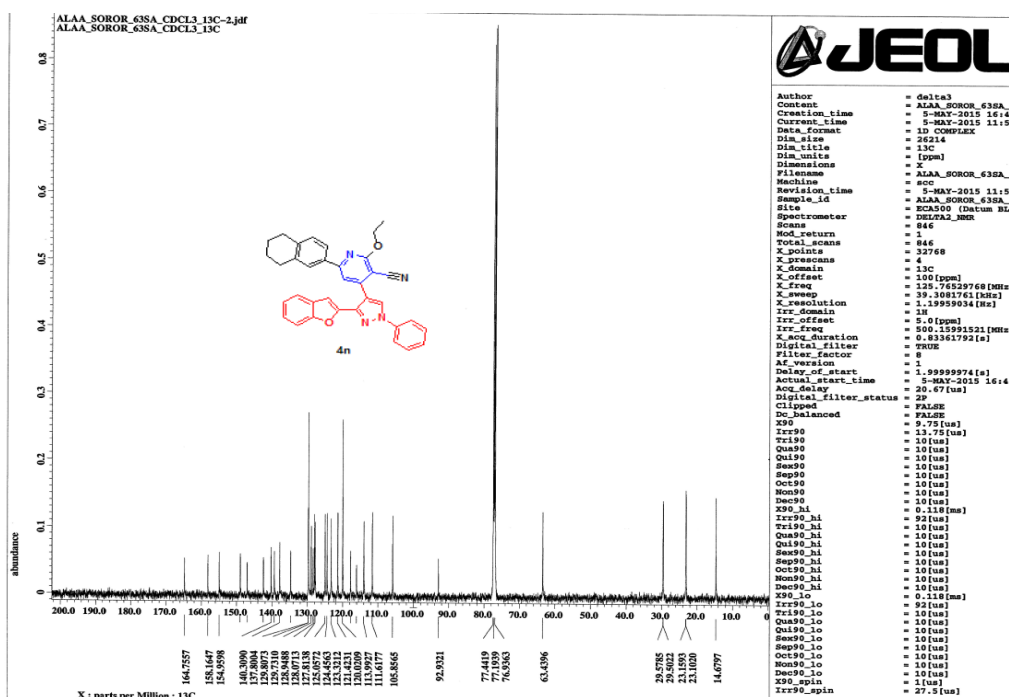


Figure S26. ^{13}C NMR spectrum of 4n.

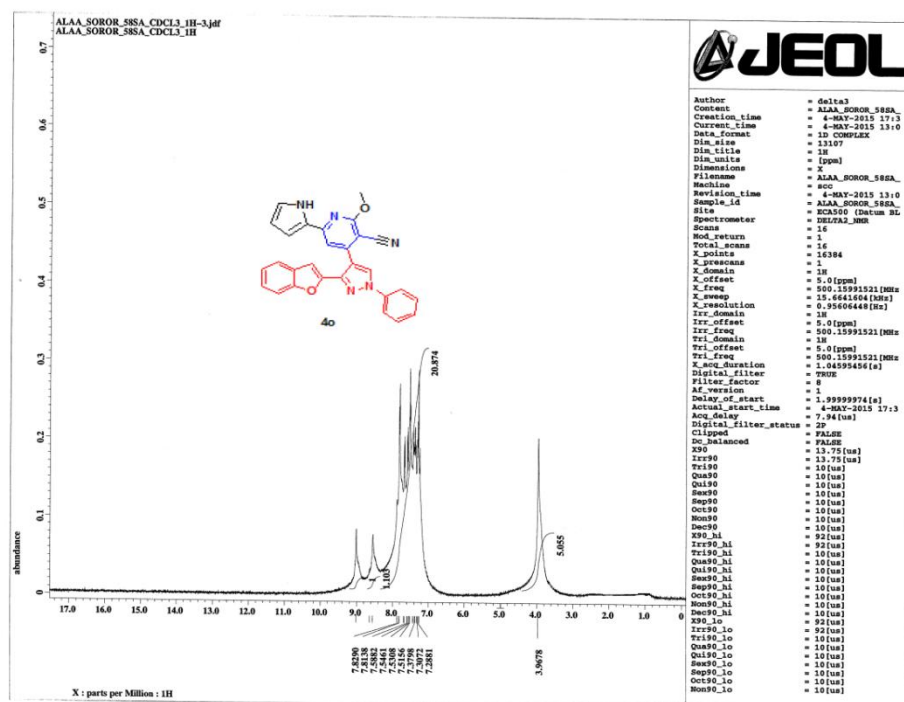


Figure S27. ^1H NMR spectrum of 4m.

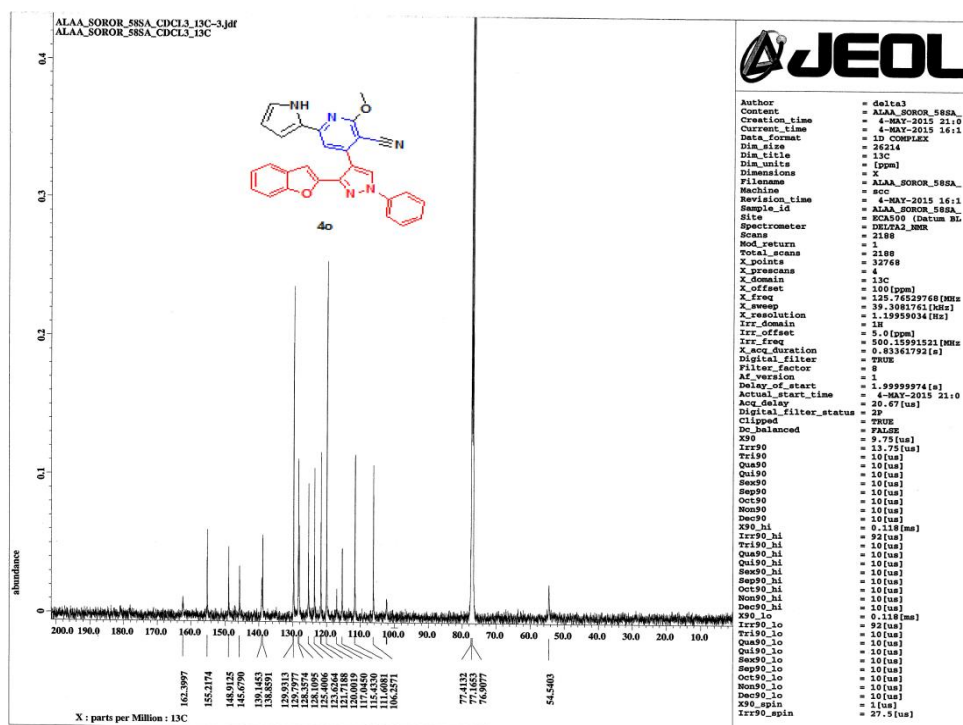


Figure S28. ^{13}C NMR spectrum of 4o.

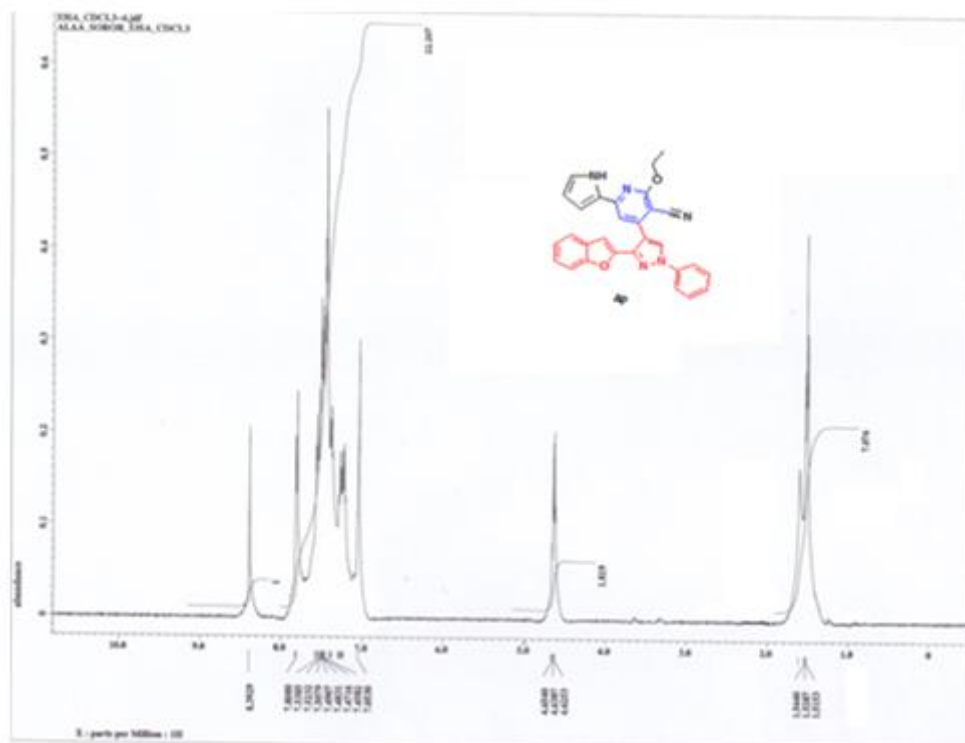


Figure S29. ¹H NMR spectrum of **4p**.

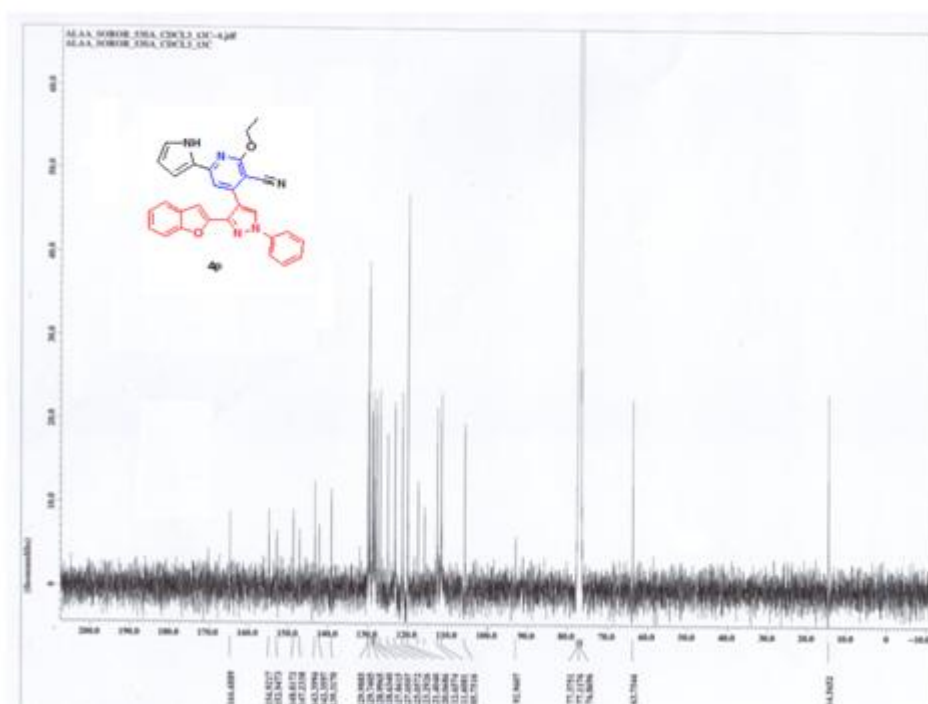


Figure S30. ¹³C NMR spectrum of **4p**.

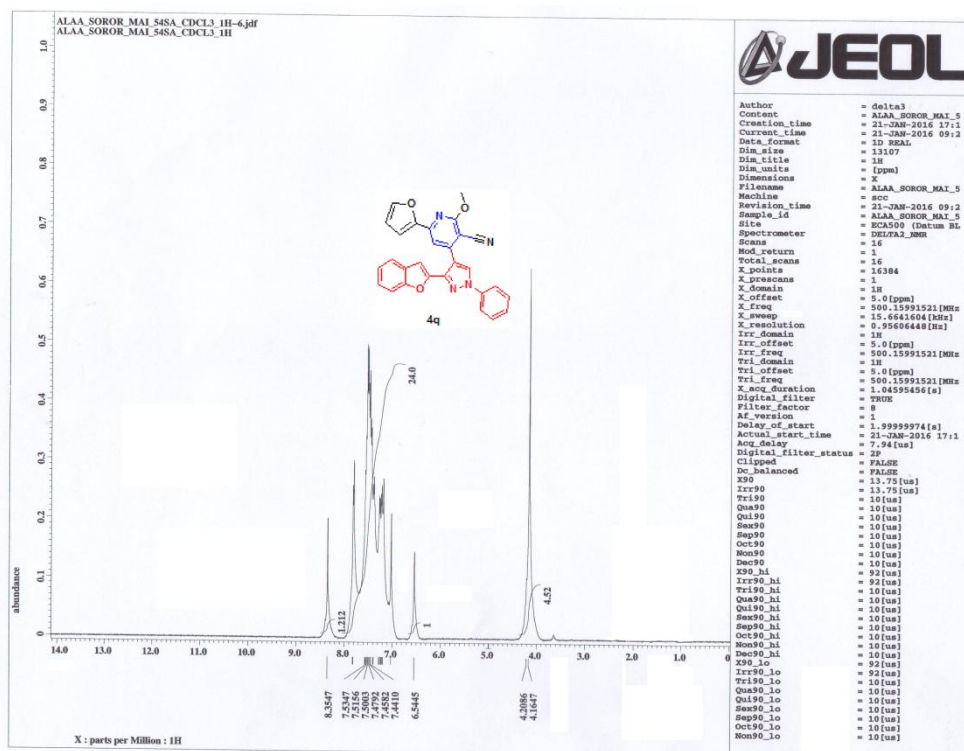


Figure S31. ^1H NMR spectrum of **4q**.

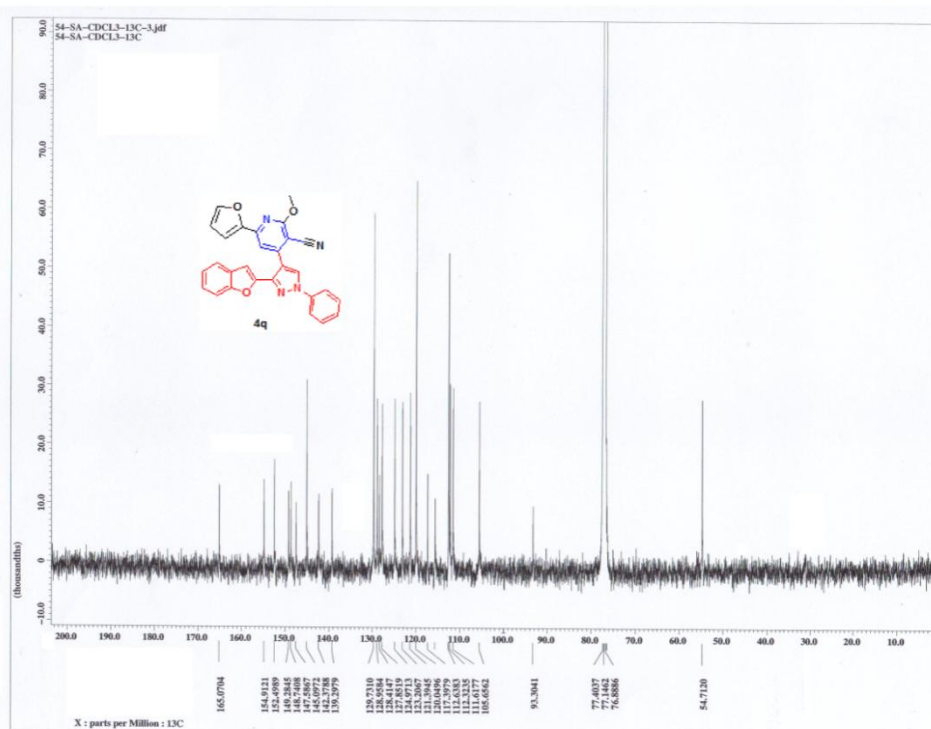


Figure S32. ^{13}C NMR spectrum of **4q**.

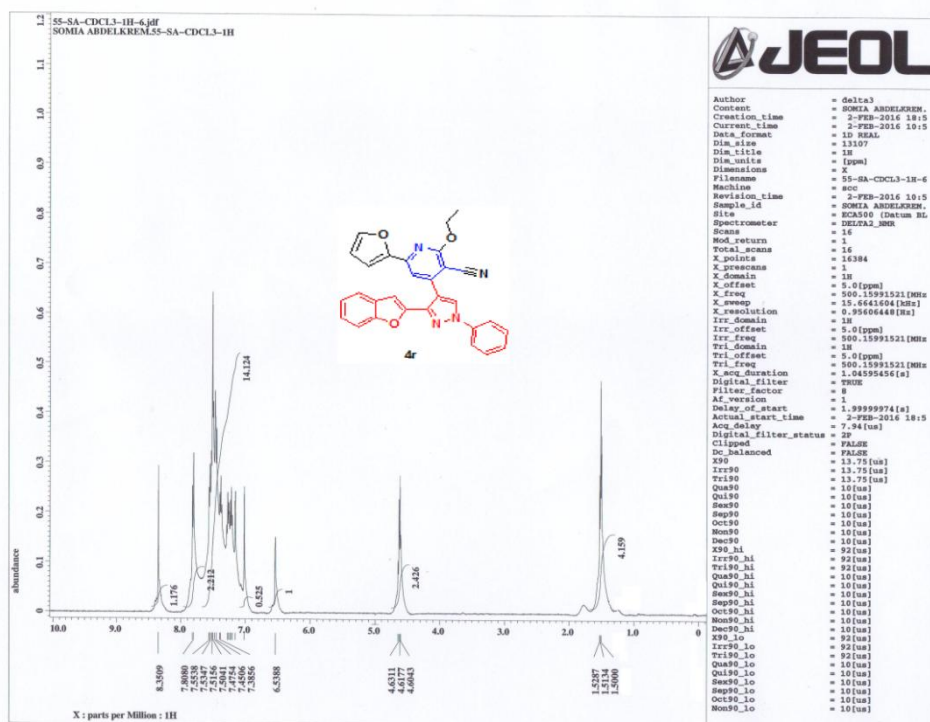


Figure S33. ^1H NMR spectrum of 4r.

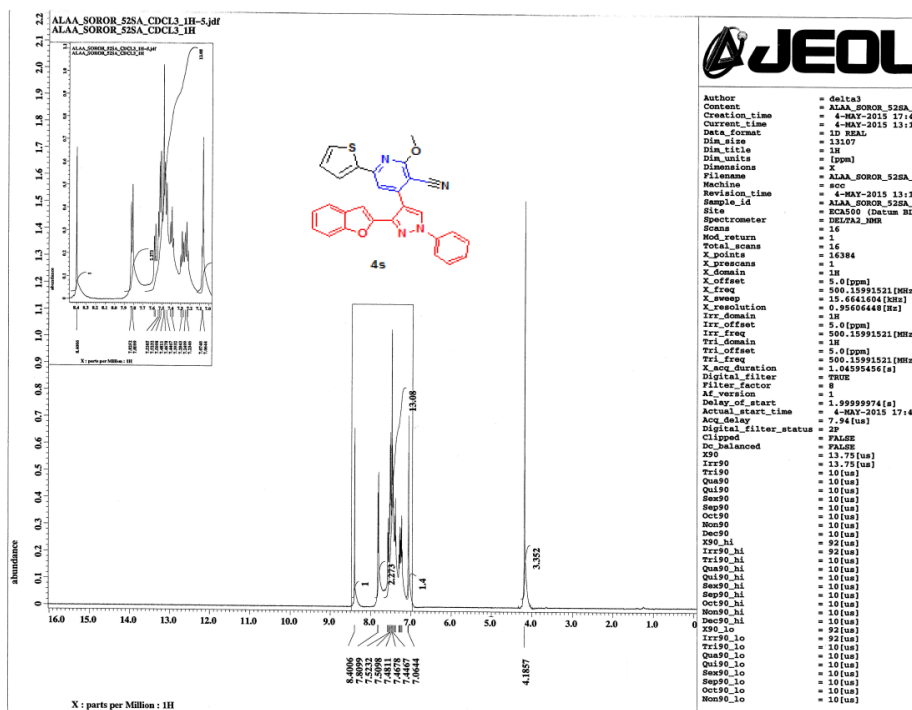


Figure S34. ^1H NMR spectrum of 4s.

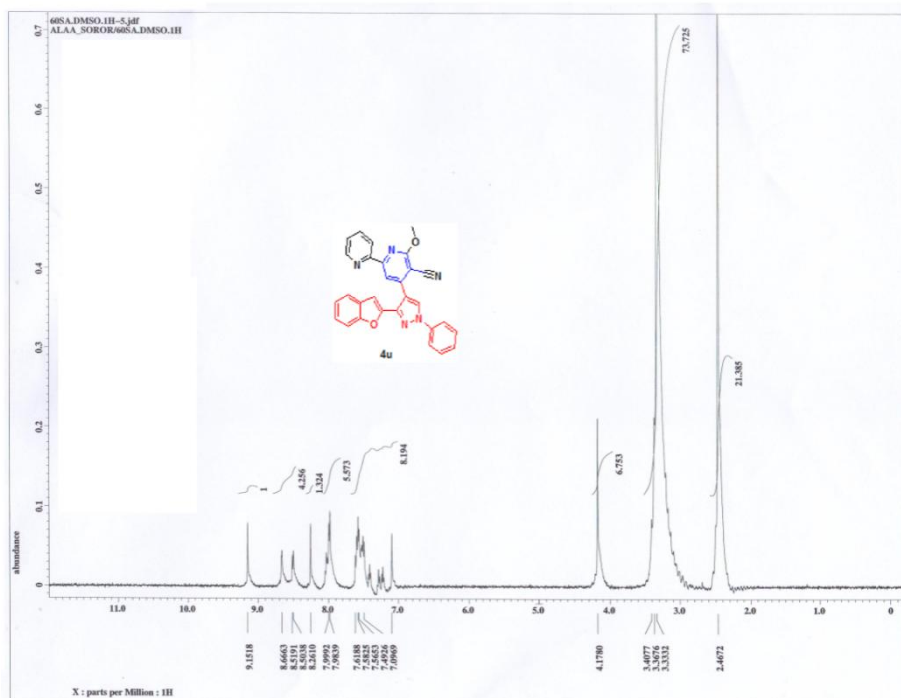


Figure S37. ^1H NMR spectrum of **4u**.

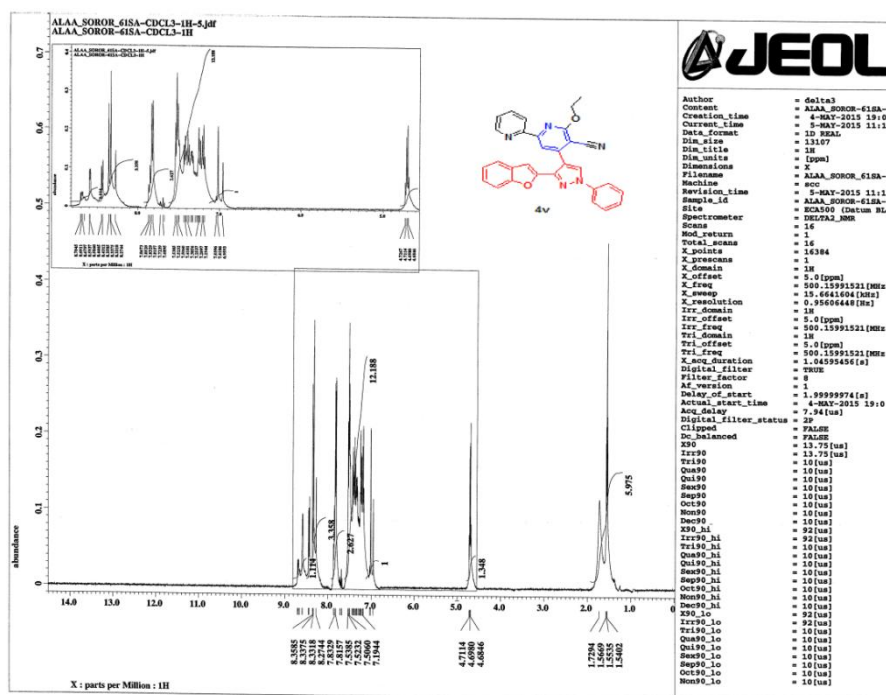


Figure S38. ^1H NMR spectrum of **4v**.

