Supplementary Material

Synthesis, characterization, antimicrobial activities and electrochemical behavior of new phenolic azo dyes from two thienocoumarin amines

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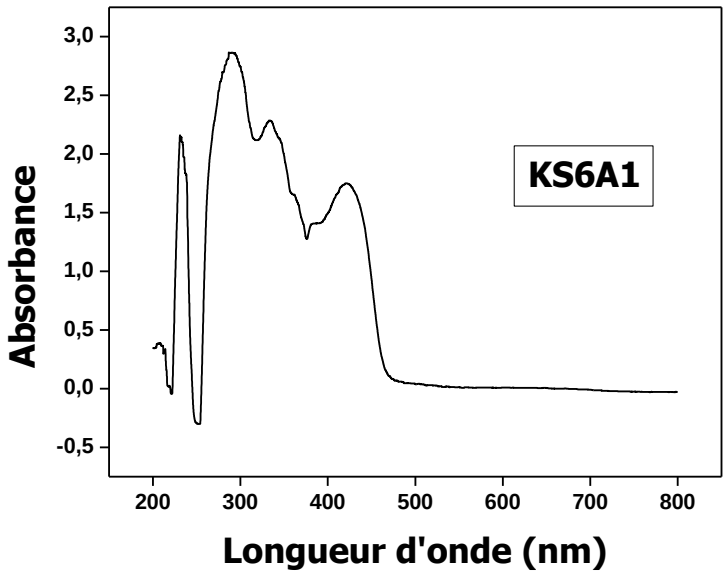


Figure 1.UV spectrum of compound **5a** in ethanol as solvent.

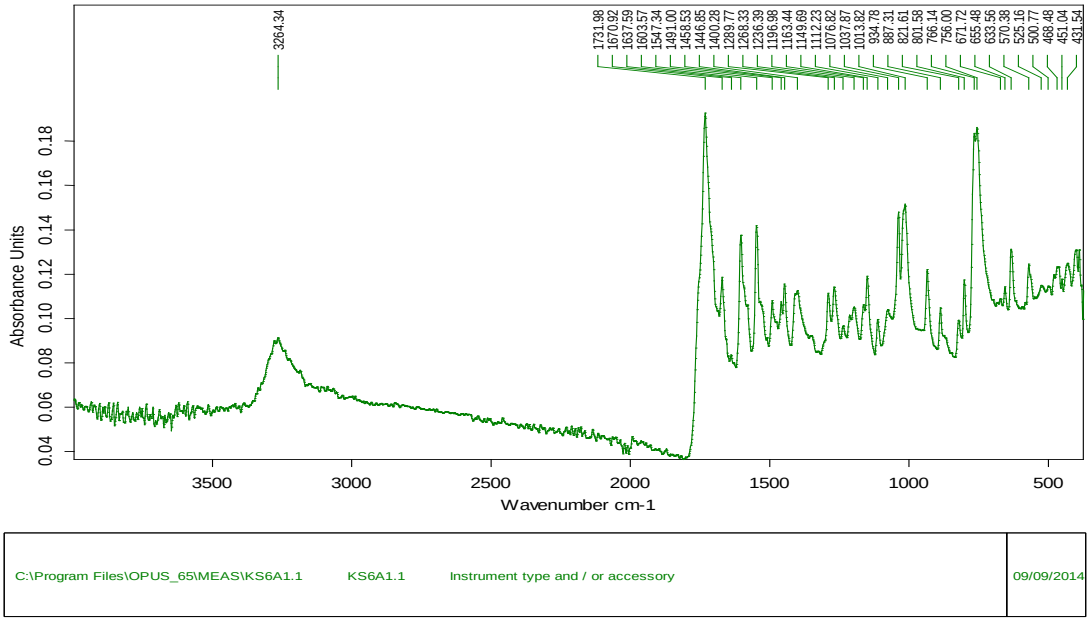


Figure 2.IR spectrum of compound **5a.**

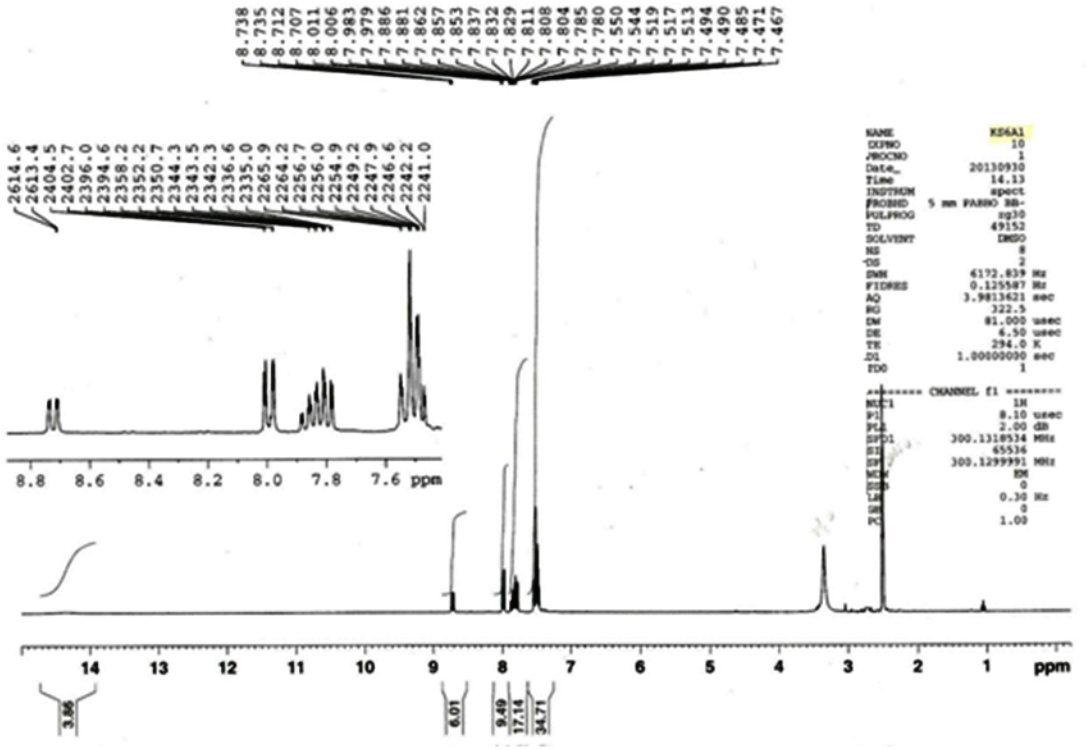


Figure 3.^{1}H-NMR (DMSO-d_6, 300 MHz) spectrum of compound **5a.**

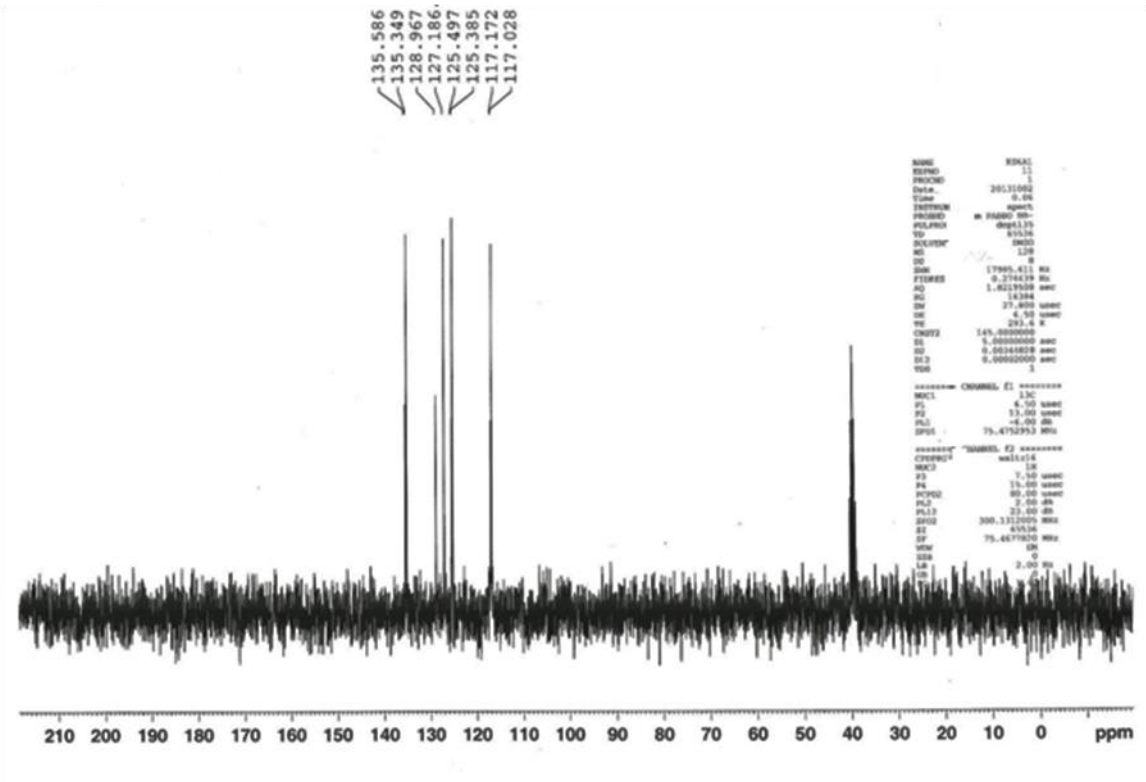


Figure 4.DEPT-135 ^{13}C(H)-NMR (DMSO-d_6, 75 MHz) spectrum of compound **5a.**

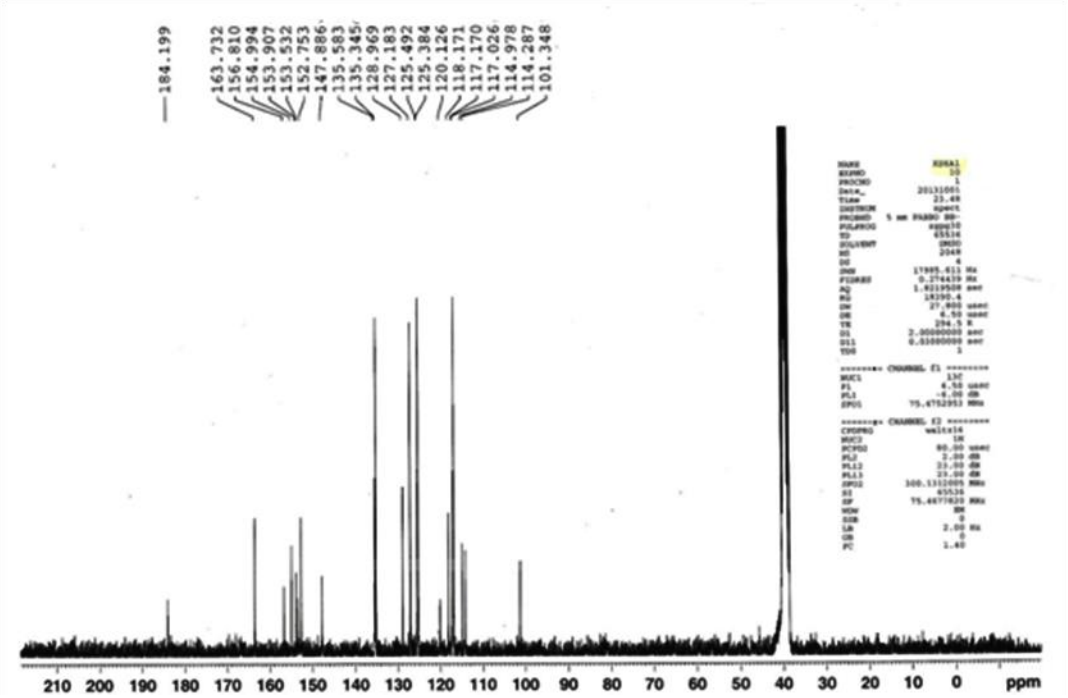


Figure 5.^{13}C(H)-NMR ^{1}H (DMSO-d_6, 75 MHz) of compound **5a.**

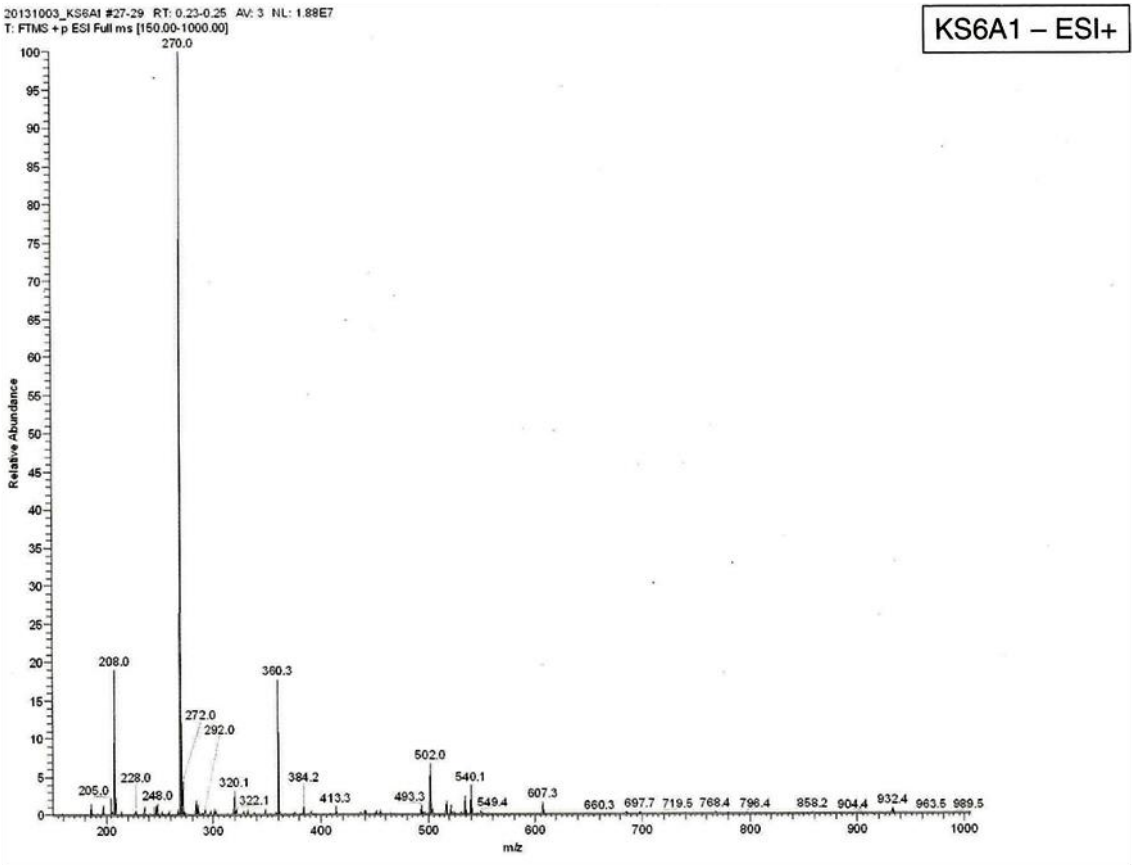


Figure 6.HRMS ESI-Positive mode of compound **5a.**

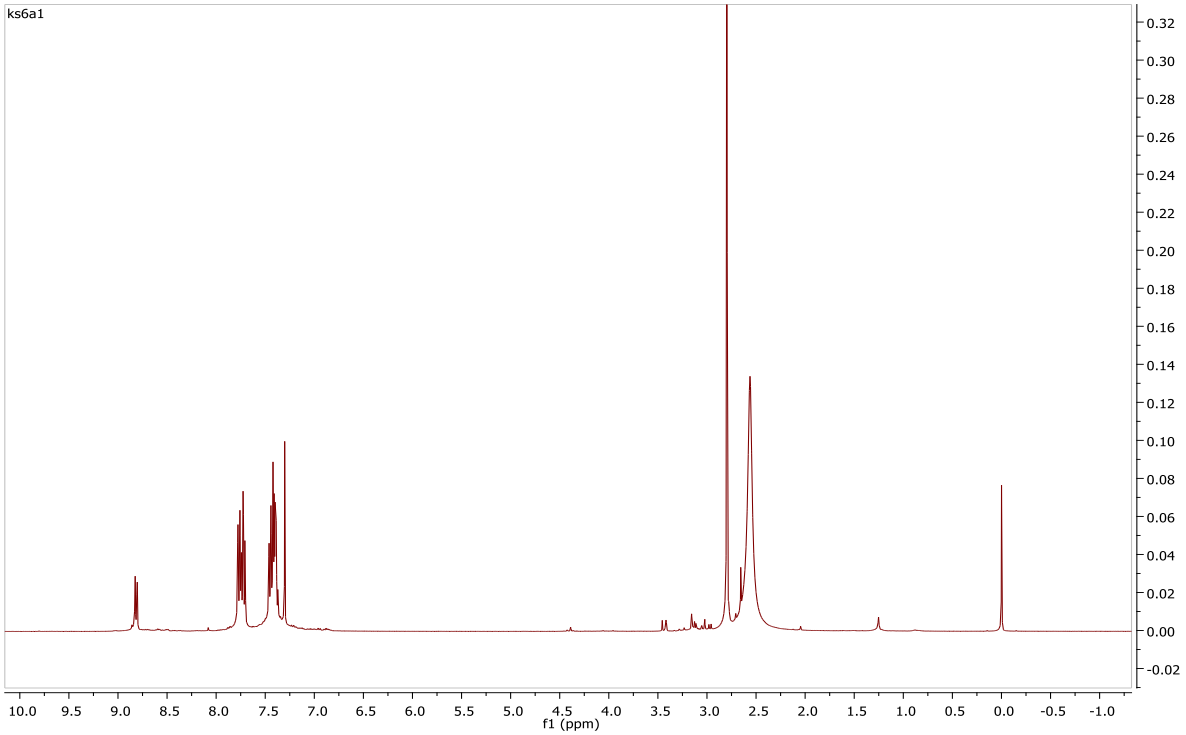


Figure 7.^{1}H-NMR (DMSO-d_6/$CDCl_3$, 400 MHz), spectrum of **5a.**

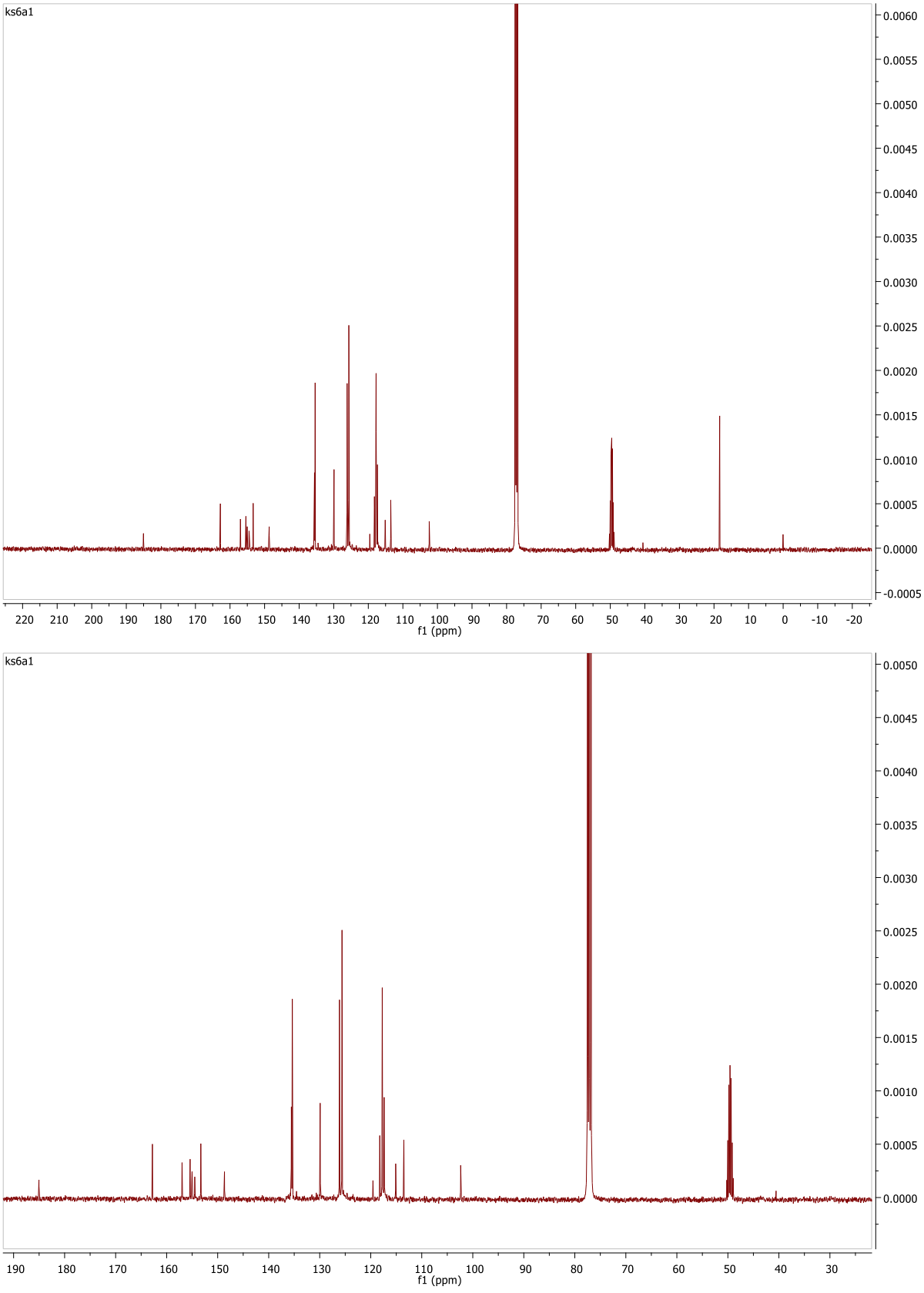


Figure 8. $^{13}C(^{1}H)$ NMR (DMSO-d_6/$CDCl_3$, 100 MHz) Spectraof**5a.**

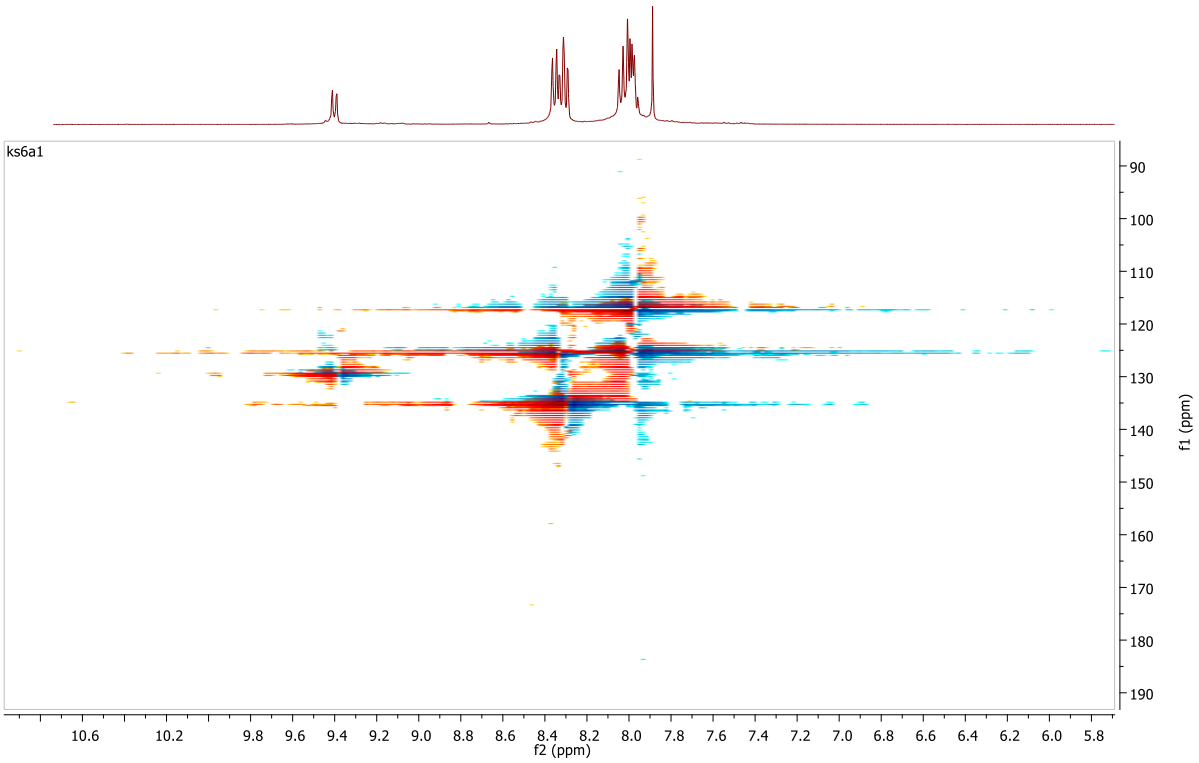


Figure 9.HSQC (DMSO-d_6/$CDCl_3$, 100 MHz) spectrum of **5a.**

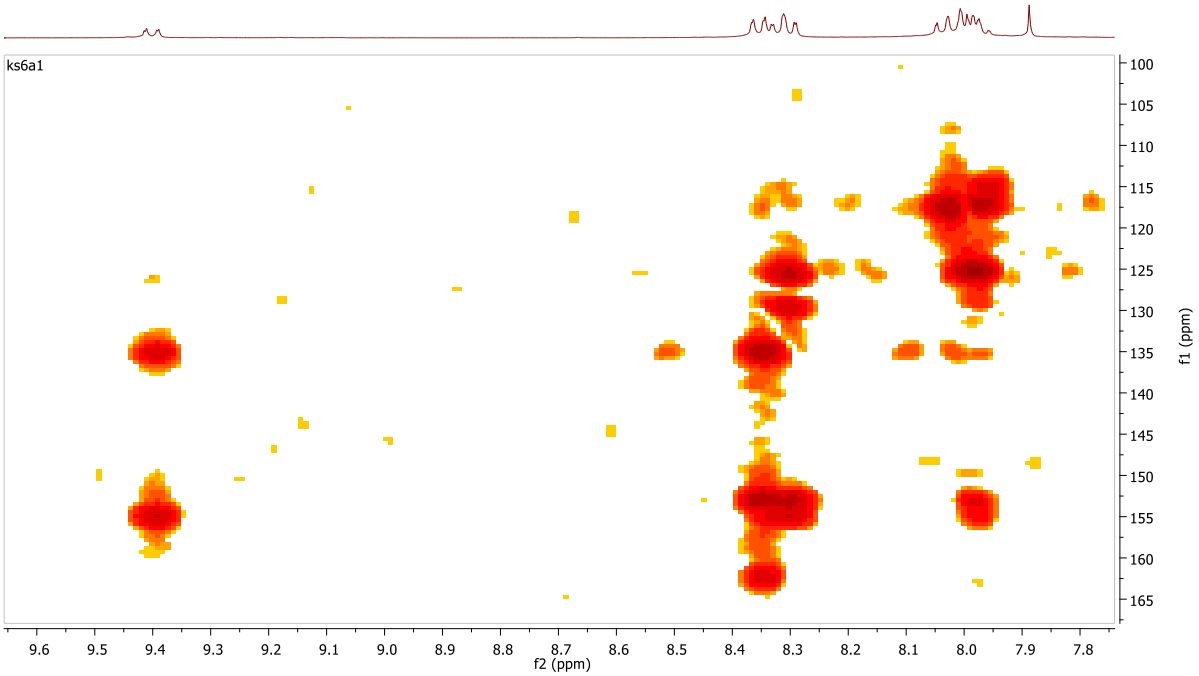


Figure 10.HMBC (DMSO-d_6/$CDCl_3$, 100 MHz) spectrum of **5a**.

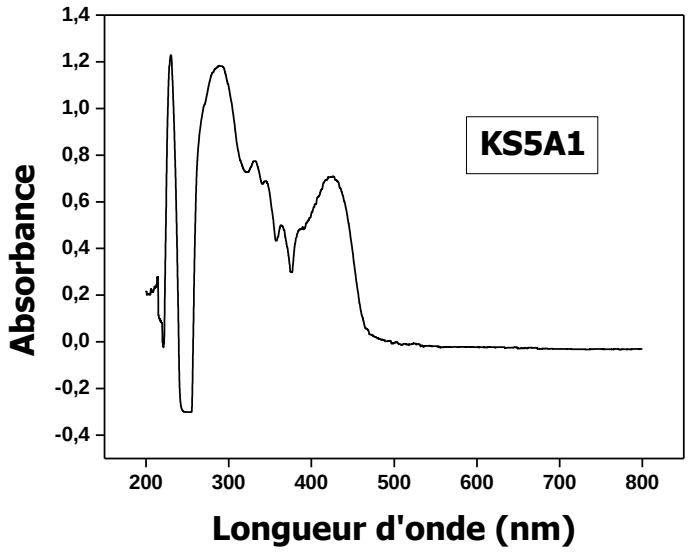
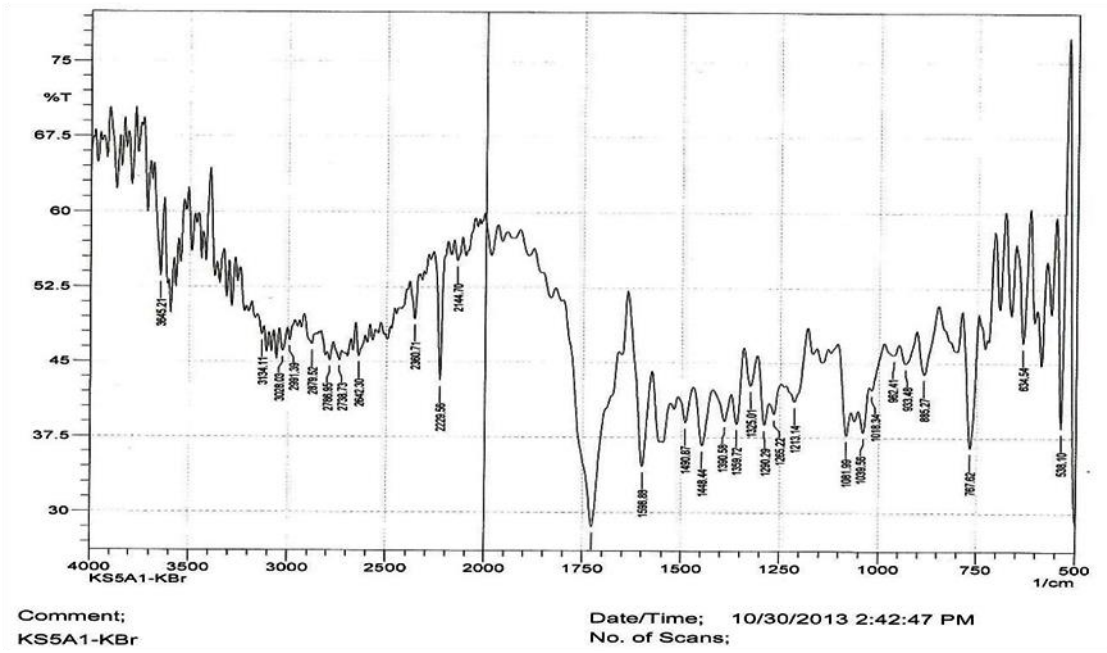


Figure 11.UV spectrum of compound **5b** in ethanol as solvent.



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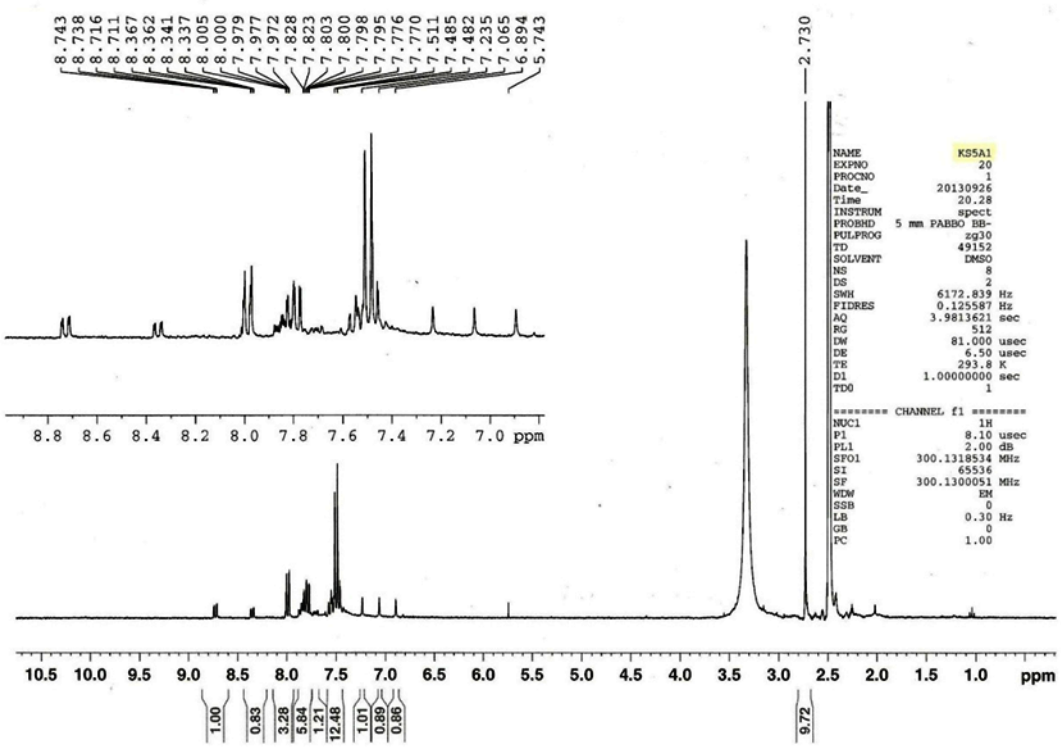


Figure 13. ^{1}H-NMR (DMSO-d_6, 300 MHz) spectrum of compound **5b.**

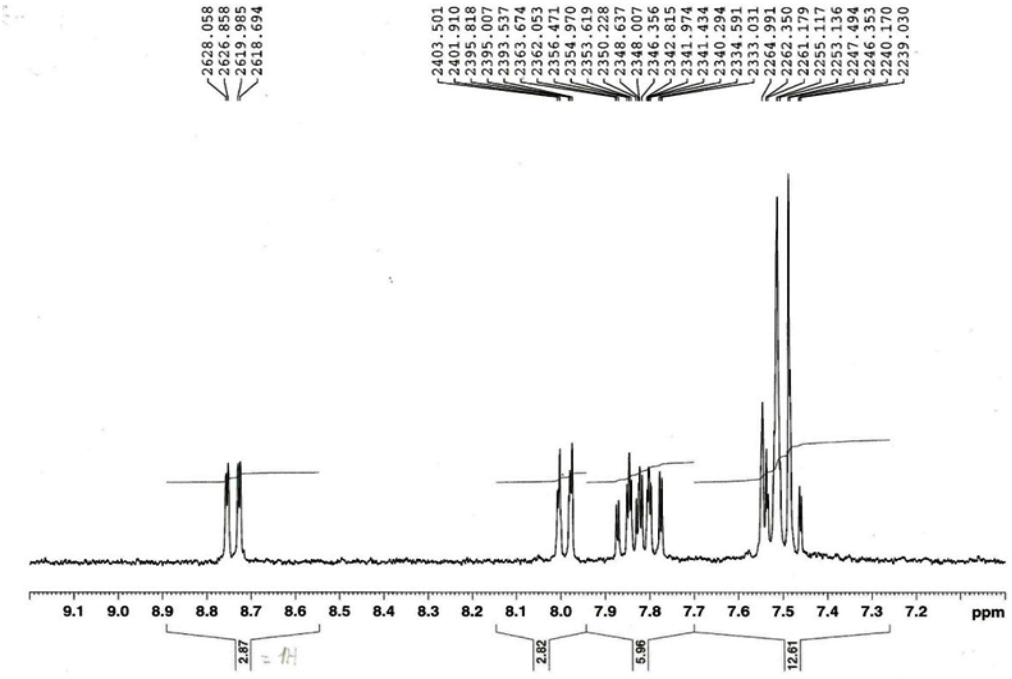


Figure 14. Enlarged ^{1}H-NMR (DMSO-d_6, 300 MHz) spectrum of compound **5b.**

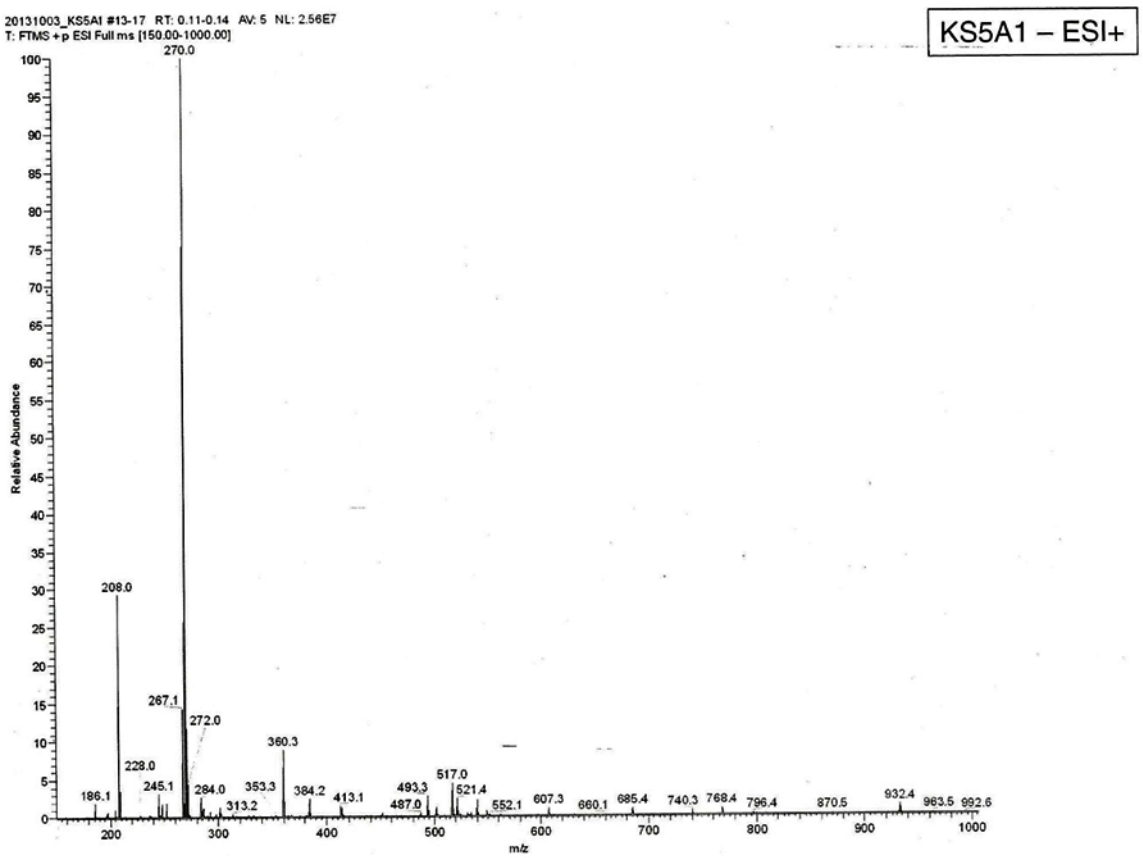


Figure 15.HRMS ESI-Positive mode of compound **5b.**

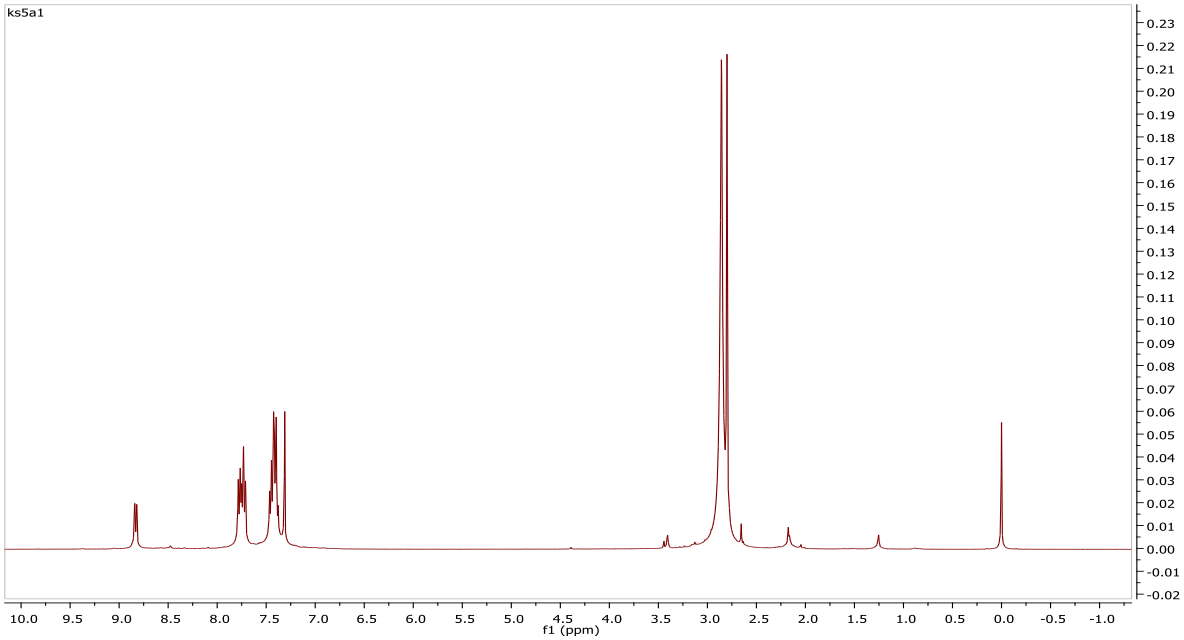


Figure 16.^{1}H-NMR (DMSO-d_6/$CDCl_3$, 400 MHz) spectrum of **5b.**

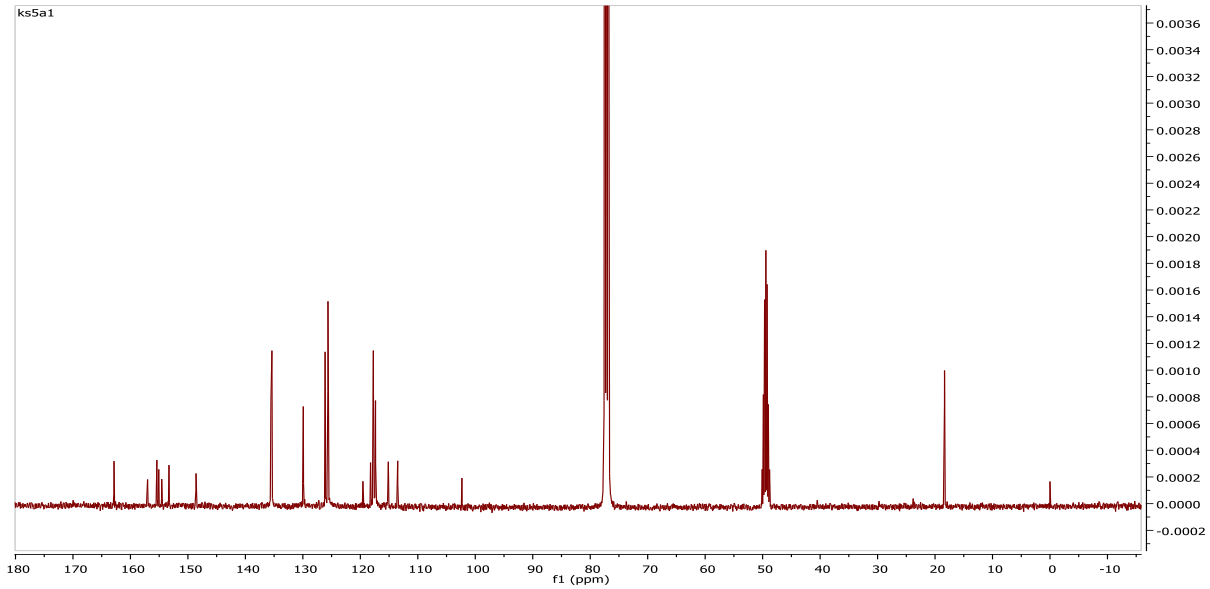


Figure 17. $^{13}C(^{1}H)$ NMR (DMSO-d_6/$CDCl_3$, 100 MHz) Spectra of **5b.**

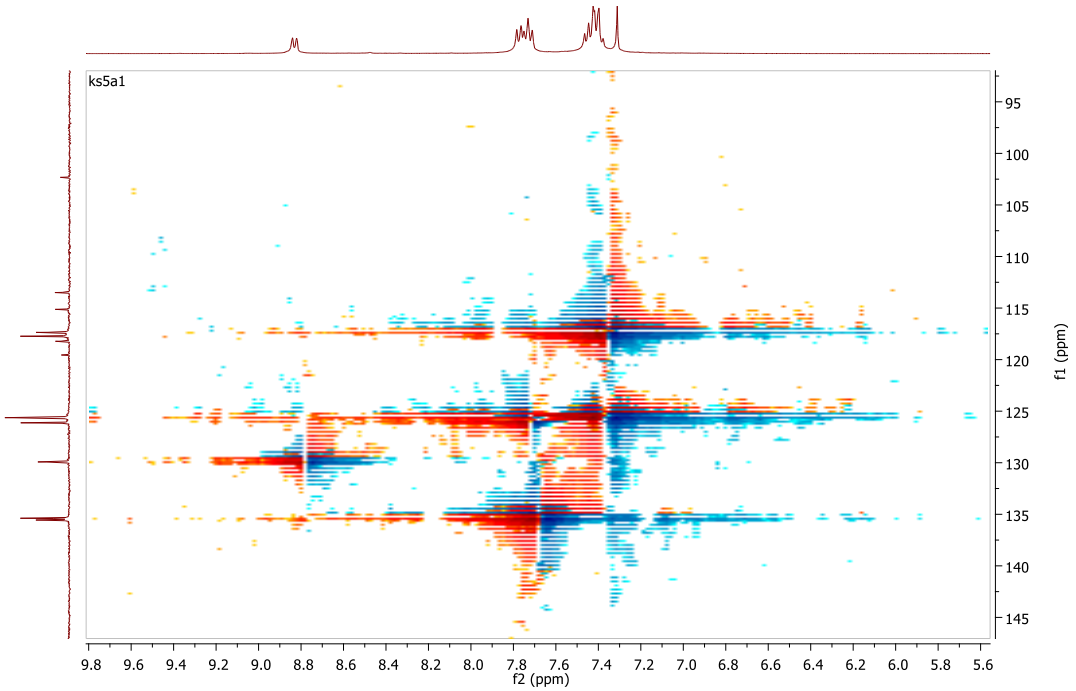
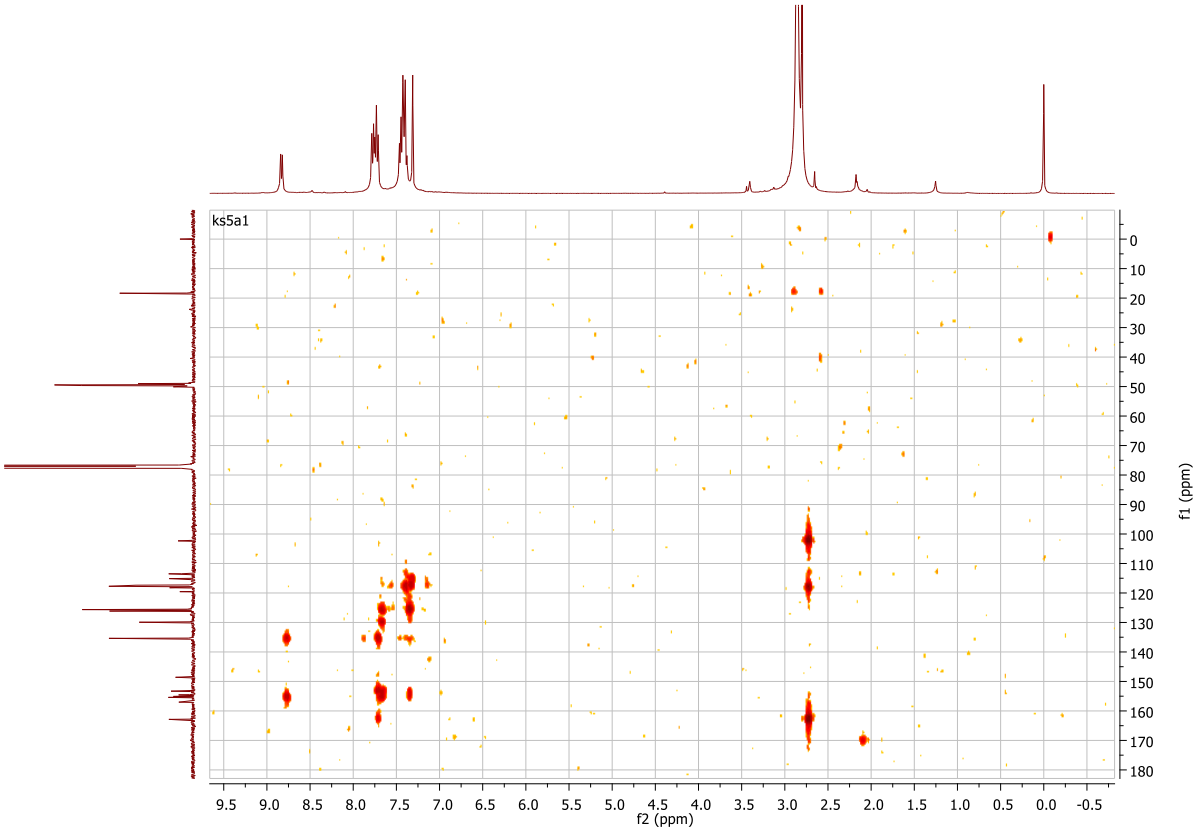


Figure 18. HSQC (DMSO-d_6/$CDCl_3$, 100 MHz) spectrum of **5b.**



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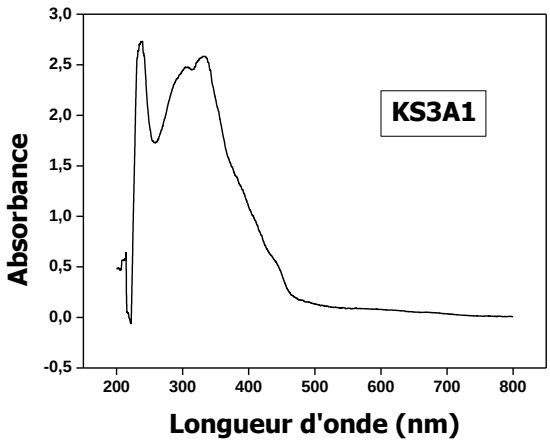


Figure 20.UV spectrum of compound **5c** in ethanol as solvent.

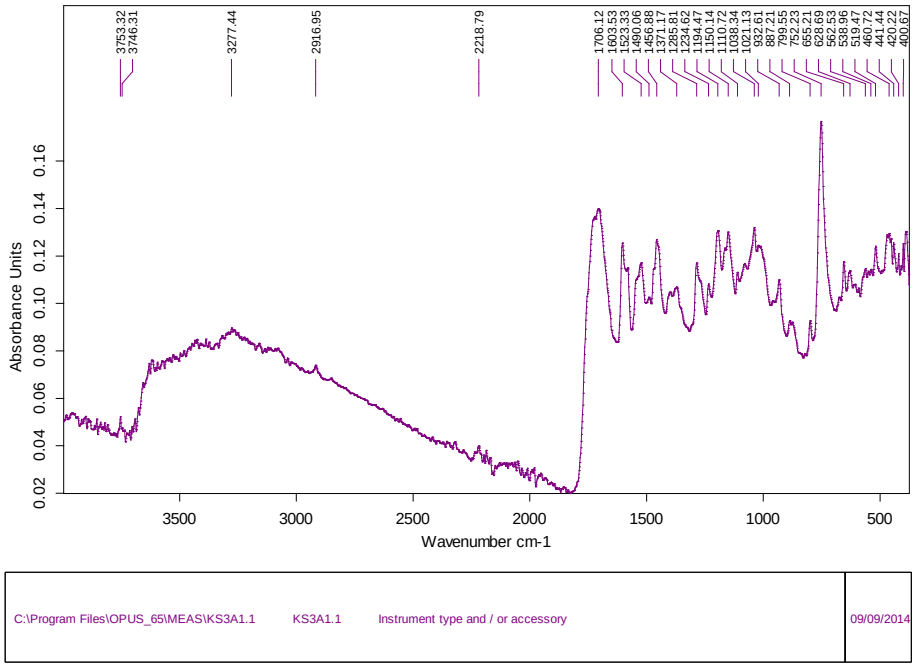


Figure 21.IR spectrum of compound **5c.**

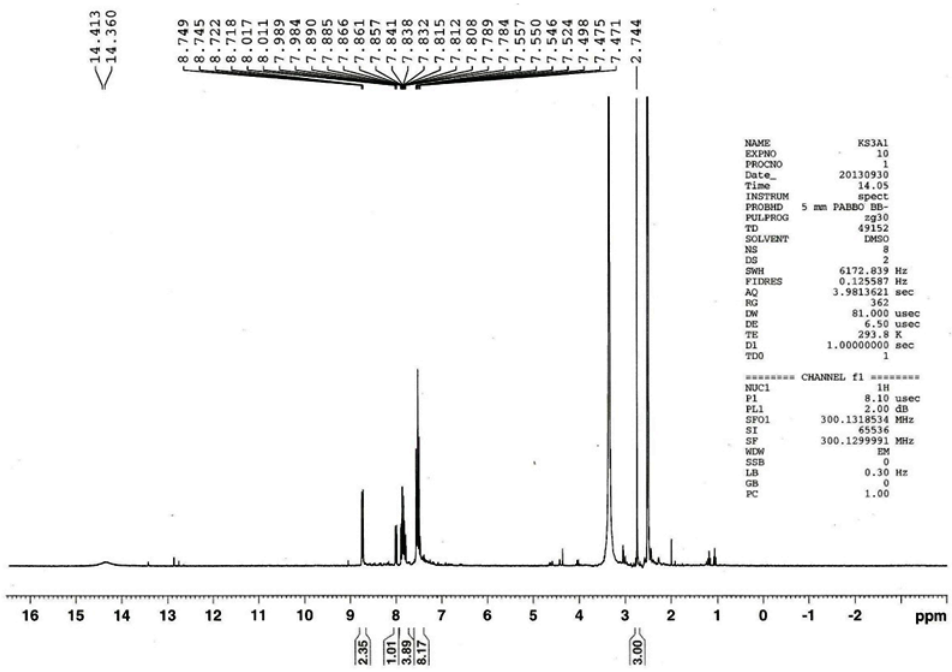


Figure 22.^{1}H-NMR (DMSO-d_6, 500 MHz) spectrum of compound **5c.**

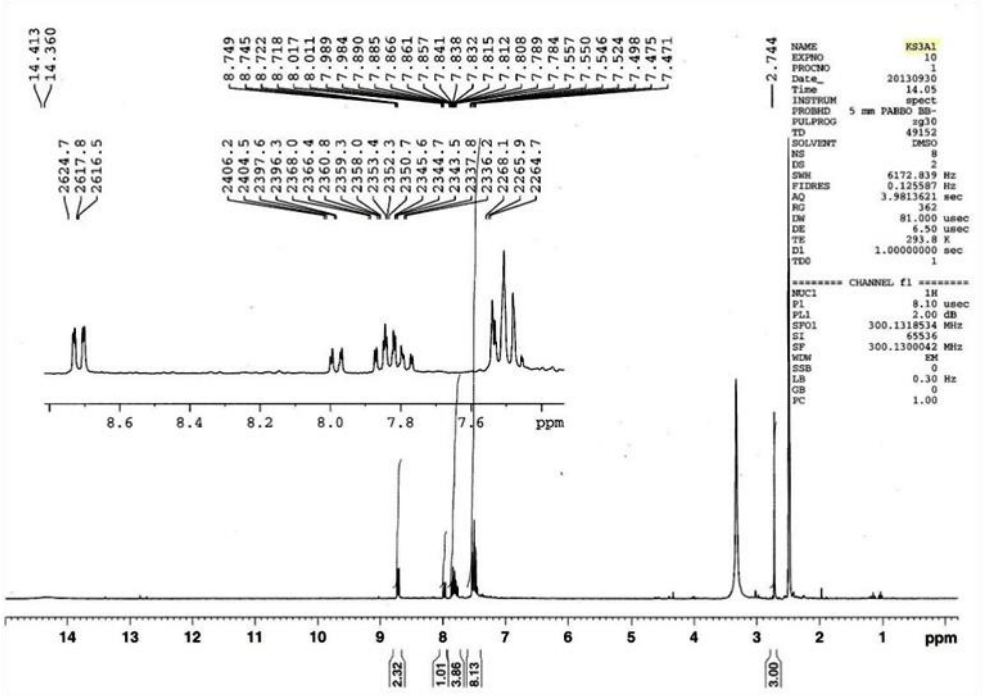


Figure 23. Enlarged ^{1}H-NMR (DMSO-d_6, 500 MHz) spectrum of compound **5c.**

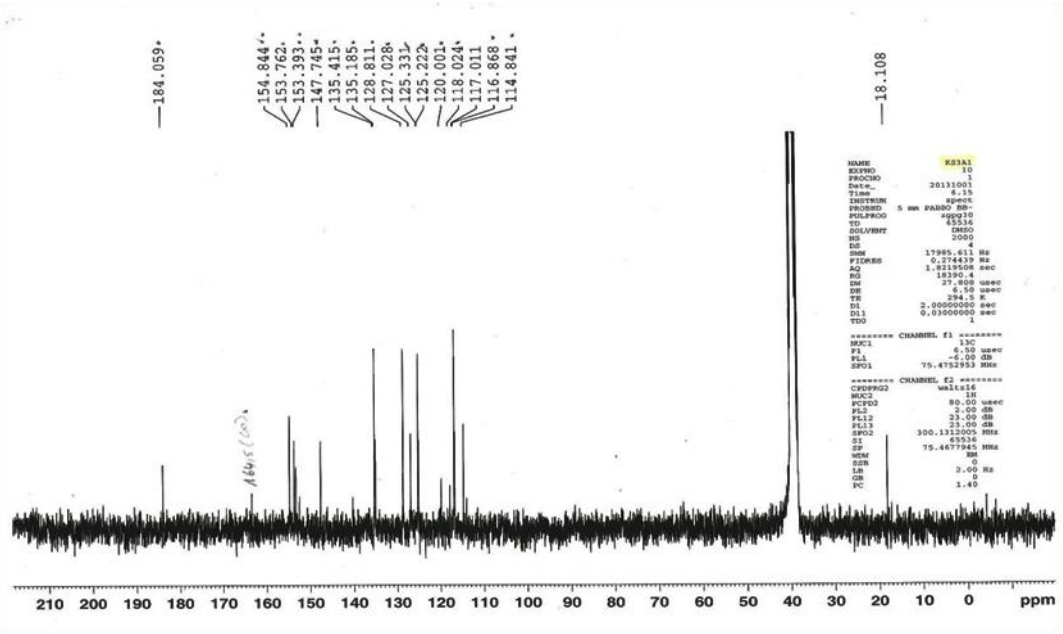


Figure 24. ^{13}C(^{1}H)-NMR (DMSO-d_6, 75 MHz) of compound **5c.**

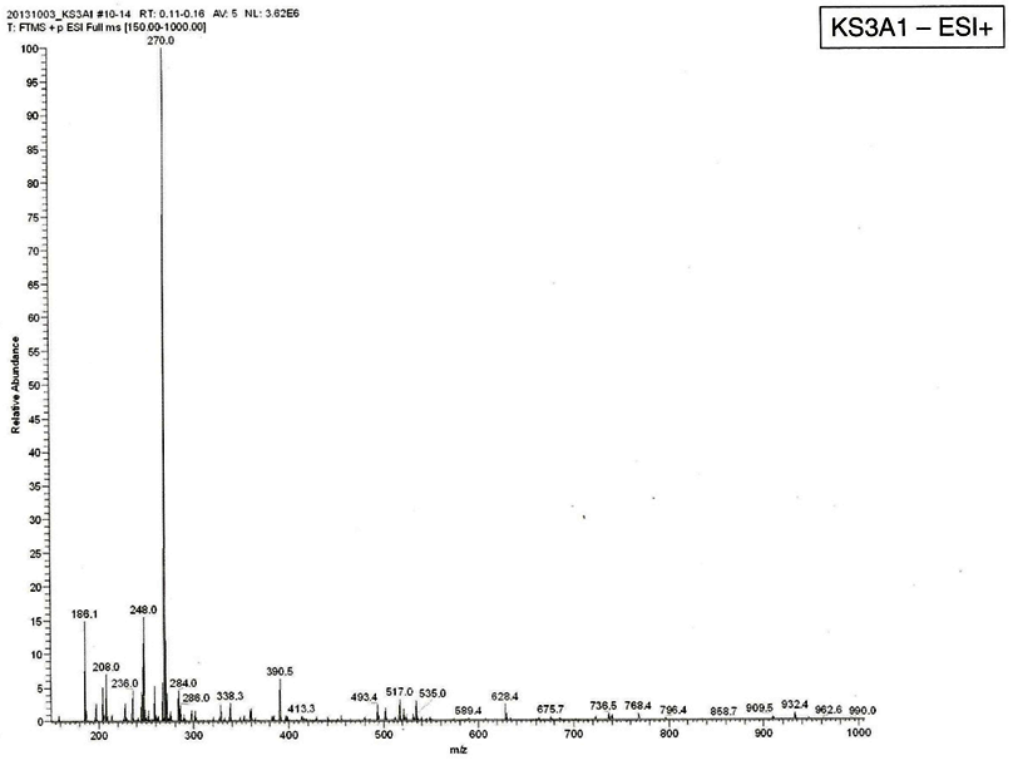


Figure 25. HRMS ESI-Positive mode of compound 5c.

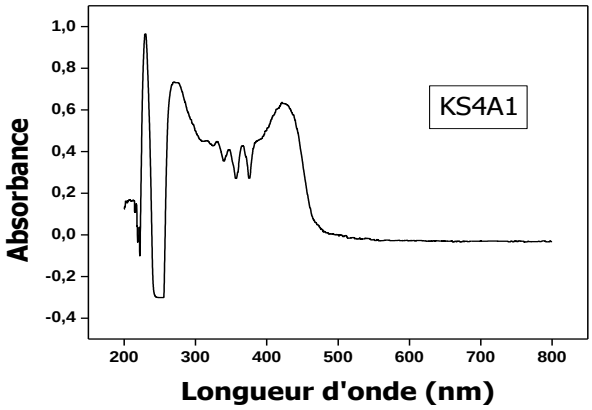


Figure 26. UV spectrum of compound **6** in ethanol as solvent.

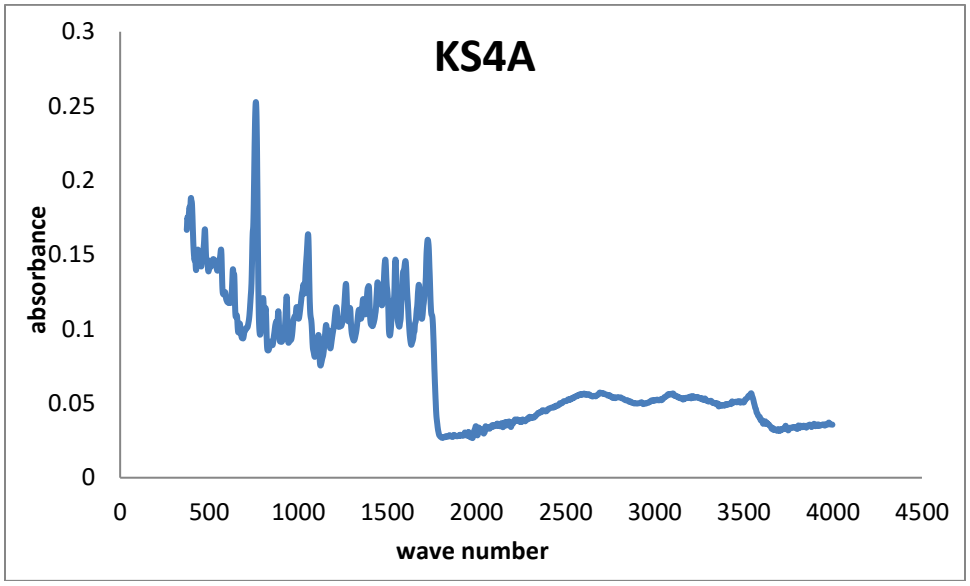


Figure 27.IR spectrum of compound **6.**

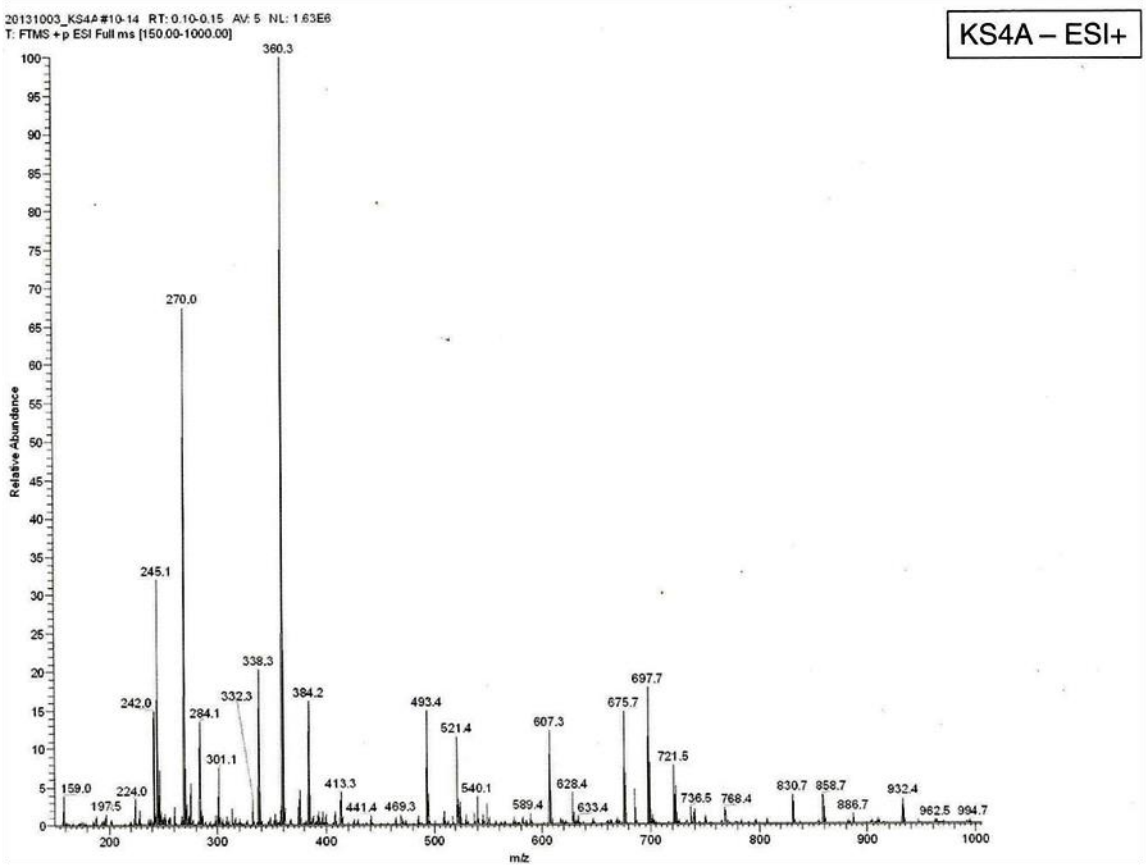


Figure 28. HRMS ESI-Positive mode of compound **6.**

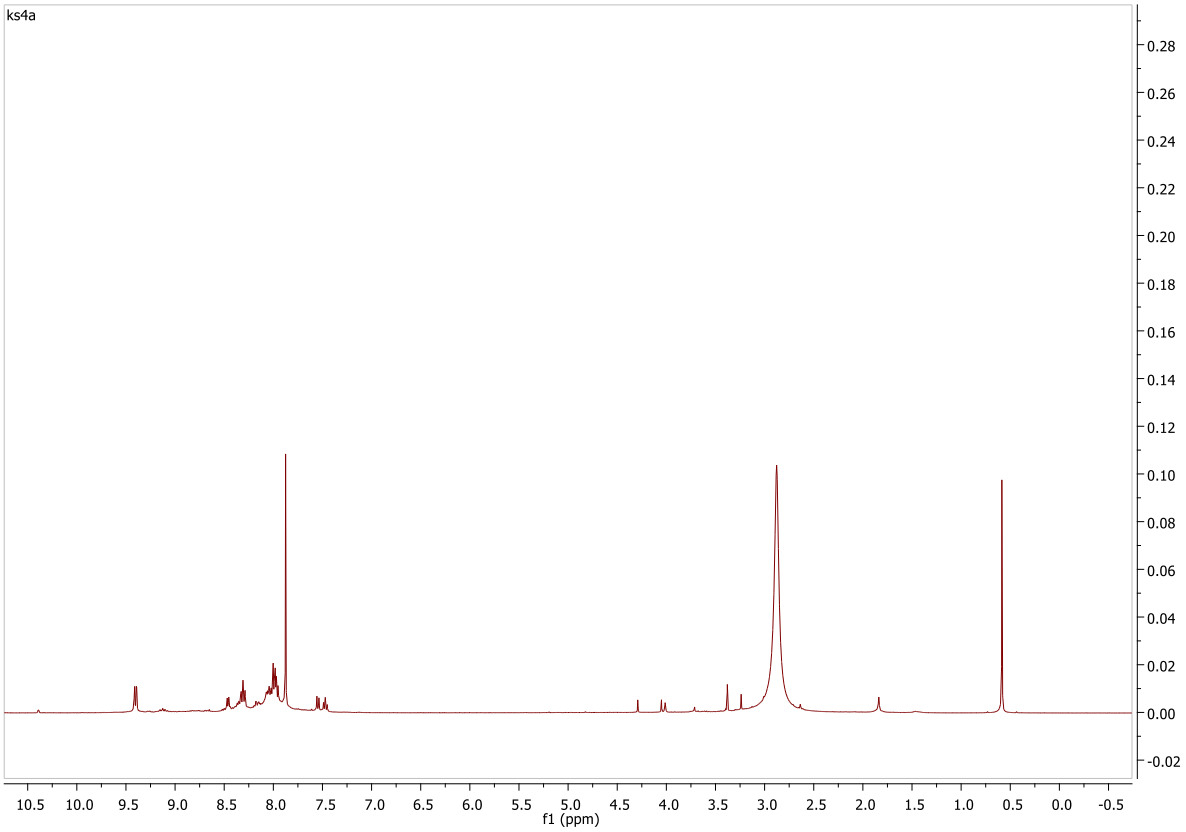


Figure 29. ^{1}H-NMR (DMSO-d_6/$CDCl_3$, 400 MHz) spectrum of **6.**

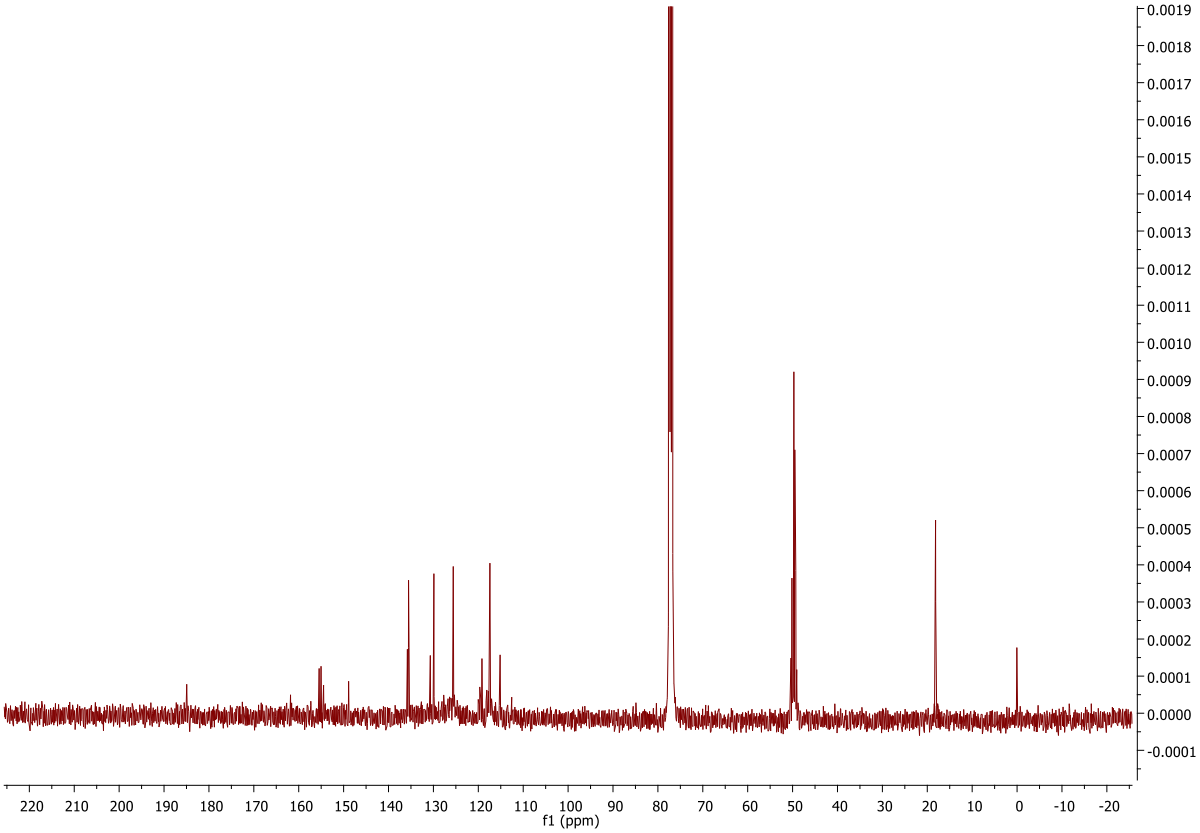


Figure 30. ^{13}C(^{1}H) NMR (DMSO-d_6/$CDCl_3$, 100 MHz) Spectrum of **6.**

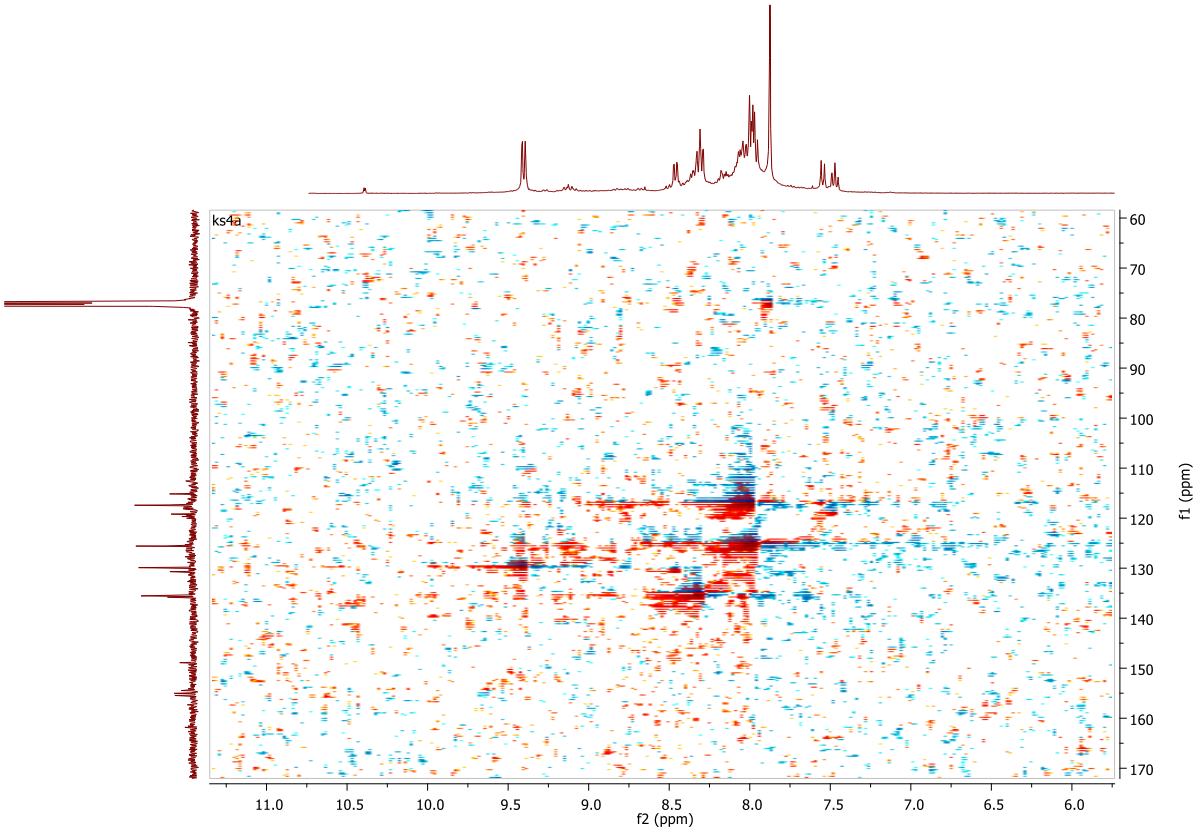


Figure 31. HSQC (DMSO-d_6/$CDCl_3$, 100 MHz) spectrum of **6.**

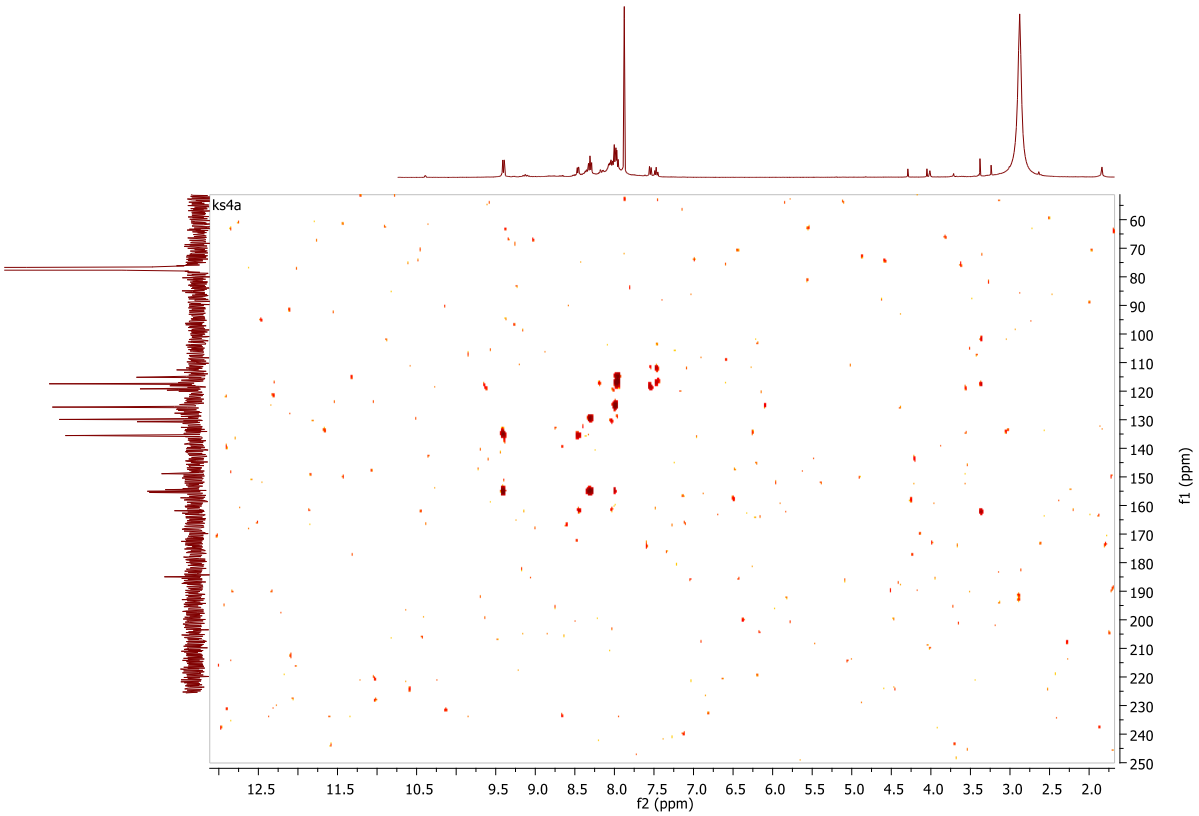


Figure32. HMBC (DMSO-d_6/$CDCl_3$, 100 MHz) spectrum of **6.**

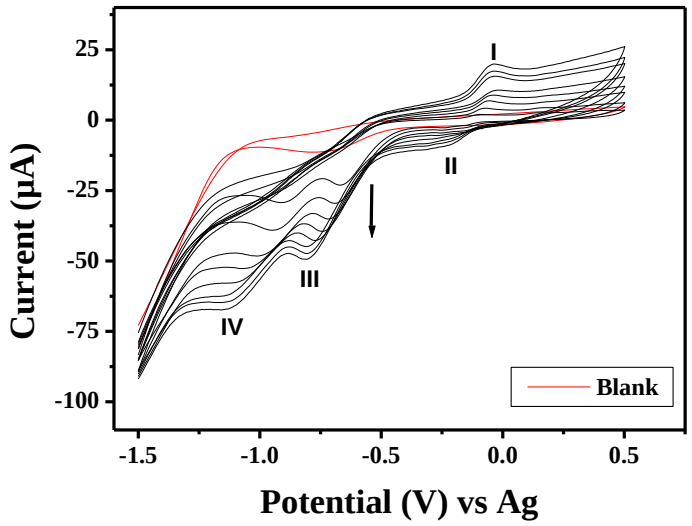


Figure 33. Cyclic voltammograms of 943 µM **5a** in 0.05 M H_2SO_4 at various scan rates: 30, 60, 90, 120, 150, 240, 270 and 300 mV/s.

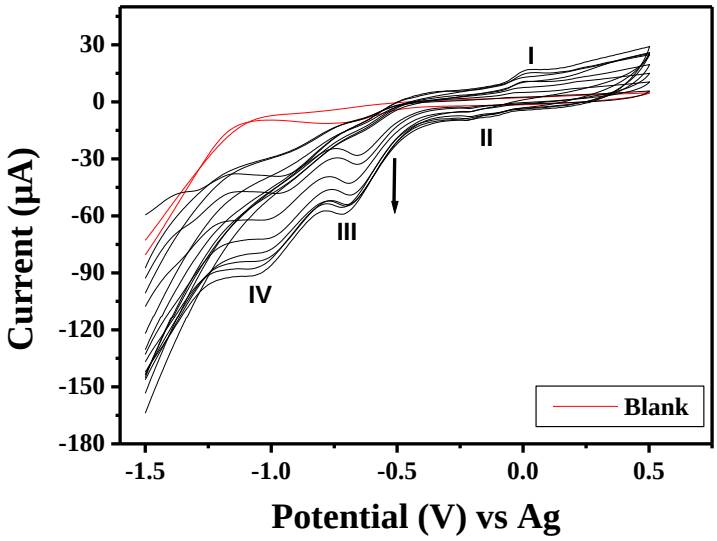


Figure 34. Cyclic voltammograms of 1120 µM **5b** in 0.05 M H_2SO_4 at various scan rates: 30, 60, 90, 120, 150, 180, 270 and 300 mV/s.

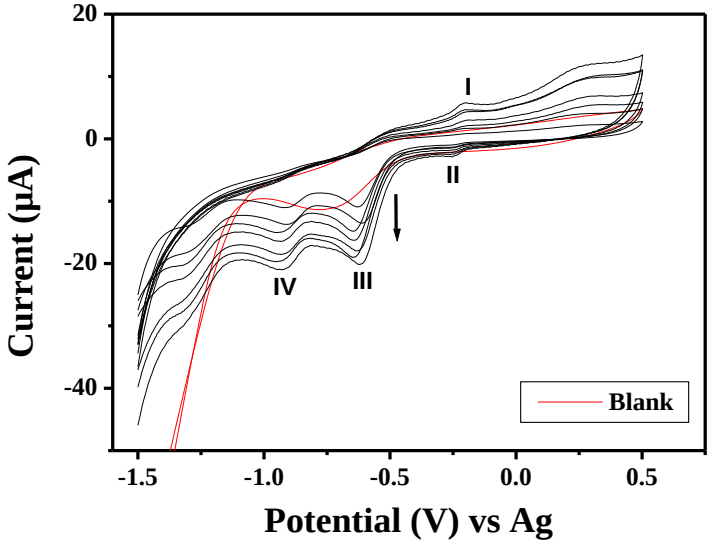


Figure 35. Cyclic voltammograms of 268 µM **5c** in 0.05 M H_2SO_4 at various scan rates: 30, 60, 90, 120, 150, 180 and 210 mV/s.

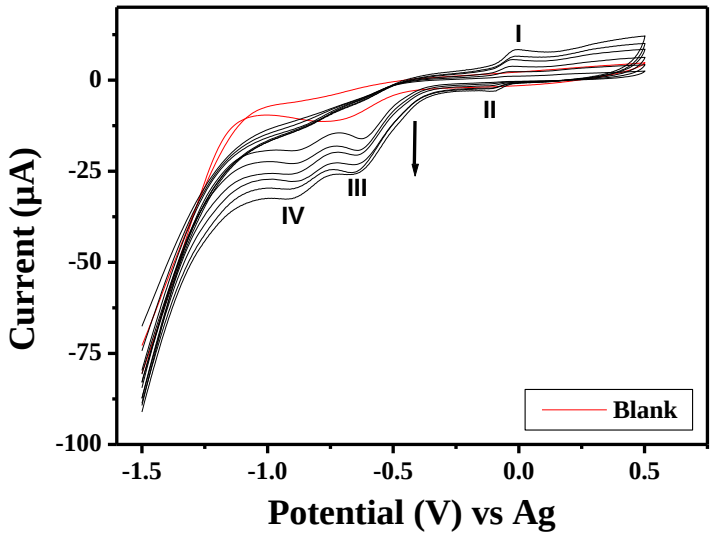
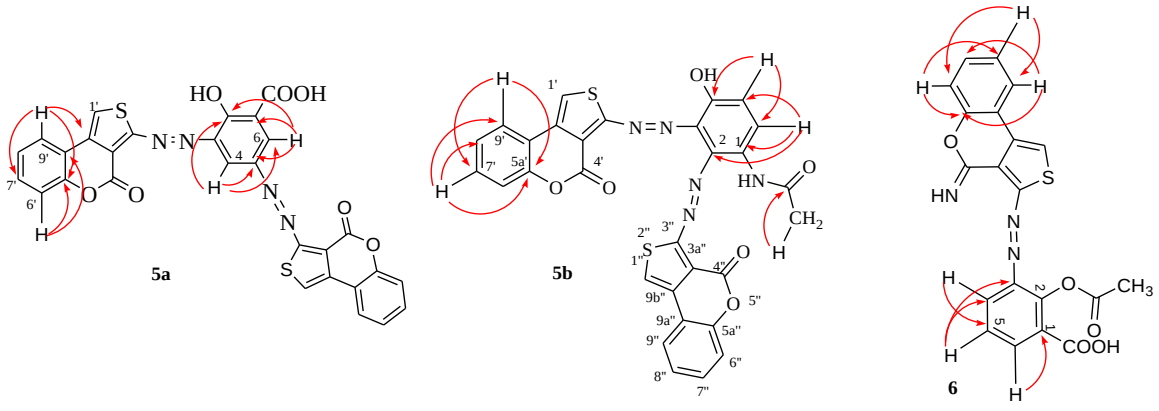


Figure 36. Cyclic voltammograms of 289 µM **6** in 0.05 M H_2SO_4 at various scan rates: 30, 60, 90, 120, 150, and 180 mV/s.

Table 1. Important HMBC interactions and ^{1}H and ^{13}C chemical shifts δ in compounds **5a**, **5b**and **6** in $CDCl_3$/DMSO-d_6 as solvent.



5a			**5b**			**6**		
N°C	δ_C	HMBC (H →C)	N°C	δ_C	HMBC(H →C)	N°C	δ_C	HMBC(H →C)
1’/1’’	125.6	H-9’ (8.80)	1’/1’’	125.6	/	1’	119.7	
3’/3’’	156.9	/	3’/3’’	155.4	/	3’	154.4	
3a’/3a’’	148.7	/	3a’/3a’’	148.6	/	3a’	148.9	/
4’/4’’	162.8	H-1’ (7.70) ; H-6’ (7.35)	4’/4’’	162.9	H-1’ (7,74)	4’	157.3	H-6’ (7.49)
5a’/5a’’	155.4	H-9’ (8.80) ; H-7’ (7.69) ; H-6’(7.35)	5a’/5a’’	155.1	H-9’ (8.82) ; H-7’ (7.71) ; H-6’ (7.39)	5a’	155.5	H-9’ (8.82) ;
6’/6’’	117.7	H-7’ (7,69) ; H-8’ (7,39)	6’/6’’	117.7	H-7’ (7.71) ; H-8’ (7.45)	6’	117,4	H-8’ (7.39)
7’/7’’	135.4	H-9’ (8.80) ; H-8’ (7.39)	7’/7’’	135.4	H-9’ (8.82) ; H-8’ (7.45);	7’	135.6	H-9’ (8.82)
8’/8’’	126.1	7.69 (H-7’) ; H-8’ (7.39)	8’/8’’	126.1	H-7’ (7.71); H-6’ (7.39)	8’	125.4	H-6’ (7.49); H-8’ (7.39)
9’/9’’	129.9	H-1’ (7.70) ; H-7’ (7.69) ; H-8’ (7.39)	9’/9’’	129.9	H-7’ (7.71)	9’	129.9	H-7’ (7.73)
9a’/9a’’	118.2	7.39 (H-8’) ; H-6’ (7.35)	9a’/9a’’	118.2	H-8’ (7.45); H-6’ (7.39)	9a’	115.8	H-8’ (7.39);
9b’/9b’’	153.6	H-9’ (8.80) ; 7.70 (H-1’)	9b’/9b’’	153.3	H-9’ (8.82); H-1’ (7,74);	9b’	155.1	H-1’ (7.40)
1	113.5	H-6 (7.37)	1	154.5	H-6 (7.37)	1	135.8	H-6 (7.88)
2	154.4	H-4 (7.72) ; H-6 (7.37)	2	113.5	H-6 (7.37)	2	154.2	
3	102.4	/	3	102.3	/	3	112.4	H-5 (6.96); H-4 (6.89)
4	117.4	H-6 (7.37)	4	157.5	H-5 (7.73)	4	119.2	H-5 (6.96);
5	119.5	H-6 (7.37) ; H-4 (7.72)	5	117.4	H-6 (7.37)	5	117.3	H-4 (6.89) ;
6	135.5	7.72 (H-4)	6	135.6	H-5 (7.73)	6	130.7	
COOH	185.1	/	C=O		H(CH_3)(2.80)	COOH	184.1	
			CH_3	18.4	/	C=O	161.8	H-6(7.88)
						CH_3	18.2	