## **Supplementary Material**

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

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as solvent	.S21



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



Seite 1 von 1 Figure 2.IR spectrum of compound 5a.



Figure 3.<sup>1</sup>H-NMR (DMSO-d<sub>6</sub>, 300 MHz) spectrum of compound 5a.



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 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 f1 (ppm)

Figure 7.<sup>1</sup>H-NMR (DMSO-d<sub>6</sub>/CDCl<sub>3</sub>, 400 MHz), spectrum of 5a.



Figure 8.<sup>13</sup>C(<sup>1</sup>H) NMR (DMSO-d<sub>6</sub>/CDCl<sub>3</sub>, 100 MHz) Spectraof5a.



Figure 9.HSQC (DMSO-d<sub>6</sub>/CDCl<sub>3</sub>, 100 MHz) spectrum of 5a.



Figure 10.HMBC (DMSO-d<sub>6</sub>/CDCl<sub>3</sub>, 100 MHz) spectrum of 5a.



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







Figure 14. Enlarged <sup>1</sup>H-NMR (DMSO-d<sub>6</sub>, 300 MHz) spectrum of compound **5b**.



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





Figure 17.<sup>13</sup>C(<sup>1</sup>H) NMR (DMSO-d<sub>6</sub>/CDCl<sub>3</sub>, 100 MHz) Spectra of 5b.



Figure 18. HSQC (DMSO-d<sub>6</sub>/CDCl<sub>3</sub>, 100 MHz) spectrum of 5b.



Figure 19. HMBC (DMSO-d<sub>6</sub>/CDCl<sub>3</sub>, 100 MHz) spectrum of 5b.



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



Seite 1 von 1 Figure 21.IR spectrum of compound 5c.



Figure 22.<sup>1</sup>H-NMR (DMSO-d<sub>6</sub>, 500 MHz) spectrum of compound 5c.



**Figure 23.** Enlarged <sup>1</sup>H-NMR (DMSO-d<sub>6</sub>, 500 MHz) spectrum of compound **5c.** 



Figure 24.<sup>13</sup>C(<sup>1</sup>H)-NMR (DMSO-d<sub>6</sub>, 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 30.<sup>13</sup>C(<sup>1</sup>H) NMR (DMSO-d<sub>6</sub>/CDCl<sub>3</sub>, 100 MHz) Spectrum of 6.



Figure 31. HSQC (DMSO-d<sub>6</sub>/CDCl<sub>3</sub>, 100 MHz) spectrum of 6.



Figure32. HMBC (DMSO-d<sub>6</sub>/CDCl<sub>3</sub>, 100 MHz) spectrum of 6.



**Figure 33.** Cyclic voltammograms of 943  $\mu$ M **5a** in 0.05 M H<sub>2</sub>SO<sub>4</sub> at various scan rates: 30, 60, 90, 120, 150, 240, 270 and 300 mV/s.



**Figure 34.** Cyclic voltammograms of 1120  $\mu$ M **5b** in 0.05 M H<sub>2</sub>SO<sub>4</sub> at various scan rates: 30, 60, 90, 120, 150, 180, 270 and 300 mV/s.



Figure 35. Cyclic voltammograms of 268  $\mu$ M 5c in 0.05 M H<sub>2</sub>SO<sub>4</sub> at various scan rates: 30, 60, 90, 120, 150, 180 and 210 mV/s.



**Figure 36.** Cyclic voltammograms of 289  $\mu$ M **6** in 0.05 M H<sub>2</sub>SO<sub>4</sub> at various scan rates: 30, 60, 90, 120, 150, and 180 mV/s.

**Table 1.** Important HMBC interactions and <sup>1</sup>H and <sup>13</sup>C chemical shifts  $\delta$  in compounds **5a**, **5b**and **6** in CDCl<sub>3</sub>/DMSO-d<sub>6</sub> as solvent.



N°C         δc         HMBC (H $\rightarrow$ C)         N°C         δc         HIMBC (H $\rightarrow$ C)         N°C         δc         HIMC (H $\rightarrow$ C)         N°C         δc         I         I         I         I         I         I         I         I         I         N°C         δc         I         I         I         I         N°C         δc         I         I         I         I         I         I         I         I         I         I         I         I         I         I         I         I         I         I         I         I         I         I         I         I         I         I         I         I         I         I         I         I         I         I         I         I         I         I         I         I <thi< th=""> <thi< th=""></thi<></thi<>	5a			5b			6		
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	N°C	δc	HMBC (H →C)	N°C	δc	HMBC(H →C)	N°C	δc	HMBC(H →C)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	1'/1''	125.6	H-9' (8.80)	1'/1''	125.6	/	1'	119.7	
3a'/3a''       148.7       /       3a'/3a''       148.6       /       3a'       3a'       148.9       /         4'/4''       162.8       H-1'(7,70); H-6'       i       162.9       H-1'(7,70); H-6'       i       157.3       H-6'(7.49)         5a'/5a''       155.4       H-9'(8.80); H-7'       5a'/5a'       155.1       H-9'(8.82); H-       5a'       155.5       H-9'(8.82); H-       i       157.3       H-6'(7.49)         5a'/5a''       155.4       H-9'(8.80); H-7'       5a'/5a'       155.1       H-9'(8.82); H-       i       155.5       H-9'(8.82); I         6'/6''       117.7       H-7'(7.69); H-8'       6'/6''       117.7       H-9'(8.82); H-       i       135.6       H-9'(8.82)         7'/7''       135.4       H-9'(8.80); H-8'       7'/7''       135.4       H-9'(8.82); H-       i       135.6       H-9'(8.82)         8'/8''       126.1       7.69 (H-7'); H-8'       8'/8''       126.1       H-7'(7.71); H-8'       8'/7       129.9       H-7'(7.73)       H       8'/7       135.6       H-9'(8.82)       H-9'/7       135.6       H-9'(8.82)       H       8'/7.39)       129.9       H-7'(7.73)       129.9       H-7'(7.73)       129.9       H-7'(7.73)       129.9	3'/3''	156.9	/	3'/3''	155.4	/	3'	154.4	
	3a'/3a''	148.7	/	3a'/3a'	148.6	/	3a'	148.9	/
$\begin{array}{cccccccccccccccccccccccccccccccccccc$				,					
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	4'/4''	162.8	H-1' (7.70) ; H-6'	4'/4''	162.9	H-1' (7,74)	4'	157.3	H-6' (7.49)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	5a'/5a''	155 4	(7.55) H-9' (8 80) · H-7'	5a'/5a'	155 1	H-9' (8 82) · H-	5a'	155 5	H-9' (8 82) ·
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	54754	100.1	(7.69): H-	, ,	100.1	7' (7.71) : H-6'	54	100.0	11 5 (0.02),
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$			6'(7.35)			(7.39)			
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	6'/6''	117.7	H-7' (7,69) ; H-8'	6'/6''	117.7	H-7' (7.71) ; H-	6'	117,4	H-8' (7.39)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$			(7,39)			8' (7.45)			
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	7'/7''	135.4	H-9' (8.80) ; H-8'	7′/7′′	135.4	H-9' (8.82) ; H-	7'	135.6	H-9' (8.82)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$			(7.39)			8' (7.45);			
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	8'/8''	126.1	7.69 (H-7') ; H-8'	8'/8''	126.1	H-7' (7.71); H-	8′	125.4	H-6' (7.49); H-
$\begin{array}{cccccccccccccccccccccccccccccccccccc$			(7.39)			6' (7.39)			8' (7.39)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	9'/9''	129.9	H-1' (7.70) ; H-7'	9'/9''	129.9	H-7' (7.71)	9'	129.9	H-7' (7.73)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$			(7.69) ; H-8'						
$\begin{array}{cccccccccccccccccccccccccccccccccccc$			(7.39)						
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	9a'/9a''	118.2	7.39 (H-8') ; H-6'	9a'/9a'	118.2	H-8' (7.45); H-	9a'	115.8	H-8' (7.39);
9b'/9b"       153.6       H-9' (8.80) ; 7.70       9b'/9b       153.3       H-9' (8.82); H-       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       2       113.5       H-6 (7.37)       2       154.2         2       154.4       H-4 (7.72) ; H-6       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       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         6       135.5       7.72 (H-4)       6       135.6       H-5 (7.73)       6       130.7         6       135.5       7.72 (H-4)       6       135.6       H-5 (7.73)       6       130.7			(7.35)	,		6' (7.39)			
(H-1')       "       1' (7,74);         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       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); H-4 (6.89)         5       119.5       H-6 (7.37); H-4       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)	9b'/9b''	153.6	H-9' (8.80) ; 7.70	9b'/9b	153.3	H-9' (8.82); H-	9b'	155.1	H-1' (7.40)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$			(H-1')	,,		1' (7,74);			
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	1	113.5	H-6 (7.37)	1	154.5	H-6 (7.37)	1	135.8	H-6 (7.88)
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       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 <sub>3</sub> 18.4       /       C=O       161.8       H-6(7.88)         CH <sub>3</sub> 18.4       /       C=O       161.8       H-6(7.88)	2	154.4	H-4 (7.72); H-6	2	113.5	H-6 (7.37)	2	154.2	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$			(7.37)			,			
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       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 <sub>3</sub> 18.4       /       C=O       161.8       H-6(7.88)         CH <sub>3</sub> 18.4       /       C=O       161.8       H-6(7.88)	3	102.4	/	3	102.3	/	3	112.4	H-5 (6.96); H-4
$\begin{array}{cccccccccccccccccccccccccccccccccccc$					4535				(6.89)
5       119.5       H-6 (7.37); H-4       5       117.4       H-6 (7.37)       5       117.3       H-4 (6.89);         (7.72)       (7.72)       6       135.5       7.72 (H-4)       6       135.6       H-5 (7.73)       6       130.7         COOH       185.1       /       C=O       H(CH <sub>3</sub> )(2.80)       COOH       184.1         CH <sub>3</sub> 18.4       /       C=O       161.8       H-6(7.88)         CH <sub>3</sub> 18.4       /       CH <sub>3</sub> 18.2	4	117.4	H-6 (7.37)	4 5	157.5	H-5 (7.73)	4	119.2	H-5 (6.96 );
6       135.5       7.72 (H-4)       6       135.6       H-5 (7.73)       6       130.7         COOH       185.1       /       C=O       H(CH <sub>3</sub> )(2.80)       COOH       184.1         CH <sub>3</sub> 18.4       /       C=O       161.8       H-6(7.88)         CH <sub>3</sub> 18.4       /       C=O       161.8       H-6(7.88)	5	119.5	н-6 (7.37); н-4 (7.72)	5	117.4	н-б(7.37)	5	117.3	H-4 (6.89) ;
COOH 185.1 / C=O H(CH <sub>3</sub> )(2.80) COOH 184.1 CH <sub>3</sub> 18.4 / C=O 161.8 H-6(7.88) CH <sub>3</sub> 18.2	6	135.5	、, 7.72 (H-4)	6	135.6	H-5 (7.73)	6	130.7	
CH <sub>3</sub> 18.4 / C=O 161.8 H-6(7.88) CH <sub>3</sub> 18.2	СООН	185.1	/	C=O		, H(CH₃)(2.80)	соон	184.1	
CH <sub>3</sub> 18.2				CH₃	18.4	/	C=O	161.8	H-6(7.88)
							CH₃	18.2	