Electronic Supplementary Material (ESI) for RSC Advances.

SUPPORTING INFORMATION

Synthesis, Antimicrobial, Anti-Cancer and Molecular Docking of Two Novel Hitherto Unreported Thiophenes

Yahia N. Mabkhot, Nabila AbdelshafyKheder, Assem Barakat, Muhammad I. Choudhary, SammerYousuf and Wolfgang Frey

Table of contents

Part 1: Copies of NMR Spectra

Figure S1:^{1}H NMR of thiophene **3a**

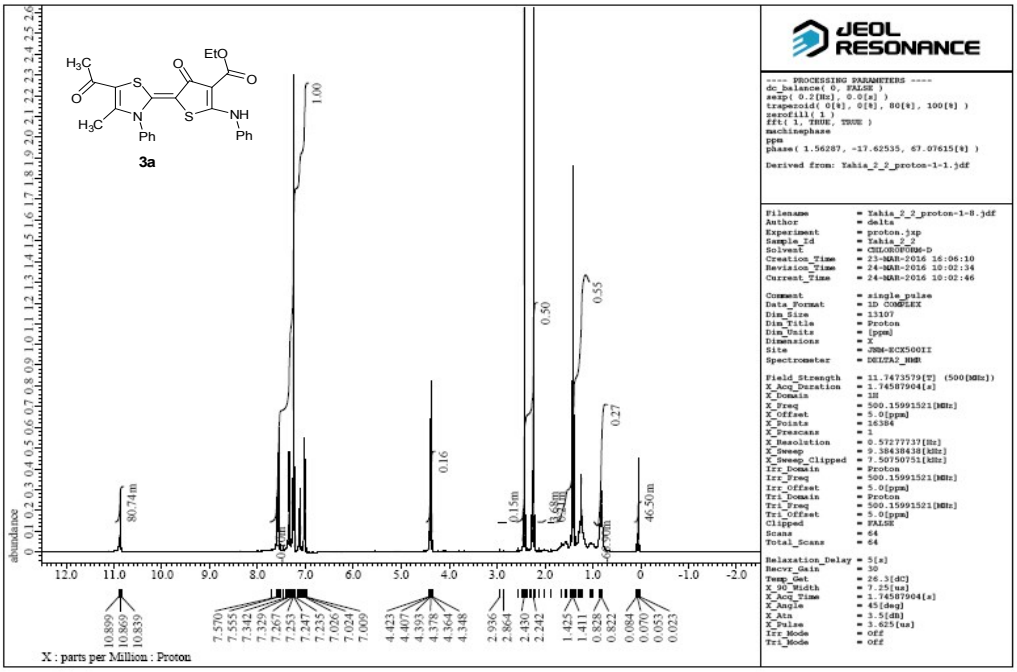


Figure S2:^{13}C NMR of thiophene **3a**

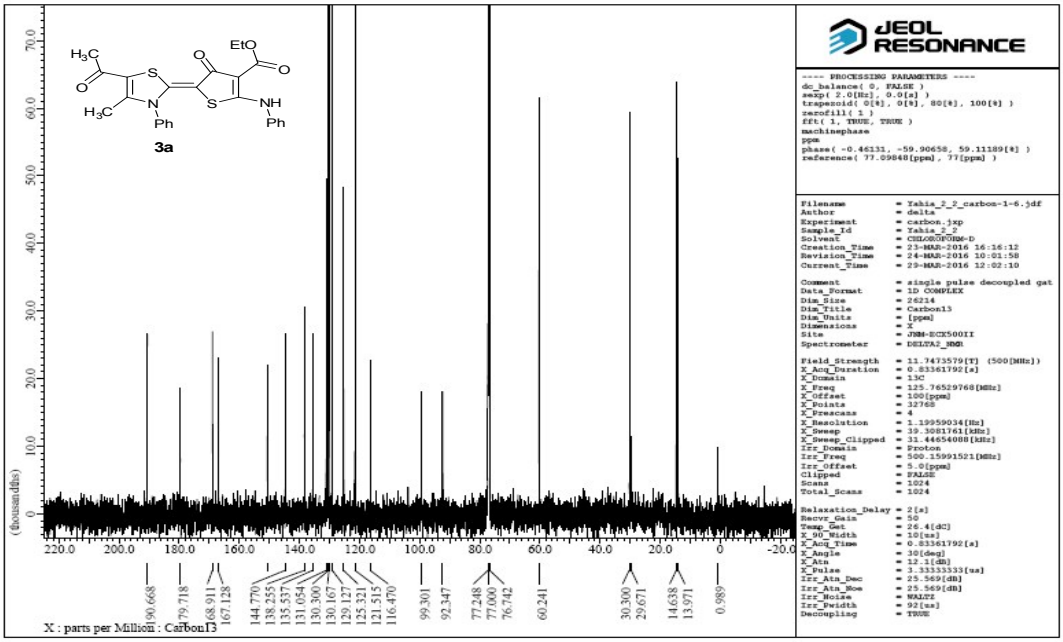


Figure S3: **NOESY** of **3a**

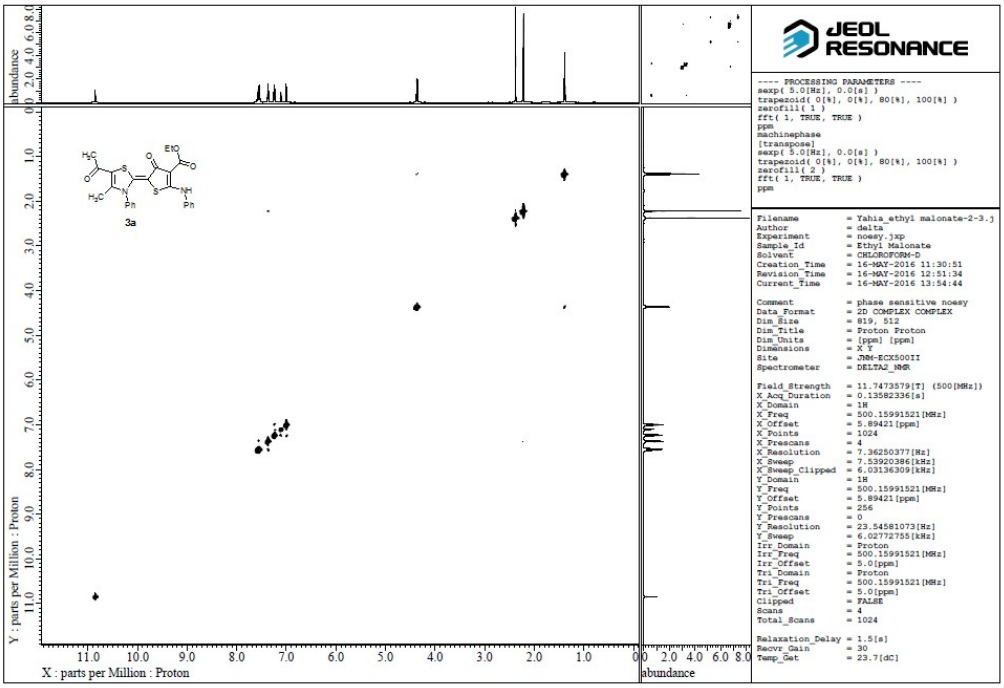


Figure S4:^{1}H NMR of thiophene **3b**

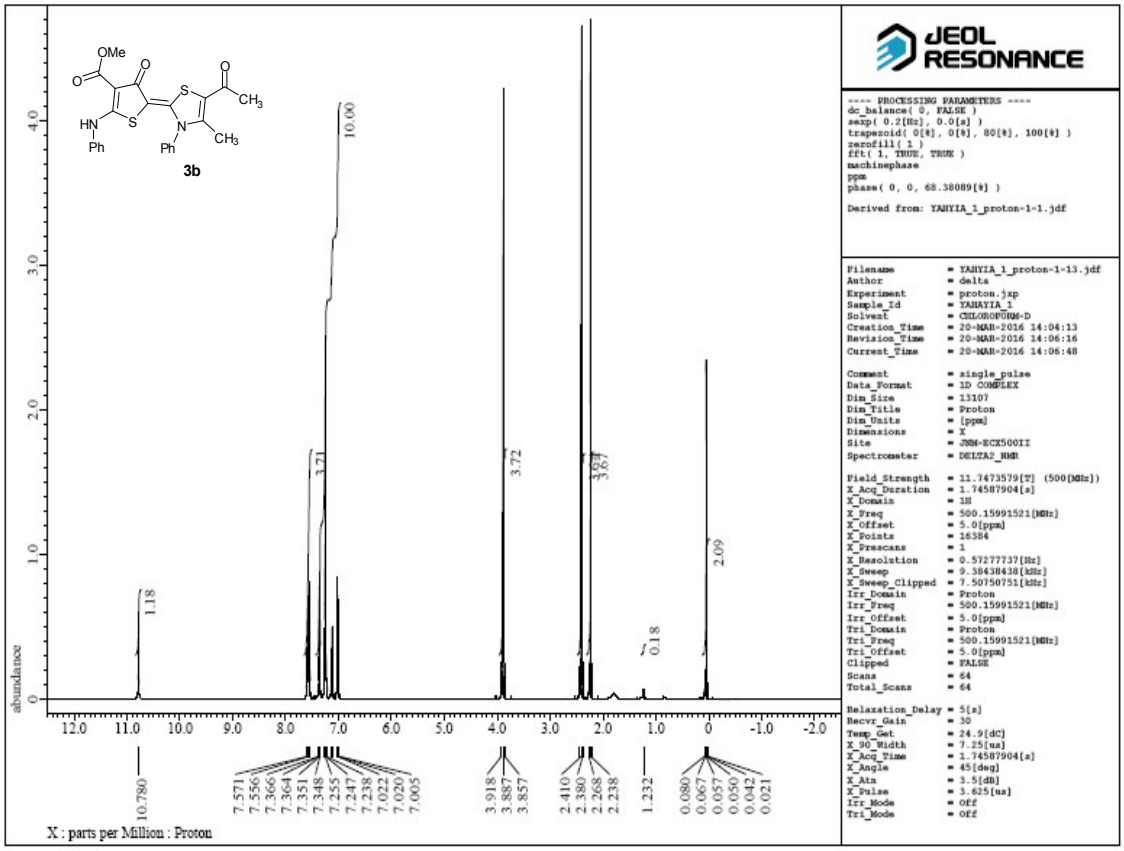


Figure S5:^{13}C NMR of thiophene **3b**

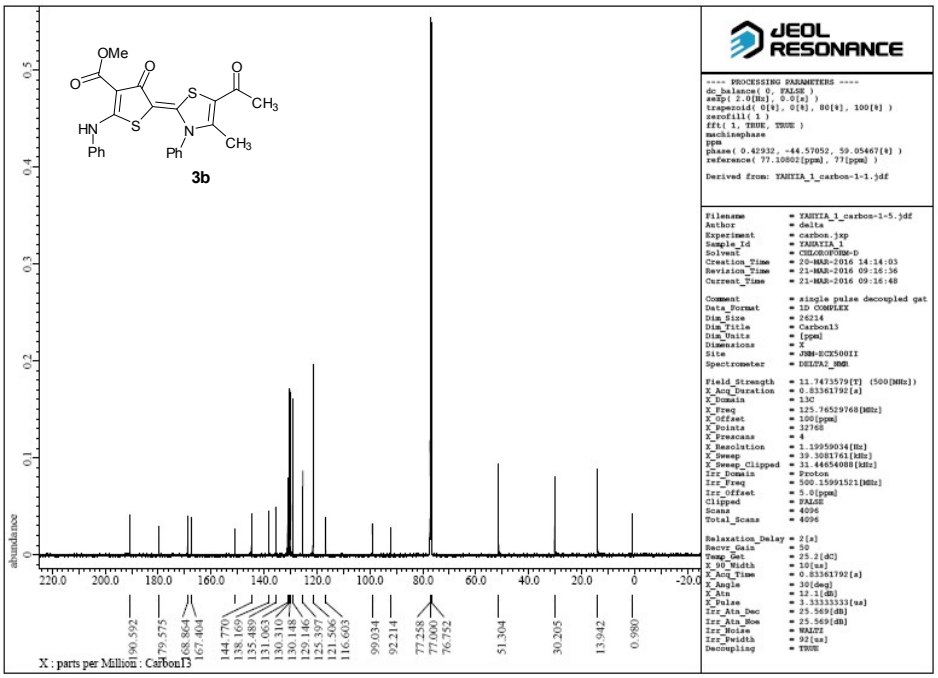
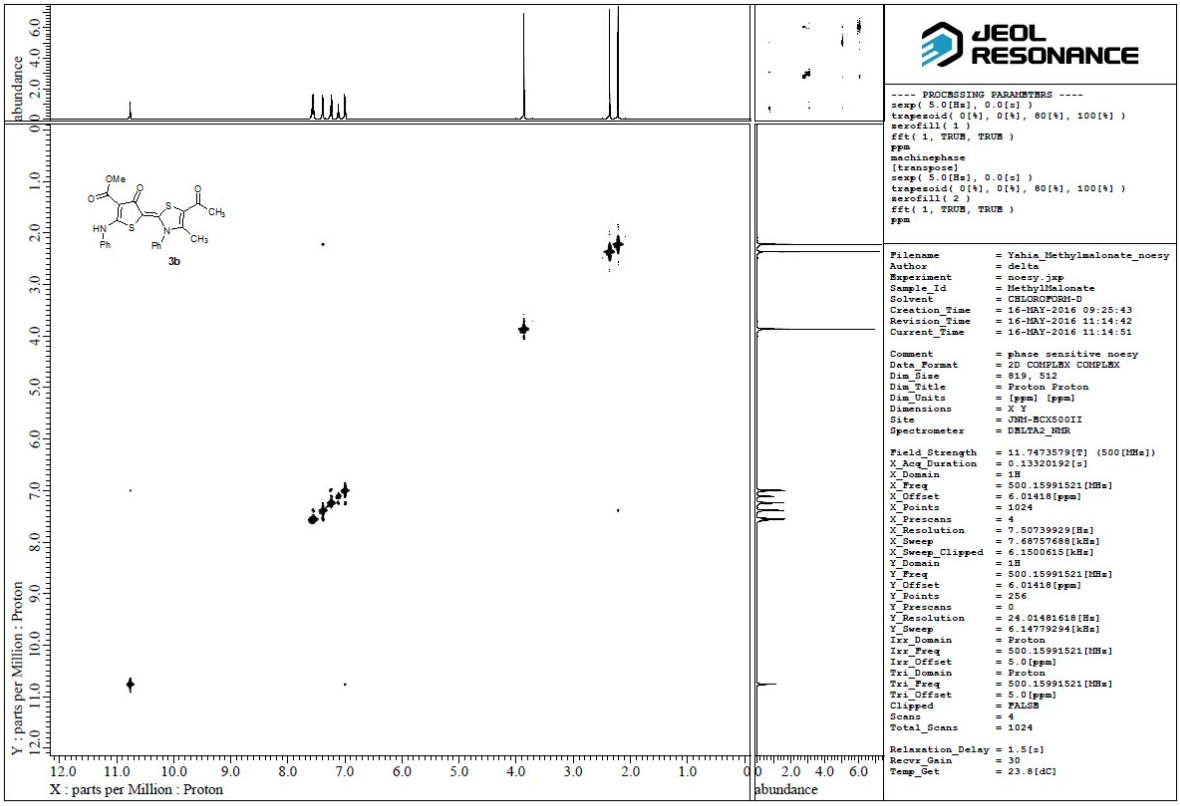
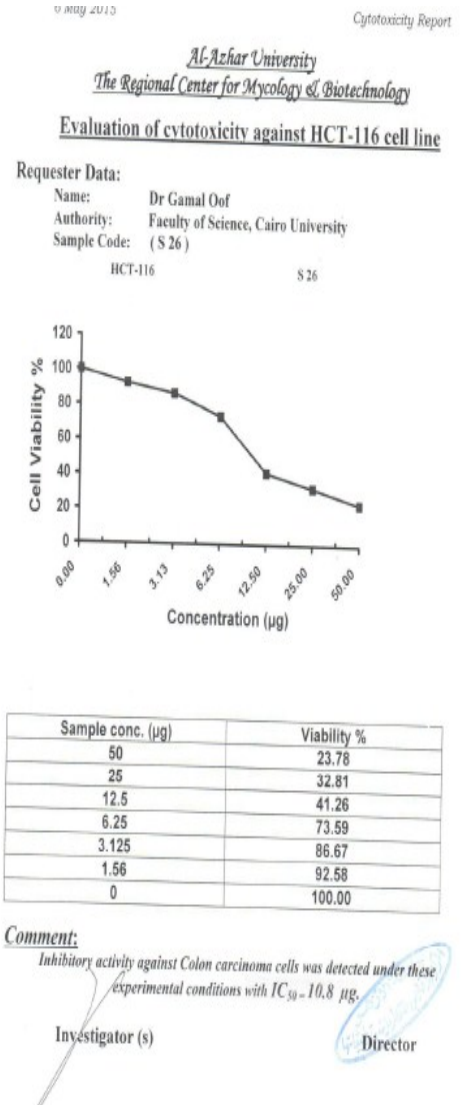


Figure S6: **NOESY** of **3b**



Part 2: Copies of the dose response curve generated for compounds

Figure S7: Dose response curve of thiophene 3a



9 May 2013 Cytotoxicity Report

Al-Azhar University
The Regional Center for Mycology & Biotechnology

Evaluation of cytotoxicity against HCT-116 cell line

Requester Data:

Name: Dr Gamal Oof
Authority: Faculty of Science, Cairo University
Sample Code: (S 26)

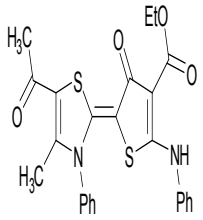
HCT-116 S 26

Sample conc. (µg)	Viability %
50	23.78
25	32.81
12.5	41.26
6.25	73.59
3.125	86.67
1.56	92.58
0	100.00

Comment:

Inhibitory activity against Colon carcinoma cells was detected under these experimental conditions with IC_{50} = 10.8 µg.

Investigator (s) Director



3a

Figure S8: Dose response curve of thiophene 3b

6 May 2015 Cytotoxicity Report

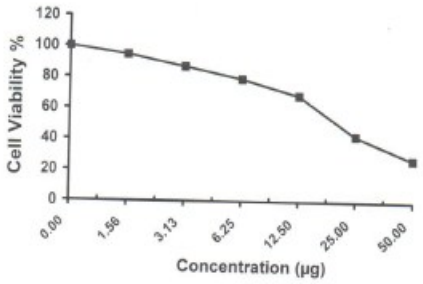
Al-Azhar University
The Regional Center for Mycology & Biotechnology

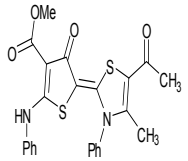
Evaluation of cytotoxicity against HCT-116 cell line

Requester Data:

Name: Dr Gamal Oof
Authority: Faculty of Science, Cairo University
Sample Code: (S 25)

HCT-116 S 25





3b

Sample conc. (µg)	Viability %
50	27.68
25	42.83
12.5	68.72
6.25	79.13
3.125	87.04
1.56	94.65
0	100.00

Comment:

Inhibitory activity against Colon carcinoma cells was detected under these experimental conditions with IC_{50} = 21.5 µg.

Investigator (s) Director

Part 3: Molecular Docking

The binding modes of thiophenes 3a,b with E. coli succinate dehydrogenase protein (PDB:1NEK).

A docking study was performed to fit the synthesized thiophenes **3a,b** into the active center of the E. coli succinate dehydrogenase in order to study the interaction between binding model and bacterial activity, all docking runs using MOE 2008.10. The binding model of compound **3a** with E. Coli Succinate Dehydrogenase protein is presented in Figure S9(A,B). As shown in figure S9(A), there is hydrogen bond interaction between the oxygen atom of the carbonyl group of the acetyl moiety of thiophene **3a**, as it acts as a hydrogen bond acceptor with the side chain of Glu388 (3 Å) with a strength of 12%. This bond enhanced the combination activity of compound **3a**.

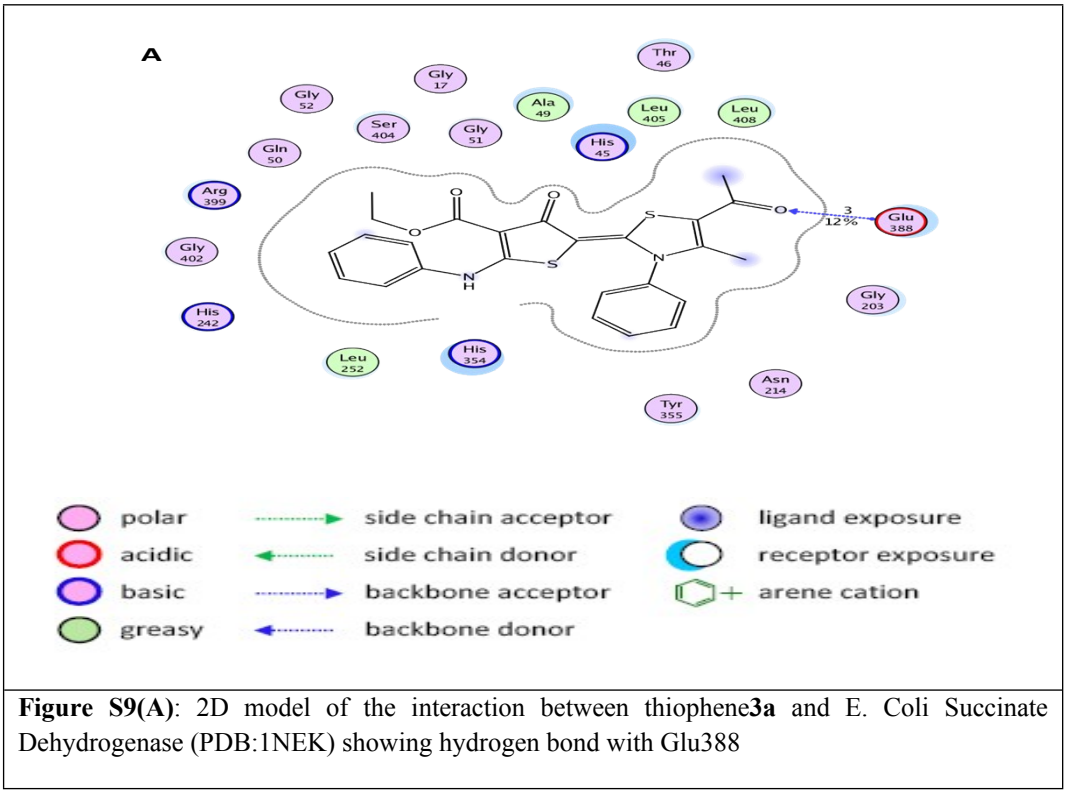


Figure S9(A): 2D model of the interaction between thiophene**3a** and E. Coli Succinate Dehydrogenase (PDB:1NEK) showing hydrogen bond with Glu388

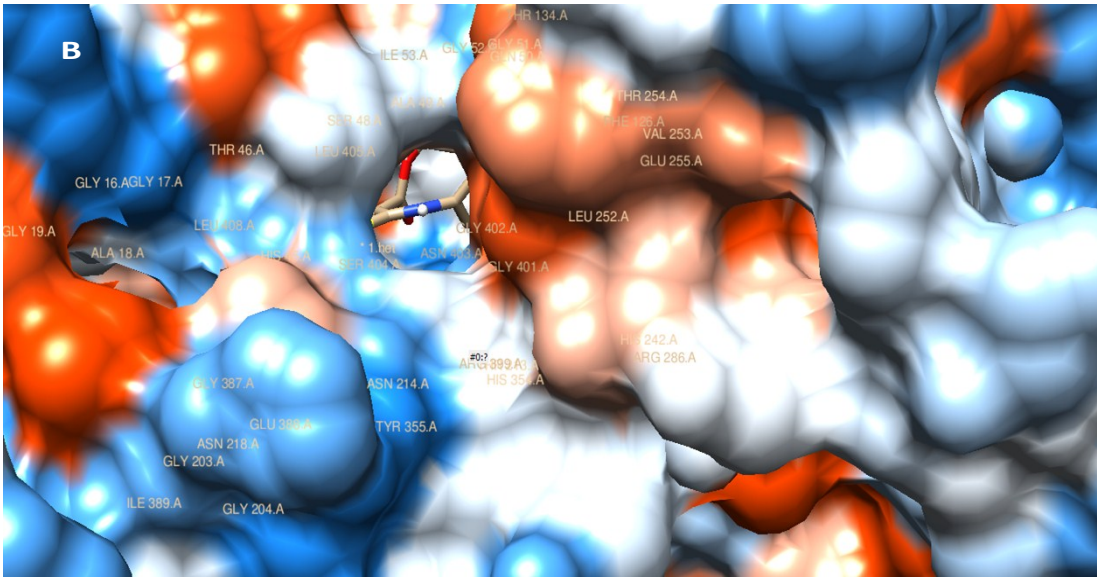


Figure S9(B): 3D model of the interaction between compound **3a** and E. Coli Succinate Dehydrogenase protein indicated that thiophene **3a** was embedded into the E. Coli Succinate Dehydrogenase protein active pocket.

Also, the binding model of compound **3b** with E. coli succinate dehydrogenase protein are presented in figure S10(A,B). In this binding model, compound **3b** was well bound to the E. coli succinate dehydrogenase protein through two hydrogen bonds, the first one between oxygen atom of the carbonyl group of the thiophene ring with His45 residue (2.53 Å) with a strength of 24%, while the second hydrogen bond between the same oxygen atom and Thr213 (2.84 Å) with a strength of 32%

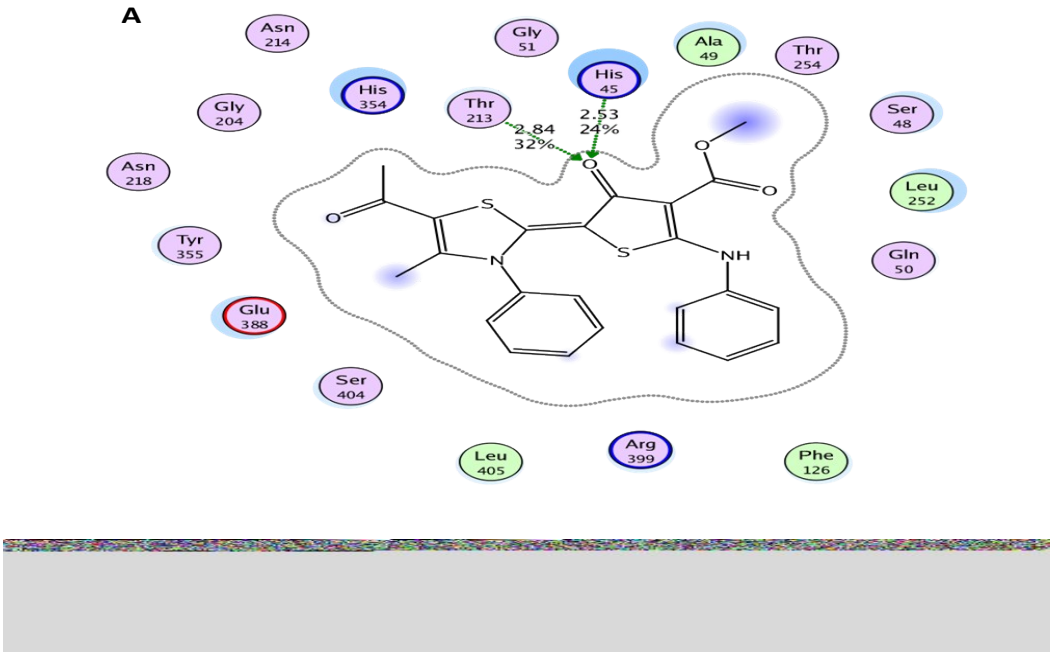


Figure S10(A): 2D model of the interaction between thiophene **3b** and E. Coli Succinate Dehydrogenase (PDB:1NEK) showing two hydrogen bonds with of His45 and Thr213 residues.

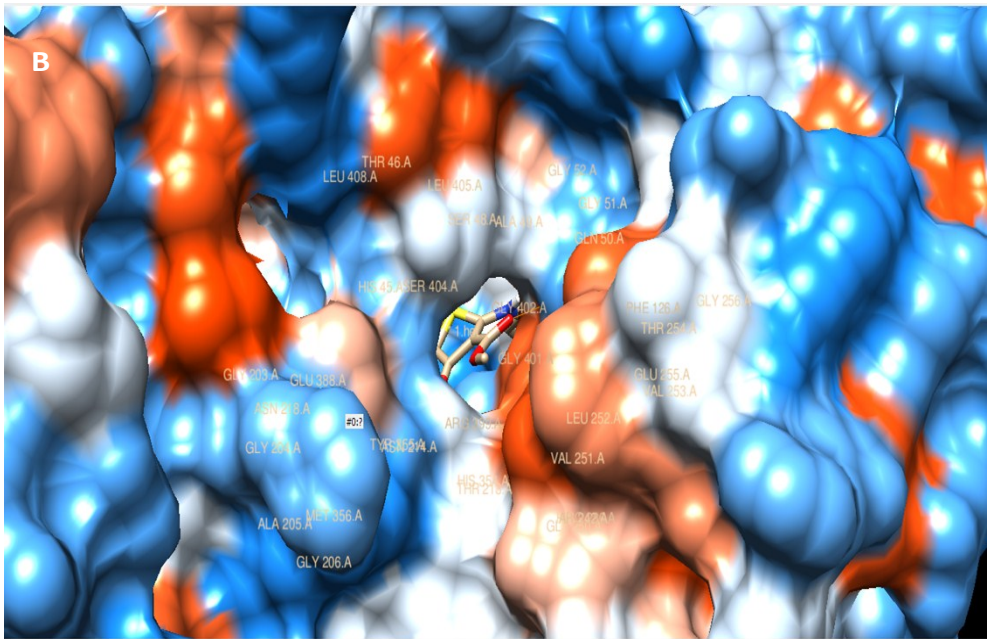


Figure S10(B): 3D model of the interaction between thiophene **3b** and E. Coli Succinate Dehydrogenase protein indicated that **3b** was embedded into the E. Coli Succinate Dehydrogenase protein active pocket.

This result indicated that these two hydrogen bonding interactions with the active site residues of E. coli succinate dehydrogenase might be one of the reasons for the good antibacterial and antifungal activities shown by this compound in the series (table 3,4).

Part 4: X-ray data for the synthesized compound **3a** and **3b**

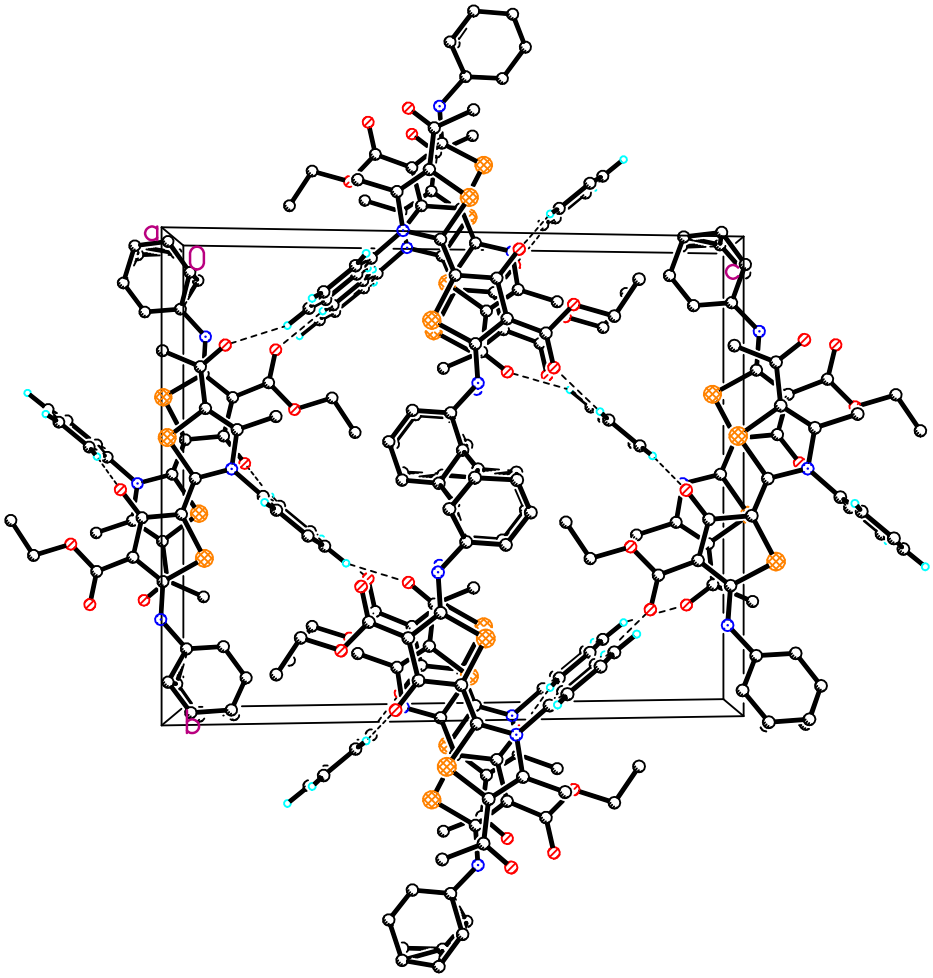


Figure S11: The packing of **3a** molecules in crystal lattice

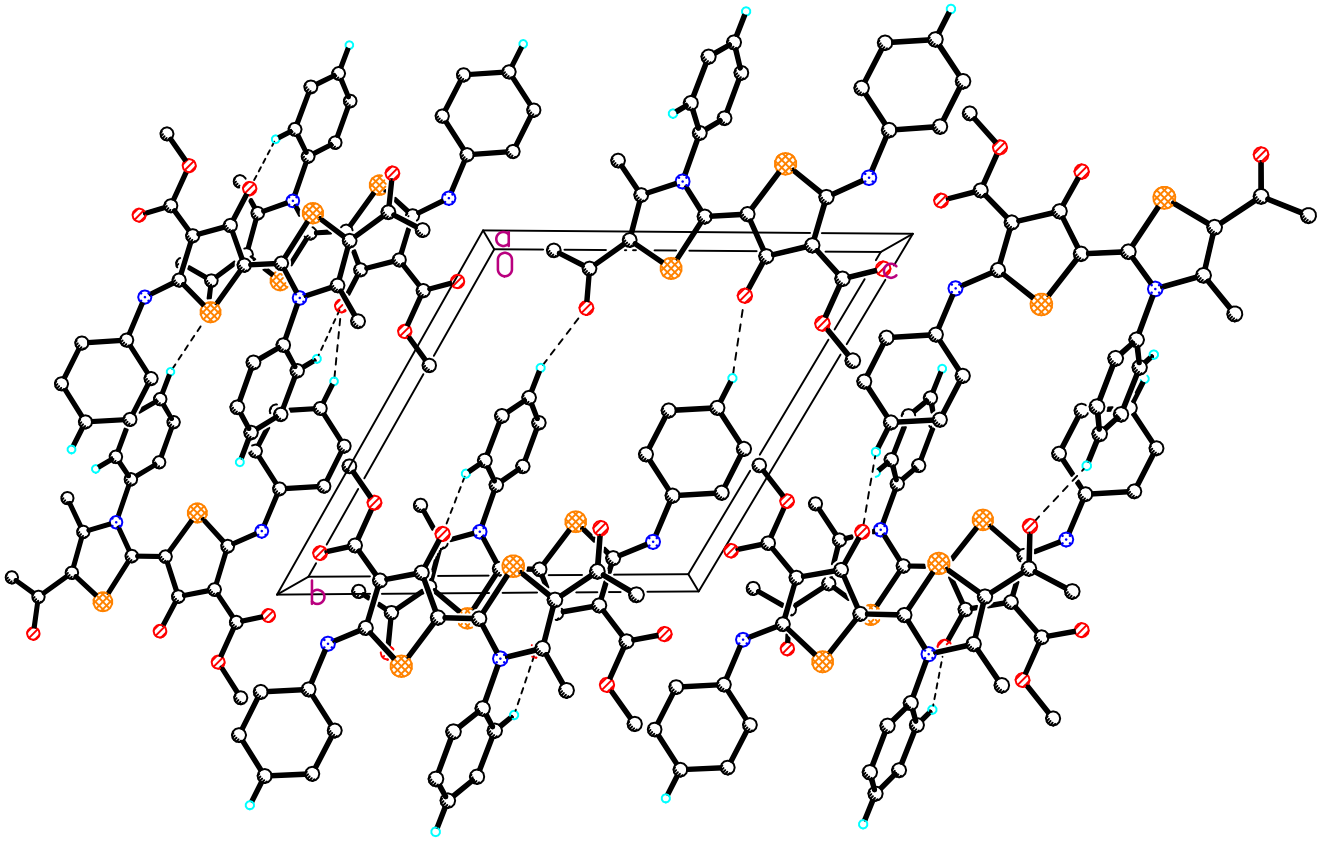


Figure S12: The packing of **3b** molecules in crystal lattice

Table S1. Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2) of **3a**

	X	*Y*	*Z*	U_{iso}*/U_{eq}	Occ. (<1)
S1	2504 (2)	10824 (1)	4807 (1)	18 (1)	
C1	2869 (6)	9955 (3)	5311 (2)	15 (1)	
O1	4332 (6)	12762 (2)	5882 (2)	32 (1)	
N1	3654 (5)	10157 (2)	5972 (2)	16 (1)	
S2	2665 (2)	8255 (1)	5463 (1)	18 (1)	
N2	1572 (6)	6937 (2)	4657 (2)	25 (1)	
O2	1317 (5)	9716 (2)	3938 (2)	26 (1)	
C2	4010 (6)	10985 (3)	6082 (2)	17 (1)	
O3	91 (5)	7240 (2)	3343 (2)	29 (1)	
C3	3475 (6)	11437 (3)	5510 (2)	18 (1)	
C4	3576 (7)	12318 (3)	5423 (2)	21 (1)	
O4	-52 (5)	8542 (2)	2999 (2)	25 (1)	
C5	2715 (7)	12666 (3)	4731 (2)	26 (1)	
C6	4880 (7)	11260 (3)	6781 (2)	25(1)	
C7	3876 (7)	9576 (3)	6533 (2)	19 (1)	
C8	5667 (7)	9293 (3)	6809 (2)	25 (1)	
C9	5810 (9)	8752 (3)	7359 (3)	35 (1)	
C10	4211 (10)	8520 (3)	7622 (3)	38 (1)	
C11	2462 (9)	8814 (3)	7336 (3)	34 (1)	
C12	2277 (7)	9398 (3)	6784 (2)	25 (1)	
C13	2382 (6)	9193 (3)	5051 (2)	1717 (1)	
C14	1583 (6)	9115 (3)	4328 (2)	20 (1)	
C15	1191 (6)	8269 (3)	4150 (2)	18 (1)	
C16	1735 (6)	7752 (3)	4702 (2)	17 (1)	
C17	373 (6)	7956 (3)	3477 (2)	20 (1)	
C18	−788 (8)	8293 (3)	2304 (2)	32 (1)	
C19	−1150 (9)	9047 (3)	1882 (3)	35 (1)	
C20	2202 (12)	6320 (3)	5134 (3)	51 (2)	
C21	2780 (9)	6376 (3)	5803 (3)	38 (1)	
C22	3395 (8)	5724 (3)	6220 (3)	34 (1)	

C23	4095 (17)	5074 (6)	5981 (7)	37 (3)	0.500
C24	4086 (15)	5027 (6)	5277 (7)	35 (2)	0.500
C25	3325 (14)	5651 (6)	4851 (6)	28 (2)	0.500
C23A	2724 (16)	4922 (7)	5982 (6)	32 (2)	0.500
C24A	1578 (15)	4857 (6)	5336 (6)	32 (2)	0.500
C25A	1148 (14)	5541 (6)	4925 (5)	26 (2)	0.500
H2	1050 (80)	6820 (40)	4230 (30)	27 (15)*	
H5A	1385	12498	4612	39(15)*	
H5B	3415	12465	4382	39*	
H5C	2787	13261	4750	39*	
H6A	6236	11131	6866	37*	
H6B	4266	10983	7121	37*	
H6C	4711	11849	6817	37*	
H8	6754	9460	6631	31*	
H9	7016	8539	7558	41*	
H10	4334	8156	8001	46*	
H11	1372	8648	7513	41*	
H12	1071	9573	6587	30*	
H18A	−1979	7982	2287	38*	
H18B	142	7943	2127	38*	
H19A	−2126	9373	2046	52*	
H19B	−1585	8900	1400	52*	
H19C	24	9364	1924	52*	
H21	2772	6897	6010	46*	
H22	3307	5749	6693	41*	
H23	4598	4644	6280	44*	0.500
H24	4605	4464	5090	41*	0.500
H25	3497	5665	4386	34*	0.500
H23A	3057	4454	6260	39*	0.500
H24A	1088	4342	5176	38*	0.500
H25A	209	5517	4521	31*	0.500

Table S2:Fractional atomic coordinates and isotropic or equivalent isotropic displacement paramet
of **3b** ($Å^2$)

	X	*Y*	*Z*	U_{iso}*/U_{eq}	Occ. (<1)
S1	2504 (2)	10824 (1)	4807 (1)	18 (1)	
C1	2869 (6)	9955 (3)	5311 (2)	15 (1)	
O1	4332 (6)	12762 (2)	5882 (2)	32 (1)	
N1	3654 (5)	10157 (2)	5972 (2)	16 (1)	
S2	2665 (2)	8255 (1)	5463 (1)	18 (1)	
N2	1572 (6)	6937 (2)	4657 (2)	25 (1)	
O2	1317 (5)	9716 (2)	3938 (2)	26 (1)	
C2	4010 (6)	10985 (3)	6082 (2)	17 (1)	
O3	91 (5)	7240 (2)	3343 (2)	29 (1)	
C3	3475 (6)	11437 (3)	5510 (2)	18 (1)	
C4	3576 (7)	12318 (3)	5423 (2)	21 (1)	
O4	-52 (5)	8542 (2)	2999 (2)	25 (1)	
C5	2715 (7)	12666 (3)	4731 (2)	26 (1)	
C6	4880 (7)	11260 (3)	6781 (2)	25(1)	
C7	3876 (7)	9576 (3)	6533 (2)	19 (1)	
C8	5667 (7)	9293 (3)	6809 (2)	25 (1)	
C9	5810 (9)	8752 (3)	7359 (3)	35 (1)	
C10	4211 (10)	8520 (3)	7622 (3)	38 (1)	
C11	2462 (9)	8814 (3)	7336 (3)	34 (1)	
C12	2277 (7)	9398 (3)	6784 (2)	25 (1)	
C13	2382 (6)	9193 (3)	5051 (2)	1717 (1)	
C14	1583 (6)	9115 (3)	4328 (2)	20 (1)	
C15	1191 (6)	8269 (3)	4150 (2)	18 (1)	
C16	1735 (6)	7752 (3)	4702 (2)	17 (1)	
C17	373 (6)	7956 (3)	3477 (2)	20 (1)	
C18	−788 (8)	8293 (3)	2304 (2)	32 (1)	
C19	−1150 (9)	9047 (3)	1882 (3)	35 (1)	
C20	2202 (12)	6320 (3)	5134 (3)	51 (2)	
C21	2780 (9)	6376 (3)	5803 (3)	38 (1)	
C22	3395 (8)	5724 (3)	6220 (3)	34 (1)	
C23	4095 (17)	5074 (6)	5981 (7)	37 (3)	0.500
C24	4086 (15)	5027 (6)	5277 (7)	35 (2)	0.500
C25	3325 (14)	5651 (6)	4851 (6)	28 (2)	0.500

C23A	2724 (16)	4922 (7)	5982 (6)	32 (2)	0.500
C24A	1578 (15)	4857 (6)	5336 (6)	32 (2)	0.500
C25A	1148 (14)	5541 (6)	4925 (5)	26 (2)	0.500
H2	1050 (80)	6820 (40)	4230 (30)	27 (15)*	
H5A	1385	12498	4612	39(15)*	
H5B	3415	12465	4382	39*	
H5C	2787	13261	4750	39*	
H6A	6236	11131	6866	37*	
H6B	4266	10983	7121	37*	
H6C	4711	11849	6817	37*	
H8	6754	9460	6631	31*	
H9	7016	8539	7558	41*	
H10	4334	8156	8001	46*	
H11	1372	8648	7513	41*	
H12	1071	9573	6587	30*	
H18A	−1979	7982	2287	38*	
H18B	142	7943	2127	38*	
H19A	−2126	9373	2046	52*	
H19B	−1585	8900	1400	52*	
H19C	24	9364	1924	52*	
H21	2772	6897	6010	46*	
H22	3307	5749	6693	41*	
H23	4598	4644	6280	44*	0.500
H24	4605	4464	5090	41*	0.500
H25	3497	5665	4386	34*	0.500
H23A	3057	4454	6260	39*	0.500
H24A	1088	4342	5176	38*	0.500
H25A	209	5517	4521	31*	0.500

Table S3:Atomic displacement parameters of **3a** (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	23 (1)	16(1)	13 (1)	1 (1)	-2 (1)	0 (1)
C1	16 (2)	19 (2)	11 (2)	4 (2)	4 (1)	0 (1)
O1	53 (2)	15 (2)	25 (2)	-5 (2)	-2 (2)	-3 (1)

N1	20 (2)	16 (2)	13 (2)	1 (1)	2 (1)	0 (1)
S2	22 (1)	15 (1)	16 (1)	-1 (1)	2 (1)	0 (1)
N2	37 (2)	14 (2)	21 (2)	-1 (2)	0 (2)	-2 (2)
O2	38 (2)	21 (2)	17 (2)	0 (1)	4 (1)	2 (14)
C2	20 (2)	17 (2)	16 (2)	-2 (2)	4 (2)	-5 (2)
O3	37 (2)	21 (2)	26 (2)	-1 (1)	2 (2)	-6 (1)
C3	19 (2)	17 (2)	17 (2)	1 (2)	1 (2)	−4 (2)
C4	24 (2)	19 (2)	21 (2)	1 (2)	7 (2)	3 (2)
O4	33 (2)	25 (2)	15 (2)	0 (1)	-2 (1)	-6 (1)
C5	27 (2)	24 (2)	26 (2)	1 (2)	3 (2)	8 (2)
C6	37 (3)	20 (2)	15 (2)	-5 (2)	0 (2)	−4 (2)
C7	27 (2)	15 (2)	13 (2)	1 (2)	1 (2)	1 (1)
C8	32 (3)	23 (2)	19 (2)	3 (2)	-1 (2)	-1 (2)
C9	52 (3)	21 (2)	24 (2)	11 (2)	-11 (2)	1 (2)
C10	76 (4)	19 (2)	16 (2)	4 (3)	-1 (2)	4 (2)
C11	56 (3)	25 (2)	23 (2)	-2 (2)	11 (2)	3 (2)
C12	30 (2)	25 (2)	20 (2)	0 (2)	5 (2)	2 (2)
C13	22 (2)	15 (2)	14 (2)	-1 (2)	3 (2)	3 (1)
C14	23 (2)	20 (2)	16 (2)	2 (2)	0 (2)	-6 (2)
C15	21 (2)	18 (2)	16 (2)	3 (2)	1 (2)	-4 (2)
C16	16 (2)	18 (2)	18 (2)	0 (2)	3 (2)	−3 (2)
C17	18 (2)	22 (2)	21 (2)	4 (2)	4 (2)	-5 (2)
C18	43 (3)	34 (3)	18 (2)	-1 (2)	1 (2)	−9 (2)
C19	51 (3)	34 (3)	19 (2)	3 (2)	4 (2)	-3 (2)
C20	96 (6)	18 (2)	30 (3)	7(3)	-12 (3)	-1 (2)
C21	57 (4)	19 (2)	34 (3)	-4 (2)	-5 (3)	-3 (2)
C22	40 (3)	33 (3)	30 (3)	-2 (2)	5 (2)	9 (2)
C23	37 (6)	19 (5)	52 (7)	3 (4)	0 (5)	8 (5)
C24	29 (5)	15 (4)	62 (6)	5 (4)	12 (5)	4 (4)
C25	21 (4)	24 (5)	42 (6)	-5 (4)	13 (4)	-2 (4)
C23A	32 (6)	28 (5)	40 (6)	8(4)	13 (5)	5 (4)
C24A	27 (5)	20 (4)	52 (6)	-4 (4)	14 (5)	-6 (4)
C25A	25 (5)	22 (4)	31 (5)	-5 (4)	5 (4)	-7 (4)

Table S4:Geometric parameters of **3a** (Å, °)

S1—C1	1.737 (4)	C11—C12	1.401 (7)
S1—C3	1.759 (4)	C11—H11	0.9500
C1—N1	1.370 (5)	C12—H12	0.9500
C1—C13	1.375 (6)	C13—C14	1.448(6)
O1—C4	1.215 (6)	C14—C15	1.451 (6)
N1—C2	1.394 (5)	C15—C16	1.384 (6)
N1—C7	1.451 (5)	C15—C17	1.451 (6)
S2—C13	1.740 (4)	C18—C19	1.492 (8)
S2—C16	1.744 (4)	C18—H18A	0.9900
N2—C16	1.347 (6)	C18—H18B	0.9900
N2—C20	1.404 (7)	C19—H19A	0.9800
N2—H2	0.88 (6)	C19—H19B	0.9800
O2—C14	1.248 (5)	C19—H19C	0.9800
C2—C3	1.352 (6)	C20—C21	1.319(8)
C2—C6	0.484(6)	C20—C25A	1.508(11)
O3—C17	1.216 (6)	C20—C25	1.527(12)
C3—C4	1.462 (6)	C21—C22	1.376(7)
C4—C5	1.512 (6)	C21—H21	0.9500
O4—C17	1.347 (6)	C22—C23	1.305(13)
O4—C18	1.442 (5)	C22—C23A	1.453(13)
C5—H5A	0.9800	C22—H22	0.9500
C5—H5B	0.9800	C23—C24	1.396(18)
C5—H5C	0.9800	C23—H23	0.9500
C6—H6A	0.9800	C24—C25	1.377(15)
C6—H6B	0.9800	C24—C24#1	1.85(2)
C6—H6C	0.9800	C24—H24	0.9500
C7—C12	1.375 (7)	C25—H25	0.9500
C7—C8	1.383 (7)	C23A—C24A	1.396(16)
C8—C9	1.396 (7)	C23A—H23A	0.9500
C8—H8	0.9500	C24A—C25A	1.390(15)
C9—C10	1.393(9)	C24A—C25A#2	2.037(14)
C9—H9	0.9500	C24A—H24A	0.9500
C10—C11	1.369(9)	C25A—C24A#2	2.037(14)
C10—H10	0.9500	C25A—H25A	0.9500

C1—S1—C3	91.1 (2)	N2—C16—C15	123.3 (4)
N1—C1—C13	127.8 (4)	N2—C16—S2	123.0 (3)
N1—C1—S1	110.0 (3)	C15—C16—S2	113.6 (3)
C13—C1—S1	122.1 (3)	O3—C17—O4	122.0 (4)
C1—N1—C2	114.7 (3)	O3—C17—C15	124.7 (4)
C1—N1—C7	122.7 (4)	O4—C17—C15	113.3(4)
C2—N1—C7	122.2 (3)	O4—C18—C19	107.2(4)
C13—S2—C16	91.2 (2)	O4—C18—H18A	110.3
C16—N2—C20	131.3 (4)	C19—C18—H18A	110.3
C16—N2—H2	107 (4)	O4—C18—H18B	110.3
C20—N2—H2	121 (4)	C19—C18—H18B	110.3
C3—C2—N1	113.0 (4)	H18A—C18—H18B	108.5
C3—C2—C6	128.5 (4)	C18—C19—H19A	109.5
N1—C2—C6	118.5 (4)	C18—C19—H19B	109.5
C2—C3—C4	129.1 (4)	H19A—C19—H19B	109.5
C2—C3—S1	111.1 (3)	C18—C19—H19C	109.5
C4—C3—S1	119.8 (3)	H19A—C19—H19C	109.5
O1—C4—C3	122.2 (4)	H19B—C19—H19C	109.5
O1—C4—C5	120.4 (4)	C21—C20—N2	129.1(5)
C3—C4—C5	117.4 (4)	C21—C20—C25A	112.8(6)
C17—O4—C18	117.8 (4)	N2—C20—C25A	110.1(6)
C4—C5—H5A	109.5	C21—C20—C25	109.0(7)
C2—C5—H5B	109.5	N2—C20—C25	113.7(6)
H5A—C5—H5B	109.5	C25A—C20—C25	63.8(6)
C4—C5—H5C	109.5	C20—C21—C22	123.9(5)
H5A—C5—H5C	109.5	C20—C21—H21	118.1
H5B—C5—H5C	109.5	C22—C21—H21	118.1
C2—C6—H6A	109.5	C23—C22—C21	121.7(7)
C2—C6—H6B	109.5	C23—C22—C23A	42.7(7)
H6A—C6—H6B	109.5	C21—C22—C23A	117.5(6)
C2—C6—H6C	109.5	C23—C22—H22	119.2
H6A—C6—H6C	109.5	C21—C22—H22	119.2
H6B—C6—H6C	109.5	C23A—C22—H22	106.3
C12—C7—C8	123.0 (4)	C22—C23—C24	118.1(9)

C12—C7—N1	117.5 (4)	C22—C23—H23	120.9
C8—C7—N1	119.5 (4)	C24—C23—H23	120.9
C7—C8—C9	117.2 (5)	C25—C24—C23	120.1(10)
C7—C8—H8	121.4	C25—C24—C24#1	85.4(9)
C9—C8—H8	121.4	C23—C24—C24#1	135.6(12)
C10—C9—C8	120.9 (5)	C25—C24—H24	120.0
C10—C9—H9	119.5	C23—C24—H24	120.0
C8—C9—H9	119.5	C24#1—C24—H24	50.6
C11—C10—C9	120.1(5)	C24—C25—C20	119.3(9)
C11—C10—H10	119.9	C24—C25—H25	120.3
C9—C10—H10	119.9	C20—C25—H25	120.3
C10—C11—C12	120.1 (6)	C24A—C23A—C22	118.2(9)
C10—C11—H11	119.9	C24A—C23A—H23A	120.9
C12—C11—H11	119.9	C22—C23A—H23A	120.9
C7—C12—C11	118.6(5)	C25A—C24A—H23A	120.5(9)
C7—C12—H12	120.7	C25A—C24A—C25A#2	90.5(7)
C11—C12—H12	120.7	C23A—C24A—H25A#2	129.7(9)
C1—C13—C14	118.7 (4)	C25A—C24A—H24A	119.7
C1—C13—S2	129.1 (3)	C23A—C24A—H24A	119.7
C14—C13—S2	112.2 (3)	C25A#2—C24A—H24A	49.3
O2—C14—C13	122.1(4)	C24A—C25A—C20	118.6(8)
O2—C14—C15	127.4 (4)	C24A—C25A—C24A#2	89.5(8)
C13—C14—C15	110.5(4)	C20—C25A—C24A#2	138.9(7)
C16—C15—C17	121.2(4)	C24A—C25A—H25A	120.7
C16—C15—C14	112.5(4)	C20—C25A—H25A	120.7
C17—C15—C14	126.3(4)	C24A#2—C25A—H25A	43.1

Table S5:Hydrogen-bond geometry of **3a**(Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O3	0.88 (6)	1.90 (6)	2.676 (5)	146 (6)
C6—H6*C*···O1	0.98	2.36	3.028 (6)	125
C8—H8···O2^{i}	0.95	2.36	3.262 (6)	159
C10—H10···O1^{ii}	0.95	2.34	3.210 (7)	152
C11—H11···O3^{iii}	0.95	2.49	3.325 (7)	146
C12—H12···O2^{iv}	0.95	2.18	3.113 (6)	167

C21—H21···S2	0.95	2.48	3.161 (5)	129

Symmetry codes: (i) −*x*+1, −*y*+2, −*z*+1; (ii) −*x*+1, *y*−1/2, −*z*+3/2; (iii) *x*, −*y*+3/2, *z*+1/2; (iv) −*x*, −*y*+2, −*z*+1.

Table S6:Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters of **3b** (Å^2)

	x	*Y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
S1	1563 (1)	1963 (1)	3926 (1)	44 (1)	
S2	2404 (1)	-875 (1)	5184 (1)	42 (1)	
O1	-2418 (3)	-1065 (2)	334 (1)	68 (1)	
O2	-2097 (3)	-2515 (2)	966 (2)	56 (1)	
O3	305 (3)	-1696 (2)	3078 (2)	54 (1)	
O4	3509 (3)	-1953 (2)	6670 (3)	68 (1)	
N1	-582 (3)	1457 (3)	1834 (3)	45 (1)	
C1	34 (3)	970 (3)	2538 (3)	39 (1)	
C2	-446 (3)	-355 (3)	2216 (3)	38 (1)	
C3	450 (3)	-616 (3)	3117 (3)	39 (1)	
C4	1607 (3)	589 (3)	4124 (3)	39 (1)	
C5	2562 (3)	576 (3)	5104 (3)	37 (1)	
C6	3731 (3)	1611 (2)	6125 (2)	**25 (1)**	
C7	4543 (3)	1280 (3)	6939 (3)	42 (1)	
C8	3962 (3)	-16 (3)	6585 (3)	43 (1)	
C9	4331 (4)	-807 (3)	7162 (3)	50 (1)	
C10	5686 (5)	-234 (4)	8319 (4)	74 (1)	
C11	5908 (4)	2335 (3)	8014 (3)	62 (1)	
C12	-1718 (4)	-1307 (3)	1100 (3)	44 (1)	
C13	-3278 (5)	-3535 (3)	-189 (4)	75 (1)	
C14	-237 (3)	2748 (3)	2009 (3)	42 (1)	
C15	321 (4)	3901 (3)	3208 (3)	54 (1)	
C16	619 (4)	5127 (3)	3272 (4)	63 (1)	
C17	330 (4)	5205 (4)	2161 (5)	68 (1)	
C18	-269 (5)	4057 (4)	967 (4)	69 (1)	
C19	−546 (4)	2830 (3)	890 (3)	56 (1)	
C20	4010 (3)	2972 (3)	6389 (3)	38 (1)	

C21	5220 (3)	3495 (3)	6013 (3)	44 (1)
C22	5458 (4)	4772 (3)	6239 (3)	54 (1)
C23	4500 (4)	5507 (3)	6826 (3)	55 (1)
C24	3309 (4)	4976 (3)	7207 (3)	50 (1)
C25	3050 (3)	3700 (3)	6995 (3)	42 (1)
H10A	5753	-896	8559	111
H10B	5546	529	9041	111
H10C	6623	29	8096	111
H11A	6359	1971	8496	93
H11B	5576	3071	8592	93
H11C	6665	2638	7644	93
H13A	-3464	-4363	-192	112
H13B	-2939	-3640	-953	112
H13C	-4218	-3279	-191	112
H15A	497	3858	3970	64
H16A	1021	5906	4081	75
H17A	539	6032	2214	81
H18A	-488	4106	211	83
H19A	-943	2054	79	67
H21A	5862	2990	5613	53
H22A	6270	5142	5996	64
H23A	4656	6368	6966	66
H24A	2673	5485	7611	60
H25A	2250	3338	7254	51
H1A	-1240 (40)	900 (30)	1230 (30)	51 (10)

Table S7:Atomic displacement parameters of **3b** (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	47 (1)	30 (1)	46 (1)	5 (1)	-8 (1)	21 (1)
S2	50 (1)	31 (1)	47 (1)	13 (1)	3 (1)	22 (1)
O1	75 (2)	52 (1)	59(2)	4 (1)	-23 (1)	27 (1)
O2	63 (2)	37 (1)	47 (1)	-4 (1)	-7 (1)	16 (1)
O3	63 (2)	30 (1)	58 (1)	7 (1)	-8 (1)	23 (1)
O4	88 (2)	52 (2)	79 (2)	26 (1)	11 (2)	45 (1)

N1	50 (2)	37 (1)	42 (2)	6 (1)	-8 (1)	22 (1)
C1	40 (2)	35 (2)	38 (2)	10 (1)	3 (1)	19 (1)
C2	42 (2)	33 (2)	34 (2)	8 (1)	1 (1)	16 (1)
C3	42 (2)	30 (2)	41 (2)	10 (1)	4 (1)	16 (1)
C4	43 (2)	30 (1)	43 (2)	9 (1)	2 (1)	20 (1)
C5	40 (2)	32 (2)	41 (2)	15 (1)	8 (1)	20 (1)
C6	29 (1)	17 (1)	26 (1)	7 (1)	-3 (1)	11 (1)
C7	45 (2)	40 (2)	41 (2)	14 (1)	2 (1)	20 (1)
C8	47 (2)	42 (2)	43 (2)	18 (1)	4 (1)	23 (1)
C9	68 (2)	48 (2)	48 (2)	32 (2)	16 (2)	29 (2)
C10	92 (3)	72 (3)	68 (2)	33 (2)	-2 (2)	45 (2)
C11	65 (2)	53 (2)	55 (2)	9 (2)	-13 (2)	26 (2)
C12	51 (2)	36 (2)	39 (2)	9 (1)	3 (1)	17 (1)
C13	74 (3)	47 (2)	57 (2)	-12 (2)	-14 (2)	8 (2)
C14	41 (2)	36 (2)	54 (2)	13(1)	6 (1)	26 (1)
C15	56 (2)	43 (2)	58 (2)	18 (2)	2 (2)	25 (2)
C16	51 (2)	39 (2)	88 (3)	14 (2)	9 (2)	26 (2)
C17	64 (2)	52 (2)	112 (3)	21 (2)	34 (2)	56 (2)
C18	88 (3)	66 (2)	85 (3)	28 (2)	32 (2)	57 (2)
C19	68 (2)	52 (2)	58 (2)	20 (2)	16 (2)	35 (2)
C20	38 (2)	31 (1)	37 (2)	8 (1)	-5 (1)	15 (1)
C21	42 (2)	45 (2)	47 (2)	11 (1)	7 (1)	24 (1)
C22	46 (2)	57 (2)	62 (2)	6 (2)	4 (2)	40 (2)
C23	57 (2)	37 (2)	67 (2)	8 (2)	-6 (2)	30 (2)
C24	47 (2)	36 (2)	56 (2)	15 (1)	1 (2)	16 (2)
C25	40 (2)	36 (2)	46 (2)	9 (1)	5 (1)	20 (1)

Table S8: Geometric parameters of **3b** (Å, °)

S1—C1	1.739 (3)	C6—C20	1.451 (3)
S1—C4	1.756 (3)	C7—C8	1.353 (4)
S2—C5	1.742 (3)	C7—C11	1.498 (4)
S2—C8	1.759 (3)	C8—C9	1.457 (4)
O1—C12	1.222 (3)	C9—C10	1.502 (5)
O2—C12	1.330 (3)	C14—C15	1.376 (4)
O2—C13	1.442 (4)	C14—C19	1.382 (4)

O3—C3	1.237 (3)	C15—C16	1.385 (4)
O4—C9	1.223 (4)	C16—C17	1.369 (5)
N1—C1	1.345 (4)	C17—C18	1.372 (6)
N1—C14	1.405 (4)	C18—C19	1.380 (4)
C1—C2	1.387 (4)	C20—C25	1.377 (4)
C2—C12	1.444 (4)	C20—C21	1.381 (4)
C2—C3	1.450 (4)	C21—C22	1.371 (4)
C3—C4	1.443 (4)	C22—C23	1.373 (5)
C4—C5	1.374(4)	C23—C24	1.376 (5)
C5—C6	1.374 (4)	C24—C25	1.375 (4)
C6—C7	1.390 (4)		
C1—S1—C4	90.86 (13)	C7—C8—C9	132.8 (3)
C5—S2—C8	90.43 (13)	C7—C8—S2	112.2 (2)
C12—O2—C13	116.1 (3)	C9—C8—S2	114.9 (2)
C1—N1—C14	131.4 (3)	O4—C9—C8	117.9 (3)
N1—C1—C2	124.0 (3)	O4—C9—C10	120.9 (3)
N1—C1—S1	122.1 (2)	C8—C9—C10	121.1 (3)
C2—C1—S1	113.9 (2)	O1—C12—O2	121.2 (3)
C1—C2—C12	120.8 (2)	O1—C12—C2	125.1 (3)
C1—C2—C3	112.4 (2)	O2—C12—C2	113.6 (2)
C12—C2—C3	126.7 (2)	C15—C14—C19	119.5 (3)
O3—C3—C4	121.9 (3)	C15—C14—N1	124.4 (3)
O3—C3—C2	127.4 (3)	C19—C14—N1	116.3 (3)
C4—C3—C2	110.7 (2)	C14—C15—C16	119.6 (3)
C5—C4—C3	120.4 (2)	C17—C16—C15	120.8 (3)
C5—C4—S1	127.5 (2)	C16—C17—C18	119.8 (3)
C3—C4—S1	112.1 (2)	C17—C18—C19	120.0 (4)
C4—C5—C6	128.1 (2)	C18—C19—C14	120.4 (3)
C4—C5—S2	121.5 (2)	C25—C20—C21	122.0 (3)
C6—C5—S2	109.98 (19)	C25—C20—C6	119.0 (3)
C5—C6—C7	115.4 (2)	C21—C20—C6	119.0 (3)
C5—C6—C20	122.0 (2)	C22—C21—C20	118.8 (3)
C7—C6—C20	122.5 (2)	C21—C22—C23	120.1 (3)
C8—C7—C6	111.9 (3)	C22—C23—C24	120.4 (3)

C8—C7—C11	129.7 (3)	C25—C24—C23	120.6 (3)
C6—C7—C11	118.3 (3)	C24—C25—C20	118.1 (3)

Table S9:Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···O1	0.78 (3)	2.01(4)	2.683(3)	144(4)
C15—H15A···S1	0.93	2.59	3.141(4)	118
C17—H17A···O3^{i}	0.93	2.46	3.308(5)	152
C23—H23A···O4^{i}	0.93	2.56	3.381(5)	148
C25—H25A···O5^{ii}	0.93	2.57	3.439(3)	156
Symmetry codes: (i) x,1+y,z; (ii) -x,1-y,1-z.				