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Supporting Information

One-pot Dilithiation-Lithium-Zinc Exchange-Negishi Coupling Approach to 2,6-Di(hetero)aryl Substituted Dithienothiazines – A Novel Class of Electronically Fine-tunable Redox Systems

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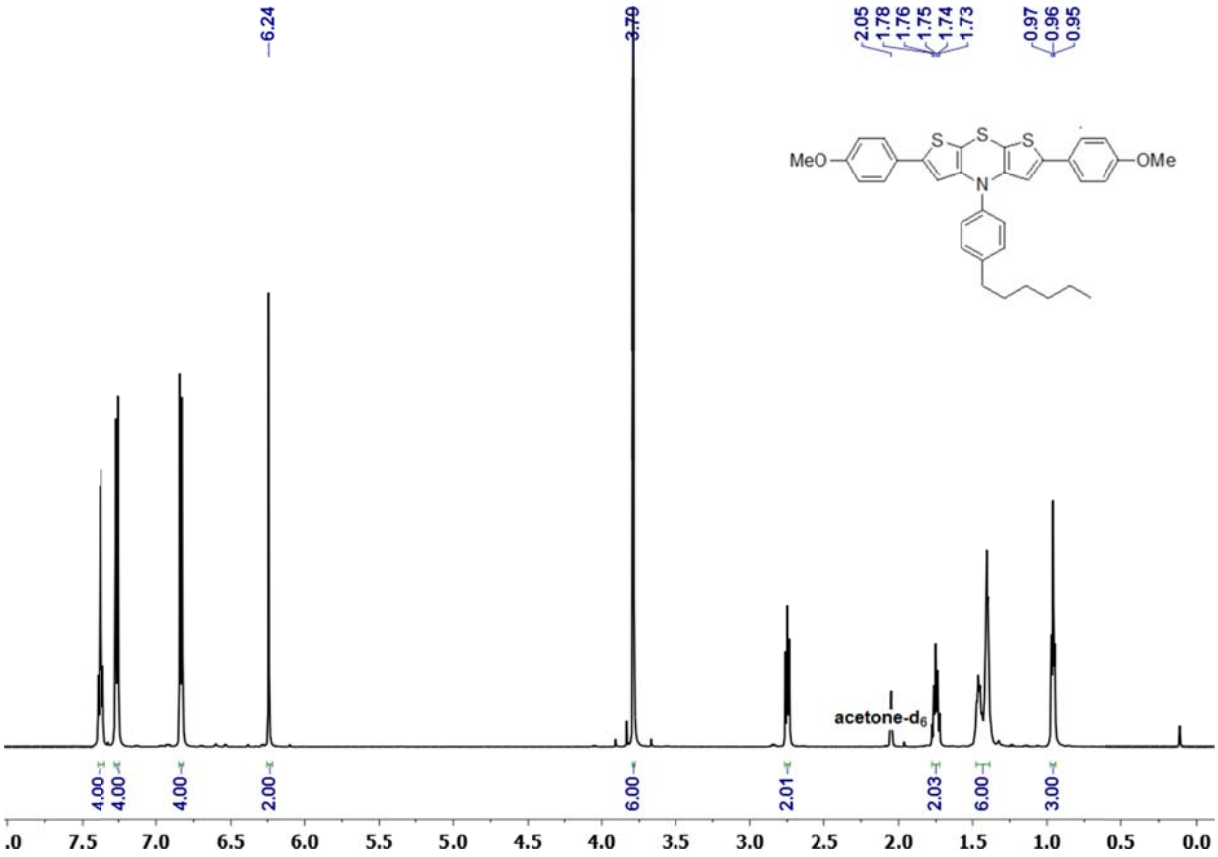
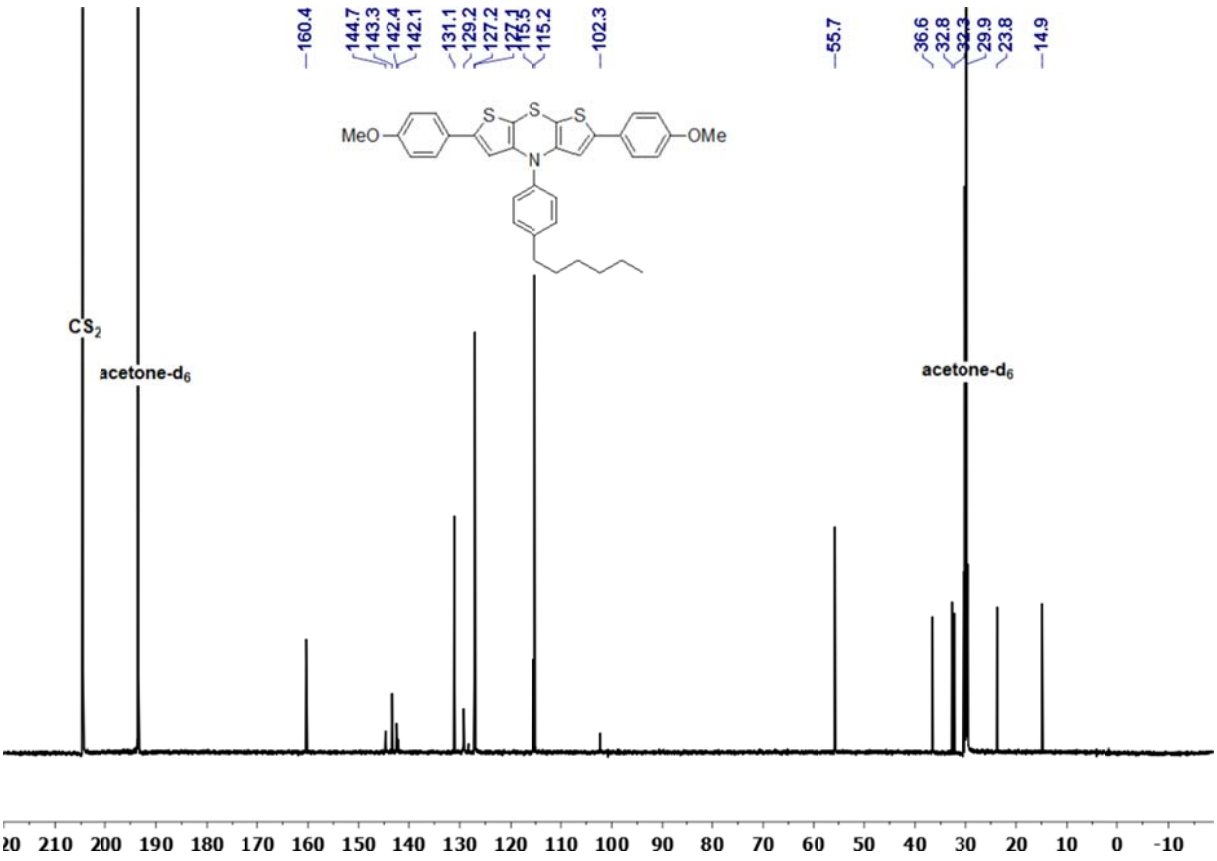
Table of contents

1 ^{1}H- and ^{13}C-NMR spectra of 2,6-di(hetero)aryl dithienothiazines 3a-3l

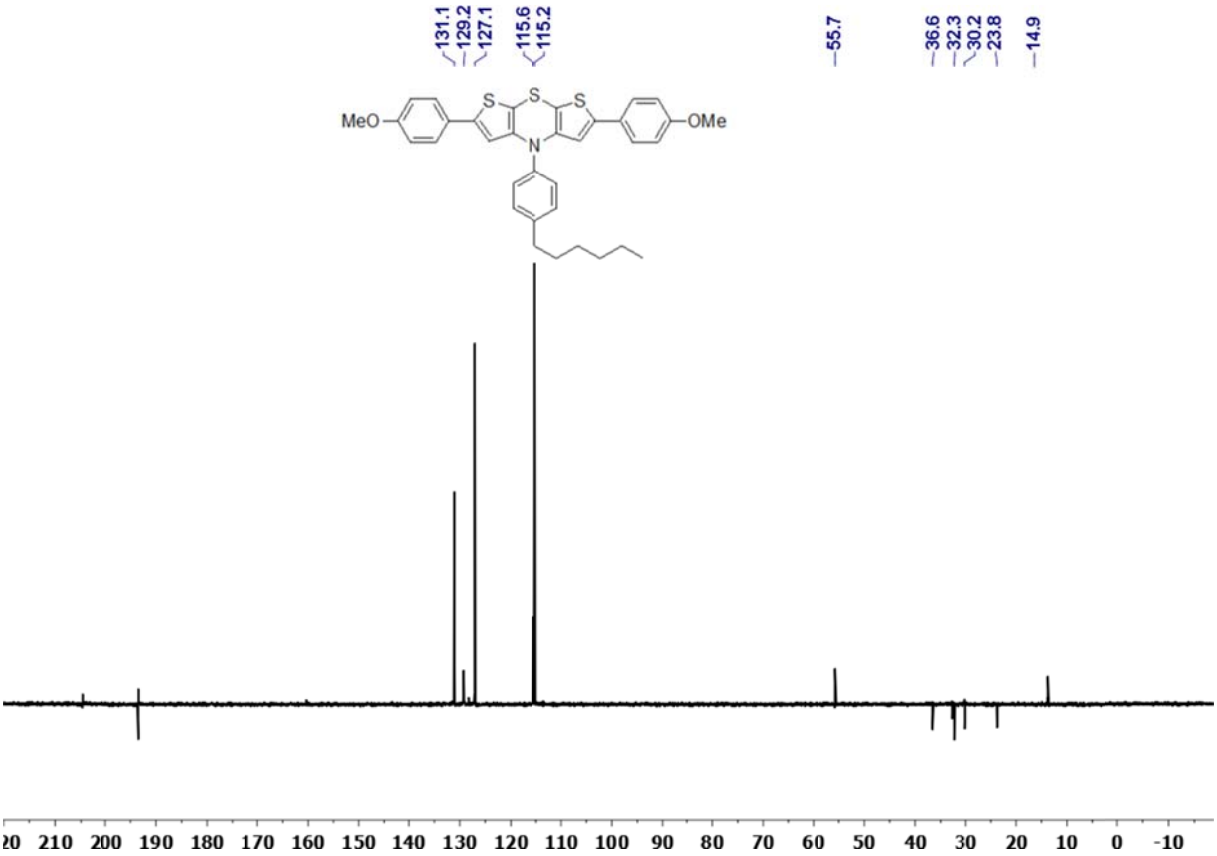
1.1 4-(4-Hexylphenyl)-2,6-bis(4-methoxyphenyl)-4H-dithieno[2,3-b:3',2'-e][1,4]thiazine (3a)



^{1}H-NMR (600 MHz) of **3a** (20 mg) in acetone-d_6/CS_2 1:1 at 313 K (δ in ppm).

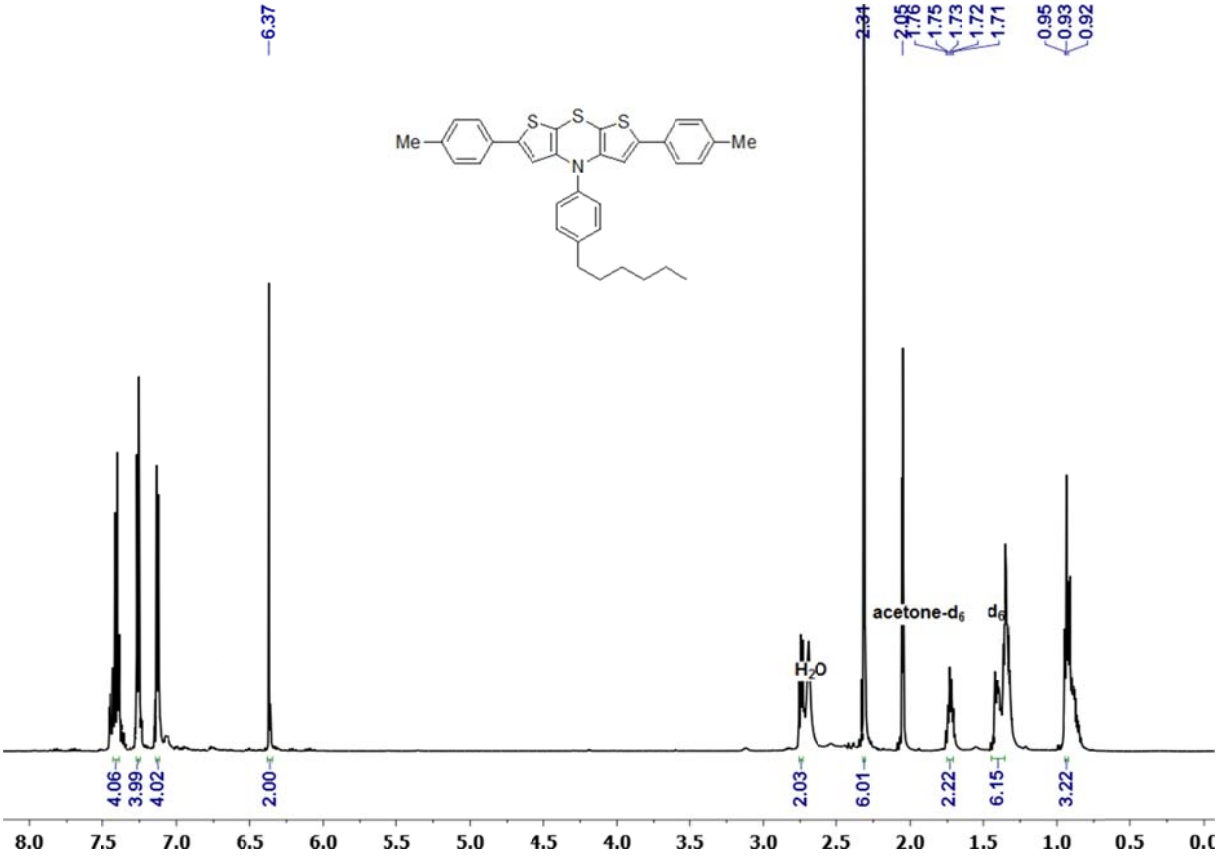


^{13}C-NMR (150 MHz) of **3a** (20 mg) in acetone-d_6/CS_2 1:1 at 313 K (δ in ppm).

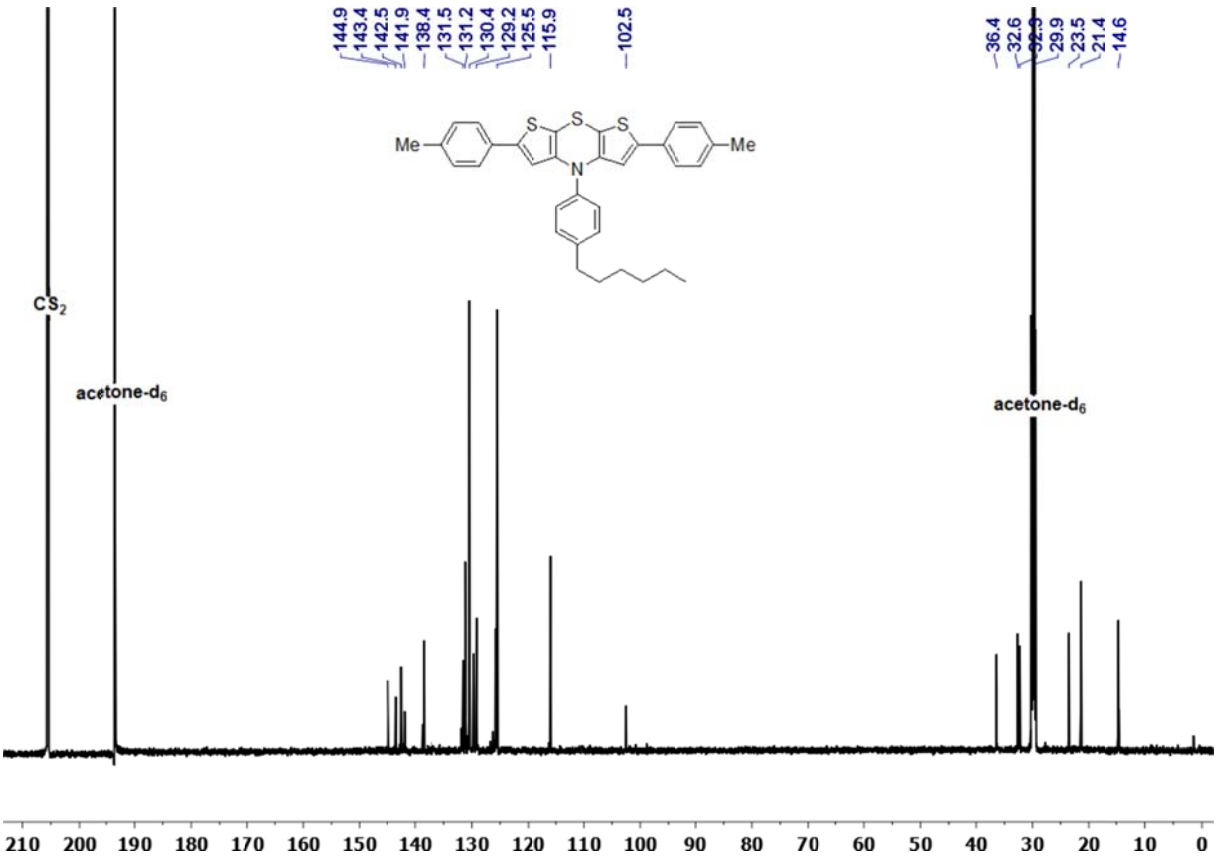


^{13}C-DEPT 135-NMR (150 MHz) of **3a** (20 mg) in acetone-d_6/CS_2 1:1 at 313 K (δ in ppm).

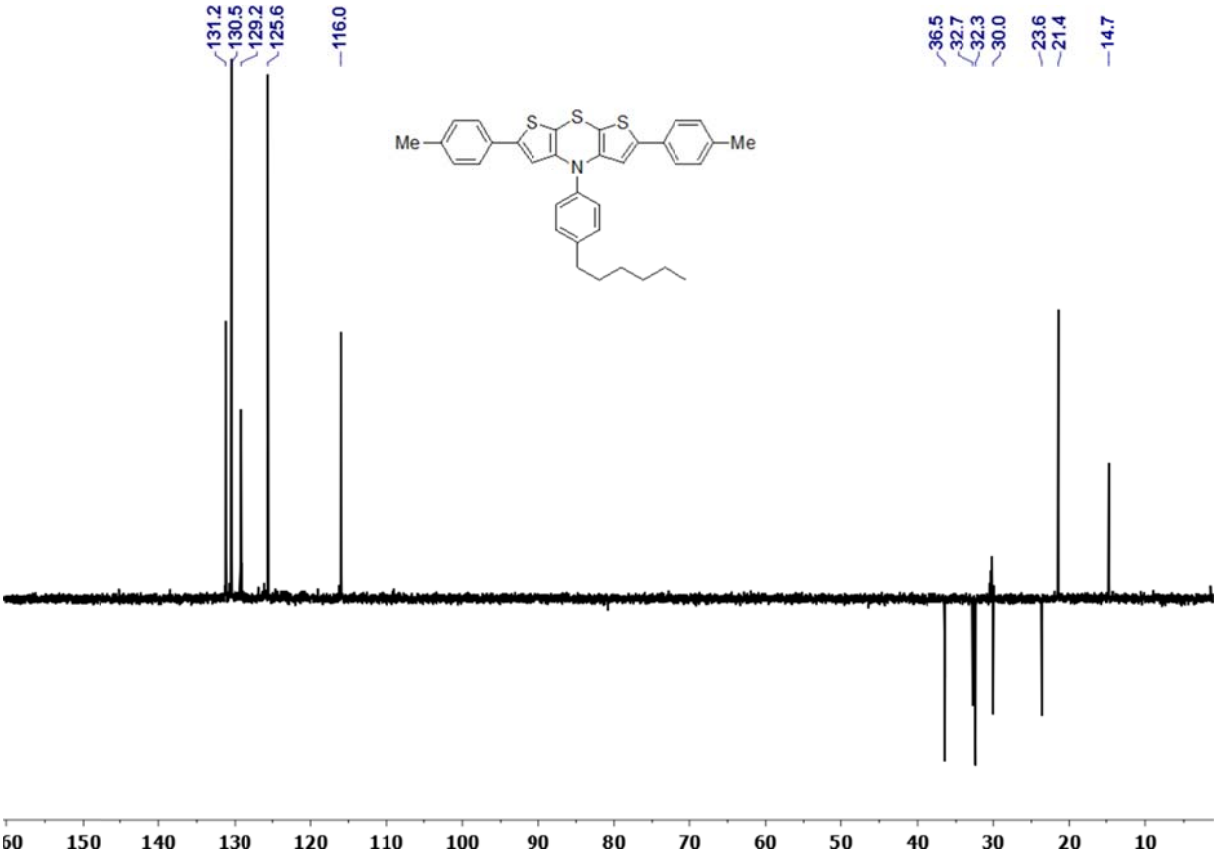
1.2 4-(4-Hexylphenyl)-2,6-di-p-tolyl-4H-dithieno[2,3-b:3',2'-e][1,4]thiazine (3b)



^{1}H-NMR (600 MHz) of **3b** (20 mg) in ace**t**one-d_6/CS_2 1:1 at 298 K (δ in ppm).

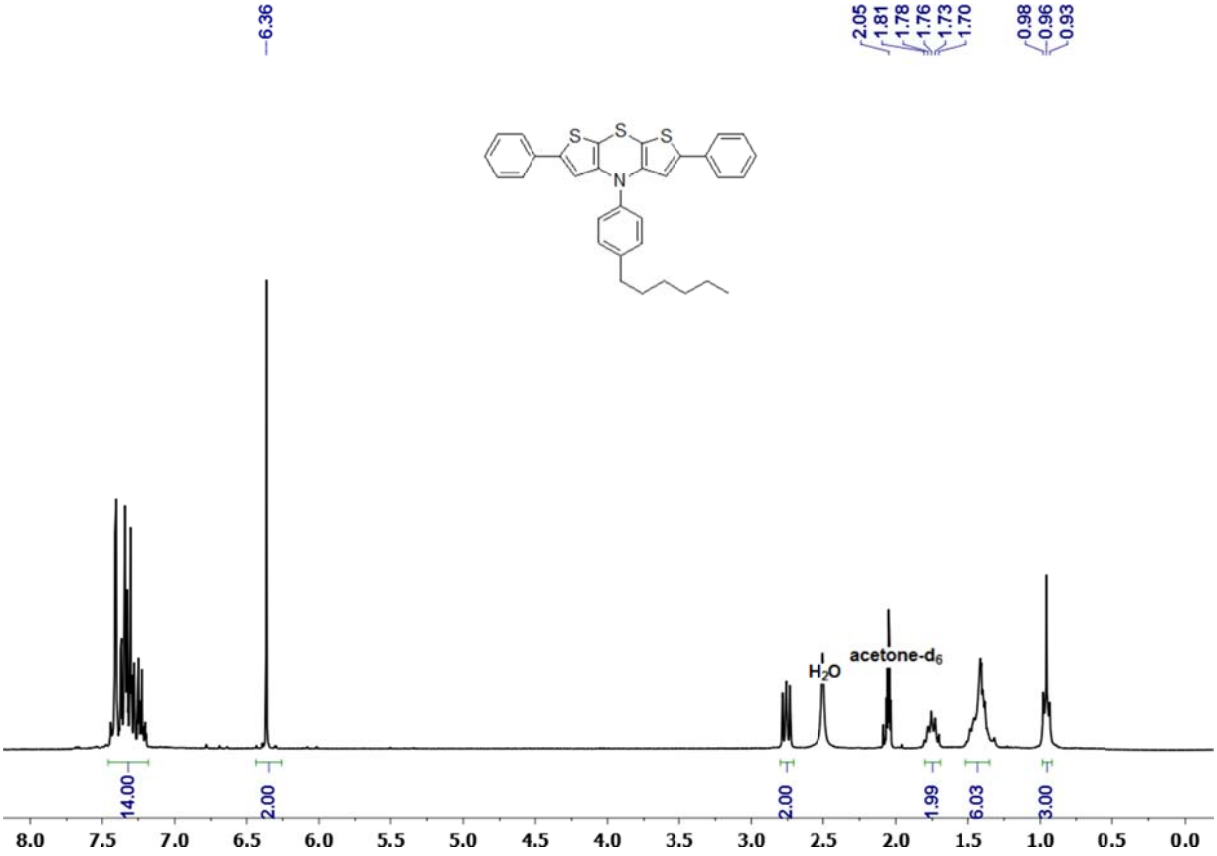


^{13}C-NMR (150 MHz) of **3b** (20 mg) in acetone-d_6/CS_2 1:1 at 298 K (δ in ppm).

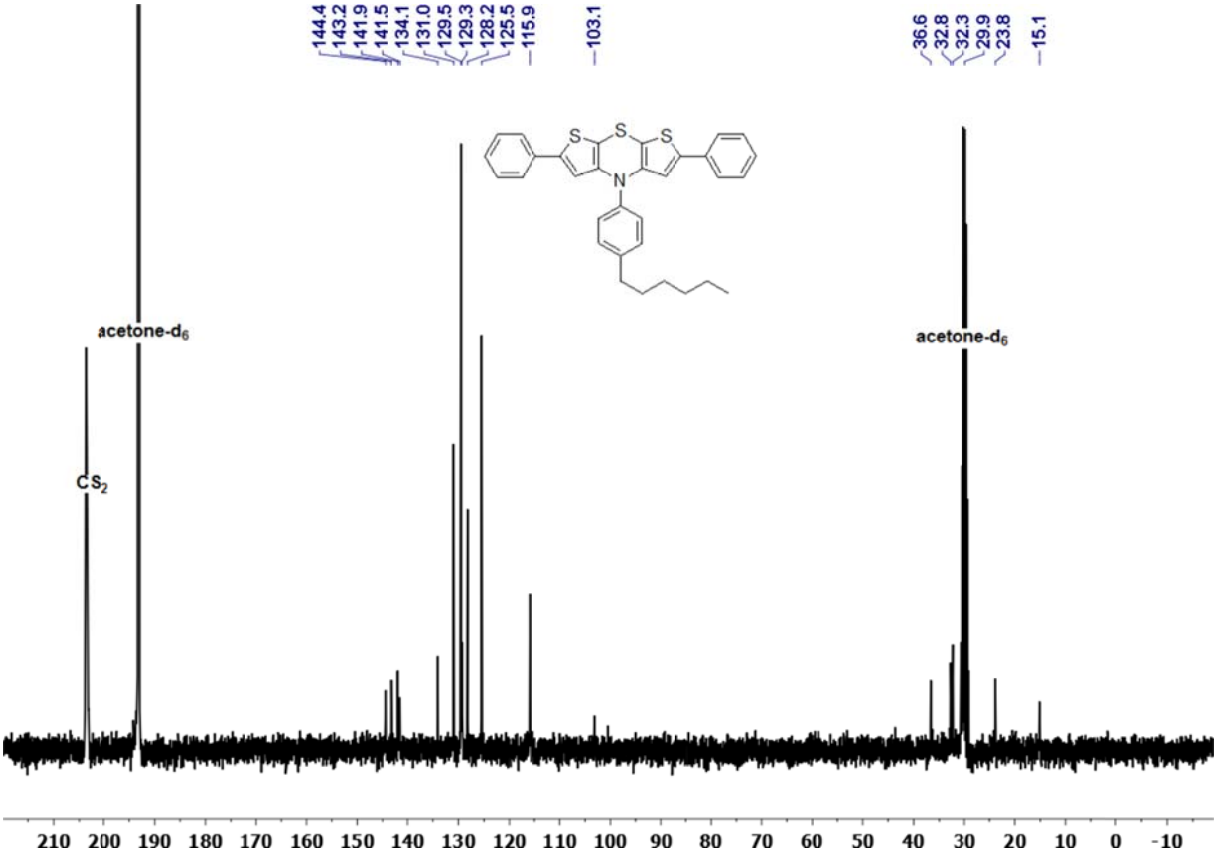


^{13}C-DEPT 135-NMR (150 MHz) of **3b** (20 mg) in acetone-d_6/CS_2 1:1 at 298 K (δ in ppm).

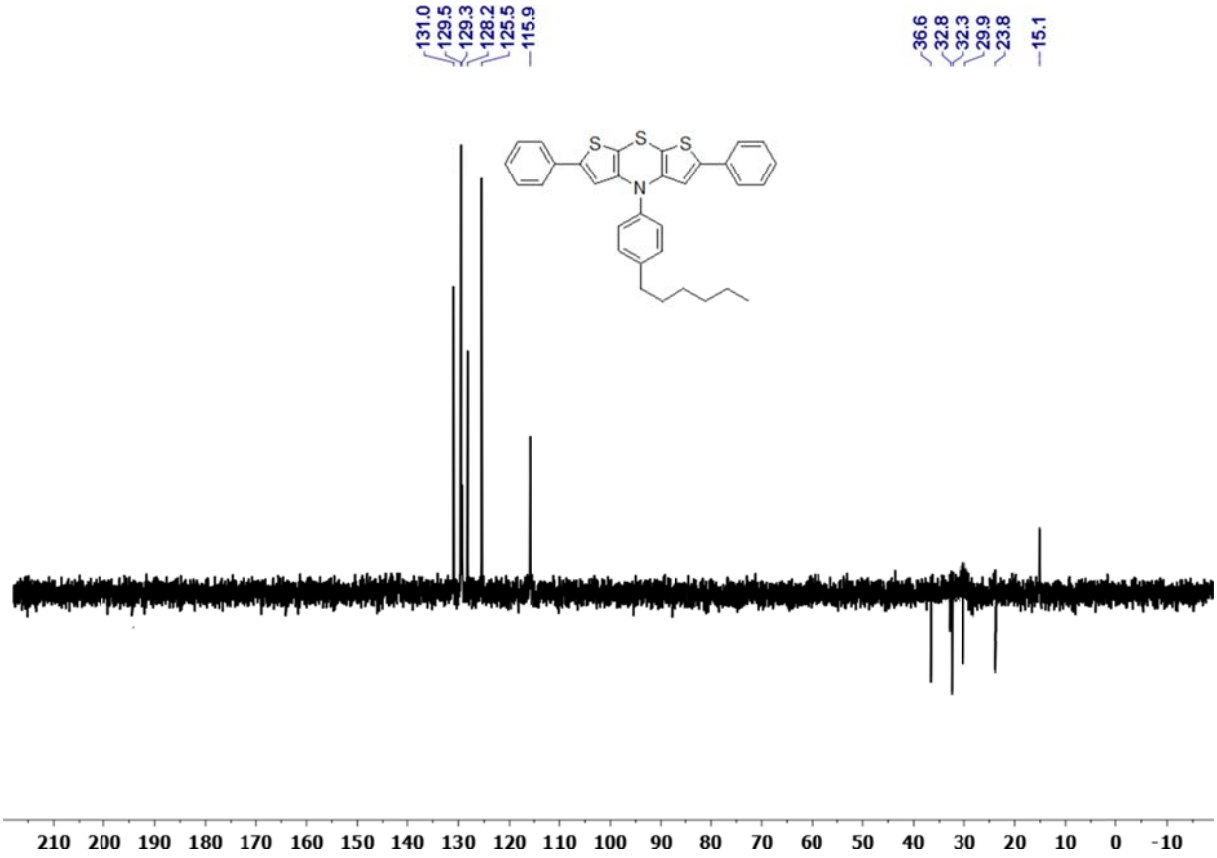
1.3 4-(4-Hexylphenyl)-2,6-diphenyl-4H-dithieno[2,3-b:3',2'-e][1,4]thiazine (3c)



[1]H-NMR (300 MHz) of **3c** (20 mg) in acetone-d_6/CS_2 2:1 at 298 K (δ in ppm).

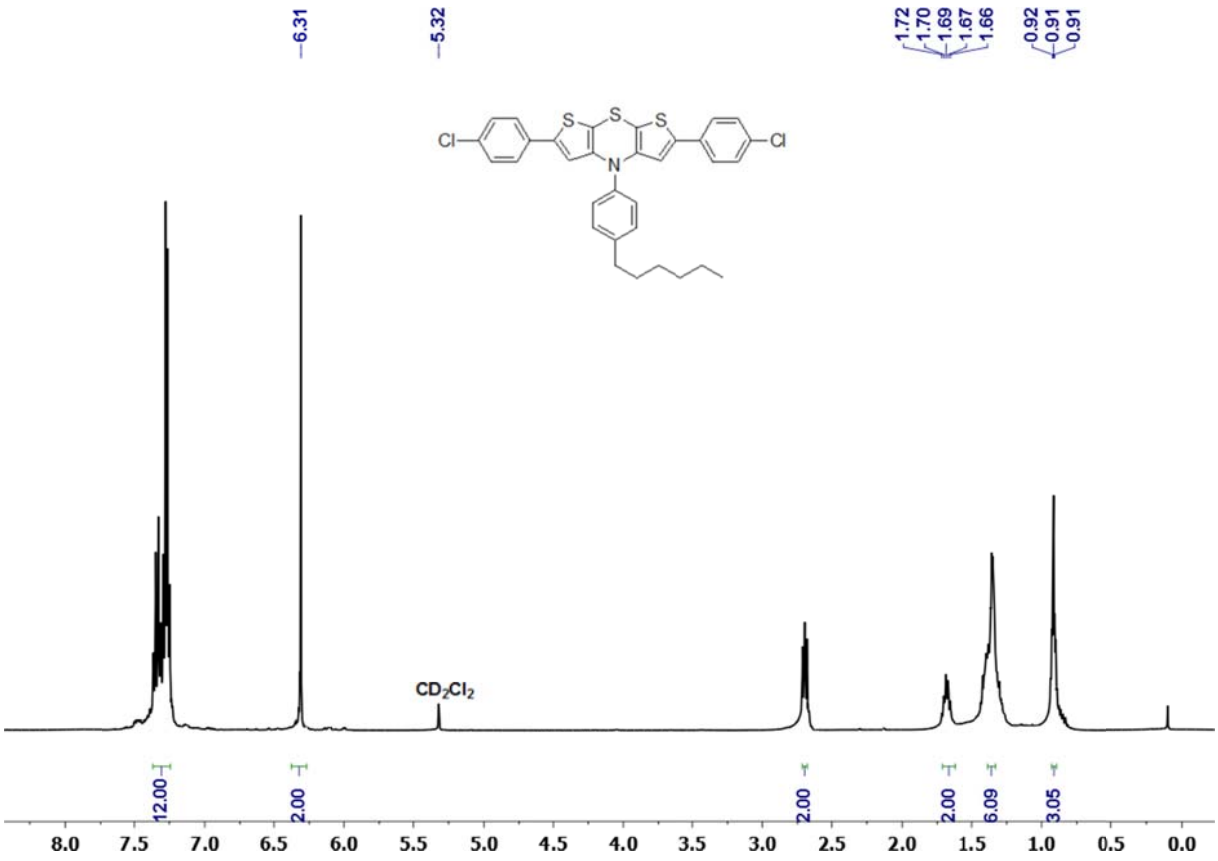


^{13}C-NMR (75 MHz) of **3c** (20 mg) in acetone-d_6/CS_2 2:1 at 298 K (δ in ppm).

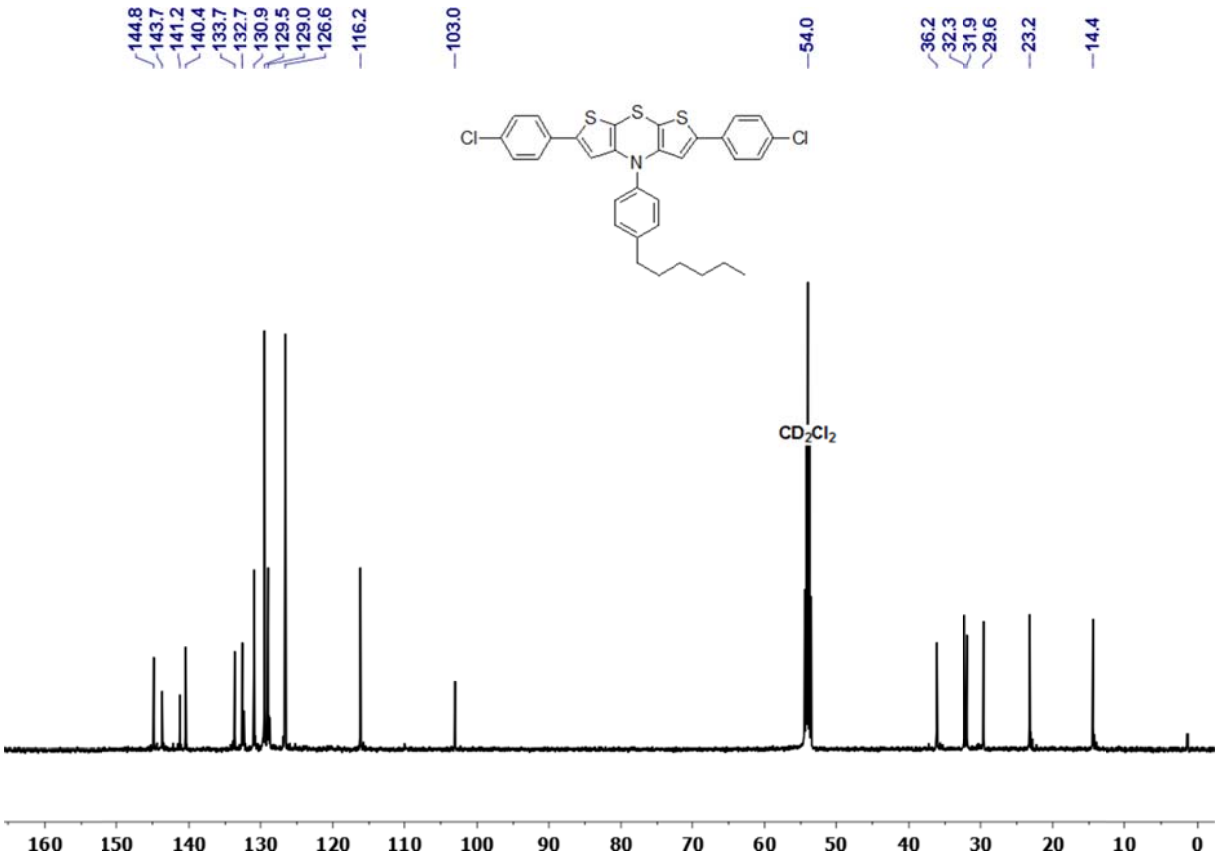


^{13}C-DEPT 135-NMR (75 MHz) of **3c** (20 mg) in acetone-d_6/CS_2 2:1 at 298 K (δ in ppm).

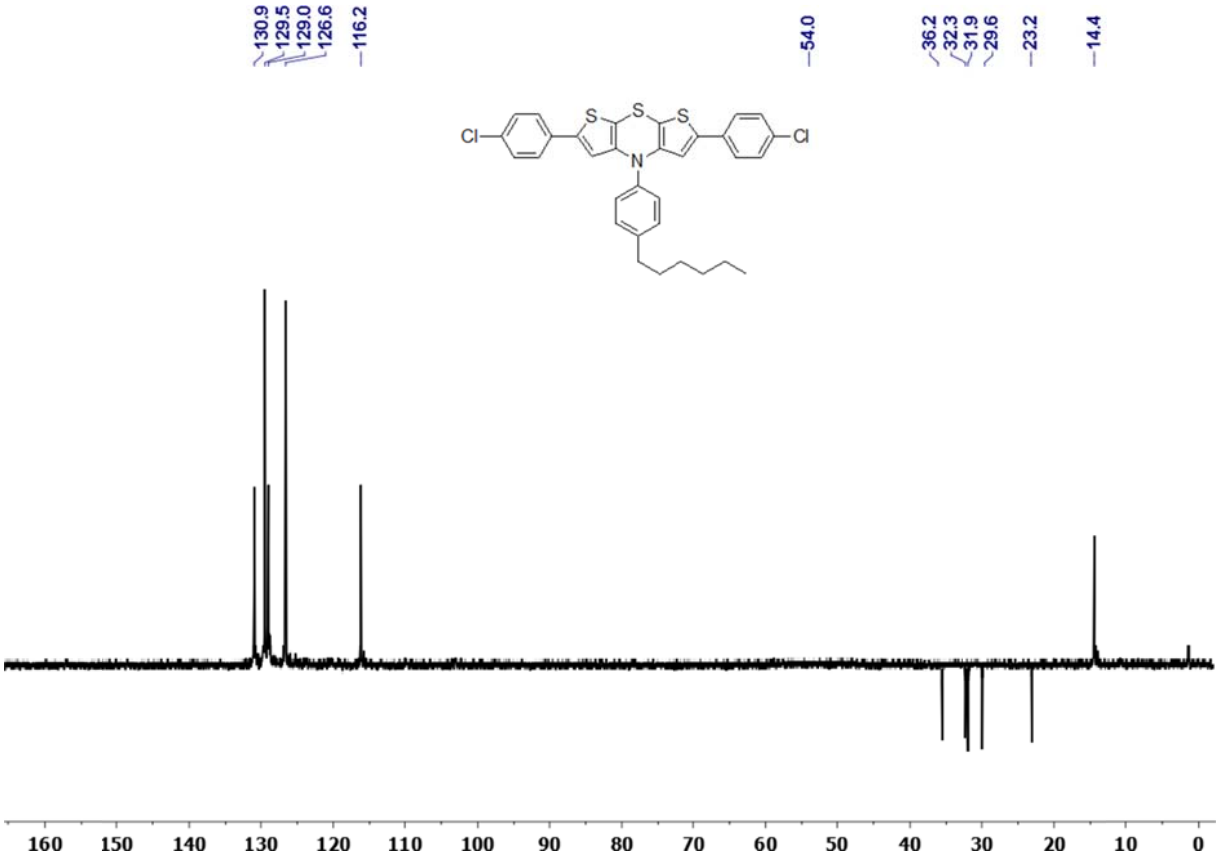
1.4 2,6-Bis(4-chlorophenyl)-4-(4-hexylphenyl)-4H-dithieno [2,3-b:3',2'-e][1,4]thiazine (3d)



[1]H-NMR (500 MHz) of **3d** (20 mg) in dichloromethane-d_2 at 298 K (δ in ppm).

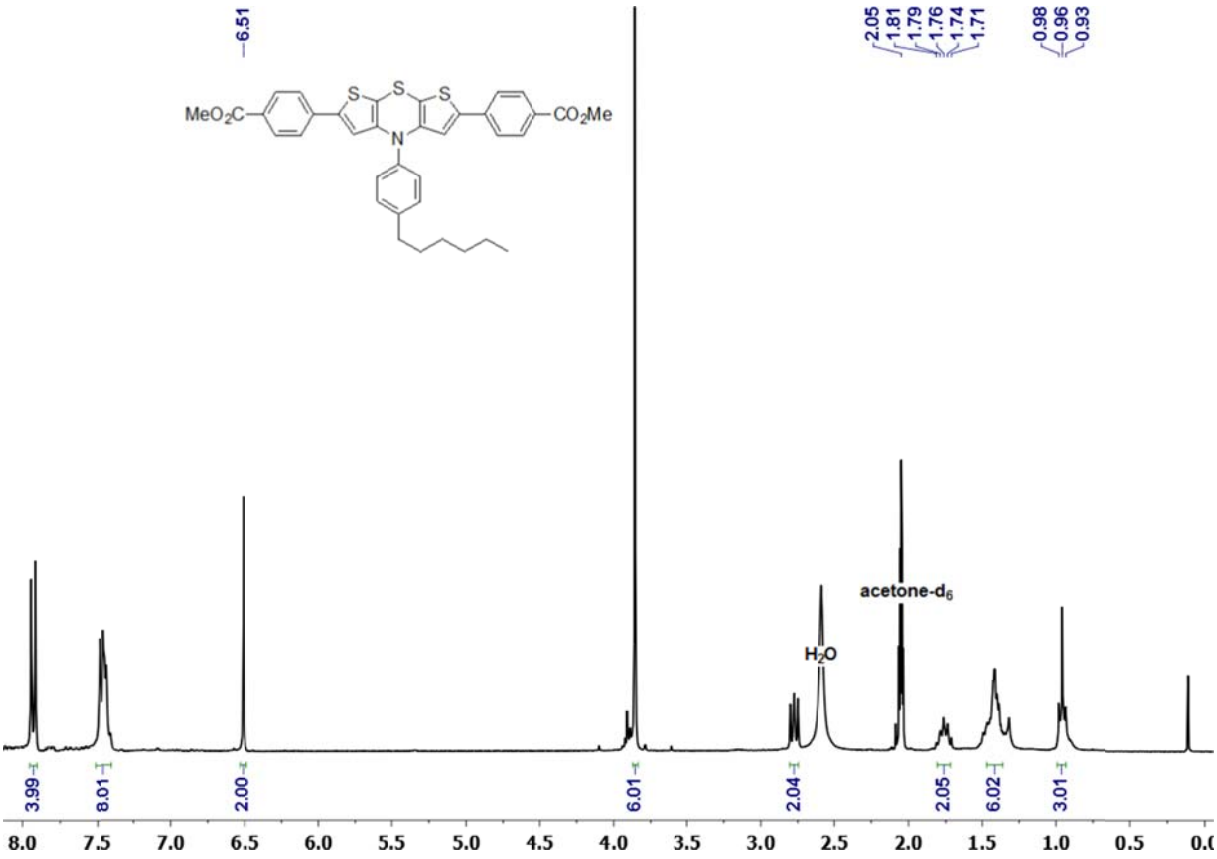


^{13}C-NMR (125 MHz) of **3d** (20 mg) in dichloromethane-d_2 at 298 K (δ in ppm).

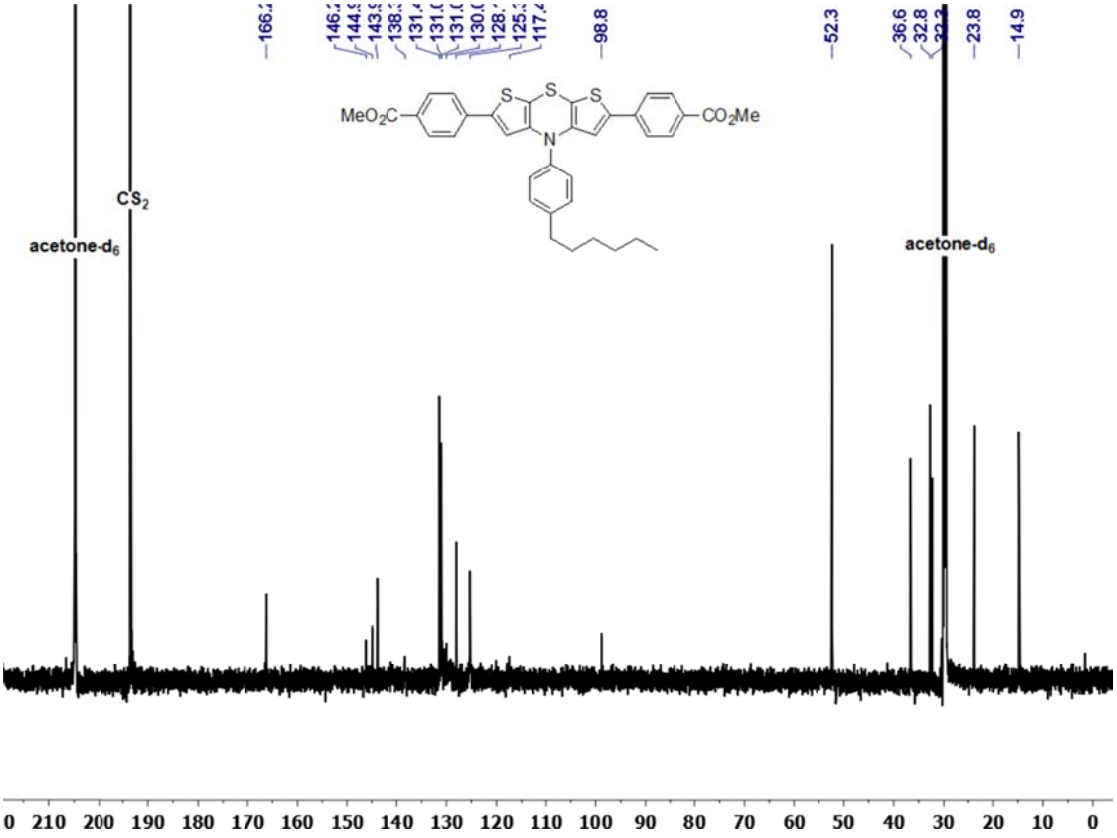


^{13}C-DEPT 135-NMR (125 MHz) of **3d** (20 mg) in dichloromethane-d_2 at 298 K (δ in ppm).

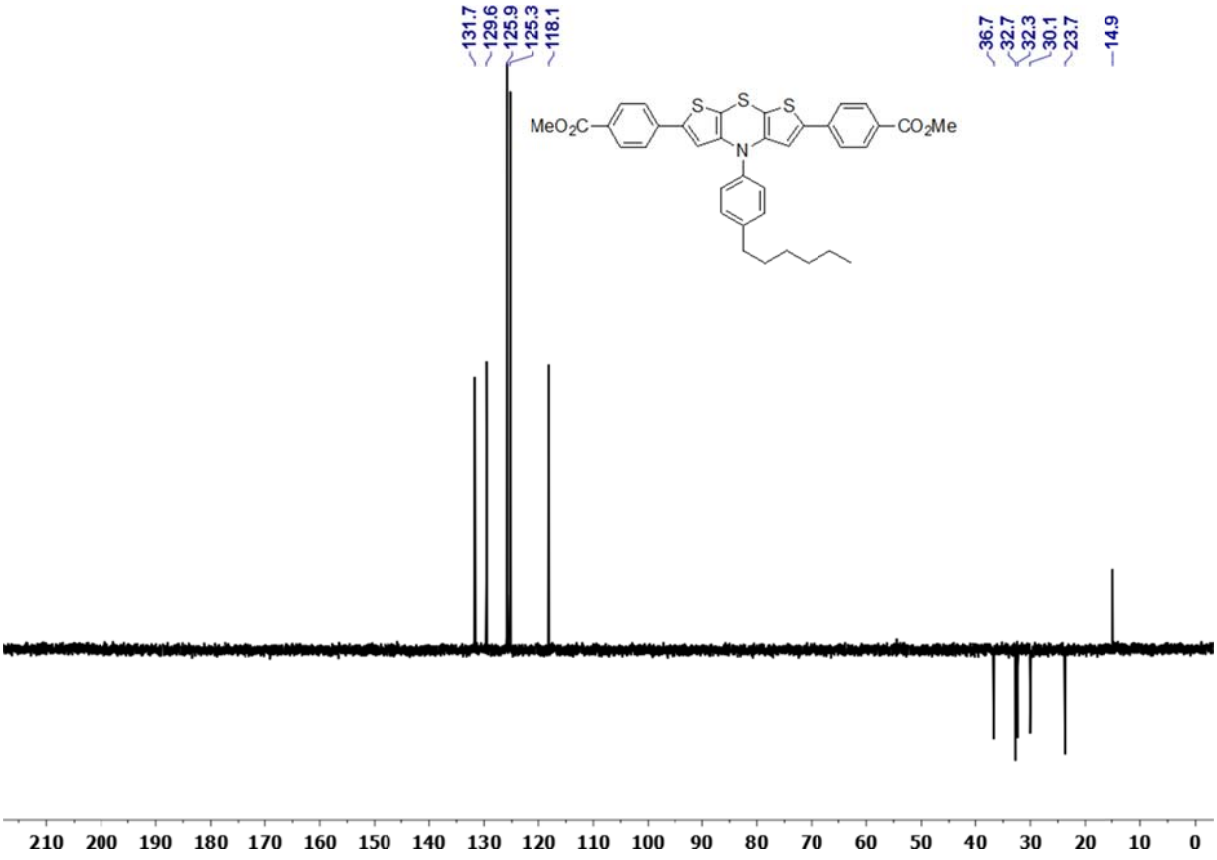
1.5 Dimethyl 4,4'-(4-(4-hexylphenyl)-4H-dithieno[2,3-b:3',2'-e][1,4]thiazine-2,6-diyl)dibenzoate (3e)



^{1}H-NMR (300 MHz) of **3e** (20 mg) in acetone-d_6/CS_2 1:1 at 293 K (δ in ppm).

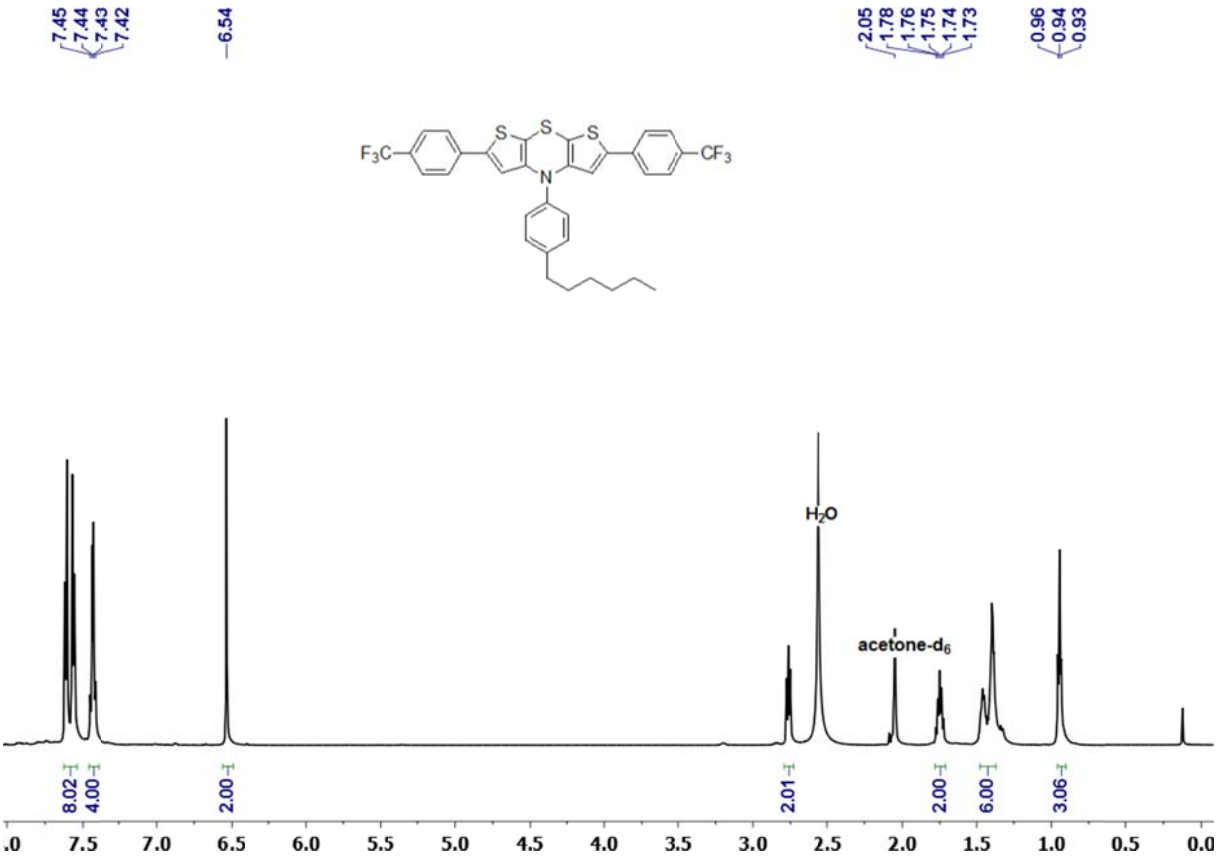


^{13}C-NMR (75 MHz) of **3e** (20 mg) in acetone-d_6/CS_2 1:1 at 293 K (δ in ppm).

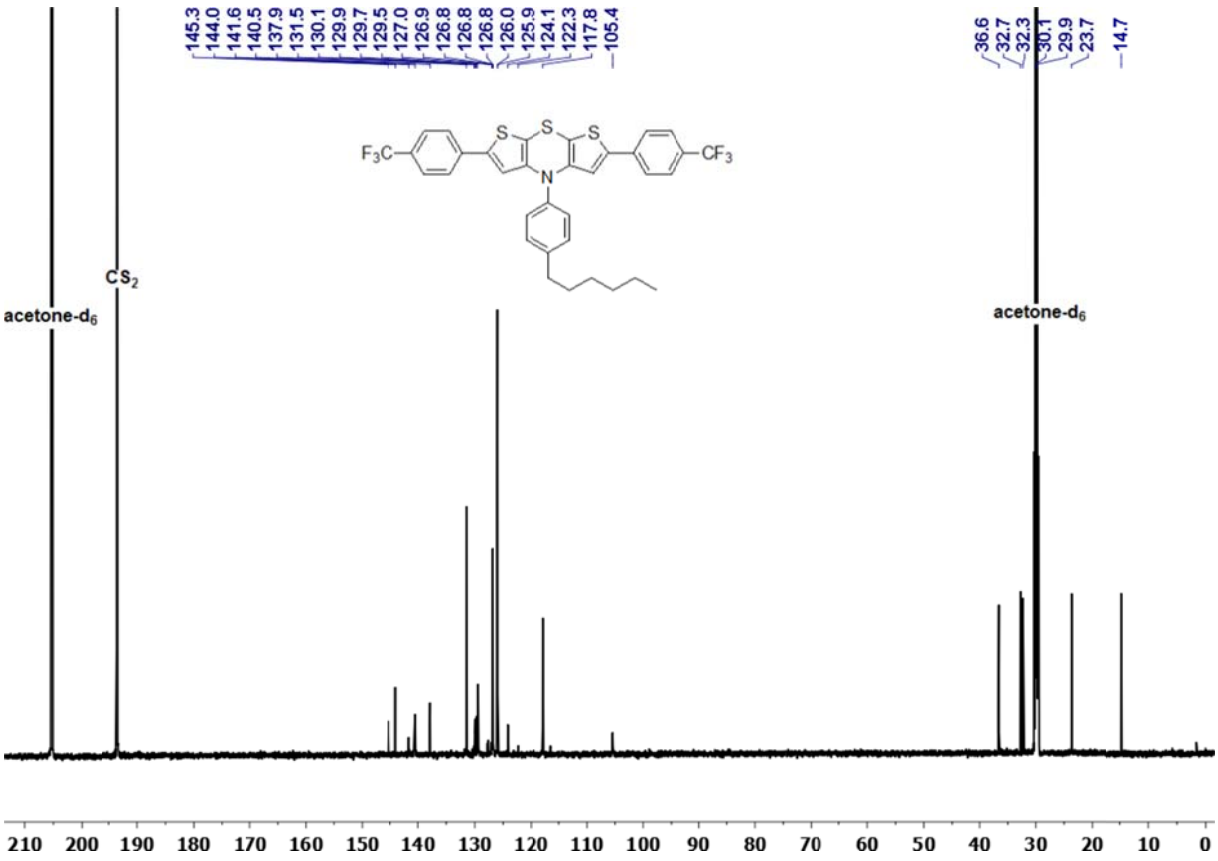


^{13}C-DEPT 135-NMR (75 MHz) of **3e** (20mg) in acetone-d_6/CS_2 1:1 at 293 K (δ in ppm).

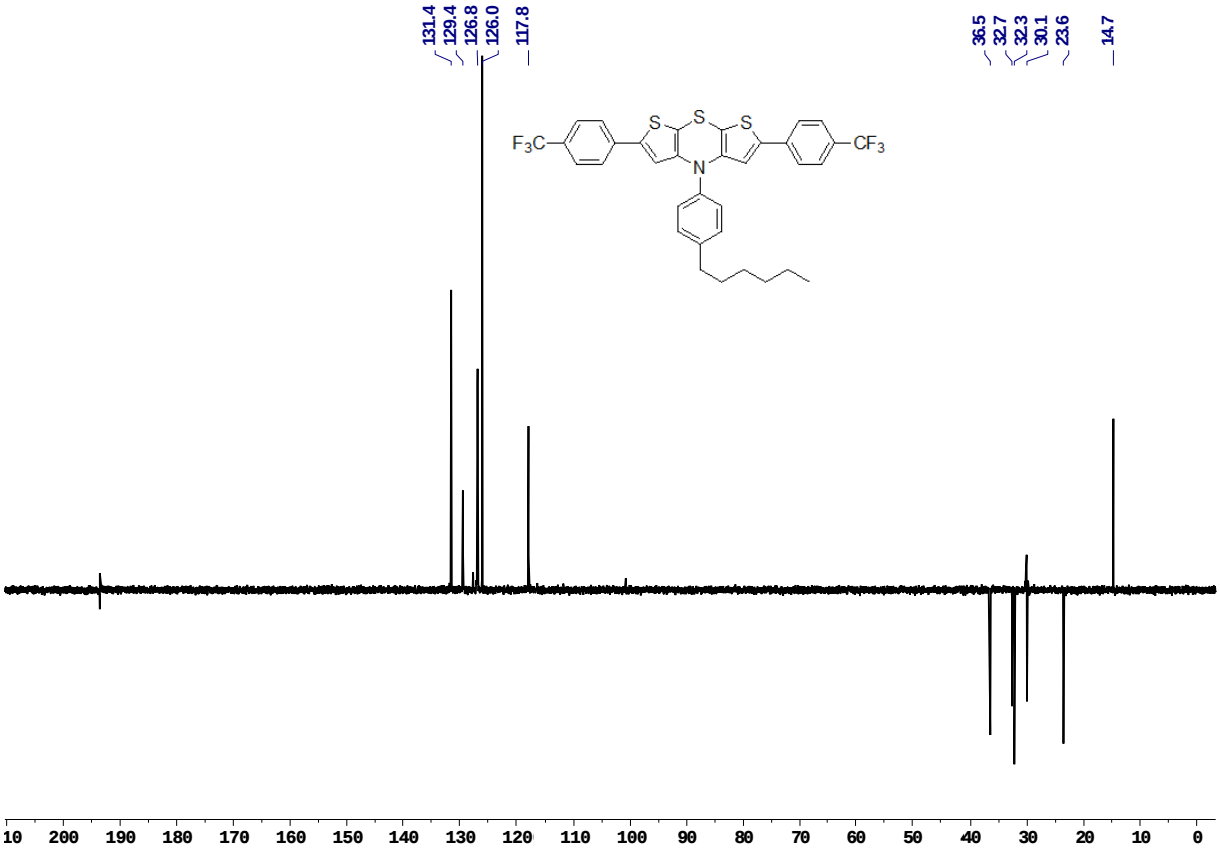
1.6 4-(4-Hexylphenyl)-2,6-bis(4-(trifluoromethyl)phenyl)-4H-dithieno[2,3-b:3',2'-e][1,4]thiazine (3f)



[1]H-NMR (600 MHz) of **3f** (20 mg) in acetone-d_6/CS_2 1:1 at 313 K (δ in ppm).

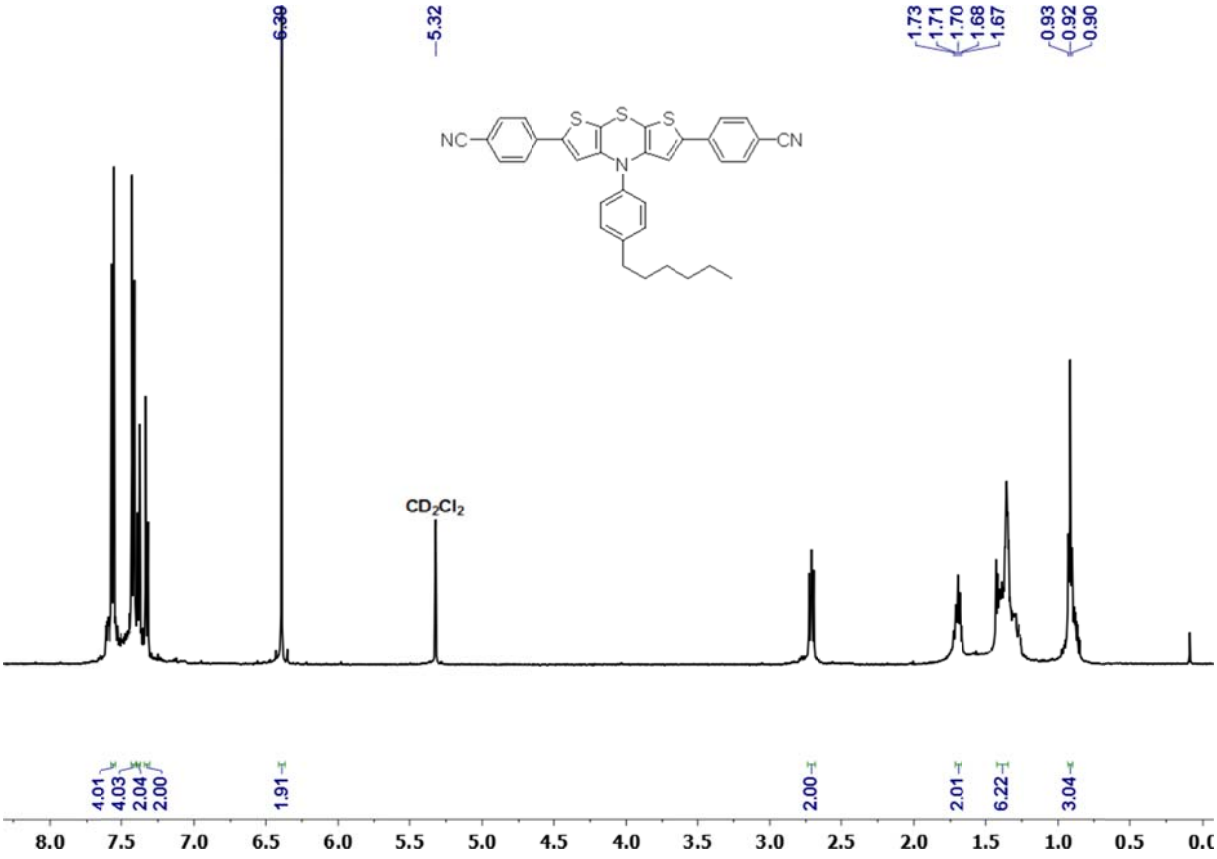


^{13}C-NMR (150 MHz) of **3f** (20 mg) in acetone-d_6/CS_2 1:1 at 313 K (δ in ppm).

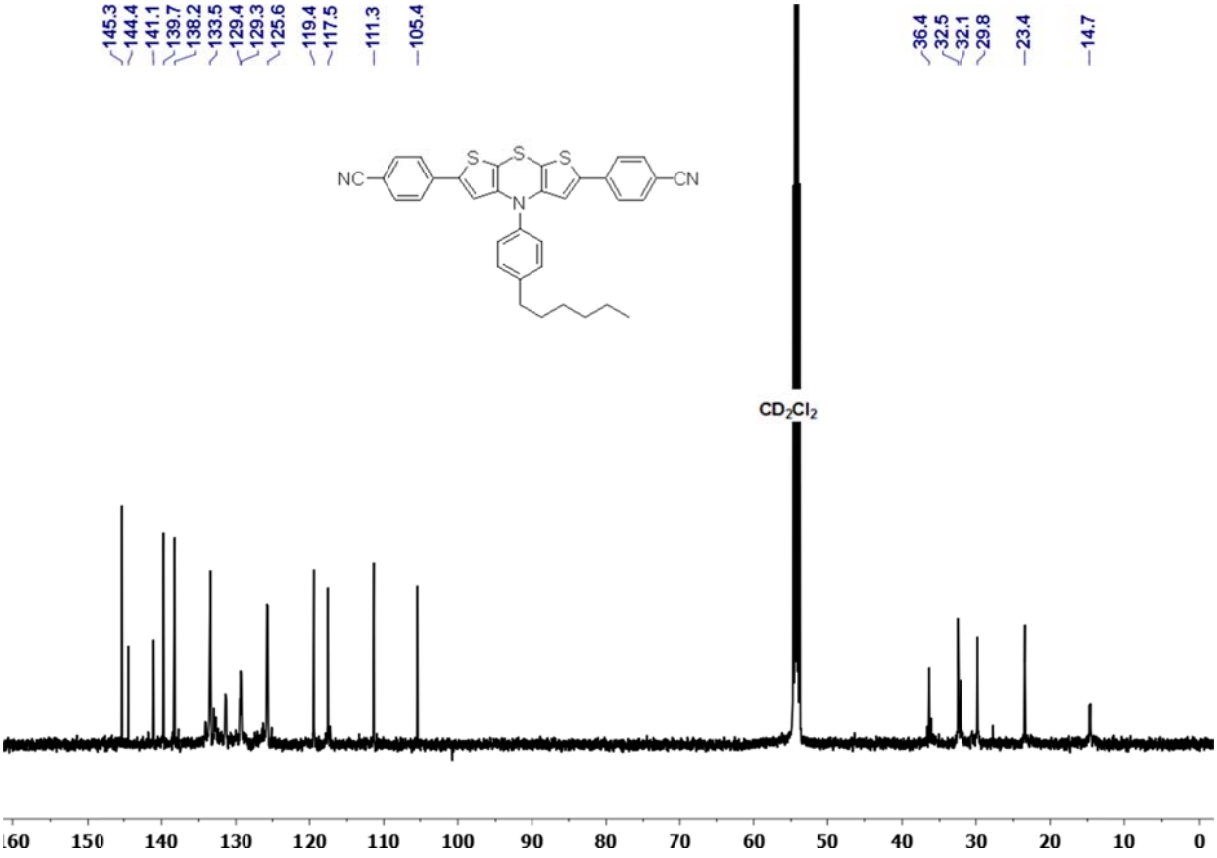


^{13}C-DEPT 135-NMR (150 MHz) of **3f** (20 mg) in acetone-d_6/CS_2 1:1 at 313 K (δ in ppm).

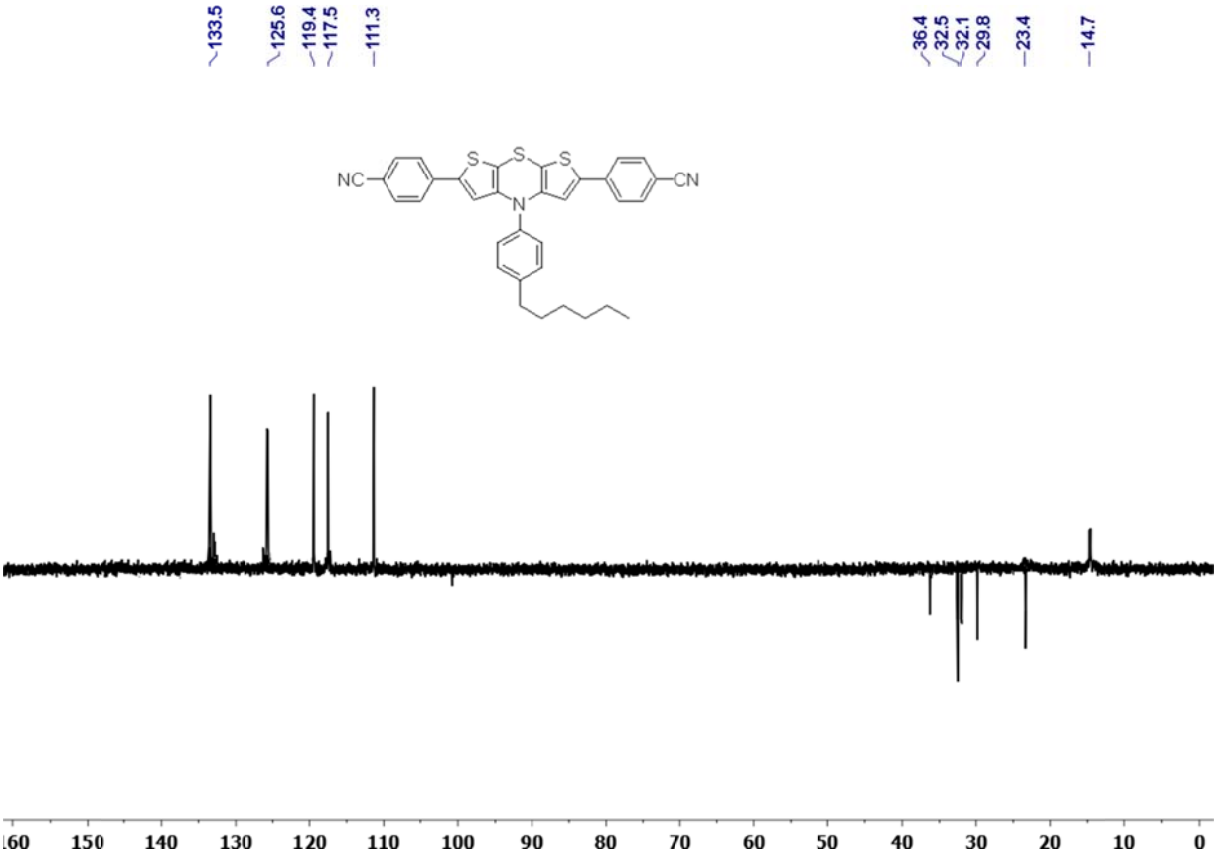
1.7 4,4'-(4-(4-Hexylphenyl)-4H-dithieno[2,3-b:3',2'-e][1,4]thiazine-2,6-diyl)dibenzonitrile (3g)



[1]H-NMR (600 MHz) of **3g** (20 mg) in dichloromethane-d_2 at 293 K (δ in ppm).

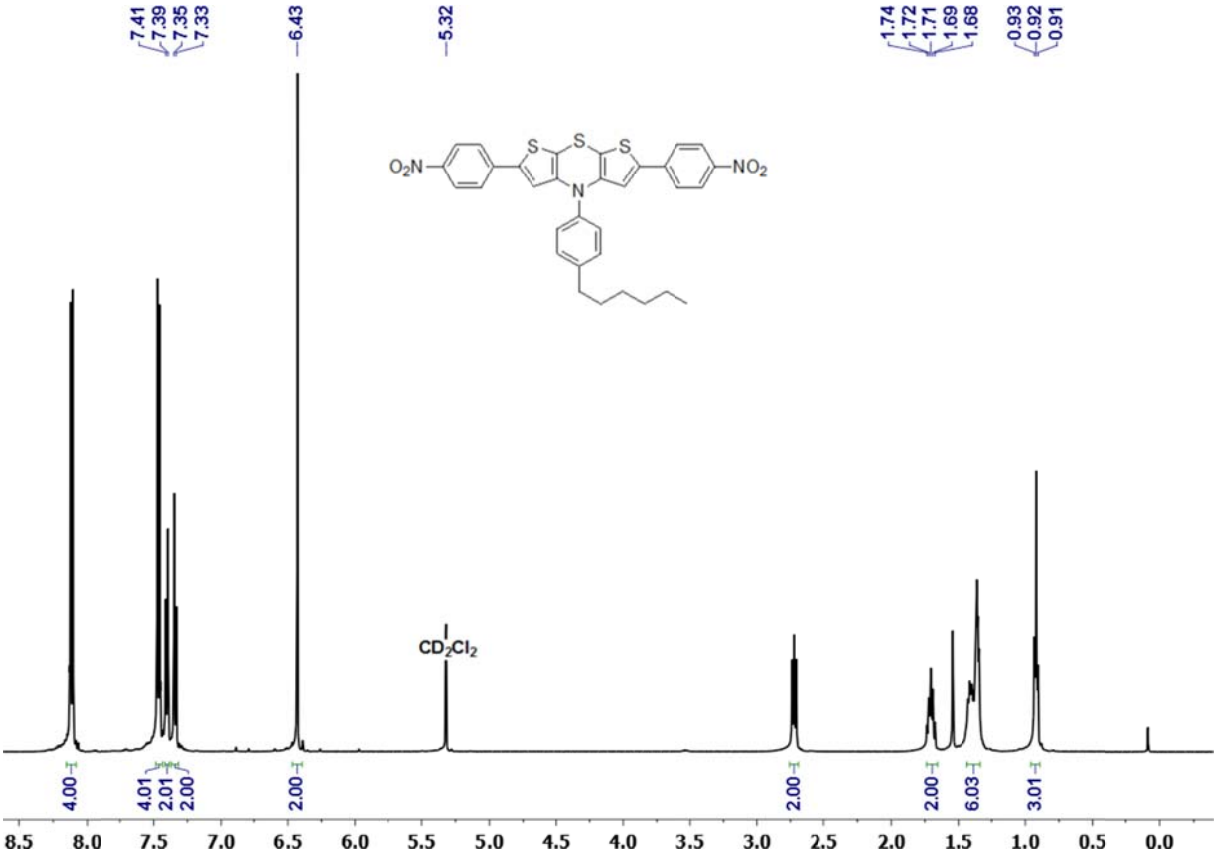


^{13}C-NMR (150 MHz) of **3g** (20 mg) in dic**h**loromethane-d_2 at 298 K (δ in ppm).

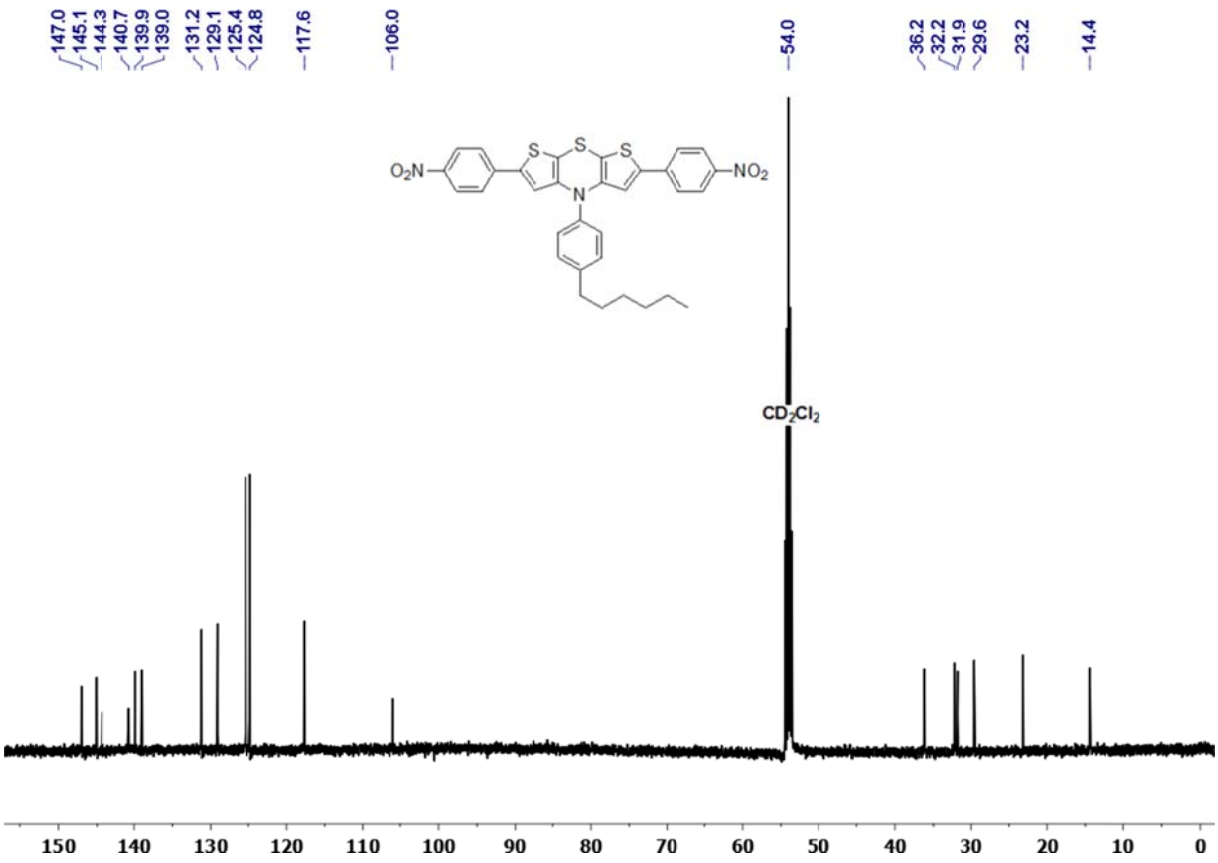


^{13}C-DEPT 135-NMR (150 MHz) of **3g** (20 mg) in dichloromethane-d_2 at 313 K (δ in ppm).

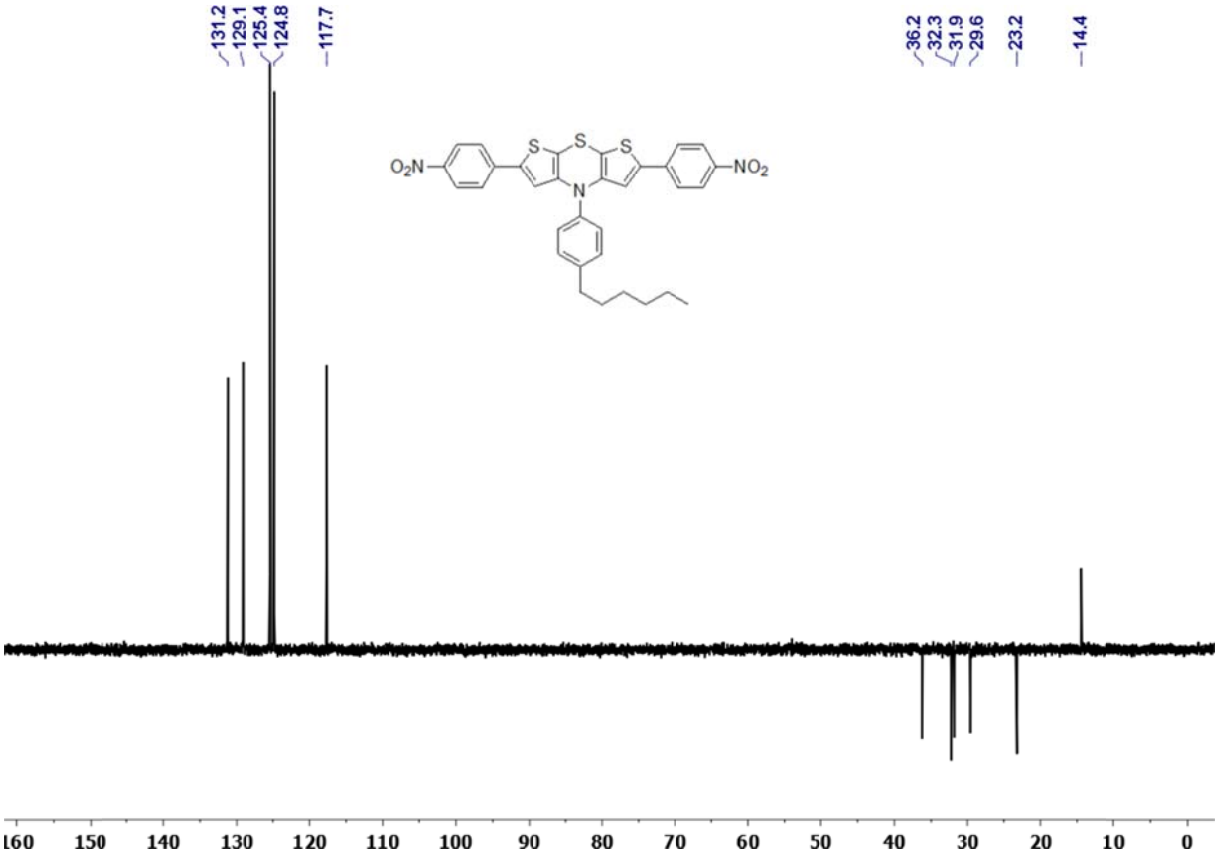
1.8 4-(4-Hexylphenyl)-2,6-bis(4-nitrophenyl)-4H-dithieno[2,3-b:3',2'-e][1,4]thiazine (3h)



[1]H-NMR (500 MHz) of **3f** (20 mg) in dichloromethane-d_2 at 298 K (δ in ppm).

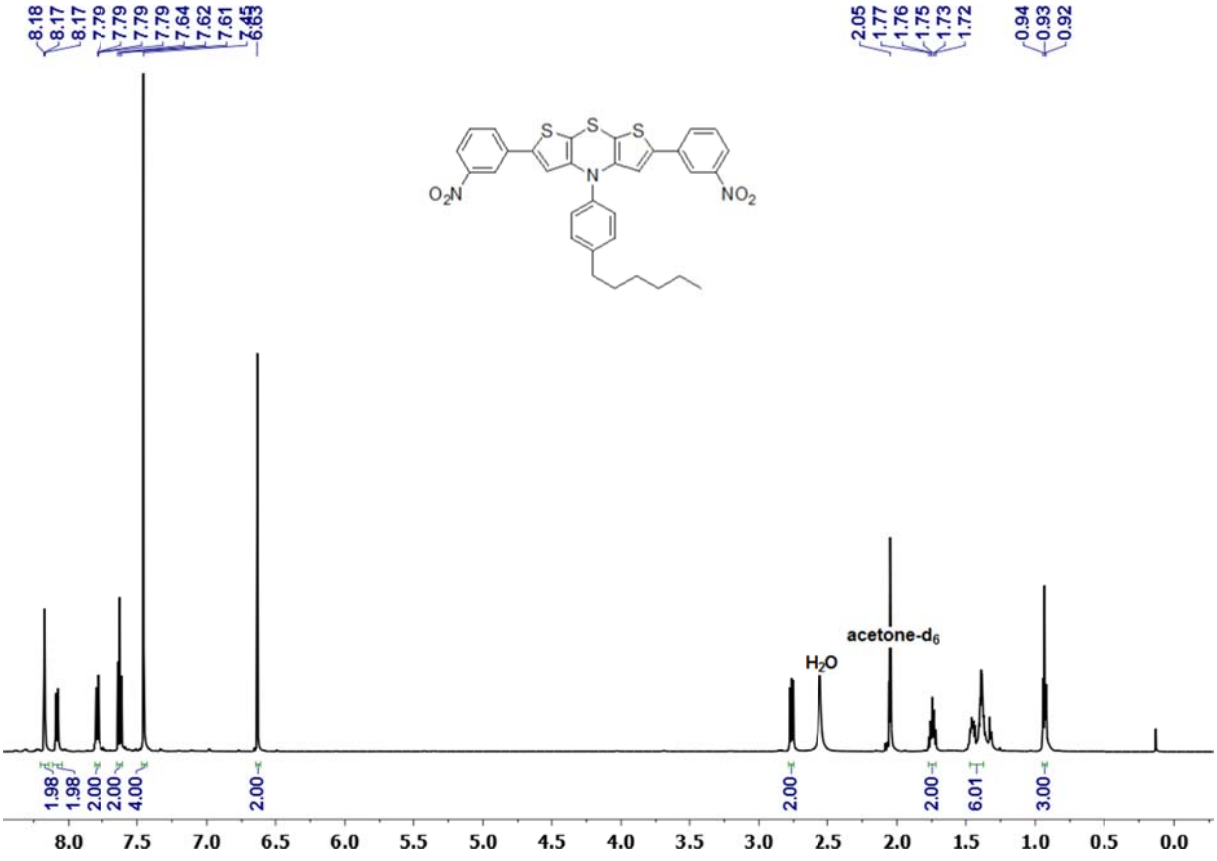


^{13}C-NMR (125 MHz) of **3f** (20 mg) in dichloromethane-d_2 at 298 K (δ in ppm).

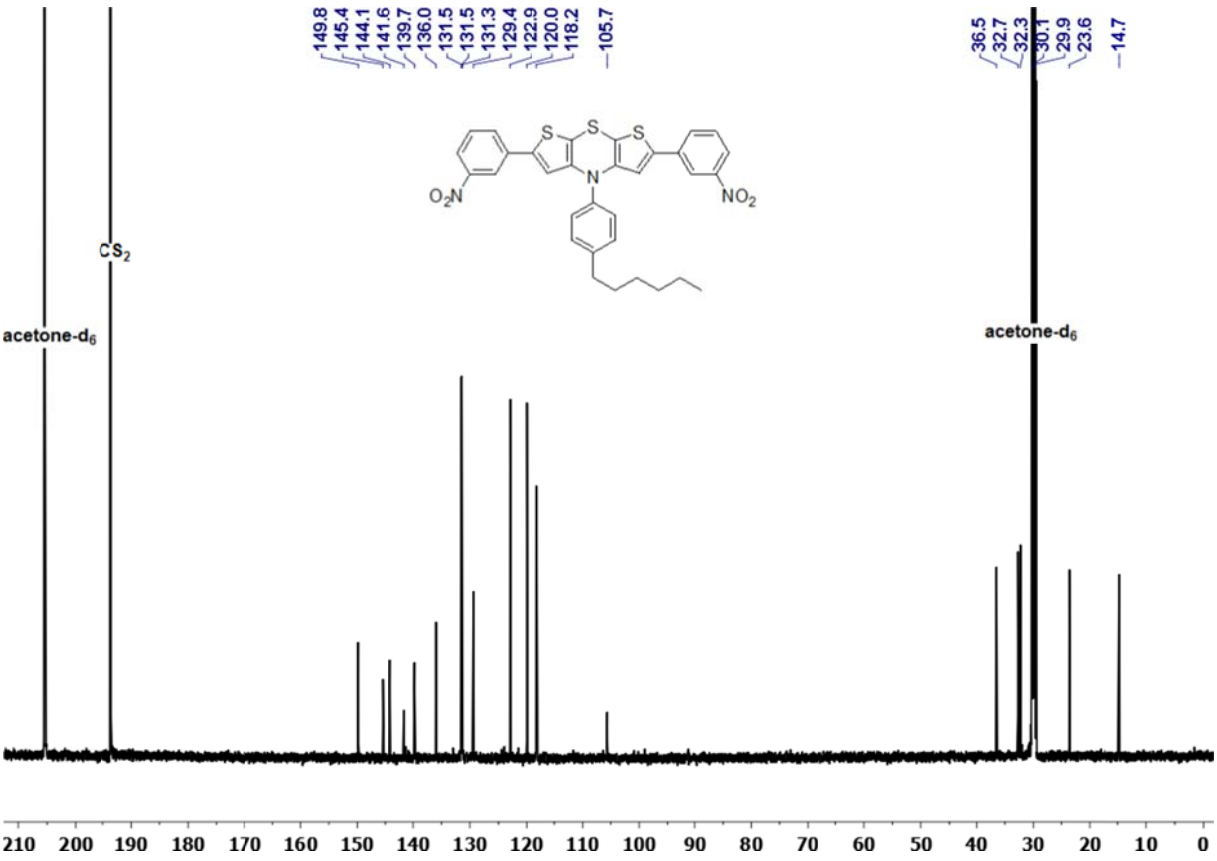


^{13}C-DEPT 135-NMR (125 MHz) of **3f** (20 mg) in dichloromethane-d_2 at 298 K (δ in ppm).

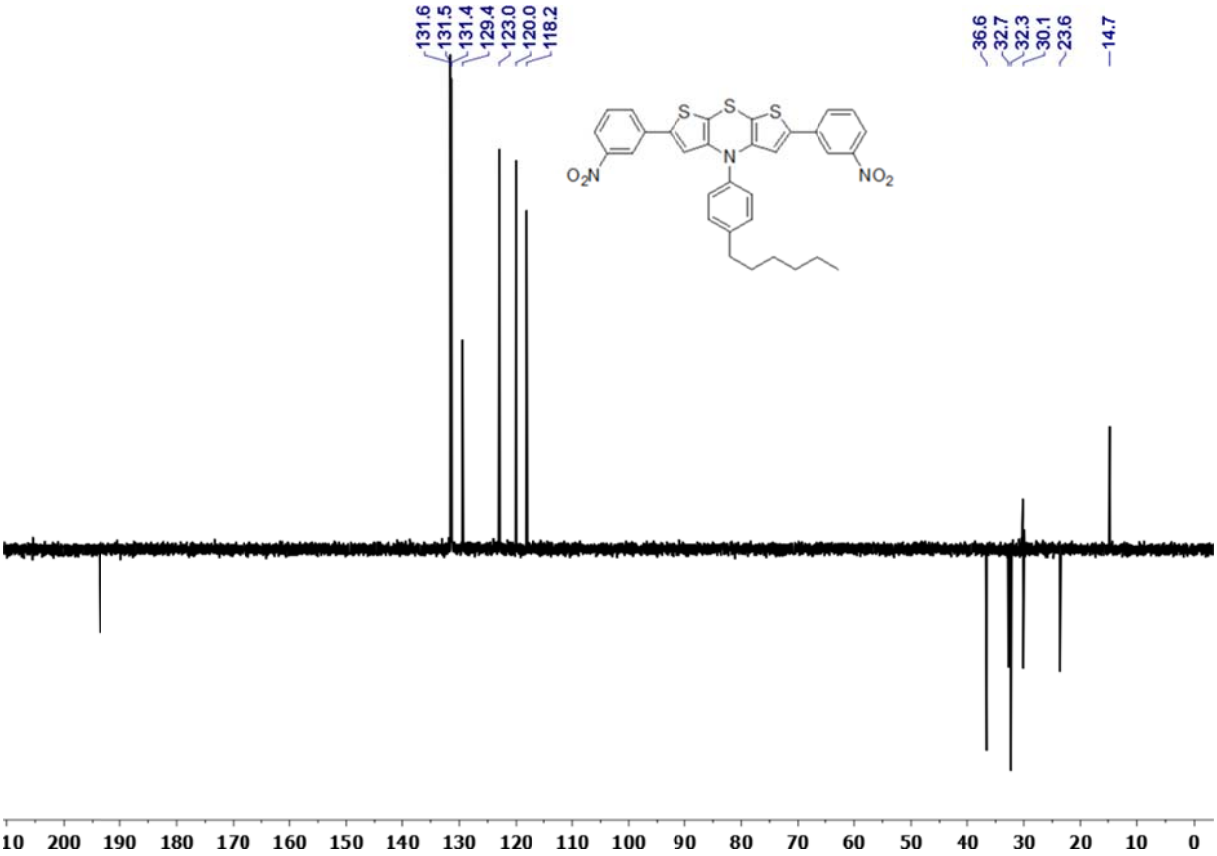
1.9 4-(4-Hexylphenyl)-2,6-bis(3-nitrophenyl)-4H-dithieno[2,3-b:3',2'-e][1,4]thiazine (3i)



[1]H-NMR (600 MHz) of **3i** (20 mg) in acetone-d_6/CS_2 1:1 at 313 K (δ in ppm).

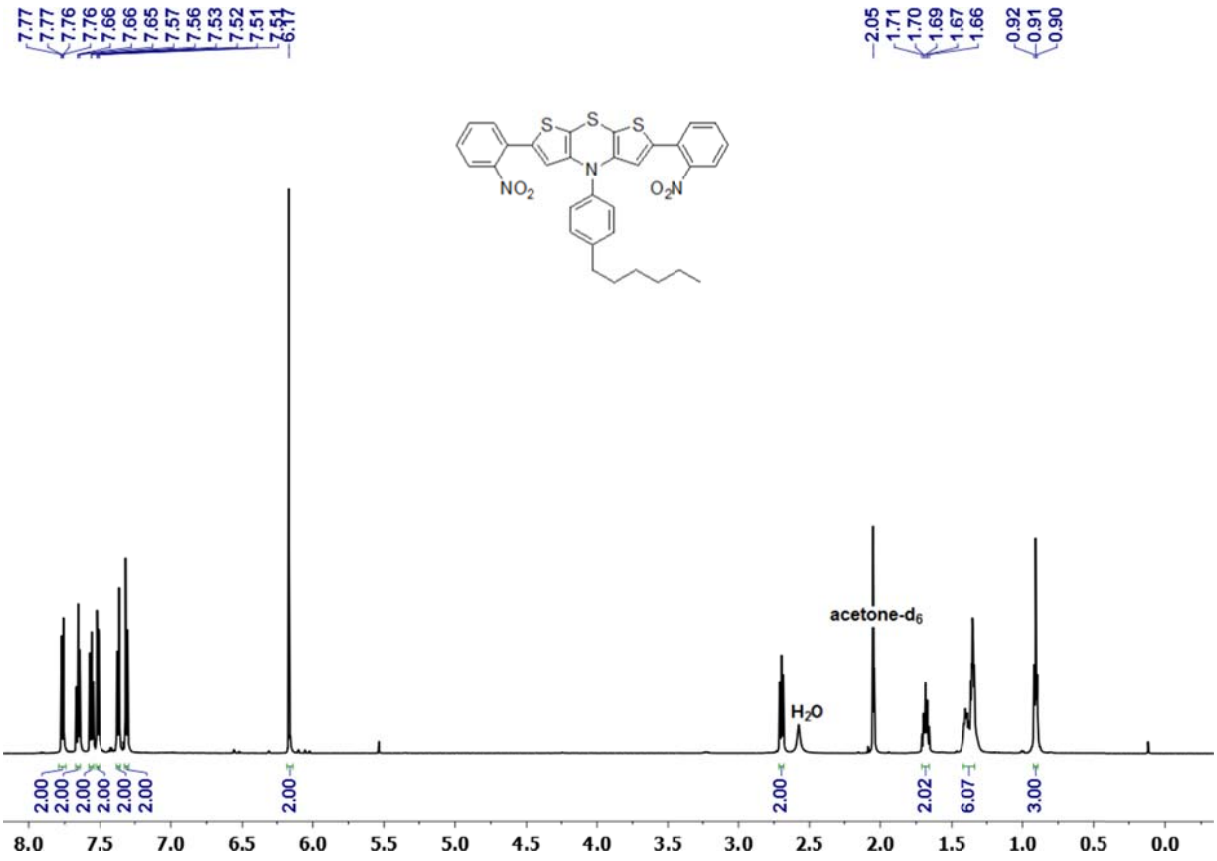


^{13}C-NMR (150 MHz) of **3i** (20 mg) in acetone-d_6/CS_2 1:1 at 313 K (δ in ppm).

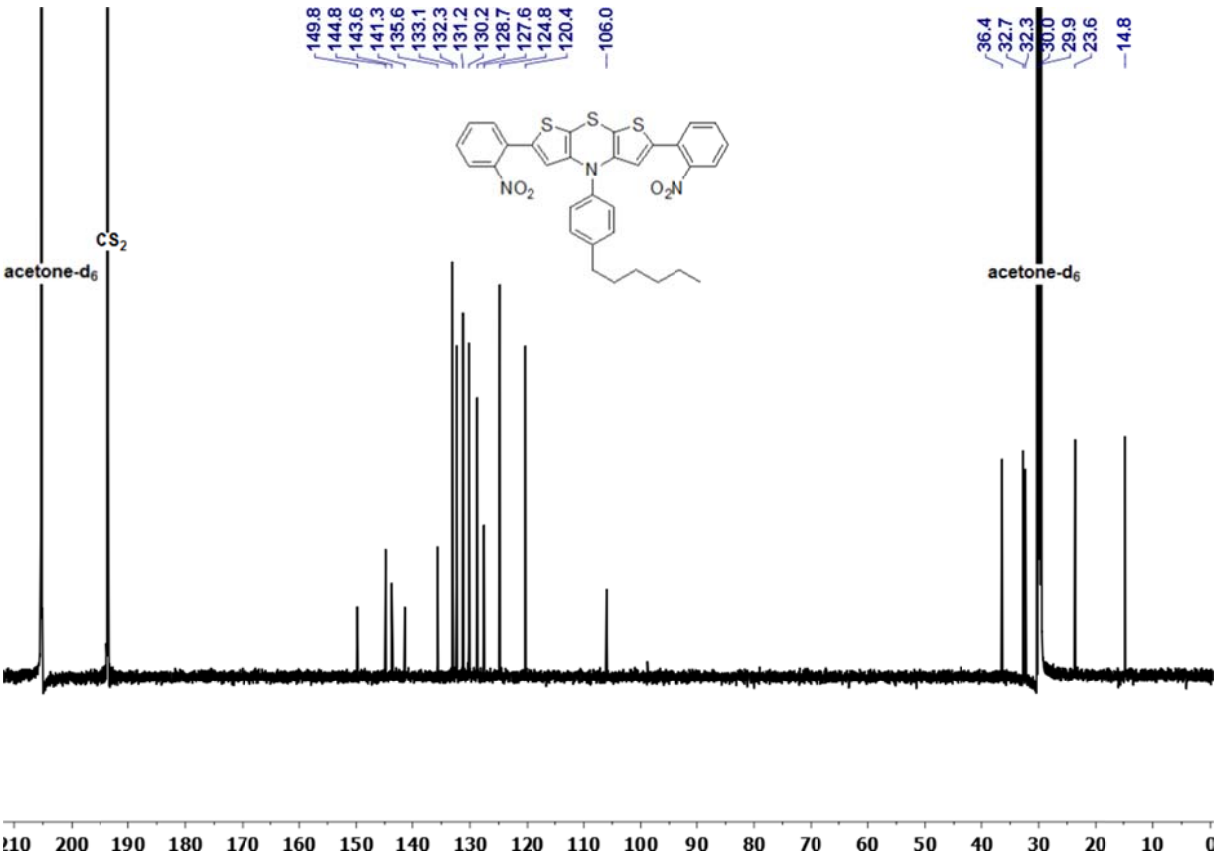


^{13}C-DEPT 135-NMR (150 MHz) of **3i** (20 mg) in acetone-d_6/CS_2 1:1 at 313 K (δ in ppm).

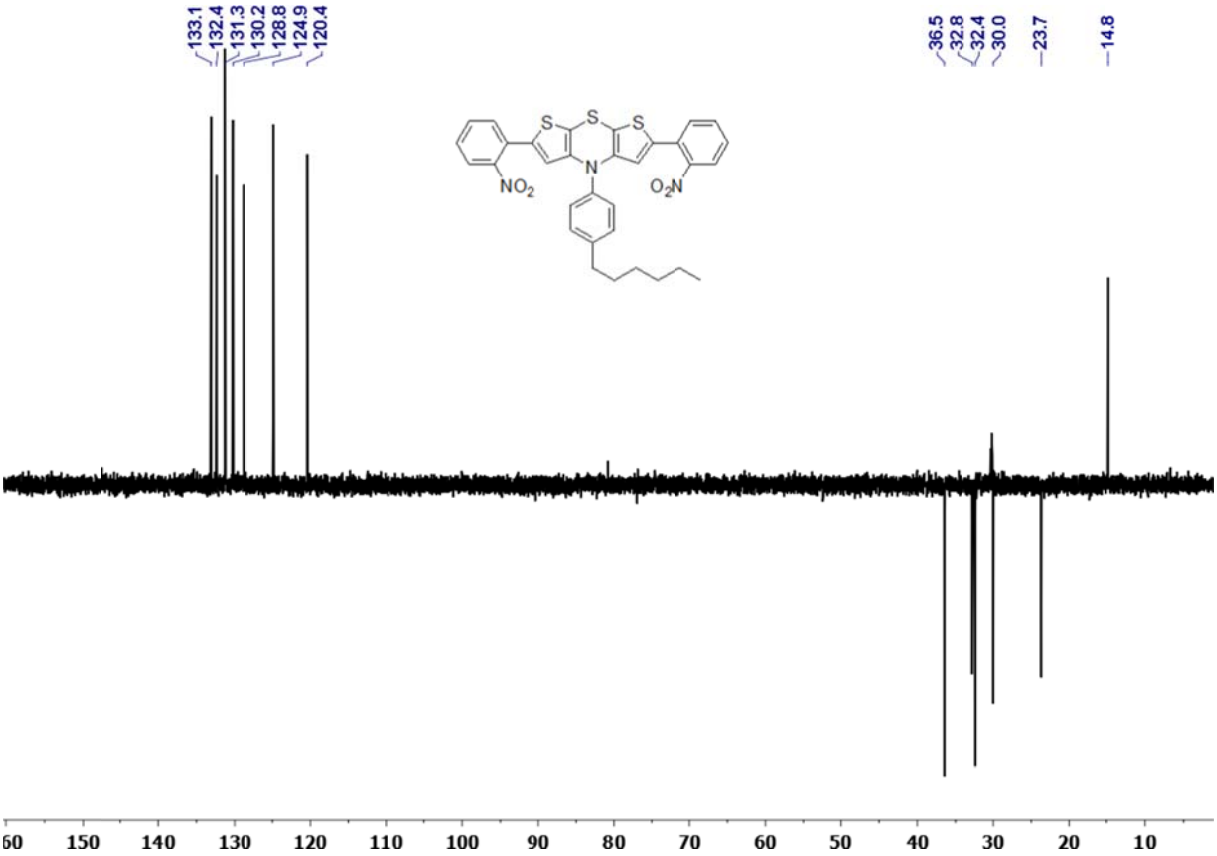
1.10 4-(4-Hexylphenyl)-2,6-bis(2-nitrophenyl)-4H-dithieno[2,3-b:3',2'-e][1,4]thiazine (3j)



[1]H-NMR (600 MHz) of **3j** (20 mg) in acetone-d_6/CS_2 1:1 at 298 K (δ in ppm).

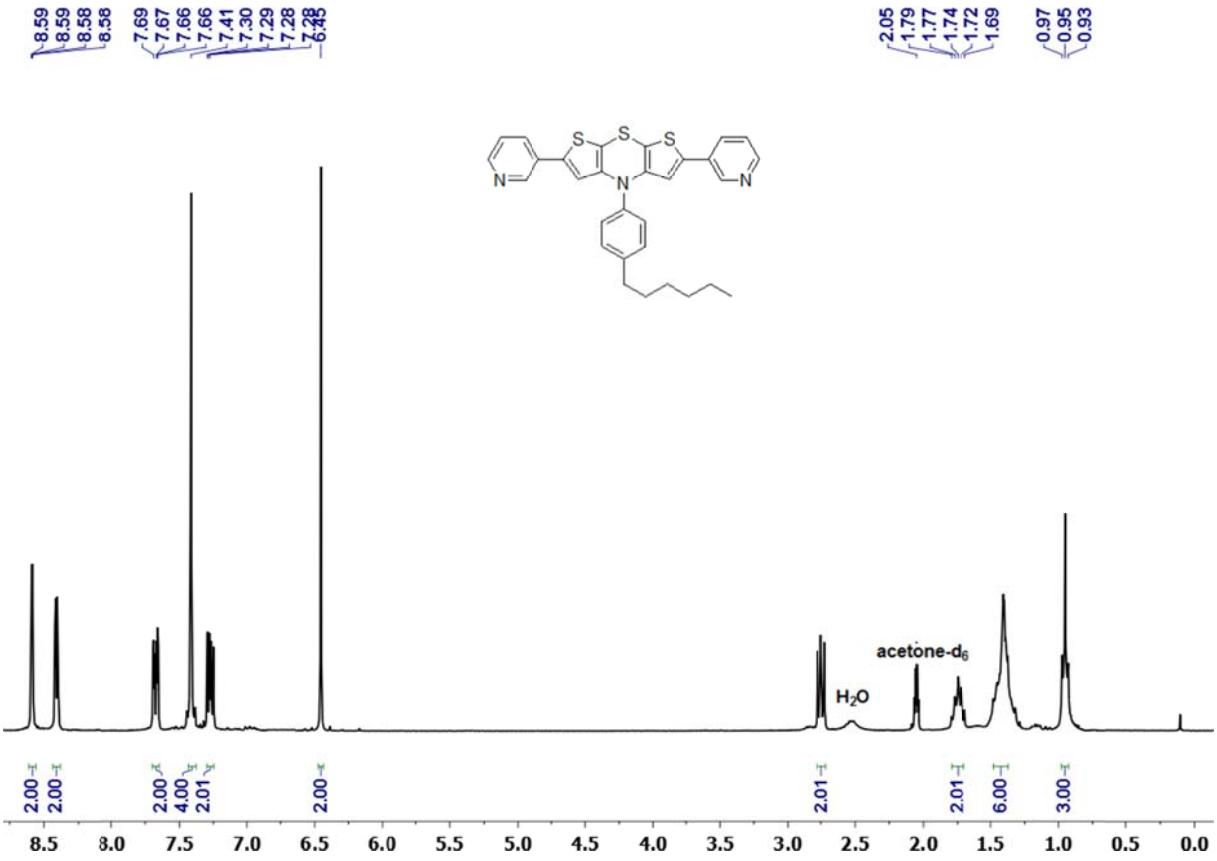


^{13}C-NMR (150 MHz) of **3j** (20 mg) in acetone-d_6/CS_2 1:1 at 298 K (δ in ppm).

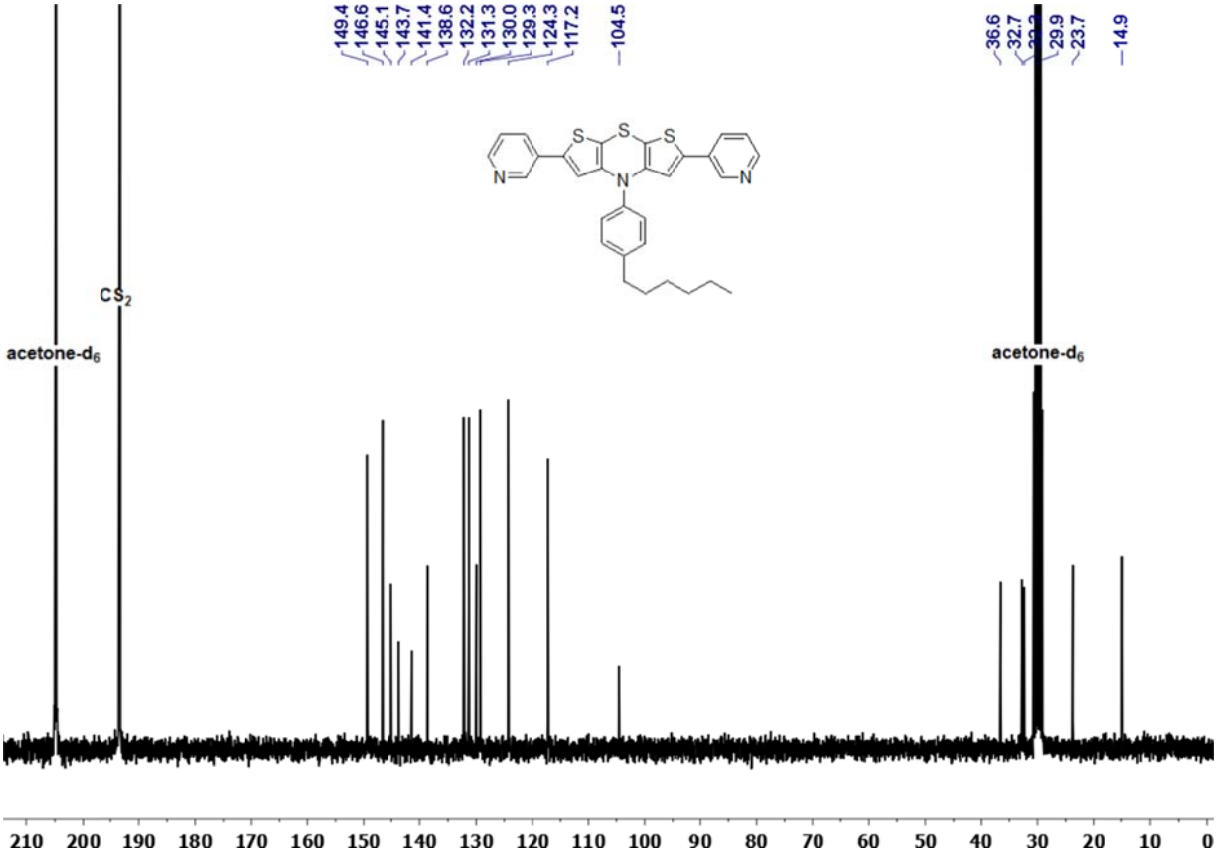


^{13}C-DEPT 135-NMR (150 MHz) of **3j** (20 mg) in acetone-d_6/CS_2 1:1 at 298 K (δ in ppm).

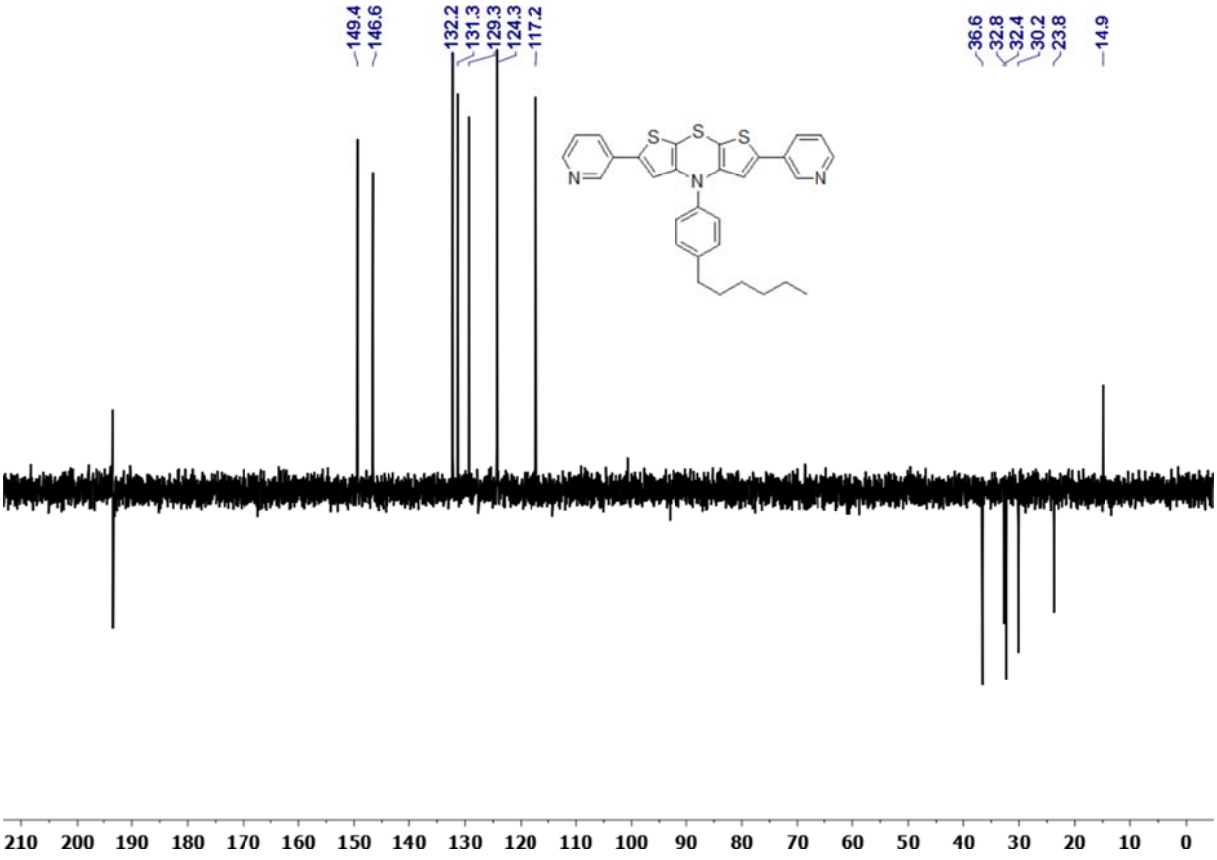
1.11 4-(4-Hexylphenyl)-2,6-di(pyridin-3-yl)-4H-dithieno[2,3-b:3',2'-e][1,4]thiazine (3k)



^{1}H-NMR (300 MHz) of **3k** (20 mg) in acetone-d_6/CS_2 1:1 at 298 K (δ in ppm).

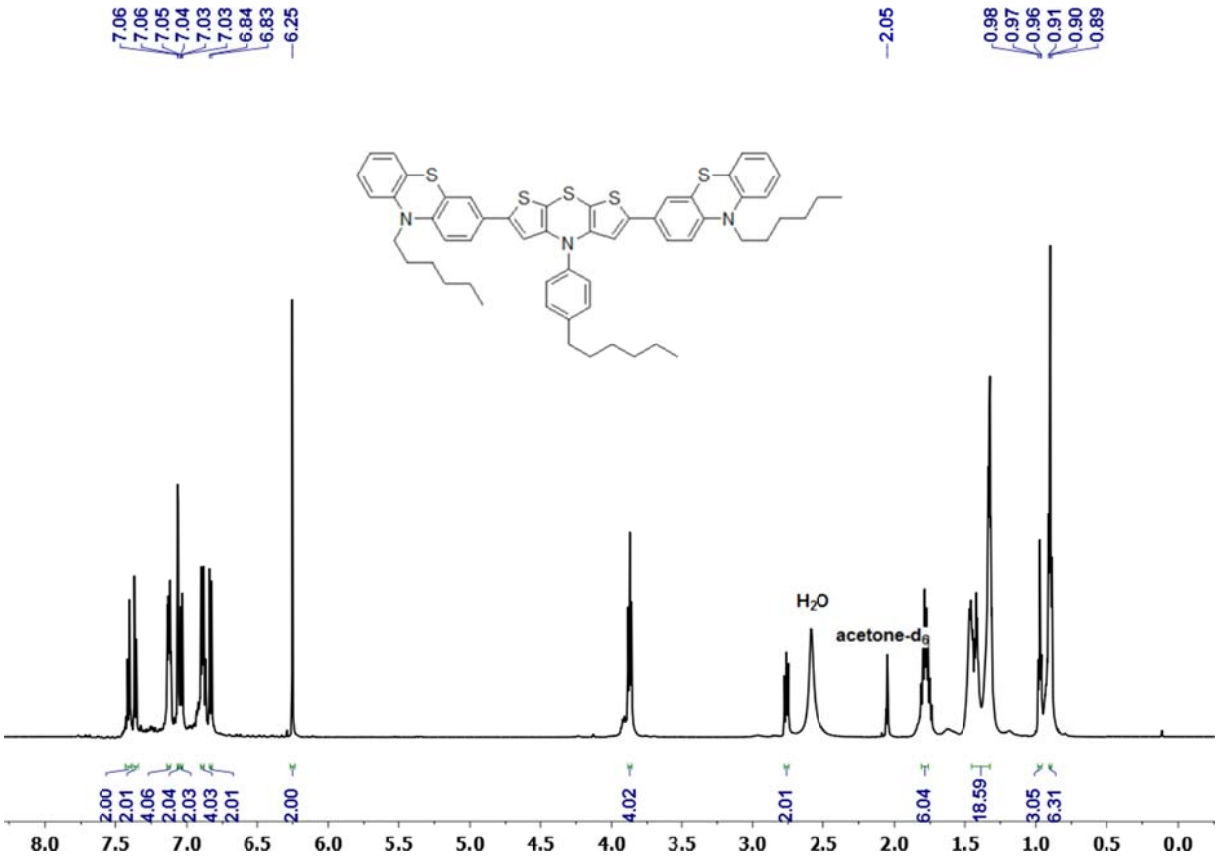


^{13}C-NMR (75 MHz) of **3k** (20 mg) in acetone-d_6/CS_2 1:1 at 298 K (δ in ppm).

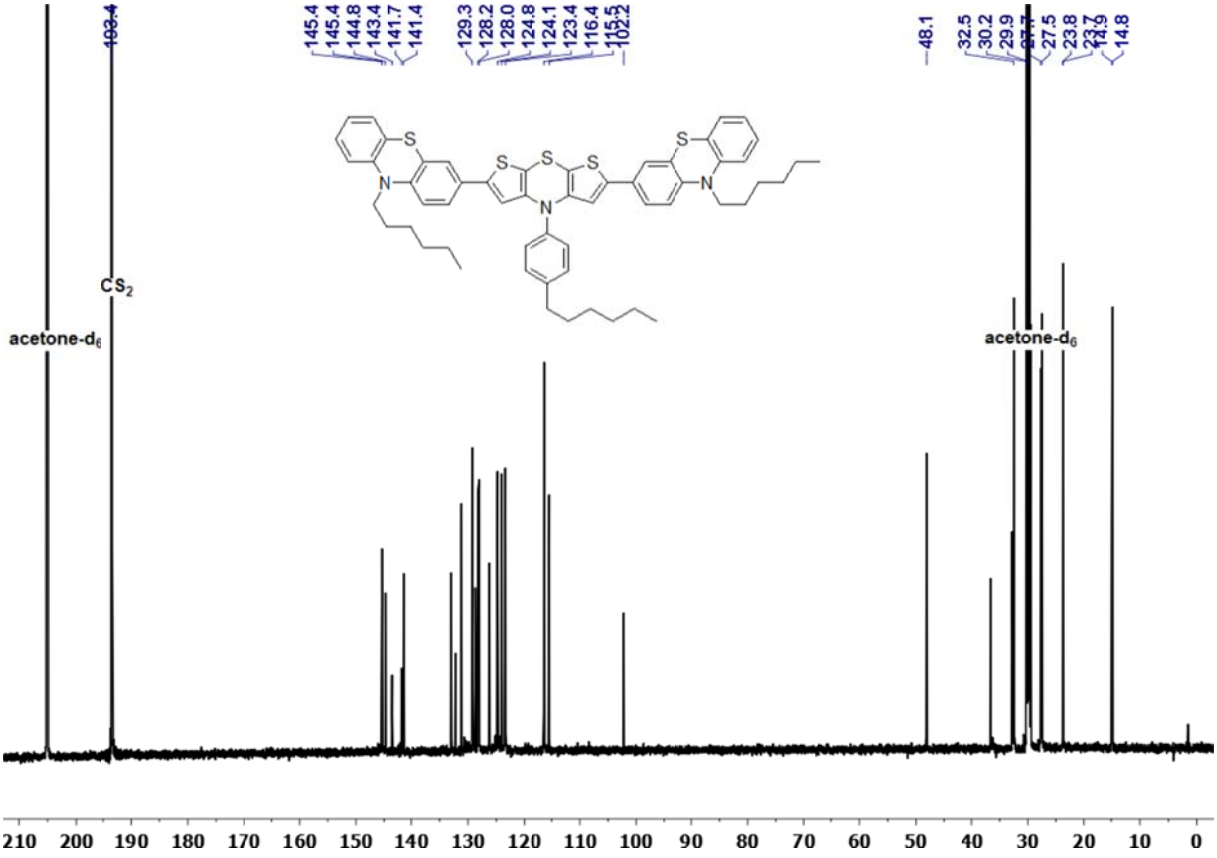


^{13}C-DEPT 135-NMR (75 MHz) of **3k** (20 mg) in acetone-d_6/CS_2 1:1 at 298 K (δ in ppm).

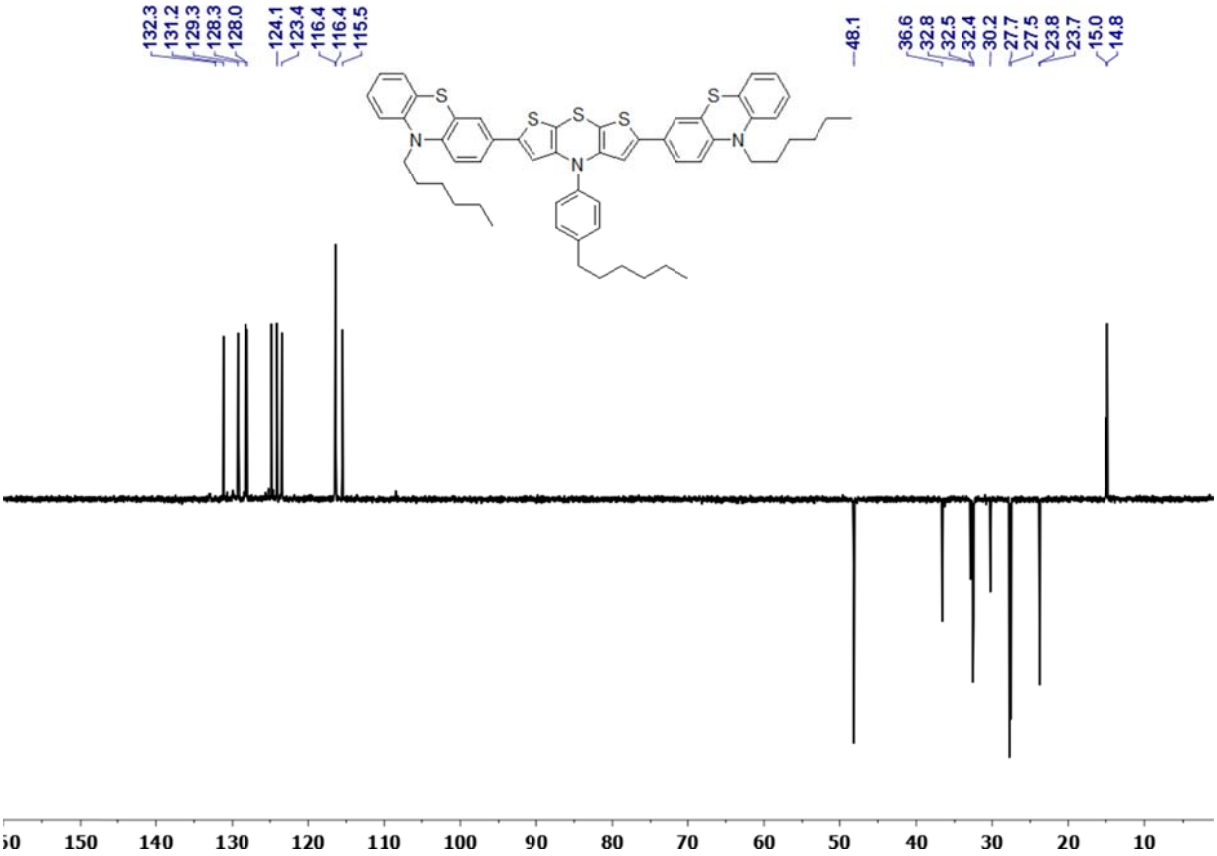
1.12 3,3'-(4-(4-Hexylphenyl)-4H-dithieno[2,3-b:3',2'-e][1,4]thiazine-2,6-diyl)bis(10-hexyl-10H-phenothiazine) (3l)



^{1}H-NMR (600 MHz) of **3l** (20 mg) in acetone-d_6/CS_2 1:2 at 298 K (δ in ppm).



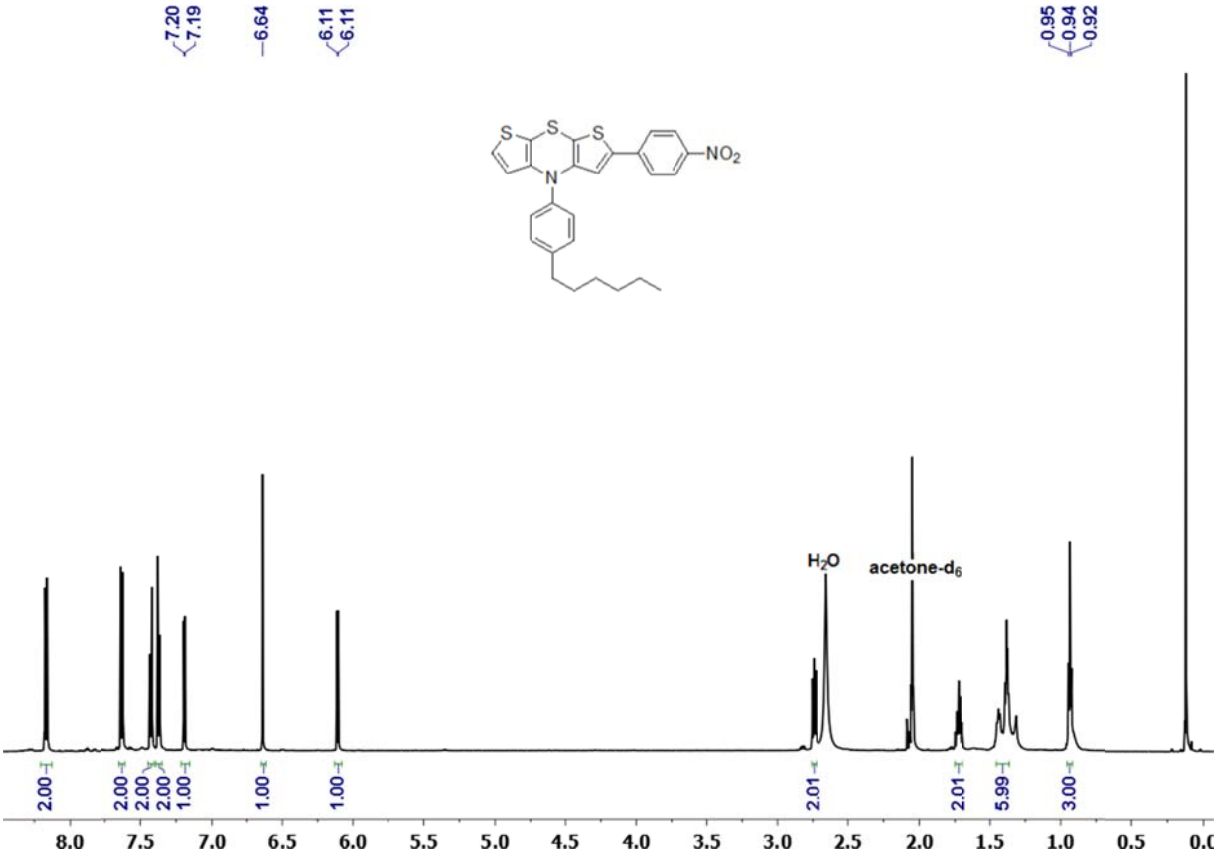
^{13}C-NMR (150 MHz) of **3l** (20 mg) in acetone-d_6/CS_2 1:2 at 298 K (δ in ppm).



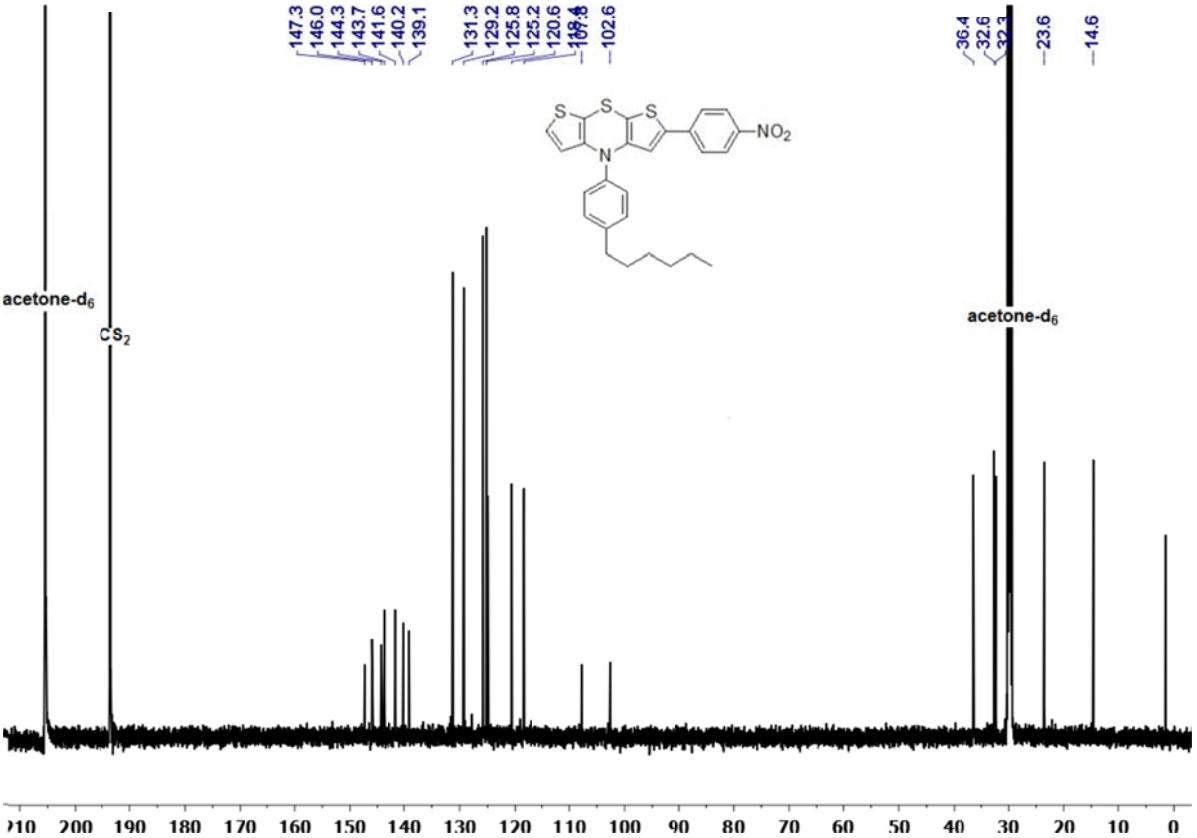
^{13}C-DEPT 135-NMR (150 MHz) of **3l** (20 mg) in acetone-d_6/CS_2 1:2 at 298 K (δ in ppm).

2 [1]H- and [13]C-NMR spectra of 2-(hetero)aryl dithienothiazines 6a-6c

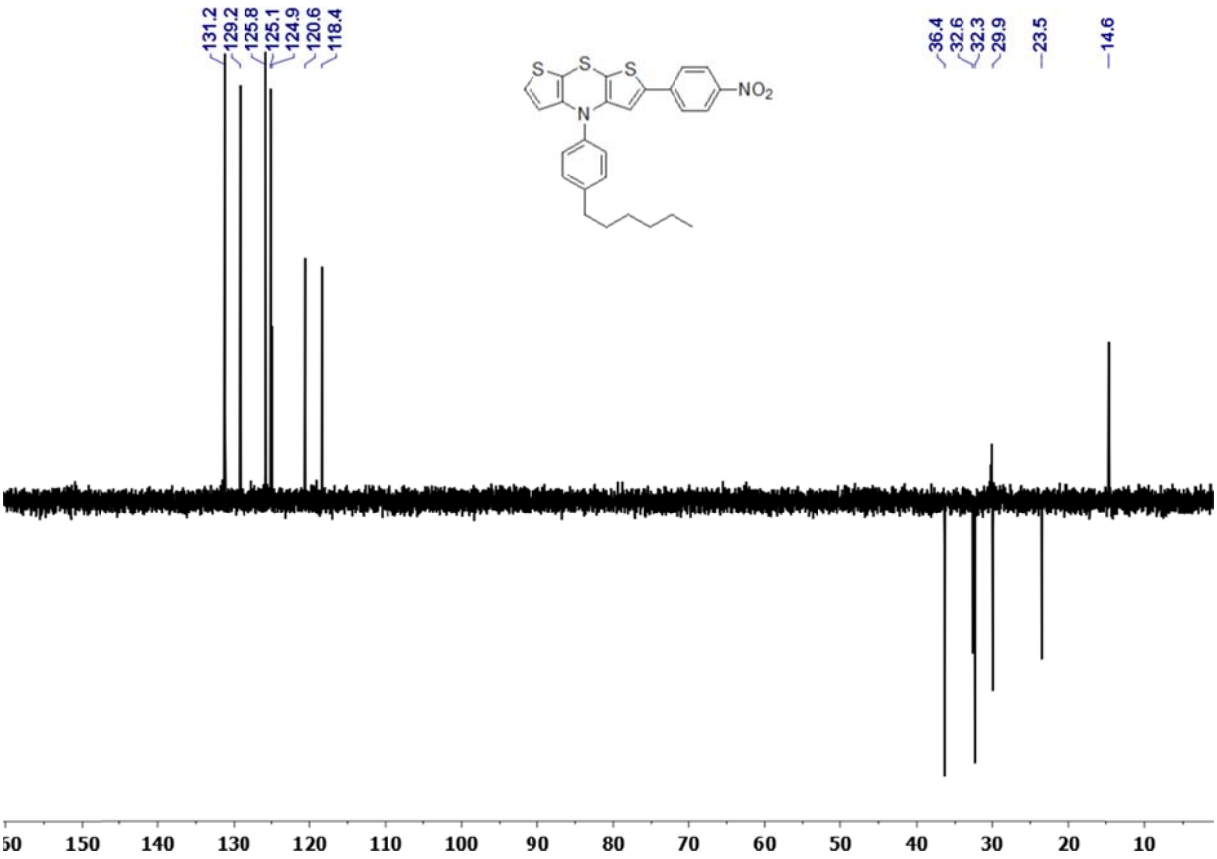
2.1 4-(4-Hexylphenyl)-2-(4-nitrophenyl)-4H-dithieno[2,3-b:3',2'-e][1,4]thiazine (6a)



[1]H-NMR (600 MHz) of **6a** (20 mg) in acetone-d_6/CS_2 2:1 at 298 K (δ in ppm).

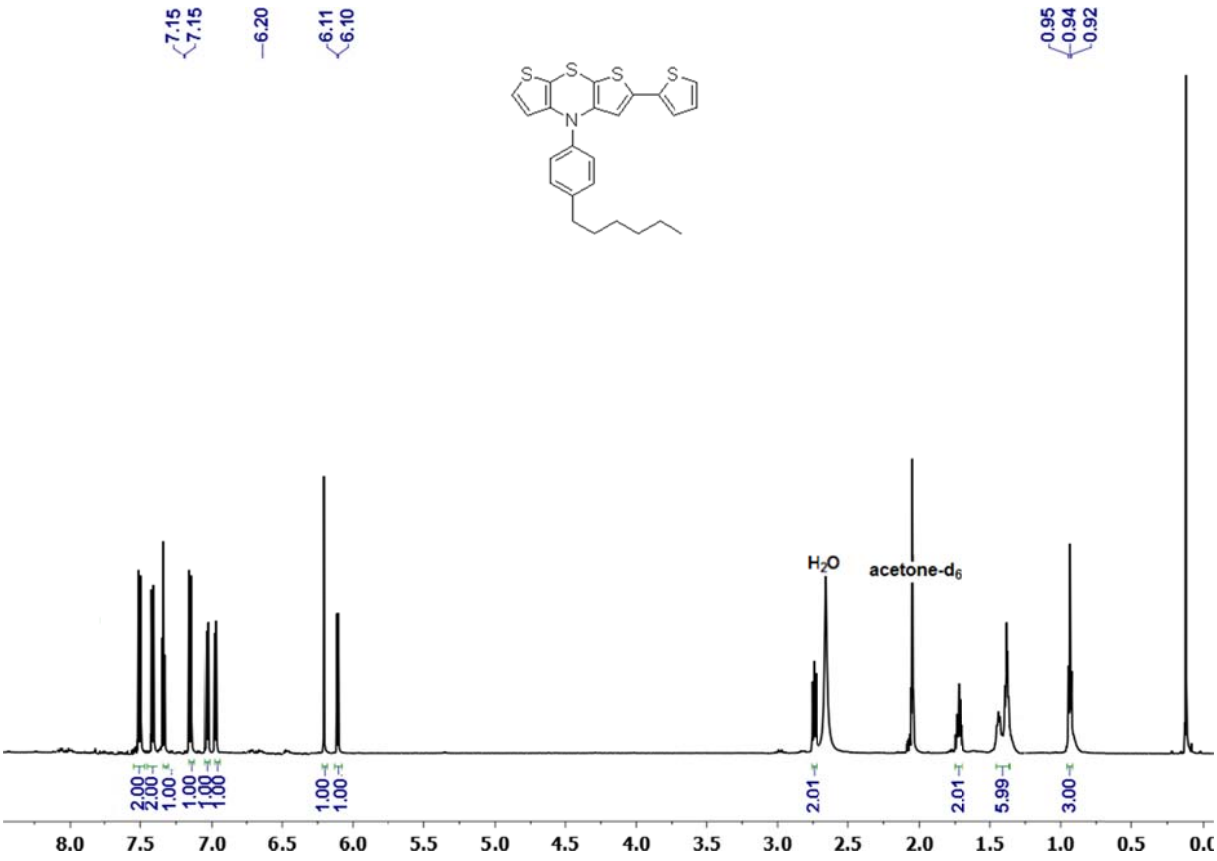


^{13}C-NMR (150 MHz) of **6a** (20 mg) in acetone-d_6/CS_2 2:1 at 298 K (δ in ppm).

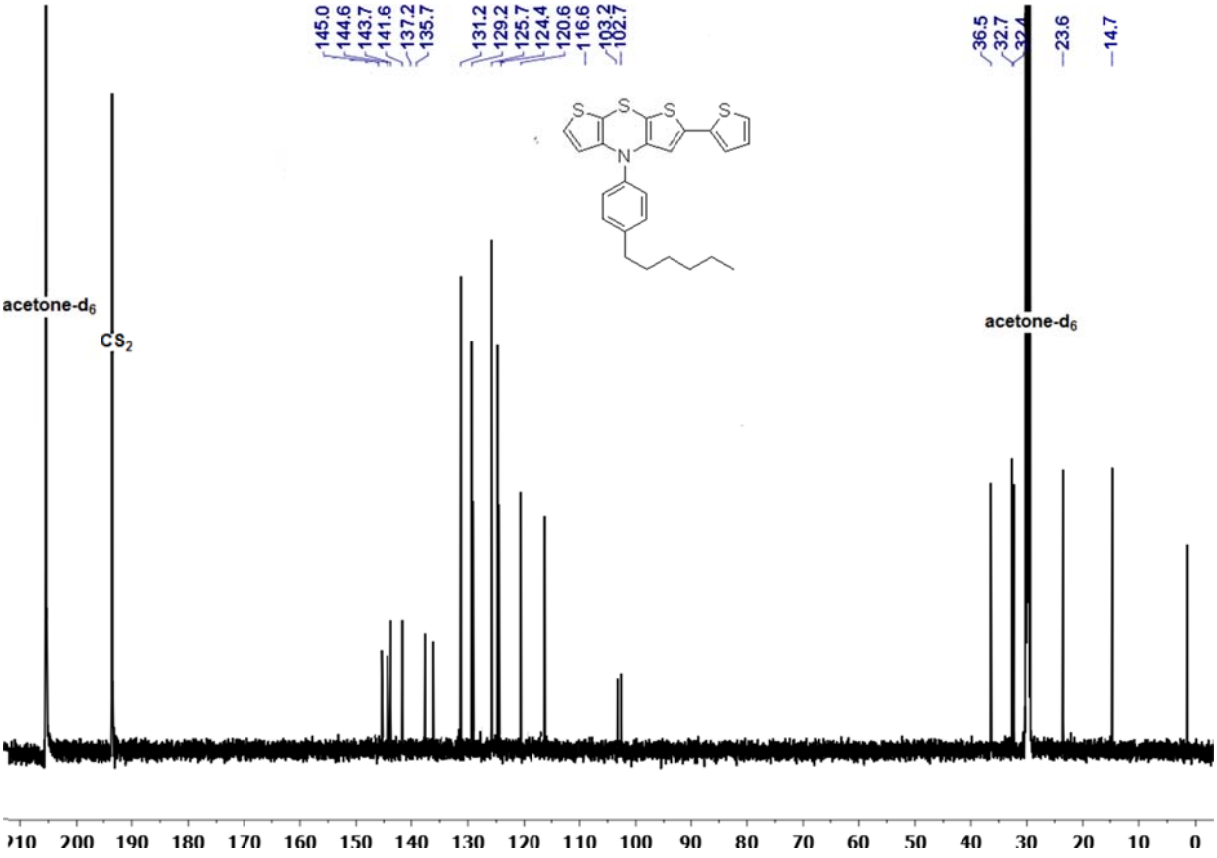


^{13}C-DEPT 135-NMR (150 MHz) of **6a** (20 mg) in acetone-d_6/CS_2 2:1 at 298 K (δ in ppm).

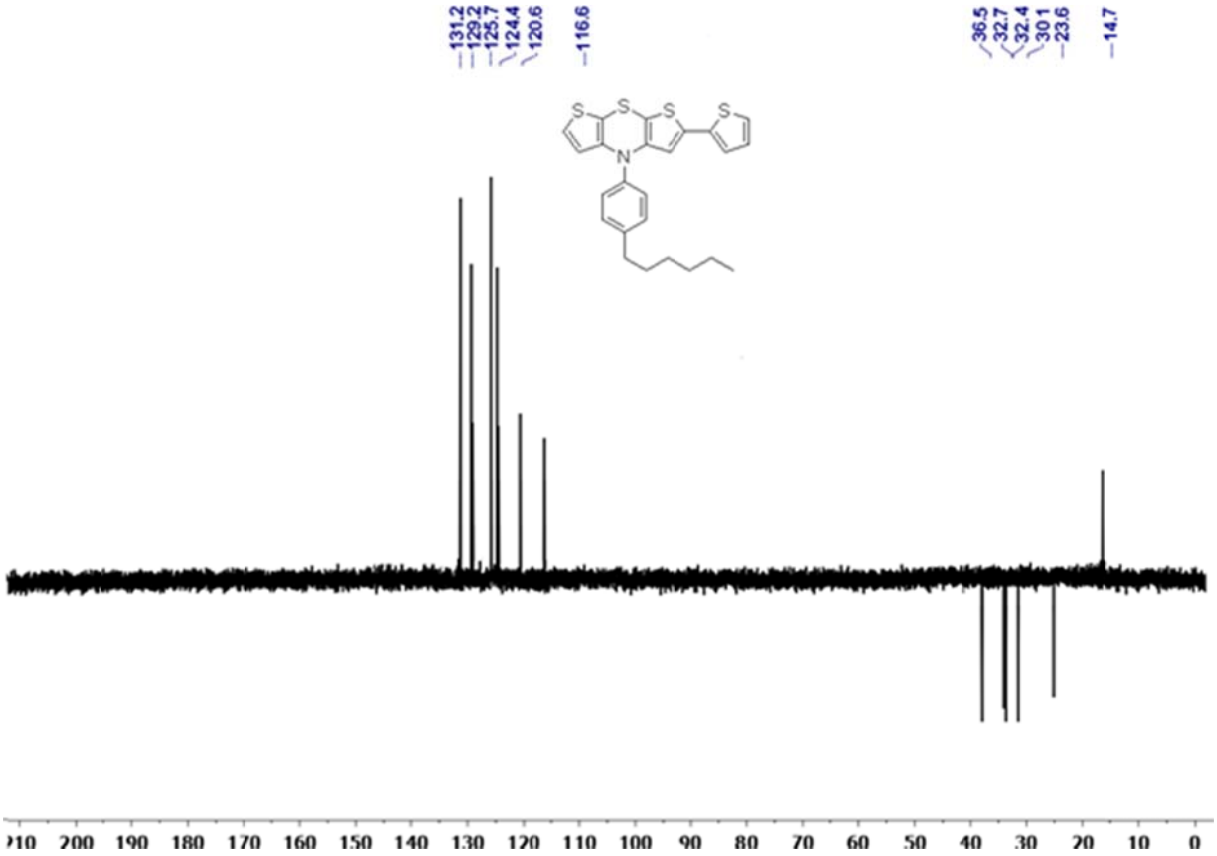
2.2 4-(4-Hexylphenyl)-2-(thiophen-2-yl)-4H-dithieno[2,3-b:3',2'-e][1,4]thiazine (6b)



^{1}H-NMR (600 MHz) of **6b** (20 mg) in ace**t**one-d_6/CS_2 5:1 at 298 K (δ in ppm).

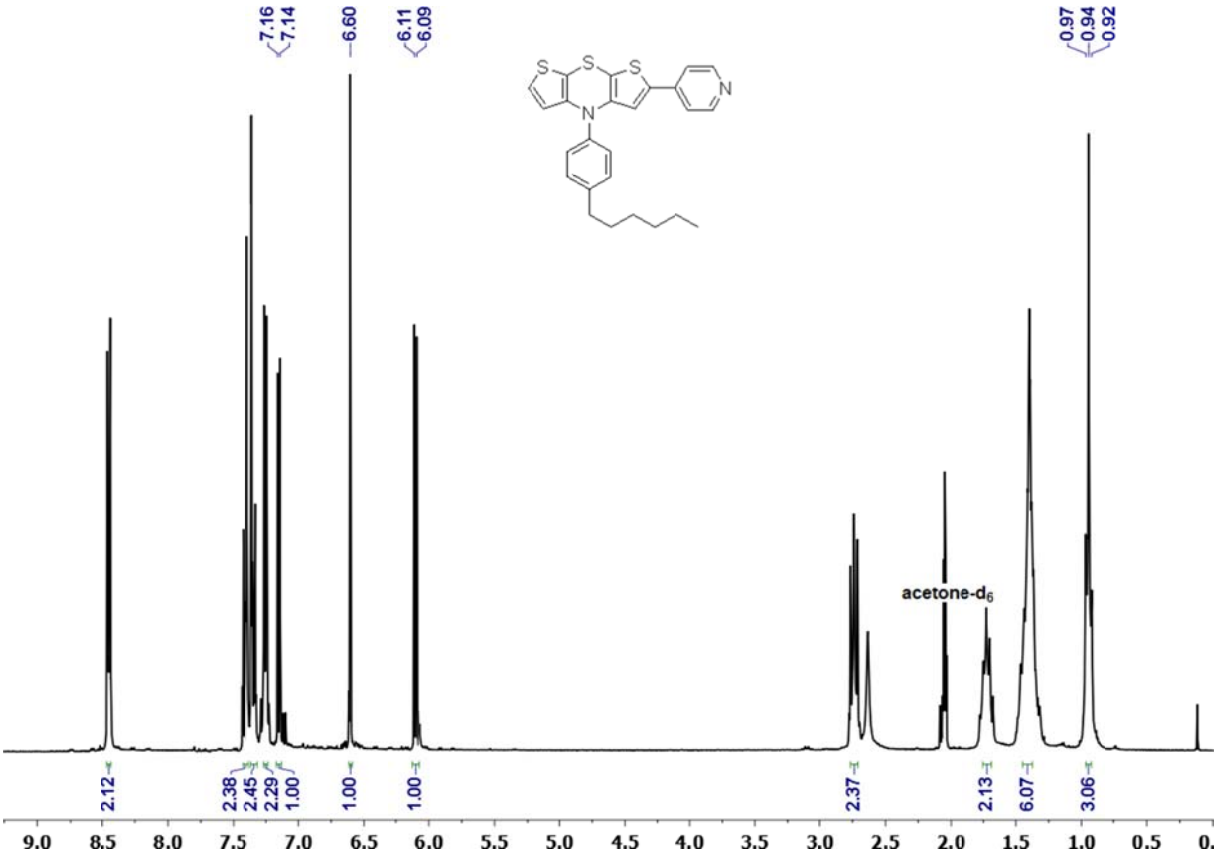


^{13}C-NMR (150 MHz) of **6b** (20 mg) in acetone-d_6/CS_2 5:1 at 298 K (δ in ppm).

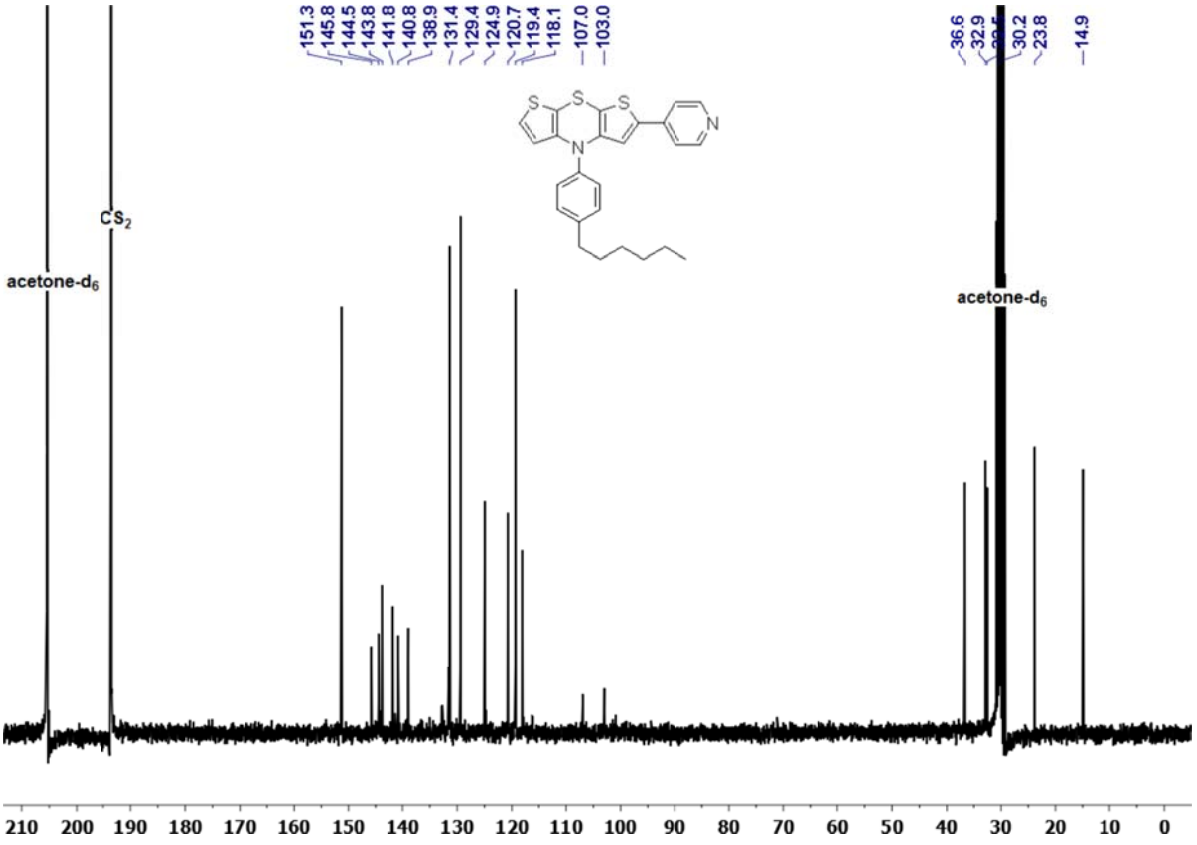


^{13}C-DEPT 135-NMR (150 MHz) of **6b** (20 mg) in acetone-d_6/CS_2 5:1 at 298 K (δ in ppm).

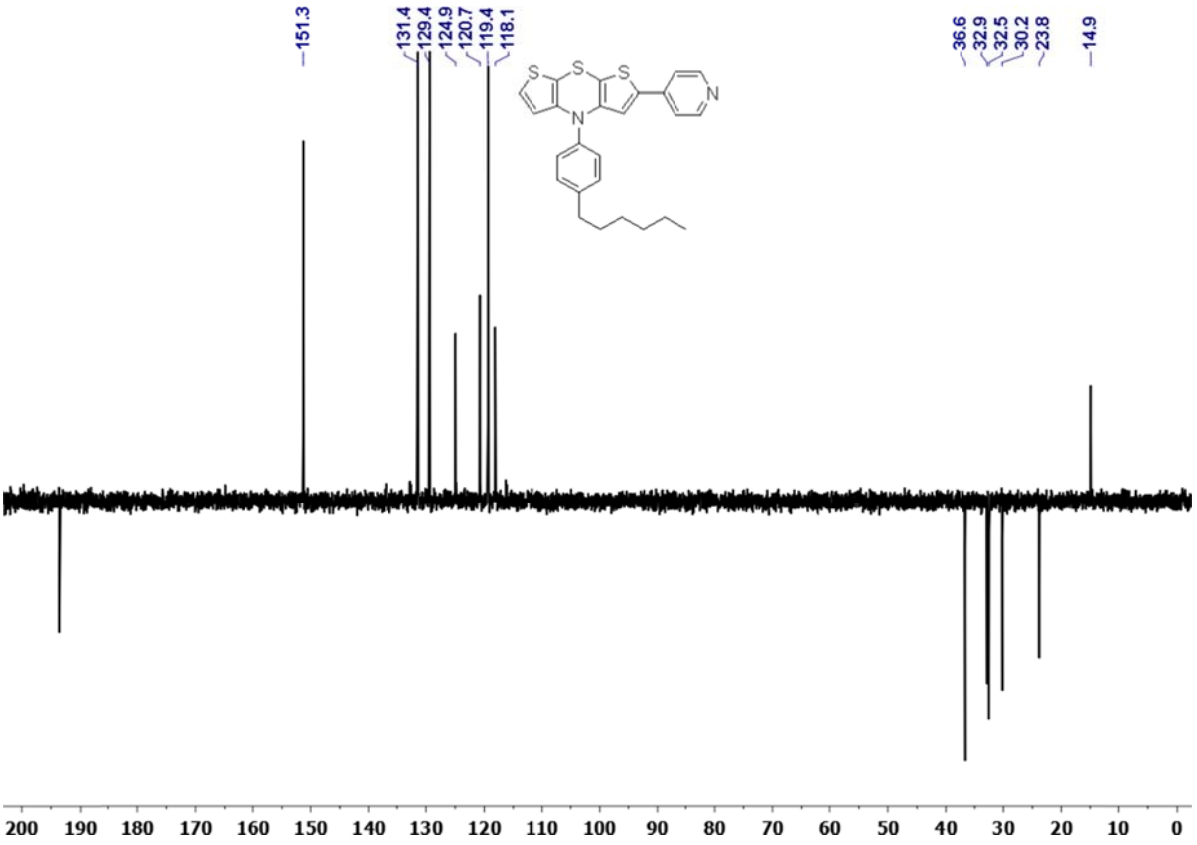
2.3 4-(4-Hexylphenyl)-2-(pyridin-4-yl)-4H-dithieno[2,3-b:3',2'-e][1,4]thiazine (6c)



^{1}H-NMR (300 MHz) of **6c** (20 mg) in acetone-d_6/CS_2 5:1 at 298 K (δ in ppm).



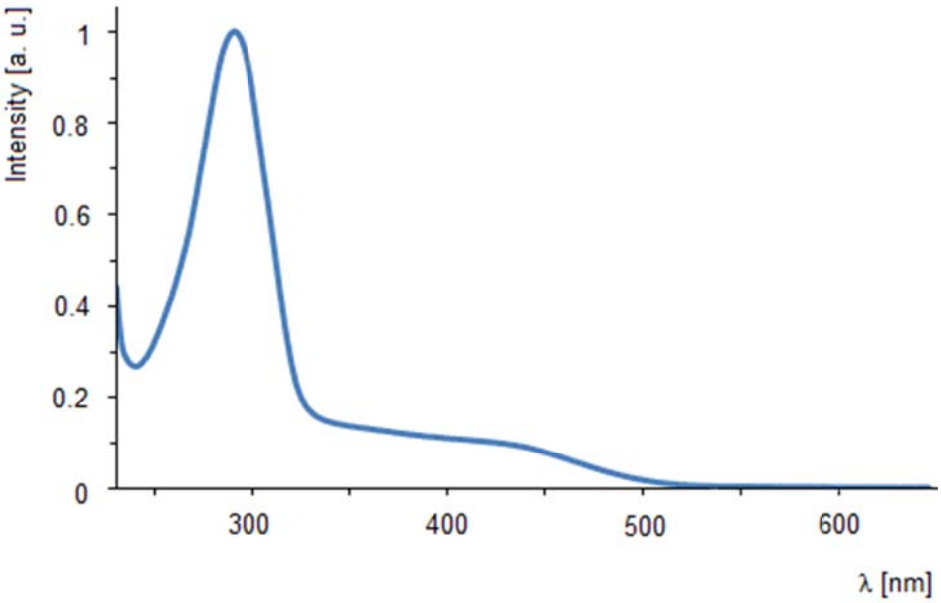
^{13}C-NMR (75 MHz) of **6c** (20 mg) in acetone-d_6/CS_2 5:1 at 298 K (δ in ppm).



^{13}C-DEPT 135-NMR (75 MHz) of **6c** (20 mg) in acetone-d_6/CS_2 5:1 at 298 K (δ in ppm).

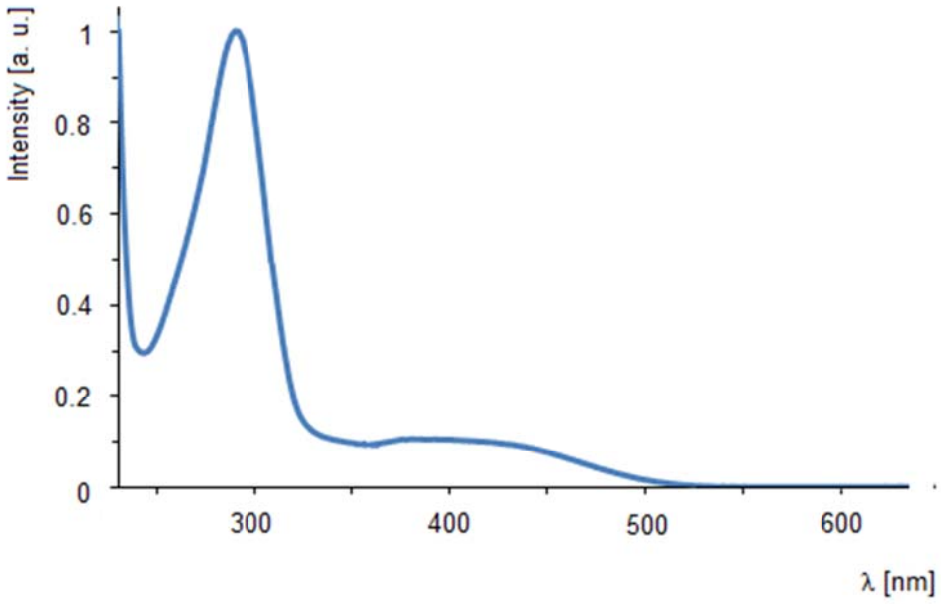
3 UV and fluorescence spectra of 2,6-di(hetero)aryl dithienothiazines 3a-3l

3.1 4-(4-Hexylphenyl)-2,6-bis(4-methoxyphenyl)-4H-dithieno[2,3-b:3',2'-e][1,4]thiazine (3a)



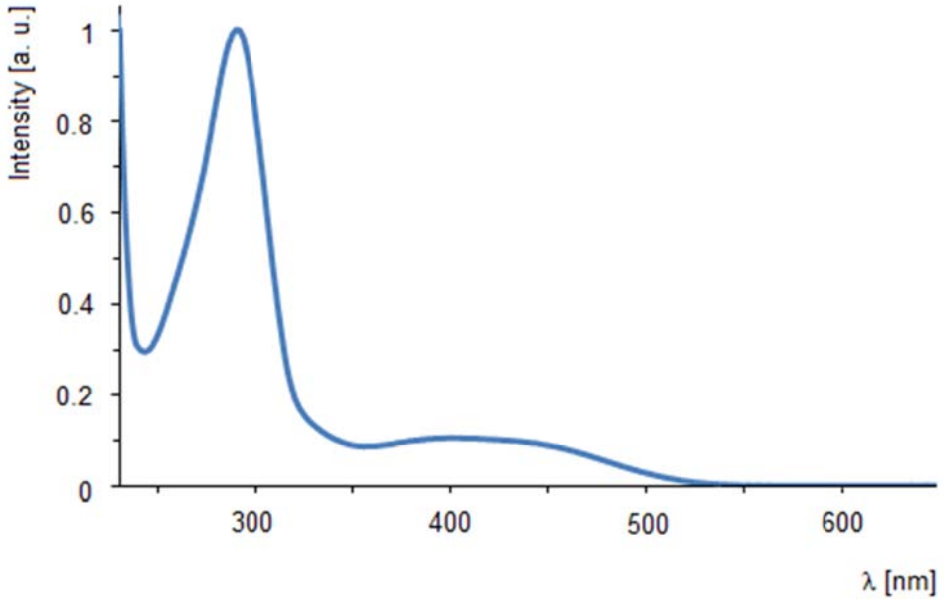
Normalized UV spectrum of **3a** in dichloromethane at 293 K.

3.2 4-(4-Hexylphenyl)-2,6-di-p-tolyl-4H-dithieno[2,3-b:3',2'-e][1,4]thiazine (3b)



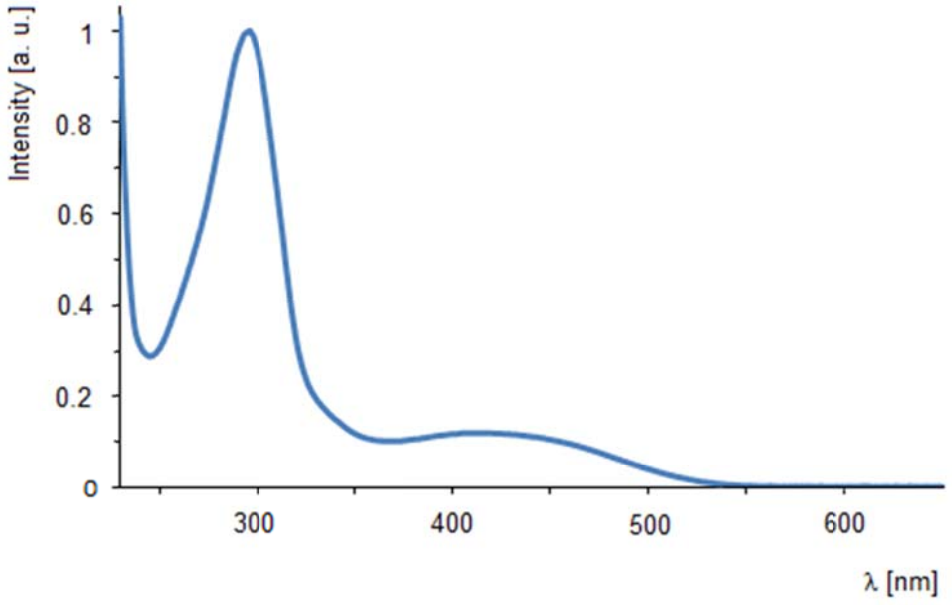
Normalized UV spectrum of **3b** in dichloromethane at 293 K.

3.3 4-(4-Hexylphenyl)-2,6-diphenyl-4H-dithieno[2,3-b:3',2'-e][1,4]thiazine (3c)



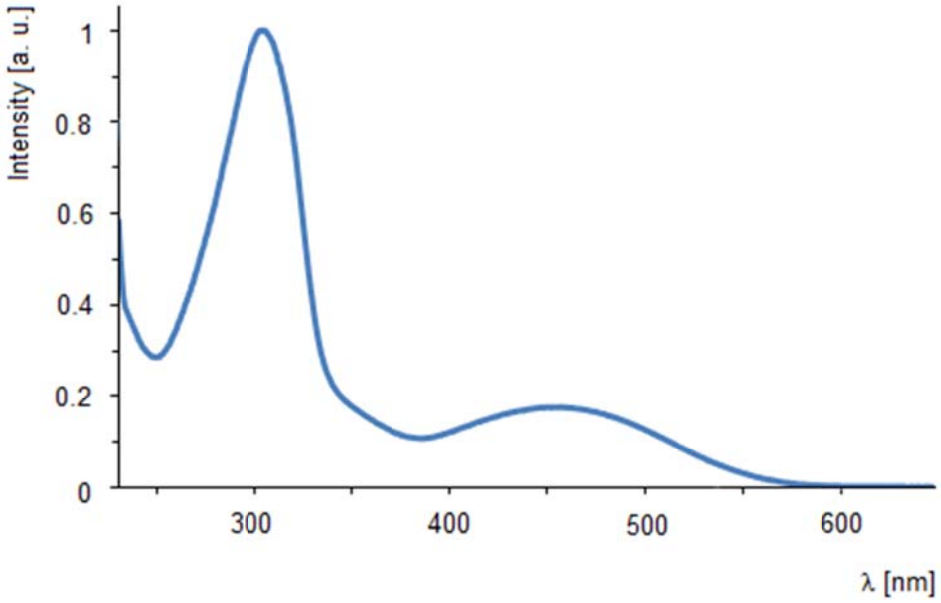
Normalized UV spectrum of **3c** in dichloromethane at 293 K.

3.4 2,6-Bis(4-chlorophenyl)-4-(4-hexylphenyl)-4H-dithieno [2,3-b:3',2'-e][1,4] thiazine (3d)



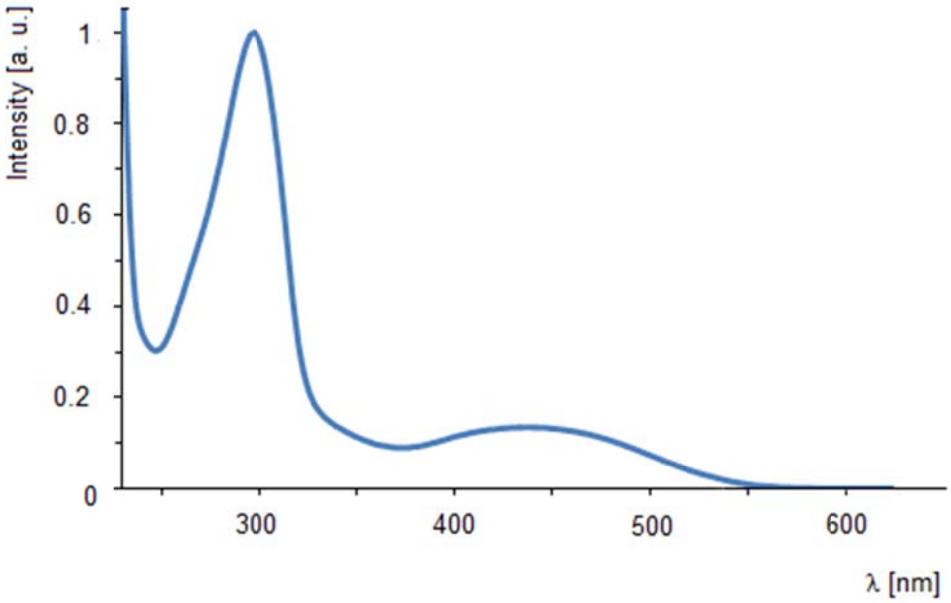
Normalized UV spectrum of **3d** in dichloromethane at 293 K.

3.5 Dimethyl 4,4'-(4-(4-hexylphenyl)-4H-dithieno[2,3-b:3',2'-e][1,4]thiazine-2,6-diyl)dibenzoate (3e)



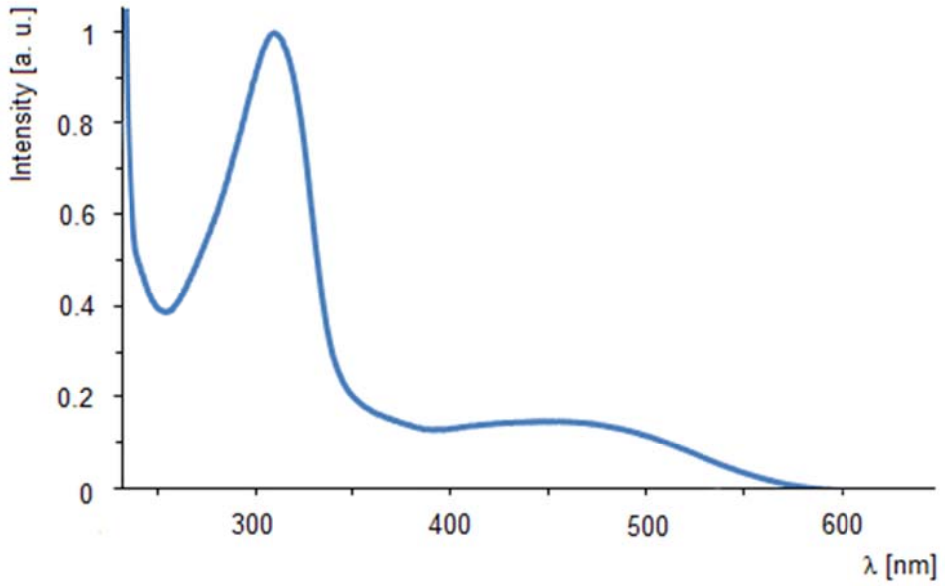
Normalized UV spectrum of **3e** in dichloromethane at 293 K.

3.6 4-(4-Hexylphenyl)-2,6-bis(4-(trifluoromethyl)phenyl)-4H-dithieno[2,3-b:3',2'-e][1,4]thiazine (3f)



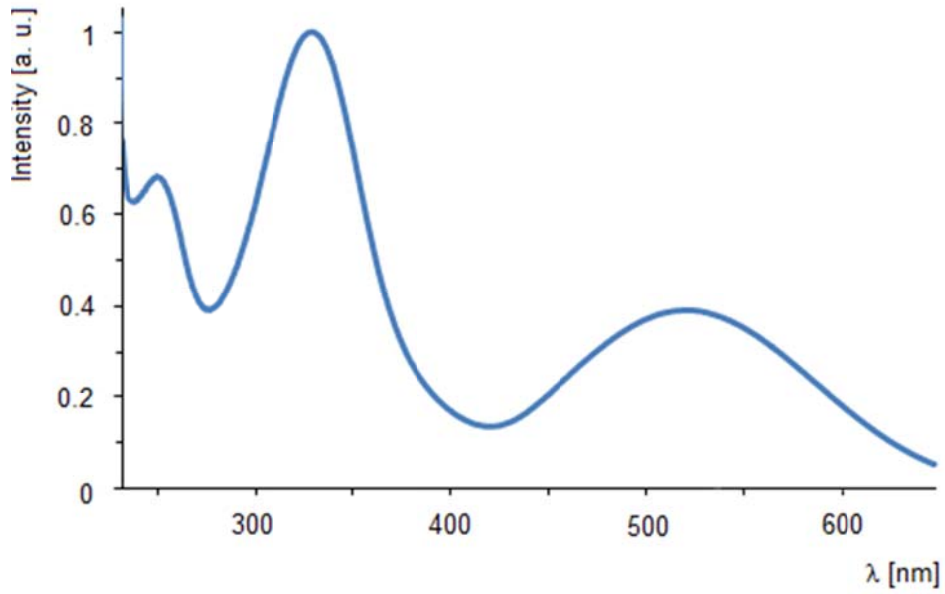
Normalized UV spectrum of **3f** in dichloromethane at 293 K.

3.7 4,4'-(4-(4-Hexylphenyl)-4H-dithieno[2,3-b:3',2'-e][1,4]thiazine-2,6-diyl)dibenzonitrile (3g)



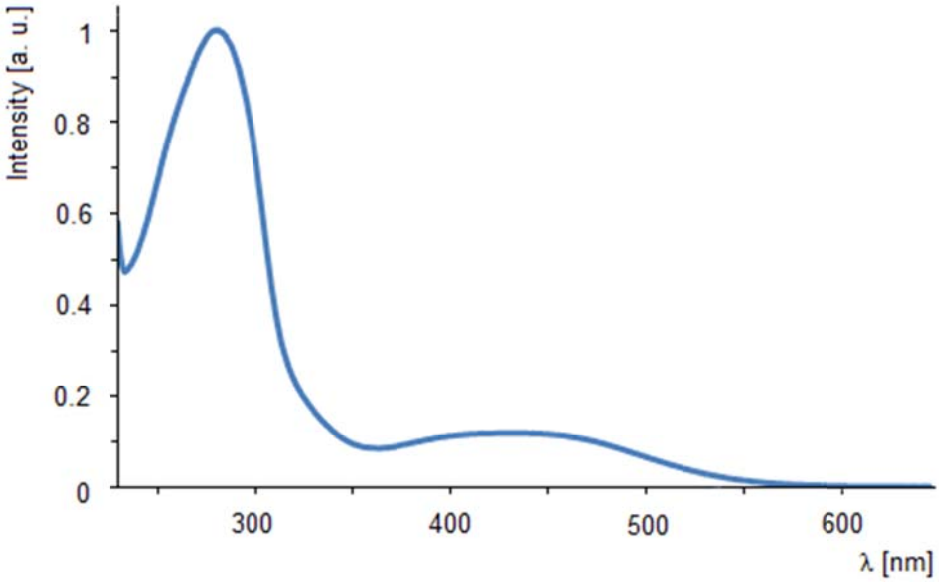
Normalized UV spectrum of **3g** in dichloromethane at 293 K.

3.8 4-(4-Hexylphenyl)-2,6-bis(4-nitrophenyl)-4H-dithieno[2,3-b:3',2'-e][1,4]thiazine (3h)



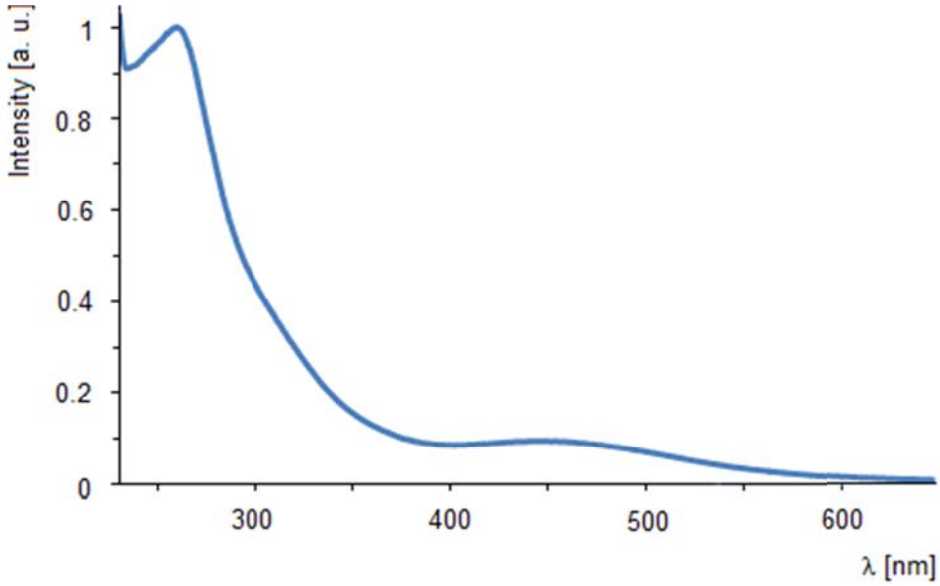
Normalized UV spectrum of **3h** in dichloromethane at 293 K.

3.9 4-(4-Hexylphenyl)-2,6-bis(3-nitrophenyl)-4H-dithieno[2,3-b:3',2'-e][1,4]thiazine (3i)



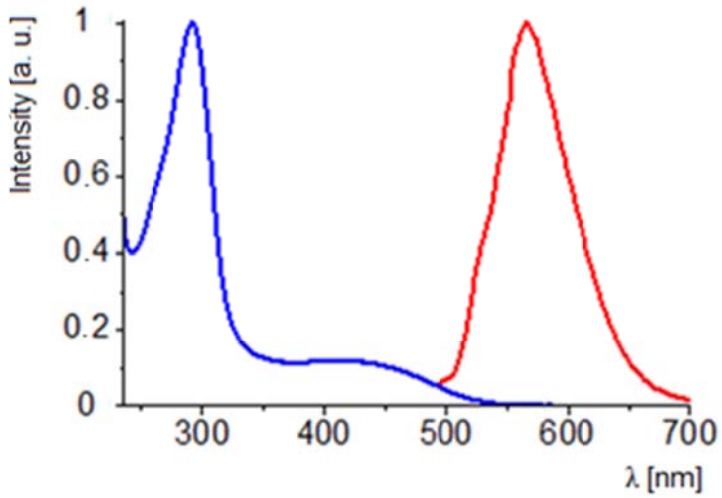
Normalized UV spectrum of **3h** in dichloromethane at 293 K.

3.10 4-(4-Hexylphenyl)-2,6-bis(2-nitrophenyl)-4H-dithieno[2,3-b:3',2'-e][1,4]thiazine (3j)



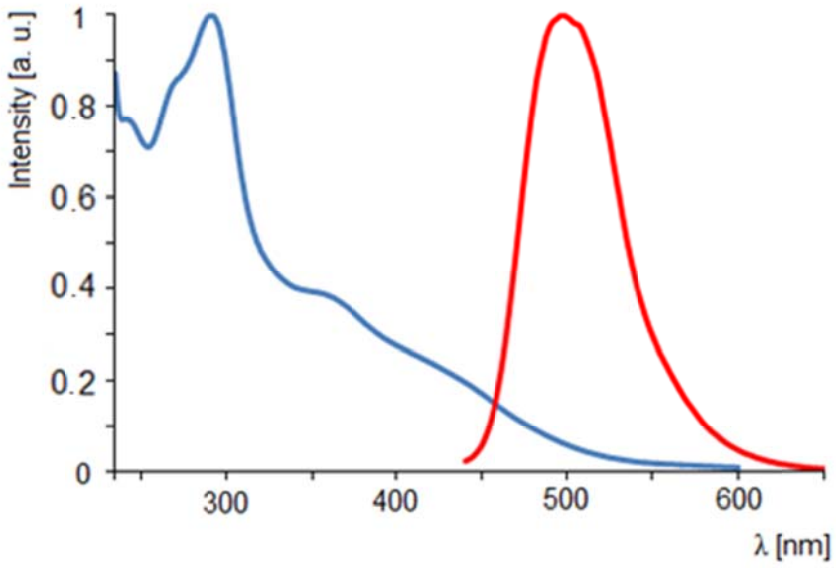
Normalized UV spectrum of **3i** in dichloromethane at 293 K.

3.11 4-(4-Hexylphenyl)-2,6-di(pyridin-3-yl)-4H-dithieno[2,3-b:3',2'-e][1,4]thiazine (3k)



Normalized absorption (blue) and emission (red) spectra of **3k** ($\lambda_{max,exc}$ = 380 nm) in dichloromethane at 293 K.

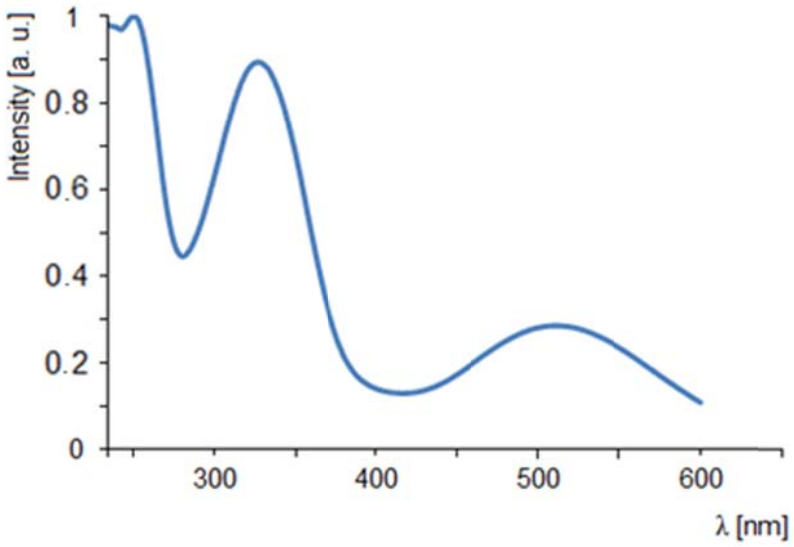
3.12 3,3'-(4-(4-Hexylphenyl)-4H-dithieno[2,3-b:3',2'-e][1,4]thiazine-2,6-diyl)bis(10-hexyl-10H-phenothiazine) (3l)



Normalized absorption (blue) and emission (red) spectra of **3l** ($\lambda_{max,exc}$ = 420 nm) in dichloromethane at 293 K.

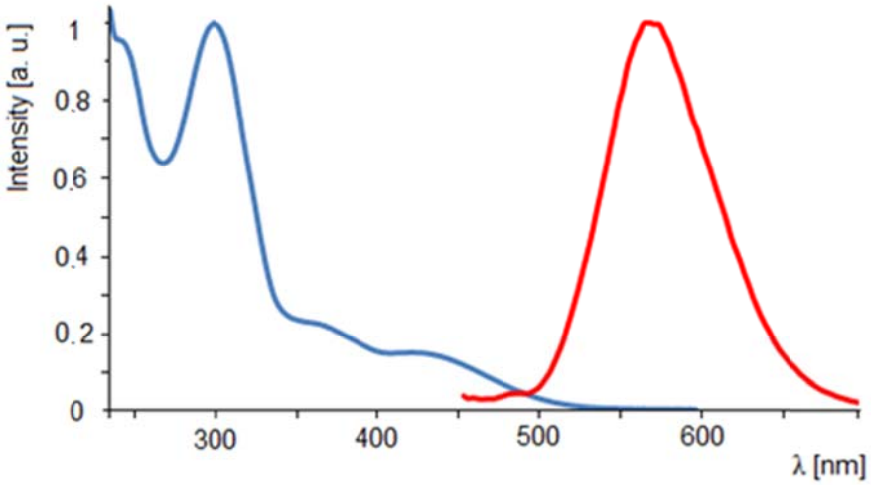
4 UV and fluorescence spectra of 2-(hetero)aryl dithienothiazines 6a-6c

4.1 4-(4-Hexylphenyl)-2-(4-nitrophenyl)-4H-dithieno[2,3-b:3',2'-e][1,4]thiazine (6a)



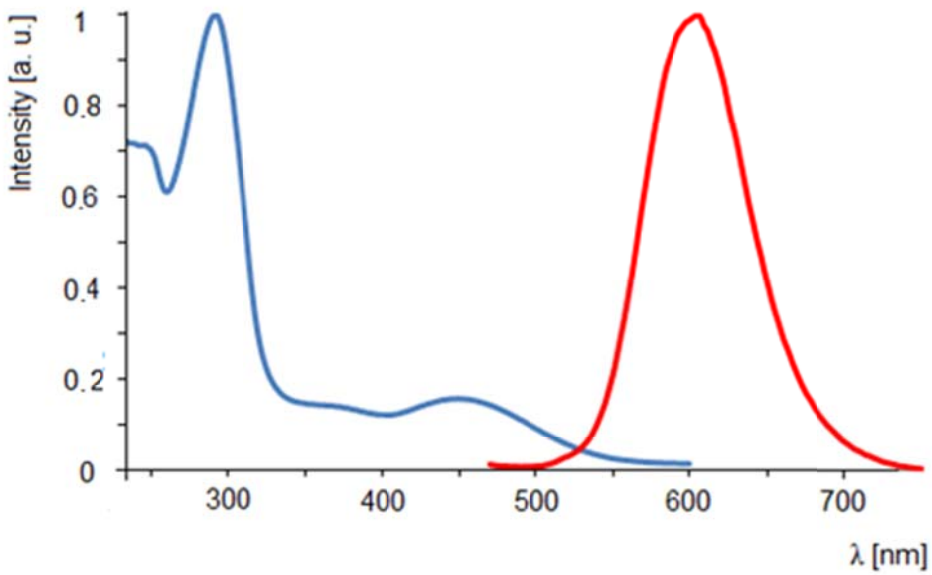
Normalized UV spectrum of **6a** in dichloromethane at 293 K.

4.2 4-(4-Hexylphenyl)-2-(thiophen-2-yl)-4H-dithieno[2,3-b:3',2'-e][1,4]thiazine (6b)



Normalized absorption (blue) and emission (red) spectra of **6b** ($\lambda_{max,exc}$ = 425 nm) in dichloromethane at 293 K.λ

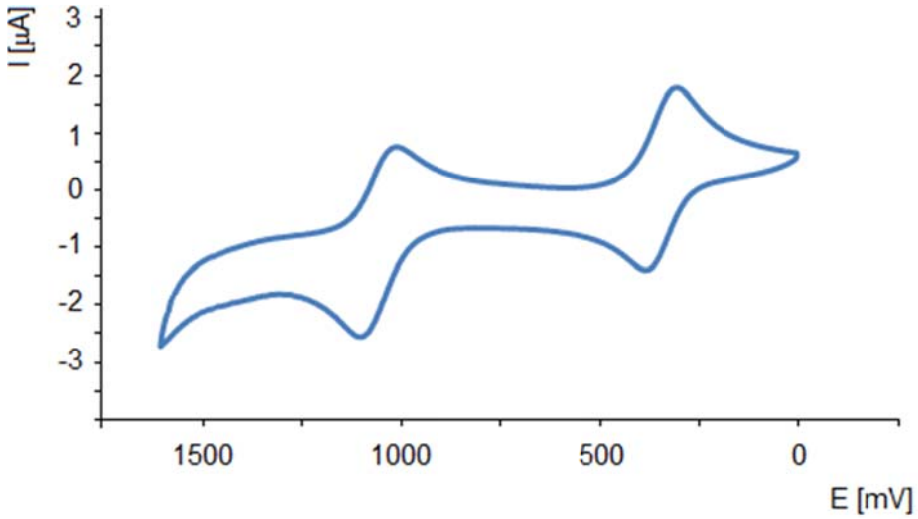
4.3 4-(4-Hexylphenyl)-2-(pyridin-4-yl)-4H-dithieno[2,3-b:3',2'-e][1,4]thiazine (6c)



Normalized absorption (blue) and emission (red) spectra of **6c** ($\lambda_{max,exc}$ = 450 nm) in dichloromethane at 293 K.

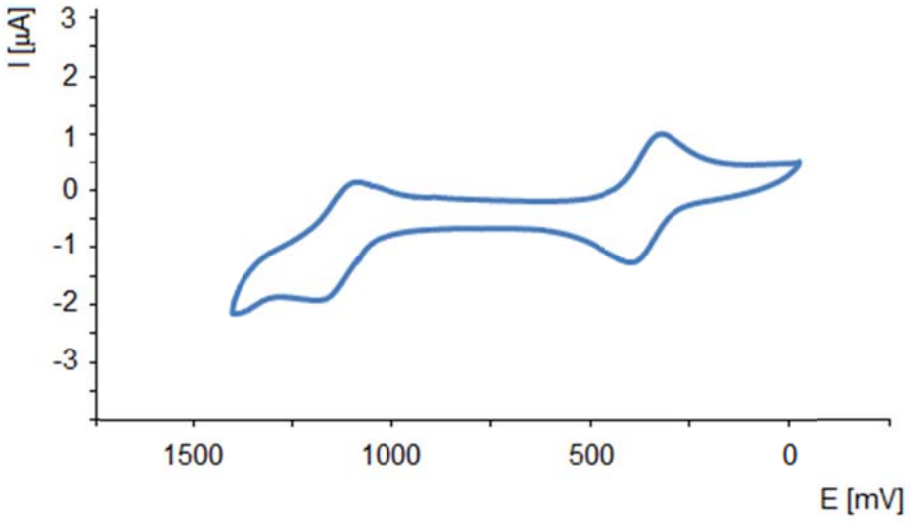
5 Cyclic voltammograms of 2,6-di(hetero)aryl dithienothiazines 3a-3l

5.1 4-(4-Hexylphenyl)-2,6-bis(4-methoxyphenyl)-4H-dithieno[2,3-b:3',2'-e][1,4]thiazine (3a)



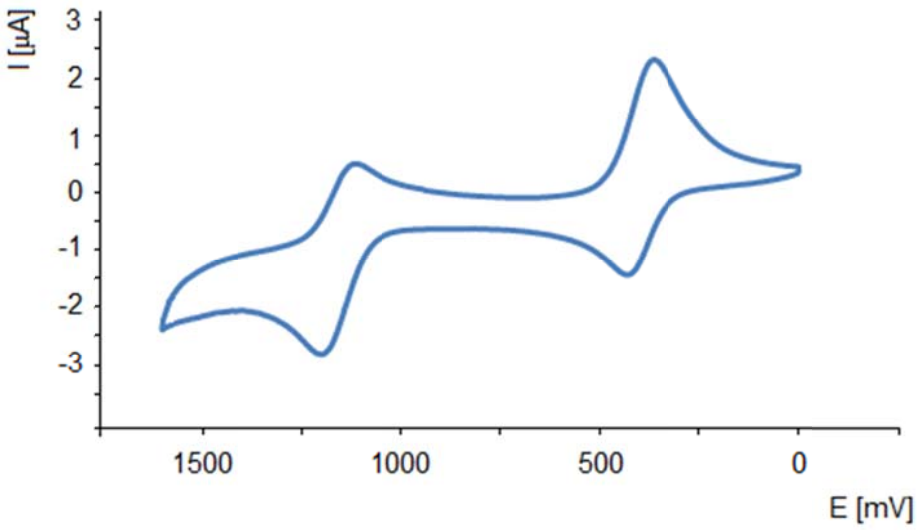
Cyclic voltammogram of **3a** recorded in dichloromethane, T = 293 K, v = 100 mV/s, 0.1 M electrolyte [^{n}Bu$_4$N$^+$][PF$_6^-$], Pt working electrode, Pt counter electrode, Ag/AgCl reference electrode.

5.2 4-(4-Hexylphenyl)-2,6-di-p-tolyl-4H-dithieno[2,3-b:3',2'-e][1,4]thiazine (3b)



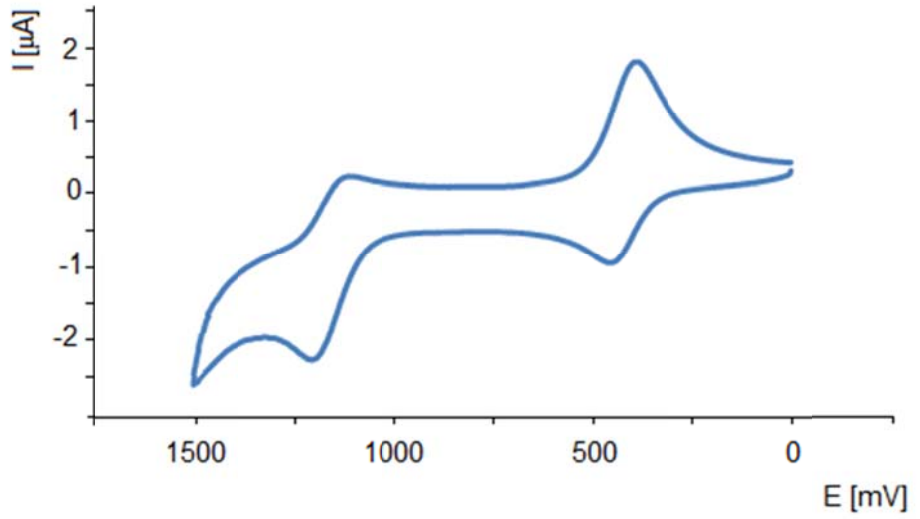
Cyclic voltammogram of **3b** recorded in dichloromethane, T = 293 K, v = 100 mV/s, 0.1 M electrolyte [^{n}Bu$_4$N$^+$][PF$_6^-$], Pt working electrode, Pt counter electrode, Ag/AgCl reference electrode.

5.3 4-(4-Hexylphenyl)-2,6-diphenyl-4H-dithieno[2,3-b:3',2'-e][1,4]thiazine (3c)



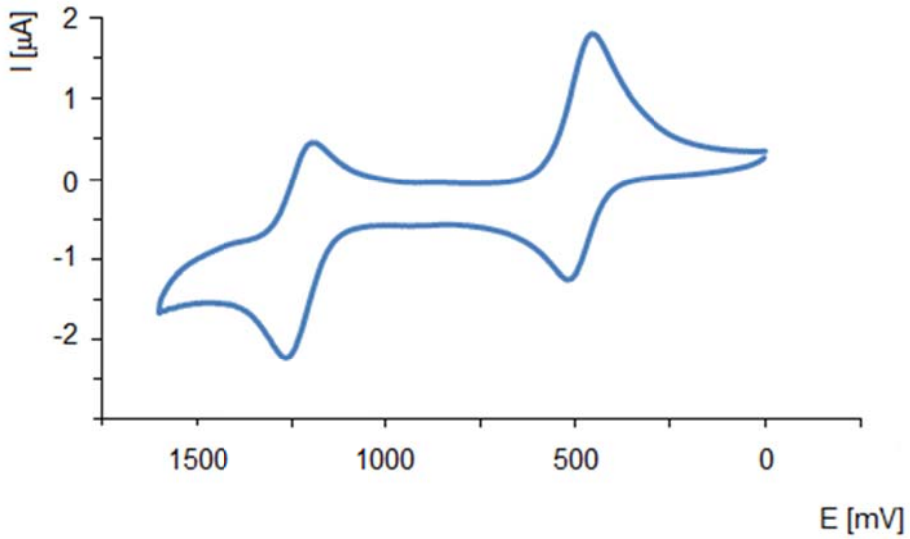
Cyclic voltammogram of **3c** recorded in dichloromethane, T = 293 K, v = 100 mV/s, 0.1 M electrolyte [$^{n}Bu_4N^+$][PF_6^-], Pt working electrode, Pt counter electrode, Ag/AgCl reference electrode.

5.4 2,6-Bis(4-chlorophenyl)-4-(4-hexylphenyl)-4H-dithieno [2,3-b:3',2'-e][1,4] thiazine (3d)



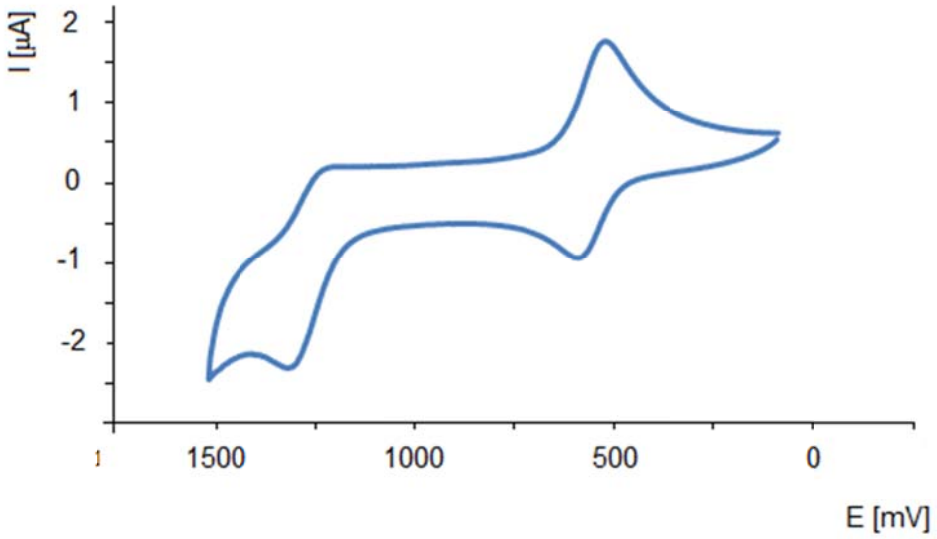
Cyclic voltammogram of **3d** recorded in dichloromethane, T = 293 K, v = 100 mV/s, 0.1 M electrolyte [$^{n}Bu_4N^+$][PF_6^-], Pt working electrode, Pt counter electrode, Ag/AgCl reference electrode.

5.5 Dimethyl 4,4'-(4-(4-hexylphenyl)-4H-dithieno[2,3-b:3',2'-e][1,4]thiazine-2,6-diyl)dibenzoate (3e)



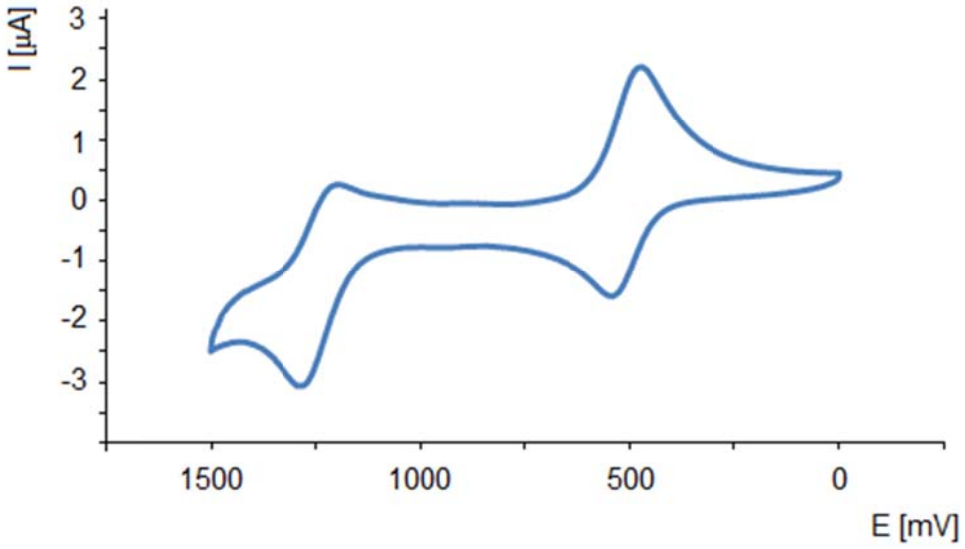
Cyclic voltammogram of **3e** recorded in dichloromethane, T = 293 K, v = 100 mV/s, 0.1 M electrolyte [$^{n}Bu_4N^+$][PF_6^-], Pt working electrode, Pt counter electrode, Ag/AgCl reference electrode.

5.6 4-(4-Hexylphenyl)-2,6-bis(4-(trifluoromethyl)phenyl)-4H-dithieno[2,3-b:3',2'-e][1,4]thiazine (3f)



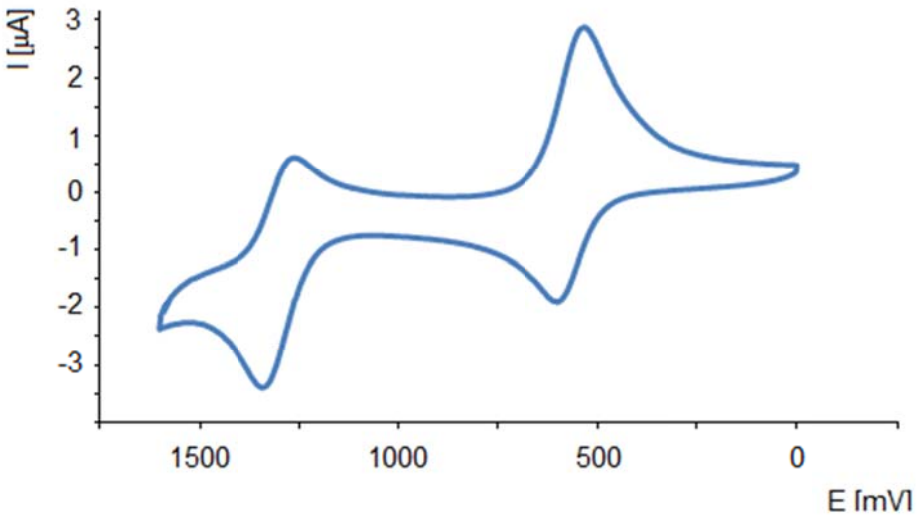
Cyclic voltammogram of **3f** recorded in dichloromethane, T = 293 K, v = 100 mV/s, 0.1 M electrolyte [$^{n}Bu_4N^+$][PF_6^-], Pt working electrode, Pt counter electrode, Ag/AgCl reference electrode.

5.7 4,4'-(4-(4-Hexylphenyl)-4H-dithieno[2,3-b:3',2'-e][1,4]thiazine-2,6-diyl)dibenzonitrile (3g)



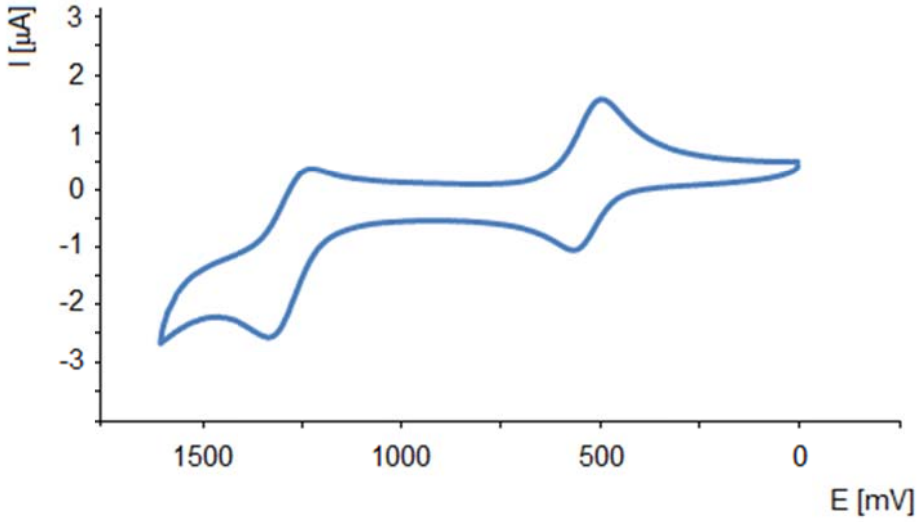
Cyclic voltammogram of **3g** recorded in dichloromethane, T = 293 K, v = 100 mV/s, 0.1 M electrolyte [$^{n}Bu_4N^+$][PF_6^-], Pt working electrode, Pt counter electrode, Ag/AgCl reference electrode.

5.8 4-(4-Hexylphenyl)-2,6-bis(4-nitrophenyl)-4H-dithieno[2,3-b:3',2'-e][1,4]thiazine (3h)



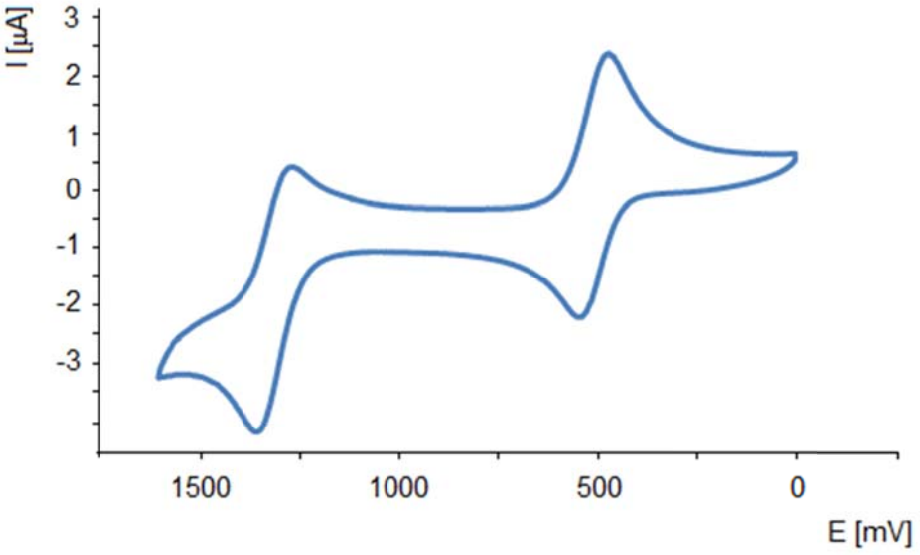
Cyclic voltammogram of **3h** recorded in dichloromethane, T = 293 K, v = 100 mV/s, 0.1 M electrolyte [$^{n}Bu_4N^+$][PF_6^-], Pt working electrode, Pt counter electrode, Ag/AgCl reference electrode.

5.9 4-(4-Hexylphenyl)-2,6-bis(3-nitrophenyl)-4H-dithieno[2,3-b:3',2'-e][1,4]thiazine (3i)



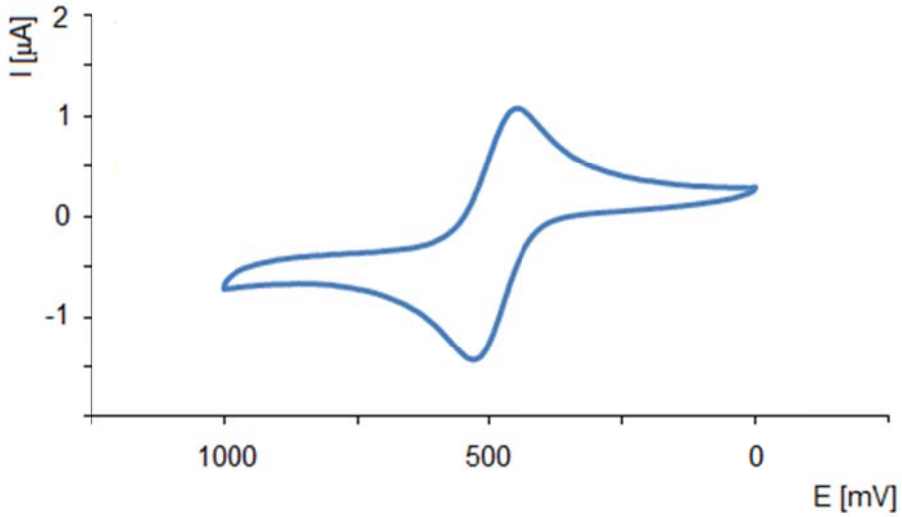
Cyclic voltammogram of **3i** recorded in dichloromethane, T = 293 K, v = 100 mV/s, 0.1 M electrolyte [$^{n}Bu_4N^+$][PF_6^-], Pt working electrode, Pt counter electrode, Ag/AgCl reference electrode.

5.10 4-(4-Hexylphenyl)-2,6-bis(2-nitrophenyl)-4H-dithieno[2,3-b:3',2'-e][1,4]thiazine (3j)



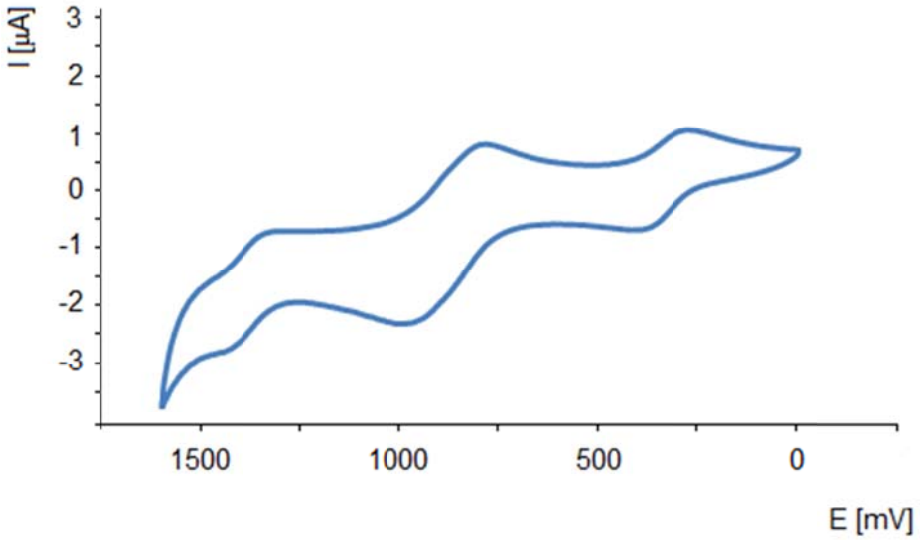
Cyclic voltammogram of **3j** recorded in dichloromethane, T = 293 K, v = 100 mV/s, 0.1 M electrolyte [$^{n}Bu_4N^+$][PF_6^-], Pt working electrode, Pt counter electrode, Ag/AgCl reference electrode.

5.11 4-(4-Hexylphenyl)-2,6-di(pyridin-3-yl)-4H-dithieno[2,3-b:3',2'-e][1,4]thiazine (3k)



Cyclic voltammogram of **3k** recorded in dichloromethane, T = 293 K, v = 100 mV/s, 0.1 M electrolyte [^{n}Bu$_4$N$^+$][PF$_6^-$], Pt working electrode, Pt counter electrode, Ag/AgCl reference electrode.

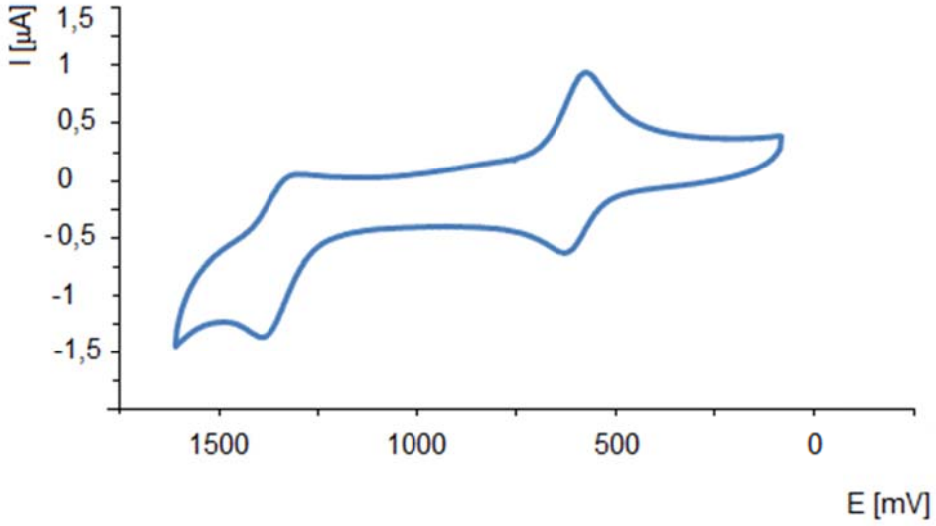
5.12 3,3'-(4-(4-Hexylphenyl)-4H-dithieno[2,3-b:3',2'-e][1,4]thiazine-2,6-diyl)bis(10-hexyl-10H-phenothiazine) (3l)



Cyclic voltammogram of **3l** recorded in dichloromethane, T = 293 K, v = 100 mV/s, 0.1 M electrolyte [^{n}Bu$_4$N$^+$][PF$_6^-$], Pt working electrode, Pt counter electrode, Ag/AgCl reference electrode.

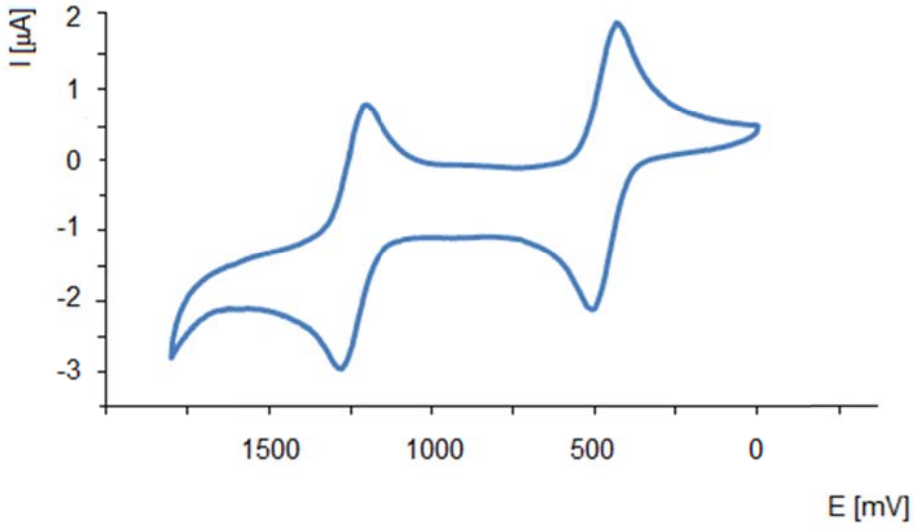
6 Cyclic voltammograms of 2-(hetero)aryl dithienothiazines 6a-6c

6.1 4-(4-Hexylphenyl)-2-(4-nitrophenyl)-4H-dithieno[2,3-b:3',2'-e][1,4]thiazine (6a)



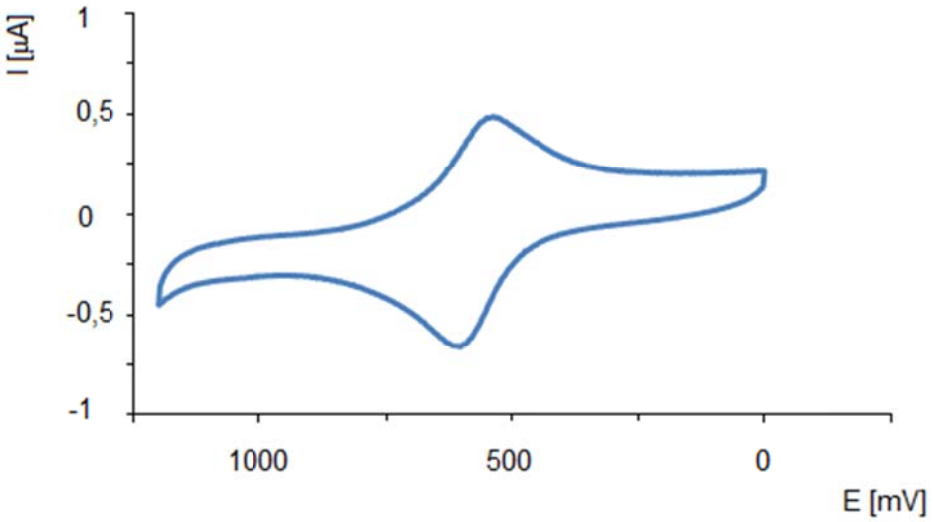
Cyclic voltammogram of **6a** recorded in dichloromethane, T = 293 K, v = 100 mV/s, 0.1 M electrolyte [$^{n}Bu_4N^+$][PF_6^-], Pt working electrode, Pt counter electrode, Ag/AgCl reference electrode.

6.2 4-(4-Hexylphenyl)-2-(thiophen-2-yl)-4H-dithieno[2,3-b:3',2'-e][1,4]thiazine (6b)



Cyclic voltammogram of **6b** recorded in dichloromethane, T = 293 K, v = 100 mV/s, 0.1 M electrolyte [$^{n}Bu_4N^+$][PF_6^-], Pt working electrode, Pt counter electrode, Ag/AgCl reference electrode.

6.3 4-(4-Hexylphenyl)-2-(pyridin-4-yl)-4H-dithieno[2,3-b:3',2'-e][1,4]thiazine (6c)



Cyclic voltammogram of **6c** recorded in dichloromethane, T = 293 K, v = 100 mV/s, 0.1 M electrolyte [$^{n}Bu_4N^+$][PF_6^-], Pt working electrode, Pt counter electrode, Ag/AgCl reference electrode.

7 Molecular modeling coordinates and FMO energies of compounds 3a, 3c and 3g-3j

7.1 XYZ-Coordinates of the S0 (Gaussian03, B3LYP/6-311G*) of compound 3a

C	4.822897	-1.168984	-1.673543
C	4.656080	-1.095909	-0.277426
C	5.777375	-1.345129	0.521772
C	7.018158	-1.653525	-0.032139
C	7.164603	-1.710519	-1.420248
C	6.051797	-1.463356	-2.235469
C	3.349208	-0.762914	0.298639
C	2.361502	0.032009	-0.222989
C	1.228156	0.175221	0.633552
C	1.355227	-0.539110	1.797074
S	2.849895	-1.429371	1.848712
N	0.023131	0.867129	0.327489
C	-1.154168	0.130080	0.636090
C	-1.251490	-0.587787	1.800299
S	0.055290	-0.664587	2.995135
C	-2.283144	-0.056623	-0.217838
C	-3.238795	-0.887966	0.306701
S	-2.711352	-1.533697	1.856055
C	-4.533259	-1.271359	-0.266169
C	-5.643473	-1.558495	0.535736
C	-6.872657	-1.915111	-0.015098
C	-7.018555	-1.983804	-1.402743
C	-5.916757	-1.699056	-2.220636
C	-4.698935	-1.356663	-1.661719
C	-0.004171	2.269346	0.119947
C	1.184603	3.012727	0.022912
C	1.147019	4.380921	-0.206953
C	-0.055351	5.083407	-0.346233
C	-1.229611	4.341650	-0.219204
C	-1.214025	2.967548	0.013005
C	-0.027473	6.577789	-0.615084
C	-1.379416	7.292188	-0.611989
O	8.325804	-1.995760	-2.070521
O	-8.169142	-2.315112	-2.050054
C	9.485743	-2.268901	-1.299447
C	-9.316972	-2.627903	-1.275964
H	3.968645	-1.013954	-2.323768
H	5.693245	-1.277812	1.601631
H	7.857168	-1.834984	0.627664
H	6.176514	-1.523441	-3.310877
H	2.447368	0.533341	-1.178237
H	-2.390079	0.439993	-1.173362
H	-5.560511	-1.483384	1.615166
H	-7.703588	-2.124517	0.646649
H	-6.040487	-1.768580	-3.295589
H	-3.851762	-1.172683	-2.313701
H	2.143591	2.529313	0.154025
H	2.089280	4.919933	-0.270564
H	-2.194571	4.831739	-0.290814
H	-2.156220	2.450071	0.135376
H	0.461405	6.752276	-1.582386
H	0.626025	7.053701	0.126360

H	-1.245796	8.361730	-0.793492
H	-2.044278	6.910468	-1.391923
H	-1.893217	7.182857	0.347332
H	10.278021	-2.471186	-2.017640
H	9.769009	-1.410002	-0.681542
H	9.345070	-3.146708	-0.659661
H	-10.101866	-2.863879	-1.991983
H	-9.142358	-3.496297	-0.631720
H	-9.631827	-1.777067	-0.662209

SCF Done: E (RB + HF-LYP) = -2558.33244230 A. U. after 7 cycles

Sum of electronic and zero-point Energies = -2557.859085

Sum of electronic and thermal Energies = -2557.826506

Sum of electronic and thermal Enthalpies = -2557.825561

Sum of electronic and thermal Free Energies = -2557.927268

LUMO+1 = -1.168 eV

LUMO = -1.211 eV

HOMO = -5.061 eV

HOMO-1 = -5.666 eV

7.2 XYZ-Coordinates of the S0 (Gaussian03, B3LYP/6-311G*) of compound 3c

C	6.951569	-2.265258	1.835631
C	6.808289	-2.320503	0.450911
C	5.591964	-1.999826	-0.142923
C	4.487845	-1.623936	0.638145
C	4.643045	-1.582048	2.033549
C	5.863131	-1.892923	2.623084
C	3.198543	-1.275083	0.028710
S	2.652727	-2.068211	-1.442690
C	1.213769	-1.092252	-1.482317
C	1.137468	-0.249613	-0.402374
C	2.264834	-0.370794	0.464305
S	-0.099469	-1.270564	-2.658750
C	-1.391212	-0.981204	-1.480652
C	-1.242306	-0.148043	-0.401030
N	-0.020614	0.543968	-0.173023
C	-2.375347	-0.171966	0.466306
C	-3.383444	-0.992911	0.031627
S	-2.908559	-1.830477	-1.439719
C	0.039600	1.960346	-0.121916
C	-1.131721	2.736568	-0.107902
C	-1.062600	4.120384	-0.029416
C	0.155932	4.805960	0.032230
C	1.312648	4.028198	-0.011266
C	1.265307	2.637597	-0.091066
C	0.162525	6.321460	0.130394
C	1.534193	6.996689	0.108852
C	-4.697252	-1.229765	0.642380
C	-5.829311	-1.515316	-0.136967
C	-7.067842	-1.731083	0.458316

C	-7.205439	-1.658416	1.842789
C	-6.089417	-1.374528	2.628528
C	-4.847952	-1.168919	2.037607
H	7.901395	-2.513418	2.297678
H	7.649624	-2.605308	-0.172664
H	5.503429	-2.018929	-1.224286
H	3.793550	-1.327866	2.658389
H	5.960498	-1.856609	3.703458
H	2.387848	0.221482	1.361633
H	-2.446856	0.429522	1.363139
H	-2.102031	2.264203	-0.184924
H	-1.992128	4.684544	-0.025416
H	2.288452	4.501152	0.007435
H	2.195488	2.088664	-0.154271
H	-0.361250	6.615535	1.049001
H	-0.444654	6.727439	-0.688197
H	1.425169	8.082212	0.174998
H	2.157851	6.679934	0.949632
H	2.080743	6.777701	-0.812892
H	-5.743250	-1.545990	-1.218276
H	-7.930285	-1.947188	-0.164006
H	-8.172434	-1.824658	2.305959
H	-6.182941	-1.325497	3.708739
H	-3.980024	-0.983549	2.661354

SCF Done: E (RB + HF-LYP) = -2329.229220214 A. U. after 9 cycles

Sum of electronic and zero-point Energies = -2328.821074

Sum of electronic and thermal Energies = -2328.793723

Sum of electronic and thermal Enthalpies = -2328.792779

Sum of electronic and thermal Free Energies = -2328.882714

LUMO+1 = -1.386 eV

LUMO = -1.451 eV

HOMO = -5.206 eV

HOMO-1 = -5.921 eV

7.3 XYZ-Coordinates of the S_0 (Gaussian03, B3LYP/6-311G*) of compound 3g

C	-0.06981	5.00414	-0.33937
C	1.13533	4.30531	-0.20654
C	1.17767	2.93579	0.01571
C	-0.00838	2.18995	0.11139
C	-1.22062	2.88261	0.00969
C	-1.24148	4.2581	-0.21484
N	0.02387	0.78269	0.31313
C	-1.14908	0.04431	0.62761
C	-1.24511	-0.66973	1.79657
S	0.0612	-0.74394	2.99042
C	1.35969	-0.61258	1.79308
C	1.22923	0.09716	0.6248
S	-2.70592	-1.60777	1.8689

C	-3.23313	-0.97546	0.31541
C	-2.27808	-0.14836	-0.22035
S	2.86056	-1.48547	1.86094
C	3.35566	-0.82931	0.30663
C	2.36356	-0.0449	-0.22605
C	-0.04782	6.50027	-0.59785
C	1.40253	7.20906	-0.59322
H	-2.38539	0.34227	-1.17878
H	2.44667	0.45075	-1.18436
H	2.13926	2.45646	0.14327
H	-2.16165	2.36276	0.13164
H	2.07537	4.84787	-0.26872
H	-2.20777	4.74571	-0.28193
H	0.4432	6.68192	-1.56251
H	0.60243	6.97273	0.14839
H	-1.27196	8.27983	-0.76809
H	-2.06437	6.8303	-1.37711
H	-1.91785	7.09319	0.36448
C	-4.52938	-1.35375	-0.25166
C	4.66585	-1.14946	-0.26406
C	5.77247	-1.44349	0.55054
C	4.84597	-1.16565	-1.65871
C	6.08111	-1.45116	-2.21708
C	7.00929	-1.73989	-0.00076
C	7.17807	-1.74332	-1.39253
H	4.0019	-0.97566	-2.31178
H	5.66983	-1.4185	1.62992
H	7.85313	-1.96007	0.6427
H	6.20227	-1.46241	-3.2941
C	8.45219	-2.04376	-1.96556
N	9.48237	-2.28572	-2.42956
C	-5.62059	-1.69284	0.56618
C	-4.71128	-1.38205	-1.64587
C	-6.84462	-2.04383	0.01837
C	-5.93412	-1.72215	-2.20079
C	-7.01584	-2.05863	-1.37304
H	-3.87738	-1.15786	-2.30118
H	-5.5169	-1.66031	1.64525
H	-7.67692	-2.29825	0.66424
H	-6.05684	-1.74193	-3.27751
C	-8.27702	-2.41532	-1.94245
N	-9.29679	-2.70275	-2.4035

SCF Done: E (RB + HF-LYP) = -2513.76143743 A. U. after 8 cycles

Sum of electronic and zero-point Energies = -2513.355987

Sum of electronic and thermal Energies = -2513.325005

Sum of electronic and thermal Enthalpies = -2513.324061

Sum of electronic and thermal Free Energies = -2513.422675

LUMO+1 = -2.331 eV

LUMO = -2.395 eV

HOMO = -5.655 eV

HOMO-1 = -6.409 eV

7.4 XYZ-Coordinates of the S0 (Gaussian03, B3LYP/6-311G*) of compound 3h

C	-7.007540	-1.915800	-1.116910
C	-6.854773	-1.859549	0.264191
C	-5.626369	-1.488267	0.789950
C	-4.540908	-1.177952	-0.048623
C	-4.729843	-1.255494	-1.441191
C	-5.955846	-1.615900	-1.977625
C	-3.242266	-0.779367	0.496710
S	-2.718331	-1.331124	2.081667
C	-1.252521	-0.407175	1.958855
C	-1.152485	0.243819	0.753516
C	-2.282365	0.012734	-0.082564
S	0.052367	-0.424596	3.156075
C	1.352251	-0.360617	1.955089
C	1.225730	0.286331	0.749828
N	0.023588	0.958804	0.401100
C	2.359839	0.092911	-0.090193
C	3.348718	-0.664952	0.486357
S	2.849371	-1.233272	2.073294
C	-0.004209	2.351569	0.113504
C	1.183539	3.083997	-0.043997
C	1.143761	4.437881	-0.347749
C	-0.060057	5.133713	-0.505612
C	-1.233007	4.402563	-0.319909
C	-1.214698	3.043102	-0.013066
C	-0.035552	6.611471	-0.853727
C	-1.386580	7.327283	-0.865038
C	4.658514	-1.019047	-0.062924
C	5.756395	-1.292030	0.772502
C	6.995026	-1.622036	0.243259
C	7.145473	-1.673988	-1.138262
C	6.081715	-1.410040	-1.995926
C	4.845887	-1.090776	-1.455999
N	8.461053	-2.019720	-1.707461
O	9.373677	-2.252088	-0.925219
O	8.559815	-2.052355	-2.927419
N	-8.312539	-2.305092	-1.682351
O	-9.214436	-2.568566	-0.897531
O	-8.413963	-2.340082	-2.902023
H	-7.694503	-2.094288	0.904272
H	-5.515766	-1.417126	1.866254
H	-3.900463	-1.054478	-2.109178
H	-6.107127	-1.680515	-3.046743
H	-2.386796	0.452658	-1.065531
H	2.444941	0.533512	-1.074713
H	2.145269	2.609238	0.098531
H	2.085133	4.970719	-0.455963
H	-2.198120	4.890143	-0.402156
H	-2.156257	2.536850	0.153845
H	0.437411	6.732200	-1.836750
H	0.631566	7.123326	-0.149613
H	-1.254113	8.385809	-1.101814
H	-2.064151	6.909242	-1.614753
H	-1.884901	7.267716	0.106672
H	5.646662	-1.224024	1.849101
H	7.844073	-1.828008	0.880943
H	6.231891	-1.470214	-3.065459
H	4.008291	-0.918384	-2.121698

SCF Done: E (RB + HF-LYP) = -2738.34454905 A. U. after 7 cycles

Sum of electronic and zero-point Energies = -2737.931407

Sum of electronic and thermal Energies = -2737.898876

Sum of electronic and thermal Enthalpies = -2737.897932

Sum of electronic and thermal Free Energies = -2738.001513

LUMO+1 = -2.897 eV

LUMO = -2.932 eV

HOMO = -5.718 eV

HOMO-1 = -6.507 eV

7.5 XYZ-Coordinates of the S0 (Gaussian03, B3LYP/6-311G*) of compound 3i

C	-4.834464	-1.307954	0.976685
C	-4.659679	-1.041352	-0.388517
C	-5.767467	-1.188044	-1.240915
C	-7.006710	-1.587448	-0.750390
C	-7.182389	-1.842095	0.605534
C	-6.083044	-1.690719	1.443321
C	-3.348374	-0.618435	-0.892134
C	-2.359495	0.060347	-0.227498
C	-1.225185	0.355479	-1.040338
C	-1.355188	-0.133743	-2.316402
S	-2.853418	-0.986690	-2.537543
N	-0.017895	0.970703	-0.613105
C	1.153642	0.297032	-1.051280
C	1.248065	-0.198241	-2.328041
S	-0.055983	-0.047202	-3.517539
C	2.279993	-0.051376	-0.248703
C	3.228587	-0.777722	-0.921596
S	2.701095	-1.123056	-2.562058
C	4.522638	-1.262328	-0.429045
C	5.615974	-1.458882	-1.290003
C	6.839428	-1.914634	-0.808985
C	7.013603	-2.177946	0.545477
C	5.928582	-1.977685	1.391644
C	4.695223	-1.538222	0.934587
C	0.018662	2.304404	-0.124204
C	-1.164738	3.015357	0.134047
C	-1.117142	4.307617	0.638215
C	0.090622	4.962253	0.904512
C	1.259408	4.258810	0.614753
C	1.233317	2.961192	0.107277
C	0.075345	6.369160	1.475359
C	1.430382	7.068593	1.589370
N	-6.243978	-1.963838	2.891735
O	-7.349370	-2.314114	3.279720
O	-5.263482	-1.819686	3.608493
N	6.087993	-2.258799	2.838675
O	7.179921	-2.657061	3.218430
O	5.119969	-2.072664	3.562668

H	-4.012497	-1.240040	1.675823
H	-5.662344	-0.968519	-2.297982
H	-7.845382	-1.691267	-1.429757
H	-8.134298	-2.149516	1.015771
H	-2.441100	0.369980	0.806189
H	2.386621	0.256078	0.783371
H	5.513042	-1.233811	-2.346121
H	7.667423	-2.055860	-1.494677
H	7.953732	-2.528356	0.948368
H	3.882277	-1.433634	1.639719
H	-2.128919	2.574513	-0.081629
H	-2.055352	4.825039	0.822366
H	2.227353	4.721330	0.773296
H	2.172128	2.478015	-0.128921
H	-0.392008	6.339599	2.467969
H	-0.592339	6.986373	0.862015
H	1.304709	8.078705	1.987040
H	2.109285	6.537190	2.262107
H	1.923828	7.156607	0.617282

SCF Done: E (RB + HF-LYP) = - 2738.34248589 A. U. after 7 cycles

Sum of electronic and zero-point Energies = -2737.931407

Sum of electronic and thermal Energies = -2737.898876

Sum of electronic and thermal Enthalpies = -2737.897932

Sum of electronic and thermal Free Energies = -2738.001513

LUMO+1 = -2.765 eV

LUMO = -2.768 eV

HOMO = -5.562 eV

HOMO-1 = -6.361 eV

7.6 XYZ-Coordinates of the S0 (Gaussian03, B3LYP/6-311G*) of compound 3j

C	5.080365	-1.622025	-1.085644
C	4.727512	-0.899951	0.071164
C	5.792435	-0.548504	0.922525
C	7.111726	-0.870582	0.632286
C	7.420869	-1.587075	-0.521551
C	6.396116	-1.975950	-1.371885
C	3.355259	-0.571808	0.506124
C	2.352662	0.137269	-0.100090
C	1.222391	0.355667	0.742660
C	1.363763	-0.226128	1.977892
S	2.878131	-1.060867	2.131516
N	0.004238	0.984628	0.367721
C	-1.157637	0.262284	0.751824
C	-1.244583	-0.328726	1.987321
S	0.063416	-0.263679	3.180329
C	-2.275365	-0.039025	-0.081953

C	-3.215868	-0.822858	0.531023
S	-2.690305	-1.276055	2.152051
C	-4.562581	-1.252888	0.105272
C	-5.645909	-0.977551	0.961301
C	-6.939712	-1.395213	0.678291
C	-7.201459	-2.135228	-0.472397
C	-6.155209	-2.451215	-1.326847
C	-4.867357	-2.001772	-1.047989
C	-0.054759	2.351693	-0.006757
C	1.115331	3.097662	-0.225405
C	1.043567	4.429342	-0.609706
C	-0.176002	5.090547	-0.792507
C	-1.331195	4.348426	-0.547540
C	-1.280780	3.011311	-0.159229
C	-0.187242	6.542221	-1.237577
C	-1.543593	7.248073	-1.209733
N	-3.838537	-2.390389	-2.033028
O	-3.888818	-3.533514	-2.465492
O	-3.026857	-1.543529	-2.377925
N	4.078037	-2.082567	-2.066766
O	4.210139	-3.217421	-2.503635
O	3.204337	-1.296784	-2.404750
H	5.564917	0.008119	1.824024
H	7.898958	-0.559799	1.310744
H	8.447134	-1.846175	-0.755813
H	6.594536	-2.559941	-2.261397
H	2.418504	0.501349	-1.112995
H	-2.378352	0.322903	-1.092639
H	-5.455000	-0.403527	1.860375
H	-7.744242	-1.140726	1.359897
H	-8.207311	-2.468680	-0.701090
H	-6.314986	-3.050444	-2.214005
H	2.088214	2.649157	-0.074390
H	1.972401	4.972424	-0.766222
H	-2.307447	4.810136	-0.647955
H	-2.209196	2.494597	0.044922
H	0.220859	6.601570	-2.254918
H	0.517574	7.103479	-0.612245
H	-1.435755	8.293047	-1.511362
H	-2.259332	6.785291	-1.894814
H	-1.984382	7.237136	-0.208766

SCF Done: E (RB + HF-LYP) = -2738.31965016 A. U. after 6 cycles

Sum of electronic and zero-point Energies = -2737.931407

Sum of electronic and thermal Energies = -2737.898876

Sum of electronic and thermal Enthalpies = -2737.897932

Sum of electronic and thermal Free Energies = -2738.001513

LUMO+1 = -2.436 eV

LUMO = -2.467 eV

HOMO = -5.330 eV

HOMO-1 = -6.184 eV

7.7 Results of the TD-DFT calculation of compound 3g

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A, 2.7252 eV, 454.96 nm, f = 0.0885
134 -> 135 0.69200

Excited State 2: Singlet-A, 2.8625 eV, 433.13 nm, f = 0.0234
134 -> 136 0.68751

Excited State 3: Singlet-A, 3.5572 eV, 348.54 nm, f = 0.5258
133 -> 135 0.68432

Excited State 4: Singlet-A, 3.6793 eV, 336.98 nm, f = 0.0393
132 -> 135 0.21770
133 -> 136 0.65319

Excited State 5: Singlet-A, 3.8533 eV, 321.76 nm, f = 0.1599
132 -> 135 0.19498
133 -> 136 -0.12300
134 -> 137 0.49287
134 -> 139 0.40656

Excited State 6: Singlet-A, 3.9341 eV, 315.15 nm, f = 0.5655
132 -> 136 0.65226
134 -> 138 0.16073

Excited State 7: Singlet-A, 3.9544 eV, 313.54 nm, f = 0.0328
132 -> 135 -0.33242
134 -> 137 0.47137
134 -> 139 -0.36578

Excited State 8: Singlet-A, 3.9659 eV, 312.63 nm, f = 0.1013
132 -> 136 -0.14166
134 -> 138 0.67307

Excited State 9: Singlet-A, 4.0385 eV, 307.00 nm, f = 0.0005

132 -> 136	0.10588
134 -> 140	0.66216
134 -> 142	-0.12672

Excited State 10: Singlet-A, 4.0559 eV, 305.69 nm, f = 0.1473

132 -> 135	0.49509
133 -> 136	-0.12412
134 -> 139	-0.40535

Excited State 11: Singlet-A, 4.3394 eV, 285.72 nm, f = 0.0049

131 -> 135	0.70247

Excited State 12: Singlet-A, 4.3890 eV, 282.49 nm, f = 0.0025

131 -> 136	0.63579
134 -> 141	0.27919

Excited State 13: Singlet-A, 4.4560 eV, 278.24 nm, f = 0.0328

131 -> 136	-0.30048
131 -> 144	0.10466
134 -> 141	0.59139

Excited State 14: Singlet-A, 4.5176 eV, 274.45 nm, f = 0.0053

133 -> 140	-0.10626
134 -> 140	0.13904
134 -> 141	0.12047
134 -> 142	0.61853
134 -> 143	-0.15920

Excited State 15: Singlet-A, 4.5242 eV, 274.04 nm, f = 0.0060

126 -> 135	-0.18300
127 -> 136	-0.18068
132 -> 138	0.26591
133 -> 137	0.54709

Excited State 16: Singlet-A, 4.5430 eV, 272.91 nm, f = 0.0093

126 -> 135	0.11698
126 -> 136	0.20247
127 -> 135	0.21497
130 -> 135	0.11046
132 -> 137	0.31923

133 -> 138 0.49142

Excited State 17: Singlet-A, 4.6076 eV, 269.08 nm, f = 0.0518
134 -> 142 0.16379
134 -> 143 0.60699
134 -> 144 -0.11223

Excited State 18: Singlet-A, 4.6754 eV, 265.18 nm, f = 0.0298
126 -> 135 0.10485
130 -> 136 -0.12669
132 -> 138 -0.16298
133 -> 137 0.15735
133 -> 139 0.59109

Excited State 19: Singlet-A, 4.6837 eV, 264.71 nm, f = 0.0610
129 -> 136 0.11208
130 -> 135 0.64033
132 -> 139 0.14748
133 -> 138 -0.11648

Excited State 20: Singlet-A, 4.7590 eV, 260.53 nm, f = 0.0362
128 -> 136 -0.12313
129 -> 135 0.21114
130 -> 136 0.59391
132 -> 140 -0.10574

133 -> 137 0.15184

Excited State 21: Singlet-A, 4.8281 eV, 256.80 nm, f = 0.0207
129 -> 135 0.62087
130 -> 136 -0.28416

Excited State 22: Singlet-A, 4.8509 eV, 255.59 nm, f = 0.0084
128 -> 135 0.13632
129 -> 136 0.45933
130 -> 135 -0.20209
132 -> 137 0.17788
132 -> 139 0.17902
133 -> 138 -0.11981
133 -> 140 0.34208

Excited State 23: Singlet-A, 4.8795 eV, 254.09 nm, f = 0.0120

129 -> 136	-0.17606
132 -> 137	-0.29909
133 -> 138	0.32093
133 -> 140	0.44276
134 -> 146	-0.10891

Excited State 24: Singlet-A, 4.8876 eV, 253.67 nm, f = 0.0071

128 -> 135	-0.34264
129 -> 136	0.39898
132 -> 137	-0.27723
133 -> 138	0.19669
133 -> 140	-0.16019

Excited State 25: Singlet-A, 4.9080 eV, 252.62 nm, f = 0.0292

126 -> 135	-0.19454
127 -> 136	-0.17326
128 -> 137	-0.11363
132 -> 138	0.39301
133 -> 137	-0.34583
133 -> 139	0.29032