Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Supporting Information

Synthesis and electronic properties of 3,7-dianilino substituted *N*-hexyl phenothiazines

Iani S. Pereţeanu,[a,b] and Thomas J. J. Müller*[a]

[a]Institut für Organische Chemie und Makromolekulare Chemie, Heinrich-Heine-Universität Düsseldorf Universitätsstraße 1, 40225 Düsseldorf, Germany
Email: ThomasJJ.Mueller@uni-duesseldorf.de

[b]Babeş-Bolyai University Cluj-Napoca, Faculty of Chemistry and Chemical Engineering, Arany Janos St 11, Cluj-Napoca 400428, Romania

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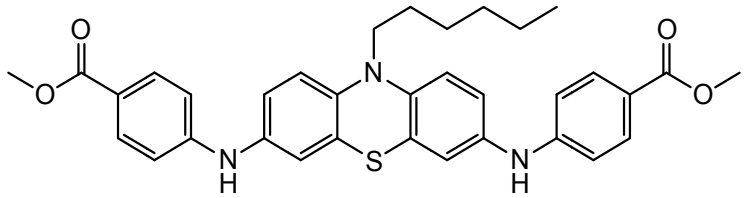
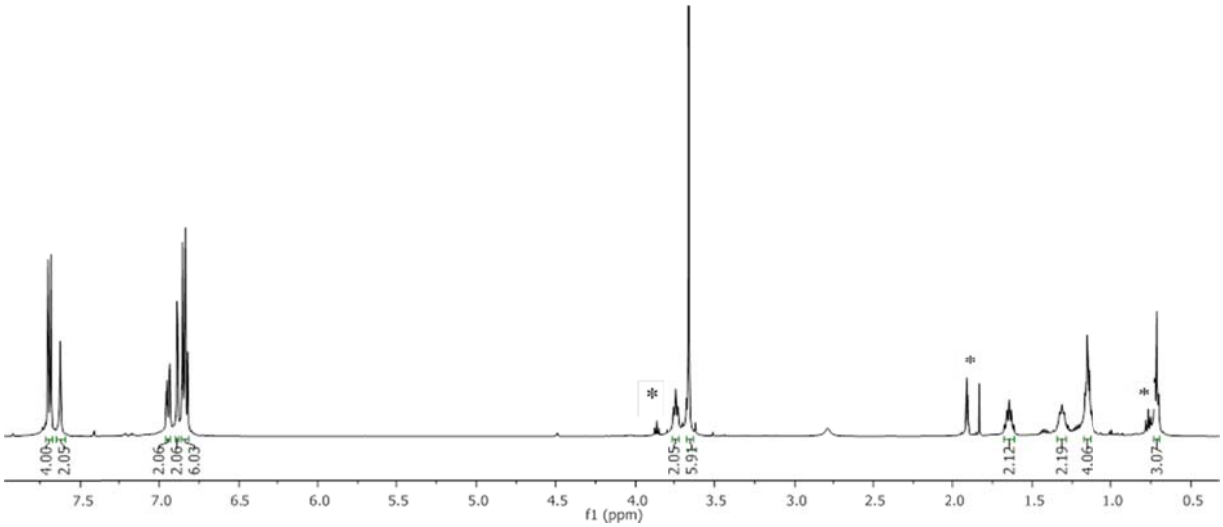
1 ^{1}H and ^{13}C NMR spectra of 3,7-dianilino substituted *N*-hexyl phenothiazines 3a-3l

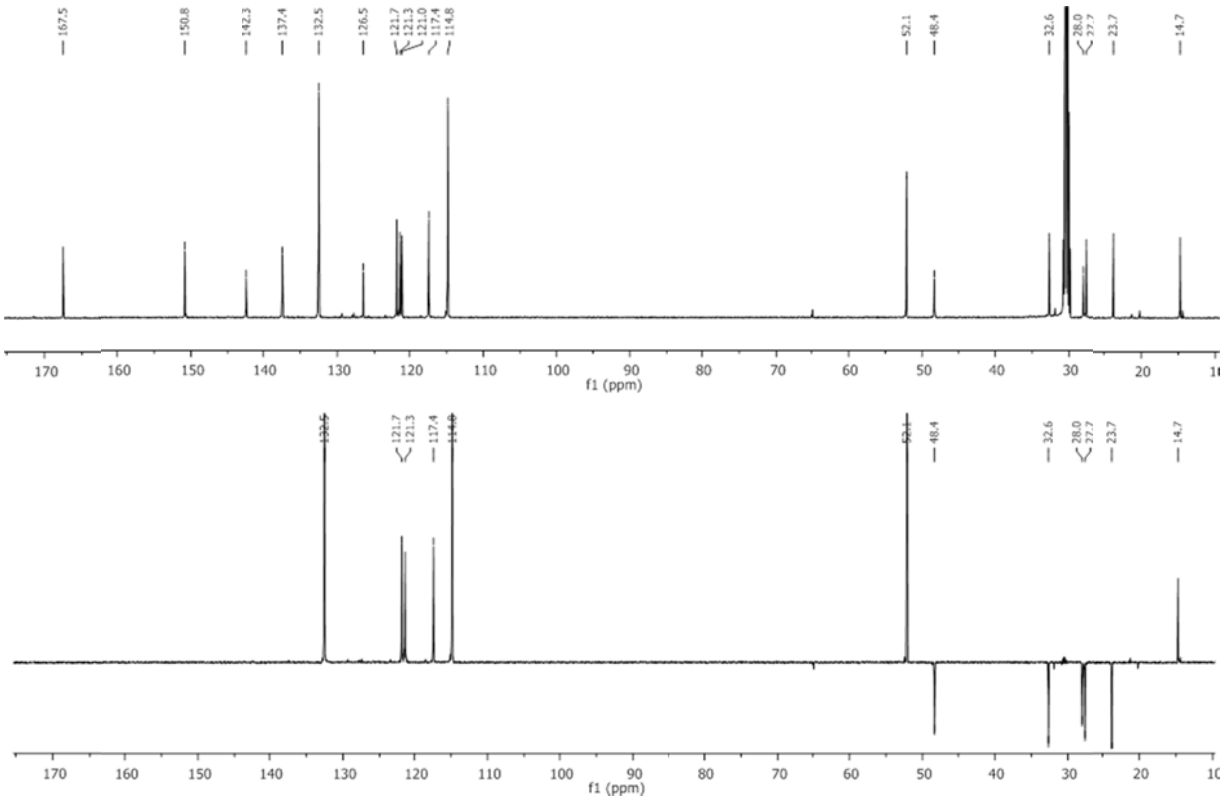
1.1 Dimethyl 4,4'-((10-hexyl-10*H*-phenothiazine-3,7-diyl)bis-(azanediyl))dibenzoate (3a)



$C_{34}H_{35}N_3O_4S$
581.72

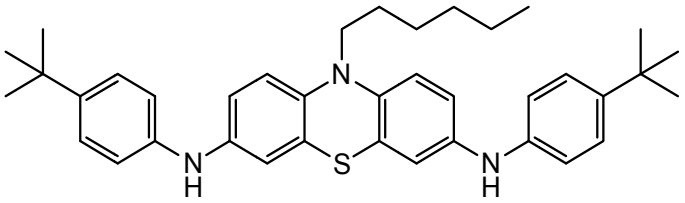


^{1}H NMR (300 MHz) of **3a** (20 mg) in acetone-d_6 at 298 K.

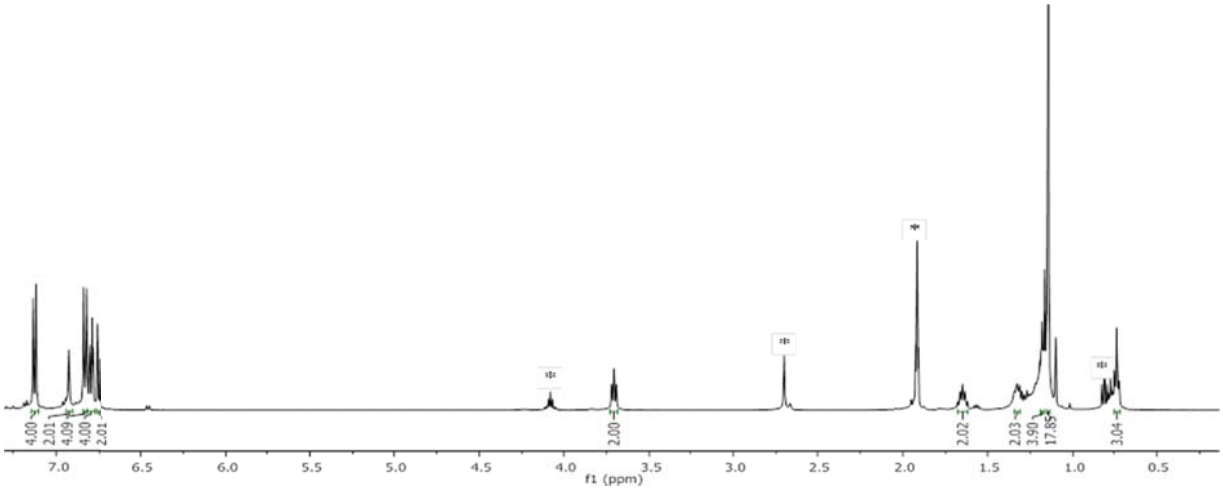


^{13}C and ^{13}C-DEPT 135 NMR (75 MHz) of **3a** (20 mg) in acetone-d_6 at 298 K.

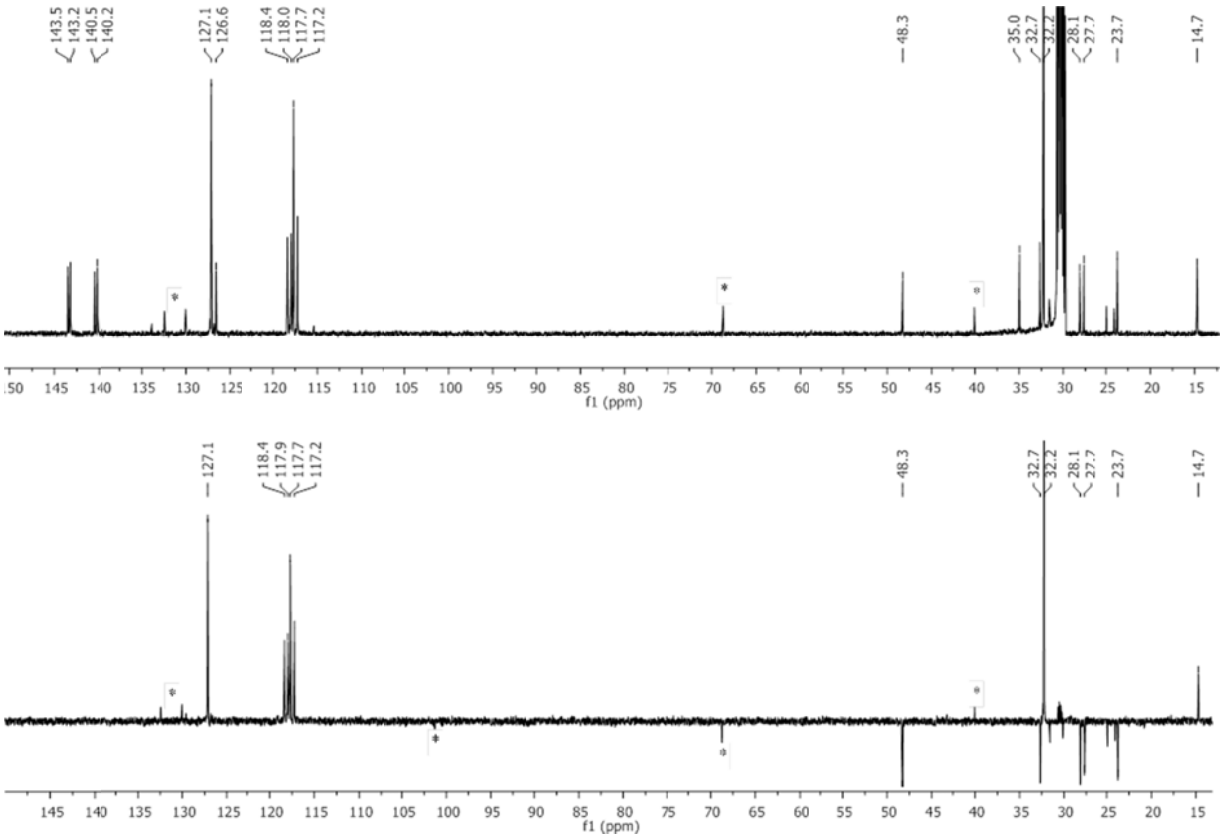
1.2 N^3,N^7-Bis(4-(*tert*-butyl)phenyl)-10-hexyl-10*H*-phenothiazine-3,7-diamine (3b)



$C_{38}H_{47}N_3S$
577.86

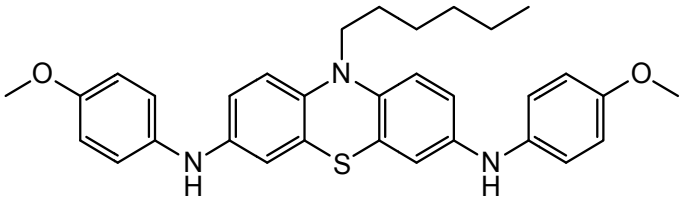


^{1}H NMR (300 MHz) of **3b** (20 mg) in acetone-d_6 at 298 K.

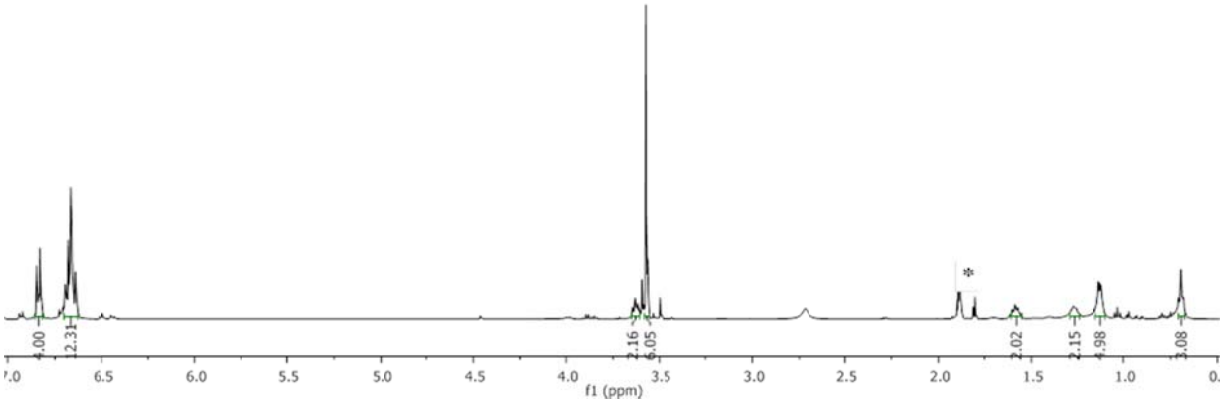


^{13}C and ^{13}C-DEPT 135 NMR (75 MHz) of **3b** (20 mg) in acetone-d_6 at 298 K.

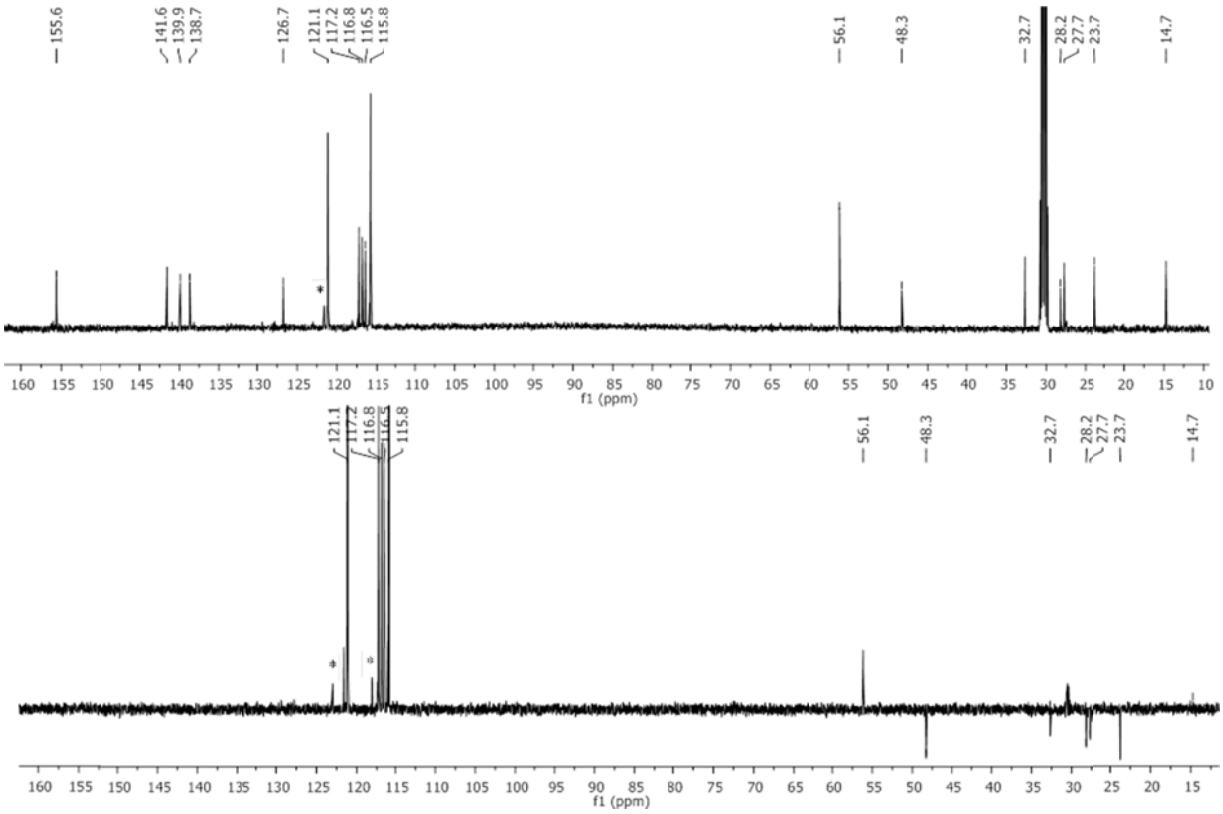
1.3 10-Hexyl-N^3,N^7-bis(4-methoxyphenyl)-10*H*-phenothiazine-3,7-diamine (3c)



$C_{32}H_{35}N_3O_2S$
525.70

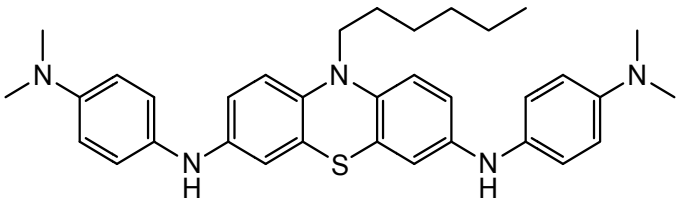


^{1}H NMR (300 MHz) of **3c** (20 mg) in acetone-d_6 at 298 K.

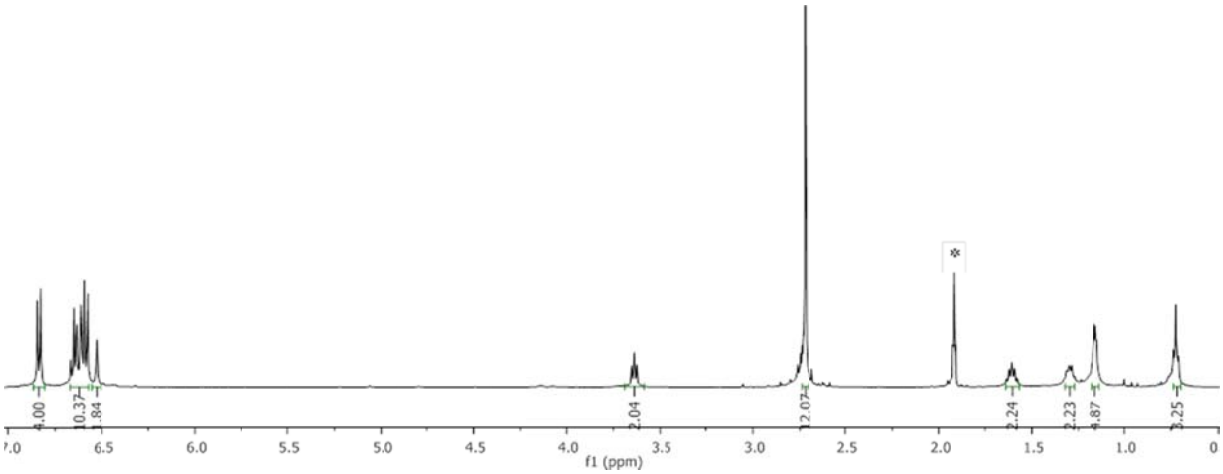


^{13}C and ^{13}C-DEPT 135 NMR (75 MHz) of **3c** (20 mg) in acetone-d_6 at 298 K.

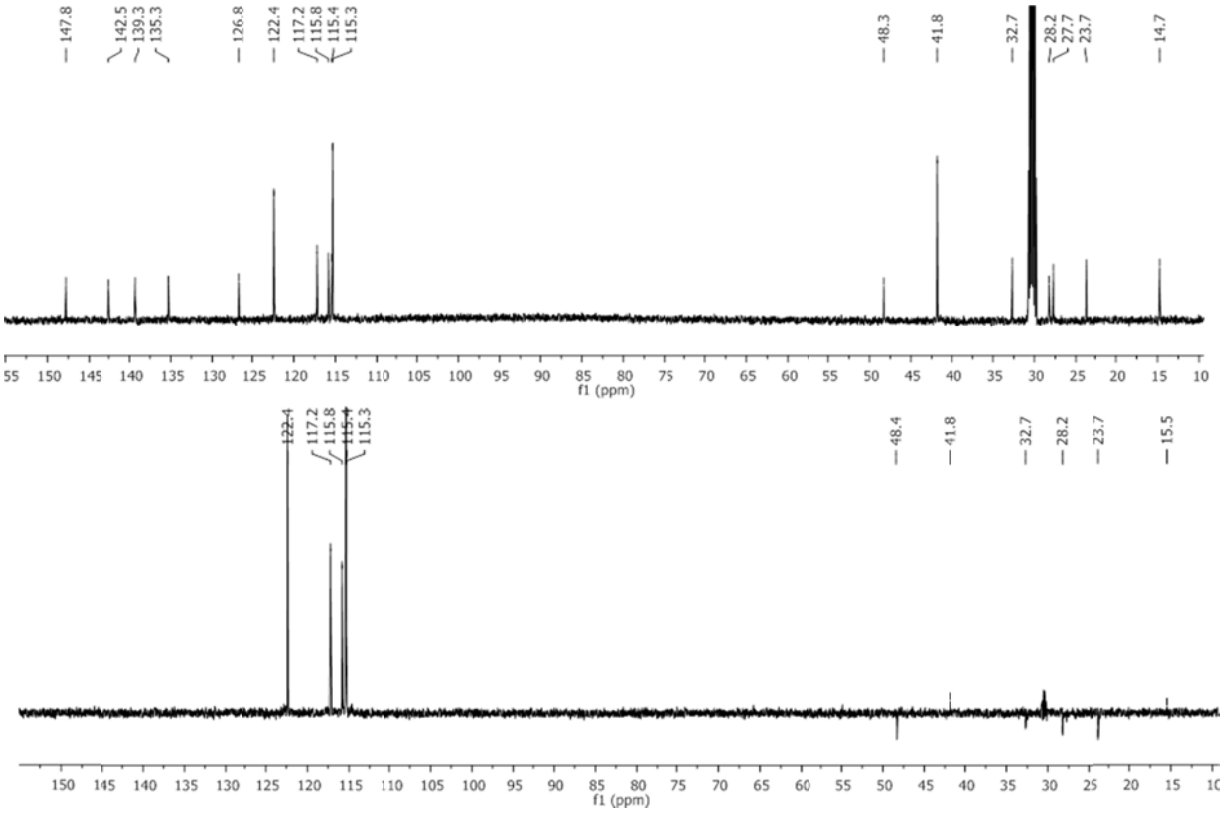
1.4 N^1,$N^{1\prime}$-(10-Hexyl-10*H*-phenothiazine-3,7-diyl)bis(N^4,$N^{4\prime}$-dimethylbenzene-1,4-diamine) (3d)



$C_{34}H_{41}N_5S$
551.79

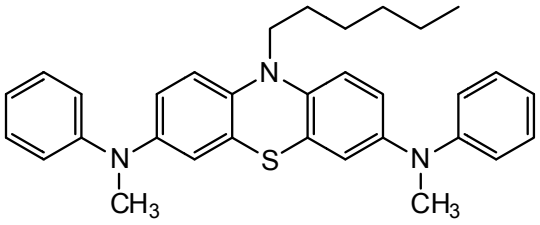


^{1}H NMR (300 MHz) of **3d** (20 mg) in acetone-d_6 at 298 K.

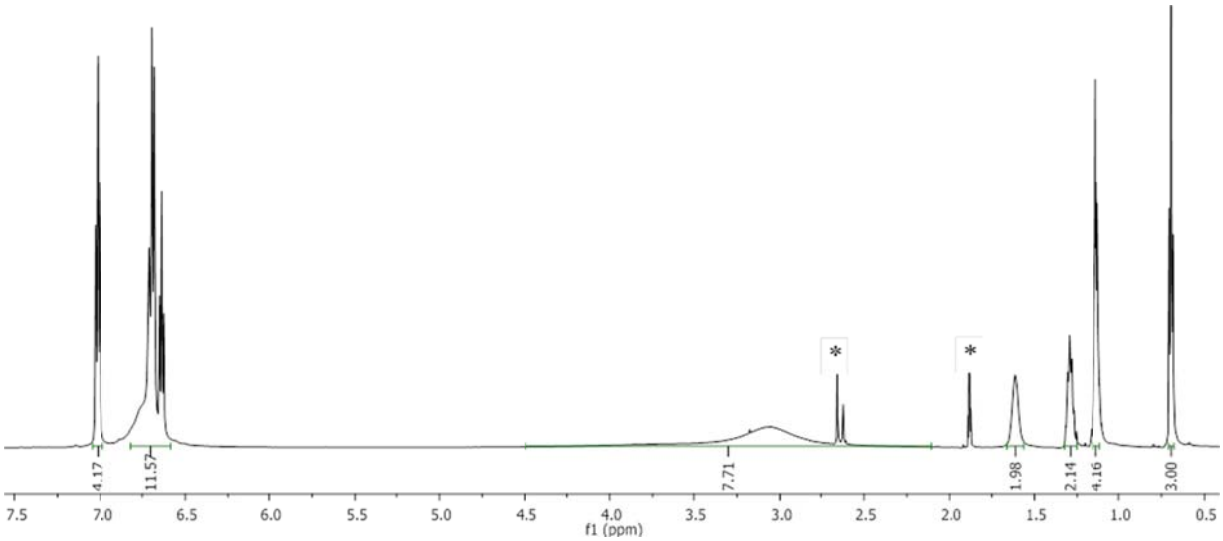


^{13}C and ^{13}C-DEPT 135 NMR (75 MHz) of **3d** (20 mg) in acetone-d_6 at 298 K.

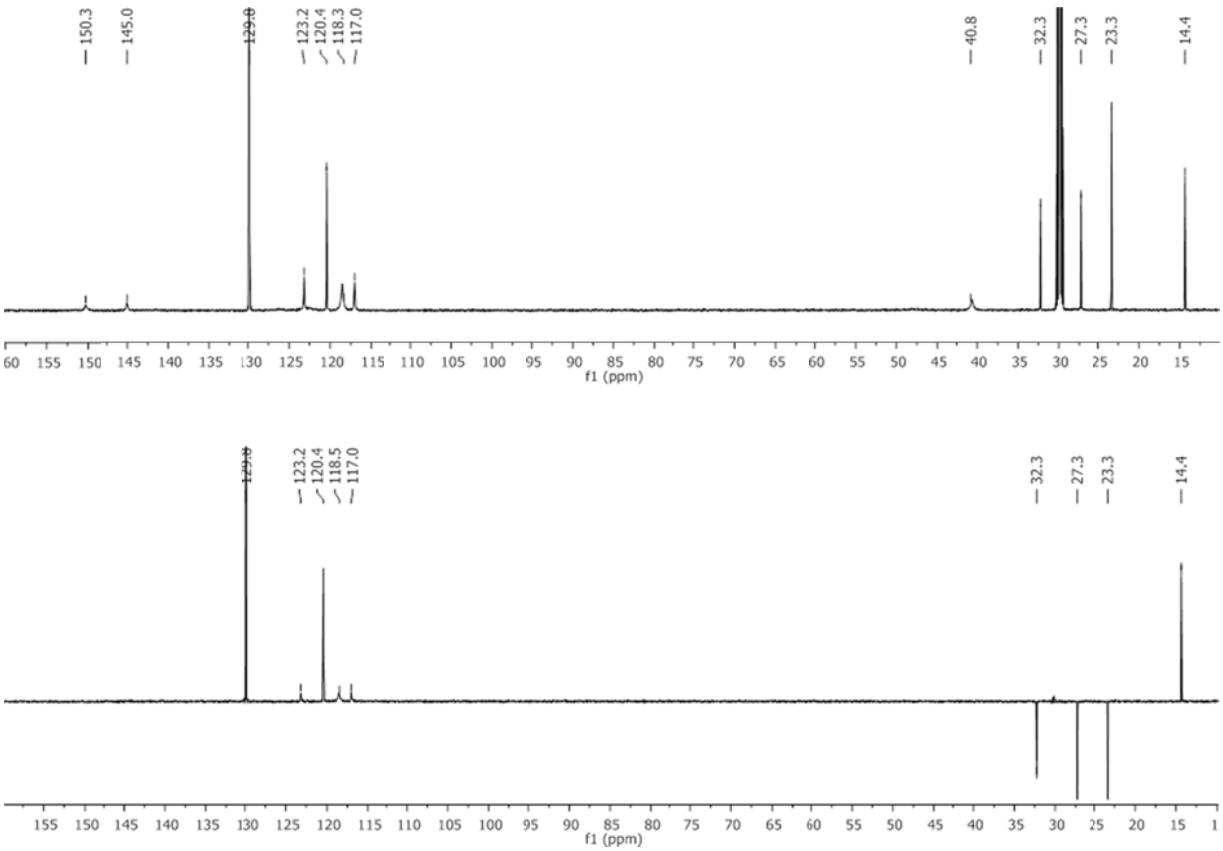
1.5 10-Hexyl-N^3,N^7-dimethyl-N^3,N^7-diphenyl-10*H*-phenothiazine-3,7-diamine (3e)



$C_{32}H_{35}N_3S$
493.71

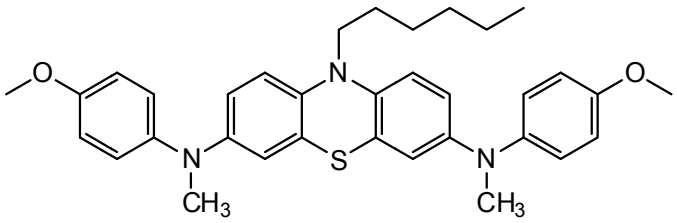


^{1}H NMR (300 MHz) of **3e** (20 mg) in acetone-d_6 at 298 K.

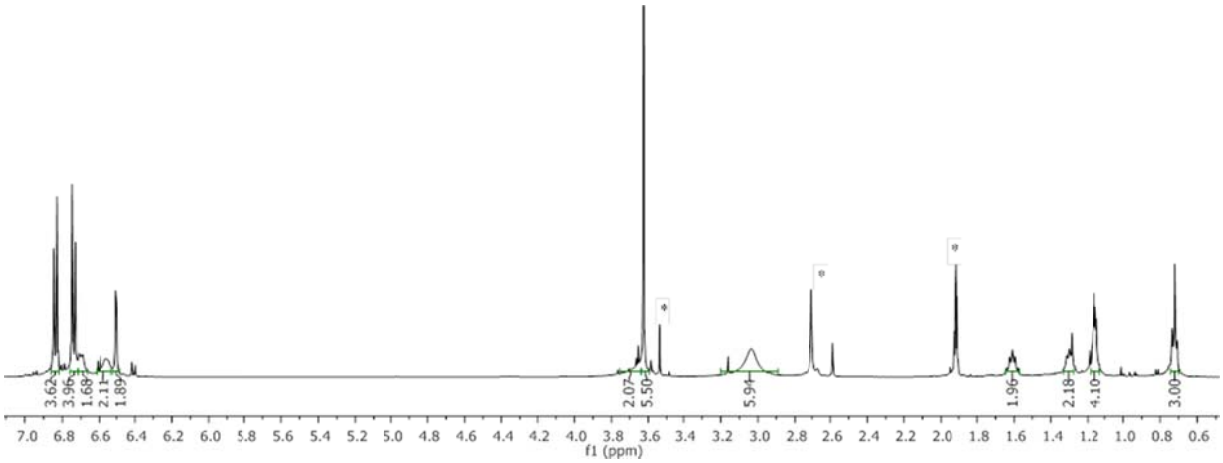


^{13}C and ^{13}C-DEPT 135 NMR (75 MHz) of **3e** (20 mg) in acetone-d_6 at 298 K.

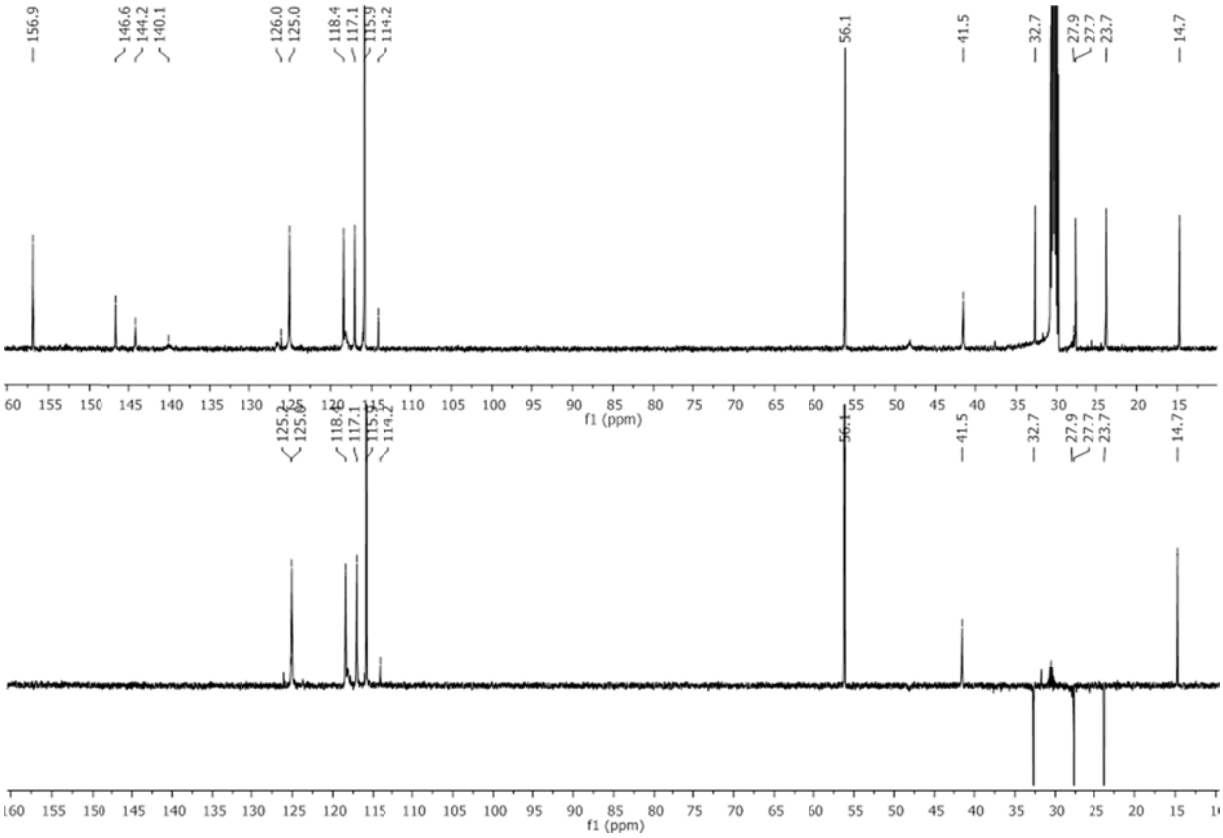
1.6 10-Hexyl-*N*^{3},*N*^{7}-bis(4-methoxyphenyl)-*N*^{3},*N*^{7}-dimethyl-10*H*-phenothiazine-3,7-diamine (3f)



$C_{34}H_{39}N_3O_2S$
553.76

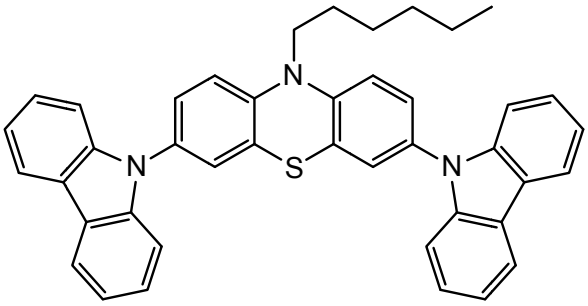


^{1}H NMR (300 MHz) of **3f** (20 mg) in acetone-d_6 at 298 K.

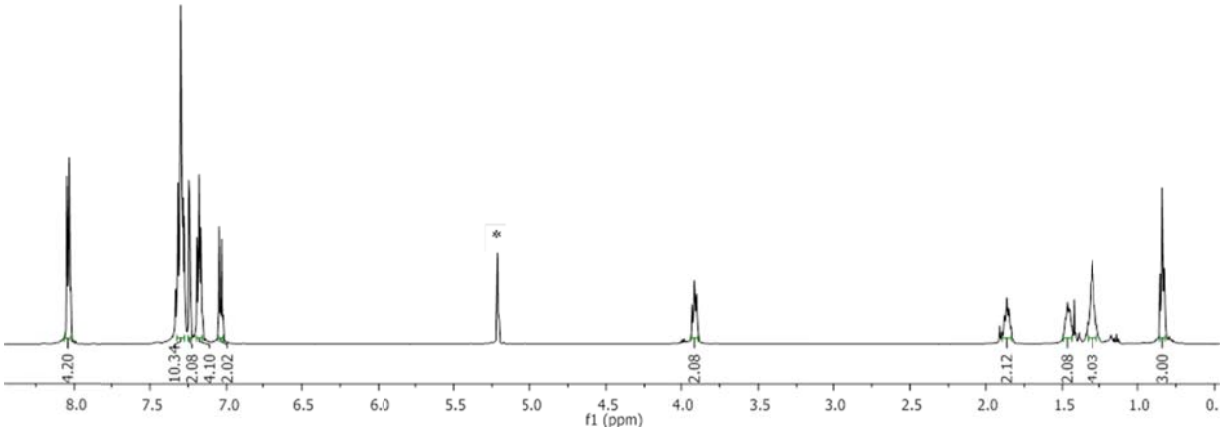


^{13}C and ^{13}C-DEPT 135 NMR (75 MHz) of **3f** (20 mg) in acetone-d_6 at 298 K.

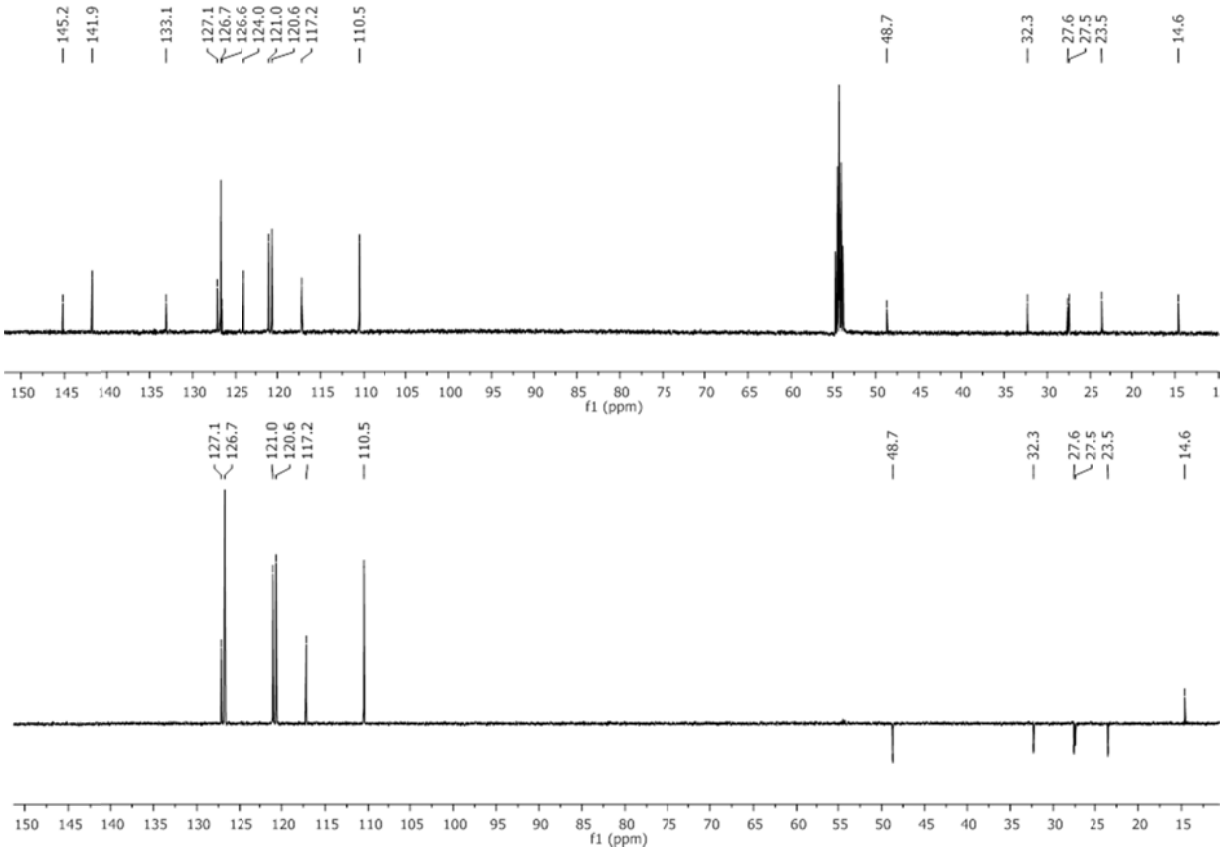
1.7 3,7-Di(9*H*-carbazol-9-yl)-10-hexyl-10*H*-phenothiazine (3g)



$C_{42}H_{35}N_3S$
613.81

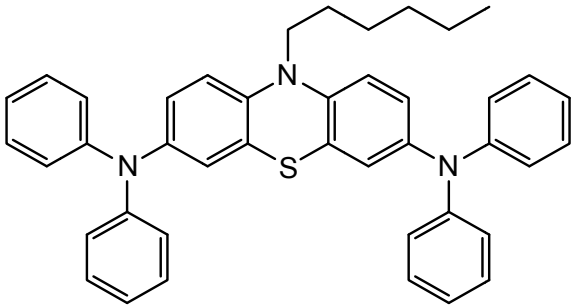


^{1}H NMR (300 MHz) of **3g** (20 mg) in CD_2Cl_2 at 298 K.

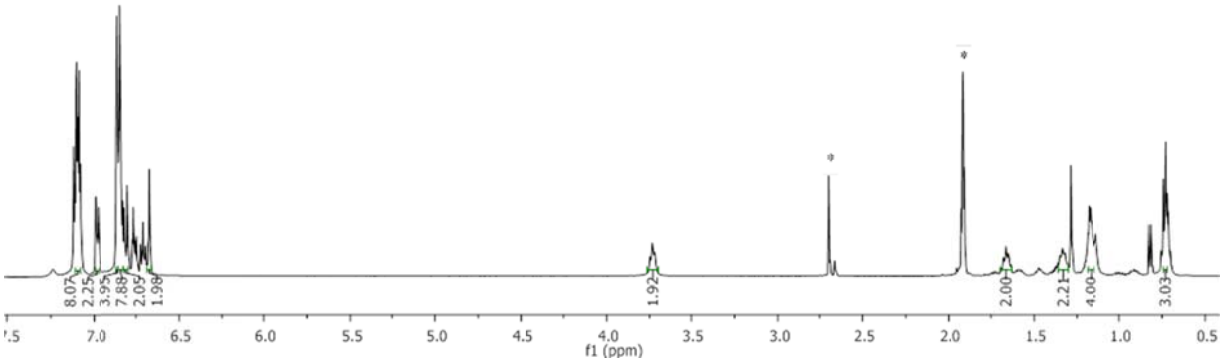


^{13}C and ^{13}C-DEPT 135 NMR (75 MHz) of **3g** (20 mg) in CD_2Cl_2 at 298 K.

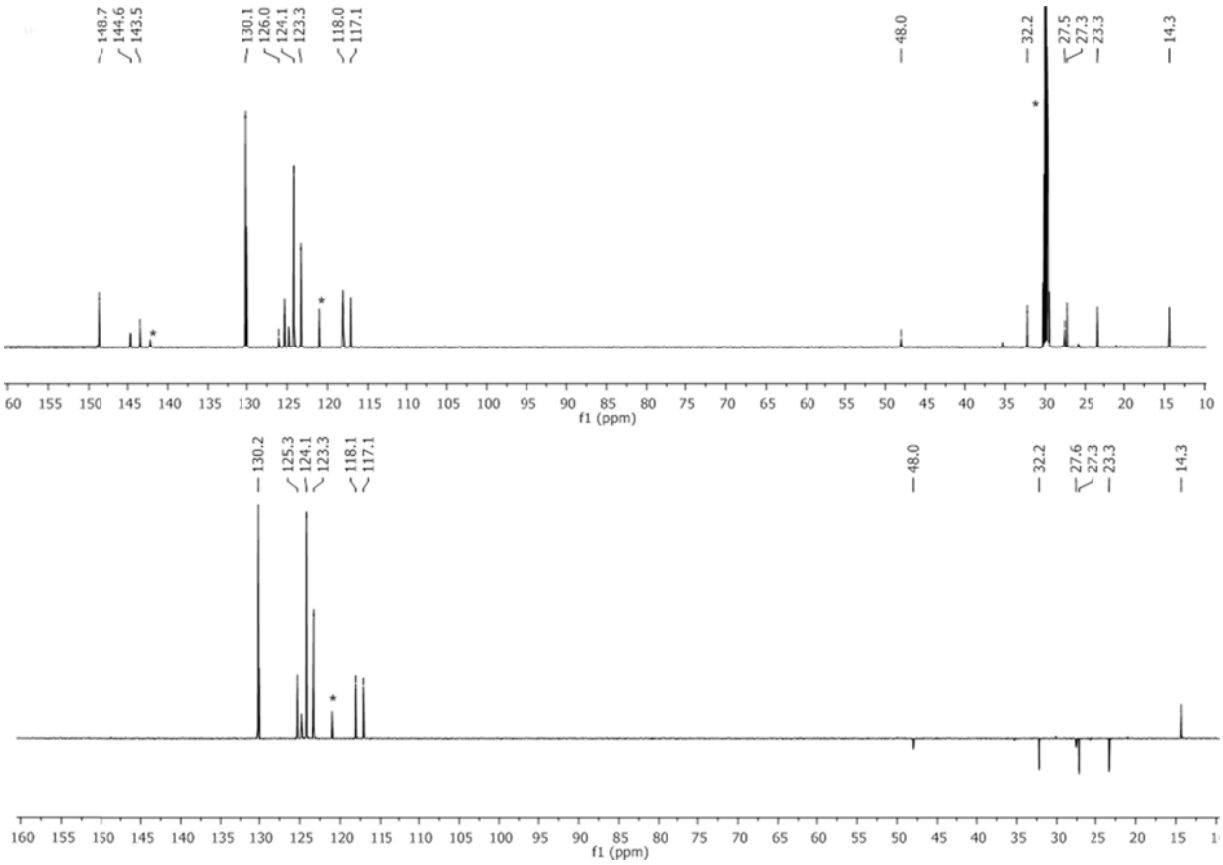
1.8 10-Hexyl-N^3,N^3,N^7,N^7-tetraphenyl-10*H*-phenothiazine-3,7-diamine (3h)



$C_{42}H_{39}N_3S$
617.84

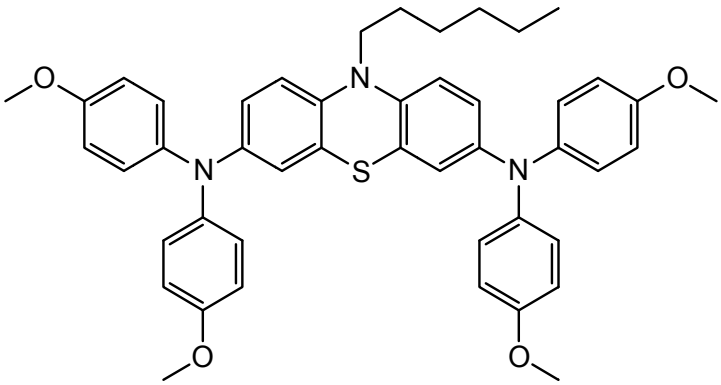


^{1}H NMR (300 MHz) of **3h** (20 mg) in acetone-d_6 at 298 K.

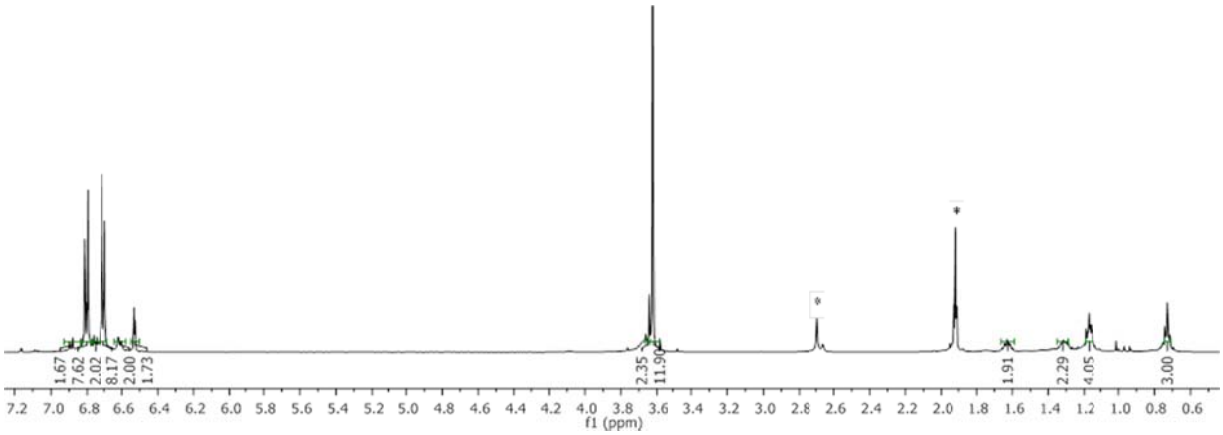


^{13}C and ^{13}C-DEPT 135 NMR (75 MHz) of **3h** (20 mg) in acetone-d_6 at 298 K.

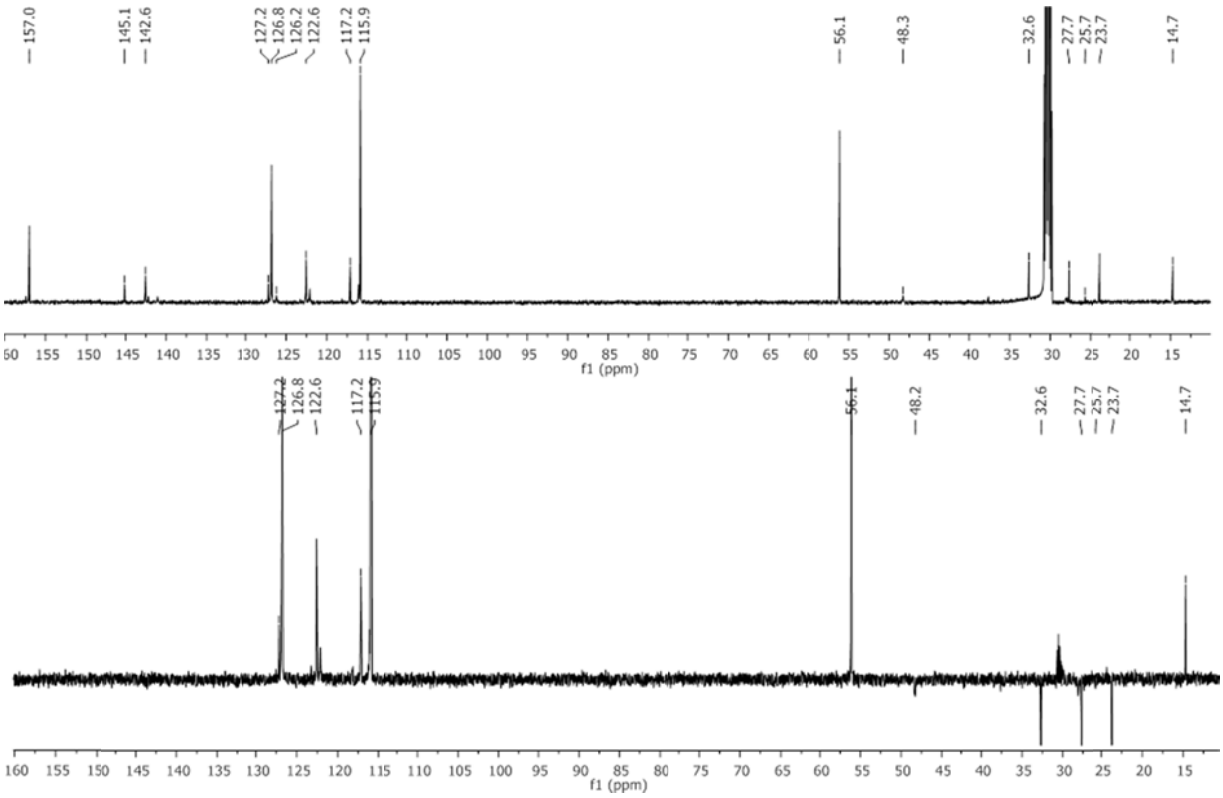
1.9 10-Hexyl-*N*^{3},*N*^{3},*N*^{7},*N*^{7}-tetrakis(4-methoxyphenyl)-10*H*-phenothiazine-3,7-diamine (3i)



$C_{46}H_{47}N_3O_4S$
737.95

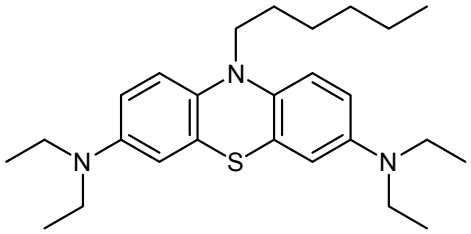


^{1}H NMR (300 MHz) of **3i** (20 mg) in acetone-d_6 at 298 K.

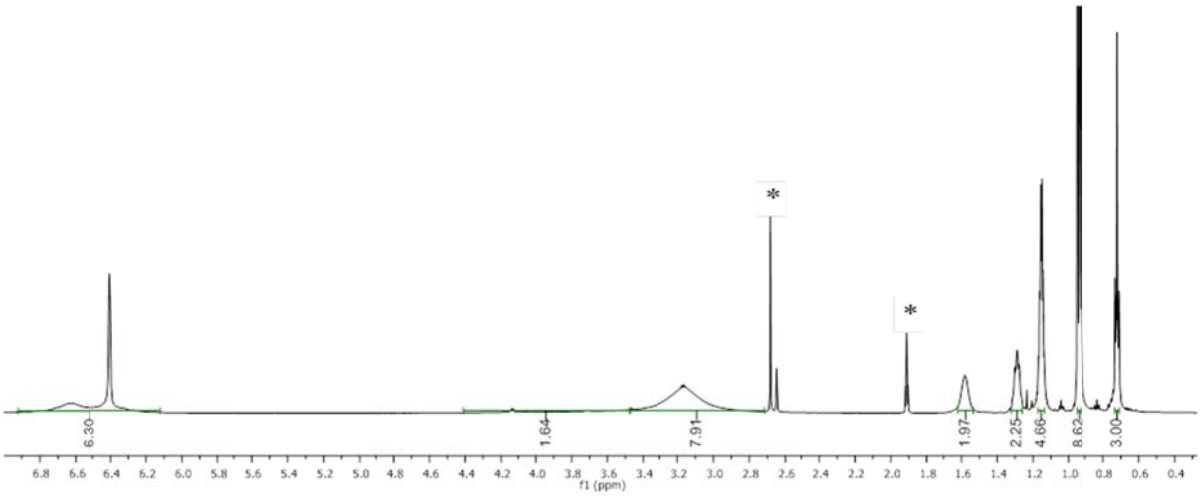


^{13}C and ^{13}C-DEPT 135 NMR (75 MHz) of **3i** (20 mg) in acetone-d_6 at 298 K.

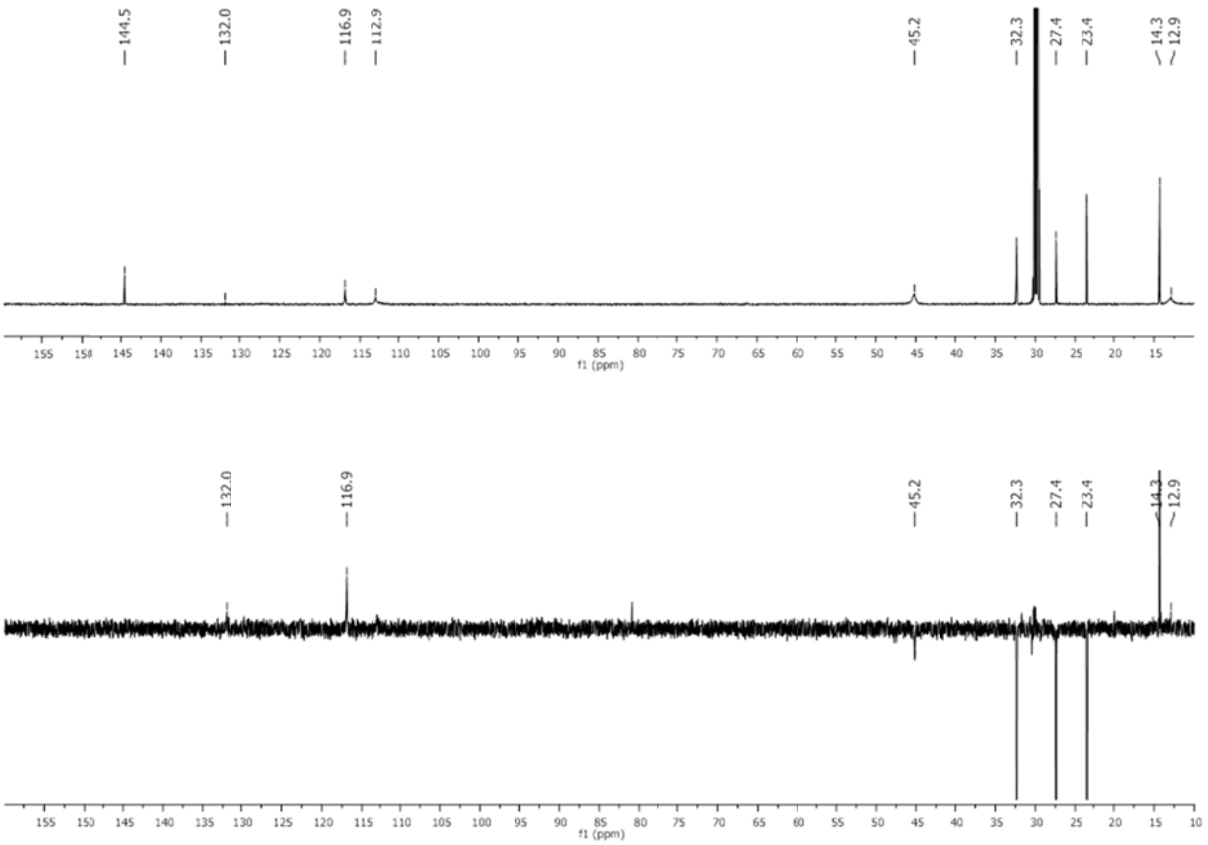
1.10 N^3,N^3,N^7,N^7-tetraethyl-10-hexyl-10*H*-phenothiazine-3,7-diamine (3j)



$C_{26}H_{39}N_3S$
425.67

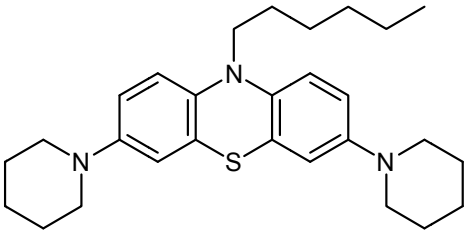


^{1}H NMR (300 MHz) of **3j** (20 mg) in acetone-d_6 at 298 K.

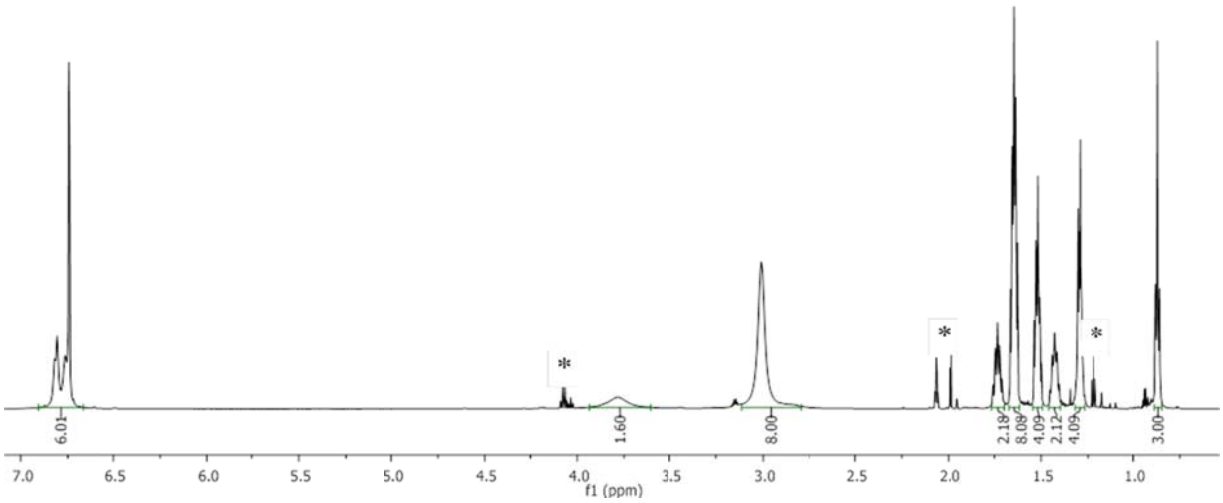


^{13}C and ^{13}C-DEPT 135 NMR (75 MHz) of **3j** (20 mg) in acetone-d_6 at 298 K.

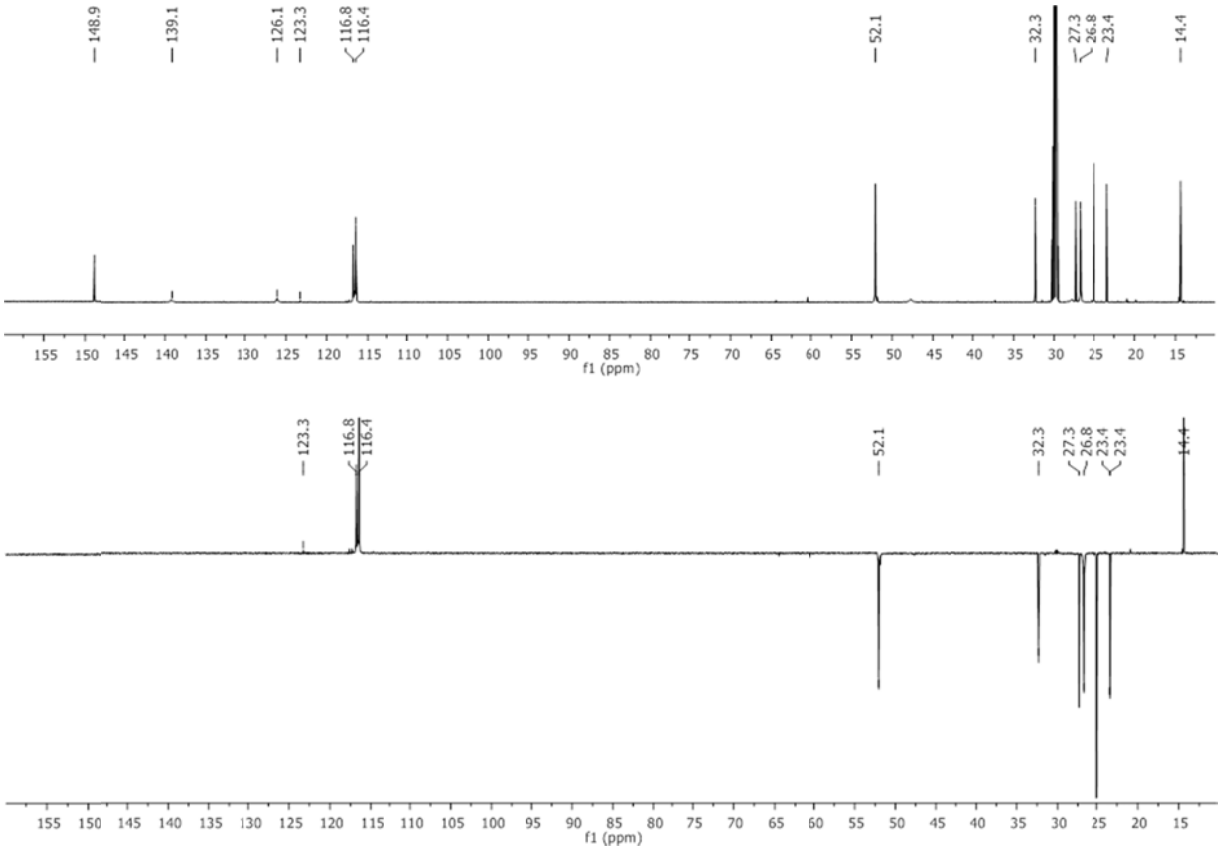
1.11 10-Hexyl-3,7-di(piperidin-1-yl)-10*H*-phenothiazine (3k)



$C_{28}H_{39}N_3S$
449.69

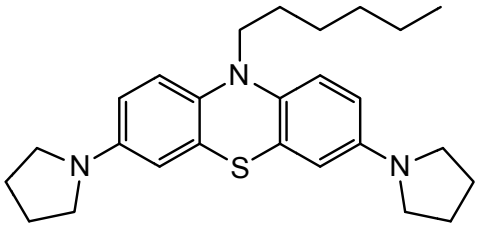


^{1}H NMR (300 MHz) of **3k** (20 mg) in acetone-d_6 at 298 K.

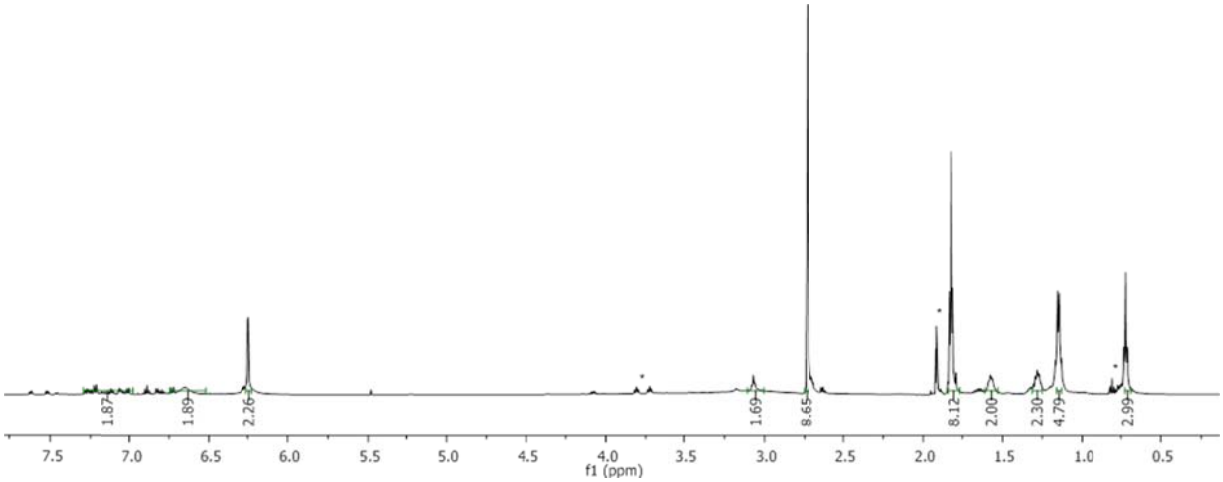


^{13}C and ^{13}C-DEPT 135 NMR (75 MHz) of **3k** (20 mg) in acetone-d_6 at 298 K.

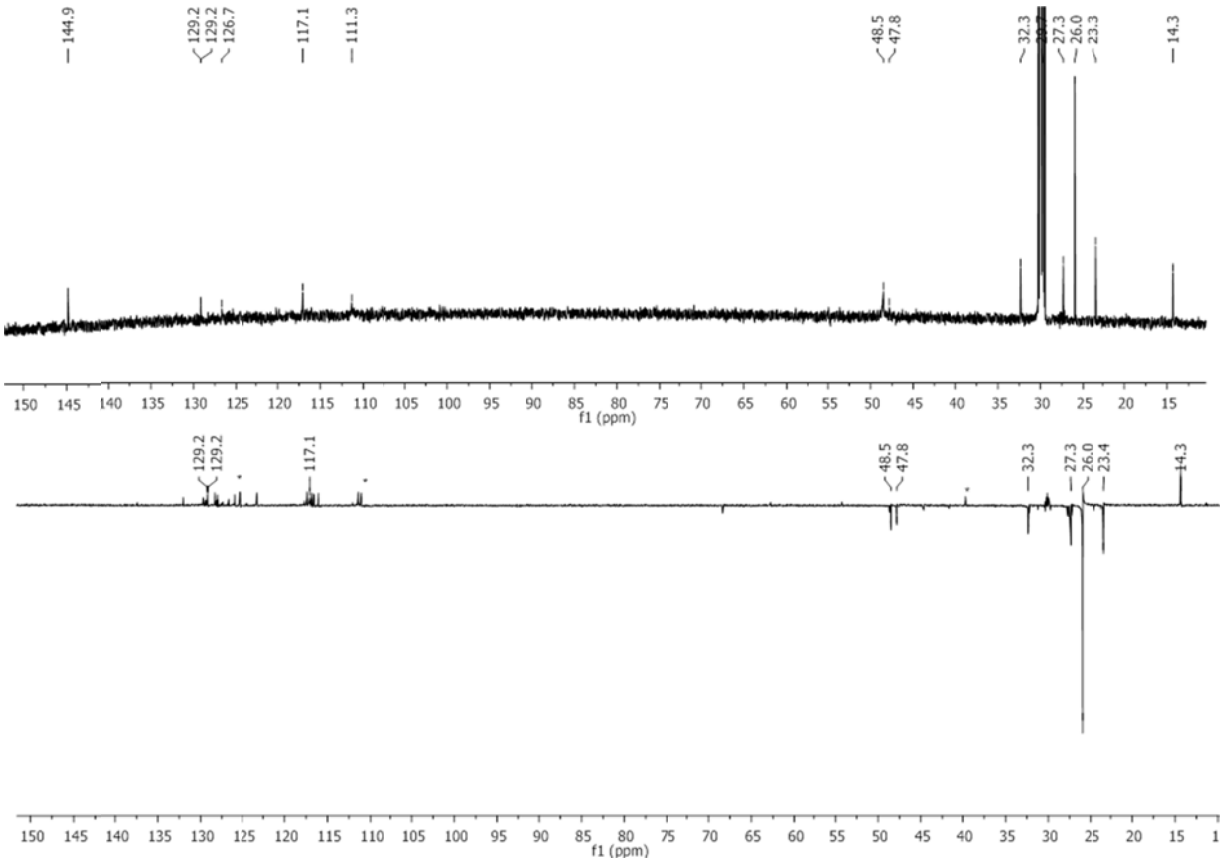
1.12 10-Hexyl-3,7-di(pyrrolidin-1-yl)-10*H*-phenothiazine (3l)



$C_{26}H_{35}N_3S$
421.64



^{1}H NMR (300 MHz) of **3l** (20 mg) in acetone-d_6 at 298 K.



^{13}C and ^{13}C-DEPT 135 NMR (75 MHz) of **3l** (20 mg) in acetone-d_6 at 298 K.

2 UV/Vis and emission spectra of 3,7-dianilino substituted *N*-hexyl phenothiazines 3a-3l

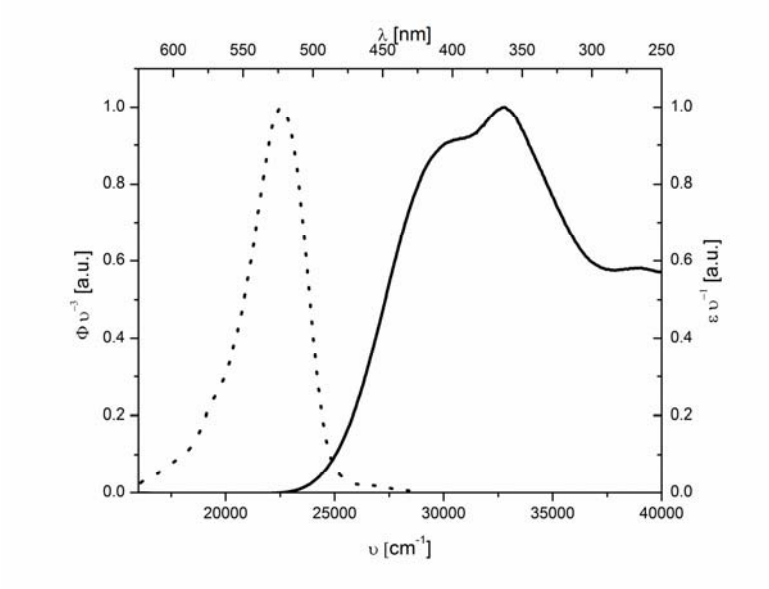


Figure 1: Normalized (arbitrary units) absorption (solid line) and emission spectra (dotted line) of Dimethyl 4,4'-((10-hexyl-10*H*-phenothiazine-3,7-diyl)bis-(azanediyl))dibenzoate **3a** (recorded in CH_2Cl_2: T = 293 K, λ_{exc} = longest wavelength λ_{max}).

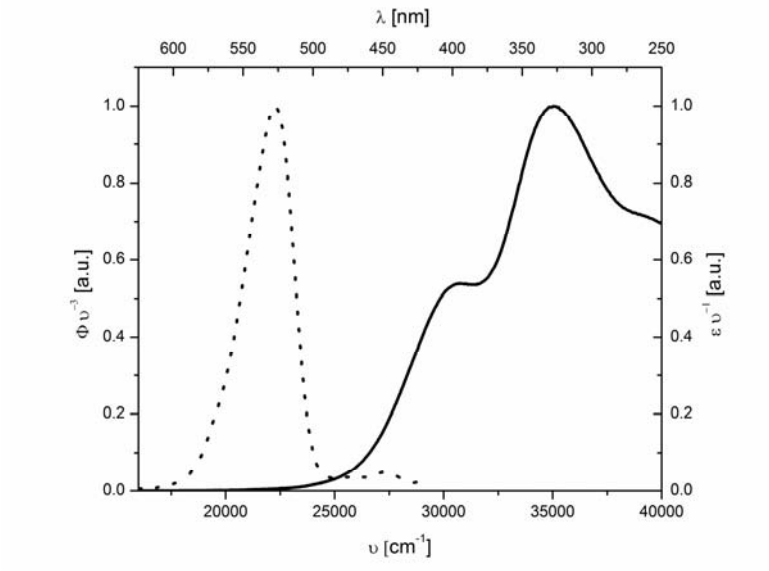


Figure 2: Normalized (arbitrary units) absorption (solid line) and emission spectra (dotted line) of N^3,N^7-Bis(4-(*tert*-butyl)phenyl)-10-hexyl-10*H*-phenothiazine-3,7-diamine **3b** (recorded in CH_2Cl_2: T = 293 K, λ_{exc} = longest wavelength λ_{max}).

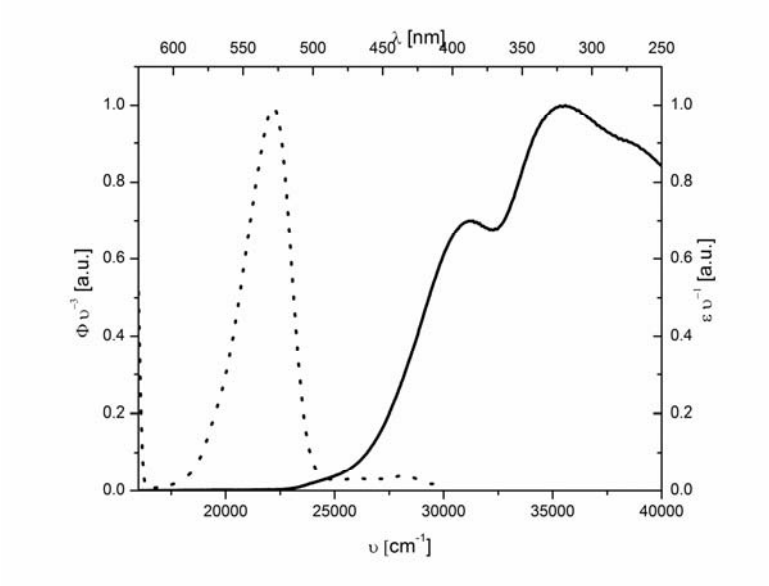


Figure 3: Normalized (arbitrary units) absorption (solid line) and emission spectra (dotted line) of 10-Hexyl-N^3,N^7-bis(4-methoxyphenyl)-10*H*-phenothiazine-3,7-diamine **3c** (recorded in CH_2Cl_2: T = 293 K, λ_{exc} = longest wavelength λ_{max}).

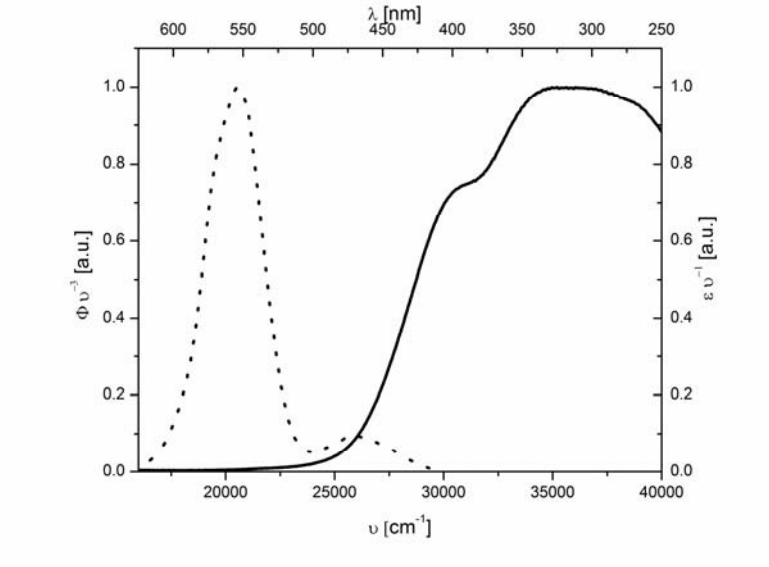


Figure 4: Normalized (arbitrary units) absorption (solid line) and emission spectra (dotted line) of N^1,$N^{1'}$-(10-Hexyl-10*H*-phenothiazine-3,7-diyl)bis(N^4,$N^{4'}$-dimethylbenzene-1,4-diamine) **3d**
(recorded in CH_2Cl_2: T = 293 K, λ_{exc} = longest wavelength λ_{max}).

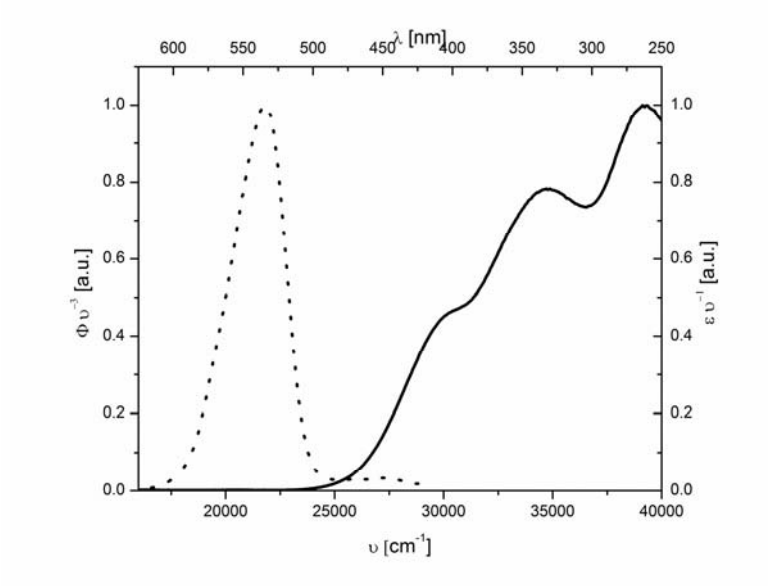


Figure 5: Normalized (arbitrary units) absorption (solid line) and emission spectra (dotted line) of 10-Hexyl-N^3,N^7-dimethyl-N^3,N^7-diphenyl-10*H*-phenothiazine-3,7-diamine **3e** (recorded in CH_2Cl_2: T = 293 K, λ_{exc} = longest wavelength λ_{max}).

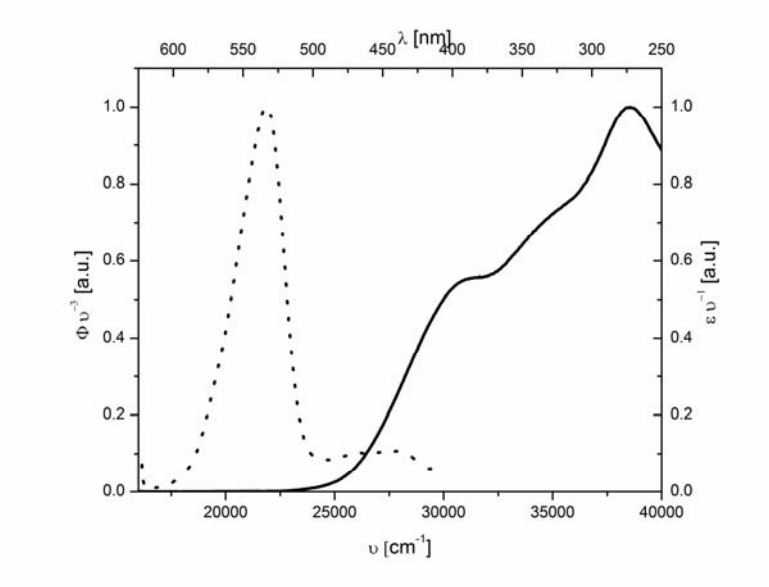


Figure 6: Normalized (arbitrary units) absorption (solid line) and emission spectra (dotted line) of 10-Hexyl-N^3,N^7-bis(4-methoxyphenyl)-N^3,N^7-dimethyl-10*H*-phenothiazine-3,7-diamine **3f**
(recorded in CH_2Cl_2: T = 293 K, λ_{exc} = longest wavelength λ_{max}).

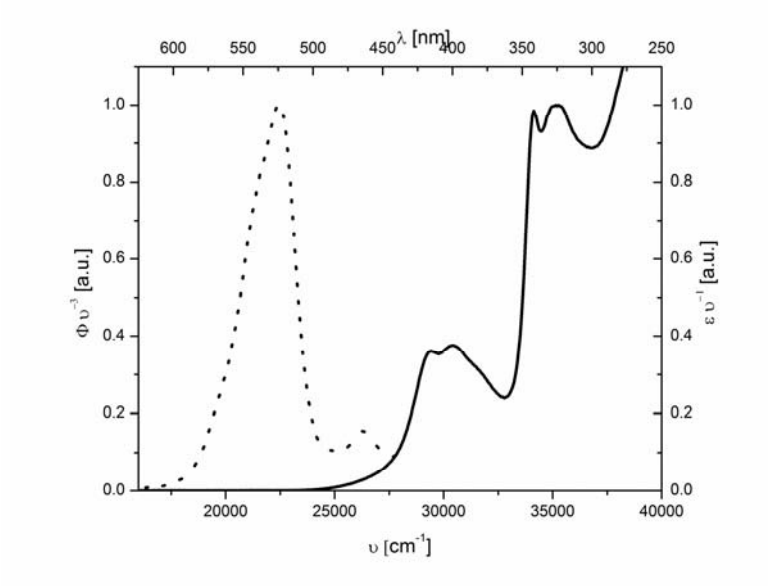


Figure 7: Normalized (arbitrary units) absorption (solid line) and emission spectra (dotted line) of 3,7-Di(9*H*-carbazol-9-yl)-10-hexyl-10*H*-phenothiazine **3g** (recorded in CH_2Cl_2: T = 293 K, λ_{exc} = longest wavelength λ_{max}).

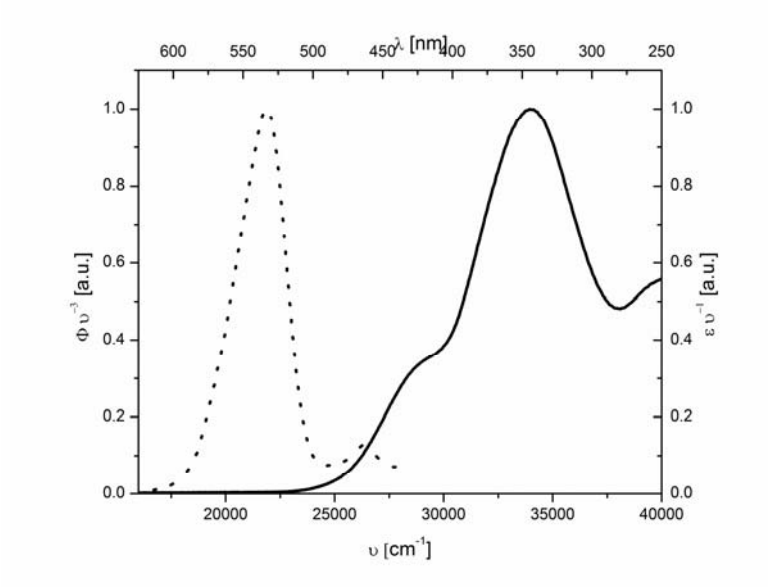


Figure 8: Normalized (arbitrary units) absorption (solid line) and emission spectra (dotted line) of 10-Hexyl-N^3,N^3,N^7,N^7-tetraphenyl-10*H*-phenothiazine-3,7-diamine **3h** (recorded in CH_2Cl_2: T = 293 K, λ_{exc} = longest wavelength λ_{max}).

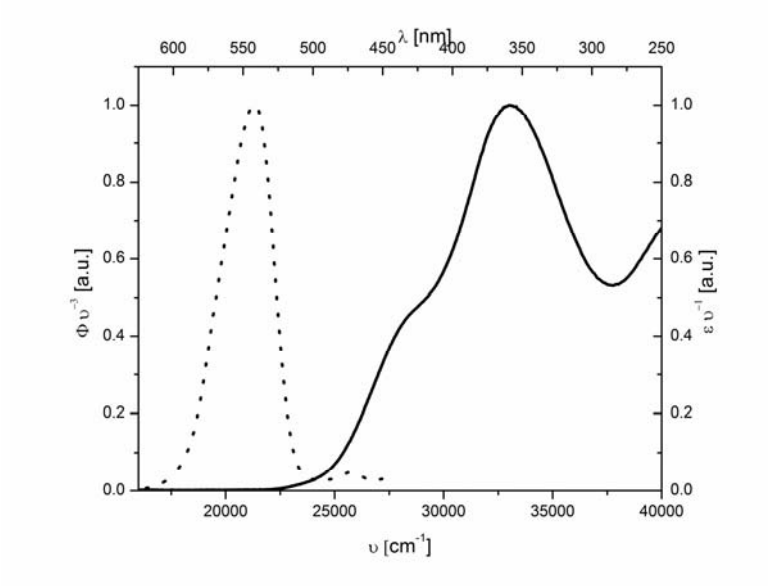


Figure 9: Normalized (arbitrary units) absorption (solid line) and emission spectra (dotted line) of 10-Hexyl-N^3,N^3,N^7,N^7-tetrakis(4-methoxyphenyl)-10*H*-phenothiazine-3,7-diamine **3i** (recorded in CH_2Cl_2: T = 293 K, λ_{exc} = longest wavelength λ_{max}).

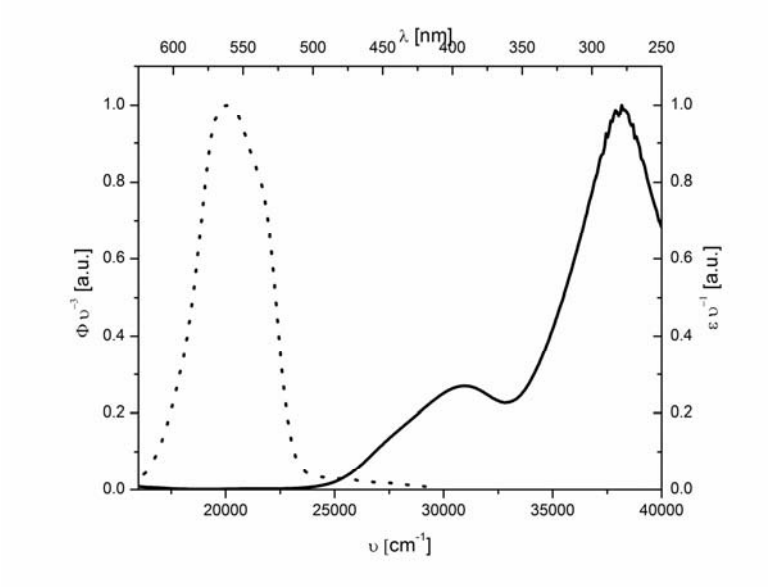


Figure 10: Normalized (arbitrary units) absorption (solid line) and emission spectra (dotted line) of N^3,N^3,N^7,N^7-tetraethyl-10-hexyl-10*H*-phenothiazine-3,7-diamine **3j** (recorded in CH_2Cl_2: T = 293 K, λ_{exc} = longest wavelength λ_{max}).

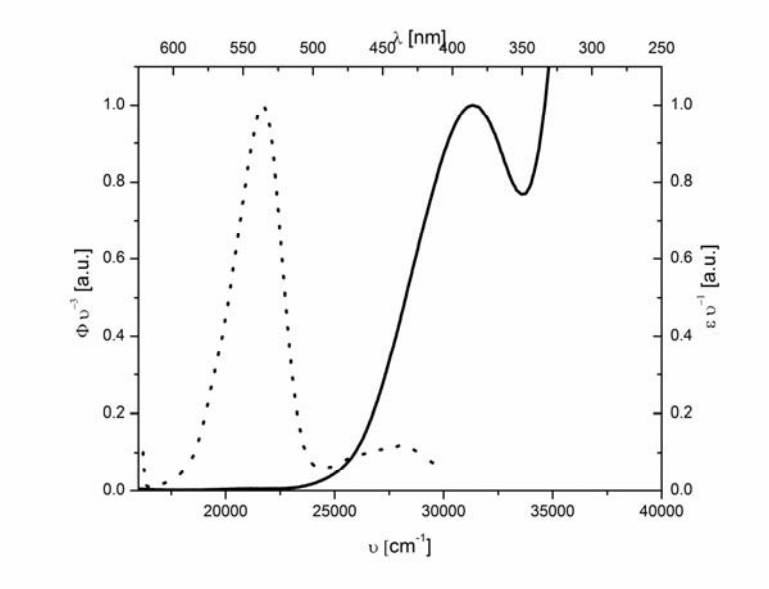


Figure 11: Normalized (arbitrary units) absorption (solid line) and emission spectra (dotted line) of 10-Hexyl-3,7-di(piperidin-1-yl)-10*H*-phenothiazine **3k** (recorded in CH_2Cl_2: T = 293 K, λ_{exc} = longest wavelength λ_{max}).

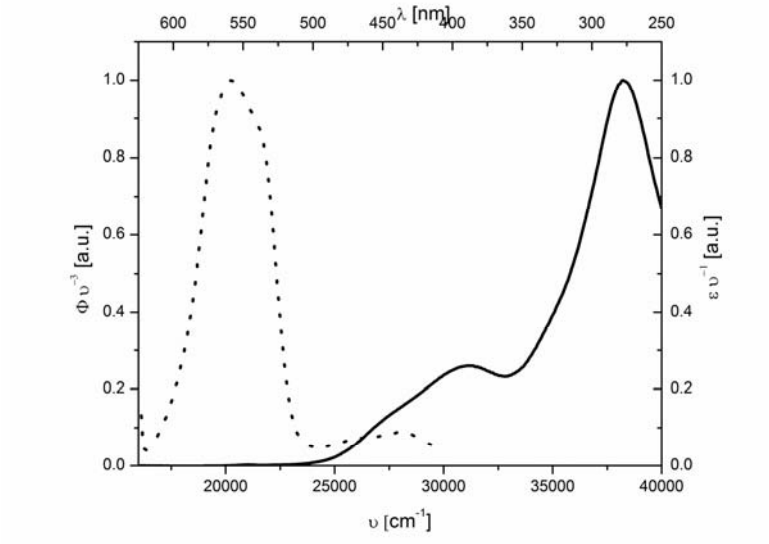


Figure 12: Normalized (arbitrary units) absorption (solid line) and emission spectra (dotted line) of 10-Hexyl-3,7-di(pyrrolidin-1-yl)-10*H*-phenothiazine **3l** (recorded in CH_2Cl_2: T = 293 K, λ_{exc} = longest wavelength λ_{max}).

3 Cyclic voltammograms of 3,7-dianilino substituted *N*-hexyl phenothiazines 3a-3l

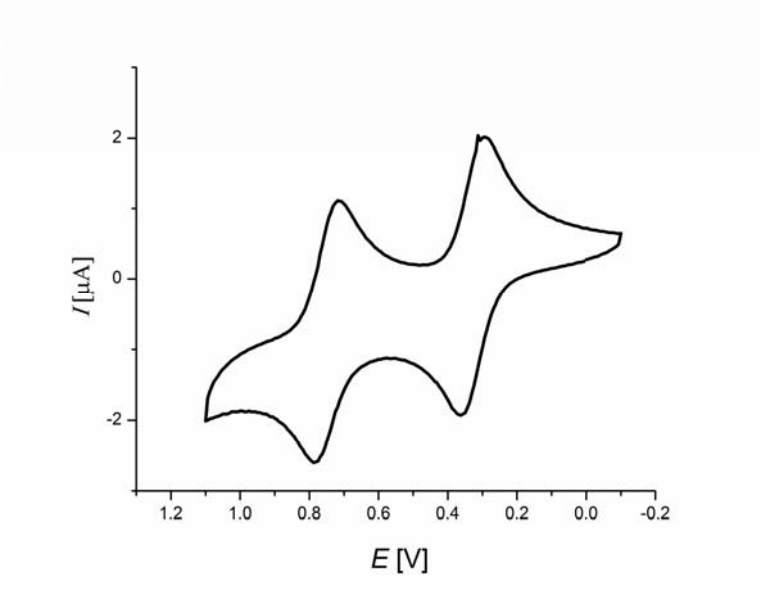


Figure 13: Cyclic voltammogram of Dimethyl 4,4'-((10-hexyl-10*H*-phenothiazine-3,7-diyl)bis-(azanediyl))dibenzoate **3a** (recorded in CH_2Cl_2 at T = 293 K, 0.1 M electrolyte $[Bu_4N][PF_6]$, v = 100 mV/s, Pt working electrode, Ag/AgCl reference and Pt counter electrode).

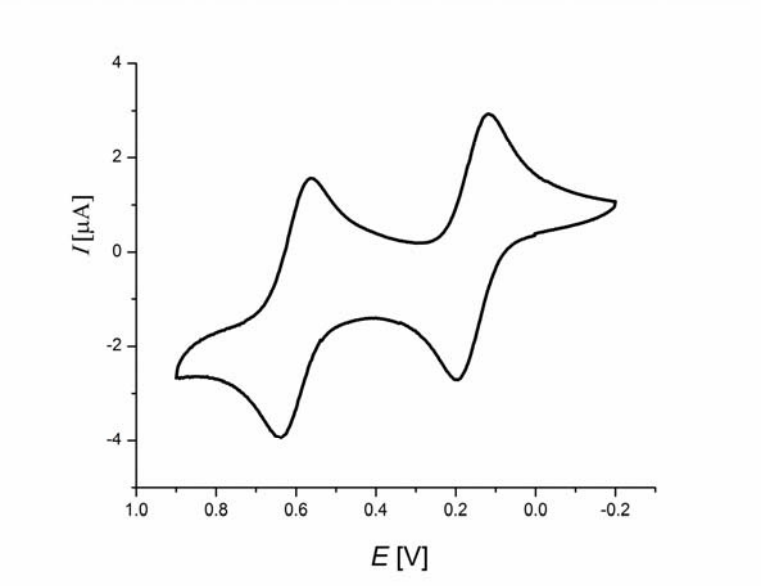


Figure 14: Cyclic voltammogram of N^3,N^7-Bis(4-(*tert*-butyl)phenyl)-10-hexyl-10*H*-phenothiazine-3,7-diamine **3b** (recorded in CH_2Cl_2 at T = 293 K, 0.1 M electrolyte $[Bu_4N][PF_6]$, v = 100 mV/s, Pt working electrode, Ag/AgCl reference and Pt counter electrode).

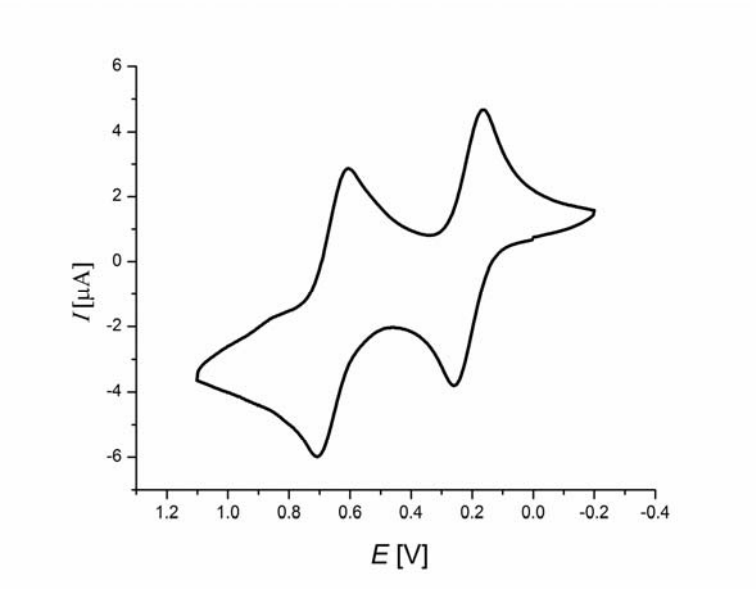


Figure 15: Cyclic voltammogram of 10-Hexyl-N^3,N^7-bis(4-methoxyphenyl)-10*H*-phenothiazine-3,7-diamine **3c** (recorded in CH_2Cl_2 at T = 293 K, 0.1 M electrolyte $[Bu_4N][PF_6]$, v = 100 mV/s, Pt working electrode, Ag/AgCl reference and Pt counter electrode).

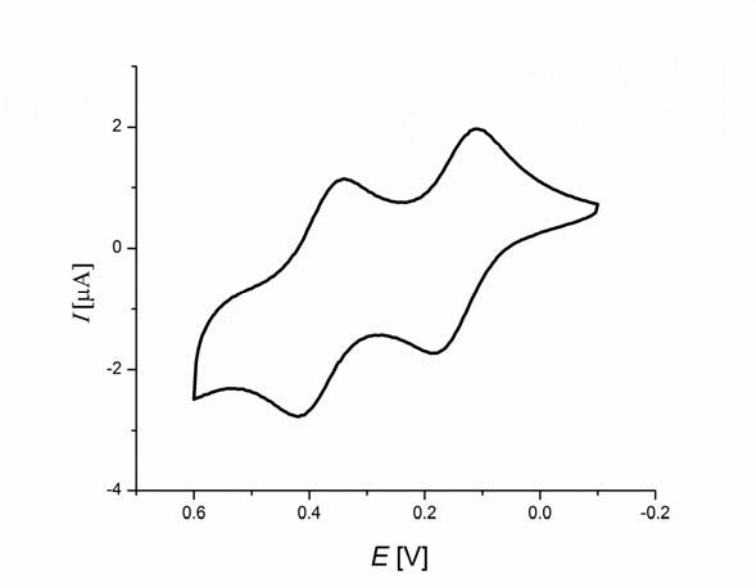


Figure 16: Cyclic voltammogram of N^1,$N^{1\prime}$-(10-Hexyl-10*H*-phenothiazine-3,7-diyl)bis(N^4,$N^{4\prime}$-dimethylbenzene-1,4-diamine) **3d** (recorded in CH_2Cl_2 at T = 293 K, 0.1 M electrolyte $[Bu_4N][PF_6]$, v = 100 mV/s, Pt working electrode, Ag/AgCl reference and Pt counter electrode).

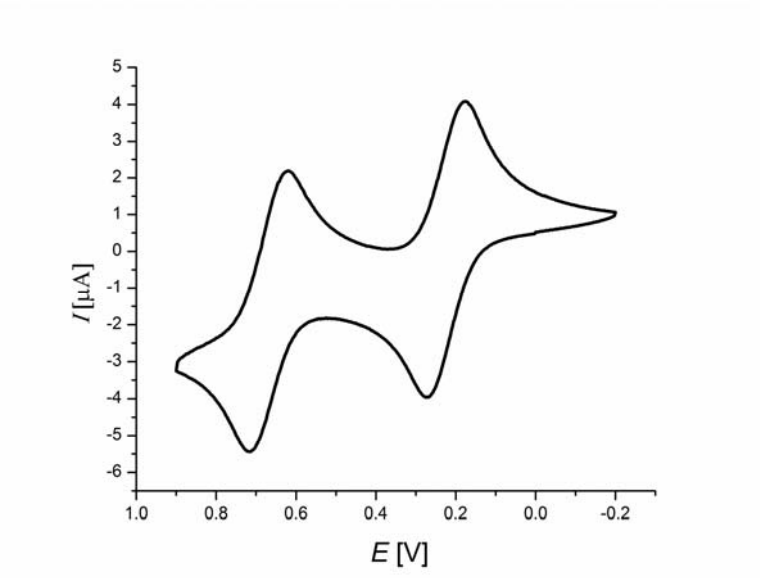


Figure 17: Cyclic voltammogram of 10-Hexyl-N^3,N^7-dimethyl-N^3,N^7-diphenyl-10*H*-phenothiazine-3,7-diamine **3e** (recorded in CH_2Cl_2 at T = 293 K, 0.1 M electrolyte $[Bu_4N][PF_6]$, v = 100 mV/s, Pt working electrode, Ag/AgCl reference and Pt counter electrode).

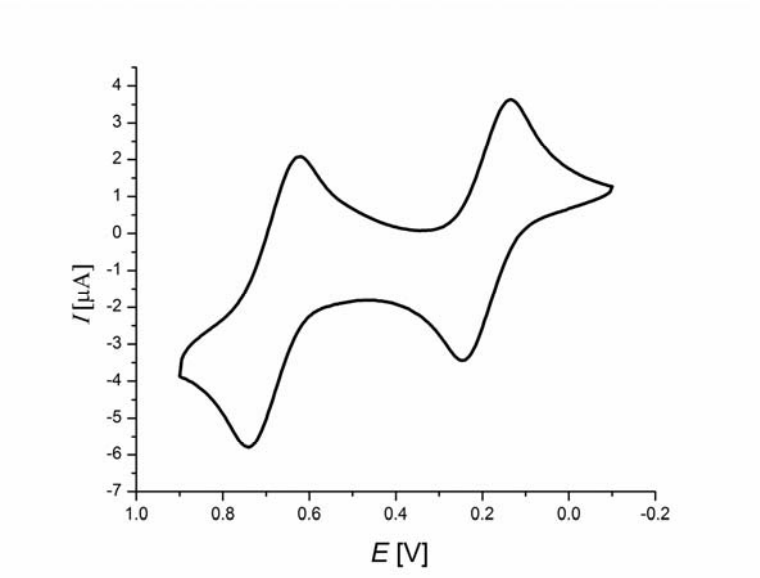


Figure 18: Cyclic voltammogram of 10-Hexyl-N^3,N^7-bis(4-methoxyphenyl)-N^3,N^7-dimethyl-10*H*-phenothiazine-3,7-diamine **3f** (recorded in CH_2Cl_2 at T = 293 K, 0.1 M electrolyte $[Bu_4N][PF_6]$, v = 100 mV/s, Pt working electrode, Ag/AgCl reference and Pt counter electrode).

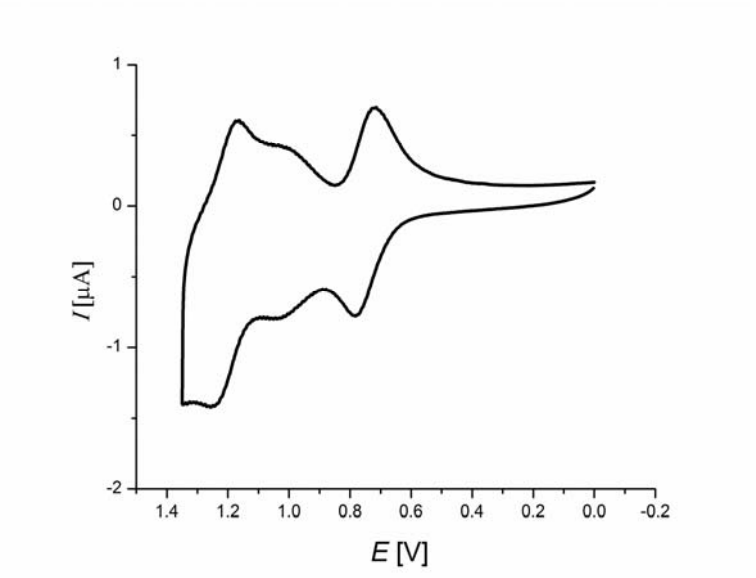


Figure 19: Cyclic voltammogram of 3,7-Di(9*H*-carbazol-9-yl)-10-hexyl-10*H*-phenothiazine **3g** (recorded in CH_2Cl_2 at T = 293 K, 0.1 M electrolyte $[Bu_4N][PF_6]$, v = 100 mV/s, Pt working electrode, Ag/AgCl reference and Pt counter electrode).

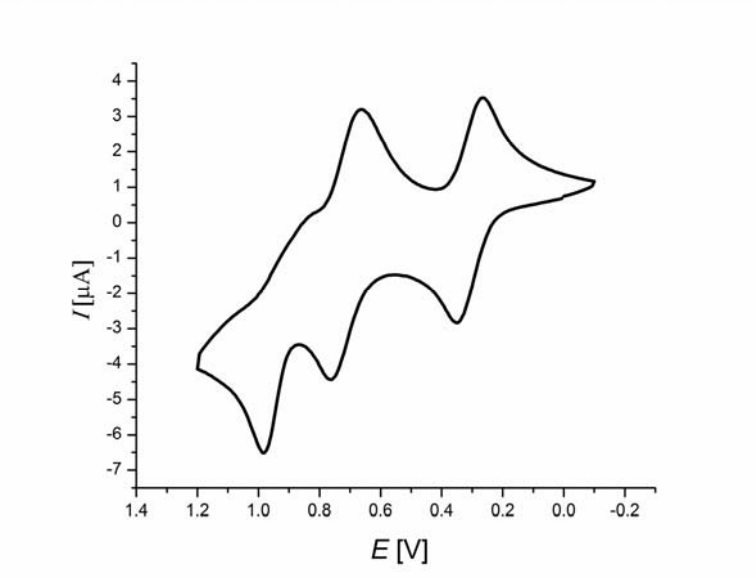


Figure 20: Cyclic voltammogram of 10-Hexyl-N^3,N^3,N^7,N^7-tetraphenyl-10*H*-phenothiazine-3,7-diamine **3h** (recorded in CH_2Cl_2 at T = 293 K, 0.1 M electrolyte $[Bu_4N][PF_6]$, v = 100 mV/s, Pt working electrode, Ag/AgCl reference and Pt counter electrode).

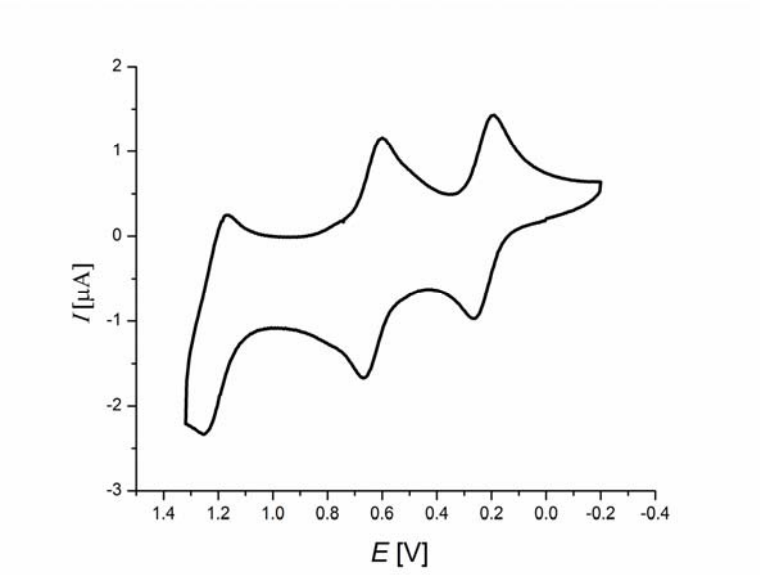


Figure 21: Cyclic voltammogram of 10-Hexyl-N^3,N^3,N^7,N^7-tetrakis(4-methoxyphenyl)-10*H*-phenothiazine-3,7-diamine **3i** (recorded in CH_2Cl_2 at T = 293 K, 0.1 M electrolyte $[Bu_4N][PF_6]$, v = 100 mV/s, Pt working electrode, Ag/AgCl reference and Pt counter electrode).

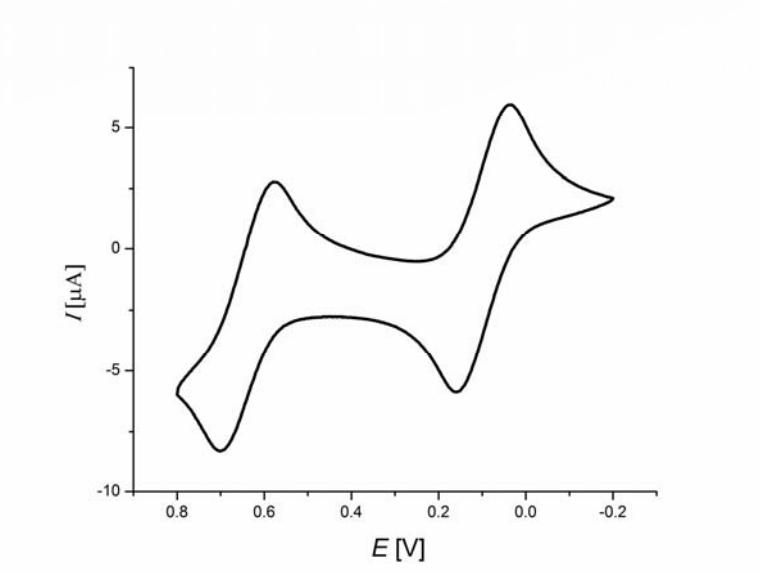


Figure 22: Cyclic voltammogram of N^3,N^3,N^7,N^7-tetraethyl-10-hexyl-10*H*-phenothiazine-3,7-diamine **3j** (recorded in CH_2Cl_2 at T = 293 K, 0.1 M electrolyte $[Bu_4N][PF_6]$, v = 100 mV/s, Pt working electrode, Ag/AgCl reference and Pt counter electrode).

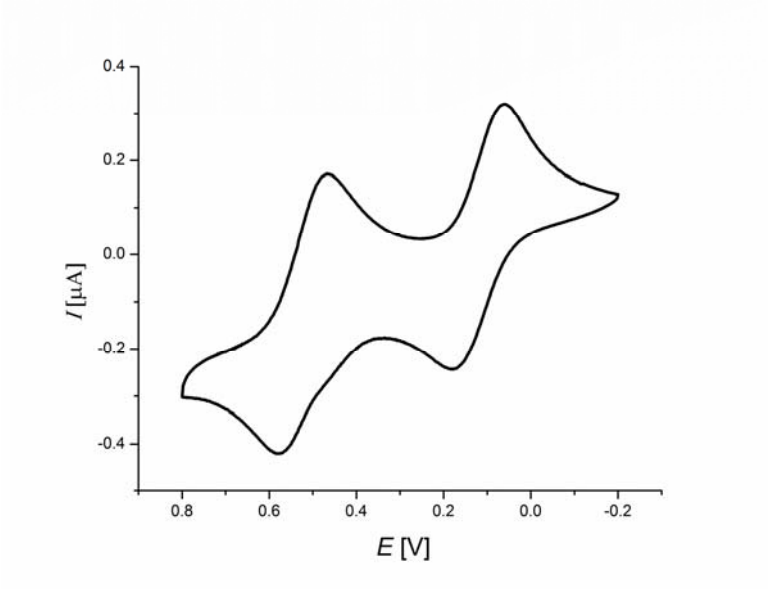


Figure 23: Cyclic voltammogram of 10-Hexyl-3,7-di(piperidin-1-yl)-10*H*-phenothiazine **3k** (recorded in CH_2Cl_2 at T = 293 K, 0.1 M electrolyte $[Bu_4N][PF_6]$, v = 100 mV/s, Pt working electrode, Ag/AgCl reference and Pt counter electrode).

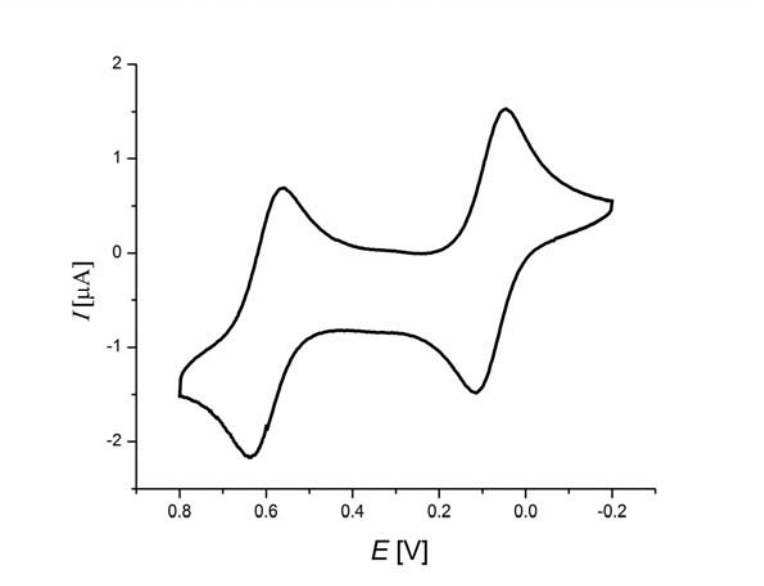


Figure 24: Cyclic voltammogram of 10-Hexyl-3,7-di(pyrrolidin-1-yl)-10*H*-phenothiazine **3l** (recorded in CH_2Cl_2 at T = 293 K, 0.1 M electrolyte $[Bu_4N][PF_6]$, v = 100 mV/s, Pt working electrode, Ag/AgCl reference and Pt counter electrode).

4 Computed xyz-coordinates and energies of 3,7-dianilino substituted *N*-hexyl phenothiazines 3a-3l

The ground state geometries of the 3,7-dianilino substituted *N*-hexyl phenothiazines **3a-3l** were optimized by DFT calculation with the B3LYP: def2-TZVP functional in the program package TURBOMOLE V6.3.

XYZ-coordinates for Dimethyl 4,4'-((10-hexyl-10*H*-phenothiazine-3,7-diyl)bis-(azanediyl))dibenzoate **3a**

H	-1.6715	-1.5018	-2.2927
C	-0.6503	-1.1506	-2.3449
C	1.9229	-0.1722	-2.5286
C	0.1764	-1.2465	-1.2207
C	-0.1962	-0.6292	-3.5478
C	1.0986	-0.1181	-3.6554
C	1.4849	-0.7566	-1.3472
H	-0.8552	-0.6256	-4.4042
H	2.9256	0.2361	-2.5764
N	-0.2783	-1.787	-5.0E-4
S	2.6202	-0.9355	-2.0E-4
C	1.4846	-0.7567	1.3466
C	-0.1968	-0.6296	3.547
C	0.1762	-1.2466	1.2198
C	1.9224	-0.1724	2.5282
C	1.098	-0.1184	3.6548
C	-0.6507	-1.1509	2.344
H	2.9251	0.236	2.5761
H	-1.6718	-1.5022	2.2916
H	-0.8558	-0.6262	4.4033
C	-1.1588	-2.9558	-6.0E-4
H	-1.8143	-2.9133	-0.8694
H	-1.8154	-2.9128	0.8674
C	-0.3934	-4.2832	2.0E-4
H	0.2598	-4.3144	0.8779
H	0.2607	-4.315	-0.8768
C	-1.3235	-5.4967	2.0E-4
H	-1.9814	-5.4513	-0.8762

H	-1.9821	-5.4509	0.876
C	-0.5811	-6.8338	8.0E-4
H	0.0764	-6.8817	0.8768
H	0.077	-6.8822	-0.8747
C	-1.5088	-8.0496	8.0E-4
H	-2.1663	-8.0009	0.8758
H	-2.1657	-8.0013	-0.8748
C	-0.7595	-9.3812	0.0013
H	-1.4499	-10.2272	0.0013
H	-0.1201	-9.4751	-0.8803
H	-0.1206	-9.4747	0.8834
N	1.6212	0.3953	4.852
H	2.6071	0.2463	4.9902
N	1.6219	0.3959	-4.8524
H	2.6078	0.2469	-4.9906
C	0.9877	1.1146	5.8499
C	-0.1781	2.6018	7.9417
C	1.6486	1.2747	7.0818
C	-0.2652	1.7256	5.6834
C	-0.8321	2.4523	6.7162
C	1.0773	2.0052	8.1022
H	2.6172	0.8093	7.2281
H	-0.7814	1.6538	4.7374
H	-1.7942	2.9221	6.5668
H	1.5909	2.1214	9.0473
C	0.9883	1.1153	-5.8502
C	-0.178	2.6023	-7.9418
C	1.6491	1.2754	-7.0821
C	-0.2646	1.7261	-5.6835
C	-0.8317	2.4528	-6.7162
C	1.0775	2.0059	-8.1025
H	2.6177	0.8102	-7.2286
H	-0.7806	1.6542	-4.7375
H	-1.7939	2.9225	-6.5667
H	1.591	2.1222	-9.0477
C	-0.7465	3.367	9.0723
O	-0.2027	3.5243	10.142
O	-1.9635	3.8886	8.7903
C	-2.5722	4.6502	9.841
H	-1.9493	5.5044	10.1069
H	-2.7207	4.0331	10.7271

H	-3.5278	4.9844	9.4448
C	-0.7467	3.3674	-9.0724
O	-0.2031	3.5248	-10.1421
O	-1.9637	3.8889	-8.7902
C	-2.5727	4.6504	-9.8408
H	-1.95	5.5045	-10.1068
H	-3.5283	4.9844	-9.4443
H	-2.7213	4.0331	-10.7267

HOMO level energy = -4.9801 eV

LUMO level energy = -1.3015 eV

HOMO-LUMO gap energy = 3.679 eV.

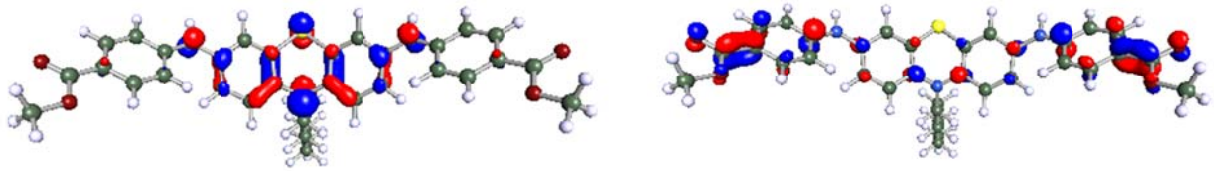


Figure 25: HOMO (left) and LUMO (right) levels of compound **3a**

XYZ-coordinates for N^3,N^7-Bis(4-(*tert*-butyl)phenyl)-10-hexyl-10*H*-phenothiazine-3,7-diamine **3b**

H	2.2409	-0.7975	2.0993
C	2.3273	-0.2286	1.1827
C	2.5623	1.3315	-1.0784
C	1.2227	-0.1262	0.3324
C	3.5315	0.4017	0.9054
C	3.6719	1.1935	-0.2389
C	1.3672	0.6768	-0.8067
H	4.3474	0.315	1.6085
H	2.6362	1.9455	-1.9693
N	6.0E-4	-0.7671	0.6285
S	0.0368	0.7968	-1.9715
C	-1.2181	-0.1395	0.2899

C	-3.6634	1.1456	-0.371
C	-2.3504	-0.2558	1.0999
C	-1.3328	0.6607	-0.8548
C	-2.5255	1.299	-1.1701
C	-3.5531	0.3572	0.7786
H	-2.2903	-0.8242	2.0189
H	-2.5764	1.9104	-2.0643
H	-4.3925	0.257	1.4513
N	-4.8278	1.8317	-0.726
H	-4.6851	2.6704	-1.263
N	4.8357	1.9073	-0.5372
H	4.7031	2.7205	-1.1145
C	-6.1535	1.5633	-0.3862
C	-8.9071	1.1077	0.1955
C	-7.0871	2.6033	-0.4201
C	-6.621	0.2829	-0.0638
C	-7.9612	0.0766	0.2239
C	-8.429	2.3744	-0.1447
H	-6.7562	3.6074	-0.6629
H	-5.9415	-0.5576	-0.0615
H	-8.2736	-0.9325	0.4641
H	-9.1031	3.2183	-0.1899
C	6.1654	1.5927	-0.2573
C	8.9265	1.069	0.227
C	6.609	0.3115	0.0762
C	7.1283	2.608	-0.3523
C	8.4669	2.3453	-0.1232
C	7.9586	0.0692	0.3158
H	5.9089	-0.5101	0.1278
H	6.8149	3.6154	-0.6048
H	9.1673	3.1667	-0.2122
H	8.2451	-0.9425	0.5675
C	10.4201	0.8263	0.4866
C	10.7154	-0.6339	0.8619
H	11.7855	-0.7573	1.0417
H	10.4342	-1.3238	0.0634
H	10.192	-0.9335	1.7726
C	11.2291	1.1675	-0.7829
H	12.2966	1.0076	-0.6102
H	11.0931	2.2082	-1.081
H	10.9222	0.5377	-1.6207

C	10.8971	1.7245	1.6479
H	11.9608	1.564	1.8423
H	10.3465	1.5009	2.5643
H	10.7562	2.7833	1.4253
C	-10.3799	0.82	0.5206
C	-11.2504	2.0838	0.4421
H	-11.2453	2.5194	-0.5593
H	-10.9217	2.848	1.1495
H	-12.2847	1.8325	0.6862
C	-10.9401	-0.2109	-0.4826
H	-10.8825	0.1695	-1.5046
H	-11.9879	-0.4298	-0.2599
H	-10.3888	-1.1515	-0.4454
C	-10.4931	0.2489	1.9501
H	-9.9305	-0.6794	2.0594
H	-11.5372	0.0367	2.195
H	-10.1098	0.9599	2.685
C	-0.0011	-2.1715	1.0418
H	-0.863	-2.3538	1.6842
H	0.8775	-2.3586	1.6588
C	-0.0203	-3.1534	-0.1355
H	0.8525	-2.9642	-0.7678
H	-0.9013	-2.9495	-0.7516
C	-0.0294	-4.6142	0.3166
H	-0.8994	-4.7909	0.96
H	0.8519	-4.8086	0.9394
C	-0.0536	-5.6116	-0.843
H	0.8161	-5.4379	-1.487
H	-0.9342	-5.4189	-1.4665
C	-0.0644	-7.0739	-0.3946
H	-0.9335	-7.2466	0.2493
H	0.8163	-7.2663	0.2277
C	-0.0901	-8.0631	-1.5591
H	-0.0972	-9.0963	-1.2052
H	0.7849	-7.9385	-2.2021
H	-0.978	-7.9189	-2.1801

HOMO level energy = -4.5836 eV

LUMO level energy = -0.6021 eV

HOMO-LUMO gap energy = 3.981 eV.

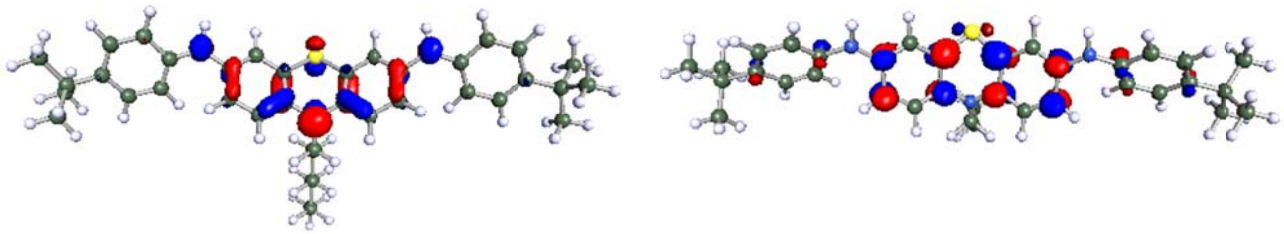


Figure 26: HOMO (left) and LUMO (right) levels of compound **3b**

XYZ-coordinates for 10-Hexyl-N^3,N^7-bis(4-methoxyphenyl)-10*H*-phenothiazine-3,7-diamine **3c**

H	-2.0443	0.673	2.2679
C	-1.1272	0.1028	2.3404
C	1.1355	-1.4579	2.5415
C	-0.2978	-0.0038	1.2211
C	-0.8297	-0.5224	3.5428
C	0.3144	-1.3186	3.6659
C	0.8439	-0.8054	1.3504
H	-1.5165	-0.4269	4.3714
H	2.0255	-2.0749	2.6001
N	-0.6179	0.6306	2.0E-4
S	1.9849	-0.9344	3.0E-4
C	0.8438	-0.8057	-1.3498
C	-0.8297	-0.5229	-3.5423
C	-0.2979	-0.0039	-1.2207
C	1.1351	-1.4587	-2.5406
C	0.3141	-1.3195	-3.6651
C	-1.1271	0.1027	-2.3401
H	2.025	-2.076	-2.5991
H	-2.0439	0.6735	-2.2679
H	-1.5166	-0.4277	-4.3709
N	0.639	-2.0245	4.8236
H	1.2386	-2.8204	4.688
N	0.6388	-2.0253	-4.8228
H	1.2381	-2.8215	-4.6874
C	0.2392	-1.7924	6.1453
C	-0.4623	-1.4263	8.8504
C	0.1851	-2.8761	7.0349

C	-0.0588	-0.5245	6.6441
C	-0.4169	-0.3419	7.9785
C	-0.1471	-2.697	8.3642
H	0.4044	-3.8735	6.6706
H	0.0044	0.339	5.9968
H	-0.641	0.6576	8.3227
H	-0.1827	-3.5387	9.0438
C	0.2394	-1.7925	-6.1446
C	-0.4623	-1.4248	-8.8493
C	0.184	-2.8759	-7.0345
C	-0.0574	-0.5241	-6.6428
C	-0.4156	-0.3407	-7.9771
C	-0.1482	-2.696	-8.3636
H	0.4023	-3.8736	-6.6705
H	0.0068	0.3391	-5.9953
H	-0.6388	0.6591	-8.321
H	-0.1848	-3.5374	-9.0435
O	-0.7968	-1.3538	10.1735
O	-0.797	-1.3516	-10.1724
C	-1.1182	-0.0869	10.7178
H	-0.2738	0.6067	10.6484
H	-1.3539	-0.2601	11.7657
H	-1.9881	0.3554	10.2212
C	-1.1171	-0.0842	-10.7163
H	-1.9864	0.3589	-10.2193
H	-1.3533	-0.2569	-11.7642
H	-0.2719	0.6084	-10.6469
C	-1.0116	2.0401	1.0E-4
H	-1.6388	2.232	0.871
H	-1.6399	2.2317	-0.87
C	0.1756	3.0102	-8.0E-4
H	0.7973	2.808	-0.8782
H	0.7985	2.808	0.8758
C	-0.2637	4.4749	-4.0E-4
H	-0.8964	4.6655	-0.8754
H	-0.8945	4.6657	0.8759
C	0.9034	5.4639	-0.0018
H	1.5369	5.2761	0.8726
H	1.5347	5.2762	-0.8778
C	0.4654	6.9294	-0.0012
H	-0.1654	7.1163	0.8746

H	-0.1678	7.1163	-0.8753
C	1.6365	7.911	-0.0028
H	1.2896	8.9466	-0.0023
H	2.2664	7.7725	-0.8852
H	2.2689	7.7724	0.8778

HOMO level energy = -4.4544 eV

LUMO level energy = -0.5139 eV

HOMO-LUMO gap energy = 3.94 eV.

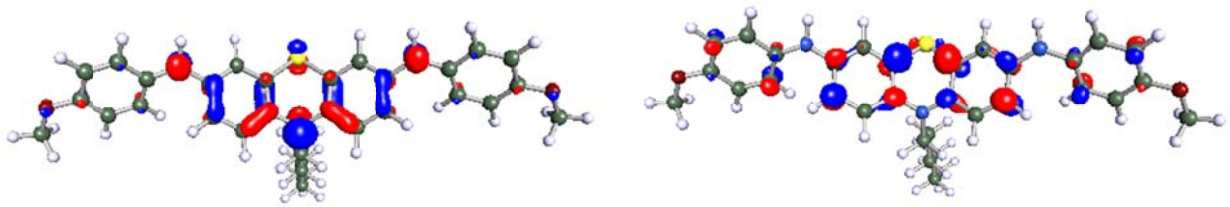


Figure 27: HOMO (left) and LUMO (right) levels of compound **3c**

XYZ-coordinates for $N^1,N^{1\prime}$-(10-Hexyl-10*H*-phenothiazine-3,7-diyl)bis($N^4,N^{4\prime}$-dimethylbenzene-1,4-diamine) **3d**

H	-2.0285	0.671	2.2646
C	-1.0758	0.1628	2.3437
C	1.2891	-1.2363	2.5539
C	-0.2468	0.0964	1.2213
C	-0.7298	-0.4187	3.5544
C	0.469	-1.1307	3.6834
C	0.9462	-0.6251	1.354
H	-1.4138	-0.3543	4.3883
H	2.2189	-1.7913	2.6163
N	-0.6194	0.7047	0.0
S	2.0874	-0.7051	-1.0E-4
C	-0.2467	0.0967	-1.2214
C	0.4688	-1.1305	-3.6835
C	-1.0757	0.1633	-2.3438
C	0.946	-0.625	-1.354

C	1.2888	-1.2363	-2.554
C	-0.7297	-0.4182	-3.5546
H	-2.0283	0.6718	-2.2648
H	2.2185	-1.7917	-2.6163
H	-1.4137	-0.3535	-4.3885
C	-1.012	2.1161	2.0E-4
H	-1.6405	2.3033	-0.8712
H	-1.6402	2.3032	0.8718
C	0.1695	3.0932	1.0E-4
H	0.7929	2.8956	-0.8772
H	0.7932	2.8954	0.8771
C	-0.2797	4.5549	3.0E-4
H	-0.9127	4.7412	0.8761
H	-0.9131	4.7413	-0.8751
C	0.8802	5.5523	1.0E-4
H	1.5137	5.3691	-0.8753
H	1.5142	5.3689	0.8751
C	0.4317	7.0145	4.0E-4
H	-0.2014	7.1968	0.8755
H	-0.2019	7.197	-0.8744
C	1.5956	8.0048	1.0E-4
H	1.2414	9.0379	3.0E-4
H	2.2275	7.8707	-0.8816
H	2.2281	7.8705	0.8814
N	0.8483	-1.7815	-4.8537
H	1.5326	-2.5098	-4.7416
N	0.8486	-1.7815	4.8536
H	1.5331	-2.5096	4.7417
C	0.4124	-1.5543	-6.1684
C	-0.3722	-1.1715	-8.8846
C	0.0596	-0.2913	-6.6494
C	0.3853	-2.6154	-7.076
C	0.0233	-2.432	-8.4015
C	-0.3298	-0.1055	-7.9674
H	0.1066	0.567	-5.993
H	0.6579	-3.6094	-6.7386
H	0.0375	-3.291	-9.0557
H	-0.5863	0.8954	-8.2816
C	0.4127	-1.5543	6.1684
C	-0.3722	-1.1714	8.8844
C	0.0596	-0.2913	6.6492

C	0.3857	-2.6154	7.076
C	0.0236	-2.4319	8.4015
C	-0.3298	-0.1055	7.9671
H	0.1065	0.5669	5.9928
H	0.6584	-3.6094	6.7387
H	0.0379	-3.2908	9.0557
H	-0.5865	0.8954	8.2813
N	-0.8005	-0.9905	10.198
N	-0.8005	-0.9906	-10.1982
C	-0.9065	0.3578	-10.7192
H	0.0526	0.8967	-10.721
H	-1.6211	0.9464	-10.1401
H	-1.275	0.3144	-11.7424
C	-0.5689	-2.0492	-11.1603
H	-1.0638	-2.9728	-10.8527
H	0.4984	-2.271	-11.31
H	-0.9936	-1.7567	-12.1188
C	-0.5689	-2.049	11.1602
H	-0.9938	-1.7565	12.1187
H	0.4984	-2.2706	11.31
H	-1.0637	-2.9727	10.8527
C	-0.9068	0.358	10.7189
H	-1.6215	0.9463	10.1397
H	0.0522	0.897	10.7208
H	-1.2755	0.3146	11.742

HOMO level energy = -4.2352 eV

LUMO level energy = -0.3221 eV

HOMO-LUMO gap energy = 3.913 eV.

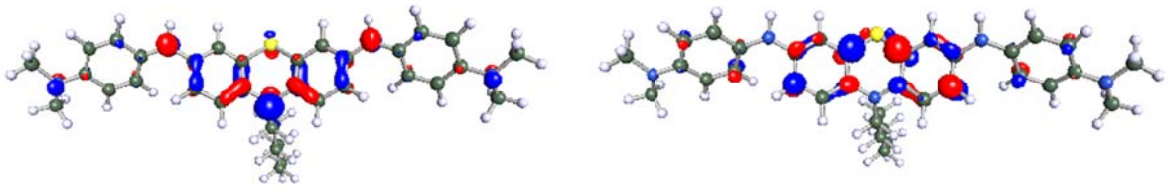


Figure 28: HOMO (left) and LUMO (right) levels of compound **3d**

XYZ-coordinates for 10-Hexyl-N^3,N^7-dimethyl-N^3,N^7-diphenyl-10*H*-phenothiazine-3,7-diamine **3e**

H	-2.355	0.6903	-2.6553
C	-2.1889	0.0675	-1.7856
C	-1.7447	-1.6173	0.3563
C	-1.0238	0.2495	-1.0305
C	-3.1254	-0.8978	-1.466
C	-2.9271	-1.7631	-0.3767
C	-0.8222	-0.6178	0.0442
H	-4.0071	-1.0056	-2.0821
H	-1.5315	-2.2645	1.1947
N	-0.0878	1.2522	-1.3757
S	0.5911	-0.4176	1.096
C	1.2897	1.0236	-1.146
C	4.0705	0.5826	-0.712
C	2.2559	1.5582	-1.9954
C	1.7477	0.241	-0.0762
C	3.1011	0.0145	0.1289
C	3.6156	1.3641	-1.7829
H	1.9404	2.1374	-2.8537
H	3.4073	-0.594	0.9687
H	4.3138	1.809	-2.4765
C	-0.5586	2.6387	-1.4732
H	-1.5018	2.6492	-2.0213
H	0.1513	3.2053	-2.0772
C	-0.7421	3.3201	-0.1123
H	-1.4451	2.7278	0.4786
H	0.2124	3.2988	0.4227
C	-1.2292	4.7656	-0.2346
H	-2.1942	4.7845	-0.7554
H	-0.5315	5.3213	-0.8713
C	-1.3652	5.5047	1.1028
H	-1.5585	6.5644	0.9013
H	-0.4058	5.4679	1.6321
C	-2.4688	4.9741	2.0219
H	-3.4222	4.9929	1.4817
H	-2.2782	3.9254	2.2667
C	-2.602	5.7734	3.3179
H	-3.4022	5.38	3.9487
H	-2.8257	6.8242	3.1149

H	-1.6765	5.7401	3.8984
N	5.4357	0.409	-0.4519
N	-3.8504	-2.7798	-0.092
C	6.3989	1.2207	-1.1795
H	6.1379	2.2789	-1.1138
H	6.4627	0.9449	-2.2413
H	7.384	1.0825	-0.7421
C	-3.4578	-3.8478	0.8148
H	-4.1994	-4.6414	0.7776
H	-3.3838	-3.5077	1.8572
H	-2.4933	-4.2633	0.5177
C	5.923	-0.7588	0.1944
C	6.9406	-3.0443	1.4627
C	6.8884	-0.647	1.1996
C	5.4757	-2.0332	-0.1679
C	5.975	-3.1624	0.4682
C	7.3973	-1.7806	1.8209
H	7.2278	0.3357	1.5034
H	4.7314	-2.1338	-0.9471
H	5.6149	-4.1409	0.175
H	8.1418	-1.6729	2.6002
H	7.3302	-3.9265	1.9544
C	-5.2406	-2.5827	-0.3019
C	-7.9998	-2.2463	-0.6933
C	-5.8666	-1.376	0.0286
C	-6.0197	-3.618	-0.8292
C	-7.3861	-3.4523	-1.0145
C	-7.2304	-1.21	-0.1744
H	-5.2781	-0.5685	0.444
H	-5.5453	-4.5506	-1.1087
H	-7.9703	-4.2657	-1.4273
H	-7.6962	-0.2678	0.0882
H	-9.0632	-2.1149	-0.8472

HOMO level energy = -4.4982 eV

LUMO level energy = -0.5810 eV

HOMO-LUMO gap energy = 3.917 eV.

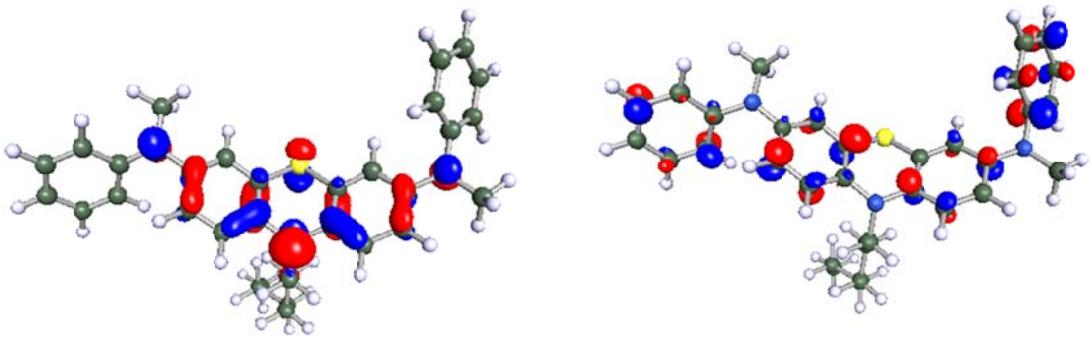


Figure 29: HOMO (left) and LUMO (right) levels of compound **3e**

XYZ-coordinates for 10-Hexyl-N^3,N^7-bis(4-methoxyphenyl)-N^3,N^7-dimethyl-10*H*-phenothiazine-3,7-diamine **3f**

H	-1.8499	-3.4032	-0.3477
C	-2.2292	-2.4111	-0.5356
C	-3.2823	0.1053	-0.9343
C	-1.3764	-1.4104	-1.0157
C	-3.5709	-2.1674	-0.2709
C	-4.1265	-0.9051	-0.4656
C	-1.9459	-0.1413	-1.2165
H	-4.1847	-2.9709	0.1156
H	-3.6787	1.0977	-1.1055
N	-0.0213	-1.6632	-1.3108
S	-1.0133	1.1477	-1.9873
C	0.9498	-0.6457	-1.242
C	2.908	1.4168	-1.1166
C	2.297	-0.9215	-0.9785
C	0.6119	0.7015	-1.4605
C	1.5636	1.7072	-1.3577
C	3.2589	0.0805	-0.9428
H	2.6193	-1.9373	-0.812
H	1.2537	2.7373	-1.4851
H	4.2907	-0.1842	-0.7542
C	0.4115	-3.0466	-1.4988
H	-0.3971	-3.5661	-2.0179
H	1.2564	-3.0299	-2.1915
C	0.8018	-3.8522	-0.2483
H	-0.0125	-3.838	0.4802

H	1.6523	-3.3853	0.253
C	1.1474	-5.2988	-0.6061
H	0.2824	-5.7685	-1.0891
H	1.9502	-5.3062	-1.3537
C	1.5725	-6.1435	0.5951
H	0.7766	-6.1277	1.3493
H	2.4472	-5.6838	1.0692
C	1.8975	-7.5945	0.2378
H	1.0214	-8.0544	-0.2318
H	2.6897	-7.6106	-0.5189
C	2.327	-8.4304	1.4419
H	1.5422	-8.4606	2.2024
H	3.2234	-8.0163	1.9102
H	2.5488	-9.4602	1.1548
N	3.8659	2.4675	-1.0837
N	-5.5079	-0.6788	-0.2282
C	-6.4425	-1.4572	-1.0273
H	-6.0394	-2.4545	-1.1842
H	-6.6305	-1.0131	-2.0157
H	-7.3954	-1.5518	-0.5044
C	4.0861	3.1813	-2.3317
H	3.1425	3.2714	-2.8647
H	4.7984	2.6695	-2.9956
H	4.463	4.1853	-2.1297
C	4.9067	2.4381	-0.1377
C	6.9366	2.4553	1.8285
C	4.6483	2.0286	1.184
C	6.2026	2.8608	-0.4373
C	7.2074	2.8767	0.5338
C	5.6409	2.0301	2.1417
H	3.6498	1.7133	1.4557
H	6.4561	3.1825	-1.4372
H	8.1944	3.2152	0.2523
H	5.4286	1.7162	3.1559
C	-5.9478	0.5495	0.3034
C	-6.8511	2.9661	1.457
C	-7.1247	1.172	-0.1384
C	-5.2425	1.1687	1.3416
C	-5.6768	2.3613	1.9068
C	-7.5697	2.3549	0.433
H	-7.7036	0.7392	-0.9418

H	-4.3388	0.7084	1.7184
H	-5.0961	2.7999	2.7058
H	-8.4795	2.8254	0.0825
O	-7.3676	4.1332	1.9489
O	7.8449	2.4237	2.851
C	-6.6779	4.7876	2.998
H	-6.6202	4.1619	3.8948
H	-7.2534	5.6831	3.224
H	-5.6658	5.0773	2.6965
C	9.1728	2.8298	2.5775
H	9.6364	2.1991	1.8113
H	9.7216	2.7211	3.5109
H	9.216	3.8755	2.2543

HOMO level energy = -4.5530 eV

LUMO level energy = -0.6901 eV

HOMO-LUMO gap energy = 3.863 eV.

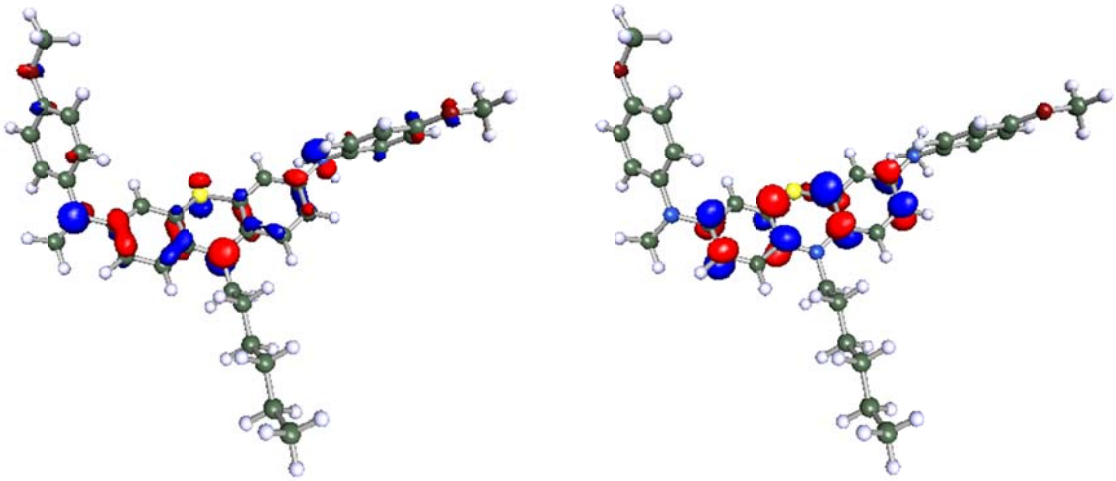


Figure 30: HOMO (left) and LUMO (right) levels of compound **3f**

XYZ-coordinates for 3,7-Di(9*H*-carbazol-9-yl)-10-hexyl-10*H*-phenothiazine **3g**

H	2.4735	-2.5495	0.8383
C	2.4614	-1.4762	0.7391
C	2.5269	1.2671	0.4396
C	1.2606	-0.7668	0.8736
C	3.6689	-0.8334	0.4962
C	3.7128	0.5442	0.3266
C	1.3306	0.6327	0.7472
H	4.5794	-1.4134	0.4266
H	2.5398	2.3416	0.3084
N	0.0432	-1.4186	1.1477
S	-0.0723	1.6437	1.0993
C	-1.3644	0.5295	0.6451
C	-3.5518	-1.1136	0.1994
C	-1.1963	-0.8612	0.7791
C	-2.5853	1.0726	0.2692
C	-3.6947	0.2589	0.0471
C	-2.3244	-1.6605	0.553
H	-2.6832	2.1468	0.178
H	-2.2578	-2.7329	0.6391
H	-4.3967	-1.7659	0.0223
N	-4.9406	0.8283	-0.3201
N	4.9349	1.2061	0.0432
C	0.0781	-2.8078	1.6123
H	-0.813	-2.9654	2.2228
H	0.9269	-2.8993	2.2926
C	0.1625	-3.9041	0.5383
H	1.0532	-3.7603	-0.0769
H	-0.6836	-3.8237	-0.1478
C	0.1881	-5.3015	1.161
H	-0.7058	-5.4409	1.7802
H	1.0423	-5.3804	1.8441
C	0.2645	-6.4272	0.1285
H	-0.5903	-6.3508	-0.5538
H	1.1585	-6.2904	-0.4907
C	0.2903	-7.8251	0.7486
H	-0.6026	-7.9608	1.3682
H	1.1456	-7.9017	1.4288
C	0.3642	-8.944	-0.2891
H	-0.4966	-8.916	-0.9624

H	0.3814	-9.927	0.1856
H	1.2649	-8.8556	-0.9019
C	-7.146	1.4317	-0.2808
C	-7.6558	0.1684	2.1426
C	-6.1272	0.7302	0.4052
C	-8.4294	1.4848	0.2637
C	-8.6788	0.8501	1.4713
C	-6.3703	0.0994	1.6231
H	-9.2211	2.0183	-0.2481
H	-9.6706	0.8843	1.9039
H	-5.5847	-0.4227	2.1525
H	-7.8691	-0.3136	3.0886
C	-5.1853	1.5876	-1.4639
C	-6.1688	3.1008	-3.5624
C	-6.5444	1.9791	-1.4748
C	-4.3181	1.9357	-2.4971
C	-4.8278	2.6965	-3.5405
C	-7.0305	2.7432	-2.5363
H	-3.2825	1.6236	-2.4923
H	-4.1726	2.9811	-4.3543
H	-8.0686	3.0516	-2.5605
H	-6.5334	3.6954	-4.3902
C	5.7393	0.9856	-1.074
C	7.6324	0.9328	-3.0923
C	6.8724	1.8289	-1.0001
C	5.5394	0.1267	-2.1522
C	6.4996	0.1117	-3.1545
C	7.8219	1.7936	-2.0218
H	4.6632	-0.5049	-2.2128
H	6.366	-0.5478	-4.0031
H	8.6951	2.4334	-1.9822
H	8.3625	0.8962	-3.8907
C	6.7446	2.5933	0.2193
C	5.9311	3.6756	2.6477
C	5.5391	2.1822	0.8347
C	7.5352	3.5624	0.8377
C	7.1229	4.1011	2.0473
C	5.1258	2.7129	2.0546
H	8.4616	3.8888	0.3808
H	7.727	4.8548	2.536
H	4.2106	2.386	2.5298

H	5.6297	4.1039	3.5955

HOMO level energy = -5.1947 eV

LUMO level energy = -1.1877 eV

HOMO-LUMO gap energy = 4.007 eV.

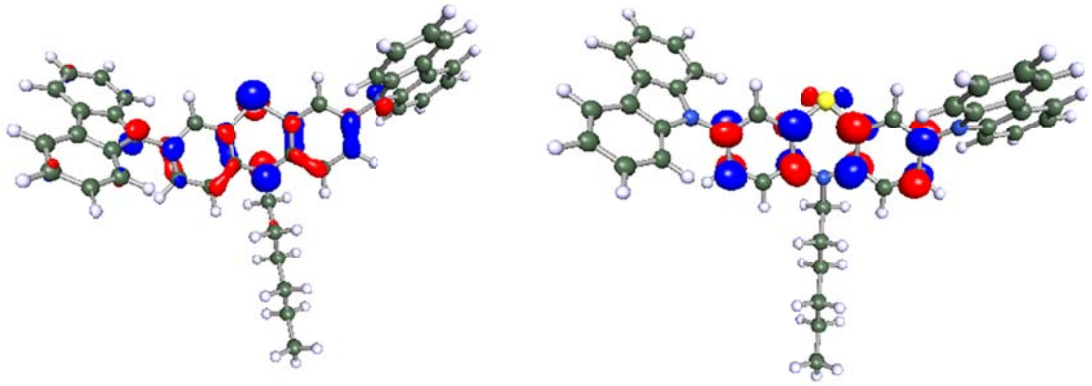


Figure 31: HOMO (left) and LUMO (right) levels of compound **3g**

XYZ-coordinates for 10-Hexyl-N^3,N^3,N^7,N^7-tetraphenyl-10*H*-phenothiazine-3,7-diamine **3h**

H	2.2732	-2.606	-0.7912
C	2.3221	-1.5375	-0.6555
C	2.5479	1.1822	-0.263
C	1.1664	-0.7558	-0.7832
C	3.562	-0.9771	-0.3763
C	3.6941	0.3914	-0.1585
C	1.321	0.6309	-0.6063
H	4.4297	-1.6192	-0.3055
H	2.6176	2.2506	-0.1038
N	-0.0854	-1.3207	-1.0991
S	-0.0177	1.7356	-0.9293
C	-1.2925	-0.7058	-0.7113
C	-3.73	0.5414	0.064

C	-1.3787	0.6854	-0.5203
C	-2.471	-1.4385	-0.5234
C	-3.6637	-0.8322	-0.1495
C	-2.5646	1.2879	-0.1257
H	-2.4731	-2.5086	-0.656
H	-4.5475	-1.4412	-0.0148
H	-2.5873	2.3607	0.0165
N	-4.9405	1.1715	0.4555
N	4.9501	0.9706	0.1627
C	-4.9336	2.1175	1.5088
C	-4.9063	4.0005	3.5907
C	-4.1241	1.9258	2.6343
C	-5.7283	3.2682	1.4413
C	-5.7178	4.1922	2.4769
C	-4.1079	2.8636	3.6579
H	-3.5064	1.0402	2.7014
H	-6.353	3.4346	0.5737
H	-6.3386	5.0769	2.4039
H	-3.4736	2.696	4.5199
H	-4.8953	4.7268	4.3931
C	-6.1486	0.8327	-0.2024
C	-8.5363	0.1467	-1.5091
C	-7.3342	0.6613	0.5214
C	-6.1767	0.6537	-1.5902
C	-7.3584	0.3079	-2.2317
C	-8.5147	0.3296	-0.13
H	-7.3256	0.7903	1.5956
H	-5.2677	0.7862	-2.1619
H	-7.3594	0.1772	-3.307
H	-9.4211	0.2002	0.4489
H	-9.4571	-0.1177	-2.0128
C	5.3713	2.1468	-0.5051
C	6.1835	4.4846	-1.8288
C	5.1441	2.3058	-1.8768
C	6.0104	3.177	0.1941
C	6.4176	4.3281	-0.4663
C	5.5407	3.4672	-2.5262
H	4.6532	1.516	-2.43
H	6.1854	3.071	1.2566
H	6.9079	5.1151	0.0939
H	5.355	3.5705	-3.5884

H	6.4957	5.3868	-2.3387
C	5.7657	0.3711	1.1527
C	7.3789	-0.8299	3.1118
C	7.1537	0.296	0.987
C	5.1982	-0.1666	2.3139
C	5.9991	-0.7658	3.2767
C	7.9482	-0.2916	1.9621
H	7.6058	0.7011	0.0915
H	4.1272	-0.1126	2.4569
H	5.5398	-1.173	4.1694
H	9.0201	-0.3402	1.8136
H	8.0011	-1.2923	3.8673
C	-0.1285	-2.6864	-1.6211
H	0.7228	-2.8022	-2.2952
H	-1.0206	-2.7652	-2.2463
C	-0.1244	-3.8323	-0.5959
H	0.7656	-3.7696	0.0341
H	-0.9735	-3.7307	0.0836
C	-0.1745	-5.1999	-1.2799
H	0.6813	-5.2995	-1.9582
H	-1.0681	-5.2576	-1.913
C	-0.1772	-6.3736	-0.2996
H	-1.0341	-6.2774	0.3774
H	0.7161	-6.3184	0.3336
C	-0.2262	-7.7411	-0.9829
H	0.6308	-7.8372	-1.6584
H	-1.1186	-7.7955	-1.616
C	-0.2301	-8.9087	0.0024
H	0.6674	-8.9021	0.6265
H	-0.2651	-9.8686	-0.517
H	-1.0953	-8.8606	0.6687

HOMO level energy = -4.6405 eV

LUMO level energy = -0.9035 eV

HOMO-LUMO gap energy = 3.737 eV.

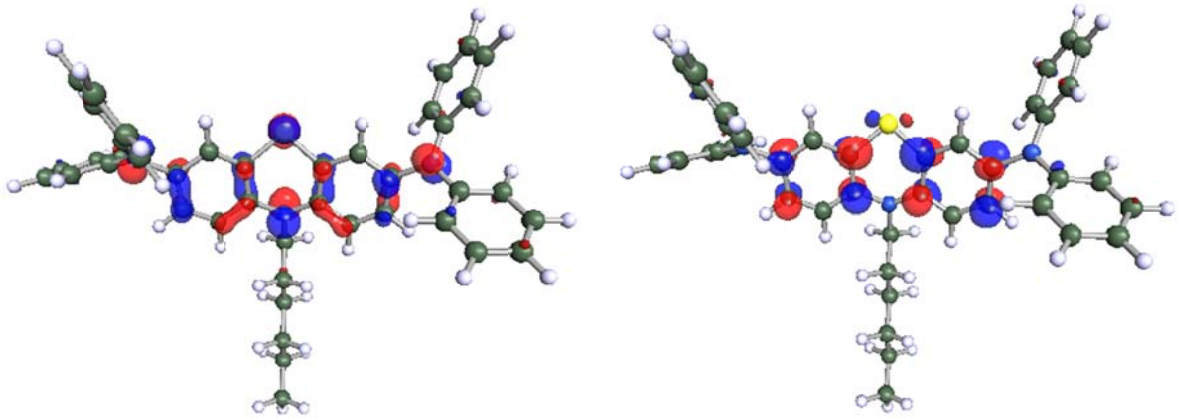


Figure 32: HOMO (left) and LUMO (right) levels of compound **3h**

XYZ-coordinates for 10-Hexyl-N^3,N^3,N^7,N^7-tetrakis(4-methoxyphenyl)-10*H*-phenothiazine-3,7-diamine **3i**

H	-2.1669	-3.1576	-0.4936
C	-2.2295	-2.1531	-0.1056
C	-2.4964	0.4245	0.8304
C	-1.0909	-1.5223	0.4102
C	-3.4658	-1.5219	-0.1547
C	-3.6233	-0.2152	0.3037
C	-1.2675	-0.2161	0.9008
H	-4.3122	-2.0535	-0.568
H	-2.5827	1.4334	1.2129
N	0.1627	-2.1649	0.4645
S	0.0384	0.6	1.7678
C	1.4324	-0.1191	0.9532
C	3.7546	-1.2579	-0.0269
C	1.368	-1.433	0.4545
C	2.6138	0.6078	0.9308
C	3.8018	0.0533	0.4428
C	2.5659	-1.9771	-0.0234
H	2.6143	1.6177	1.3199
H	2.5885	-2.98	-0.4193
H	4.6515	-1.7255	-0.4096
C	0.2172	-3.61	0.2558
H	-0.6489	-4.0433	0.7608

H	1.095	-3.9826	0.7885
C	0.2564	-4.1068	-1.1992
H	1.1347	-3.7054	-1.7095
H	-0.6047	-3.7206	-1.7496
C	0.2712	-5.6346	-1.2762
H	-0.6135	-6.0337	-0.7654
H	1.1364	-6.0197	-0.723
C	0.3094	-6.1718	-2.7072
H	1.1954	-5.7771	-3.2184
H	-0.555	-5.7866	-3.261
C	0.3194	-7.699	-2.7896
H	-0.5658	-8.0931	-2.2783
H	1.184	-8.0842	-2.2378
C	0.355	-8.2257	-4.2232
H	1.2477	-7.8781	-4.75
H	0.3602	-9.3174	-4.2473
H	-0.5154	-7.8858	-4.7908
N	5.0032	0.7995	0.4392
N	-4.8728	0.4434	0.2456
C	4.9959	2.168	0.0623
C	4.9872	4.8854	-0.6671
C	5.7678	3.1044	0.7633
C	4.2271	2.621	-1.0079
C	4.2081	3.9666	-1.3667
C	5.7721	4.4379	0.3992
H	6.3713	2.7765	1.5997
H	3.6232	1.9176	-1.5662
H	3.5915	4.2767	-2.1983
H	6.3691	5.1586	0.9433
C	6.2374	0.1521	0.71
C	8.6772	-1.1368	1.2568
C	6.3662	-0.7098	1.8077
C	7.3529	0.3557	-0.0994
C	8.5674	-0.2705	0.1715
C	7.5616	-1.3516	2.0713
H	5.5149	-0.8769	2.455
H	7.2785	1.0186	-0.9517
H	9.4092	-0.0824	-0.4795
H	7.6581	-2.017	2.9197
C	-6.0686	-0.2816	0.491
C	-8.4379	-1.7145	0.9862

C	-6.1737	-1.1396	1.5938
C	-7.1709	-0.1577	-0.3521
C	-8.3511	-0.8553	-0.1072
C	-7.3343	-1.8517	1.8327
H	-5.3318	-1.2477	2.2654
H	-7.113	0.4994	-1.2103
H	-9.1838	-0.7284	-0.7842
H	-7.4127	-2.514	2.6855
C	-4.9431	1.8171	-0.1038
C	-5.098	4.5373	-0.8058
C	-4.1742	2.3344	-1.155
C	-5.7863	2.6885	0.5831
C	-5.877	4.0333	0.234
C	-4.2421	3.6734	-1.4935
H	-3.5135	1.6773	-1.7053
H	-6.3889	2.3124	1.3997
H	-6.5464	4.6737	0.7904
H	-3.6447	4.0703	-2.3044
O	5.0497	6.2214	-0.9394
O	9.812	-1.8107	1.6045
O	-9.539	-2.4522	1.3118
O	-5.1012	5.8372	-1.2222
C	4.2618	6.7311	-2.0008
H	4.5436	6.2858	-2.9604
H	4.4553	7.8013	-2.0319
H	3.1944	6.5622	-1.8254
C	-5.9412	6.7587	-0.5503
H	-5.7825	7.7197	-1.0352
H	-5.6796	6.842	0.5095
H	-6.9963	6.4799	-0.6397
C	-10.6869	-2.3522	0.4877
H	-11.0766	-1.3293	0.4638
H	-11.4327	-3.0097	0.9297
H	-10.4771	-2.6811	-0.5353
C	10.9753	-1.6245	0.8178
H	10.8174	-1.9478	-0.2161
H	11.7477	-2.2416	1.2723
H	11.2998	-0.5789	0.822

HOMO level energy = -4.3061 eV

LUMO level energy = -0.6946 eV

HOMO-LUMO gap energy = 3.612 eV.

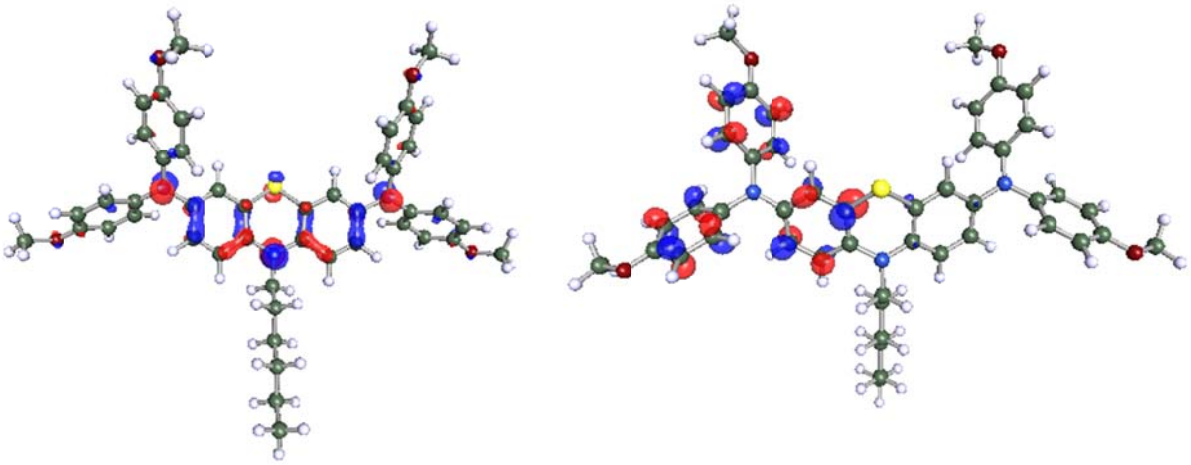


Figure 33: HOMO (left) and LUMO (right) levels of compound **3i**

XYZ-coordinates for N^3,N^3,N^7,N^7-tetraethyl-10-hexyl-10*H*-phenothiazine-3,7-diamine **3j**

H	3.3761	0.5844	-0.0487
C	2.6319	0.6749	0.7324
C	0.8002	0.8494	2.7862
C	1.3209	0.2623	0.4786
C	3.0102	1.2134	1.9508
C	2.1005	1.3218	3.019
C	0.4156	0.3652	1.5377
H	4.0284	1.5559	2.0668
H	0.0638	0.8396	3.5759
N	0.9427	-0.2662	-0.7763
S	-1.28	-0.0932	1.294
C	-0.0198	-1.2993	-0.8337
C	-1.9479	-3.412	-0.9361
C	0.0485	-2.3117	-1.79
C	-1.0737	-1.3746	0.0852

C	-1.9932	-2.4152	0.0538
C	-0.8996	-3.3234	-1.8675
H	0.8571	-2.3067	-2.5099
H	-2.749	-2.4481	0.8257
H	-0.8065	-4.0409	-2.6684
N	-2.8979	-4.4395	-0.9495
N	2.4971	1.8758	4.2421
C	1.499	2.0773	5.2851
H	1.3088	1.1435	5.841
H	0.563	2.3507	4.8003
C	1.8478	3.1889	6.2721
H	2.7521	2.9762	6.8436
H	1.0305	3.3024	6.9874
H	1.9842	4.1405	5.7554
C	3.8721	1.6426	4.6922
H	4.2787	0.7876	4.1475
H	3.8428	1.3397	5.7434
C	4.8115	2.8401	4.5378
H	5.8167	2.5763	4.8784
H	4.4683	3.6941	5.1224
H	4.8783	3.1587	3.4966
C	-4.2575	-4.1332	-0.4979
H	-4.4025	-3.051	-0.5328
H	-4.963	-4.5515	-1.2226
C	-4.6034	-4.6497	0.9002
H	-4.5364	-5.7368	0.9515
H	-5.623	-4.3586	1.1668
H	-3.9263	-4.2413	1.6518
C	-2.7636	-5.5159	-1.9226
H	-1.7011	-5.7093	-2.0599
H	-3.1617	-5.2153	-2.9064
C	-3.4171	-6.8277	-1.4946
H	-3.2314	-7.5862	-2.2582
H	-4.4982	-6.7418	-1.3789
H	-2.9983	-7.1829	-0.5516
C	1.2792	0.4702	-1.9944
H	2.2856	0.8788	-1.8931
H	1.3222	-0.2307	-2.8295
C	0.2977	1.6011	-2.3234
H	0.2662	2.2983	-1.4801
H	-0.708	1.1796	-2.4162

C	0.6673	2.3507	-3.6038
H	1.6809	2.7586	-3.5086
H	0.7036	1.6441	-4.4421
C	-0.2987	3.4857	-3.9464
H	-0.3329	4.1953	-3.1113
H	-1.313	3.0805	-4.0391
C	0.0634	4.2355	-5.2294
H	1.0779	4.6388	-5.1372
H	0.0947	3.5266	-6.0643
C	-0.9058	5.3691	-5.5612
H	-0.9324	6.1134	-4.7607
H	-1.9233	4.9923	-5.6932
H	-0.6201	5.8829	-6.4817

HOMO level energy = -4.3362 eV

LUMO level energy = -0.2550 eV

HOMO-LUMO gap energy = 4.081 eV.

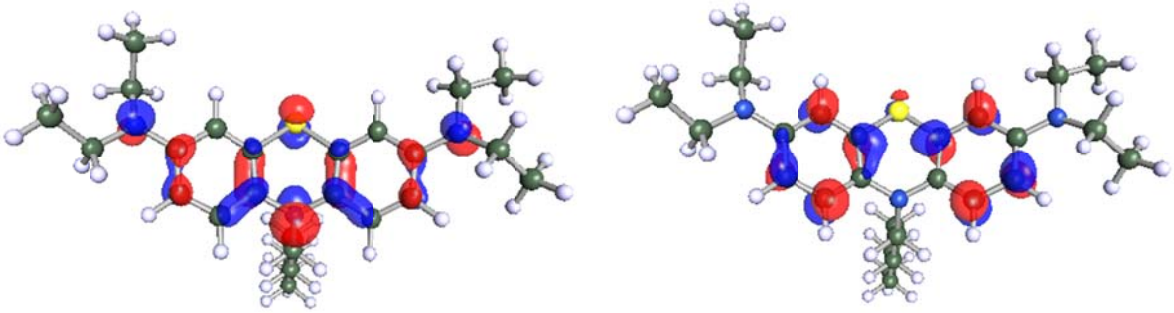


Figure 34: HOMO (left) and LUMO (right) levels of compound **3j**

XYZ-coordinates for 10-Hexyl-3,7-di(piperidin-1-yl)-10*H*-phenothiazine **3k**

H	2.2227	-1.1762	2.4543
C	2.2872	-0.5226	1.5938
C	2.4738	1.2449	-0.5193
C	1.1641	-0.349	0.776
C	3.4755	0.1428	1.3504
C	3.6007	1.047	0.2842
C	1.2873	0.55	-0.2862
H	4.3041	-0.0020	2.0312
H	2.5063	1.9265	-1.3573
N	-0.0491	-1.02	1.0341
S	-0.0624	0.7551	-1.4199
C	-1.4171	0.5236	-0.2973
C	-3.5995	0.0907	1.3433
C	-1.2765	-0.367	0.7717
C	-2.6096	1.1971	-0.5375
C	-3.7443	0.9842	0.2652
C	-2.3925	-0.5451	1.5914
H	-2.6535	1.8669	-1.3845
H	-2.3166	-1.1871	2.4601
H	-4.4176	-0.0758	2.0289
N	-4.9405	1.6349	0.0142
N	4.8111	1.7476	0.0911
C	-6.1857	1.1776	0.6182
H	-6.3418	1.617	1.6161
H	-6.128	0.0965	0.7579
C	-4.9954	2.7966	-0.8648
H	-5.0909	2.5042	-1.9225
H	-4.0564	3.3465	-0.7757
C	-7.3753	1.4997	-0.2853
H	-8.2864	1.1012	0.1664
H	-7.2368	0.9663	-1.2296
C	-6.1494	3.7176	-0.4718
H	-5.9701	4.0689	0.5482
H	-6.1351	4.6022	-1.1119
C	-7.514	3.0099	-0.5511
H	-8.1974	3.4607	0.1726
H	-7.9634	3.1641	-1.5353
C	4.8024	2.8752	-0.8324
H	3.8972	3.4574	-0.6586

H	4.7757	2.5354	-1.884
C	6.0253	0.9331	-0.0261
H	5.9762	0.1158	0.6899
H	6.0763	0.4746	-1.0302
C	7.2827	1.7648	0.2128
H	7.2899	2.1069	1.2526
H	8.1628	1.1314	0.072
C	6.0271	3.7665	-0.6228
H	5.9584	4.2288	0.3667
H	6.0079	4.5749	-1.3591
C	7.3275	2.9702	-0.7271
H	8.1867	3.606	-0.4993
H	7.4589	2.6206	-1.7579
C	-0.034	-2.4575	1.3007
H	-0.9558	-2.724	1.818
H	0.7775	-2.6896	1.9926
C	0.1088	-3.3131	0.036
H	1.0291	-3.0269	-0.483
H	-0.7169	-3.0776	-0.6423
C	0.1272	-4.8126	0.3344
H	-0.7934	-5.0909	0.862
H	0.9503	-5.0377	1.0231
C	0.2698	-5.6809	-0.9169
H	-0.5519	-5.457	-1.6066
H	1.1904	-5.405	-1.4448
C	0.2878	-7.1823	-0.6254
H	-0.6332	-7.4583	-0.0999
H	1.1086	-7.4056	0.0648
C	0.4329	-8.0402	-1.8817
H	0.4425	-9.1052	-1.6397
H	1.3619	-7.812	-2.4109
H	-0.3925	-7.8648	-2.5765

HOMO level energy = -4.3244 eV

LUMO level energy = -0.2176 eV

HOMO-LUMO gap energy = 4.107 eV.

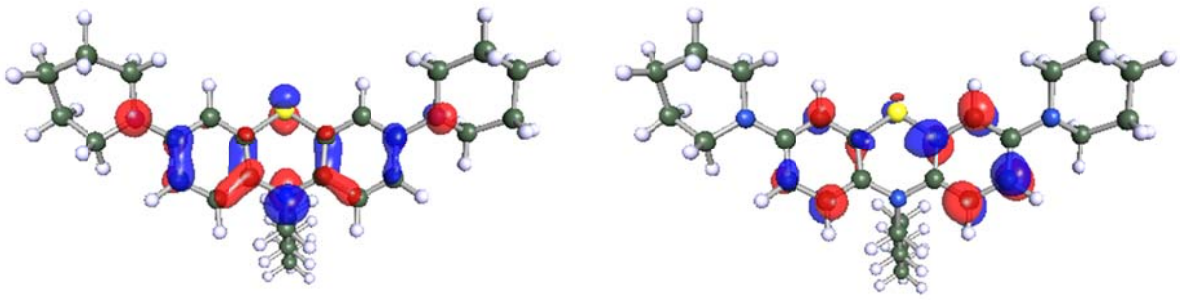


Figure 35: HOMO (left) and LUMO (right) levels of compound **3k**

XYZ-coordinates for 10-Hexyl-3,7-di(pyrrolidin-1-yl)-10*H*-phenothiazine **3l**

C	-7.1143	-0.1285	1.0847
C	-7.1072	-0.9366	-0.065
C	-6.0036	-0.8131	-0.9294
C	-4.99	0.0997	-0.6706
C	-4.9971	0.9056	0.4755
C	-6.0745	0.7536	1.3495
S	-3.6693	0.2956	-1.838
C	-2.3491	0.6012	-0.6937
C	-2.6192	1.3472	0.4612
N	-3.9348	1.8149	0.6972
C	-1.0741	0.1334	-0.9812
C	0.0128	0.4204	-0.1352
C	-0.2609	1.1522	1.0326
C	-1.5488	1.5827	1.3255
C	-4.1412	2.9488	1.5891
C	-5.2084	3.9334	1.0958
C	-4.8492	4.6249	-0.2203
C	-5.9202	5.6075	-0.6958
C	-5.5698	6.306	-2.0108
C	-6.6432	7.2877	-2.4792
N	-8.1313	-1.8173	-0.3352
N	1.2856	-0.0131	-0.4347
C	-9.3245	-1.9386	0.4886
C	-10.242	-2.8465	-0.335

C	-9.2583	-3.7322	-1.1085
C	-8.0984	-2.7825	-1.4253
C	1.6051	-0.8413	-1.5881
C	3.0641	-1.2427	-1.3537
C	3.6333	-0.0604	-0.5608
C	2.4637	0.3624	0.3335
H	-7.9267	-0.199	1.7938
H	-5.936	-1.4185	-1.8221
H	-6.1185	1.3364	2.2593
H	-0.9291	-0.4458	-1.8822
H	0.5293	1.3674	1.7378
H	-1.711	2.1114	2.255
H	-3.1936	3.4829	1.6464
H	-4.377	2.6259	2.6139
H	-5.3436	4.6852	1.8815
H	-6.1703	3.426	0.9901
H	-4.6804	3.8672	-0.9904
H	-3.8975	5.1569	-0.1012
H	-6.092	6.3649	0.0789
H	-6.8716	5.0753	-0.8141
H	-5.4031	5.5499	-2.7851
H	-4.6174	6.8351	-1.8951
H	-6.3634	7.7671	-3.4199
H	-6.8066	8.0768	-1.7404
H	-7.5994	6.7815	-2.6366
H	-9.7765	-0.9597	0.6765
H	-9.0968	-2.3852	1.4681
H	-10.9339	-3.4144	0.2871
H	-10.833	-2.2442	-1.0295
H	-9.6916	-4.1747	-2.0056
H	-8.9064	-4.547	-0.4708
H	-7.1389	-3.3077	-1.4607
H	-8.237	-2.2926	-2.3999
H	1.4907	-0.2835	-2.5292
H	0.9457	-1.7128	-1.6455
H	3.106	-2.1539	-0.7521
H	3.5982	-1.4328	-2.2849
H	3.8948	0.7551	-1.2395
H	4.525	-0.3161	0.0122
H	2.4949	-0.1555	1.3029
H	2.4746	1.4374	0.5404

HOMO level energy = -4.2404 eV

LUMO level energy = -0.1274 eV

HOMO-LUMO gap energy = 4.113 eV.

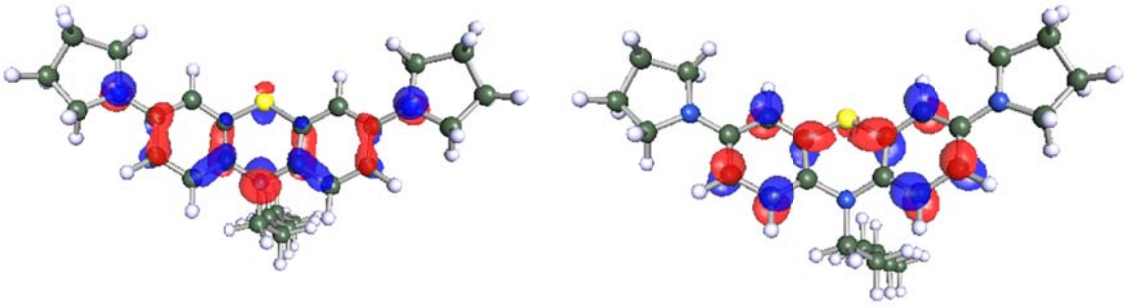


Figure 36: HOMO (left) and LUMO (right) levels of compound **3l**

5 Correlation graphs of selected experimental and computational electronic data of the structures 3a-3l

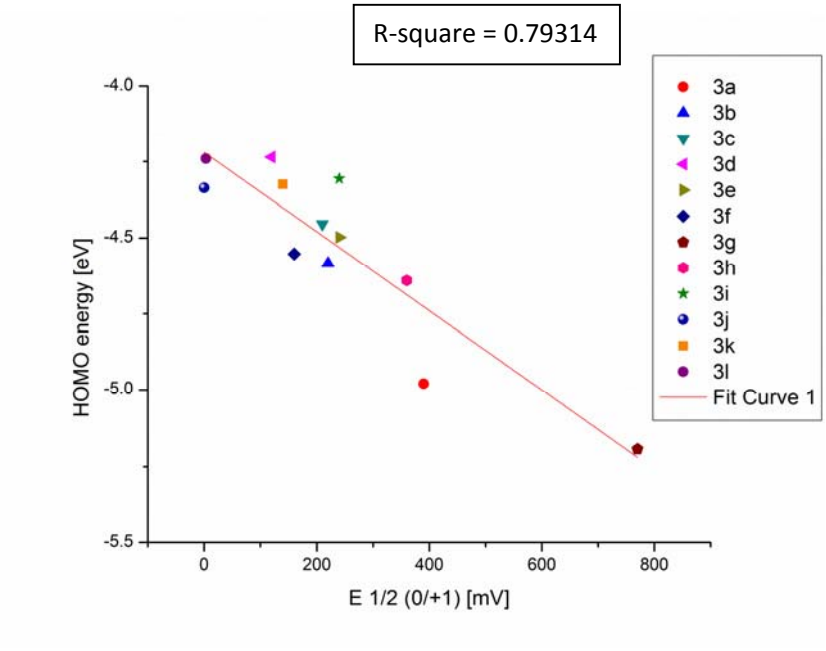


Figure 37: Correlation between the HOMO energy and the first oxidation potential for the 3,7-dianilino substituted *N*-hexyl phenothiazines **3a-3l**

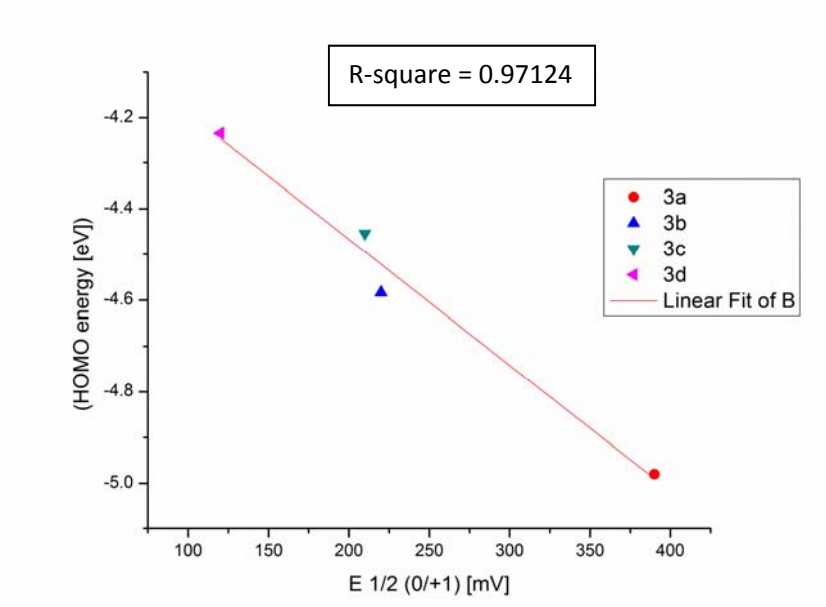


Figure 38: Correlation between the HOMO energy and the first oxidation potential for the consanguineous series **3a-3d**

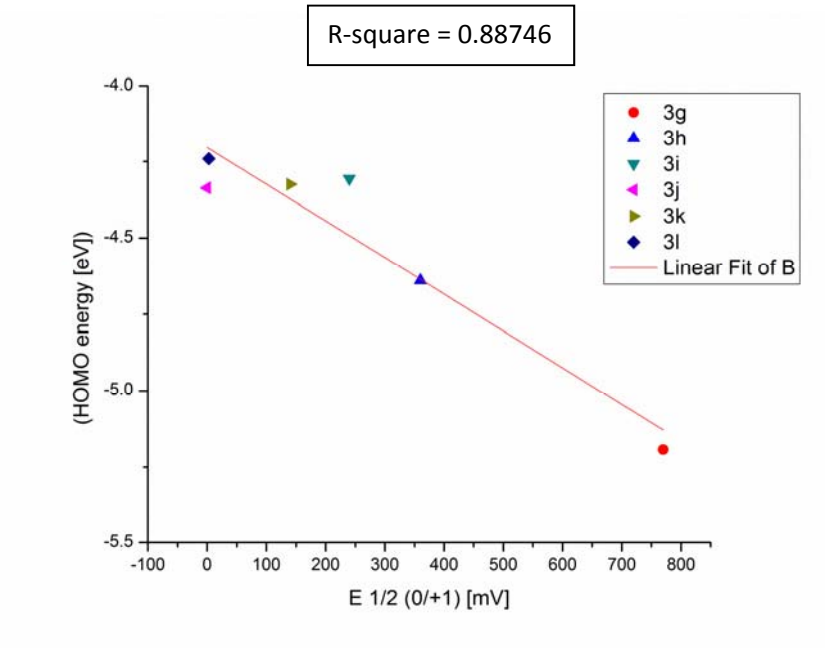


Figure 39: Correlation between the HOMO energy and the first oxidation potential for the consanguineous series **3g-3l**

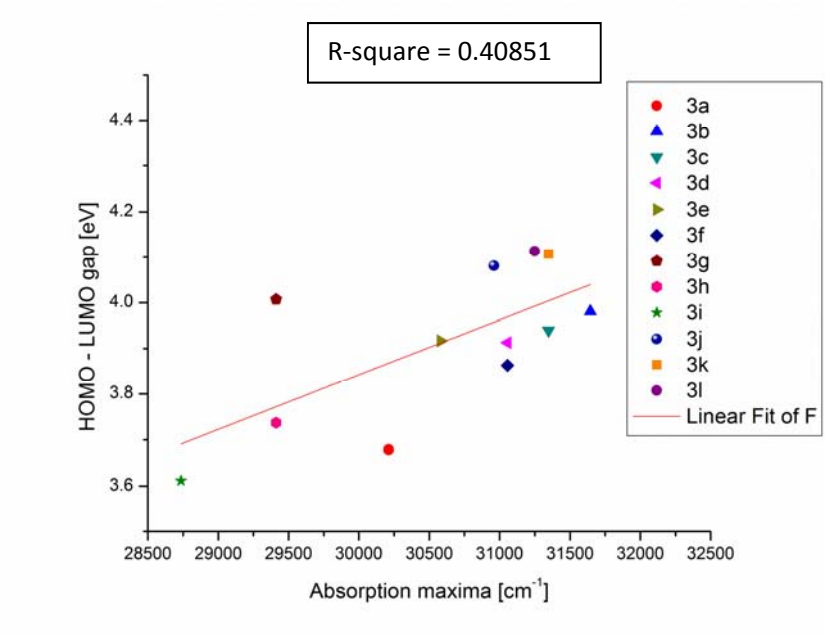


Figure 40: Correlation between the HOMO – LUMO energy gap and the absorption maxima energy for the 3,7-dianilino substituted *N*-hexyl phenothiazines **3a-3l**

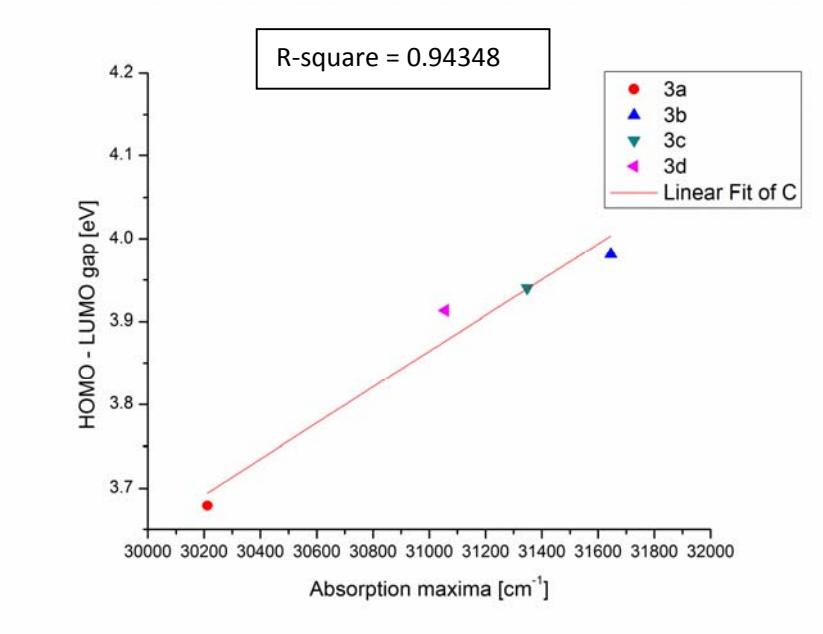


Figure 41: Correlation between the HOMO – LUMO energy gap and the absorption maxima energy for the consanguineous series **3a-3d**

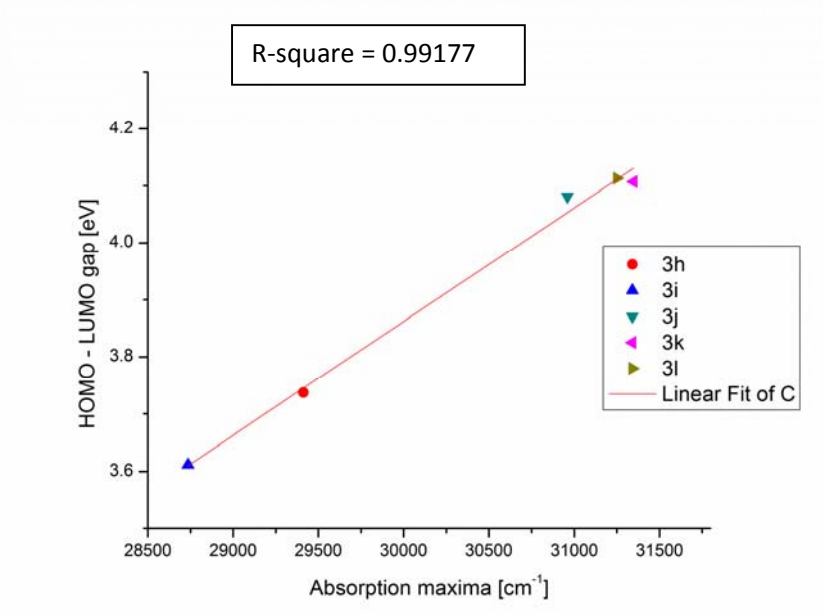


Figure 42: Correlation between the HOMO – LUMO energy gap and the absorption maxima energy for the consanguineous series **3h-3l**