Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Synthesis and Structure–Property Relationships of Luminescent, Redoxactive *N*-Aryl Phenothiazines

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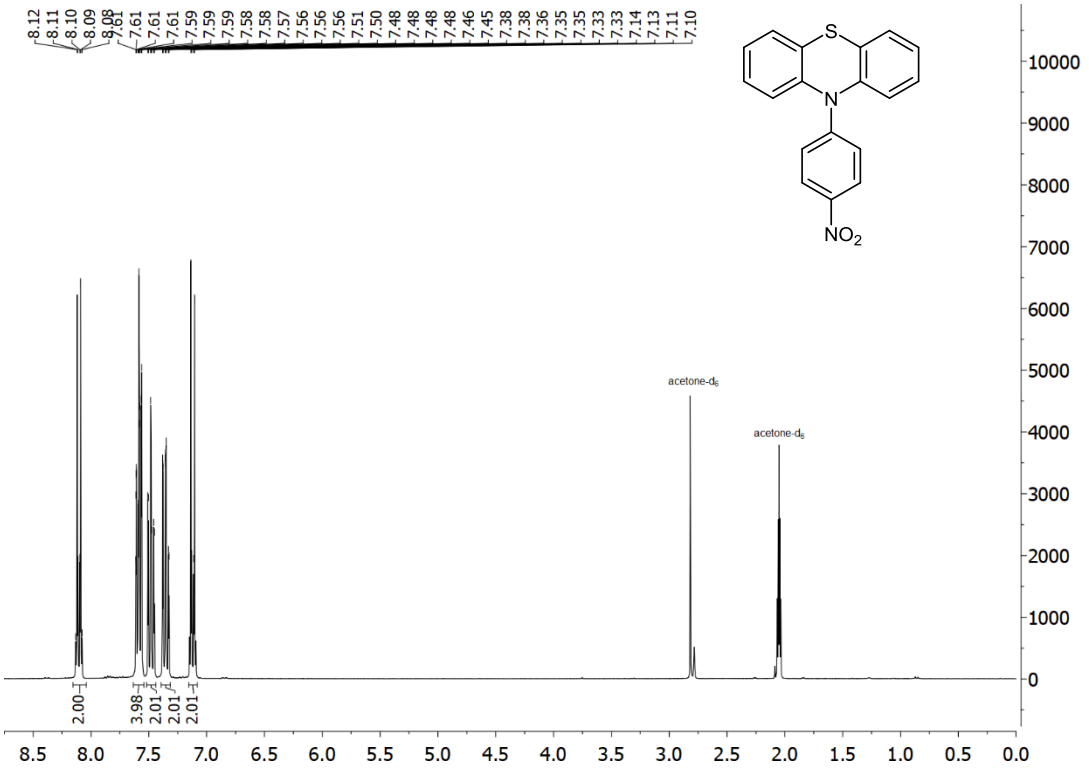
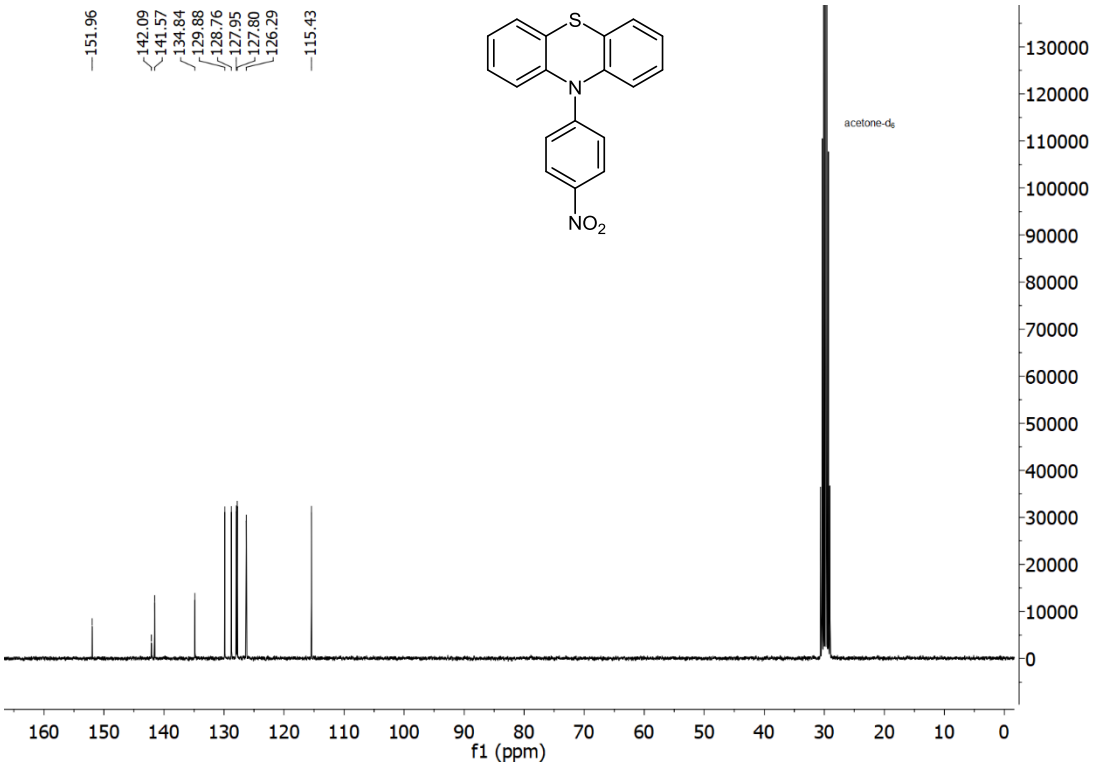
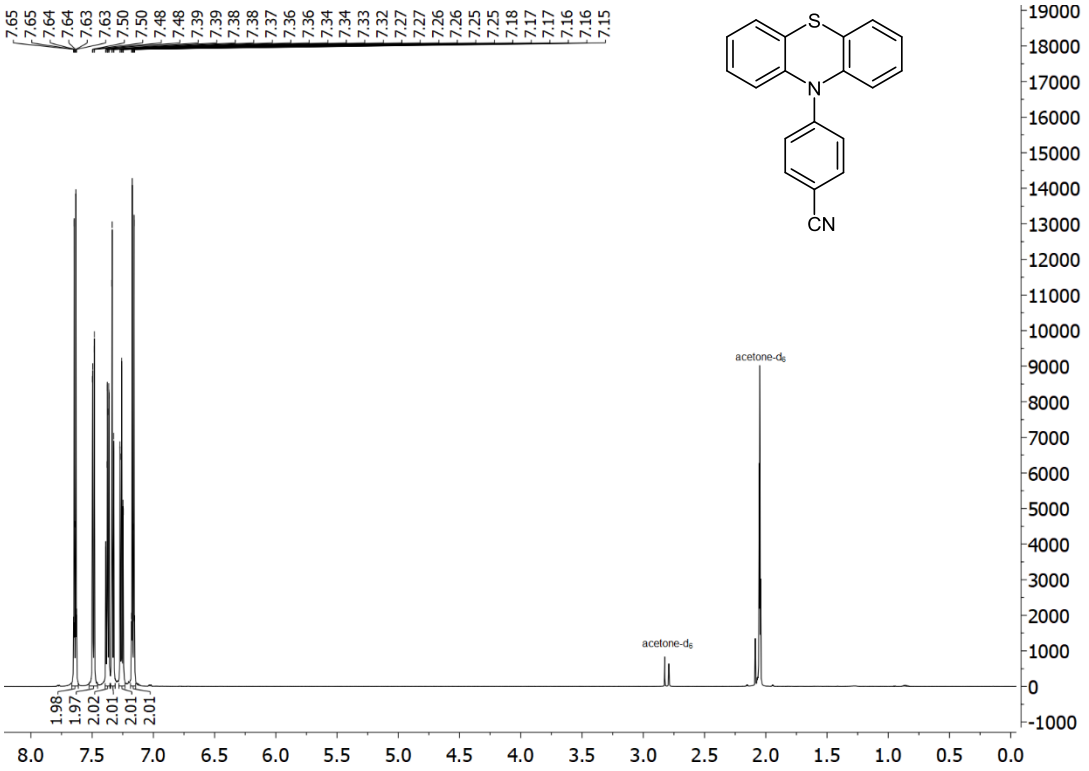


^{13}C NMR spectrum of 10-(4-Nitrophenyl)-10*H*-phenothiazine (3a) (acetone-d_6, 75 MHz, 293 K)



1.2 ^{1}H NMR spectrum of 4-(10*H*-Phenothiazin-10-yl)benzonitrile (3b) (acetone-d_6, 600 MHz, 293 K)



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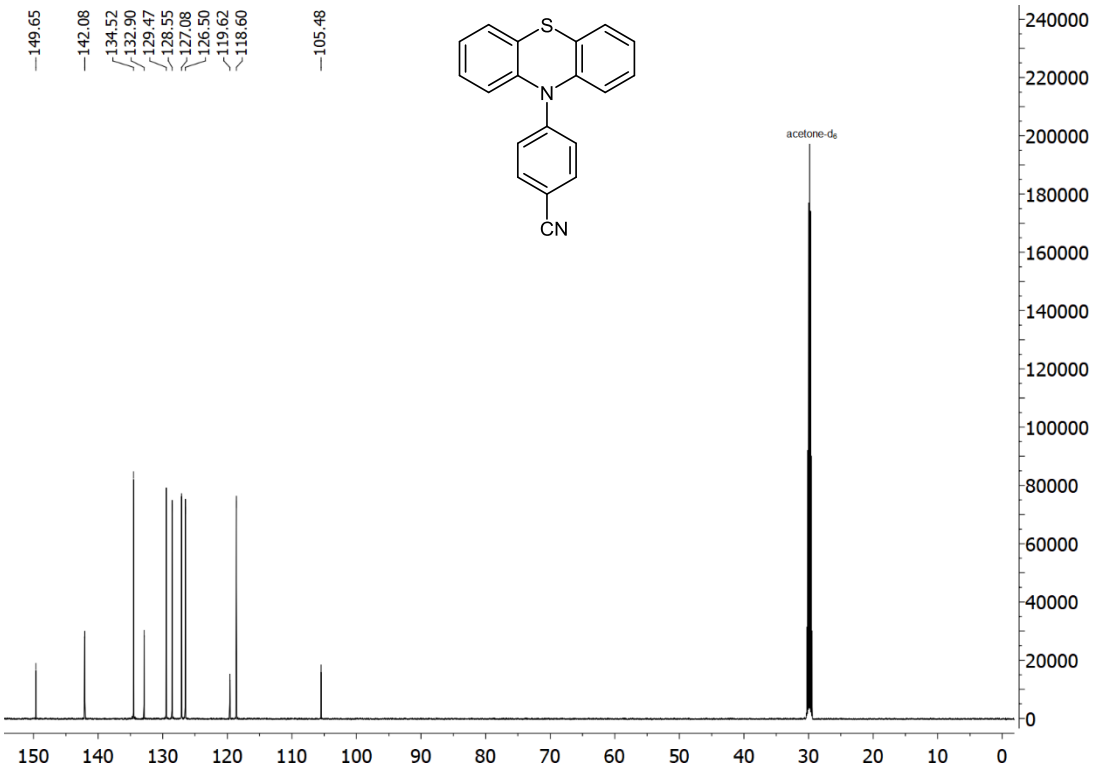
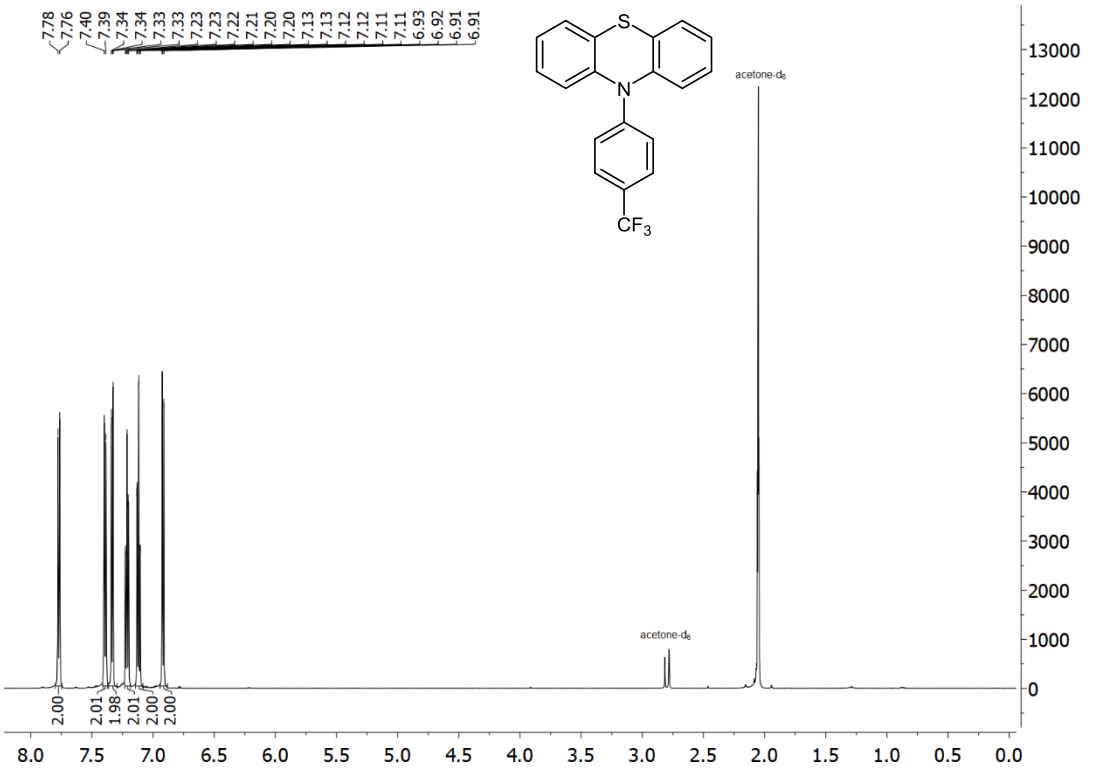
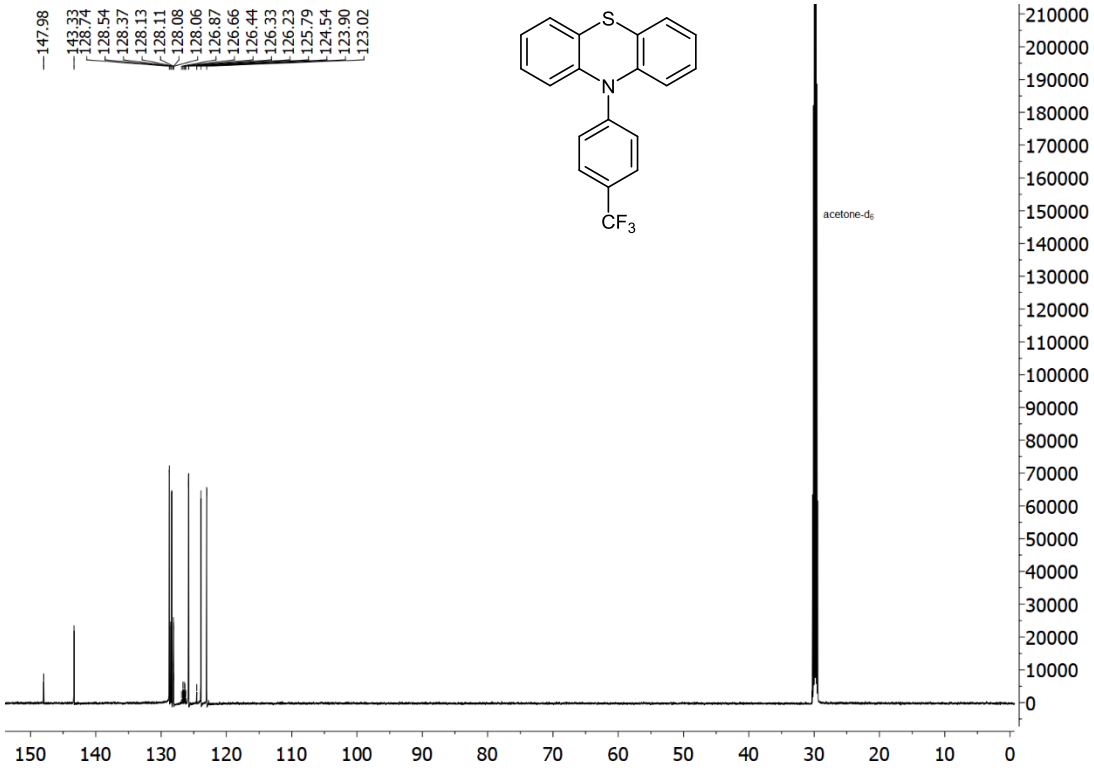


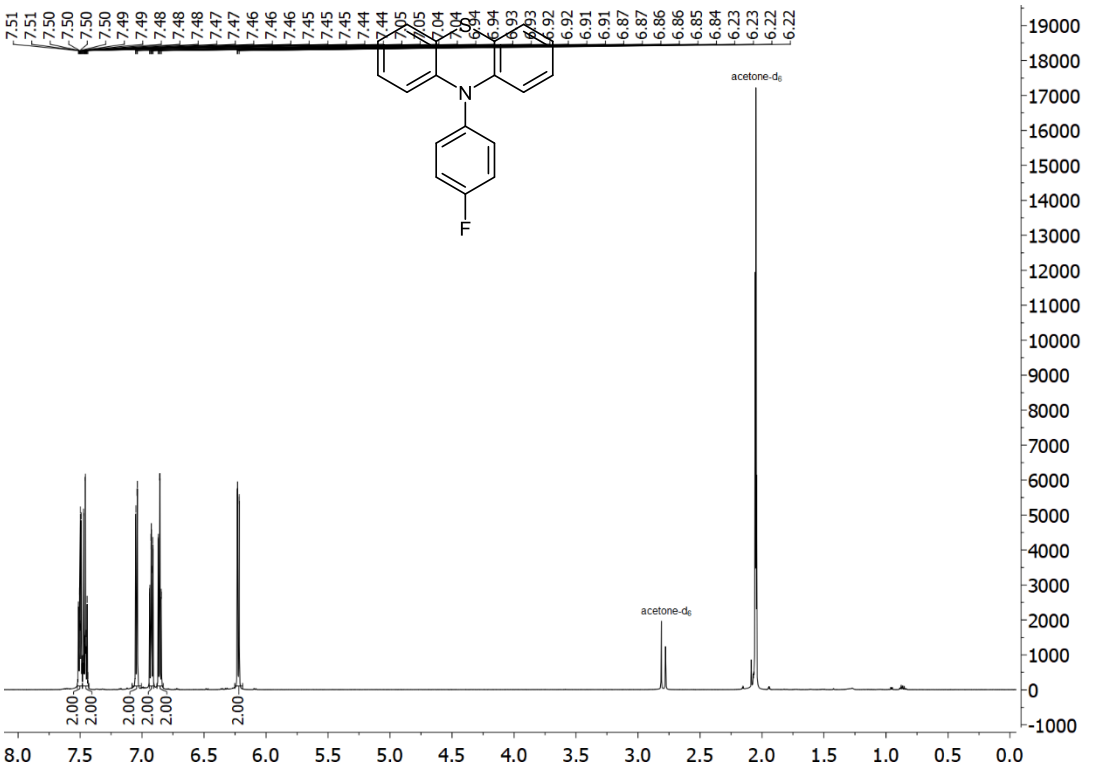
1.3 ^{1}H NMR spectrum of 10-(4-(Trifluoromethyl)phenyl)-10*H*-phenothiazine (3c) (acetone-d_6, 600 MHz, 293 K)



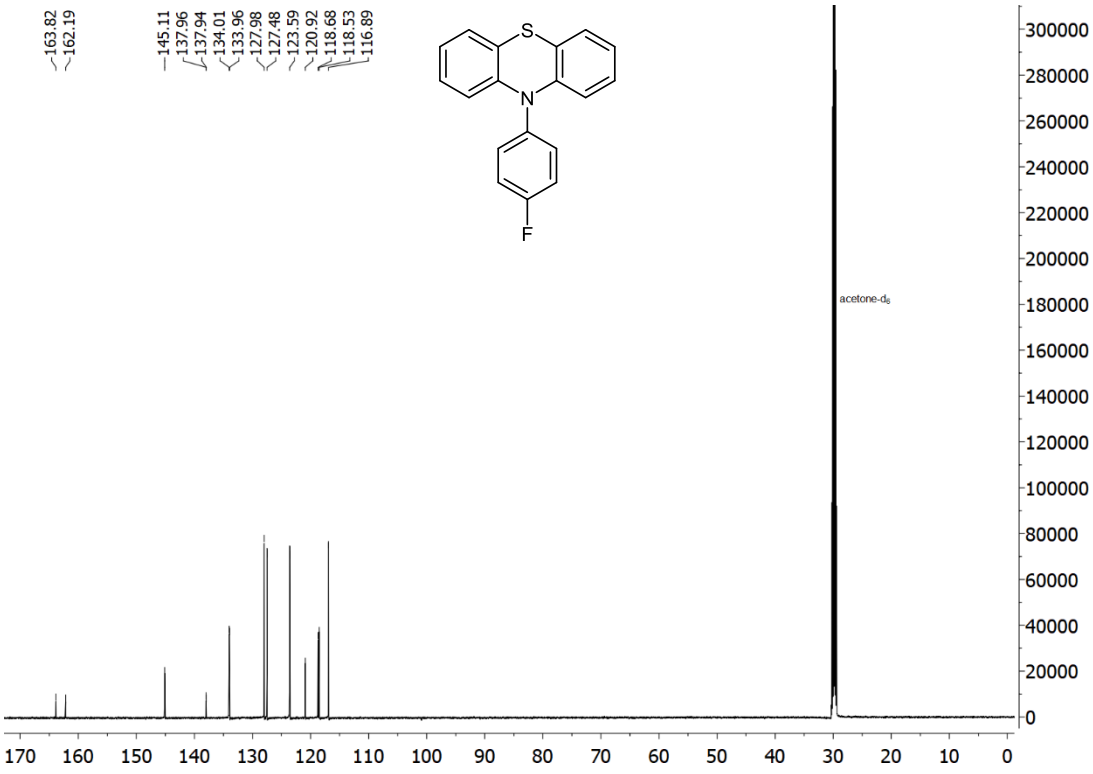
^{13}C NMR spectrum of 10-(4-(Trifluoromethyl)phenyl)-10*H*-phenothiazine (3c) (acetone-d_6, 150 MHz, 293 K)



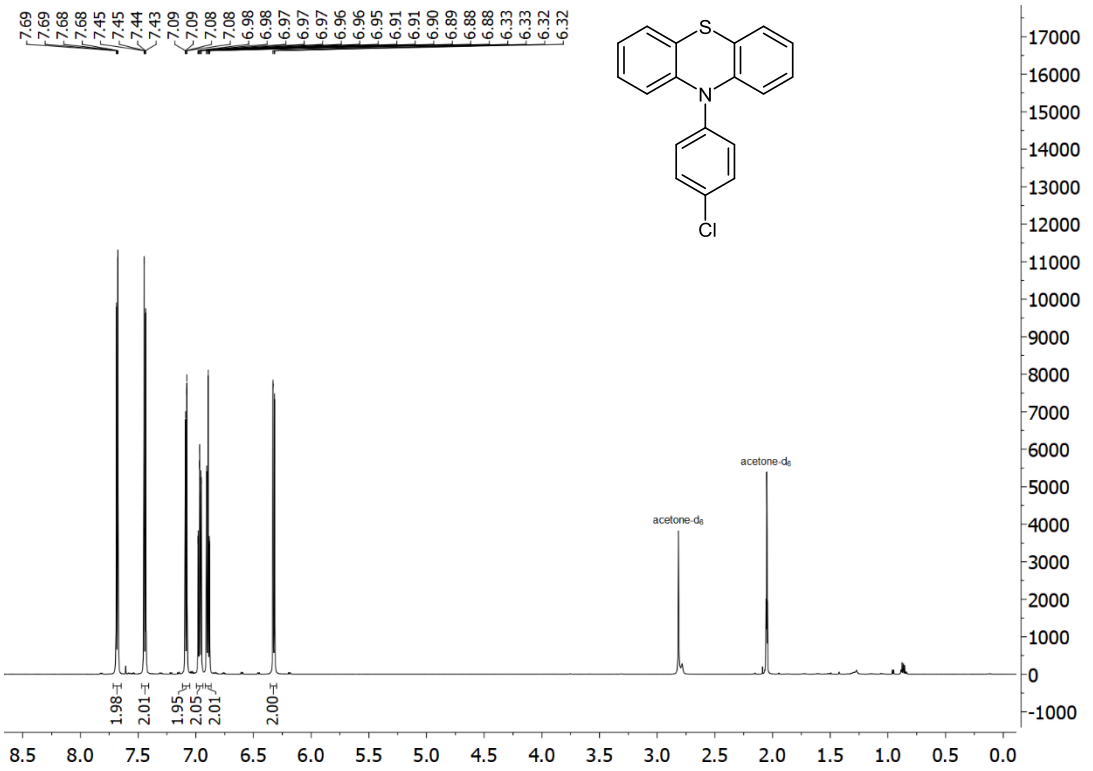
1.4 ^{1}H NMR spectrum of 10-(4-Fluorophenyl)-10*H*-phenothiazine (3d) (acetone-d_6, 600 MHz, 293 K)



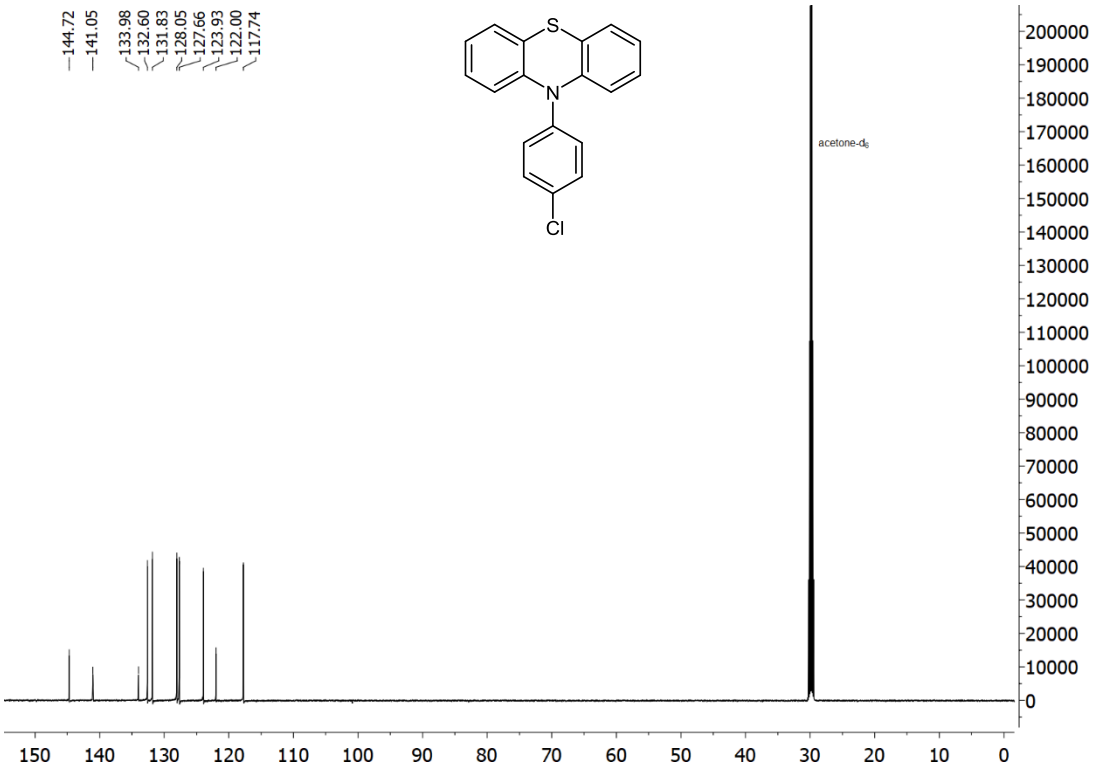
^{13}C NMR spectrum of 10-(4-Fluorophenyl)-10*H*-phenothiazine (3d) (acetone-d_6, 150 MHz, 293 K)



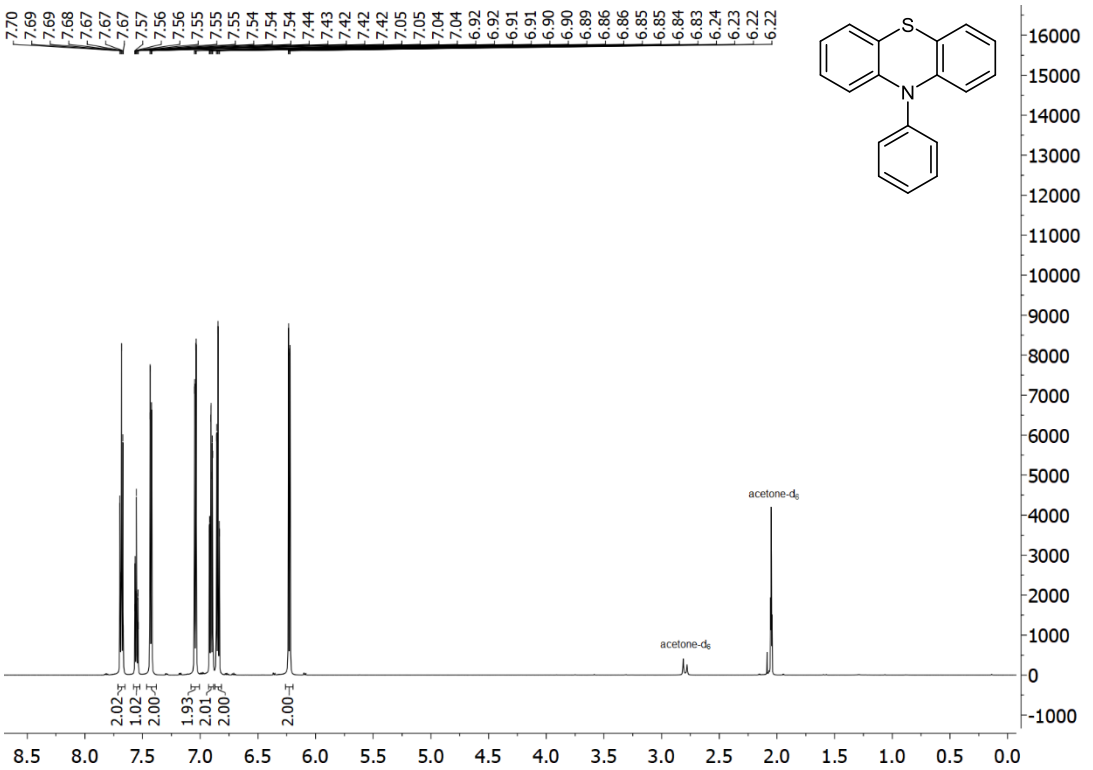
1.5 ^{1}H NMR spectrum of 10-(4-Chlorophenyl)-10*H*-phenothiazine (3e) (acetone-d_6, 600 MHz, 293 K)



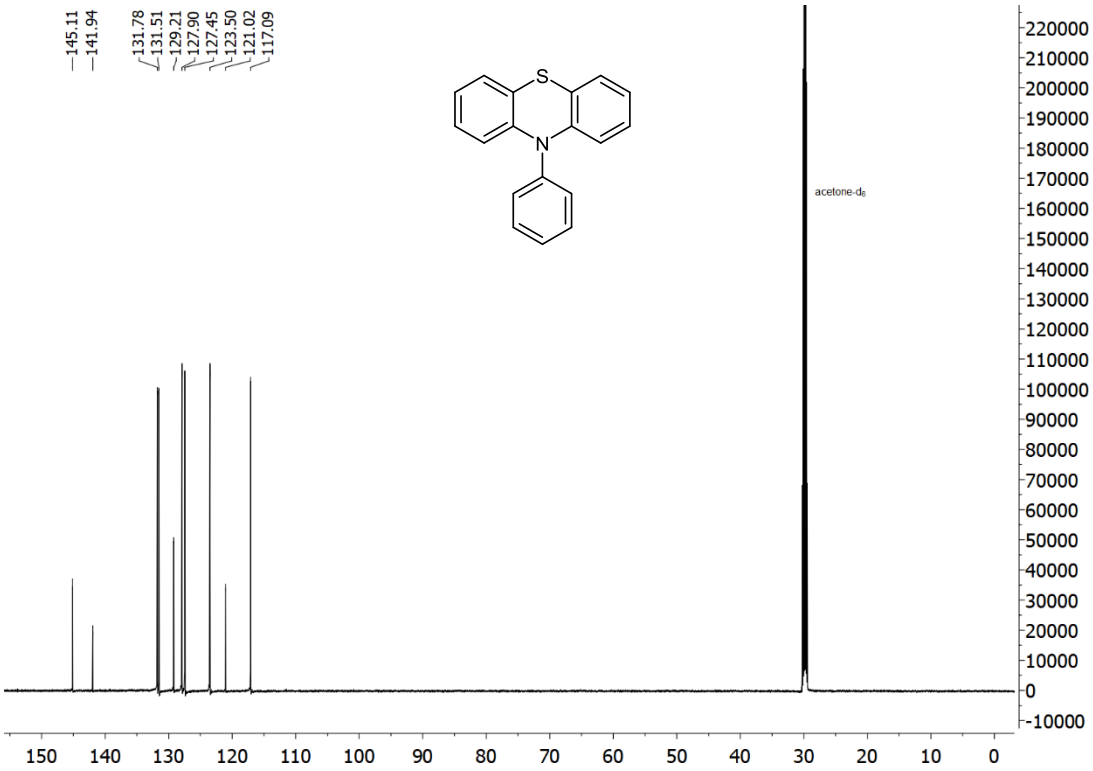
^{13}C NMR spectrum of 10-(4-Chlorophenyl)-10*H*-phenothiazine (3e) (acetone-d_6, 150 MHz, 293 K)



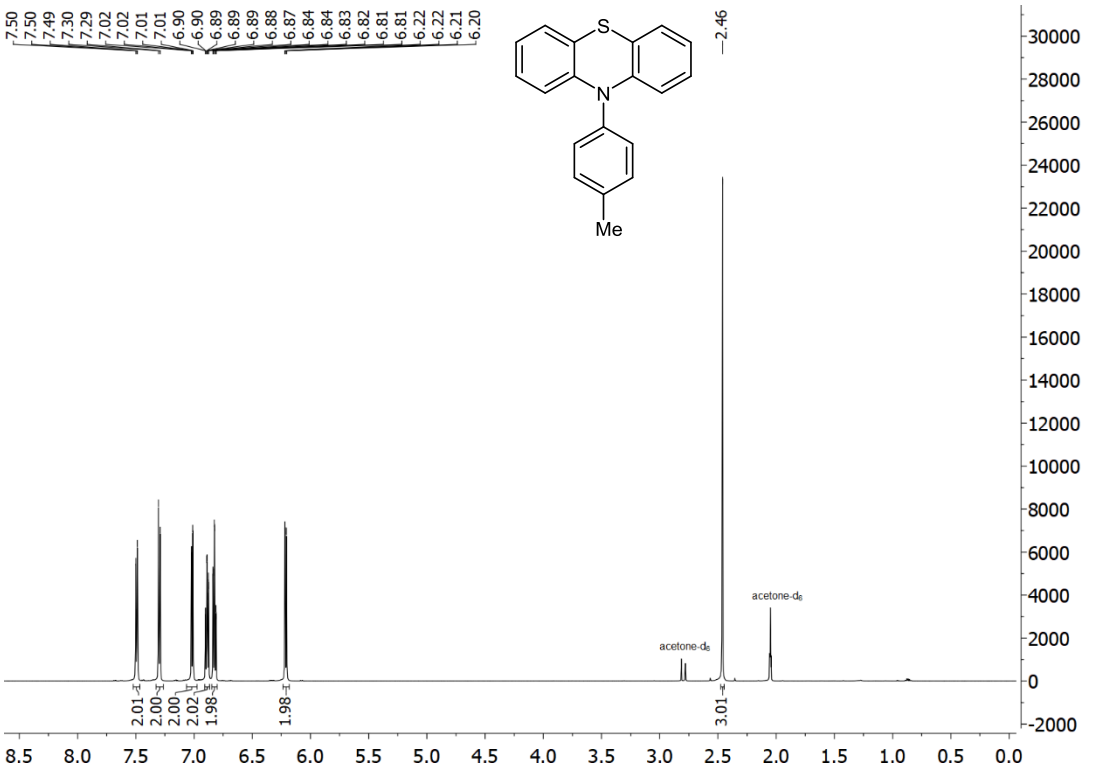
1.6 ^{1}H NMR spectrum of 10-Phenyl-10*H*-phenothiazine (3f) (acetone-d_6, 600 MHz, 293 K)



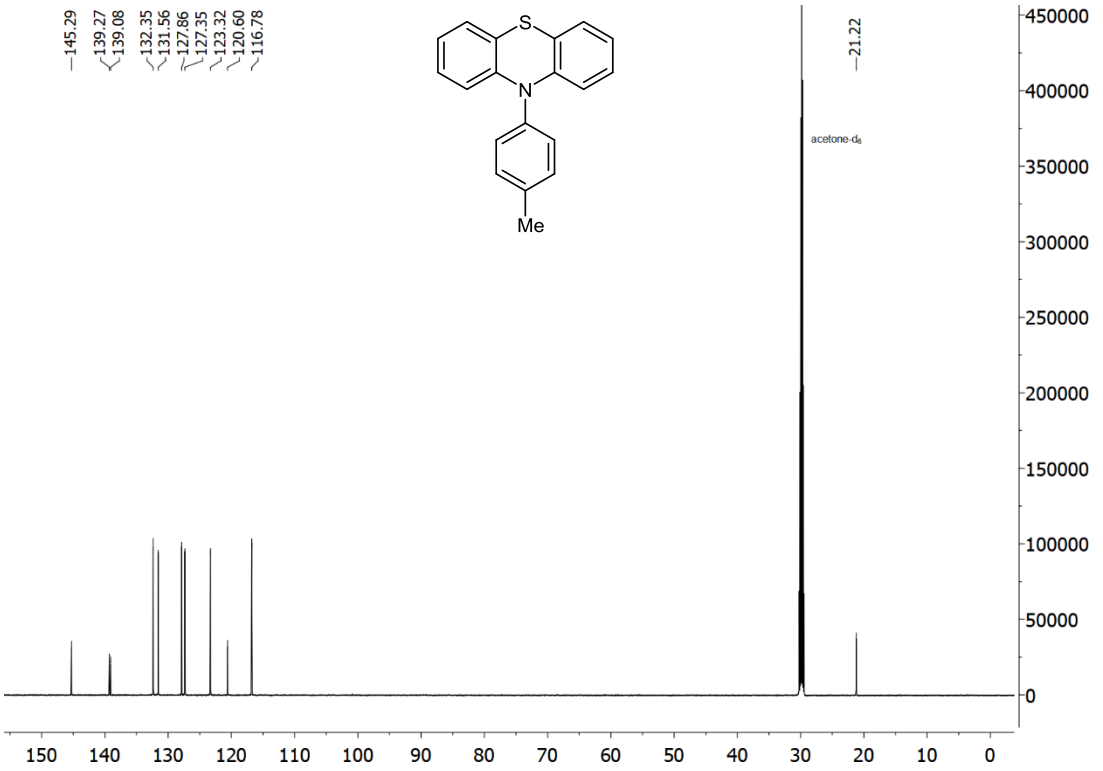
^{13}C NMR spectrum of 10-Phenyl-10*H*-phenothiazine (3f) (acetone-d_6, 150 MHz, 293 K)



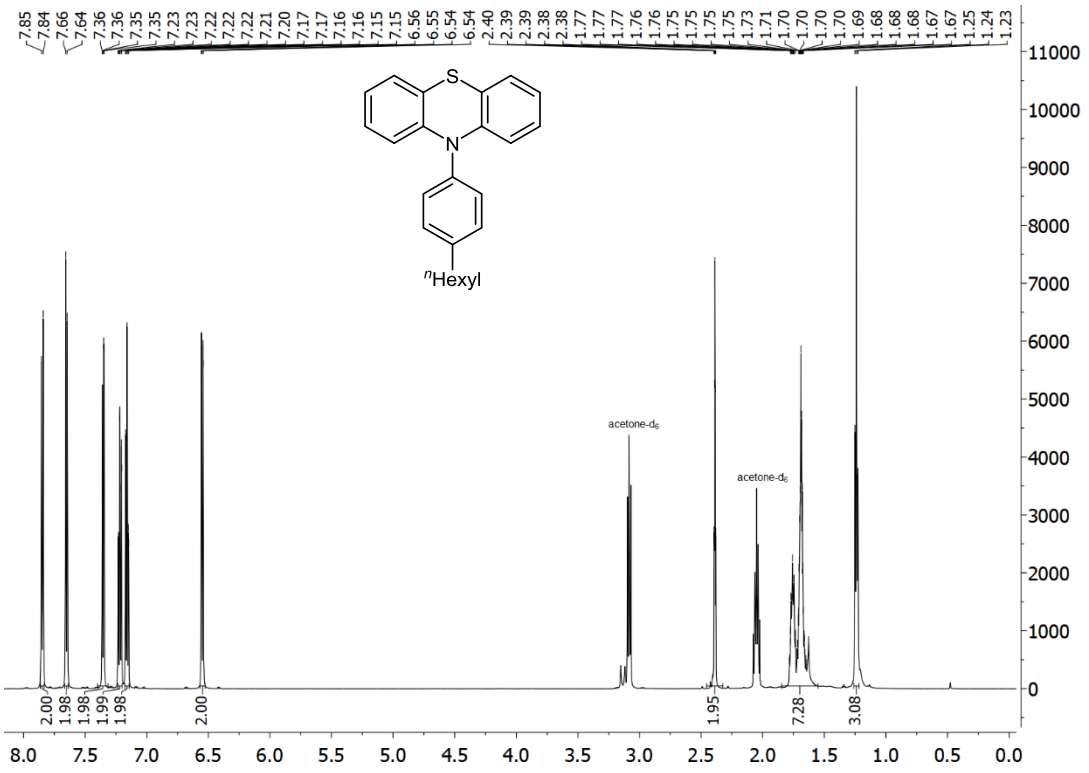
1.7 ^{1}H NMR spectrum of 10-(*p*-Tolyl)-10*H*-phenothiazine (3g) (acetone-d_6, 600 MHz, 293 K)



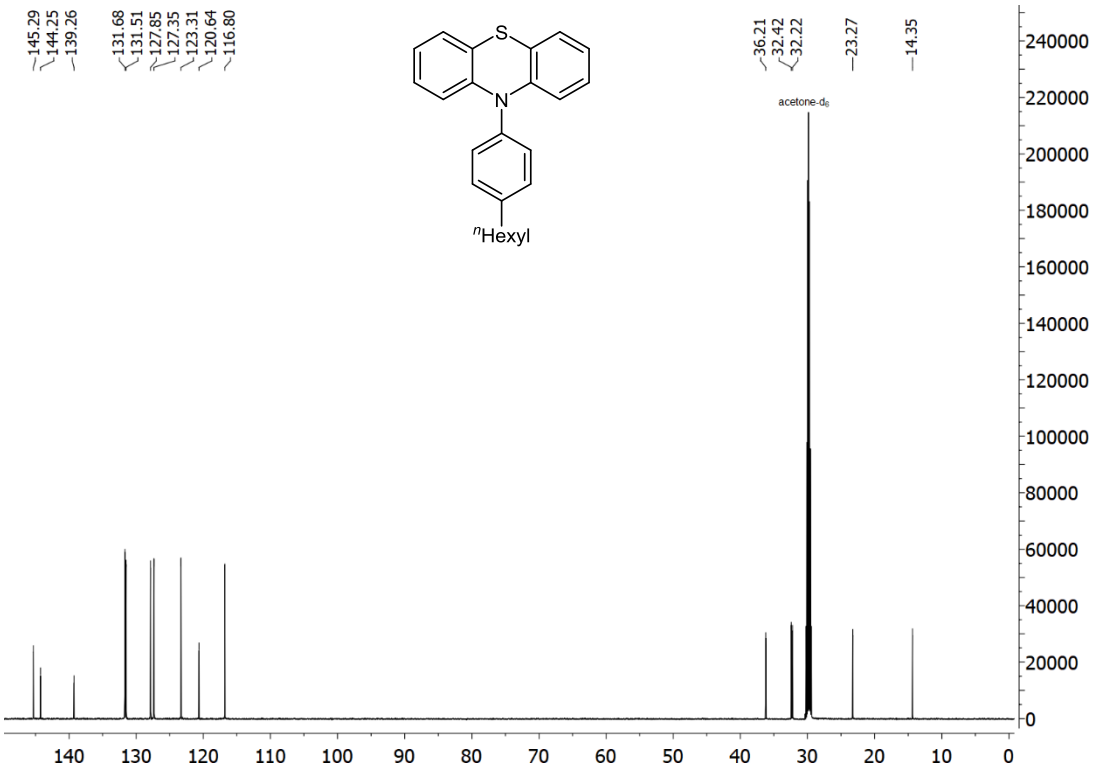
^{13}C NMR spectrum of 10-(*p*-Tolyl)-10*H*-phenothiazine (3g) (acetone-d_6, 150 MHz, 293 K)



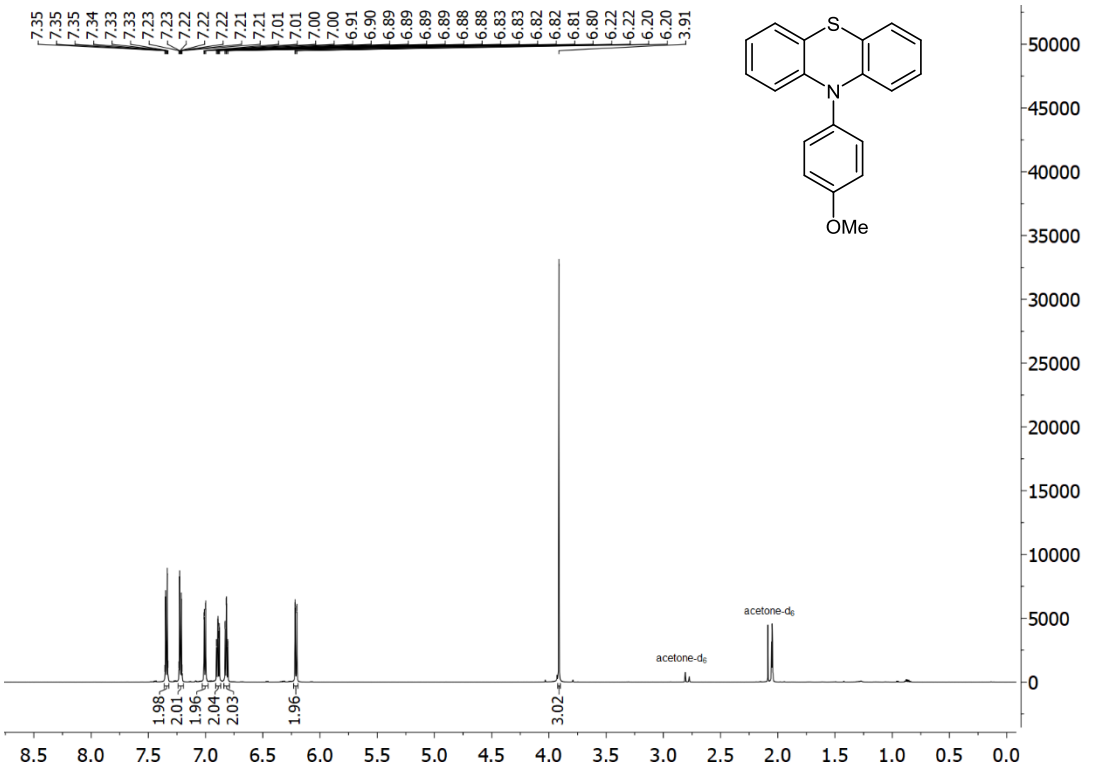
1.8 ^{1}H NMR spectrum of 10-(4-Hexylphenyl)-10*H*-phenothiazine (3h) (acetone-d$_6$, 600 MHz, 293 K)



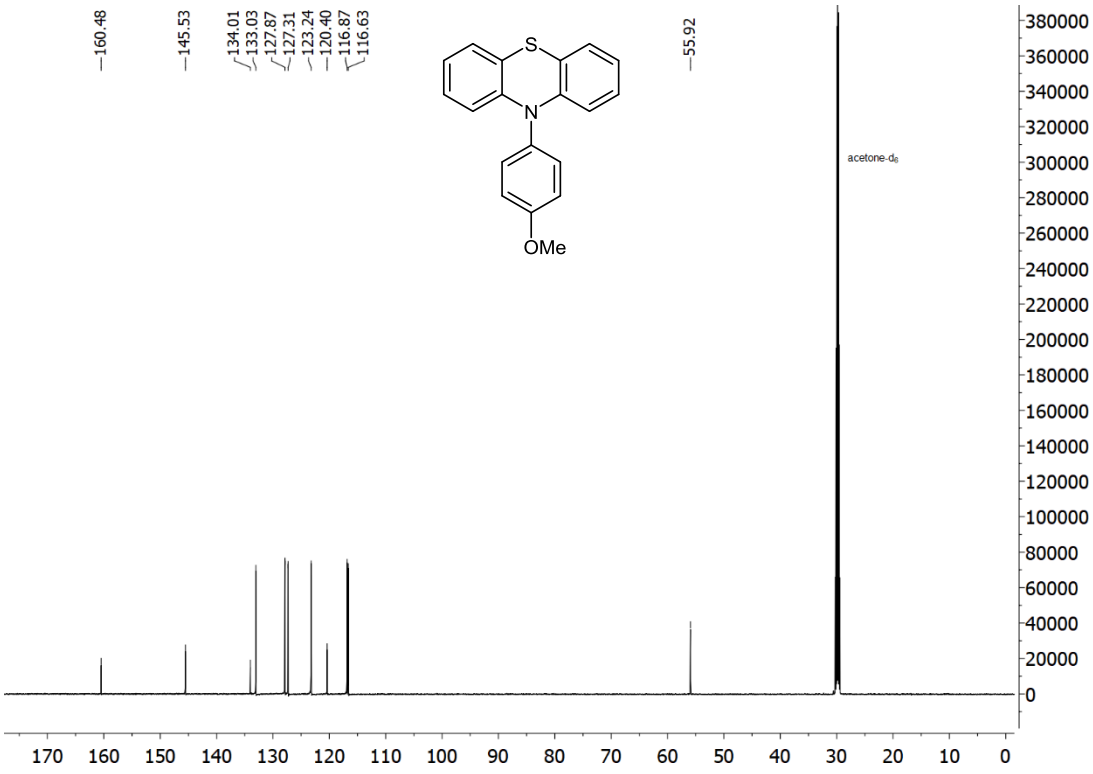
^{1}H NMR spectrum of 10-(4-Hexylphenyl)-10*H*-phenothiazine (3h) (acetone-d$_6$, 150 MHz, 293 K)



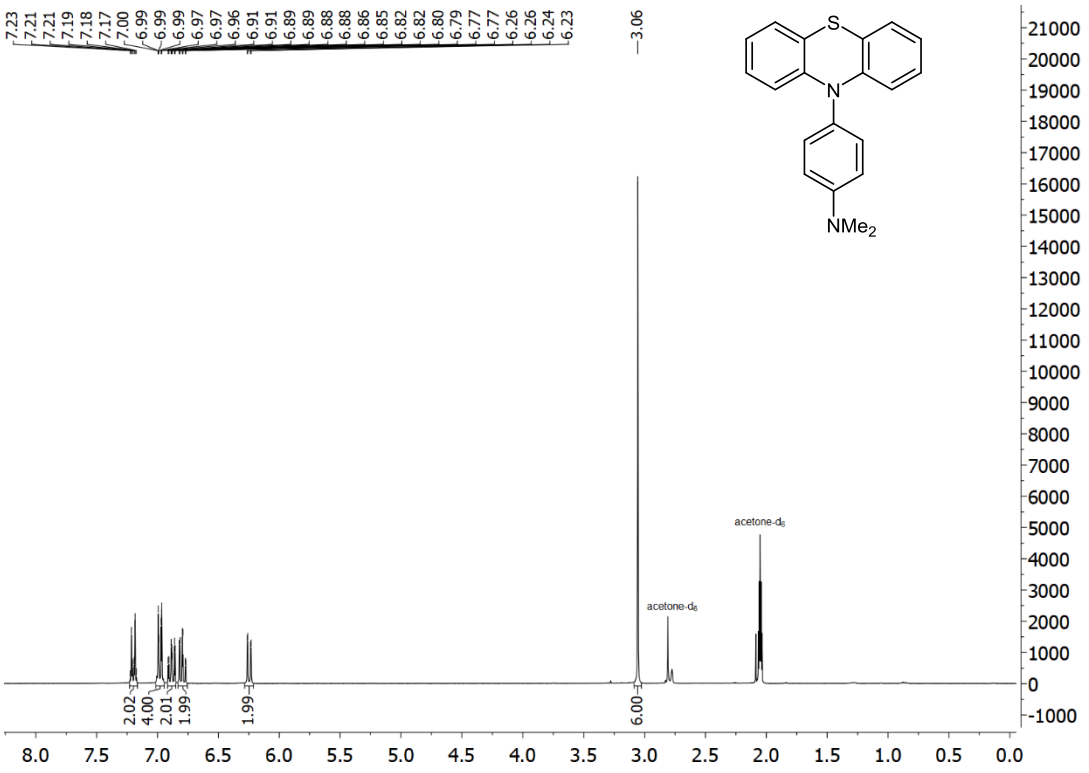
1.9 ^{1}H NMR spectrum of 10-(4-Methoxyphenyl)-10*H*-phenothiazine (3i) (acetone-d_6, 600 MHz, 293 K)



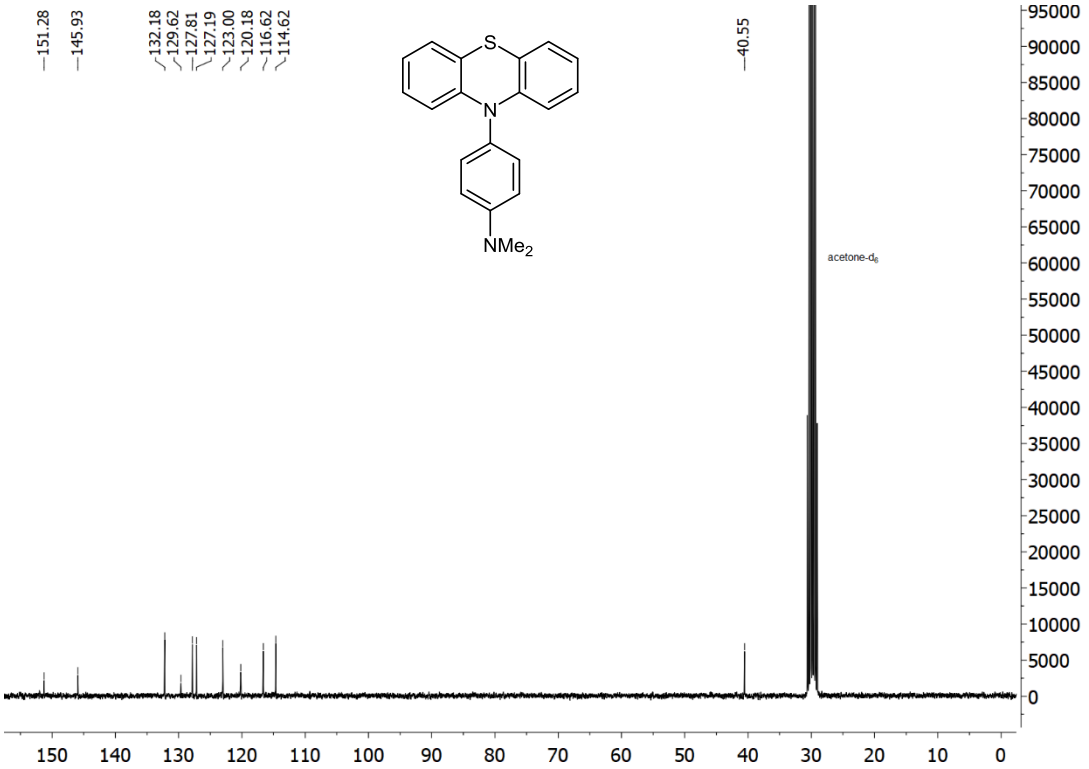
^{13}C NMR spectrum of 10-(4-Methoxyphenyl)-10*H*-phenothiazine (3i) (acetone-d_6, 150 MHz, 293 K)



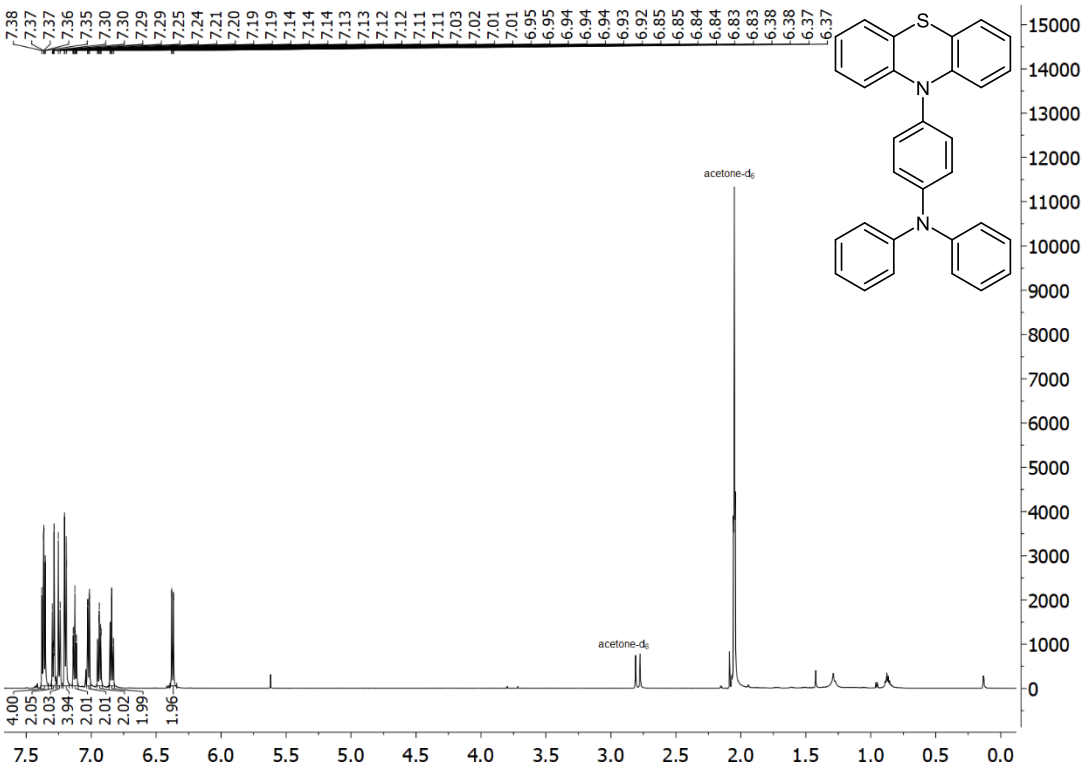
1.10 ^{1}H NMR spectrum of *N*,*N*-Dimethyl-4-(10*H*-phenothiazin-10-yl)aniline (3j) (acetone-d_6, 300 MHz, 293 K)



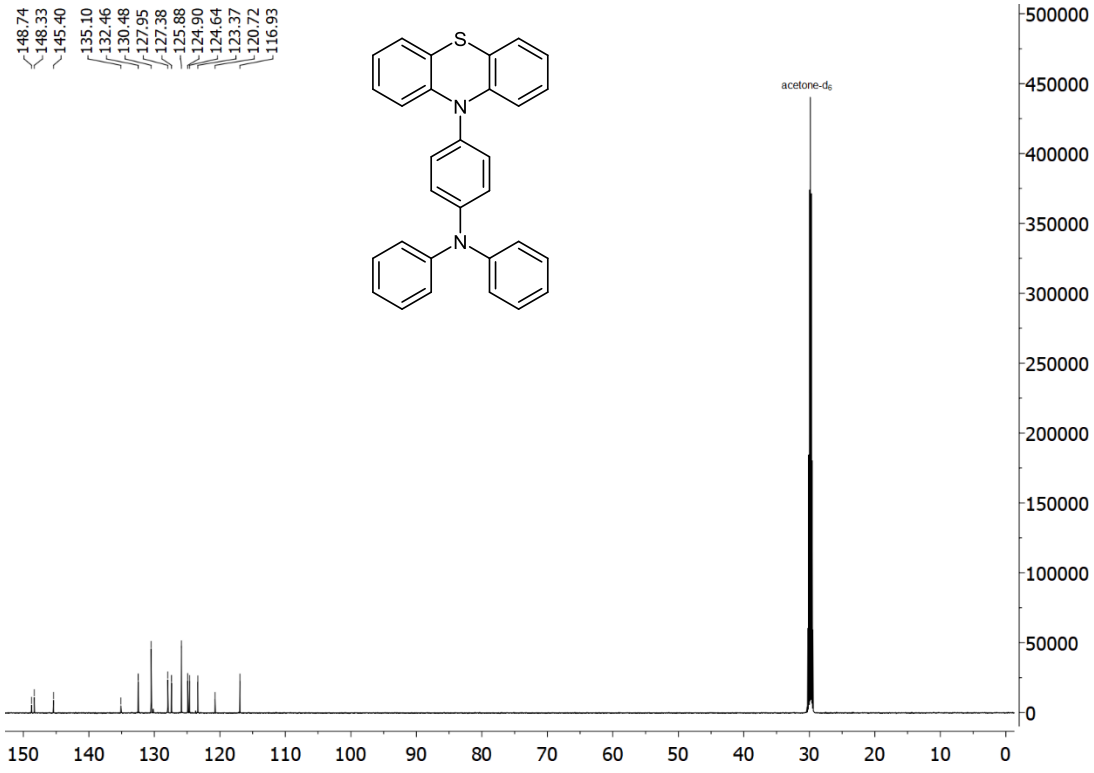
^{13}C NMR spectrum of *N*,*N*-Dimethyl-4-(10*H*-phenothiazin-10-yl)aniline (3j) (acetone-d_6, 75 MHz, 293 K)



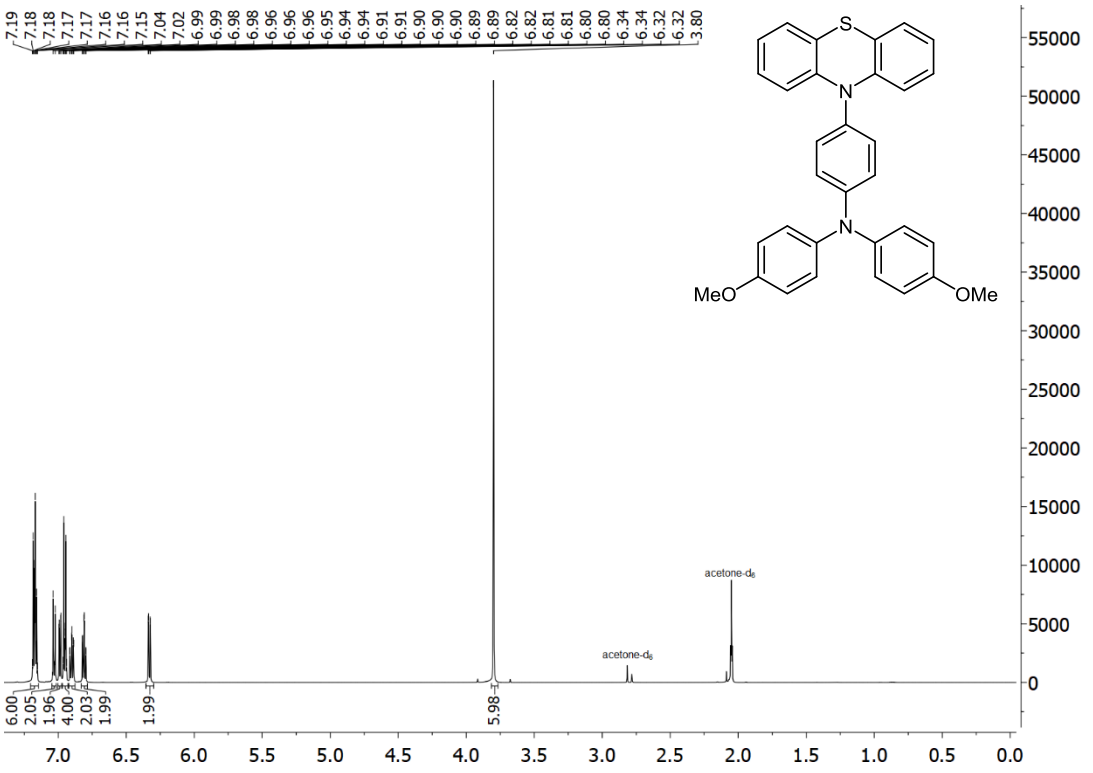
1.11 ^{1}H NMR spectrum of 4-(10*H*-Phenothiazin-10-yl)-*N*,*N*-diphenylaniline (3k) (acetone-d_6, 600 MHz, 293 K)



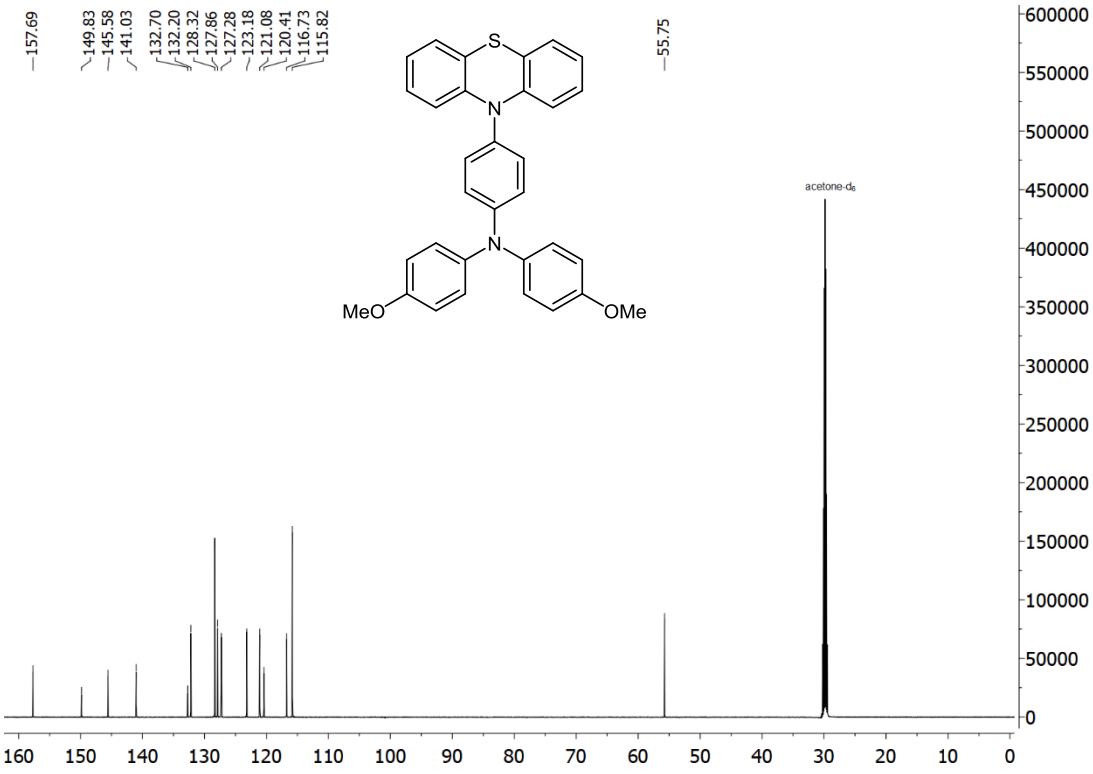
^{13}C NMR spectrum of 4-(10*H*-Phenothiazin-10-yl)-*N*,*N*-diphenylaniline (3k) (acetone-d_6, 150 MHz, 293 K)



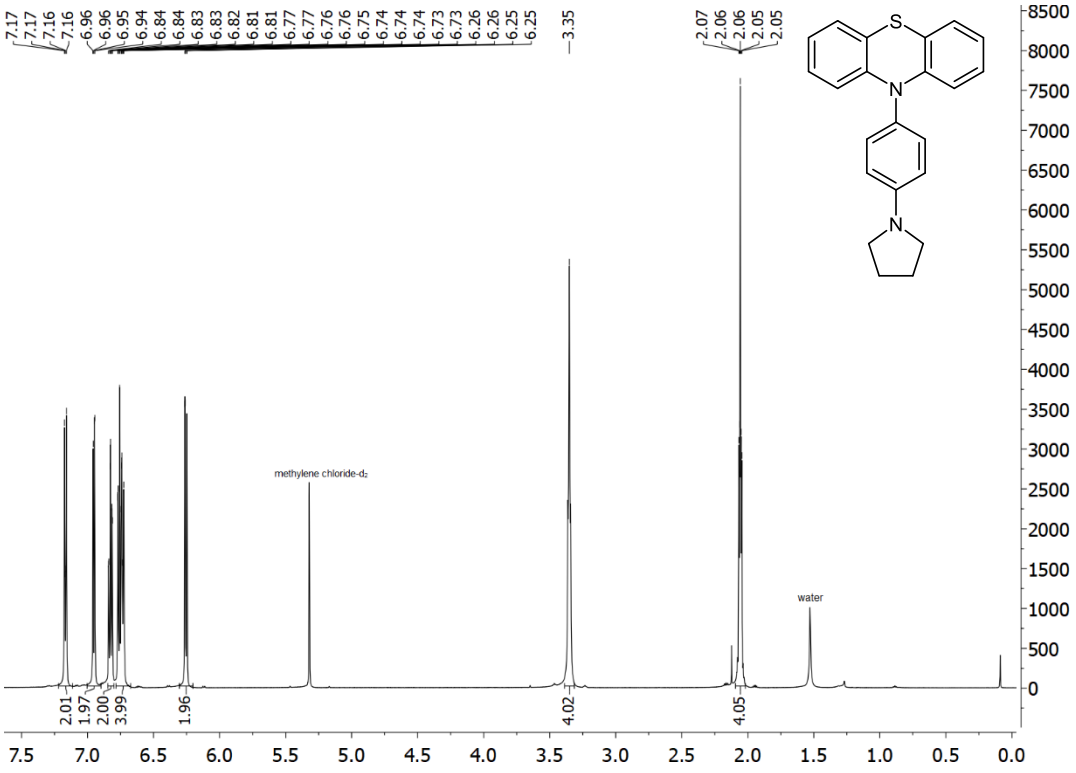
1.12 ^{1}H NMR spectrum of *N*-(4-(10*H*-Phenothiazin-10-yl)phenyl)-4-methoxy-*N*-(4-methoxyphenyl)aniline (3l) (acetone-d_6, 600 MHz, 293 K)



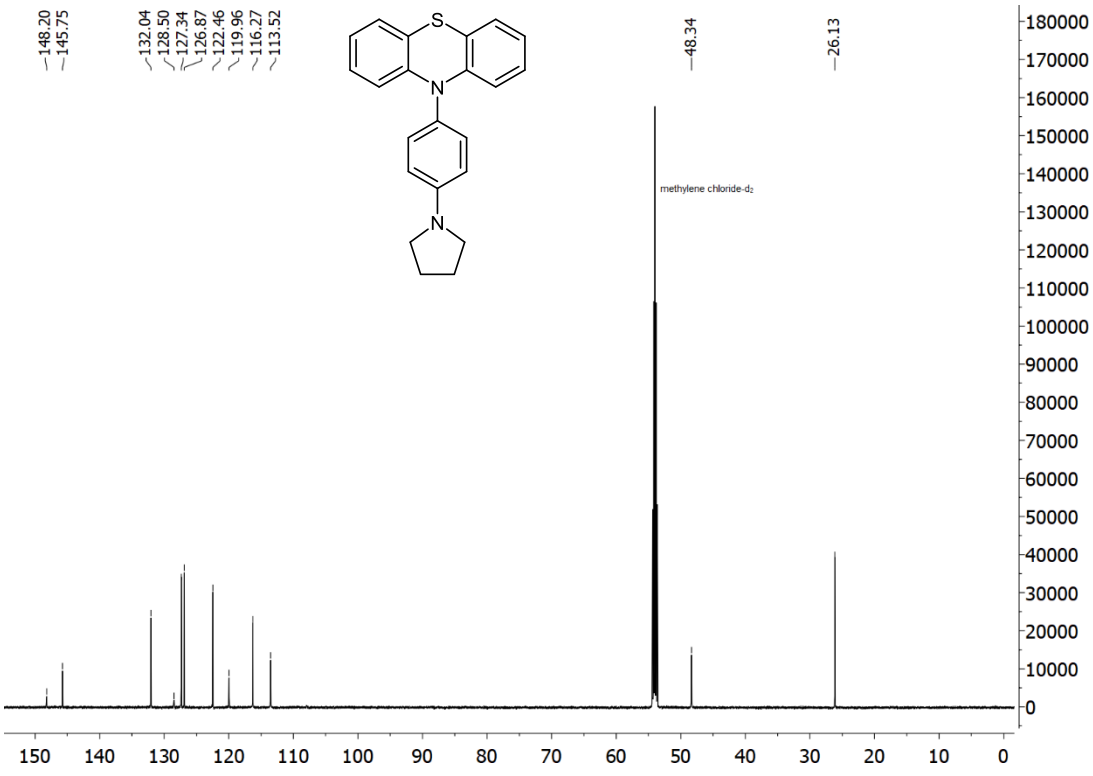
^{13}C NMR spectrum of *N*-(4-(10*H*-Phenothiazin-10-yl)phenyl)-4-methoxy-*N*-(4-methoxyphenyl)aniline (3l) (acetone-d_6, 150 MHz, 293 K)



1.13 ^{1}H NMR spectrum of 10-(4-(Pyrrolidin-1-yl)phenyl)-10*H*-phenothiazine (3m) (methylene chloride-d_2, 600 MHz, 293 K)

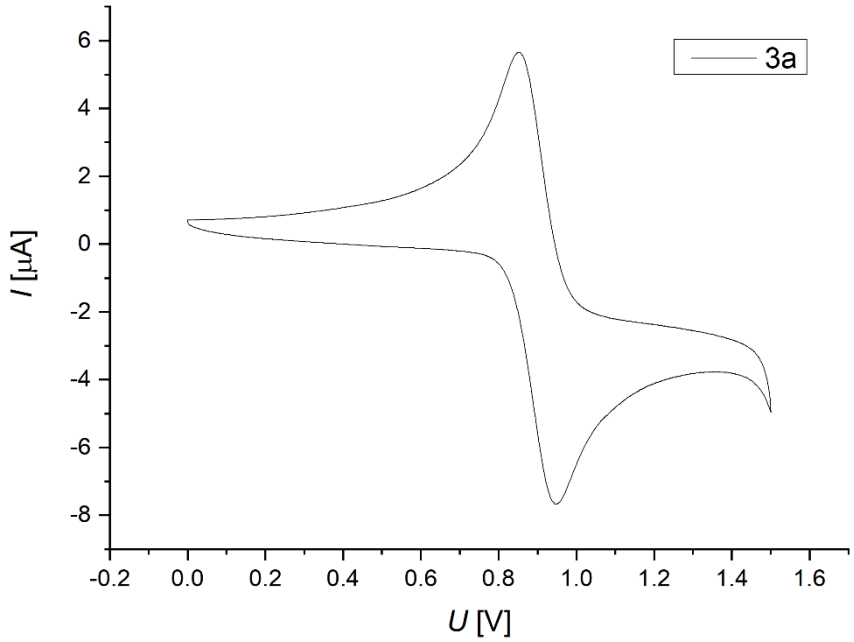


^{13}C NMR spectrum of 10-(4-(Pyrrolidin-1-yl)phenyl)-10*H*-phenothiazine (3m) (methylene chloride-d_2, 600 MHz, 293 K)



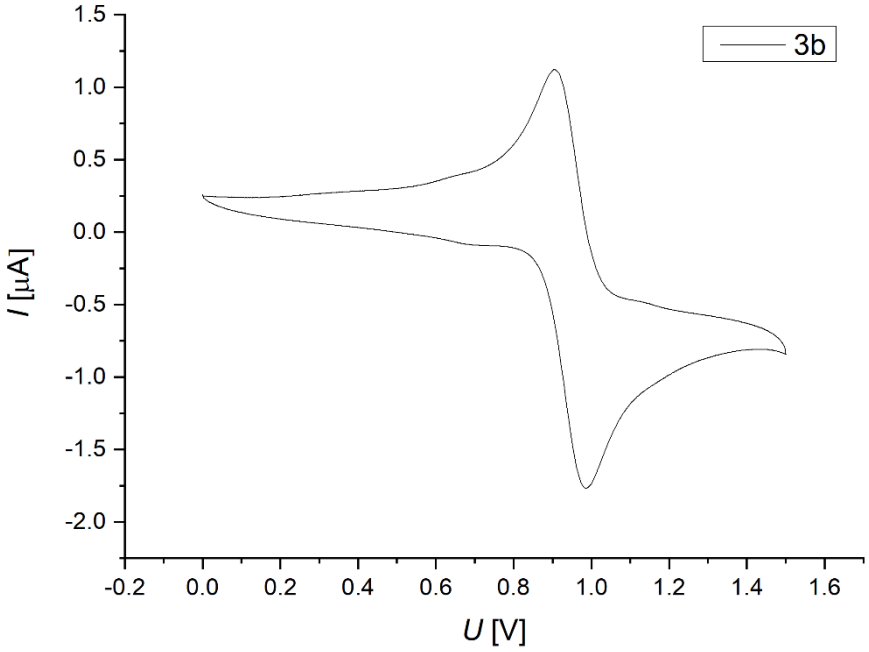
2 Cyclic voltammogram

2.1 Cyclic voltammogram of 10-(4-Nitrophenyl)-10*H*-phenothiazine (3a)



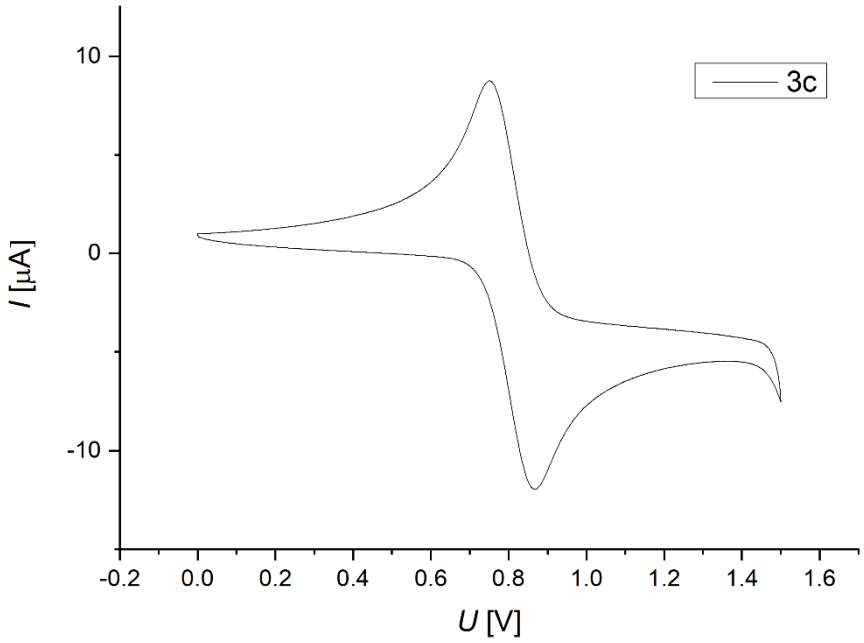
Recorded in dichloromethane, T = 293 K, electrolyte: $[Bu_4N][PF_6]$, Pt working electrode, Pt counter electrode, Ag/AgCl reference electrode, v = 100 mV/s, standard: $[Fe(Cp)_2]/[Fe(Cp)_2]^+$.

2.2 Cyclic voltammogram of 4-(10*H*-Phenothiazin-10-yl)benzonitrile (3b)



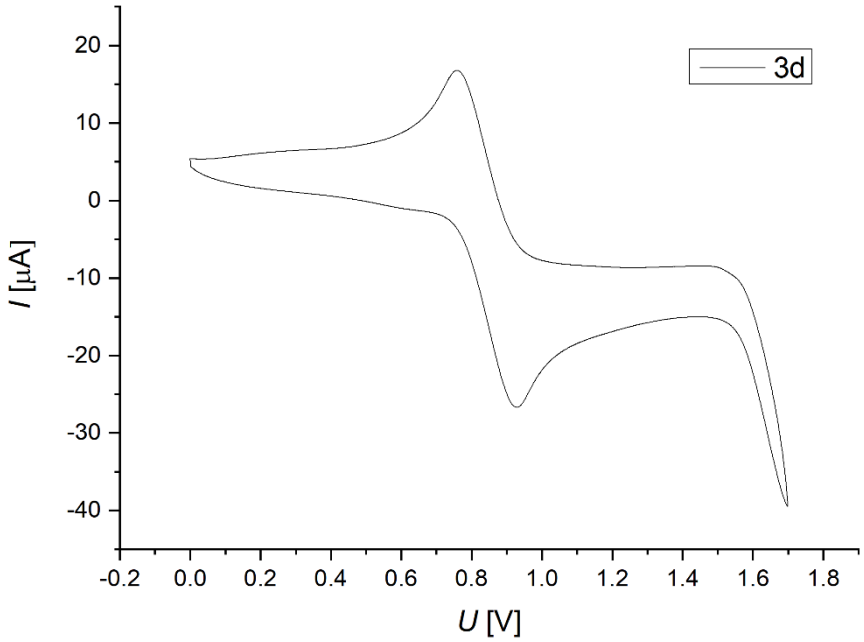
Recorded in dichloromethane, T = 293 K, electrolyte: $[Bu_4N][PF_6]$, Pt working electrode, Pt counter electrode, Ag/AgCl reference electrode, v = 100 mV/s, standard: $[Fe(Cp)_2]/[Fe(Cp)_2]^+$.

2.3 Cyclic voltammogram of 10-(4-(Trifluoromethyl)phenyl)-10*H*-phenothiazine (3c)



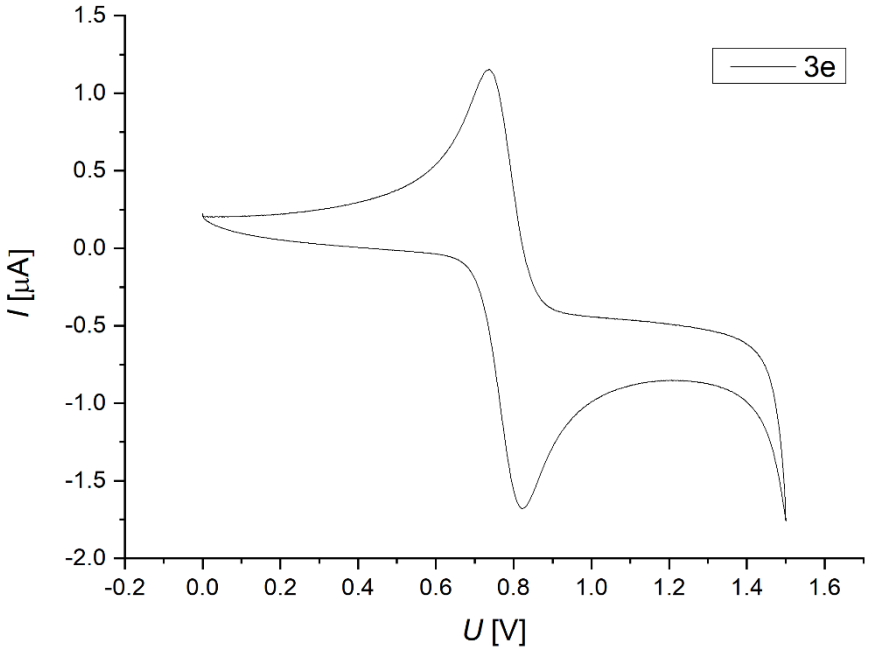
Recorded in dichloromethane, T = 293 K, electrolyte: $[Bu_4N][PF_6]$, Pt working electrode, Pt counter electrode, Ag/AgCl reference electrode, v = 100 mV/s, standard: $[Fe(Cp)_2]/[Fe(Cp)_2]^+$.

2.4 Cyclic voltammogram of 10-(4-Fluorophenyl)-10*H*-phenothiazine (3d)



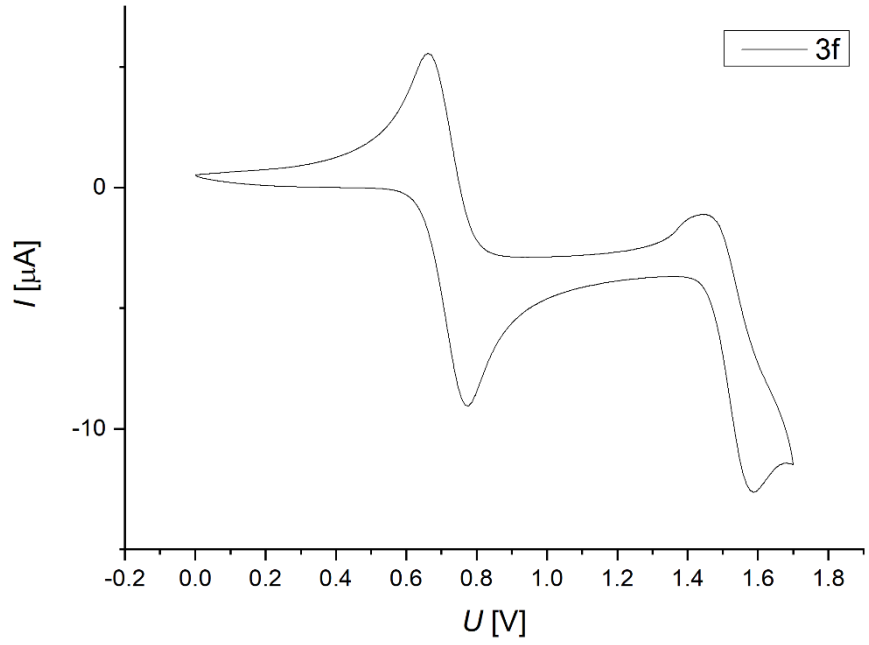
Recorded in dichloromethane, T = 293 K, electrolyte: $[Bu_4N][PF_6]$, Pt working electrode, Pt counter electrode, Ag/AgCl reference electrode, v = 100 mV/s, standard: $[Fe(Cp)_2]/[Fe(Cp)_2]^+$.

2.5 Cyclic voltammogram of 10-(4-Chlorophenyl)-10*H*-phenothiazine (3e)



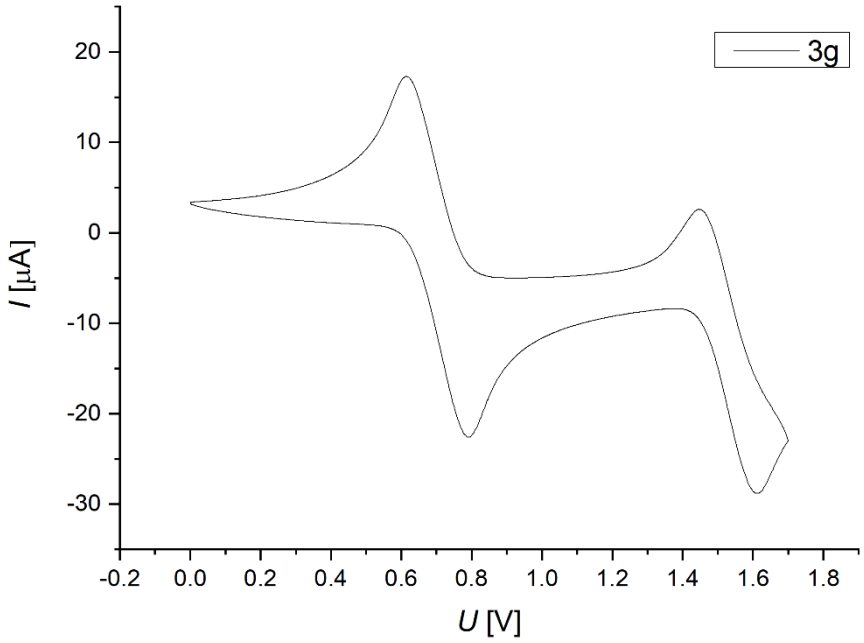
Recorded in dichloromethane, T = 293 K, electrolyte: $[Bu_4N][PF_6]$, Pt working electrode, Pt counter electrode, Ag/AgCl reference electrode, v = 100 mV/s, standard: $[Fe(Cp)_2]/[Fe(Cp)_2]^+$.

2.6 Cyclic voltammogram of 10-Phenyl-10*H*-phenothiazine (3f)



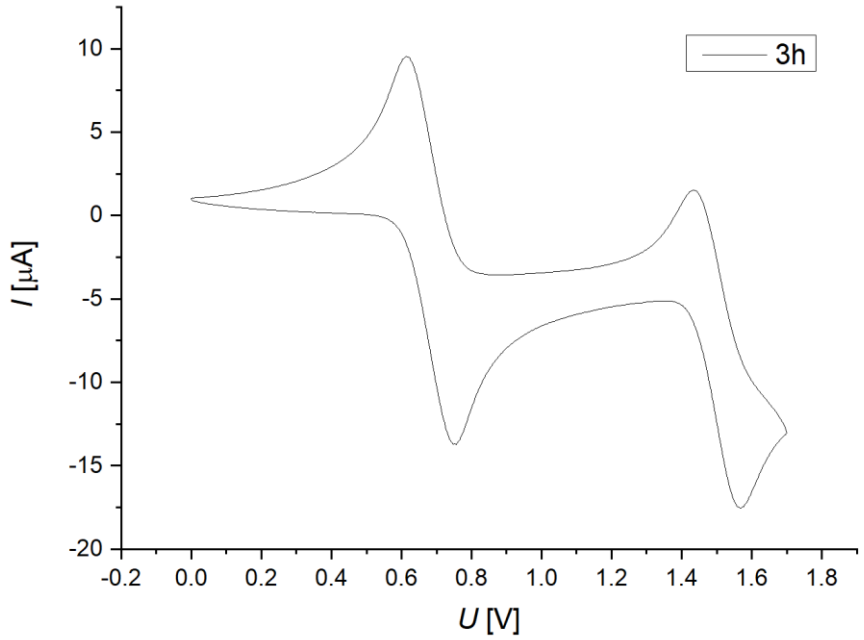
Recorded in dichloromethane, T = 293 K, electrolyte: $[Bu_4N][PF_6]$, Pt working electrode, Pt counter electrode, Ag/AgCl reference electrode, v = 100 mV/s, standard: $[Fe(Cp)_2]/[Fe(Cp)_2]^+$.

2.7 Cyclic voltammogram of 10-(*p*-Tolyl)-10*H*-phenothiazine (3g)



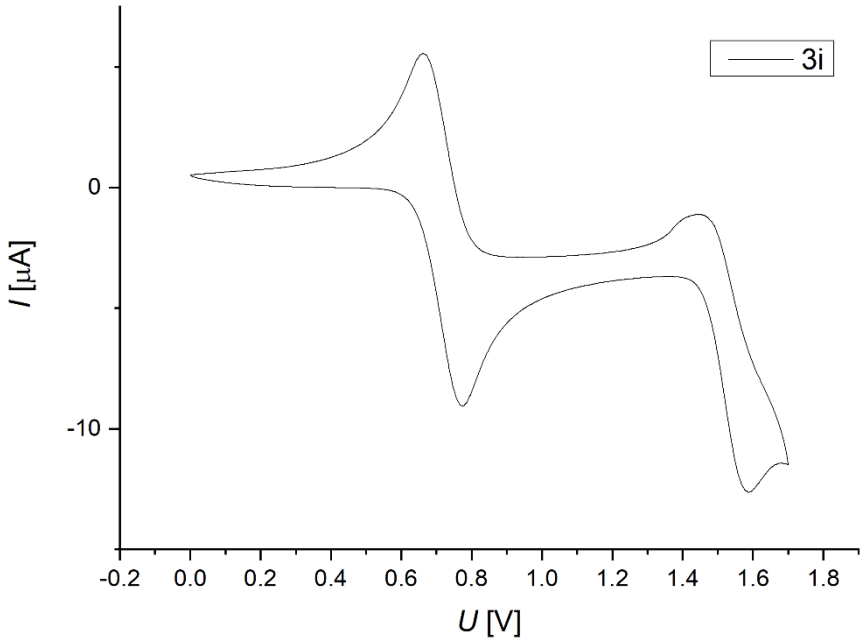
Recorded in dichloromethane, T = 293 K, electrolyte: $[Bu_4N][PF_6]$, Pt working electrode, Pt counter electrode, Ag/AgCl reference electrode, v = 100 mV/s, standard: $[Fe(Cp)_2]/[Fe(Cp)_2]^+$.

2.8 Cyclic voltammogram of 10-(4-Hexylphenyl)-10*H*-phenothiazine (3h)



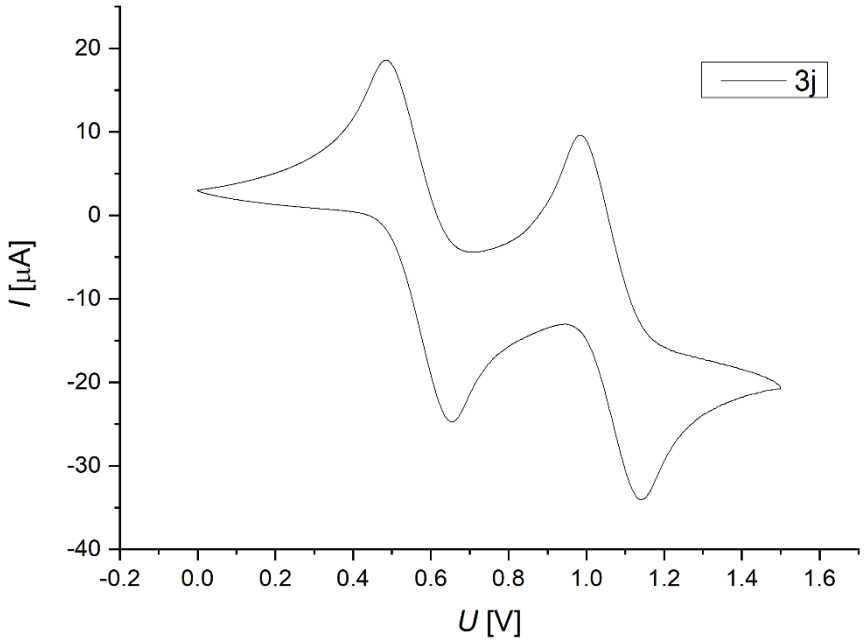
Recorded in dichloromethane, T = 293 K, electrolyte: $[Bu_4N][PF_6]$, Pt working electrode, Pt counter electrode, Ag/AgCl reference electrode, v = 100 mV/s, standard: $[Fe(Cp)_2]/[Fe(Cp)_2]^+$.

2.9 Cyclic voltammogram of 10-(4-Methoxyphenyl)-10*H*-phenothiazine (3i)



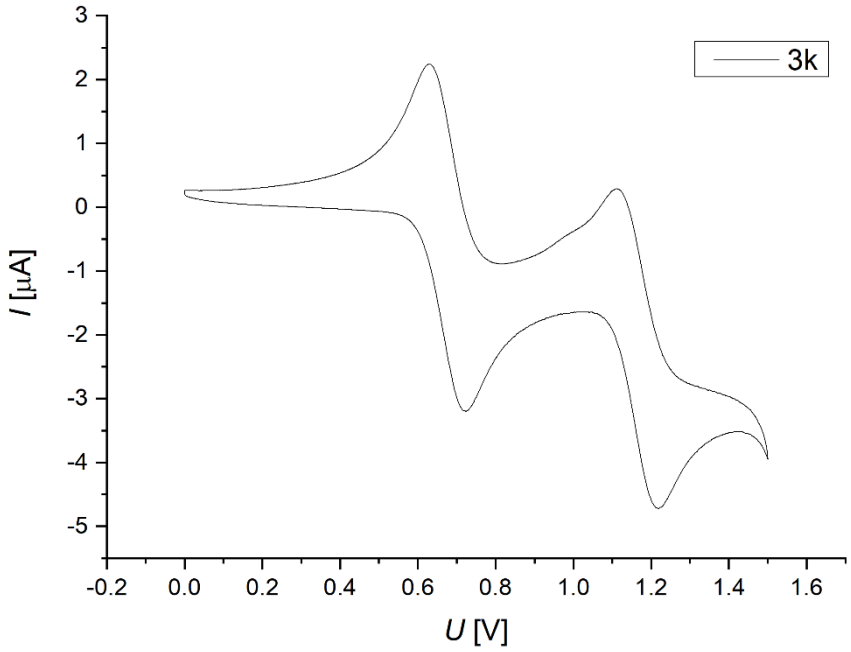
Recorded in dichloromethane, T = 293 K, electrolyte: $[Bu_4N][PF_6]$, Pt working electrode, Pt counter electrode, Ag/AgCl reference electrode, v = 100 mV/s, standard: $[Fe(Cp)_2]/[Fe(Cp)_2]^+$.

2.10 Cyclic voltammogram of *N*,*N*-Dimethyl-4-(10*H*-phenothiazin-10-yl)aniline (3j)



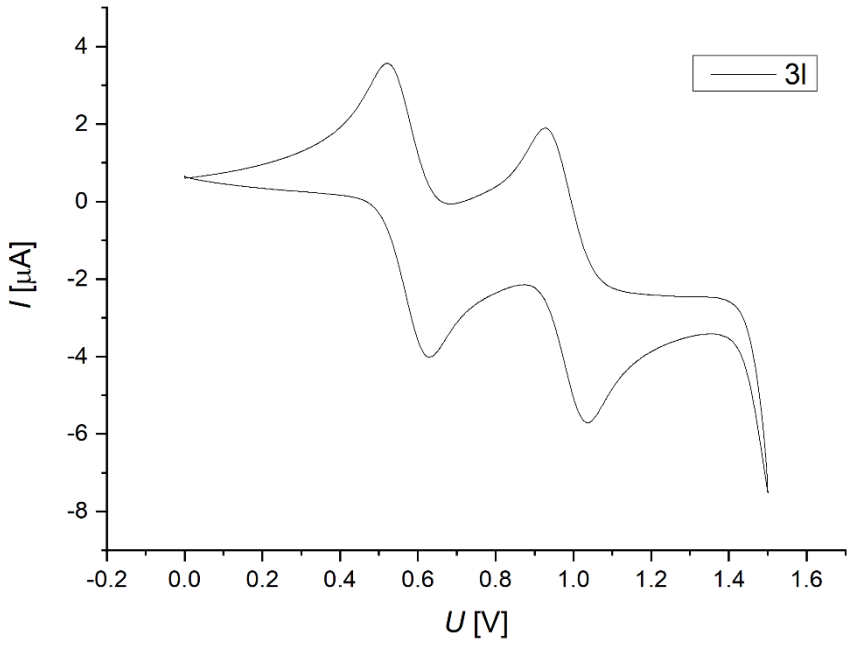
Recorded in dichloromethane, T = 293 K, electrolyte: $[Bu_4N][PF_6]$, Pt working electrode, Pt counter electrode, Ag/AgCl reference electrode, v = 100 mV/s, standard: $[FeCp^*_2]/[FeCp^*_2]^+$.

2.11 Cyclic voltammogram of 4-(10*H*-Phenothiazin-10-yl)-*N*,*N*-diphenylaniline (3k)



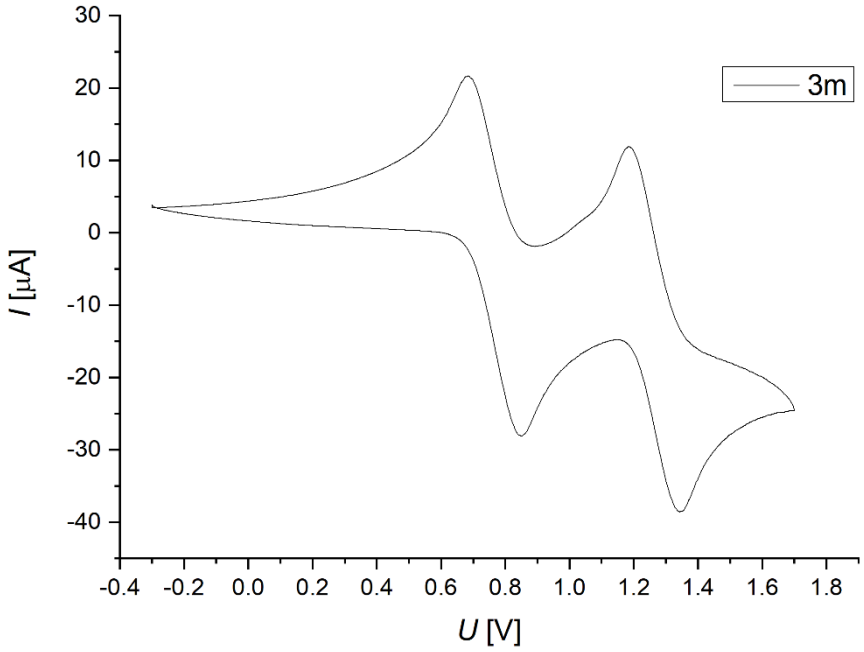
Recorded in dichloromethane, T = 293 K, electrolyte: $[Bu_4N][PF_6]$, Pt working electrode, Pt counter electrode, Ag/AgCl reference electrode, v = 100 mV/s, standard: $[FeCp^*_2]/[FeCp^*_2]^+$.

2.12 Cyclic voltammogram of *N*-(4-(10*H*-Phenothiazin-10-yl)phenyl)-4-methoxy-*N*-(4-methoxyphenyl)aniline (3l)



Recorded in dichloromethane, T = 293 K, electrolyte: $[Bu_4N][PF_6]$, Pt working electrode, Pt counter electrode, Ag/AgCl reference electrode, v = 100 mV/s, standard: $[FeCp^*_2]/[FeCp^*_2]^+$.

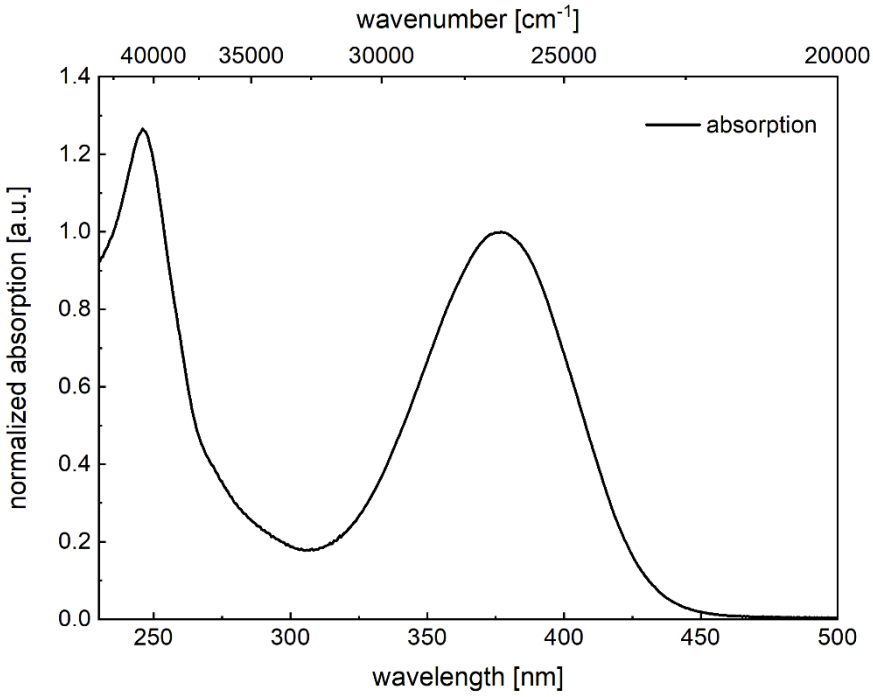
2.13 Cyclic voltammogram of 10-(4-(Pyrrolidin-1-yl)phenyl)-10*H*-phenothiazine (3m)



Recorded in dichloromethane, T = 293 K, electrolyte: $[Bu_4N][PF_6]$, Pt working electrode, Pt counter electrode, Ag/AgCl reference electrode, v = 100 mV/s, standard: $[FeCp^*_2]/[FeCp^*_2]^+$.

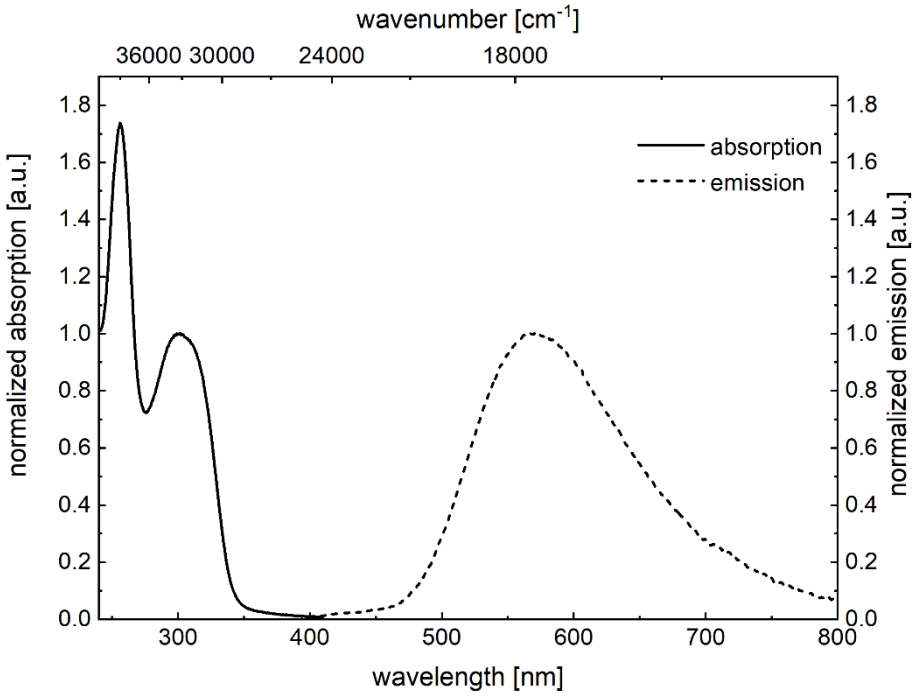
3 Absorption and emission spectra

3.1 Absorption spectra of 10-(4-Nitrophenyl)-10*H*-phenothiazine (3a)



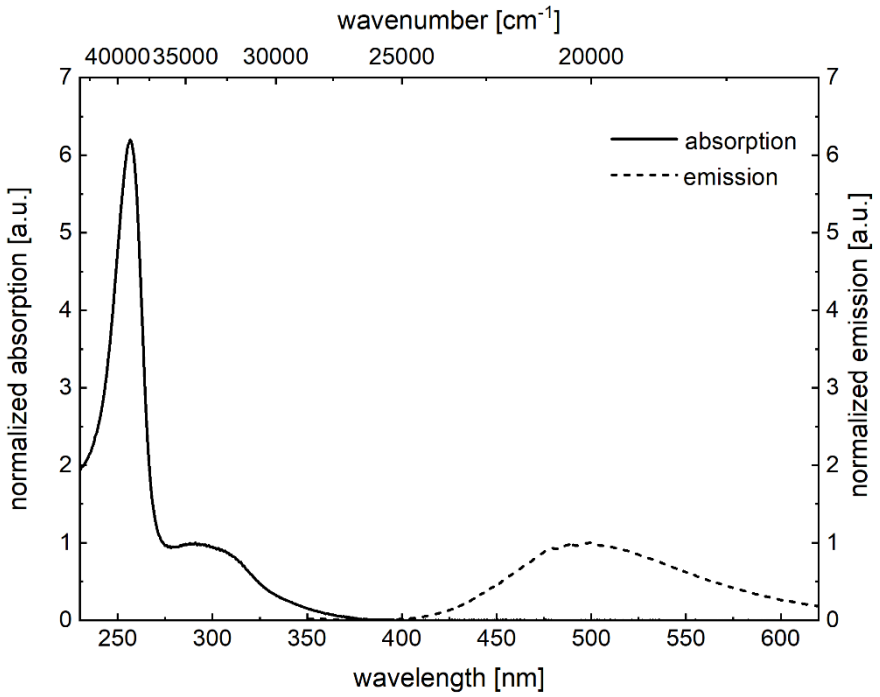
Recorded in dichloromethane, T = 293 K, c(**3**) = 10^{-5} M, $\lambda_{ex} = \lambda_{max,abs}$.

3.2 Absorption and emission spectra of 4-(10*H*-Phenothiazin-10-yl)benzonitrile (3b)



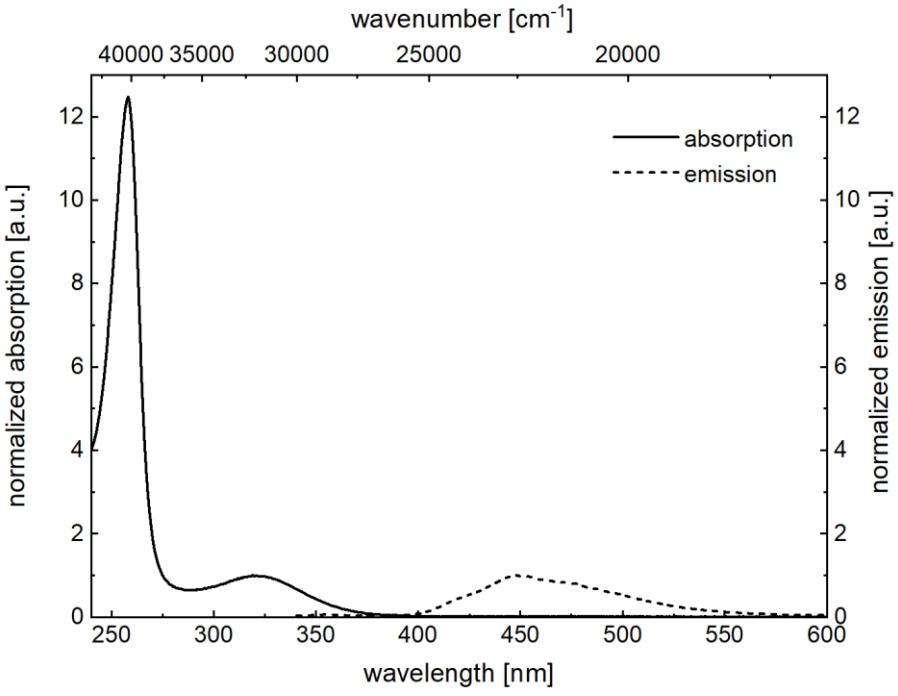
Recorded in dichloromethane, T = 293 K, c(**3**) = 10^{-5} M, $\lambda_{ex} = \lambda_{max,abs}$.

3.3 Absorption and emission spectra of 10-(4-(Trifluoromethyl)phenyl)-10*H*-phenothiazine (3c)



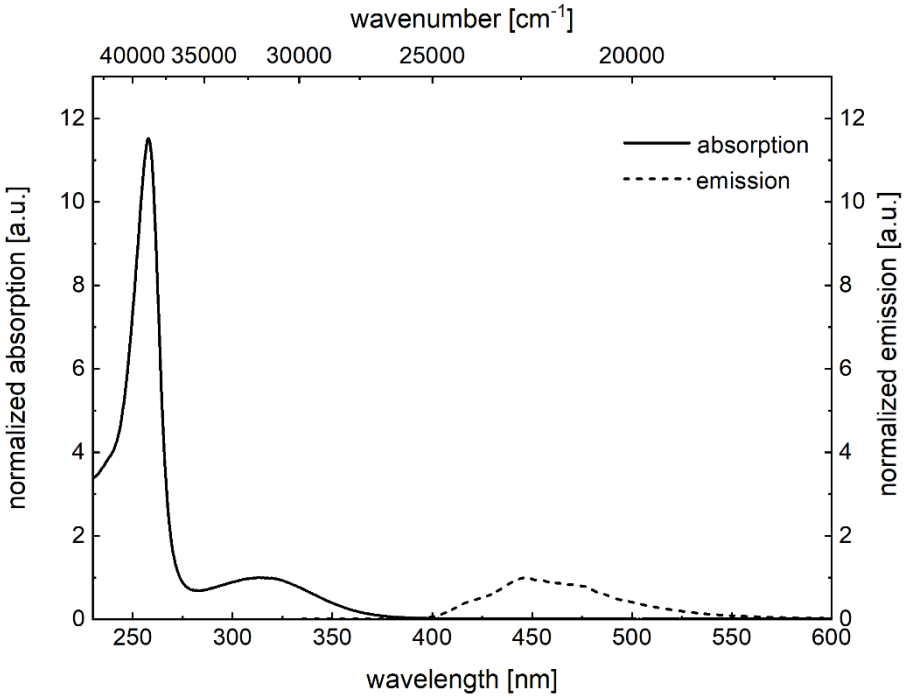
Recorded in dichloromethane, T = 293 K, c(**3**) = 10^{-5} M, $\lambda_{ex} = \lambda_{max,abs}$.

3.4 Absorption and emission spectra of 10-(4-Fluorophenyl)-10*H*-phenothiazine (3d)



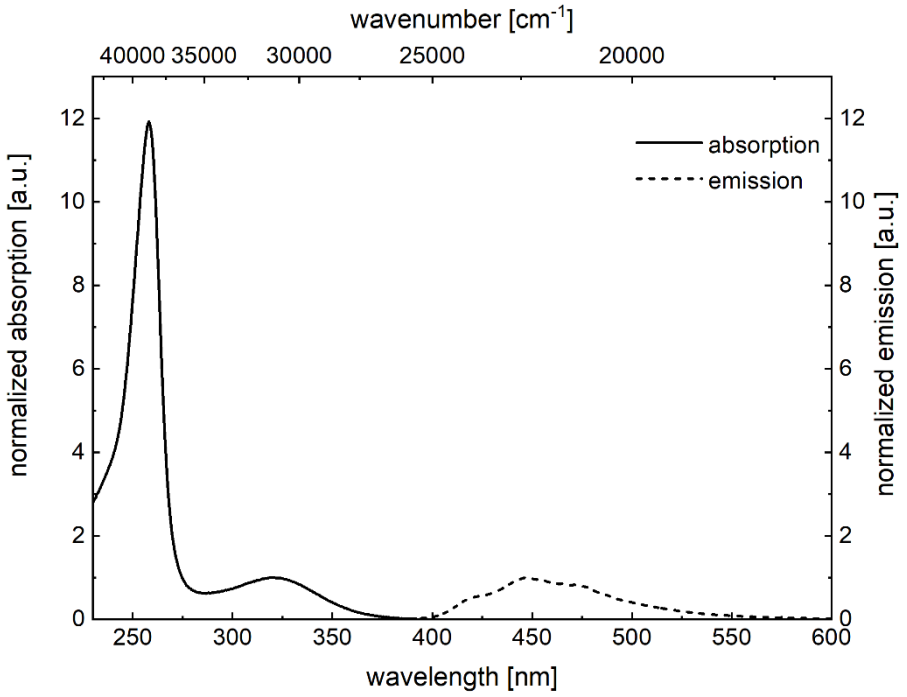
Recorded in dichloromethane, T = 293 K, c(**3**) = 10^{-5} M, $\lambda_{ex} = \lambda_{max,abs}$.

3.5 Absorption and emission spectra of 10-(4-Chlorophenyl)-10*H*-phenothiazine (3e)



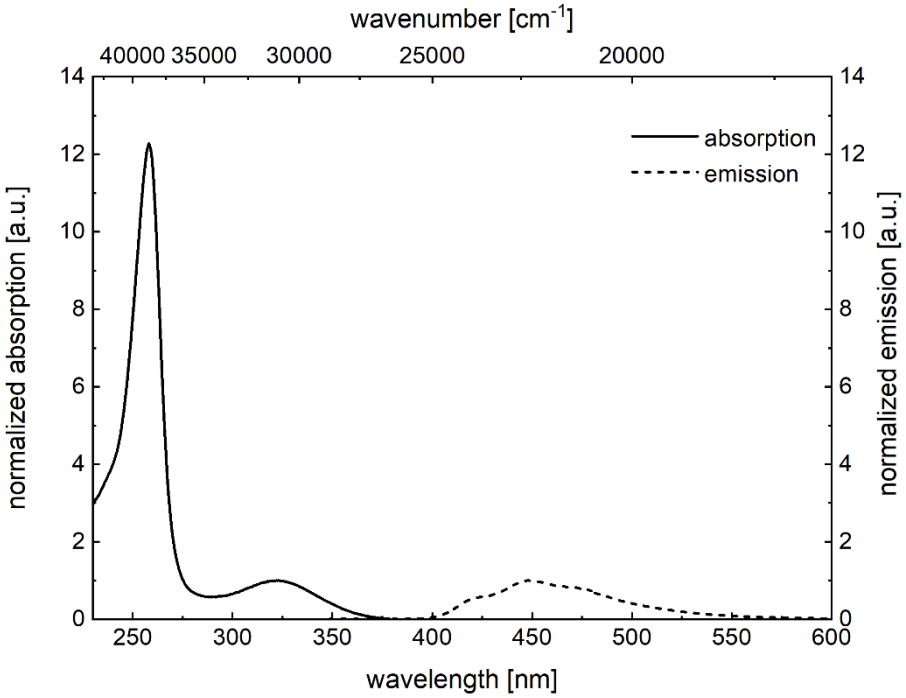
Recorded in dichloromethane, T = 293 K, c(**3**) = 10^{-5} M, $\lambda_{ex} = \lambda_{max,abs}$.

3.6 Absorption and emission spectra of 10-Phenyl-10*H*-phenothiazine (3f)



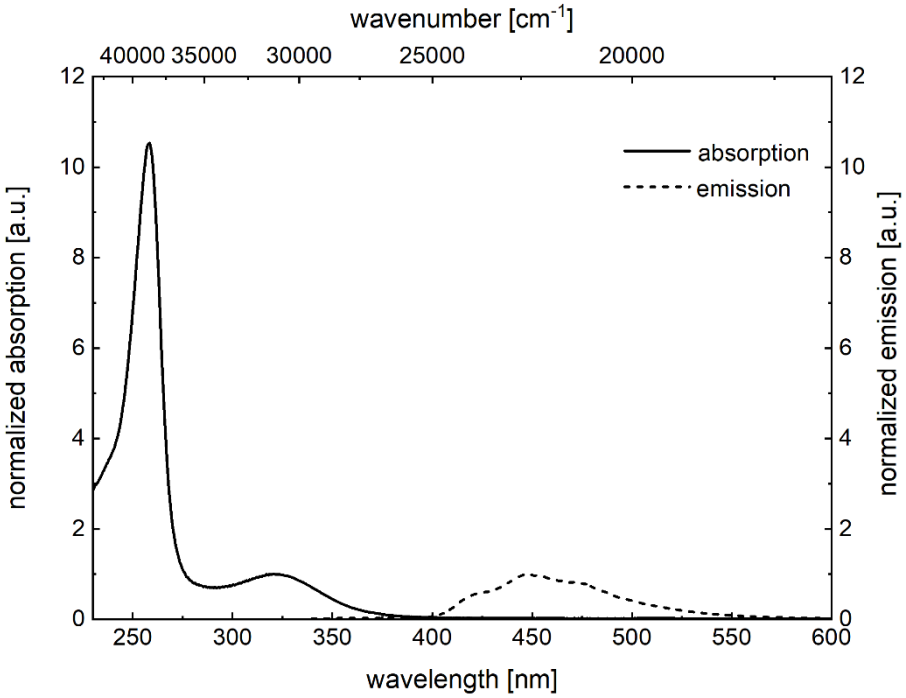
Recorded in dichloromethane, T = 293 K, c(**3**) = 10^{-5} M, $\lambda_{ex} = \lambda_{max,abs}$.

3.7 Absorption and emission spectra of 10-(*p*-Tolyl)-10*H*-phenothiazine (3g)



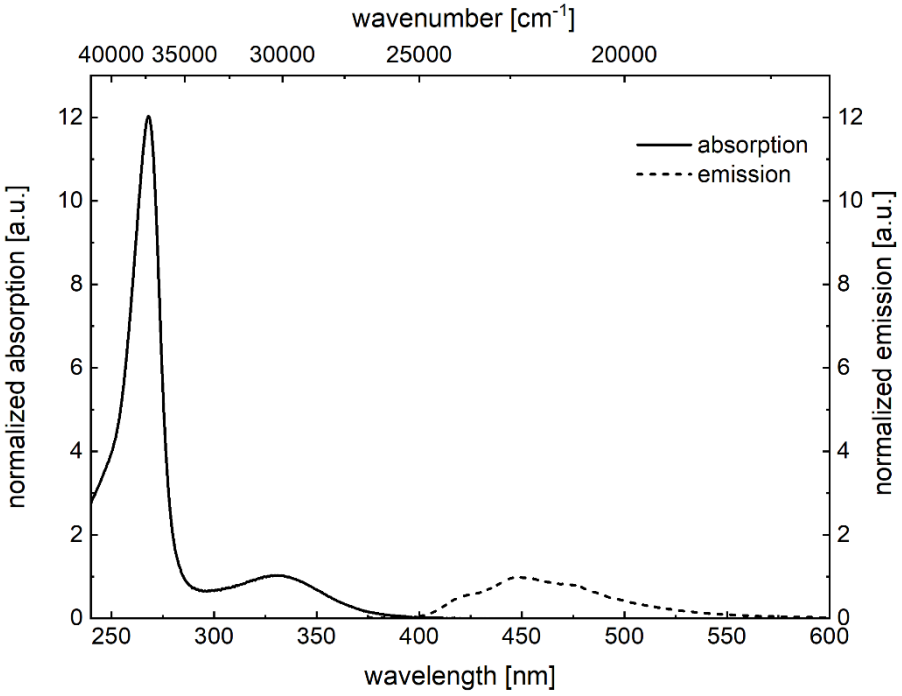
Recorded in dichloromethane, T = 293 K, c(**3**) = 10^{-5} M, $\lambda_{ex} = \lambda_{max,abs}$.

3.8 Absorption and emission spectra of 10-(4-Hexylphenyl)-10*H*-phenothiazine (3h)



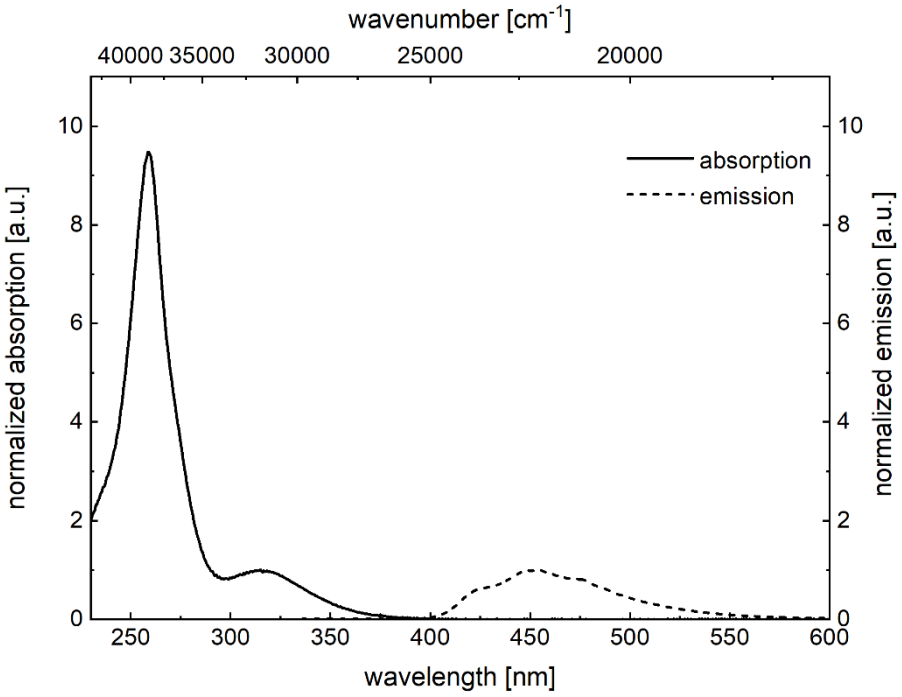
Recorded in dichloromethane, T = 293 K, c(**3**) = 10^{-5} M, $\lambda_{ex} = \lambda_{max,abs}$.

3.9 Absorption and emission spectra of 10-(4-Methoxyphenyl)-10*H*-phenothiazine (3i)



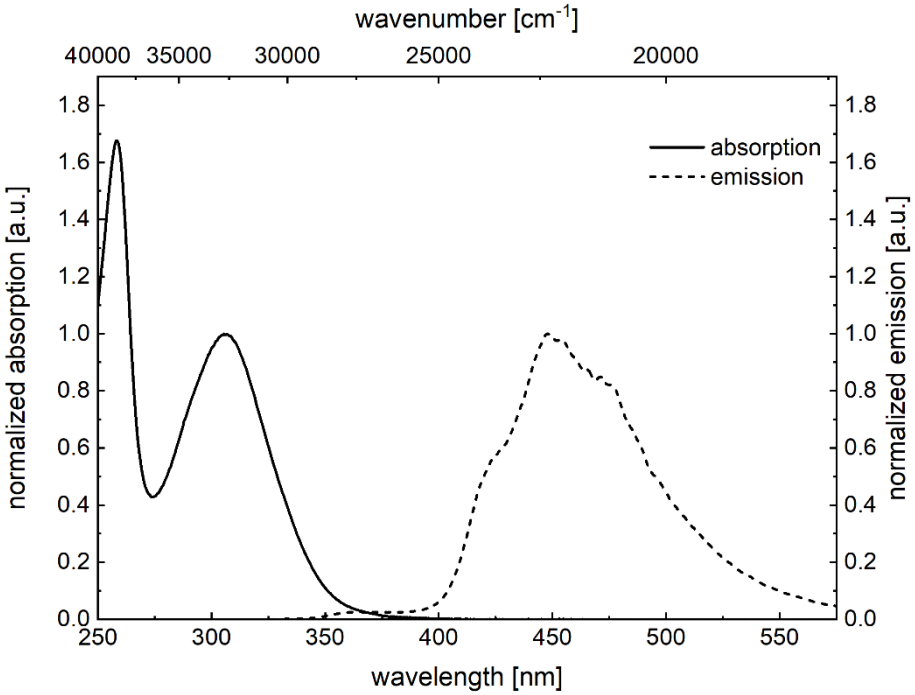
Recorded in dichloromethane, T = 293 K, c(**3**) = 10^{-5} M, $\lambda_{ex} = \lambda_{max,abs}$.

3.10 Absorption and emission spectra of *N*,*N*-Dimethyl-4-(10*H*-phenothiazin-10-yl)aniline (3j)



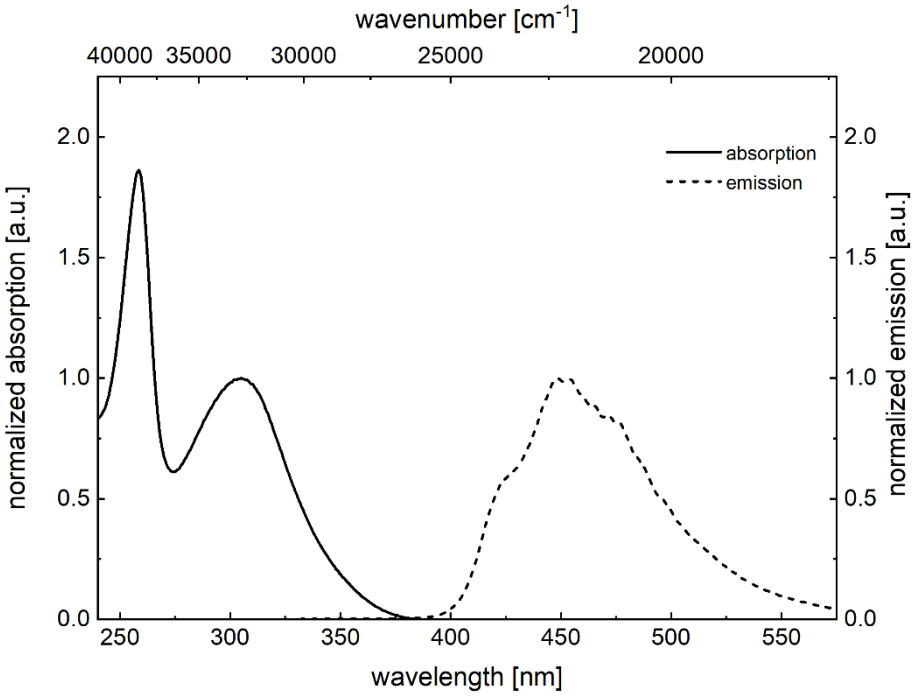
Recorded in dichloromethane, T = 293 K, c(**3**) = 10^{-5} M, $\lambda_{ex} = \lambda_{max,abs}$.

3.11 Absorption and emission spectra of 4-(10*H*-Phenothiazin-10-yl)-*N*,*N*-diphenylaniline (3k)



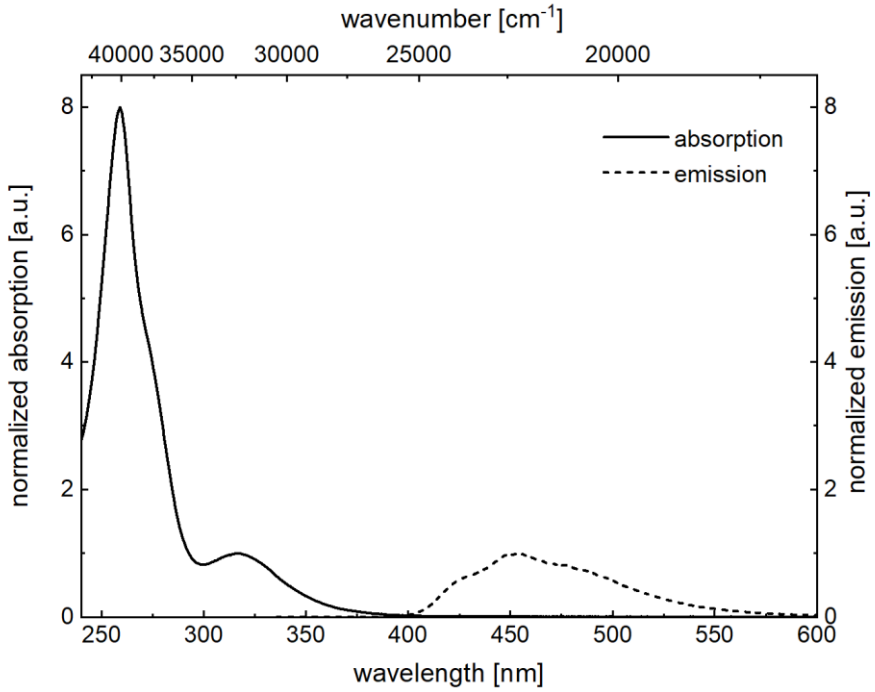
Recorded in dichloromethane, T = 293 K, c(**3**) = 10^{-5} M, $\lambda_{ex} = \lambda_{max,abs}$.

3.12 Absorption and emission spectra of *N*-(4-(10*H*-Phenothiazin-10-yl)phenyl)-4-methoxy-*N*-(4-methoxyphenyl)aniline (3l)



Recorded in dichloromethane, T = 293 K, c(**3**) = 10^{-5} M, $\lambda_{ex} = \lambda_{max,abs}$.

3.13 Absorption and emission spectra of 10-(4-(Pyrrolidin-1-yl)phenyl)-10*H*-phenothiazine (3m)



Recorded in dichloromethane, T = 293 K, c(**3**) = 10^{-5} M, $\lambda_{ex} = \lambda_{max,abs}$.

4 Solvatochromism

solvent	refractive index[1] n_D^{20}	permittivity[1] ε_r	orientation polarizability Δf	$\lambda_{max,abs}$ [a] [nm]	$\lambda_{max,em}$ [a] [nm]	$\Delta\tilde{\nu}$ [b] [cm^{-1}]
cyclohexane	1.4262	2.02	-0.0016497	290	441	11800
toluene	1.4969	2.38	0.013235	293	455	12200
tetrahydrofuran	1.4072	7.58	0.20957	290	478	13500
ethyl acetate	1.3724	6.02	0.19964	289	477	13700
dichloromethane	1.4242	8.93	0.21710	291	499	14400
acetonitrile	1.3441	35.94	0.30457	290	531	15700

[a] recorded in different solvents, T = 293 K, c(**3**) = 10^{-5} M. [b] $\Delta\tilde{\nu} = \frac{1}{\lambda_{max,Abs}} - \frac{1}{\lambda_{max,Em}}$.

5 Hammett correlations

Table S1: Tabular overview of the utilized parameters[2]

	σ_p	σ_I	σ_R	σ_p^+	σ_p^-	$E_0^{0/+1}$ [V]	$\Delta\Delta G_{extra\text{-}intra}$ [kcal/mol][a]
R = NO_2 **3a**	0.78	0.76	0.02	0.79	1.27	0.91	2.89
R = CN **3b**	0.66	0.53	0.13	0.66	1.00	0.86	1.41
R = CF_3 **3c**	0.54	0.42	0.12	0.61	0.65	0.83	0.71
R = F **3d**	0.06	0.52	-0.46	-0.07	-0.03	0.77	-1.31
R = Cl **3e**	0.23	0.47	-0.24	0.11	0.19	0.78	-2.15
R = H **3f**	0.00	0.00	0.00	0.00	0.00	0.72	-1.83
R = Me **3g**	-0.17	-0.04	-0.13	-0.31	0.17	0.71	-2.62
R = OMe **3i**	-0.27	0.27	-0.54	-0.78	-0.26	0.70	-3.26
R = NMe_2 **3j**	-0.83	0.06	-0.89	-1.70	-0.12	0.57	-4.41

[a] Gaussian 09 B3LYP/6-311++G** PCM (CH_2Cl_2).

5.1 Linear correlation between the calculated C-N bond lengths and the Hammett parameters σ_p

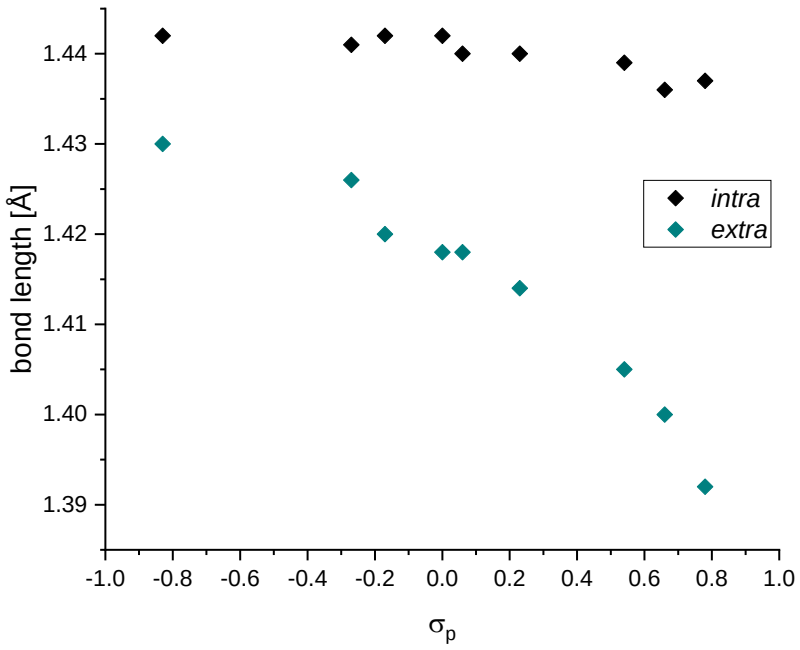


Figure S1: Linear correlation between the bond length (B3LYP/6-311++G**, PCM CH_2Cl_2) and the Hammett parameters σ_p ($\Delta\Delta G_{extra\text{-}intra}$ = 4.49 kcal/mol · σ_p + 1.67 kcal/mol; R^2 = 0.93).

5.2 Linear correlation between the difference of free energy $\Delta\Delta G_{extra\text{-}intra}$ and the Hammett parameters σ

$\Delta\Delta G_{extra\text{-}intra}$ vs. σ_p: $\Delta\Delta G_{extra\text{-}intra}$ = 4.49 kcal/mol · σ_p − 1.67 kcal/mol; R^2 = 0.93

$\Delta\Delta G_{extra\text{-}intra}$ vs. σ_I: $\Delta\Delta G_{extra\text{-}intra}$ = 6.51 kcal/mol · σ_I − 3.34 kcal/mol; R^2 = 0.58

$\Delta\Delta G_{extra\text{-}intra}$ vs. σ_R: $\Delta\Delta G_{extra\text{-}intra}$ = 5.53 kcal/mol · σ_R + 0.05 kcal/mol; R^2 = 0.65

$\Delta\Delta G_{extra\text{-}intra}$ vs. σ_p^+.: $\Delta\Delta G_{extra\text{-}intra}$ = 2.74 kcal/mol · σ_p^+ − 0.96 kcal/mol; R^2 = 0.83

$\Delta\Delta G_{extra\text{-}intra}$ vs. σ_p^-: $\Delta\Delta G_{extra\text{-}intra}$ = 4.26 kcal/mol · σ_p^- − 2.53 kcal/mol; R^2 = 0.91

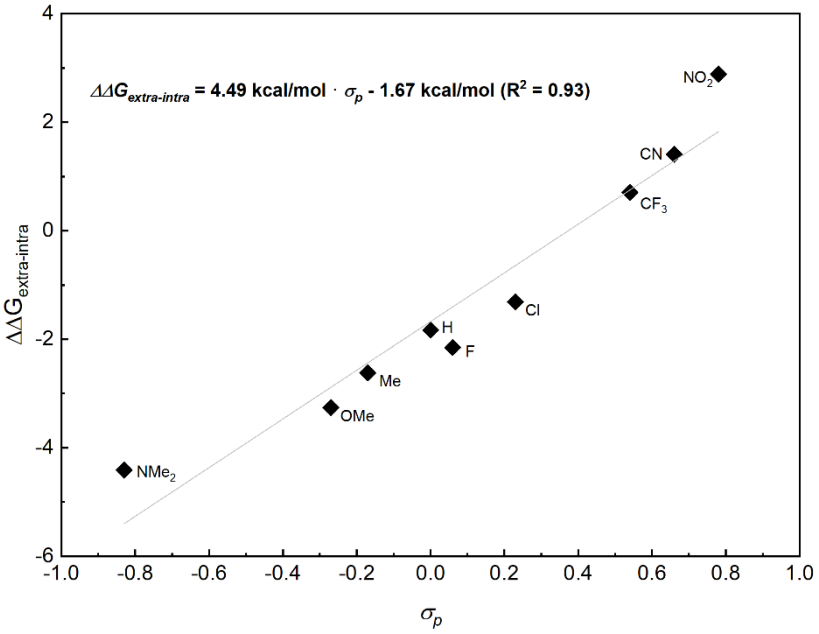


Figure S2: Linear correlation between the difference of DFT-computed free energy $\Delta\Delta G_{extra\text{-}intra}$ (B3LYP/6-311++G**, PCM CH_2Cl_2) and the Hammett parameters σ_p ($\Delta\Delta G_{extra\text{-}intra}$ = 4.49 kcal/mol · σ_p + 1.67 kcal/mol; R^2 = 0.93).

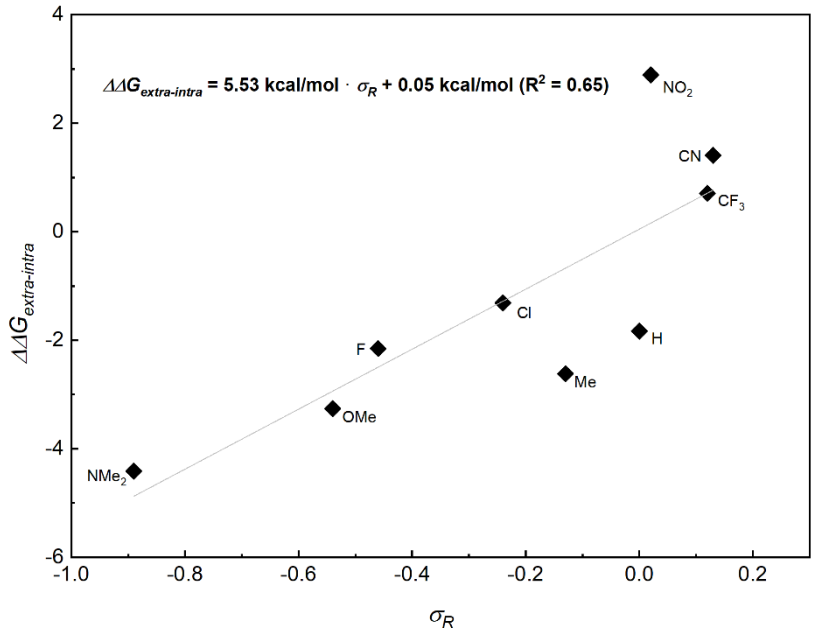


Figure S3: Linear correlation between the difference of DFT-computed free energy $\Delta\Delta G_{extra\text{-}intra}$ (B3LYP/6-311++G**, PCM CH_2Cl_2) and the Hammett parameters σ_I ($\Delta\Delta G_{extra\text{-}intra}$ = 6.51 kcal/mol · σ_I − 3.34 kcal/mol; R^2 = 0.58).

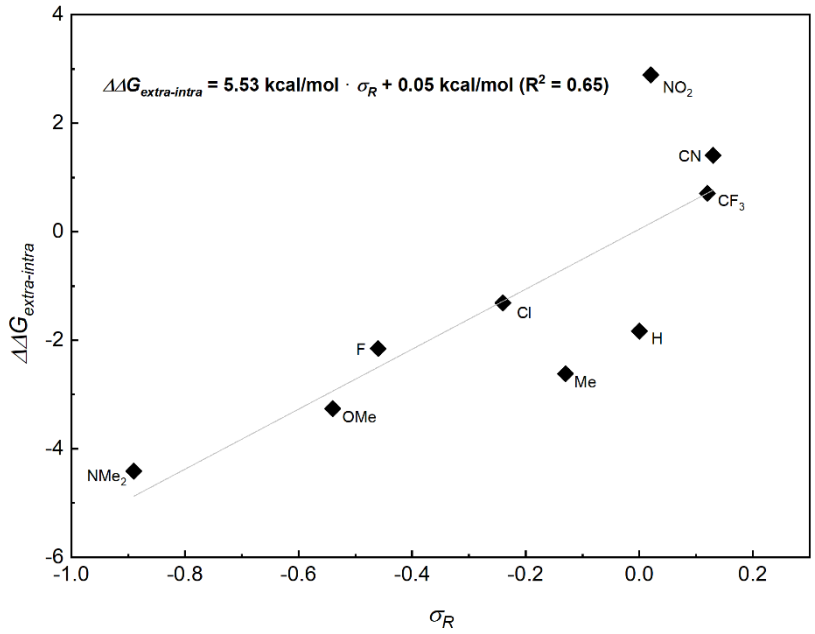


Figure S4: Linear correlation between the difference of DFT-computed free energy $\Delta\Delta G_{extra\text{-}intra}$ (B3LYP/6-311++G**, PCM CH_2Cl_2) and the Hammett parameters σ_R ($\Delta\Delta G_{extra\text{-}intra}$ = 5.53 kcal/mol · σ_R + 0.05 kcal/mol; R^2 = 0.65).

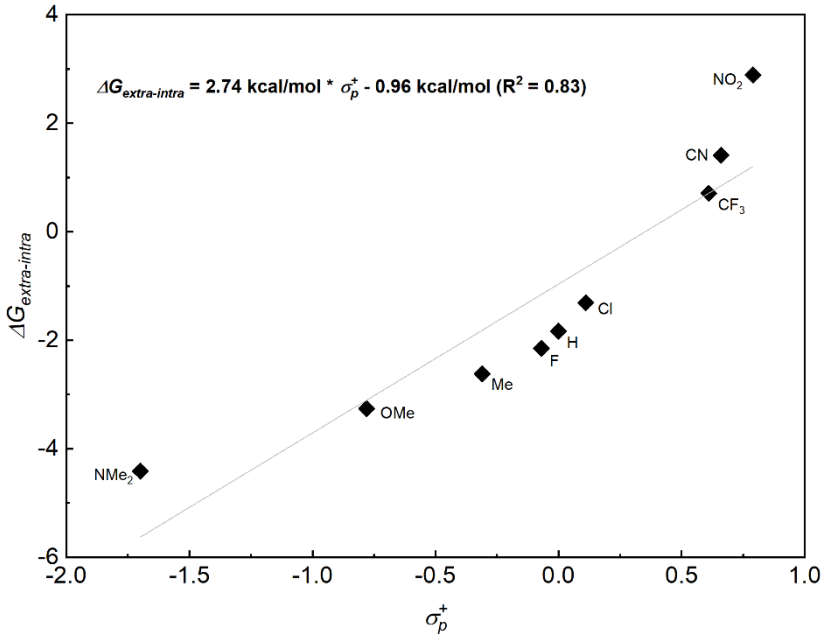


Figure S5: Linear correlation between the difference of DFT-computed free energy $\Delta\Delta G_{extra\text{-}intra}$ (B3LYP/6-311++G**, PCM CH_2Cl_2) and the Hammett parameters σ_p^+ ($\Delta\Delta G_{extra\text{-}intra}$ = 2.74 kcal/mol · σ_p^+ – 0.96 kcal/mol; R^2 = 0.83).

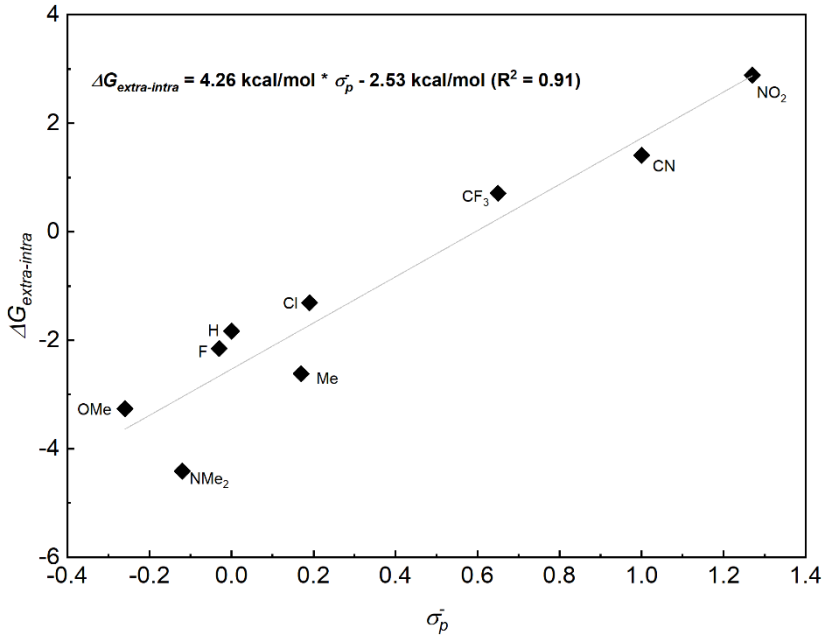


Figure S6: Linear correlation between the difference of DFT-computed free energy $\Delta\Delta G_{extra\text{-}intra}$ (B3LYP/6-311++G**, PCM CH_2Cl_2) and the Hammett parameters σ_p^- ($\Delta\Delta G_{extra\text{-}intra}$ = 4.26 kcal/mol · σ_p^- – 2.53 kcal/mol; R^2 = 0.91).

5.3 Linear correlation between the first oxidation potentials $E_0^{0/+1}$ and the Hammett parameters σ

$E_0^{0/+1}$ vs. σ_p: $E_0^{0/+1}$ = 0.197 V · σ_p + 0.739 V; R^2 = 0.982

$E_0^{0/+1}$ vs. σ_I: $E_0^{0/+1}$ = 0.300 V · σ_I + 0.661 V; R^2 = 0.674

$E_0^{0/+1}$ vs. σ_R: $E_0^{0/+1}$ = 0.233 V · σ_R + 0.812 V; R^2 = 0.640

$E_0^{0/+1}$ vs. σ_p^+: $E_0^{0/+1}$ = 0.123 V · σ_p^+ + 0.770 V; R^2 = 0.924

$E_0^{0/+1}$ vs. σ_p^-: $E_0^{0/+1}$ = 0.161 V · σ_p^- + 0.709 V; R^2 = 0.724

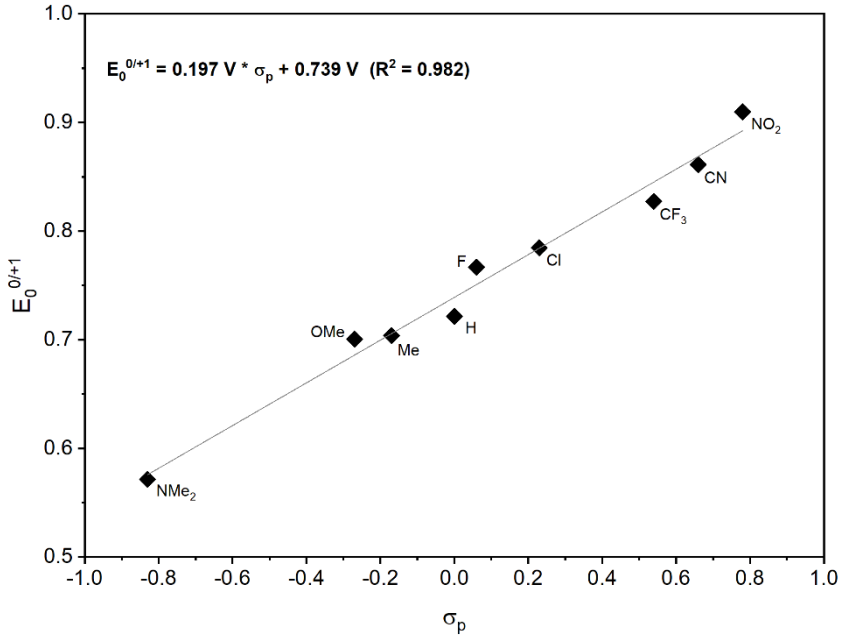


Figure S7: Linear correlation between the first oxidation potentials $E_0^{0/+1}$ and the Hammett parameters σ_p ($E_0^{0/+1}$ = 0.197 V · σ_p + 0.739 V; R^2 = 0.982).

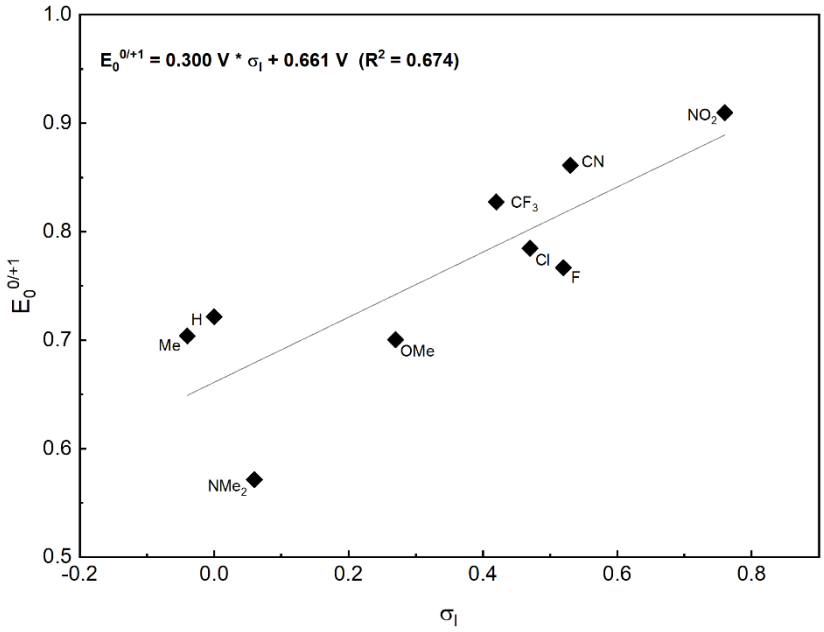


Figure S8: Linear correlation between the first oxidation potentials $E_0^{0/+1}$ and the Hammett parameters σ_I ($E_0^{0/+1}$ = 0.300 V · σ_I + 0.661 V; R^2 = 0.674).

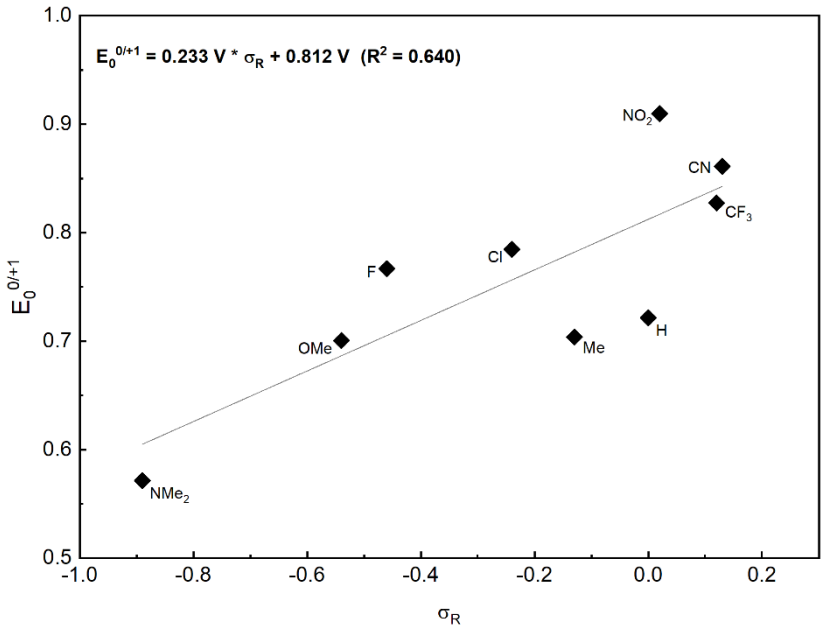


Figure S9: Linear correlation between the first oxidation potentials $E_0^{0/+1}$ and the Hammett parameters σ_R ($E_0^{0/+1}$ = 0.233 V · σ_R + 0.812 V; R^2 = 0.640).

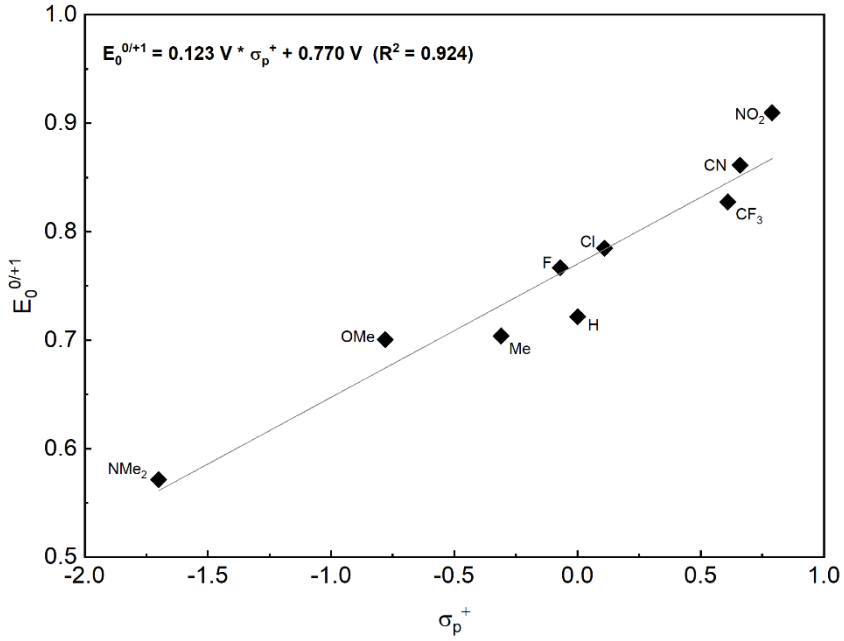


Figure S10: Linear correlation between the first oxidation potentials $E_0^{0/+1}$ and the Hammett parameters σ_p^+ ($E_0^{0/+1}$ = 0.123 V · σ_p^+ + 0.770 V; R^2 = 0.924).

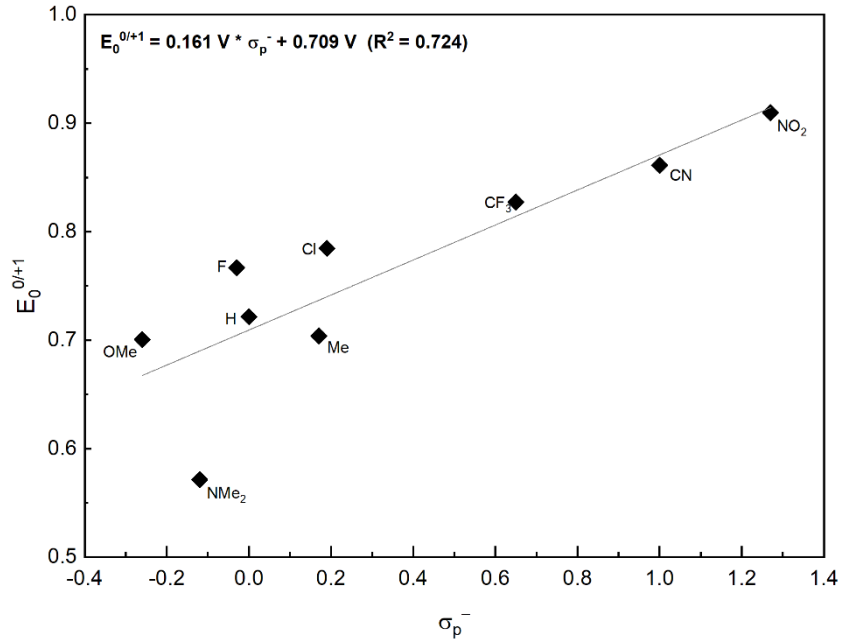


Figure S11: Linear correlation between the first oxidation potentials $E_0^{0/+1}$ and the Hammett parameters σ_p^- ($E_0^{0/+1}$ = 0.161 V · σ_p^- + 0.709 V; R^2 = 0.724).

6 Data of quantum chemical calculations

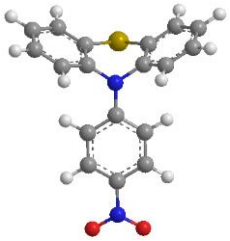
Table S2: TD-DFT calculations on the absorption UV/vis absorption spectra for the *N*-aryl phenothiazines.

R	$\lambda_{max,Abs}$ [a] [nm] (ε [$M^{-1}cm^{-1}$])	$\lambda_{max,calcd}$ [nm]	Oscillator strength	Most dominant contribution	Functional
NO_2	378 (15300)	389	0.4474	HOMO → LUMO (98%)	PBEh1PBE
		342	0.1894	HOMO-1 → LUMO (98%)	
	246 (19300)	247	0.2757	HOMO-1 → LUMO+4 (48%) HOMO → LUMO+5 (30%)	
CN	301 (14800)	307	0.4619	HOMO → LUMO (87%)	PBEh1PBE
	256 (25700)	260	0.172	HOMO → LUMO+4 (72%)	
		251	0.227	HOMO-1 → LUMO+3 (65%)	
CF_3	291 (6520)	298	0.1708	HOMO → LUMO (95%)	PBEh1PBE
		281	0.1185	HOMO → LUMO+2 (45%) HOMO → LUMO+1 (39%)	
	257 (40500)	260	0.0414	HOMO-1 → LUMO (80%)	
		251	0.2163	HOMO → LUMO+3 (44%) HOMO → LUMO+4 (28%)	
Cl	314 (4250)	312	0.086	HOMO → LUMO+3 (96%)	B3LYP
	258 (47600)	264	0.2305	HOMO-1 → LUMO (92%)	
		257	0.0985	HOMO-1 → LUMO+6 (88%)	
F	319 (3570)	322	0.013	HOMO → LUMO+3 (81%)	B3LYP
	258 (44800)	263	0.1764	HOMO → LUMO+7 (58%) HOMO-1 → LUMO (22%)	
		262	0.1481	HOMO-1 → LUMO (69%) HOMO → LUMO+7 (22%)	
		257	0.0803	HOMO → LUMO+6 (88%)	
H	319 (3750)	325	0.010	HOMO → LUMO+1 (87%)	B3LYP
		315	0.036	HOMO → LUMO+3 (85%)	
		314	0.029	HOMO → LUMO+2 (95%)	
	258 (44600)	259	0.413	HOMO-1 → LUMO (85%)	
Me	321 (3720)	318	0.0265	HOMO → LUMO+3 (41%) HOMO → LUMO+1 (28%) HOMO → LUMO+2 (25%)	B3LYP
	258 (46900)	258	0.4605	HOMO-1 → LUMO (83%)	
Hexyl	319 (4620)	314	0.0544	HOMO → LUMO+3 (68%)	B3LYP
	258 (49200)	257	0.4926	HOMO-1 → LUMO (82%)	

OMe	321 (3770)	318	0.0362	HOMO → LUMO+1 (90%)	B3LYP
	258 (44300)	257	0.4679	HOMO-1 → LUMO (83%)	
NMe_2	314 (6530)	313	0.008	HOMO → LUMO (85%)	cam-B3LYP
	259 (59000)	275	0.119	HOMO → LUMO+3 (56%)	
		251	0.246	HOMO-1 → LUMO+1 (56%)	
NPh_2	306 (25600)	312	0.0062	HOMO → LUMO (32%) HOMO → LUMO+3 (31%)	cam-B3LYP
		292	0.5144	HOMO-1 → LUMO+1 (75%)	
	259 (42800)	261	0.0174	HOMO → LUMO+1 (55%)	
$N(4\text{-}MeOPh)_2$	305 (26700)	309	0.0495	HOMO → LUMO (74%)	cam-B3LYP
		291	0.6447	HOMO → LUMO+1 (34%) HOMO → LUMO+3 (25%)	
	258 (49700)	265	0.1005	HOMO → LUMO+15 (27%)	
		254	0.0116	HOMO-1 → LUMO+3 (24%) HOMO-1 → LUMO+1 (23%)	
Pyrrolidin	317 (7680)	314	0.0089	HOMO → LUMO (85%)	cam-B3LYP
	259 (61200)	275	0.1200	HOMO → LUMO+4 (40%)	
		253	0.0247	HOMO-1 → LUMO+1 (77%)	

[a] recorded in CH_2Cl_2, T = 293 K, c(**3**) = 10^{-5} M

6.1 Computed xyz-coordinates (B3LYP/6-311++G IEFPCM CH_2Cl_2) and Excitation energies (PBEh1PBE/6-311++G**) of 10-(4-Nitrophenyl)-10*H*-phenothiazine (3a)**



C	-2.85969	3.52553	-0.21821
C	-1.97629	3.36875	-1.28736
C	-1.22371	2.20313	-1.40641
C	-1.32881	1.20438	-0.43740
C	-2.24607	1.34576	0.61150
C	-3.01178	2.50830	0.72069
N	-0.55313	-0.00009	-0.50786
C	-1.32915	-1.20435	-0.43740
C	-2.24644	-1.34546	0.61150
S	-2.44537	0.00018	1.77164
C	-1.22444	-2.20308	-1.40647
C	-1.97738	-3.36847	-1.28744
C	-2.86078	-3.52502	-0.21825
C	-3.01252	-2.50777	0.72068
C	0.82250	-0.00019	-0.29673
C	1.54313	-1.21275	-0.17781
C	2.90969	-1.21181	0.01995
C	3.59943	-0.00023	0.10925
C	2.90976	1.21138	0.01966
C	1.54320	1.21234	-0.17809
N	5.03136	-0.00024	0.30960
O	5.61595	1.08449	0.39100
O	5.61589	-1.08499	0.39129
H	-3.45079	4.42927	-0.12830
H	-1.88042	4.14798	-2.03392
H	-0.54457	2.06695	-2.23947
H	-3.72751	2.60855	1.52805
H	-0.54532	-2.06707	-2.23958
H	-1.88180	-4.14769	-2.03405
H	-3.45217	-4.42857	-0.12836

H	-3.72827	-2.60781	1.52805
H	1.02743	-2.15972	-0.23020
H	3.44769	-2.14510	0.11123
H	3.44782	2.14465	0.11071
H	1.02754	2.15933	-0.23074

SCF Done: E(RB3LYP) = -1351.46978880 A.U. after 23 cycles
Sum of electronic and zero-point Energies = -1351.210213
Sum of electronic and thermal Energies = -1351.192624
Sum of electronic and thermal Enthalpies = -1351.191680
Sum of electronic and thermal Free Energies = -1351.257472

Excitation energies and oscillator strengths (PBEh1PBE/6-311++G** TD=NStates=15):

Excited State 1: Singlet-A 3.1889 eV 388.80 nm f=0.4474 <S**2>=0.000
83 -> 84 0.70290
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -1350.22156325
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.6229 eV 342.22 nm f=0.1894 <S**2>=0.000
82 -> 84 0.70281

Excited State 3: Singlet-A 3.8521 eV 321.86 nm f=0.0000 <S**2>=0.000
77 -> 84 0.69232

Excited State 4: Singlet-A 4.2842 eV 289.40 nm f=0.0071 <S**2>=0.000
79 -> 84 0.46810
80 -> 84 -0.26021
81 -> 84 -0.16359
82 -> 86 -0.11441
83 -> 86 -0.39891

Excited State 5: Singlet-A 4.3338 eV 286.09 nm f=0.0077 <S**2>=0.000
83 -> 85 0.68679

Excited State 6: Singlet-A 4.4245 eV 280.22 nm f=0.0025 <S**2>=0.000
81 -> 84 0.65118
83 -> 86 -0.22644
83 -> 88 0.10780

Excited State 7: Singlet-A 4.4628 eV 277.81 nm f=0.0221 <S**2>=0.000

81 -> 84 -0.11182
83 -> 88 0.67846

Excited State 8: Singlet-A 4.5110 eV 274.85 nm f=0.0011 <S**2>=0.000
79 -> 84 0.35638
80 -> 84 -0.22559
81 -> 84 0.16402
83 -> 86 0.51478
83 -> 89 -0.11939

Excited State 9: Singlet-A 4.5175 eV 274.45 nm f=0.0042 <S**2>=0.000
74 -> 84 0.66976
78 -> 84 0.16037

Excited State 10: Singlet-A 4.6000 eV 269.53 nm f=0.0283 <S**2>=0.000
82 -> 85 0.25132
83 -> 87 0.64213

Excited State 11: Singlet-A 4.6782 eV 265.03 nm f=0.0015 <S**2>=0.000
79 -> 84 0.32822
80 -> 84 0.60418
83 -> 89 -0.10243

Excited State 12: Singlet-A 4.7910 eV 258.79 nm f=0.0392 <S**2>=0.000
74 -> 84 -0.15919
78 -> 84 0.67018
82 -> 85 -0.11419

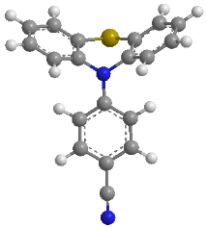
Excited State 13: Singlet-A 4.8739 eV 254.39 nm f=0.0442 <S**2>=0.000
78 -> 84 0.11115
81 -> 88 -0.11787
82 -> 85 0.61887
83 -> 87 -0.25979

Excited State 14: Singlet-A 4.8823 eV 253.94 nm f=0.0000 <S**2>=0.000
79 -> 84 0.17809
82 -> 86 0.28240
82 -> 88 0.42368
83 -> 89 0.39372

Excited State 15: Singlet-A 5.0293 eV 246.52 nm f=0.2757 <S**2>=0.000

82 -> 86	-0.22687
82 -> 88	0.48891
83 -> 89	-0.38697
83 -> 91	-0.11015

6.2 Computed xyz-coordinates (B3LYP/6-311++G IEFPCM CH_2Cl_2) and Excitation energies (PBEh1PBE/6-311++G**) of 4-(10*H*-Phenothiazin-10-yl)benzonitrile (3b)**



C	-2.52346	3.53061	-0.22706
C	-1.62994	3.37547	-1.28798
C	-0.88009	2.20770	-1.40454
C	-0.99545	1.20402	-0.44123
C	-1.92112	1.34668	0.60040
C	-2.68619	2.50999	0.70644
N	-0.22179	-0.00011	-0.51352
C	-0.99588	-1.20398	-0.44120
C	-1.92161	-1.34627	0.60043
S	-2.13070	0.00025	1.75815
C	-0.88103	-2.20765	-1.40457
C	-1.63134	-3.37513	-1.28802
C	-2.52486	-3.52994	-0.22705
C	-2.68715	-2.50927	0.70648
C	1.15640	-0.00026	-0.26930
C	1.87376	1.20855	-0.13619
C	3.23840	1.20668	0.09157
C	3.94699	-0.00038	0.20190
C	3.23825	-1.20738	0.09187
C	1.87362	-1.20915	-0.13590
C	5.35267	-0.00044	0.42849
N	6.49624	-0.00046	0.61260
H	-3.11331	4.43542	-0.13927
H	-1.52466	4.15743	-2.03053
H	-0.19379	2.07268	-2.23200
H	-3.40884	2.60886	1.50788
H	-0.19475	-2.07288	-2.23209
H	-1.52643	-4.15710	-2.03060
H	-3.11508	-4.43451	-0.13926
H	-3.40982	-2.60785	1.50792

H	1.36088	2.15665	-0.20206
H	3.76185	2.14992	0.18989
H	3.76159	-2.15066	0.19043
H	1.36064	-2.15721	-0.20151

SCF Done: E(RB3LYP) = -1239.17071967 A.U. after 22 cycles
Sum of electronic and zero-point Energies = -1238.914703
Sum of electronic and thermal Energies = -1238.897918
Sum of electronic and thermal Enthalpies = -1238.896974
Sum of electronic and thermal Free Energies = -1238.960139

Excitation energies and oscillator strengths (PBEh1PBE/6-311++G** TD=NStates=10):

Excited State 1: Singlet-A 4.0390 eV 306.96 nm f=0.4619 <S**2>=0.000
78 -> 79 0.65956
78 -> 80 0.21422
78 -> 83 0.10626
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -1237.98097874
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 4.3214 eV 286.91 nm f=0.0001 <S**2>=0.000
78 -> 81 0.66594
78 -> 82 -0.15978

Excited State 3: Singlet-A 4.3691 eV 283.78 nm f=0.1159 <S**2>=0.000
77 -> 79 0.13122
78 -> 79 -0.17599
78 -> 80 0.62730
78 -> 83 -0.16366

Excited State 4: Singlet-A 4.3743 eV 283.44 nm f=0.0086 <S**2>=0.000
78 -> 81 0.16470
78 -> 82 0.67259

Excited State 5: Singlet-A 4.5890 eV 270.18 nm f=0.0066 <S**2>=0.000
77 -> 79 0.57801
77 -> 80 0.12531
78 -> 79 0.11958
78 -> 80 -0.19518
78 -> 83 -0.29214

Excited State 6: Singlet-A 4.7656 eV 260.16 nm f=0.1718 <S**2>=0.000

76 -> 82	0.10361
77 -> 79	0.31187
78 -> 79	-0.10407
78 -> 83	0.59807

Excited State 7: Singlet-A 4.7754 eV 259.63 nm f=0.0053 <S**2>=0.000

73 -> 79	-0.16354
77 -> 81	0.25814
77 -> 82	-0.30778
78 -> 84	0.52730

Excited State 8: Singlet-A 4.9237 eV 251.81 nm f=0.0903 <S**2>=0.000

77 -> 79	-0.16031
77 -> 80	0.67503

Excited State 9: Singlet-A 4.9490 eV 250.52 nm f=0.2268 <S**2>=0.000

77 -> 82	0.57262
78 -> 84	0.29959
78 -> 86	0.10637

Excited State 10: Singlet-A 5.0253 eV 246.72 nm f=0.0055 <S**2>=0.000

77 -> 81	0.61831
78 -> 84	-0.30307

Computed xyz-coordinates of S_1 state (B3LYP/6-311G* IEFPCM CH_2Cl_2) and Excitation energies ($S_0^* \rightarrow S_1$) (PBEh1PBE/6-311++G) of 4-(10*H*-Phenothiazin-10-yl)benzonitrile (3b)**

C	1.86411	1.36057	0.04467
C	0.44941	1.23089	0.03284
N	-0.20430	-0.00001	0.02656
C	0.44946	-1.23087	0.03283
C	1.86417	-1.36049	0.04467
S	2.94927	0.00006	0.05075
C	-0.31254	-2.42352	0.02745
C	0.29844	-3.65908	0.03395
C	1.69796	-3.77052	0.04618
C	2.46950	-2.62678	0.05133
C	2.46939	2.62689	0.05134

C	1.69780	3.77060	0.04619
C	0.29828	3.65909	0.03396
C	-0.31265	2.42351	0.02746
C	-1.65438	-0.00004	0.01445
C	-2.37706	-0.00005	1.23698
C	-3.74774	-0.00008	1.23182
C	-4.48999	-0.00009	-0.00892
C	-3.72738	-0.00008	-1.23717
C	-2.35677	-0.00005	-1.21989
C	-5.88330	-0.00012	-0.02038
N	-7.05667	-0.00015	-0.03013
H	-1.38892	-2.35056	0.01826
H	-0.31557	-4.55188	0.02961
H	2.17232	-4.74436	0.05152
H	3.55163	-2.69516	0.06072
H	3.55151	2.69531	0.06073
H	2.17212	4.74445	0.05154
H	-0.31577	4.55187	0.02963
H	-1.38902	2.35050	0.01826
H	-1.83786	-0.00004	2.17928
H	-4.28910	-0.00009	2.17163
H	-4.25328	-0.00009	-2.18577
H	-1.80210	-0.00004	-2.15318

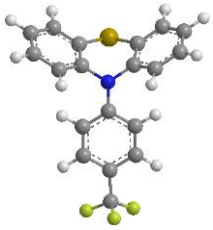
SCF Done: E(RB3LYP) = -1239.12180929 A.U. after 8 cycles

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.1681 eV 571.85 nm f=0.0000 <S**2>=0.000

78 -> 79 0.70259

6.3 Computed xyz-coordinates (B3LYP/6-311++G IEFPCM CH_2Cl_2) and Excitation energies (PBEh1PBE/6-311++G**) of 10-(4-(Trifluoromethyl)phenyl)-10*H*-phenothiazine (3c)**



C	-3.16795	-3.54065	-0.17493
C	-2.32250	-3.38324	-1.27426
C	-1.58592	-2.21107	-1.42656
C	-1.66488	-1.20437	-0.46253
C	-2.54194	-1.35134	0.62000
C	-3.29520	-2.51853	0.76255
N	-0.90029	0.00184	-0.57442
C	-1.67242	1.20313	-0.46052
C	-2.54990	1.34278	0.62275
S	-2.70298	-0.00594	1.78646
C	-1.60055	2.21183	-1.42300
C	-2.34418	3.37924	-1.26817
C	-3.18960	3.52969	-0.16788
C	-3.31005	2.50515	0.76785
C	0.48769	0.00593	-0.35416
C	1.20429	1.21365	-0.23934
C	2.57630	1.21252	-0.03239
C	3.28022	0.01265	0.07691
C	2.57927	-1.19167	-0.02157
C	1.20870	-1.19949	-0.22931
C	4.76299	0.00560	0.24650
F	5.23943	1.16340	0.76482
F	5.19159	-0.99369	1.06093
F	5.42937	-0.17566	-0.93437
H	-3.74812	-4.44860	-0.05913
H	-2.24473	-4.16697	-2.01839
H	-0.93624	-2.07421	-2.28281
H	-3.98072	-2.61978	1.59572
H	-0.95108	2.08027	-2.28022
H	-2.27185	4.16463	-2.01109

H	-3.77513	4.43393	-0.05002
H	-3.99573	2.60074	1.60156
H	0.69013	2.16149	-0.30003
H	3.09526	2.15888	0.05517
H	3.10083	-2.13640	0.07484
H	0.69721	-2.14928	-0.28214

SCF Done: E(RB3LYP) = -1484.04912436 A.U. after 11 cycles
Sum of electronic and zero-point Energies = -1483.787766
Sum of electronic and thermal Energies = -1483.769032
Sum of electronic and thermal Enthalpies = -1483.768088
Sum of electronic and thermal Free Energies = -1483.837398

Excitation energies and oscillator strengths (PBEh1PBE/6-311++G** TD=NStates=10):

Excited State 1: Singlet-A 4.1582 eV 298.17 nm f=0.1708 <S**2>=0.000
88 -> 89 0.68867
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -1482.66733619
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 4.3415 eV 285.58 nm f=0.0004 <S**2>=0.000
88 -> 90 0.43954
88 -> 91 -0.40604
88 -> 92 0.33734

Excited State 3: Singlet-A 4.3540 eV 284.76 nm f=0.0085 <S**2>=0.000
88 -> 90 -0.23790
88 -> 91 0.24674
88 -> 92 0.60534

Excited State 4: Singlet-A 4.4132 eV 280.94 nm f=0.1185 <S**2>=0.000
87 -> 89 0.19786
88 -> 89 0.10108
88 -> 90 0.44310
88 -> 91 0.47598
88 -> 93 -0.10645

Excited State 5: Singlet-A 4.7708 eV 259.88 nm f=0.0414 <S**2>=0.000

87 -> 89 0.63267

88 -> 90 -0.15772

88 -> 91 -0.14818

Excited State 6: Singlet-A 4.7968 eV 258.47 nm f=0.0046 <S**2>=0.000

84 -> 89 -0.12167

87 -> 90 0.13731

87 -> 91 -0.14428

87 -> 92 0.35067

88 -> 94 0.53025

Excited State 7: Singlet-A 4.9483 eV 250.56 nm f=0.2163 <S**2>=0.000

87 -> 91 0.11164

87 -> 92 0.47166

88 -> 93 -0.37265

88 -> 94 -0.25350

Excited State 8: Singlet-A 4.9554 eV 250.20 nm f=0.1798 <S**2>=0.000

87 -> 90 -0.14043

87 -> 92 0.28491

88 -> 93 0.54956

88 -> 94 -0.20934

Excited State 9: Singlet-A 5.0246 eV 246.75 nm f=0.0959 <S**2>=0.000

87 -> 90 0.57358

87 -> 91 0.36487

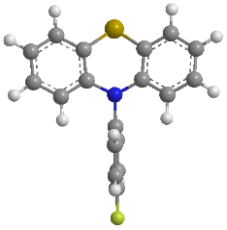
Excited State 10: Singlet-A 5.0451 eV 245.75 nm f=0.0113 <S**2>=0.000

87 -> 90 -0.31530

87 -> 91 0.54965

88 -> 94 0.26507

6.4 Computed xyz-coordinates (B3LYP/6-311++G IEFPCM CH_2Cl_2) and Excitation energies (B3LYP/6-311++G**) of 10-(4-Fluorophenyl)-10*H*-phenothiazine (3d)**



C	2.09178	3.67975	-0.47597
C	0.72825	3.58400	-0.73813
C	0.05495	2.37578	-0.56526
C	0.72534	1.23569	-0.09793
C	2.09616	1.35452	0.19682
C	2.77301	2.55415	-0.01648
N	0.05367	-0.00005	0.09336
C	0.72555	-1.23567	-0.09802
C	2.09639	-1.35427	0.19674
S	2.95749	0.00018	0.96990
C	0.05539	-2.37586	-0.56543
C	0.72892	-3.58395	-0.73836
C	2.09245	-3.67947	-0.47619
C	2.77347	-2.55376	-0.01663
C	-1.38626	-0.00012	0.10966
C	-2.04086	-0.00035	1.34180
C	-3.43321	-0.00041	1.40238
C	-4.14202	-0.00021	0.21218
C	-3.52355	0.00005	-1.02848
C	-2.13133	0.00010	-1.07277
F	-5.50067	-0.00025	0.26214
H	2.62101	4.61385	-0.62077
H	0.17685	4.44804	-1.09065
H	-1.00196	2.32611	-0.78542
H	3.83357	2.60743	0.20210
H	-1.00152	-2.32640	-0.78559
H	0.17768	-4.44807	-1.09093
H	2.62186	-4.61346	-0.62103
H	3.83403	-2.60686	0.20196
H	-1.45647	-0.00049	2.25389

H	-3.95840	-0.00059	2.34912
H	-4.11833	0.00021	-1.93313
H	-1.62446	0.00031	-2.03031

SCF Done: E(RB3LYP) = -1246.16698116 A.U. after 22 cycles
Sum of electronic and zero-point Energies = -1245.918189
Sum of electronic and thermal Energies = -1245.902257
Sum of electronic and thermal Enthalpies = -1245.901313
Sum of electronic and thermal Free Energies = -1245.962717

Excitation energies and oscillator strengths (B3LYP/6-311++G** TD=NStates=10):

Excited State 1: Singlet-A 3.4980 eV 354.44 nm f=0.0004 <S**2>=0.000
76 -> 77 0.66931
76 -> 78 -0.17272
76 -> 79 -0.12075
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -1246.03843117
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.7935 eV 326.83 nm f=0.0119 <S**2>=0.000
76 -> 77 0.20751
76 -> 78 0.62013
76 -> 79 0.24864

Excited State 3: Singlet-A 3.8538 eV 321.72 nm f=0.0130 <S**2>=0.000
76 -> 78 -0.27863
76 -> 79 0.63642

Excited State 4: Singlet-A 3.9667 eV 312.56 nm f=0.0289 <S**2>=0.000
76 -> 80 0.69160

Excited State 5: Singlet-A 4.1909 eV 295.84 nm f=0.0972 <S**2>=0.000
75 -> 77 0.11804
75 -> 79 -0.13100
76 -> 81 0.67380

Excited State 6: Singlet-A 4.6397 eV 267.23 nm f=0.0051 <S**2>=0.000
76 -> 82 0.67196
76 -> 85 0.14264

Excited State 7: Singlet-A 4.7232 eV 262.50 nm f=0.1764 <S**2>=0.000

75 -> 77	0.33473
75 -> 79	-0.10120
76 -> 84	0.54332
76 -> 88	0.19173
76 -> 90	0.10819

Excited State 8: Singlet-A 4.7380 eV 261.68 nm f=0.1481 <S**2>=0.000

75 -> 77	0.58989
76 -> 81	-0.10199
76 -> 84	-0.33223
76 -> 88	-0.10391

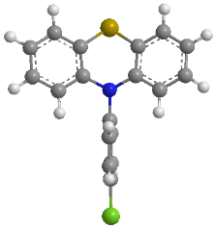
Excited State 9: Singlet-A 4.8324 eV 256.57 nm f=0.0803 <S**2>=0.000

75 -> 80	0.13476
76 -> 82	0.10152
76 -> 83	0.66215

Excited State 10: Singlet-A 4.9521 eV 250.37 nm f=0.1705 <S**2>=0.000

75 -> 78	0.65456
75 -> 79	0.16046
76 -> 81	0.10057
76 -> 84	0.11224

6.5 Computed xyz-coordinates (B3LYP/6-311++G IEFPCM CH_2Cl_2) and Excitation energies (B3LYP/6-311++G**) of 10-(4-Chlorophenyl)-10*H*-phenothiazine (3e)**



C	-2.41793	-3.67886	-0.46415
C	-1.05754	-3.58344	-0.74202
C	-0.38187	-2.37555	-0.57613
C	-1.04664	-1.23593	-0.10000
C	-2.41393	-1.35421	0.21049
C	-3.09354	-2.55347	0.00409
N	-0.37306	-0.00006	0.08529
C	-1.04637	1.23594	-0.09995
C	-2.41364	1.35452	0.21053
S	-3.26559	0.00024	0.99403
C	-0.38133	2.37538	-0.57608
C	-1.05671	3.58344	-0.74195
C	-2.41708	3.67917	-0.46408
C	-3.09296	2.55394	0.00413
C	1.06665	-0.00014	0.08418
C	1.73706	-0.00032	1.30685
C	3.12992	-0.00036	1.34945
C	3.83985	-0.00019	0.15348
C	3.19053	0.00004	-1.07755
C	1.79812	0.00007	-1.10591
Cl	5.60125	-0.00022	0.19618
H	-2.94905	-4.61271	-0.60349
H	-0.51056	-4.44738	-1.10158
H	0.67243	-2.32632	-0.80858
H	-4.15153	-2.60659	0.23476
H	0.67297	2.32589	-0.80853
H	-0.50953	4.44725	-1.10150
H	-2.94799	4.61314	-0.60341
H	-4.15094	2.60730	0.23479
H	1.16569	-0.00045	2.22730

H	3.65125	-0.00052	2.29793
H	3.75960	0.00020	-1.99818
H	1.28167	0.00027	-2.05848

SCF Done: E(RB3LYP) = -1606.52070568 A.U. after 18 cycles
Sum of electronic and zero-point Energies = -1606.273236
Sum of electronic and thermal Energies = -1606.256903
Sum of electronic and thermal Enthalpies = -1606.255959
Sum of electronic and thermal Free Energies = -1606.318684

Excitation energies and oscillator strengths (B3LYP/6-311++G** TD=NStates=10):

Excited State 1: Singlet-A 3.4700 eV 357.30 nm f=0.0002 <S**2>=0.000
80 -> 81 0.68317
80 -> 83 -0.15911
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -1606.39318586
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.6695 eV 337.88 nm f=0.0006 <S**2>=0.000
80 -> 82 0.67683
80 -> 83 -0.18024

Excited State 3: Singlet-A 3.8049 eV 325.86 nm f=0.0194 <S**2>=0.000
80 -> 81 0.15944
80 -> 82 0.18378
80 -> 83 0.65259

Excited State 4: Singlet-A 3.9707 eV 312.25 nm f=0.0281 <S**2>=0.000
80 -> 84 0.69146

Excited State 5: Singlet-A 4.1816 eV 296.50 nm f=0.1000 <S**2>=0.000
79 -> 81 0.11839
79 -> 83 -0.15928
80 -> 85 0.67243

Excited State 6: Singlet-A 4.6105 eV 268.92 nm f=0.0039 <S**2>=0.000
80 -> 86 0.67806
80 -> 90 -0.11716

Excited State 7: Singlet-A 4.6928 eV 264.20 nm f=0.2305 <S**2>=0.000

79 -> 81 0.67768

80 -> 85 -0.11772

Excited State 8: Singlet-A 4.7338 eV 261.91 nm f=0.0331 <S**2>=0.000

79 -> 83 -0.13892

80 -> 88 0.63004

80 -> 93 -0.22023

80 -> 95 0.12307

Excited State 9: Singlet-A 4.8233 eV 257.06 nm f=0.0354 <S**2>=0.000

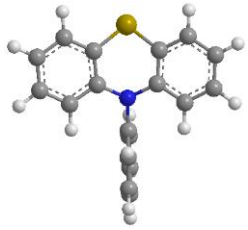
79 -> 82 0.69035

Excited State 10: Singlet-A 4.8310 eV 256.64 nm f=0.0985 <S**2>=0.000

79 -> 84 0.13239

80 -> 87 0.66228

6.6 Computed xyz-coordinates (B3LYP/6-311++G IEFPCM CH_2Cl_2) and Excitation energies (B3LYP/6-311++G**) of 10-Phenyl-10*H*-phenothiazine (3f)**



C	1.77638	-3.68054	-0.49220
C	0.40727	-3.58497	-0.72385
C	-0.26210	-2.37650	-0.53842
C	0.41824	-1.23510	-0.08803
C	1.79541	-1.35418	0.17671
C	2.46745	-2.55406	-0.04976
N	-0.24937	-0.00010	0.11511
C	0.41777	1.23515	-0.08800
C	1.79489	1.35477	0.17674
S	2.67326	0.00046	0.93067
C	-0.26303	2.37628	-0.53840
C	0.40586	3.58501	-0.72382
C	1.77493	3.68113	-0.49215
C	2.46646	2.55492	-0.04972
C	-1.69130	-0.00031	0.15527
C	-2.45302	-0.00026	-1.01601
C	-3.84487	-0.00044	-0.94036
C	-4.47876	-0.00065	0.30260
C	-3.71743	-0.00066	1.47078
C	-2.32457	-0.00048	1.39803
H	2.30228	-4.61491	-0.64719
H	-0.15186	-4.44965	-1.06252
H	-1.32351	-2.32602	-0.73546
H	3.53260	-2.60688	0.14553
H	-1.32442	2.32535	-0.73546
H	-0.15361	4.44947	-1.06250
H	2.30046	4.61571	-0.64714
H	3.53158	2.60816	0.14558
H	-1.95689	-0.00008	-1.97973
H	-4.43252	-0.00041	-1.85122

H	-5.56126	-0.00078	0.35949
H	-4.20490	-0.00081	2.43894
H	-1.72204	-0.00049	2.29890

SCF Done: E(RB3LYP) = -1146.89843675 A.U. after 24 cycles

Excitation energies and oscillator strengths (B3LYP/6-311++G** TD=NStates=10):

Excited State 1: Singlet-A 3.5199 eV 352.24 nm f=0.0015 <S**2>=0.000
72 -> 73 0.68561
72 -> 76 -0.13151
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -1146.76908360
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.8120 eV 325.25 nm f=0.0102 <S**2>=0.000
72 -> 74 0.65810
72 -> 76 -0.20768

Excited State 3: Singlet-A 3.9345 eV 315.12 nm f=0.0358 <S**2>=0.000
71 -> 73 -0.10052
72 -> 73 0.10564
72 -> 74 0.22864
72 -> 76 0.64748

Excited State 4: Singlet-A 3.9531 eV 313.64 nm f=0.0294 <S**2>=0.000
72 -> 75 0.69193

Excited State 5: Singlet-A 4.2173 eV 293.99 nm f=0.0802 <S**2>=0.000
71 -> 73 -0.12389
71 -> 76 0.11482
72 -> 77 0.67590

Excited State 6: Singlet-A 4.6013 eV 269.45 nm f=0.0038 <S**2>=0.000
72 -> 78 0.66396
72 -> 79 -0.11001
72 -> 81 -0.16488

Excited State 7: Singlet-A 4.7040 eV 263.57 nm f=0.0576 <S**2>=0.000

71 -> 73	-0.10597
71 -> 76	0.10050
72 -> 80	0.63002
72 -> 84	-0.20954
72 -> 86	0.12968

Excited State 8: Singlet-A 4.7963 eV 258.50 nm f=0.4128 <S**2>=0.000

71 -> 73	0.65451
72 -> 76	0.10635
72 -> 77	0.13528
72 -> 80	0.13329

Excited State 9: Singlet-A 4.8221 eV 257.12 nm f=0.0783 <S**2>=0.000

71 -> 75	-0.12715
72 -> 78	0.12629
72 -> 79	0.65718

Excited State 10: Singlet-A 4.9491 eV 250.52 nm f=0.0196 <S**2>=0.000

71 -> 75	0.10409
72 -> 78	0.17352
72 -> 81	0.64411
72 -> 82	-0.15355

Computed xyz-coordinates of S_1 state (B3LYP/6-311G* IEFPCM CH_2Cl_2) and Excitation energies ($S_0^* \rightarrow S_1$) (B3LYP/6-311++G) of 10-Phenyl-10*H*-phenothiazine (3f)**

C	1.84230	1.35553	0.12095
C	0.39728	1.23957	0.02757
N	-0.23428	-0.00000	0.01484
C	0.39733	-1.23955	0.02757
C	1.84235	-1.35545	0.12095
S	2.85228	0.00006	0.46497
C	-0.34653	-2.44353	-0.04628
C	0.26796	-3.67587	-0.06633
C	1.69105	-3.77771	-0.00916
C	2.44477	-2.63558	0.09674
C	2.44466	2.63568	0.09674
C	1.69089	3.77779	-0.00916

C	0.26780	3.67589	-0.06631
C	-0.34664	2.44351	-0.04626
C	-1.68284	-0.00004	0.02063
C	-2.35686	-0.00006	1.23756
C	-3.75332	-0.00009	1.24227
C	-4.45546	-0.00010	0.03594
C	-3.76842	-0.00007	-1.17670
C	-2.37081	-0.00004	-1.18930
H	-1.42534	-2.39406	-0.10360
H	-0.33920	-4.57167	-0.12981
H	2.17365	-4.74760	-0.05139
H	3.52747	-2.69858	0.15786
H	3.52735	2.69874	0.15784
H	2.17345	4.74770	-0.05139
H	-0.33940	4.57166	-0.12979
H	-1.42544	2.39400	-0.10358
H	-1.79467	-0.00005	2.16457
H	-4.28803	-0.00010	2.18572
H	-5.54037	-0.00012	0.04247
H	-4.31430	-0.00008	-2.11380
H	-1.81940	-0.00003	-2.12261

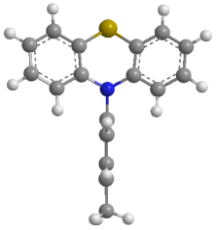
SCF Done: E(RB3LYP) = -1146.85305843   A.U. after   7 cycles

Excitation energies and oscillator strengths:

Excited State   1:   Singlet-A   2.6874 eV 461.35 nm f=0.0001 <S**2>=0.000

72 -> 73   0.70008

6.7 Computed xyz-coordinates (B3LYP/6-311++G IEFPCM CH_2Cl_2) and Excitation energies (B3LYP/6-311++G**) of 10-(*p*-Tolyl)-10*H*-phenothiazine (3g)**



C	2.12471	-3.67584	-0.47282
C	0.75977	-3.58365	-0.72962
C	0.08403	-2.37697	-0.55642
C	0.75278	-1.23355	-0.09363
C	2.12525	-1.34940	0.19633
C	2.80449	-2.54757	-0.01760
N	0.07760	-0.00090	0.09616
C	0.74579	1.23555	-0.09379
C	2.11753	1.35922	0.19639
S	2.98544	0.00736	0.96671
C	0.07061	2.37510	-0.55680
C	0.73944	3.58566	-0.72979
C	2.10374	3.68569	-0.47255
C	2.78990	2.56130	-0.01730
C	-1.36477	-0.00471	0.10834
C	-2.10943	-0.00779	-1.07312
C	-3.50110	-0.01414	-1.02138
C	-4.18131	-0.01541	0.20313
C	-3.42067	-0.01635	1.37753
C	-2.02742	-0.01011	1.33435
C	-5.68950	0.00947	0.25197
H	2.65578	-4.60886	-0.61808
H	0.20921	-4.44977	-1.07857
H	-0.97377	-2.32840	-0.77246
H	3.86598	-2.59759	0.19749
H	-0.98679	2.32034	-0.77326
H	0.18402	4.44861	-1.07888
H	2.62947	4.62178	-0.61756
H	3.85103	2.61744	0.19802
H	-1.60075	-0.00856	-2.03053

H	-4.06641	-0.02050	-1.94758
H	-3.92158	-0.02426	2.33997
H	-1.44807	-0.01261	2.25055
H	-6.12402	-0.53875	-0.58692
H	-6.06466	-0.42732	1.17973
H	-6.06274	1.03786	0.19830

SCF Done: E(RB3LYP) = -1186.22632821 A.U. after 9 cycles
Sum of electronic and zero-point Energies = -1185.942144
Sum of electronic and thermal Energies = -1185.925137
Sum of electronic and thermal Enthalpies = -1185.924193
Sum of electronic and thermal Free Energies = -1185.988686

Excitation energies and oscillator strengths (B3LYP/6-311++G** TD=NStates=10):

Excited State 1: Singlet-A 3.5283 eV 351.40 nm f=0.0023 <S**2>=0.000
76 -> 77 0.68706
76 -> 80 0.13315
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -1186.09666696
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.8912 eV 318.63 nm f=0.0265 <S**2>=0.000
75 -> 77 -0.10531
76 -> 78 -0.37255
76 -> 79 0.35670
76 -> 80 0.45392

Excited State 3: Singlet-A 3.9451 eV 314.28 nm f=0.0290 <S**2>=0.000
76 -> 78 0.58434
76 -> 79 0.27650
76 -> 80 0.24595

Excited State 4: Singlet-A 3.9478 eV 314.06 nm f=0.0261 <S**2>=0.000
76 -> 79 0.52973
76 -> 80 -0.43931

Excited State 5: Singlet-A 4.2248 eV 293.47 nm f=0.0750 <S**2>=0.000
75 -> 77 -0.12517
75 -> 80 -0.11511
76 -> 81 0.67711

Excited State 6: Singlet-A 4.5885 eV 270.21 nm f=0.0038 <S**2>=0.000

76 -> 82 0.64308

76 -> 83 0.18153

76 -> 85 0.18768

Excited State 7: Singlet-A 4.6915 eV 264.27 nm f=0.0520 <S**2>=0.000

75 -> 77 0.10415

76 -> 84 0.63454

76 -> 89 0.20684

76 -> 90 -0.12319

Excited State 8: Singlet-A 4.8116 eV 257.68 nm f=0.0820 <S**2>=0.000

76 -> 82 -0.17142

76 -> 83 0.63334

Excited State 9: Singlet-A 4.8128 eV 257.61 nm f=0.4605 <S**2>=0.000

75 -> 77 0.64140

76 -> 80 0.11998

76 -> 81 0.13923

76 -> 84 -0.13790

Excited State 10: Singlet-A 4.9172 eV 252.14 nm f=0.0341 <S**2>=0.000

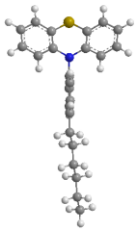
76 -> 82 -0.20789

76 -> 85 0.62784

76 -> 86 -0.14741

76 -> 88 0.10746

6.8 Computed xyz-coordinates (B3LYP/6-311++G IEFPCM CH_2Cl_2) and Excitation energies (B3LYP/6-311++G**) of 10-(4-Hexylphenyl)-10*H*-phenothiazine (3h)**



C	-3.90048	3.77362	0.25465
C	-2.62434	3.59219	0.77988
C	-1.99748	2.34933	0.71019
C	-2.62152	1.25818	0.08649
C	-3.89731	1.46415	-0.47123
C	-4.53629	2.69814	-0.36301
N	-1.99131	-0.00939	-0.00217
C	-2.75214	-1.20603	0.00923
C	-4.04155	-1.23979	-0.55446
S	-4.65841	0.17758	-1.44079
C	-2.24877	-2.39460	0.55955
C	-3.00472	-3.56561	0.55364
C	-4.29233	-3.57671	0.02515
C	-4.80890	-2.40281	-0.52035
C	-0.58093	-0.09182	0.29013
C	0.32745	-0.10163	-0.76361
C	1.69925	-0.17353	-0.51228
C	2.19246	-0.23647	0.79428
C	1.26201	-0.22482	1.84502
C	-0.10529	-0.15508	1.60324
C	3.67257	-0.32853	1.12016
C	4.65217	-0.09388	-0.03367
C	6.11543	-0.13873	0.42224
C	7.11757	0.07976	-0.71649
C	8.58064	0.04861	-0.26008
C	9.57634	0.26318	-1.40387
H	-4.39598	4.73498	0.31743
H	-2.10800	4.41595	1.25933
H	-1.01054	2.23139	1.13437
H	-5.52687	2.81806	-0.78714

H	-1.25537	-2.40950	0.98478
H	-2.57972	-4.46841	0.97723
H	-4.88741	-4.48198	0.03027
H	-5.80604	-2.38948	-0.94579
H	-0.04073	-0.05108	-1.78192
H	2.38138	-0.17743	-1.35330
H	1.61679	-0.26864	2.87002
H	-0.80554	-0.14513	2.43090
H	3.88841	0.38707	1.92248
H	3.86641	-1.31812	1.55426
H	4.49882	-0.84887	-0.81353
H	4.44860	0.87838	-0.49843
H	6.27589	0.62307	1.19593
H	6.31641	-1.10639	0.89984
H	6.96409	-0.68729	-1.48682
H	6.91209	1.04358	-1.20038
H	8.73475	0.81762	0.50673
H	8.78576	-0.91275	0.22658
H	10.60905	0.23826	-1.04455
H	9.47165	-0.51263	-2.16921
H	9.41662	1.23101	-1.89010

SCF Done: E(RB3LYP) = -1382.84622586 A.U. after 10 cycles
Sum of electronic and zero-point Energies = -1382.420265
Sum of electronic and thermal Energies = -1382.396581
Sum of electronic and thermal Enthalpies = -1382.395637
Sum of electronic and thermal Free Energies = -1382.476851

Excitation energies and oscillator strengths (B3LYP/6-311++G** TD=NStates=10):
Excited State 1: Singlet-A 3.5375 eV 350.49 nm f=0.0026 <S**2>=0.000
96 -> 97 0.69095
96 ->100 -0.10660
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -1382.71622603
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.9034 eV 317.63 nm f=0.0074 <S**2>=0.000
96 -> 98 0.62898
96 ->100 0.30145

Excited State 3: Singlet-A 3.9456 eV 314.23 nm f=0.0320 <S**2>=0.000

96 -> 99 0.66255

96 ->100 0.17293

Excited State 4: Singlet-A 3.9494 eV 313.93 nm f=0.0544 <S**2>=0.000

95 -> 97 -0.12665

96 -> 97 0.10231

96 -> 98 -0.29230

96 -> 99 -0.20000

96 ->100 0.58416

Excited State 5: Singlet-A 4.2595 eV 291.08 nm f=0.0619 <S**2>=0.000

95 -> 97 -0.12155

95 ->100 0.10723

96 ->101 0.67719

Excited State 6: Singlet-A 4.5863 eV 270.34 nm f=0.0040 <S**2>=0.000

96 ->102 0.59393

96 ->103 -0.33685

96 ->106 0.11291

Excited State 7: Singlet-A 4.6871 eV 264.52 nm f=0.0486 <S**2>=0.000

95 -> 97 0.10601

96 ->104 0.15617

96 ->105 0.61520

96 ->111 0.20137

96 ->113 -0.11228

Excited State 8: Singlet-A 4.8083 eV 257.85 nm f=0.0755 <S**2>=0.000

95 -> 99 -0.11205

96 ->102 0.21518

96 ->103 0.25314

96 ->104 0.56494

96 ->105 -0.13685

Excited State 9: Singlet-A 4.8260 eV 256.91 nm f=0.4926 <S**2>=0.000

92 -> 99 0.11736

95 -> 97 0.64350

96 ->100 0.13427

96 ->101 0.13695

96 ->105 -0.13779

Excited State 10: Singlet-A 4.9146 eV 252.28 nm f=0.0383 <S**2>=0.000

95 -> 99 -0.10566

96 ->102 -0.26775

96 ->103 -0.34214

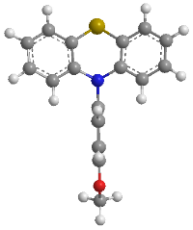
96 ->104 0.25197

96 ->106 0.41639

96 ->107 0.15504

96 ->108 -0.12574

6.9 Computed xyz-coordinates (B3LYP/6-311++G IEFPCM CH_2Cl_2) and Excitation energies (B3LYP/6-311++G**) of 10-(4-Methoxyphenyl)-10*H*-phenothiazine (3i)**



C	2.44692	-3.68013	-0.40751
C	1.09957	-3.58365	-0.74358
C	0.41843	-2.37519	-0.60837
C	1.06227	-1.23408	-0.10626
C	2.41533	-1.35412	0.26240
C	3.10230	-2.55426	0.08767
N	0.37972	-0.00002	0.04523
C	1.06218	1.23408	-0.10630
C	2.41522	1.35424	0.26234
S	3.23369	0.00011	1.08147
C	0.41824	2.37511	-0.60846
C	1.09928	3.58362	-0.74373
C	2.44663	3.68022	-0.40767
C	3.10210	2.55442	0.08756
C	-1.05991	-0.00005	-0.02737
C	-1.73759	0.00002	-1.25302
C	-3.12384	0.00000	-1.28969
C	-3.86113	-0.00008	-0.09665
C	-3.19150	-0.00014	1.13046
C	-1.79537	-0.00012	1.15301
O	-5.21583	-0.00011	-0.23569
C	-6.02513	-0.00001	0.94253
H	2.98284	-4.61462	-0.52236
H	0.56779	-4.44778	-1.12508
H	-0.62500	-2.32322	-0.88494
H	4.14924	-2.60771	0.36439
H	-0.62519	2.32304	-0.88503
H	0.56743	4.44768	-1.12527
H	2.98247	4.61475	-0.52256
H	4.14904	2.60797	0.36427
H	-1.17589	0.00010	-2.18012

H	-3.65541	0.00006	-2.23377
H	-3.73511	-0.00021	2.06517
H	-1.27313	-0.00016	2.10274
H	-7.05557	0.00009	0.59332
H	-5.84405	-0.89459	1.54528
H	-5.84386	0.89455	1.54526

SCF Done: E(RB3LYP) = -1261.45689947 A.U. after 22 cycles
Sum of electronic and zero-point Energies = -1261.167532
Sum of electronic and thermal Energies = -1261.149828
Sum of electronic and thermal Enthalpies = -1261.148884
Sum of electronic and thermal Free Energies = -1261.214084

Excitation energies and oscillator strengths (B3LYP/6-311++G** TD=NStates=10):

Excited State 1: Singlet-A 3.5399 eV 350.25 nm f=0.0023 <S**2>=0.000
80 -> 81 0.68062
80 -> 82 -0.16499
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -1261.32681043
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.9012 eV 317.81 nm f=0.0362 <S**2>=0.000
79 -> 81 0.11403
80 -> 81 0.16659
80 -> 82 0.67056

Excited State 3: Singlet-A 3.9463 eV 314.18 nm f=0.0293 <S**2>=0.000
80 -> 83 0.69212

Excited State 4: Singlet-A 4.0457 eV 306.46 nm f=0.0369 <S**2>=0.000
80 -> 84 0.68530

Excited State 5: Singlet-A 4.2773 eV 289.86 nm f=0.0537 <S**2>=0.000
79 -> 81 -0.10634
80 -> 85 0.68269

Excited State 6: Singlet-A 4.5829 eV 270.53 nm f=0.0035 <S**2>=0.000
80 -> 86 0.63678
80 -> 87 0.20380
80 -> 89 0.17883

Excited State 7: Singlet-A 4.6899 eV 264.36 nm f=0.0495 <S**2>=0.000

79 -> 81	0.10121
80 -> 88	0.63579
80 -> 93	-0.20322
80 -> 94	0.12631

Excited State 8: Singlet-A 4.8124 eV 257.64 nm f=0.0698 <S**2>=0.000

78 -> 81	-0.13922
79 -> 83	0.11277
80 -> 86	-0.15858
80 -> 87	0.59747
80 -> 89	-0.21198

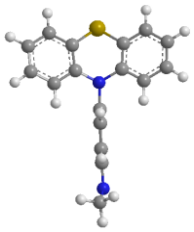
Excited State 9: Singlet-A 4.8209 eV 257.18 nm f=0.4679 <S**2>=0.000

77 -> 83	0.11085
79 -> 81	0.64481
80 -> 84	-0.11366
80 -> 85	0.11859
80 -> 88	-0.13661

Excited State 10: Singlet-A 4.8420 eV 256.06 nm f=0.0426 <S**2>=0.000

75 -> 84	-0.12560
78 -> 81	0.61455
78 -> 82	0.21013
80 -> 87	0.13731

6.10 Computed xyz-coordinates (B3LYP/6-311++G IEFPCM CH_2Cl_2) and Excitation energies (cam-B3LYP/6-311++G**) of *N*,*N*-Dimethyl-4-(10*H*-phenothiazin-10-yl)aniline (3j)**



C	-2.66457	3.70795	-0.46316
C	-1.30536	3.58707	-0.73898
C	-0.65237	2.36701	-0.57329
C	-1.33735	1.23712	-0.10000
C	-2.70330	1.38227	0.20830
C	-3.36071	2.59413	0.00287
N	-0.68175	-0.00687	0.07941
C	-1.37922	-1.22876	-0.09394
C	-2.74942	-1.32573	0.21473
S	-3.58064	0.04472	0.99304
C	-0.73329	-2.38401	-0.56088
C	-1.42769	-3.58179	-0.72051
C	-2.79031	-3.65472	-0.44484
C	-3.44799	-2.51535	0.01527
C	0.75985	-0.03146	0.06870
C	1.49559	-0.05080	-1.11779
C	2.88457	-0.07240	-1.10117
C	3.60185	-0.08587	0.11972
C	2.84177	-0.04753	1.31295
C	1.45269	-0.02657	1.27845
N	4.98208	-0.14536	0.14446
C	5.68798	0.06849	1.40136
C	5.73279	0.03245	-1.09188
H	-3.17833	4.65164	-0.60190
H	-0.74205	4.44142	-1.09672
H	0.40126	2.29414	-0.80254
H	-4.41774	2.66635	0.23331
H	0.32231	-2.34890	-0.78985
H	-0.89375	-4.45677	-1.07344
H	-3.33604	-4.58096	-0.57896

H	-4.50691	-2.54994	0.24575
H	0.97888	-0.04437	-2.07135
H	3.41065	-0.07953	-2.04523
H	3.33271	-0.03506	2.27570
H	0.89482	-0.00114	2.20806
H	5.51743	1.07250	1.81442
H	5.38605	-0.66653	2.15185
H	6.75609	-0.05511	1.23179
H	5.58623	1.02752	-1.53504
H	6.79331	-0.09626	-0.88264
H	5.44996	-0.71805	-1.83441

SCF Done: E(RB3LYP) = -1280.90443757 A.U. after 8 cycles
Sum of electronic and zero-point Energies = -1280.574966
Sum of electronic and thermal Energies = -1280.555392
Sum of electronic and thermal Enthalpies = -1280.554448
Sum of electronic and thermal Free Energies = -1280.624171

Excitation energies and oscillator strengths (cam-B3LYP/6-311++G** TD=NStates=10):

Excited State 1: Singlet-A 3.9550 eV 313.48 nm f=0.0084 <S**2>=0.000
84 -> 85 0.65142
84 -> 88 -0.16036
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -1280.25403872
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 4.3886 eV 282.51 nm f=0.0389 <S**2>=0.000
84 -> 87 0.65681

Excited State 3: Singlet-A 4.5026 eV 275.36 nm f=0.1191 <S**2>=0.000
82 -> 85 0.21035
84 -> 85 0.11669
84 -> 88 0.52585
84 -> 90 0.20030
84 -> 92 -0.19632
84 -> 93 0.10749
84 -> 94 0.15045

Excited State 4: Singlet-A 4.5495 eV 272.52 nm f=0.0517 <S**2>=0.000

83 -> 85	0.35851
83 -> 88	0.41848
83 -> 89	0.10086
83 -> 92	0.29212
83 -> 93	-0.13913
83 -> 94	-0.18366

Excited State 5: Singlet-A 4.9385 eV 251.05 nm f=0.2462 <S**2>=0.000

83 -> 85	0.13700
83 -> 86	0.52567
83 -> 89	-0.21263
83 -> 92	-0.20503
83 -> 94	-0.13577
83 -> 96	0.18105

Excited State 6: Singlet-A 5.0385 eV 246.07 nm f=0.0088 <S**2>=0.000

83 -> 86	-0.12441
84 -> 86	0.37297
84 -> 89	0.41699
84 -> 91	0.12271
84 -> 95	0.23773
84 ->100	0.13017
84 ->101	-0.10743
84 ->106	-0.10724

Excited State 7: Singlet-A 5.0606 eV 245.00 nm f=0.2210 <S**2>=0.000

82 -> 85	-0.21673
84 -> 88	-0.10681
84 -> 90	0.34966
84 -> 93	0.13275
84 -> 94	0.24297
84 -> 99	0.19141
84 ->102	-0.22320
84 ->107	0.16139
84 ->110	-0.12308

Excited State 8: Singlet-A 5.1386 eV 241.28 nm f=0.0332 <S**2>=0.000

82 -> 85	-0.13139
82 -> 88	0.15259
84 -> 88	0.28380
84 -> 89	0.15237
84 -> 92	0.50769
84 ->102	-0.11324

Excited State 9: Singlet-A 5.1588 eV 240.33 nm f=0.4484 <S**2>=0.000

83 -> 85	-0.14987
83 -> 86	0.32522
83 -> 90	-0.16032
83 -> 92	0.36914
83 -> 94	0.19392
83 -> 96	-0.24530
84 -> 97	-0.13646

Excited State 10: Singlet-A 5.2223 eV 237.41 nm f=0.0228 <S**2>=0.000

82 -> 85	0.15222
82 -> 88	-0.16274
84 -> 85	-0.11914
84 -> 88	-0.17232
84 -> 90	-0.17958
84 -> 93	0.18068
84 -> 94	0.38813
84 -> 96	-0.31369

Computed xyz-coordinates of S_1 state (B3LYP/6-311G* IEFPCM CH_2Cl_2) and Excitation energies (S_0* → S_1) (B3LYP/6-311++G) of *N*,*N*-Dimethyl-4-(10*H*-phenothiazin-10-yl)aniline (3j)**

C	1.98368	1.34292	0.10544
C	0.53559	1.25678	0.00693
N	-0.12596	0.03237	0.01535
C	0.48180	-1.21786	0.07623
C	1.92304	-1.36352	0.19883
S	2.95525	-0.02018	0.52749
C	-0.28645	-2.40815	0.02412
C	0.30040	-3.65373	0.04952

C	1.72006	-3.78500	0.13309
C	2.49669	-2.65626	0.22073
C	2.61522	2.60714	0.03990
C	1.88850	3.76276	-0.10534
C	0.46282	3.69254	-0.15756
C	-0.17971	2.47540	-0.10114
C	-1.57279	0.06243	-0.01759
C	-2.29645	0.10298	1.16988
C	-3.68579	0.13513	1.14751
C	-4.39866	0.11837	-0.07720
C	-3.63627	0.08924	-1.27076
C	-2.24662	0.05821	-1.23480
N	-5.77553	0.12441	-0.10533
C	-6.47402	0.25684	-1.37485
C	-6.52621	0.30611	1.12794
H	-1.36262	-2.33395	-0.05263
H	-0.32544	-4.53775	0.00175
H	2.18207	-4.76586	0.12446
H	3.57672	-2.74075	0.30254
H	3.69918	2.64688	0.10203
H	2.39397	4.71902	-0.18124
H	-0.12344	4.60019	-0.24620
H	-1.25930	2.44623	-0.15746
H	-1.77227	0.11367	2.11957
H	-4.21450	0.17424	2.09000
H	-4.12519	0.09126	-2.23532
H	-1.68355	0.03416	-2.16167
H	-7.54674	0.21756	-1.19830
H	-6.22239	-0.56206	-2.05532
H	-6.24622	1.20326	-1.88276
H	-7.59069	0.25515	0.90915
H	-6.32202	1.27361	1.60529
H	-6.30092	-0.48306	1.85133

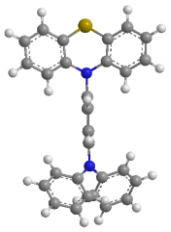
SCF Done: E(RB3LYP) = -1280.85139307 A.U. after 7 cycles

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.6966 eV 459.78 nm f=0.0022 <S**2>=0.000

84 -> 85 0.70275

6.11 Computed xyz-coordinates (B3LYP/6-311++G IEFPCM CH_2Cl_2) and Excitation energies (cam-B3LYP/6-311++G**) of 4-(10*H*-Phenothiazin-10-yl)-*N*,*N*-diphenylaniline (3k)**



C	4.57326	3.49629	-1.22610
C	3.21893	3.54533	-0.90837
C	2.53974	2.39416	-0.51309
C	3.19334	1.15420	-0.45124
C	4.55410	1.11206	-0.80841
C	5.23833	2.27316	-1.16402
N	2.51384	-0.02804	-0.06073
C	3.19154	-1.06259	0.63391
C	4.55239	-1.32039	0.38343
S	5.38783	-0.45787	-0.93316
C	2.53582	-1.87073	1.57490
C	3.21347	-2.88854	2.24383
C	4.56806	-3.11045	2.01260
C	5.23506	-2.31313	1.08433
C	1.07298	-0.01340	-0.03220
C	0.35967	0.51504	1.04670
C	-1.03024	0.50702	1.04771
C	-1.74355	-0.01885	-0.04196
C	-1.02099	-0.54037	-1.12632
C	0.36953	-0.54212	-1.11436
N	-3.15789	-0.02297	-0.04505
C	-3.87353	-1.11480	-0.61543
C	-4.97697	-0.88092	-1.44702
C	-5.68487	-1.94933	-1.99195
C	-5.29673	-3.26363	-1.73034
C	-4.19448	-3.49894	-0.90763
C	-3.49191	-2.43617	-0.34571
C	-3.88142	1.06600	0.52106
C	-3.50964	2.38882	0.24520
C	-4.21925	3.44895	0.80340
C	-5.31877	3.20908	1.62839

C	-5.69736	1.89312	1.89585
C	-4.98234	0.82758	1.35464
H	5.10728	4.39118	-1.52222
H	2.68003	4.48474	-0.95491
H	1.49063	2.45958	-0.26181
H	6.29107	2.20917	-1.41536
H	1.48661	-1.71137	1.77913
H	2.67330	-3.50044	2.95720
H	5.10076	-3.89276	2.53981
H	6.28792	-2.47338	0.88116
H	0.89339	0.92170	1.89818
H	-1.56749	0.90814	1.89781
H	-1.54991	-0.94391	-1.98045
H	0.91849	-0.94435	-1.95800
H	-5.27809	0.13727	-1.66223
H	-6.53610	-1.75128	-2.63384
H	-5.84591	-4.09289	-2.16073
H	-3.88647	-4.51533	-0.68871
H	-2.64568	-2.62737	0.30315
H	-2.66634	2.58304	-0.40660
H	-3.91929	4.46667	0.57945
H	-5.87358	4.03617	2.05576
H	-6.54664	1.69175	2.53930
H	-5.27592	-0.19192	1.57414

SCF Done: E(RB3LYP) = -1664.47513887 A.U. after 10 cycles
Sum of electronic and zero-point Energies = -1664.041403
Sum of electronic and thermal Energies = -1664.015592
Sum of electronic and thermal Enthalpies = -1664.014648
Sum of electronic and thermal Free Energies = -1664.100653

Excitation energies and oscillator strengths (cam-B3LYP/6-311++G** TD=NStates=10):
Excited State 1: Singlet-A 3.9776 eV 311.71 nm f=0.0062 <S**2>=0.000
116 ->117 0.39705
116 ->118 -0.16075
116 ->119 -0.24637
116 ->120 -0.39083
116 ->121 0.22832

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-KS) = -1663.60522446

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 4.1802 eV 296.60 nm f=0.0501 <S**2>=0.000

115 ->117 0.59055

115 ->118 0.21258

115 ->120 0.13440

115 ->121 -0.17331

Excited State 3: Singlet-A 4.2442 eV 292.13 nm f=0.5144 <S**2>=0.000

115 ->117 -0.16841

115 ->118 0.61085

115 ->119 -0.12217

115 ->120 -0.16241

Excited State 4: Singlet-A 4.4021 eV 281.65 nm f=0.2748 <S**2>=0.000

115 ->119 0.51272

115 ->120 -0.39477

115 ->121 -0.16936

Excited State 5: Singlet-A 4.4124 eV 280.99 nm f=0.0639 <S**2>=0.000

116 ->122 0.63541

Excited State 6: Singlet-A 4.4931 eV 275.94 nm f=0.0972 <S**2>=0.000

111 ->122 -0.10257

114 ->117 -0.14775

114 ->120 0.10817

116 ->117 -0.26236

116 ->118 0.11352

116 ->120 -0.14608

116 ->121 0.18307

116 ->125 0.47285

116 ->130 -0.13853

Excited State 7: Singlet-A 4.7431 eV 261.40 nm f=0.0174 <S**2>=0.000

114 ->118	0.10952
116 ->118	0.52513
116 ->119	-0.11586
116 ->120	-0.20457
116 ->125	-0.23982

Excited State 8: Singlet-A 4.8312 eV 256.63 nm f=0.0365 <S**2>=0.000

107 ->117	0.11291
108 ->118	-0.13338
115 ->120	0.18605
115 ->125	0.30880
115 ->126	0.13877
115 ->130	0.43643

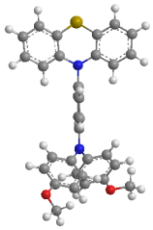
Excited State 9: Singlet-A 4.9131 eV 252.36 nm f=0.0359 <S**2>=0.000

115 ->129	0.58993

Excited State 10: Singlet-A 4.9890 eV 248.51 nm f=0.0557 <S**2>=0.000

116 ->117	-0.37719
116 ->118	-0.22390
116 ->123	-0.11476
116 ->125	-0.14210
116 ->128	0.11745
116 ->130	0.39137

6.12 Computed xyz-coordinates (B3LYP/6-311++G IEFPCM CH_2Cl_2) and Excitation energies (cam-B3LYP/6-311++G**) of *N*-(4-(10*H*-Phenothiazin-10-yl)phenyl)-4-methoxy-*N*-(4-methoxyphenyl)aniline (3l)**



C	-5.37311	-2.80501	-2.42105
C	-4.01347	-2.96093	-2.16654
C	-3.32952	-2.04261	-1.37190
C	-3.98328	-0.92519	-0.83057
C	-5.35002	-0.76059	-1.12456
C	-6.03839	-1.70309	-1.88671
N	-3.29753	0.02177	-0.02798
C	-3.96557	0.71270	1.01457
C	-5.33018	1.03879	0.90029
S	-6.18833	0.73230	-0.63127
C	-3.29547	1.10869	2.18227
C	-3.96187	1.79503	3.19583
C	-5.31957	2.08175	3.08488
C	-6.00103	1.69039	1.93387
C	-1.85616	0.00124	-0.02394
C	-1.12959	-0.90111	0.75662
C	0.25981	-0.89922	0.73802
C	0.96867	0.00518	-0.07529
C	0.22878	0.91026	-0.85807
C	-1.16090	0.90629	-0.82586
N	2.37350	-0.00004	-0.10555
C	3.10670	1.19143	-0.39643
C	4.09440	1.19119	-1.39166
C	4.82848	2.33637	-1.66210
C	4.58136	3.52001	-0.95434
C	3.59332	3.53414	0.03434
C	2.87427	2.37065	0.31268
C	3.10616	-1.20056	0.14602
C	2.81474	-2.38007	-0.55548

C	3.53566	-3.54070	-0.32063
C	4.58481	-3.54797	0.60872
C	4.89248	-2.37558	1.30381
C	4.14703	-1.21737	1.07466
O	5.35069	4.59498	-1.29827
O	5.24253	-4.73544	0.75976
C	5.15312	5.82550	-0.60186
C	6.32357	-4.80080	1.68988
H	-5.91093	-3.52302	-3.02842
H	-3.47376	-3.80681	-2.57679
H	-2.27613	-2.18982	-1.18069
H	-7.09517	-1.55572	-2.07921
H	-2.24336	0.88863	2.29506
H	-3.41038	2.09454	4.07976
H	-5.84359	2.60479	3.87581
H	-7.05676	1.91028	1.82146
H	-1.65304	-1.60571	1.39326
H	0.80141	-1.60139	1.35864
H	0.74474	1.61461	-1.49775
H	-1.71658	1.60519	-1.44075
H	4.28906	0.28381	-1.95118
H	5.59331	2.33514	-2.42983
H	3.38326	4.42971	0.60312
H	2.12051	2.38765	1.09119
H	2.01658	-2.38413	-1.28852
H	3.31023	-4.45133	-0.86320
H	5.69552	-2.34859	2.02785
H	4.38848	-0.31443	1.62311
H	5.86231	6.52845	-1.03449
H	5.35859	5.71276	0.46698
H	4.13555	6.20228	-0.74299
H	6.69533	-5.82243	1.64176
H	5.98423	-4.58437	2.70737
H	7.12489	-4.10835	1.41464

SCF Done: E(RB3LYP) = -1893.58935998 A.U. after 23 cycles

Sum of electronic and zero-point Energies = -1893.091435

Sum of electronic and thermal Energies = -1893.060244

Sum of electronic and thermal Enthalpies = -1893.059300

Sum of electronic and thermal Free Energies = -1893.157837

Excitation energies and oscillator strengths (cam-B3LYP/6-311++G** TD=NStates=10):

Excited State 1: Singlet-A 3.9669 eV 312.55 nm f=0.0058 <S**2>=0.000

131 ->133 -0.36436

131 ->134 0.42314

131 ->136 0.36648

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-KS) = -1892.63050761

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 4.0173 eV 308.63 nm f=0.0495 <S**2>=0.000

132 ->133 0.60982

132 ->134 0.19252

132 ->135 -0.13188

132 ->136 0.14943

Excited State 3: Singlet-A 4.2666 eV 290.59 nm f=0.6447 <S**2>=0.000

132 ->134 0.41065

132 ->135 -0.30332

132 ->136 -0.35503

132 ->137 0.13159

132 ->139 0.14407

Excited State 4: Singlet-A 4.4020 eV 281.66 nm f=0.0617 <S**2>=0.000

130 ->152 0.10152

131 ->136 0.18739

131 ->137 0.61620

Excited State 5: Singlet-A 4.4971 eV 275.70 nm f=0.0773 <S**2>=0.000

130 ->133	-0.12304
130 ->134	0.12543
131 ->133	-0.20730
131 ->136	-0.21053
131 ->139	0.11867
131 ->142	0.47566
131 ->148	-0.11629
132 ->138	0.10120
132 ->140	-0.13234
132 ->141	-0.16106

Excited State 6: Singlet-A 4.5031 eV 275.33 nm f=0.2833 <S**2>=0.000

131 ->142	0.17436
132 ->138	-0.24826
132 ->140	0.32612
132 ->141	0.38961
132 ->142	-0.13377
132 ->143	-0.15548

Excited State 7: Singlet-A 4.6300 eV 267.78 nm f=0.0486 <S**2>=0.000

129 ->133	-0.13569
132 ->143	0.40548
132 ->144	-0.33762
132 ->145	-0.26422
132 ->148	-0.12459

Excited State 8: Singlet-A 4.6805 eV 264.90 nm f=0.1005 <S**2>=0.000

128 ->133	-0.16633
132 ->134	0.13512
132 ->136	0.15639
132 ->142	0.31882
132 ->143	0.11184
132 ->147	0.23136
132 ->148	0.36886

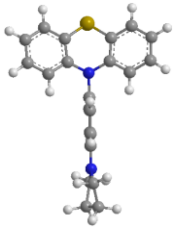
Excited State 9: Singlet-A 4.8821 eV 253.95 nm f=0.0116 <S**2>=0.000

131 ->134	-0.34222
131 ->135	0.28391
131 ->136	0.34529
131 ->137	-0.14161
131 ->139	-0.10296
131 ->142	0.21595
131 ->160	0.10580

Excited State 10: Singlet-A 4.9651 eV 249.71 nm f=0.0014 <S**2>=0.000

132 ->134	0.26179
132 ->135	0.51549
132 ->136	-0.17054
132 ->138	-0.11683
132 ->144	-0.10936
132 ->146	-0.15780

6.13 Computed xyz-coordinates (B3LYP/6-311++G IEFPCM CH_2Cl_2) and Excitation energies (cam-B3LYP/6-311++G**) of 10-(4-(Pyrrolidin-1-yl)phenyl)-10*H*-phenothiazine (3m)**



C	3.28549	3.69320	-0.41164
C	1.92747	3.59014	-0.70046
C	1.25983	2.37569	-0.55347
C	1.92806	1.23323	-0.08614
C	3.29308	1.35999	0.23423
C	3.96546	2.56666	0.04763
N	1.25580	-0.00419	0.07544
C	1.94014	-1.23235	-0.10395
C	3.30749	-1.34815	0.21140
S	4.14960	0.00386	1.01003
C	1.28392	-2.37621	-0.58466
C	1.96578	-3.57999	-0.75277
C	3.32621	-3.67077	-0.47158
C	3.99385	-2.54342	0.00354
C	-0.18611	-0.00854	0.05304
C	-0.88844	0.00631	1.25840
C	-2.27737	0.00897	1.28235
C	-3.02555	-0.00827	0.08014
C	-2.30033	-0.02537	-1.13705
C	-0.91167	-0.02221	-1.14097
N	-4.39393	-0.00818	0.09254
C	-5.22037	0.06114	-1.11635
C	-6.63060	0.33236	-0.57750
C	-6.61916	-0.33655	0.80538
C	-5.19740	-0.07253	1.31711
H	3.81063	4.63273	-0.53527
H	1.37660	4.45447	-1.05365
H	0.20741	2.31630	-0.79215
H	5.02130	2.62446	0.28747
H	0.22988	-2.32693	-0.81787
H	1.42388	-4.44548	-1.11685

H	3.86245	-4.60151	-0.61270
H	5.05107	-2.59211	0.23929
H	-0.33627	0.02092	2.19175
H	-2.78508	0.03162	2.23740
H	-2.82700	-0.04766	-2.08181
H	-0.38526	-0.03460	-2.08927
H	-5.17917	-0.88414	-1.67534
H	-4.87464	0.85655	-1.78355
H	-6.78725	1.41001	-0.47332
H	-7.40685	-0.05804	-1.23734
H	-6.78318	-1.41339	0.70430
H	-7.38059	0.05788	1.47991
H	-5.14043	0.87285	1.87450
H	-4.84288	-0.86928	1.97800

SCF Done: E(RB3LYP) = -1358.34863477 A.U. after 10 cycles
Sum of electronic and zero-point Energies = -1357.982494
Sum of electronic and thermal Energies = -1357.962264
Sum of electronic and thermal Enthalpies = -1357.961320
Sum of electronic and thermal Free Energies = -1358.032683

Excitation energies and oscillator strengths (cam-B3LYP/6-311++G** TD=NStates=10):

Excited State 1: Singlet-A 3.9500 eV 313.88 nm f=0.0089 <S**2>=0.000
91 -> 92 0.65268
91 -> 96 0.11125
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -1357.65590854
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 4.3837 eV 282.83 nm f=0.0370 <S**2>=0.000
86 -> 92 0.10178
91 -> 94 0.65287

Excited State 3: Singlet-A 4.4489 eV 278.69 nm f=0.0566 <S**2>=0.000

90 -> 92	0.35265
90 -> 95	0.23991
90 -> 96	-0.33730
90 -> 99	-0.24497
90 ->100	0.23165
90 ->102	-0.15948
90 ->103	0.10345

Excited State 4: Singlet-A 4.5010 eV 275.46 nm f=0.1200 <S**2>=0.000

87 -> 94	-0.10001
89 -> 92	-0.20898
91 -> 92	-0.10457
91 -> 95	-0.25708
91 -> 96	0.44590
91 -> 97	-0.23046
91 -> 99	-0.16696
91 ->100	0.13321
91 ->102	-0.14577

Excited State 5: Singlet-A 4.8926 eV 253.41 nm f=0.0247 <S**2>=0.000

90 -> 93	0.62247
90 -> 95	-0.10332
90 -> 96	-0.11869
90 ->105	0.11232
90 ->107	-0.10364

Excited State 6: Singlet-A 5.0000 eV 247.97 nm f=0.5085 <S**2>=0.000

90 -> 92	0.16009
90 -> 97	0.10599
90 -> 99	0.25880
90 ->100	-0.19526
90 ->102	-0.25231
90 ->103	0.14740
90 ->106	-0.16454
91 -> 93	0.19495
91 -> 95	0.23586
91 -> 96	0.12026
91 ->103	-0.15750
91 ->105	-0.11698
91 ->108	0.10041

Excited State 7: Singlet-A 5.0441 eV 245.80 nm f=0.2730 <S**2>=0.000

90 -> 92	-0.12929
90 -> 99	-0.19417
90 ->100	0.14748
90 ->102	0.16298
90 ->103	-0.11981
90 ->106	0.11946
91 -> 93	0.29950
91 -> 95	0.32874
91 -> 96	0.17330
91 ->102	-0.14358
91 ->107	0.13202

Excited State 8: Singlet-A 5.0582 eV 245.11 nm f=0.2262 <S**2>=0.000

89 -> 92	-0.22476
91 -> 96	0.11489
91 -> 97	0.34123
91 ->101	-0.15149
91 ->102	0.14724
91 ->103	-0.12463
91 ->106	-0.12345
91 ->109	-0.26453
91 ->114	-0.17493
91 ->118	0.15472

Excited State 9: Singlet-A 5.1600 eV 240.28 nm f=0.0327 <S**2>=0.000

89 -> 92	0.15555
89 -> 95	-0.10061
89 -> 96	0.14360
91 -> 92	-0.10825
91 -> 95	-0.18380
91 -> 96	0.26675
91 -> 99	0.37059
91 ->100	-0.33210
91 ->109	0.13679

Excited State 10: Singlet-A 5.2715 eV 235.20 nm f=0.0147 <S**2>=0.000

89 -> 92	0.13336
91 -> 97	-0.18477
91 -> 99	-0.13030
91 ->101	-0.11048
91 ->102	0.40214
91 ->103	-0.27754
91 ->106	0.21922

7 Literature

(1) C. Reichardt, T. Welton, Appendix A. Properties, Purification, and Use of Organic Solvents. In *Solvents and Solvent Effects in Organic Chemistry*, Wiley-VCH: Weinheim, 2010; pp 549-586.
(2) C. Hansch, A. Leo, R. W. Taft, Chem. Rev., 1991, 91, 165-195.