Supporting Information

Phenoxazine-containing polyaniline derivatives with improved electrochemical stability and processability

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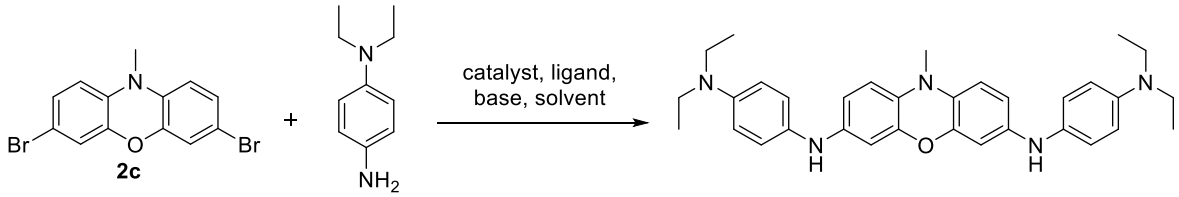
Table S1: Screened conditions for Buchwald/Hartwig reaction with the synthesis of the small molecule.



Entry	catalyst	ligand	base	solvent	temp (°C)	time (h)	isolated yield (%)
1	Pd_2dba_3	BINAP	KO *t*But	THF	85	24	none
2	$Pd(OAc)_2$	Xphos	Cs_2CO_3	THF	85	72	mono
3	Pd_2dba_3	Xantphos	Cs_2CO_3	Dioxane	100	24	none
4	$Pd(OAc)_2$	Xphos	Cs_2CO_3	Toluene	100	48	none
5	$Pd(OAc)_2$	Xphos	Cs_2CO_3	Dioxane	100	48	none
6	$Pd(OAc)_2$	Xphos	KO ^{t}But	Toluene	100	72	traces
7	**$Pd(OAc)_2$**	**Xphos**	**NaO ^{t}But**	**THF**	**85**	**18**	**72**

1 equiv. dibromide, 2 equiv. N,N-diethyl-PPDA.

Figure S1: ^{1}H NMR of crude product of small molecule and the dibrominated xanthene starting material. Peaks “a” and “b” shifted up-field in the product and no residual peaks were seen in the crude.

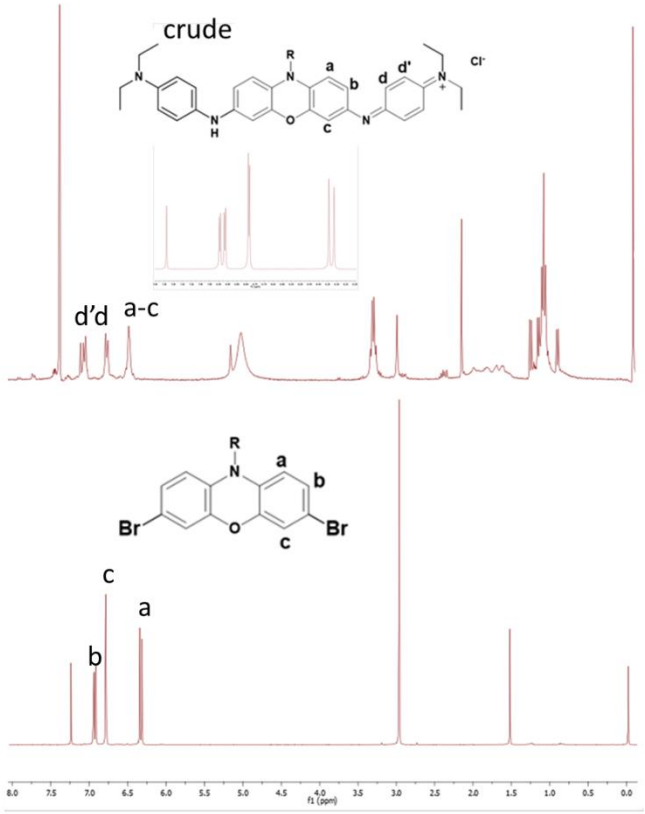
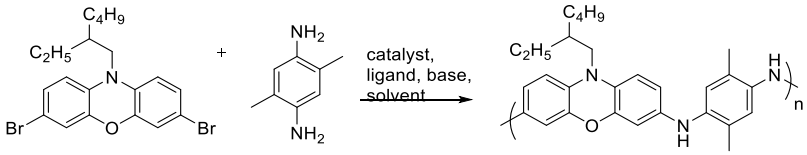


Table S2: Condition optimization of the polymers.



Entry	Pd	Ligand	Base	Solvent	M_n (g/mol)[a]	M_w (g/mol)[a]	Đ [a]
Opt-1	**$Pd(OAc)_2$**	**Xphos**	**NaO^{t}Bu**	**THF**	**12300**	**25350**	**2.06**
Opt-2	$Pd(dba)_2$	BINAP	NaO^{t}Bu	THF	9280	15710	1.69
Opt-3	$Pd(OAc)_2$	dppf	NaO^{t}Bu	THF	3190	5260	1.65
Opt-4	$Pd(dba)_2$	dppf	NaO^{t}Bu	THF	2230	3060	1.371

[a] M_n, M_w, and PDI of the polymers were determined by gel permeation chromatography using polystyrene standards in THF at 40 °C.

Figure S2: GPC data for polymer optimization. GPC traces of polymers eluted with THF at 40 °C at a flow rate of 0.7 mL/min.

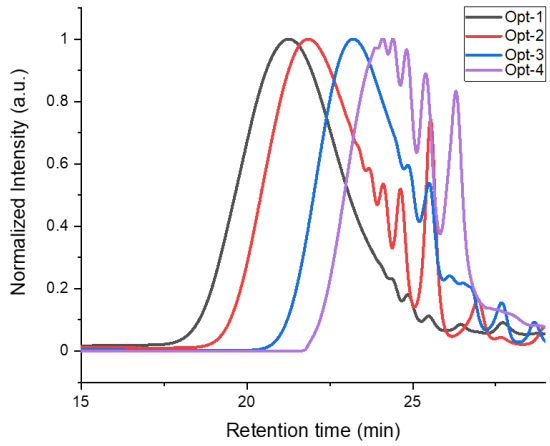


Figure S3: ^{1}H NMR of small molecule

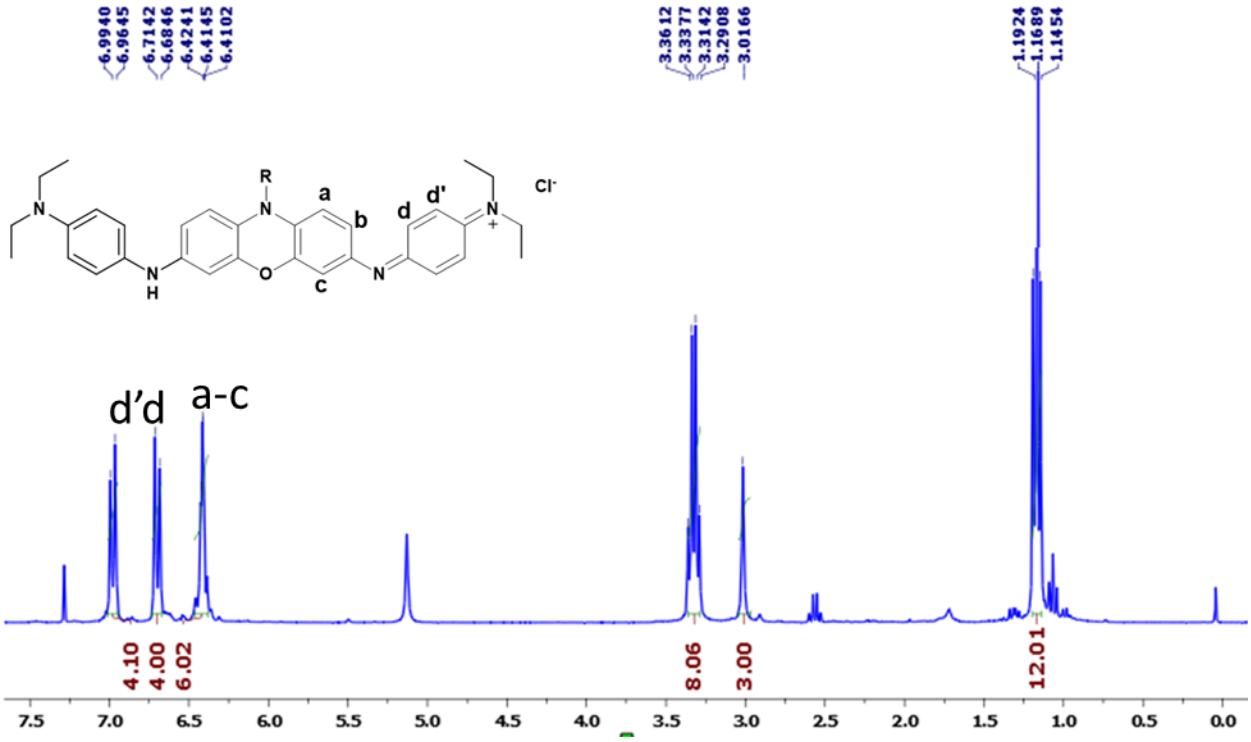
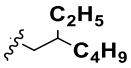
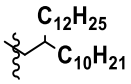


Table S3: Molecular weight distribution of different R-groups on **P1** and **P2.**

P1 R-group	Mn	Mw	Mw/Mn
CH_3	700	5860	8.23
	12360	20260	1.64
	45180	60990	1.35

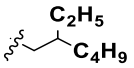
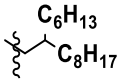
P2 R-group	Mn	Mw	Mw/Mn
CH_3	-	-	-
	12000	16960	1.41
	18050	24630	1.37

Figure S4: Solubility chart showing the effect of the size of the alkyl group on solubility of **P1** and **P2**.

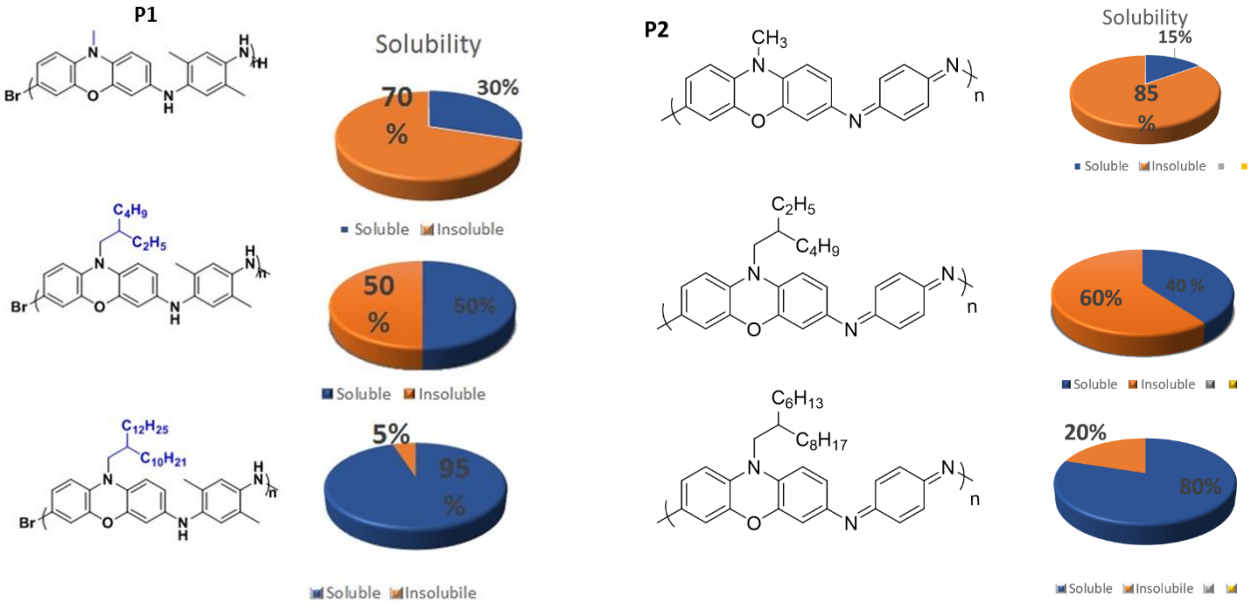
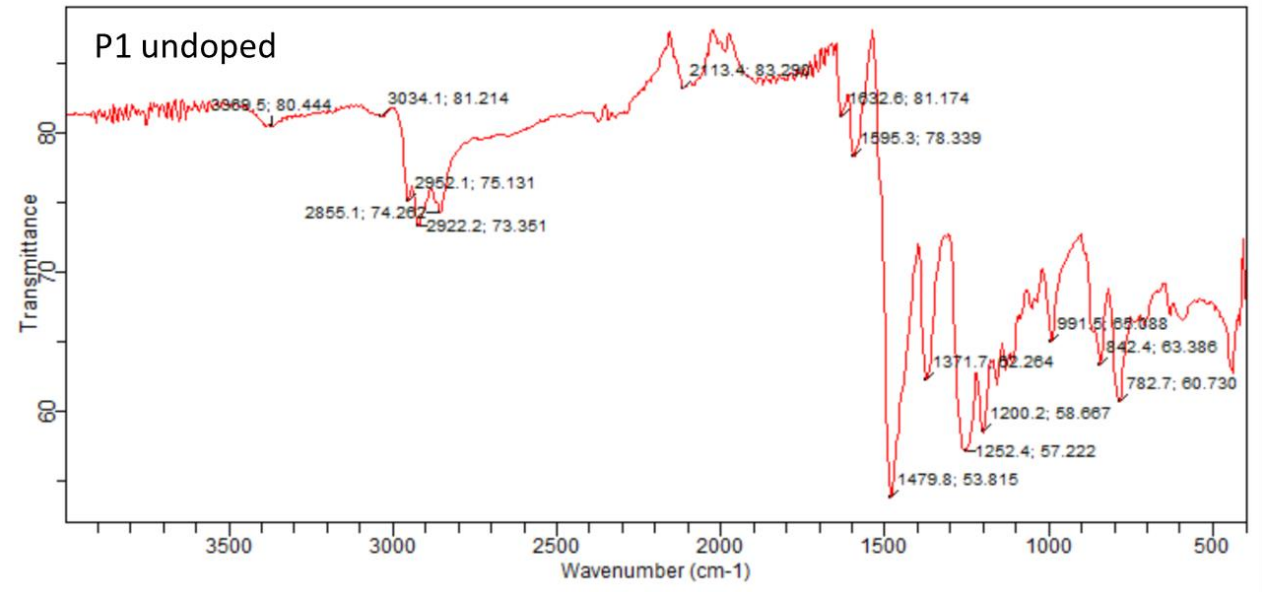
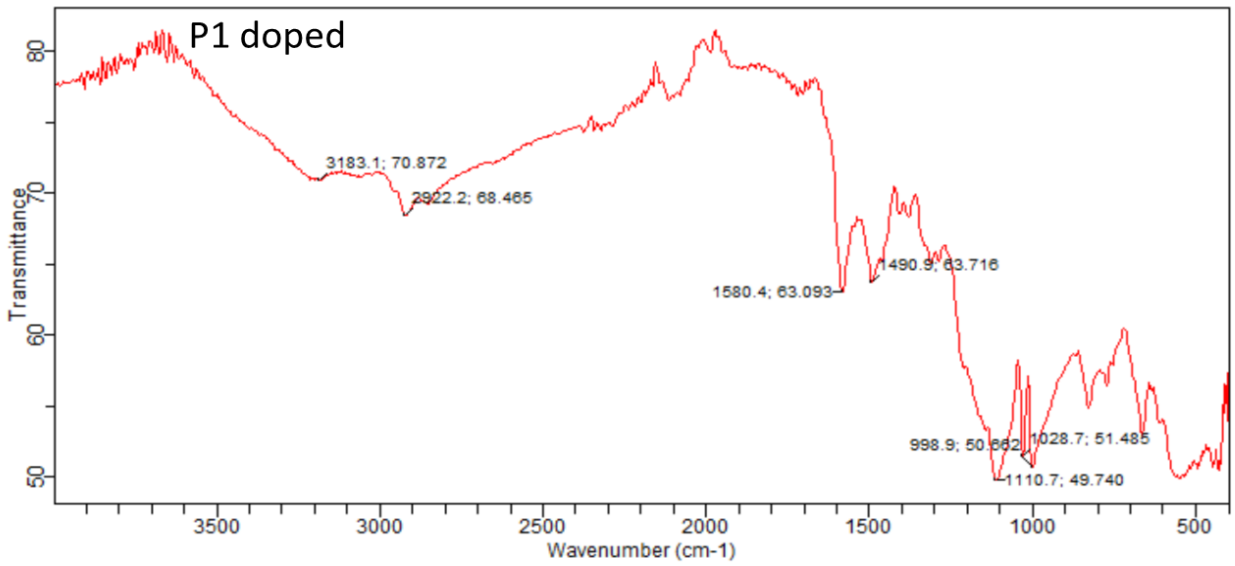


Figure S5: FTIR spectra of doped and undoped **P1** and **P2.**





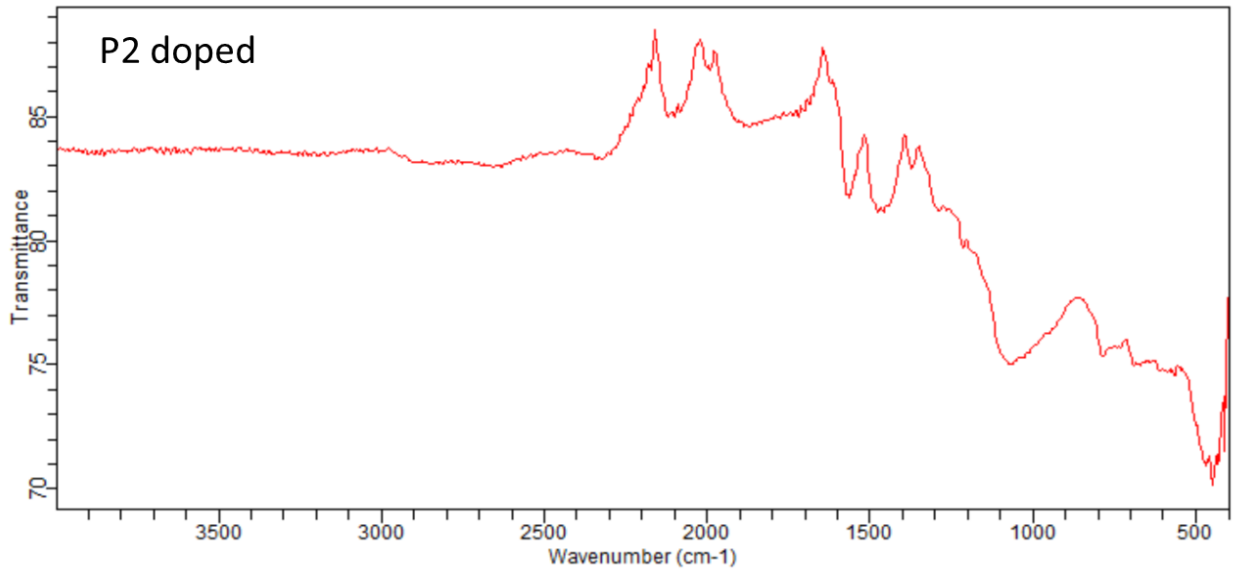


Table S4: EPR data for **P1** and **P2.**

P1				P2		
dopants	**a/b**	**g-factor**		**dopants**	**a/b**	**g-factor**
CSA	1.63	2.0045		CSA	1.36	2.0039
PSS	1.08	2.0034		PSS	1.78	2.0054
DBS	1.19	2.0036		DBS	1.18	2.0040
HCl	1.05	2.0033		HCl	1.05	2.0035

Table S5: Summary of conductivity studies for **P1.**

Entry	Sample preparation	Conductivity (S/cm)	Average
1	P1-CSA	0.0012	-
2	P1-CSA	0.019	-
3	P1-CSA-*m*-cresol/no heat	4.48	
4	P1-CSA-*m*-cresol/no heat	1.39	2.82
5	P1-CSA-*m*-cresol/no heat	2.58	
3	P1-CSA-*m*-cresol/no heat	4.58	
6	P1-CSA-*m*-cresol /heat 1 min	4.08	
7	P1-CSA-*m*-cresol/heat 2 min	2.85	-
8	P1-CSA-*m*-cresol/heat 3 min	2.56	
9	P1-CSA-*m*-cresol/heat 4 min	2.38	

Entry 1 was spin-coated; entry 2 was drop-casted; entries 3-12 were drop-casted. All films were prepared on glass slides. Entries 3-12 were slowly dried in the presence of *m*-cresol vapor. All samples were air-dried for 24 h following preparation. For entries 9-12, heating was provided by a heating gun.

Table S6: Summary of conductivity studies for **P2.**

Entry	Sample Preparation	Conductivity (S/cm)	Average
1	P2-CSA-*m*-cresol	0.350	
2	P2-CSA-*m*-cresol	0.350	0.408
3	P2-CSA-*m*-cresol	0.431	
4	P2-CSA-*m*-cresol	0.499	

All samples were drop casted on glass slides and the solvent slowly removed in the presence of *m*-cresol vapor, followed by 24 h air drying.

Figure S6: SEM images of **P1** at different length scale.

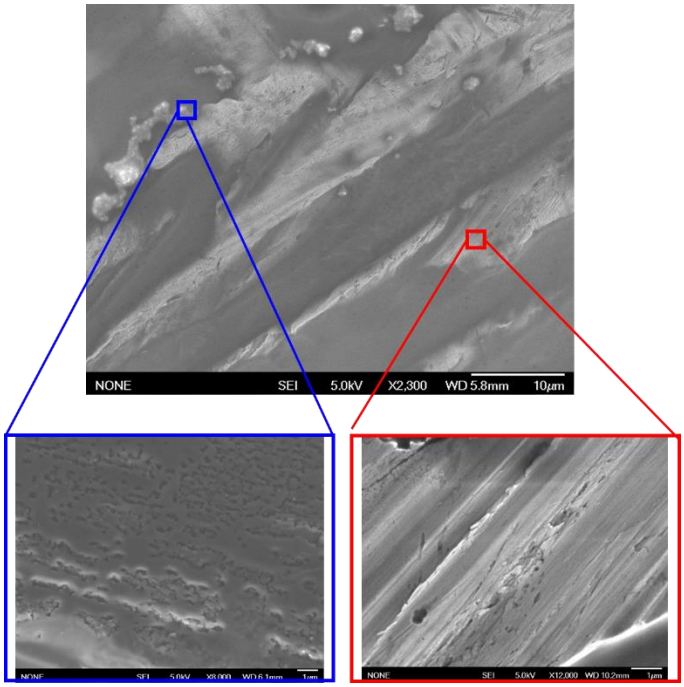


Figure S7: XRD data for **P1** and **P2** crushed films casted from EtOH in the presence and absence of *m*-cresol (temp. at 100 K).

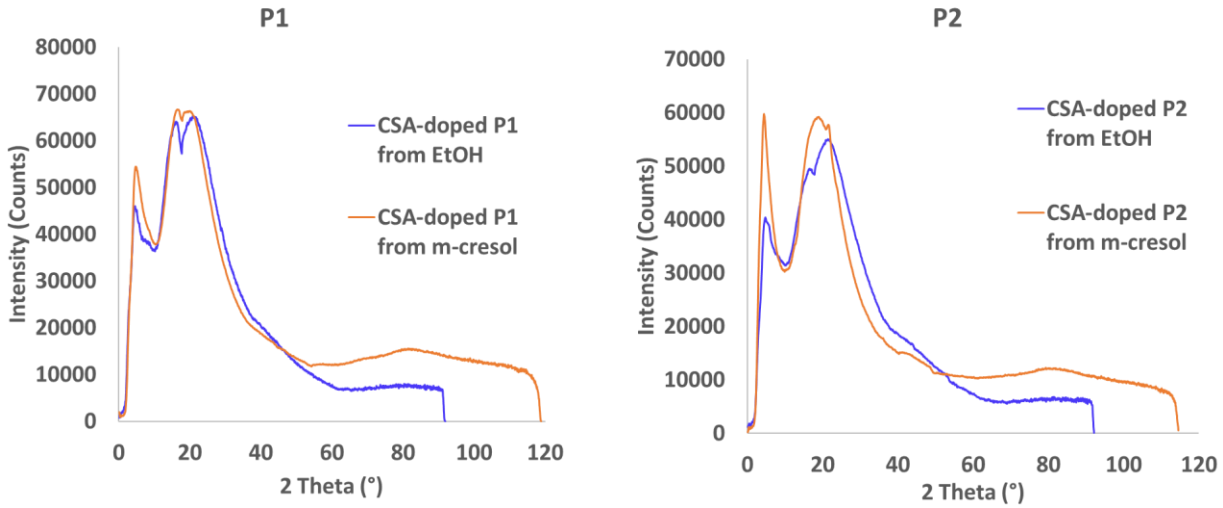


Table S7: XRD values for **P1** absence of *m*-cresol

Index	***2 theta (deg)***	***D-spacing (Å)***	***Intensity (counts)***
1	4.715	18.72445	33614.7
2	16.093	5.50316	29389.9
3	21.167	4.19389	26976.5

Table S8: XRD values for **P1** presence of *m*-cresol

Index	***2 theta (deg)***	***D-spacing (Å)***	***Intensity (counts)***
1	4.701	18.78396	48643.3
2	16.538	5.35589	49379.9
3	19.709	4.5008	47205.4
4	81.963	1.17457	256.738

Table S9: XRD values for **P2** absence of *m*-cresol

Index	***2 theta (deg)***	***D-spacing (Å)***	***Intensity (counts)***
1	1	4.879	18.09659
2	2	16.584	5.34128
3	3	21.577	4.11526

Table S10: XRD values for **P2** presence of *m*-cresol

Index	***2 theta (deg)***	***D-spacing (Å)***	***Intensity (counts)***
1	4.255	20.74743	54007.3
2	18.697	4.74211	59113.3
3	21.474	4.13468	57623.6
4	42.427	2.12881	14900.5
5	48.132	1.88897	12521.9
6	81.137	1.18442	11958.1

Figure S8: TUNA AFM of **P1**. 10 × 10 μm imaged region. Height Sensor, Peak Force Error, and Contact Current.

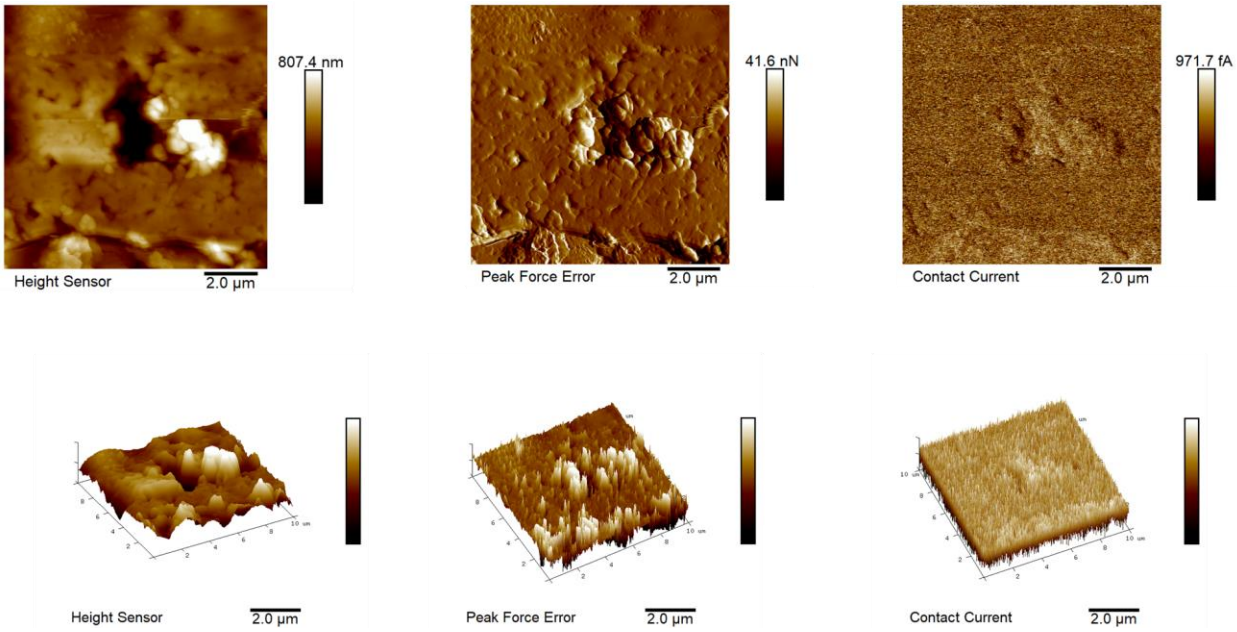


Figure S9: 100 cyclic voltammetry cycles of doped **P1** on spray-cast films on ITO/glass in 0.1 M $TBAPF_6$/acetonitrile.

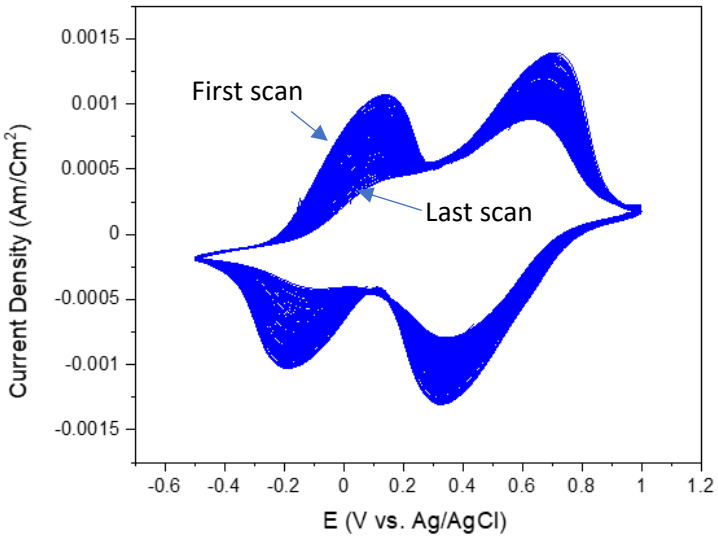
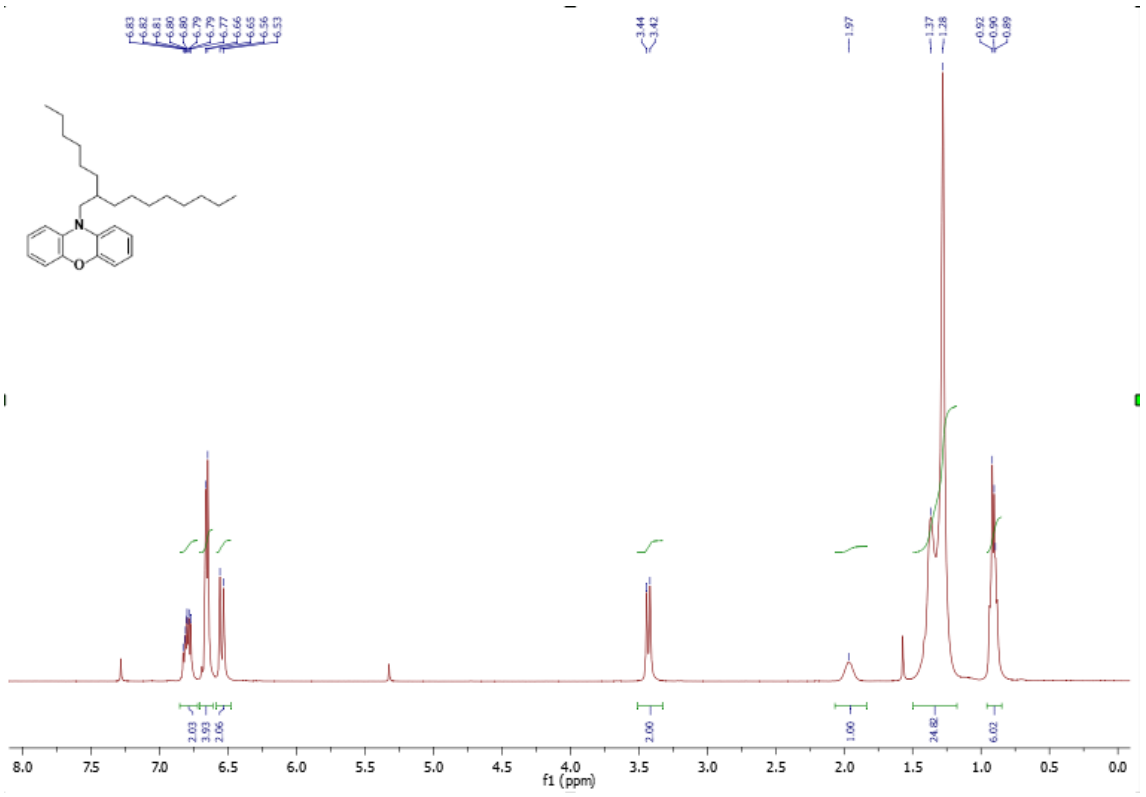


Figure S10: ^{1}H and ^{13}C NMR spectra of **1b**



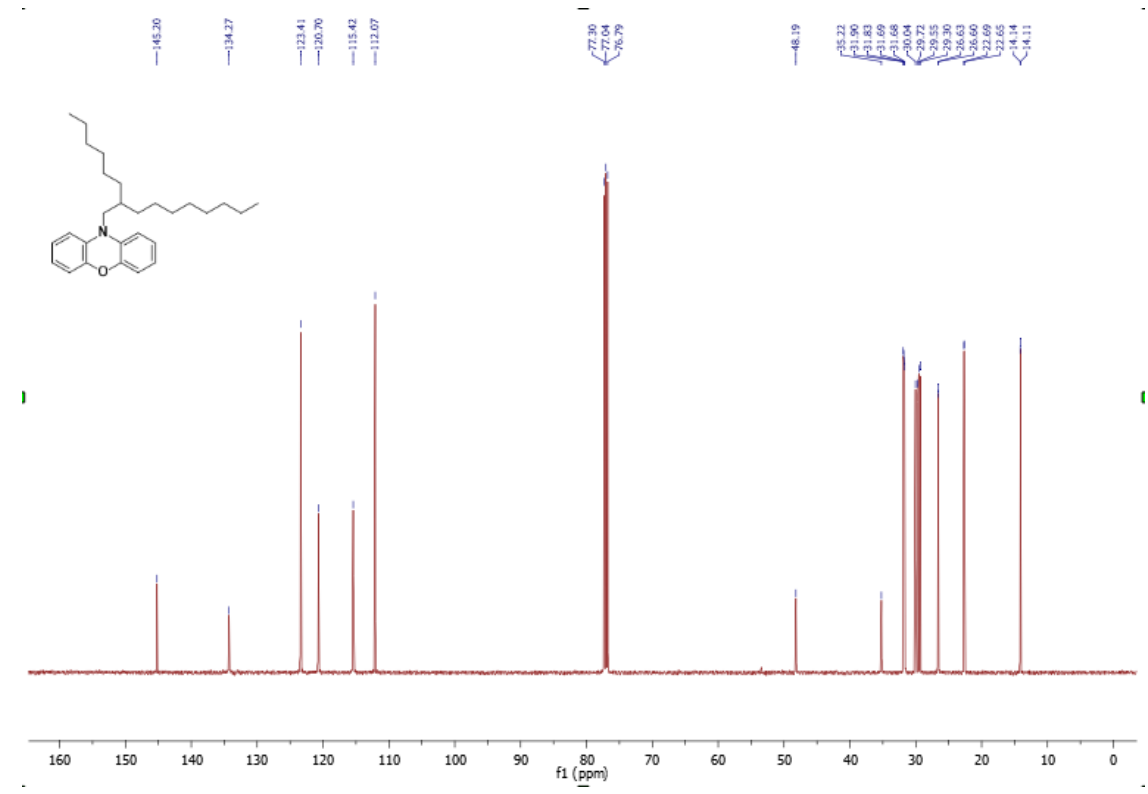


Figure S11: ^{1}H and ^{13}C NMR spectra of **1c**

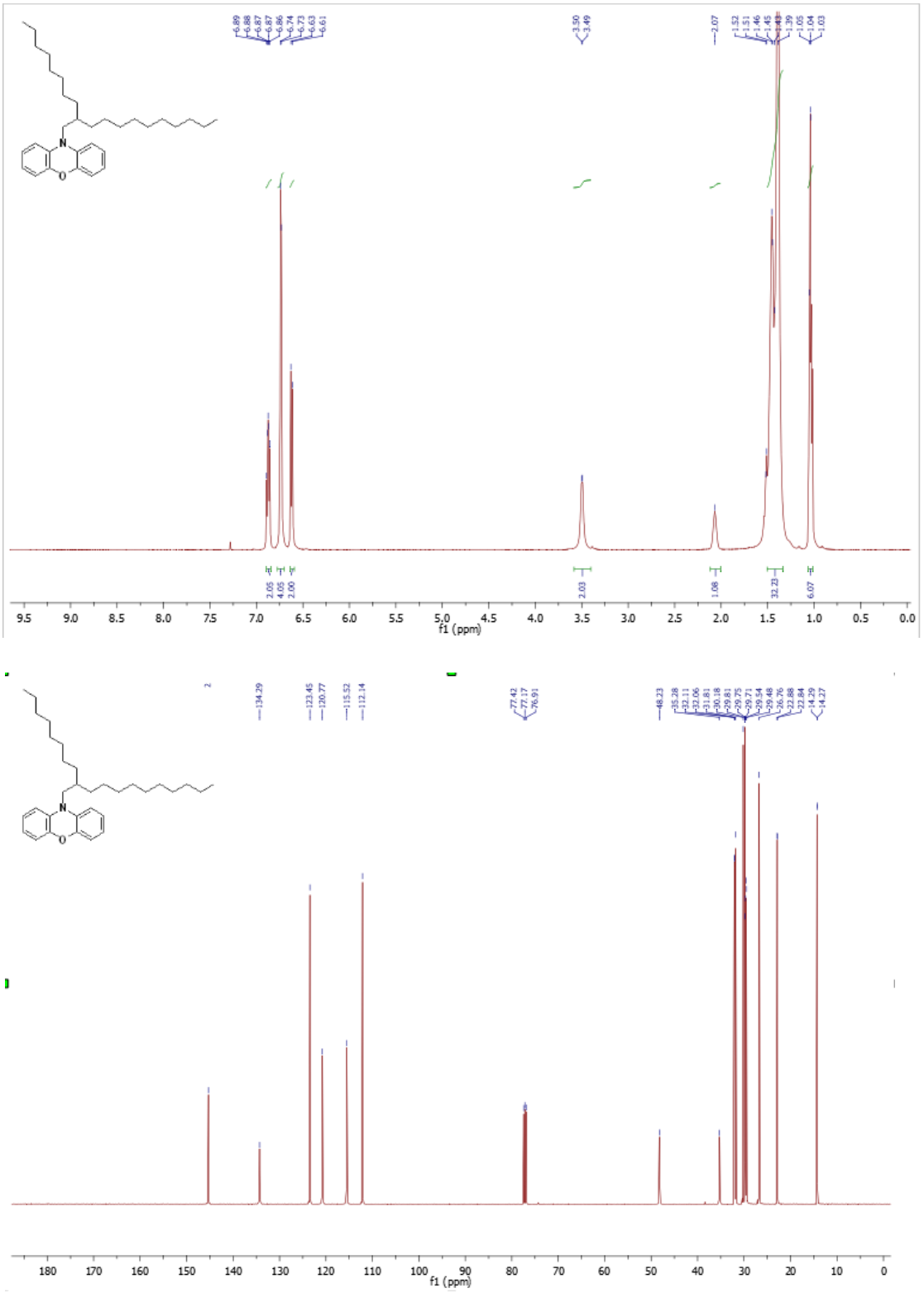
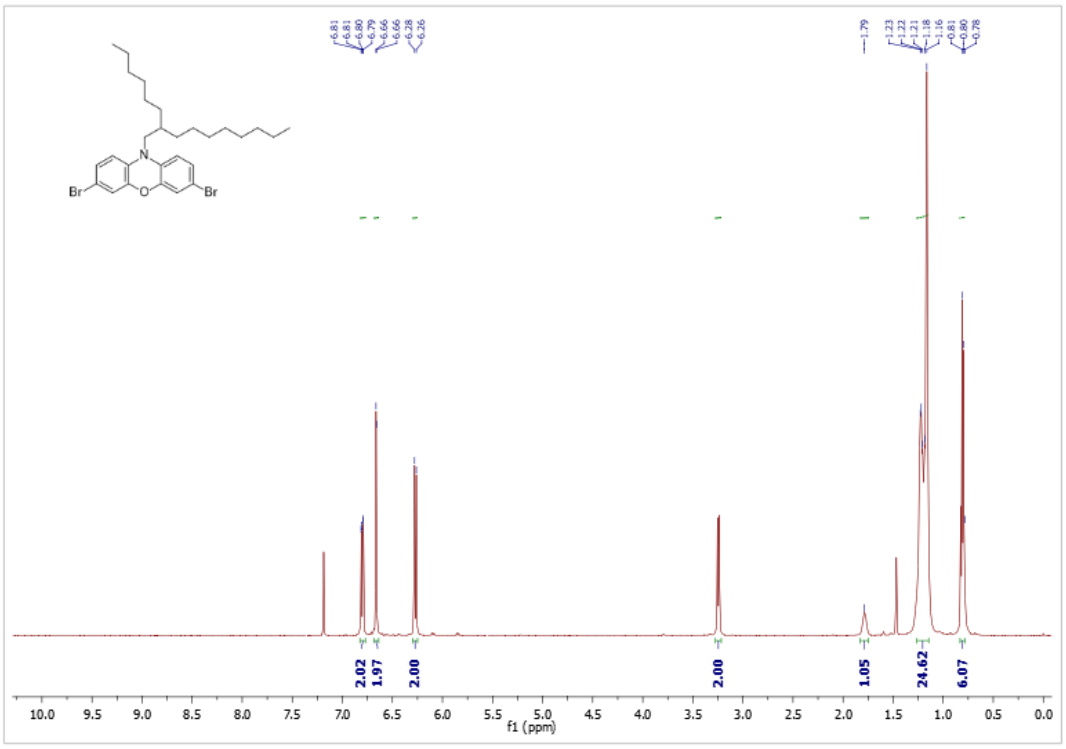


Figure S12: ^{1}H and ^{13}C NMR spectra of **2b**



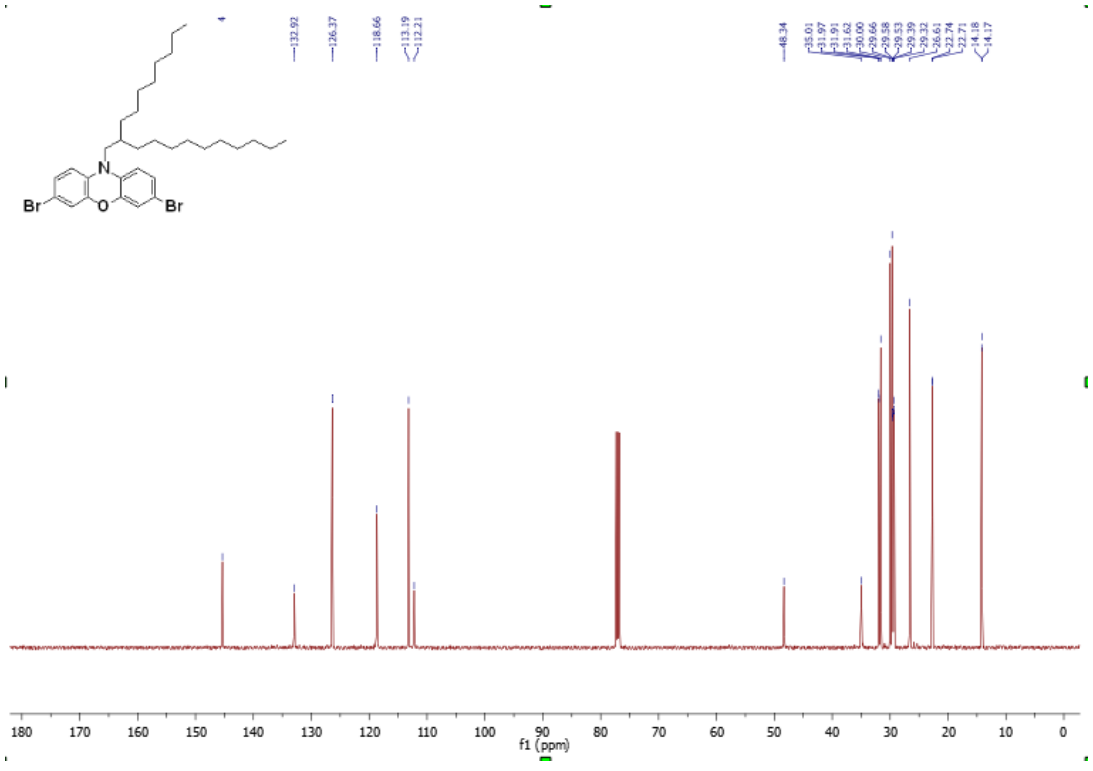


Figure S13: ^{1}H and ^{13}C NMR spectra of **2c**