A Comprehensive Scope of Peripheral and Axial Substituent Effect on the Spectroelectrochemistry of Boron Subphthalocyanines.

Supporting Information

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Table S1. Extinction Coefficients of Investigated BsubPcs Measured in 1,2-Dichlorobezene.

Compound	**Extinction Coefficient ($\varepsilon \times 10^4$ M^{-1} cm^{-1})**	
	Soret Band Peak (~300 nm)	**Q Band Max Peak (~560 – 590 nm)**
PhO-BsubPc (**1**)	4.20 ± 1.10	8.63 ± 1.28
$3F_1$PhO-BsubPc (**2**)	4.29 ± 1.17	9.40 ± 1.17
$35F_2$PhO-BsubPc (**3**)	3.59 ± 1.77	7.30 ± 1.77
$246F_3$PhO-BsubPc (**4**)	2.89 ± 1.49	5.69 ± 1.49
$345F_3$PhO-BsubPc (**5**)	4.30 ± 1.42	8.71 ± 1.42
$2356F_4$PhO-BsubPc (**6**)	5.08 ± 3.10	10.20 ± 3.10
F_5BsubPc (**7**)	4.33 ± 0.82	8.51 ± 0.82
3-MePhO-BsubPc (**8**)	4.01 ± 1.68	8.93 ± 1.68
PhO-Cl_6BsubPc (**9**)	6.25 ± 4.10	15.6 ± 4.10
PhO-Cl_{12}BsubPc (**10**)	3.86 ± 1.05	10.9 ± 1.10
Ph-BsubPc (**11**)	6.20 ± 3.55	10.0 ± 3.55
F-BsubPc (**12**)	4.55 ± 2.72	9.78 ± 2.72
Cl-BsubPc (**13**)	3.73 ± 1.28	7.35 ± 1.28
Cl-Cl_6BsubPc (**14**)	4.57 ± 1.62	9.99 ± 1.62

Table S2. UV-visible Spectral Data of Neutral and Anion Radicals of Investigated Fluorophenoxy-BsubPcs in CH_2Cl_2 Containing 0.1 M TBAP.[a]

Compound	λ_{max} (nm)							
	Neutral			Anion Radical				
PhO-BsubPc (**1**)	307	513[sh]	561	301	483	513	566	600-800[br]
$3F_1$PhO-BsubPc (**2**)	307	515[sh]	562	301	483	515	569	600-800[br]
$35F_2$PhO-BsubPc (**3**)	307	515[sh]	561	302	484	515	564	600-800[br]
$246F_3$PhO-BsubPc (**4**)	307	515[sh]	561	304	483	515	567	600-800[br]
$345F_3$PhO-BsubPc (**5**)	307	517[sh]	561	304	488	517	563	600-800[br]
$2356F_4$PhO-BsubPc (**6**)	307	517[sh]	561	305	488	517	563	600-800[br]
F_5BsubPc (**7**)	307	515[sh]	561	301	483	515	567	600-800[br]

[a]sh = shoulder peak, br = broad peak

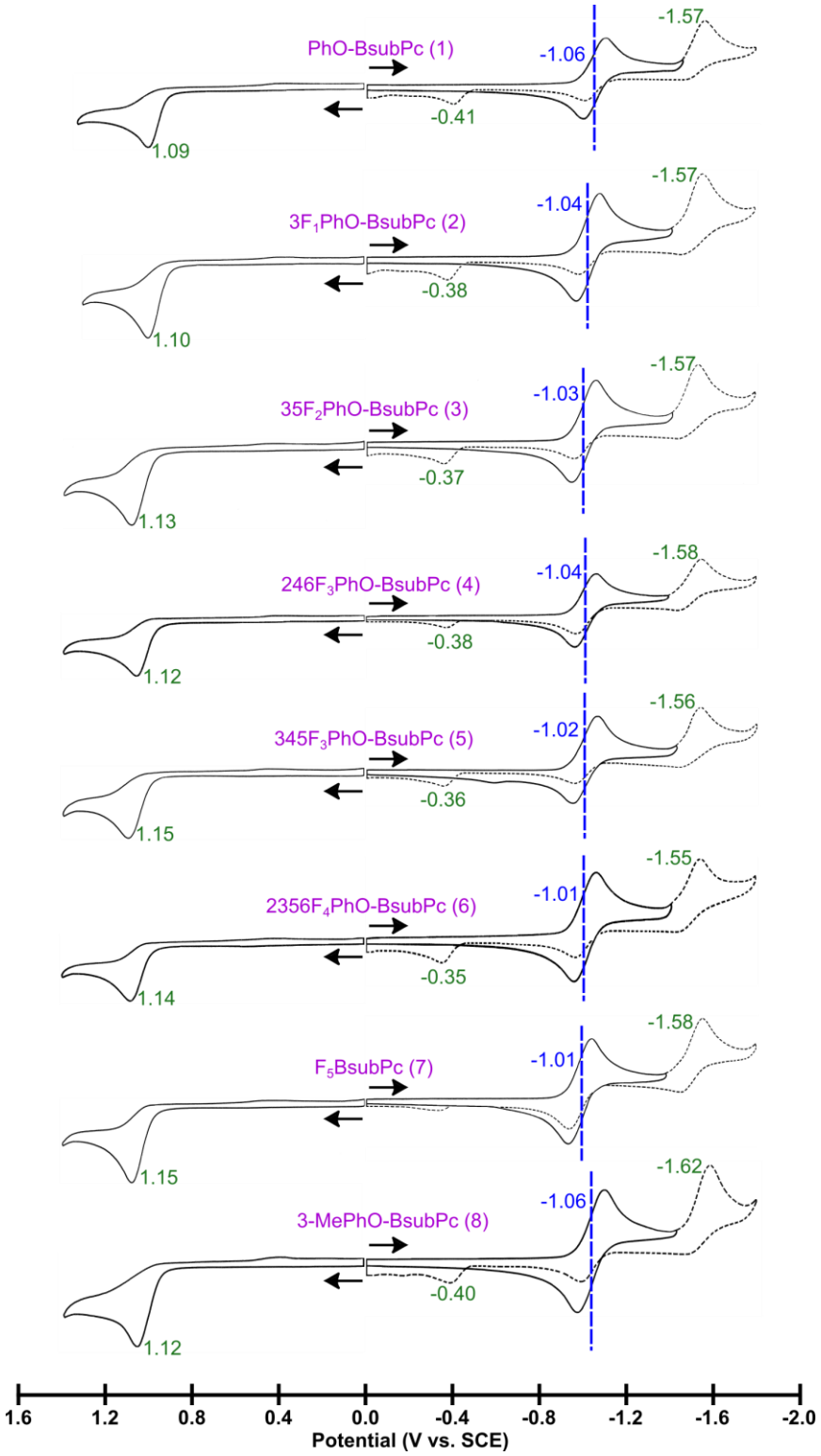

Figure S1. Cyclic voltammograms of axial phenoxy-substituted BsubPcs (PhO-BsubPc, **1**; $3F_1$PhO-BsubPc, **2**; $35F_2$PhO-BsubPc, **3**; $246F_3$PhO-BsubPc, **4**; $345F_3$PhO-BsubPc, **5**; $2356F_4$PhO-BsubPc, **6**; F_5BsubPc, **7**; and 3-MePhO-BsubPc, **8**) in CH_2Cl_2 containing 0.1 M TBAP.

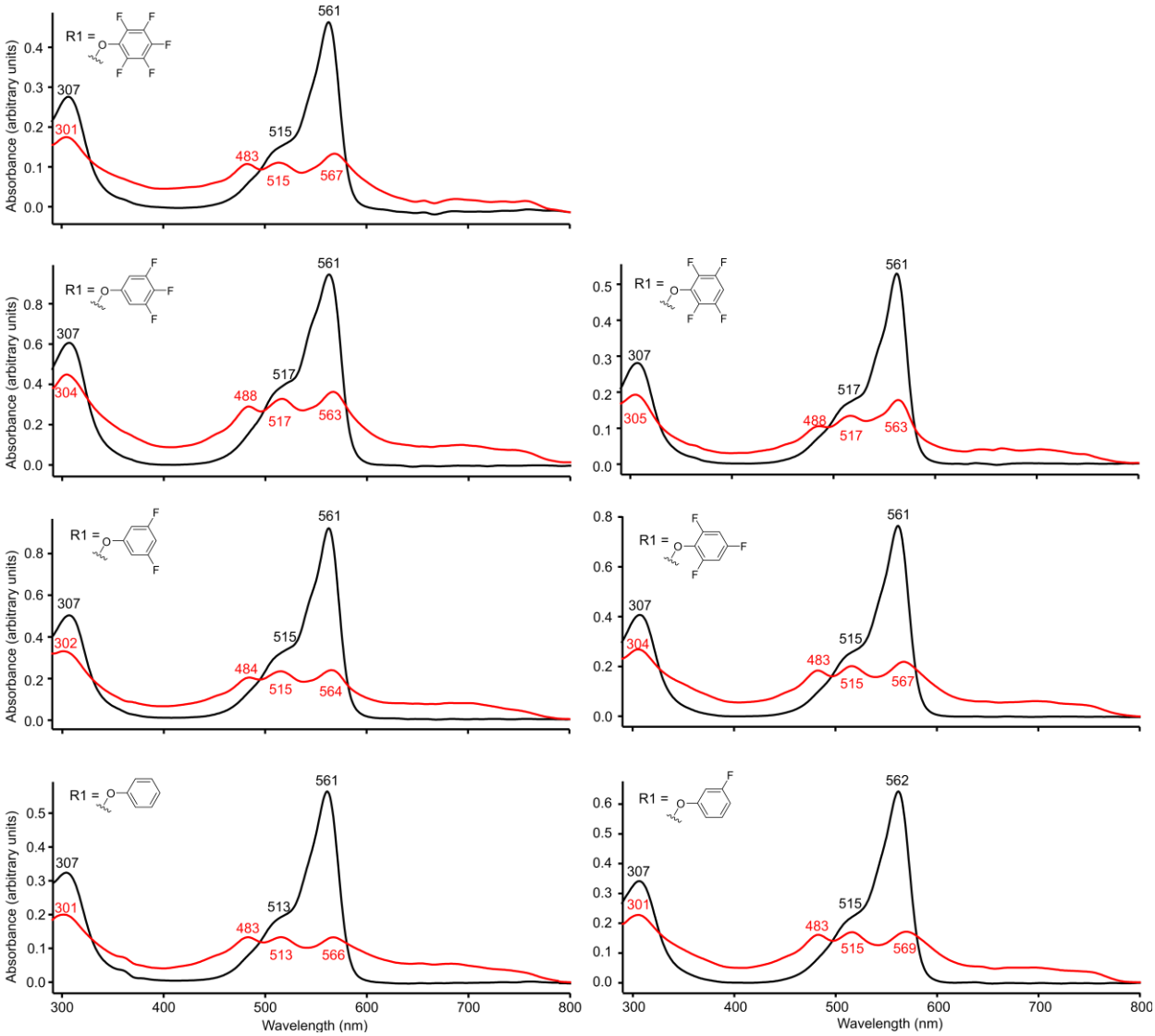

Figure S2. UV-vis spectra of neutral (black line) and singly reduced (red line) fluorophenoxy-BsubPcs at -1.4 V (-1.3 V for F_5BsubPc), where n = 0-5, in CH_2Cl_2 containing 0.1 M TBAP.

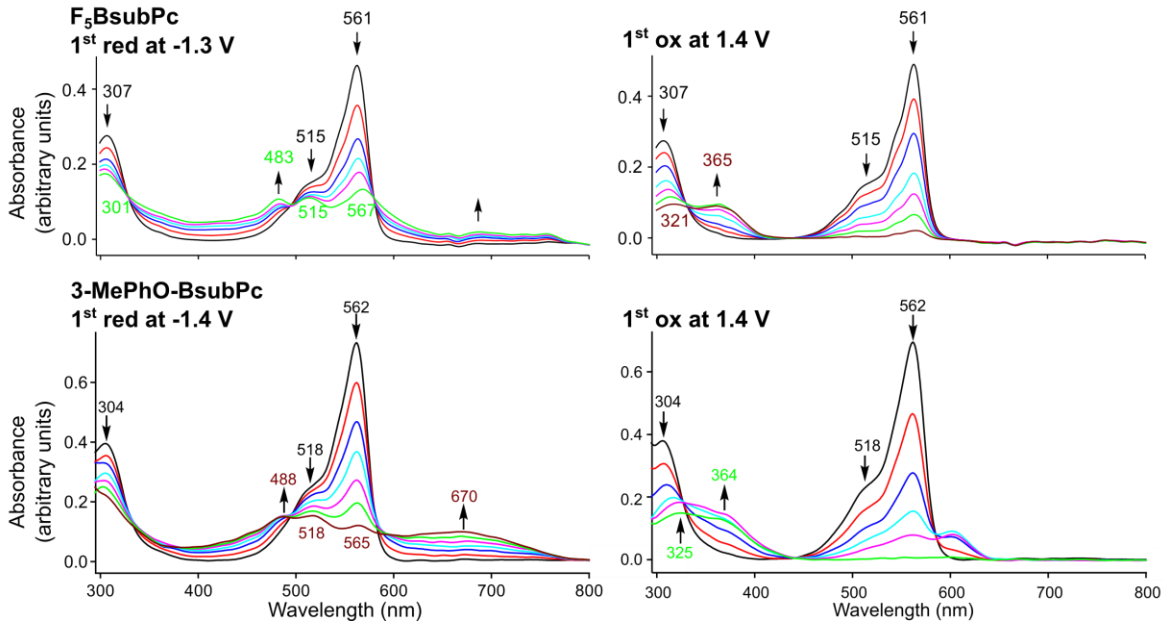

Figure S3. UV-vis spectral changes of F_5BsubPc (top, **7**) and 3-MePhO-BsubPc (bottom, **8**) during first reduction (left spectra) and first oxidation (right spectra) at the respective potentials, in CH_2Cl_2 containing 0.1 M TBAP.