

Supporting Information

For

Organoboron copolymers containing thienothiophene and selenophenothiophene analogues: Optical, electrochemical and fluoride sensing properties

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NMR and Mass Spectra

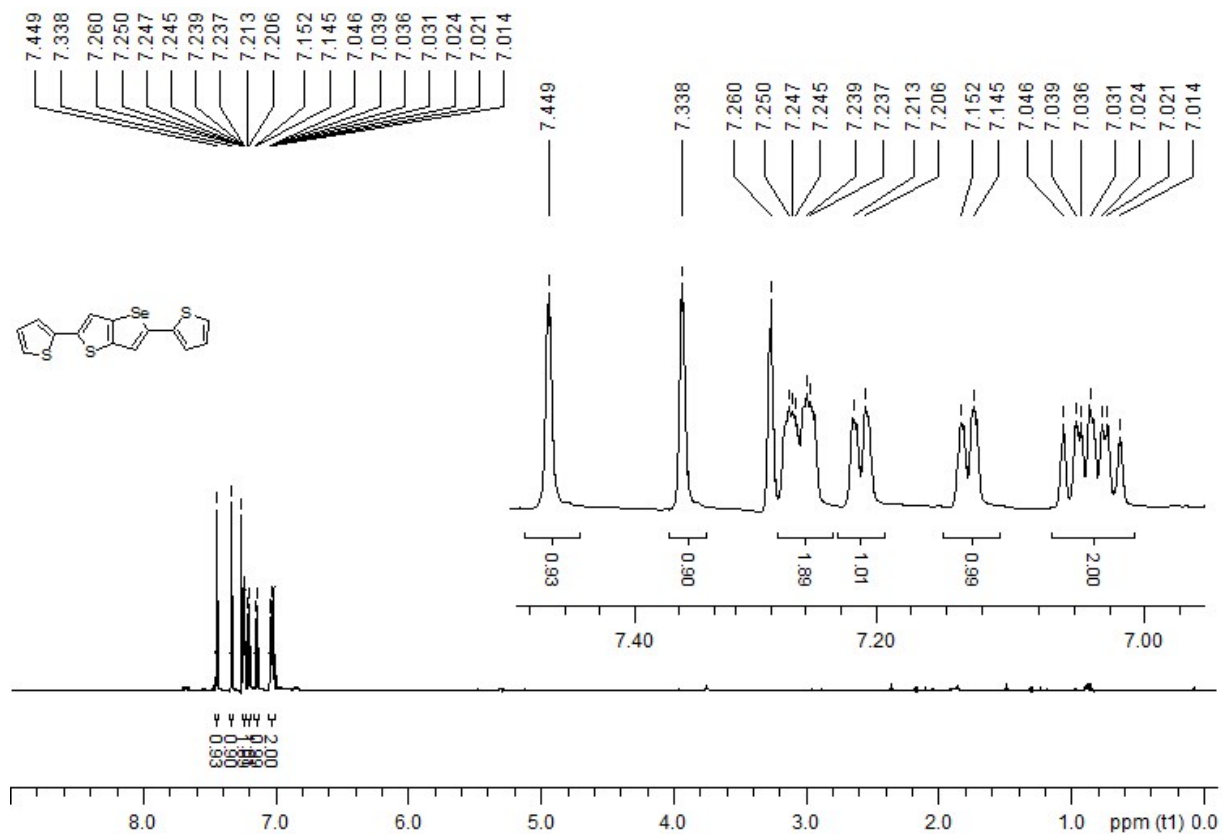


Figure S1. ¹H-NMR (500 MHz, CDCl₃) spectrum of **5**.

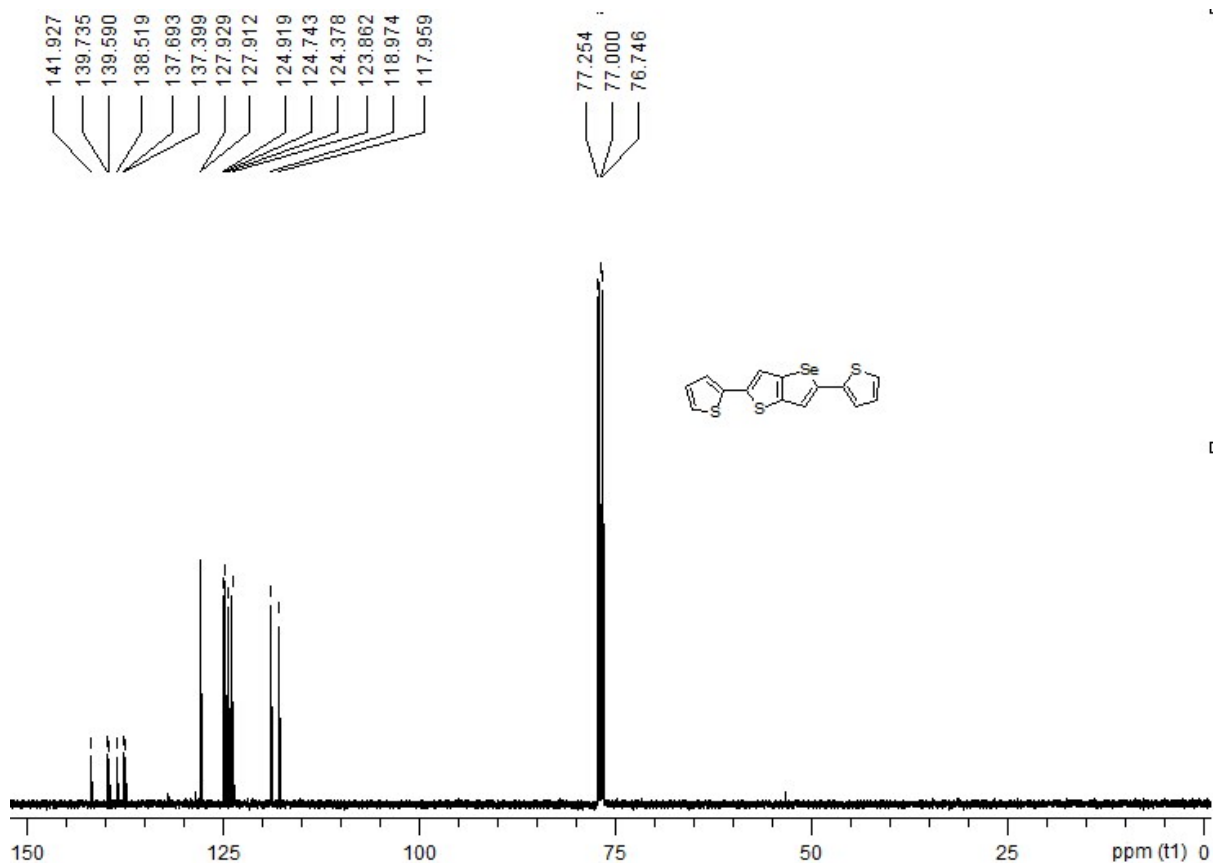


Figure S2. ¹³C-NMR (125 MHz, CDCl₃) spectrum of **5**.

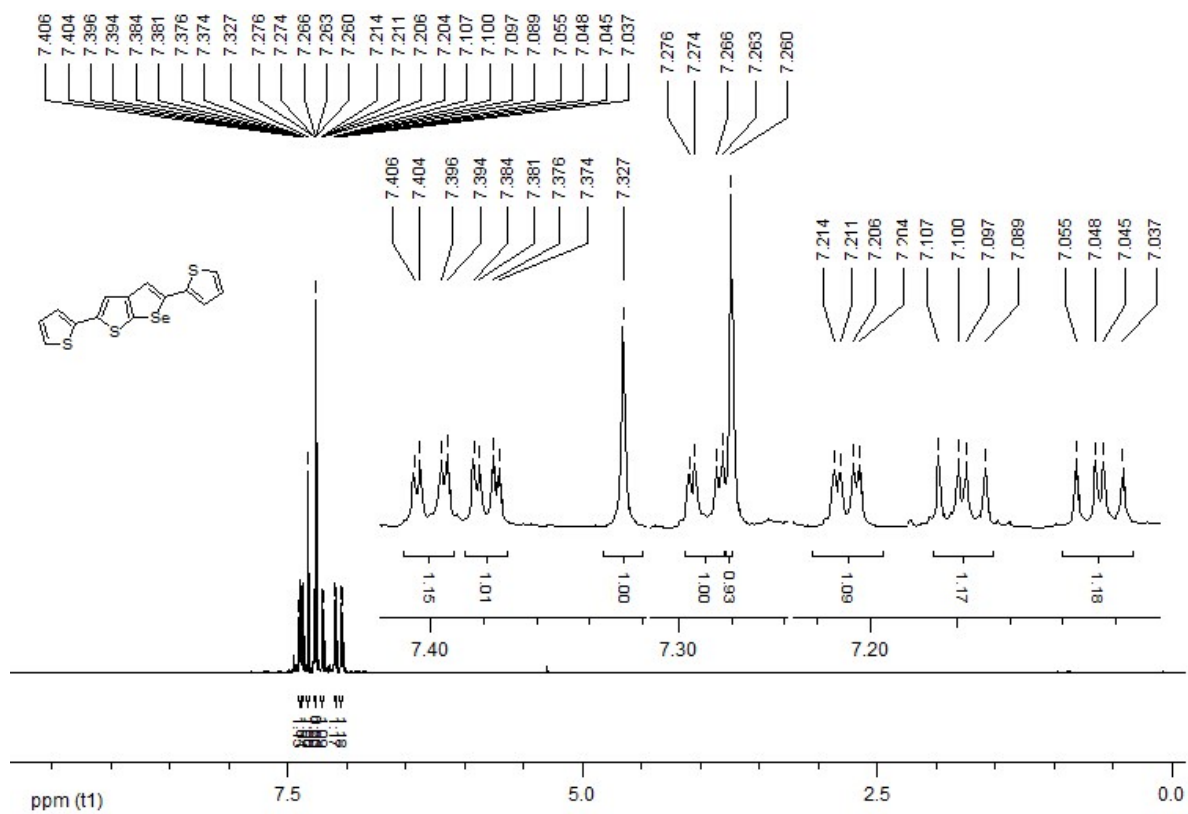


Figure S3. ¹H-NMR (500 MHz, CDCl₃) spectrum of 6.

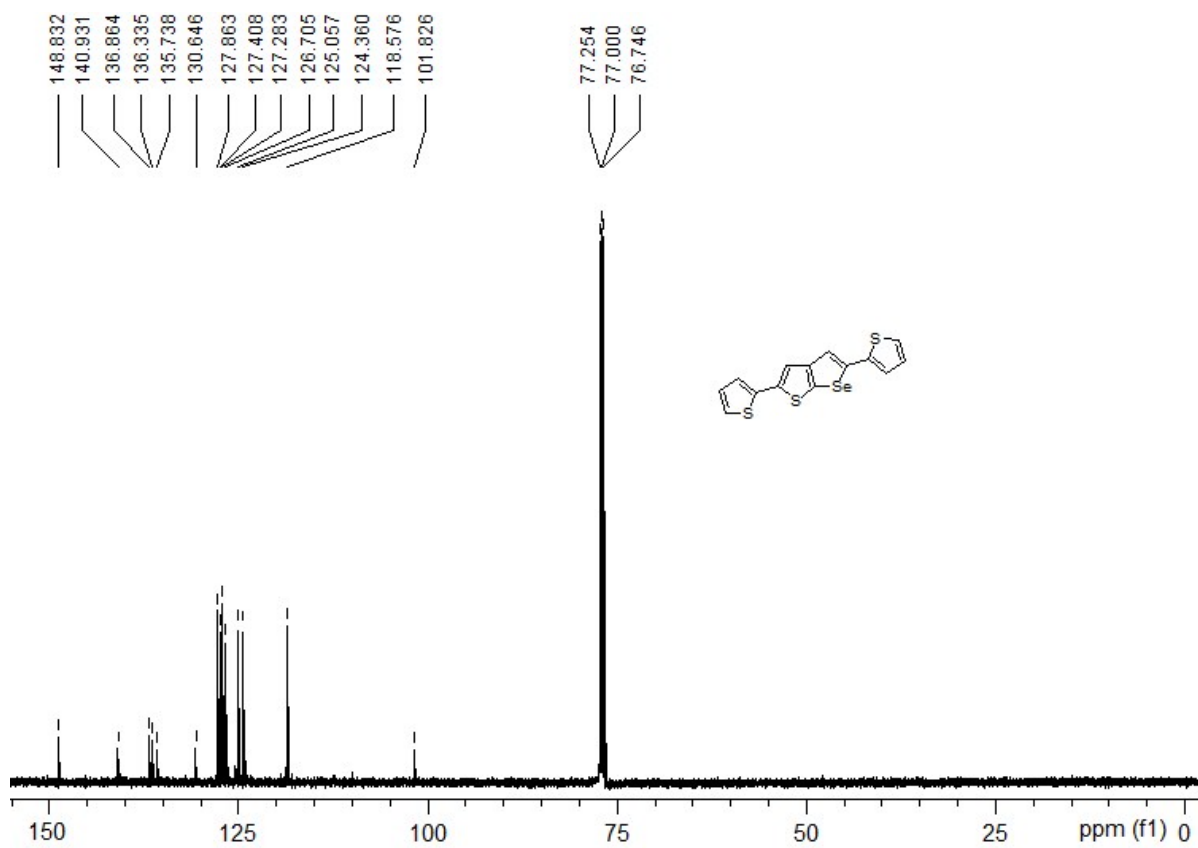
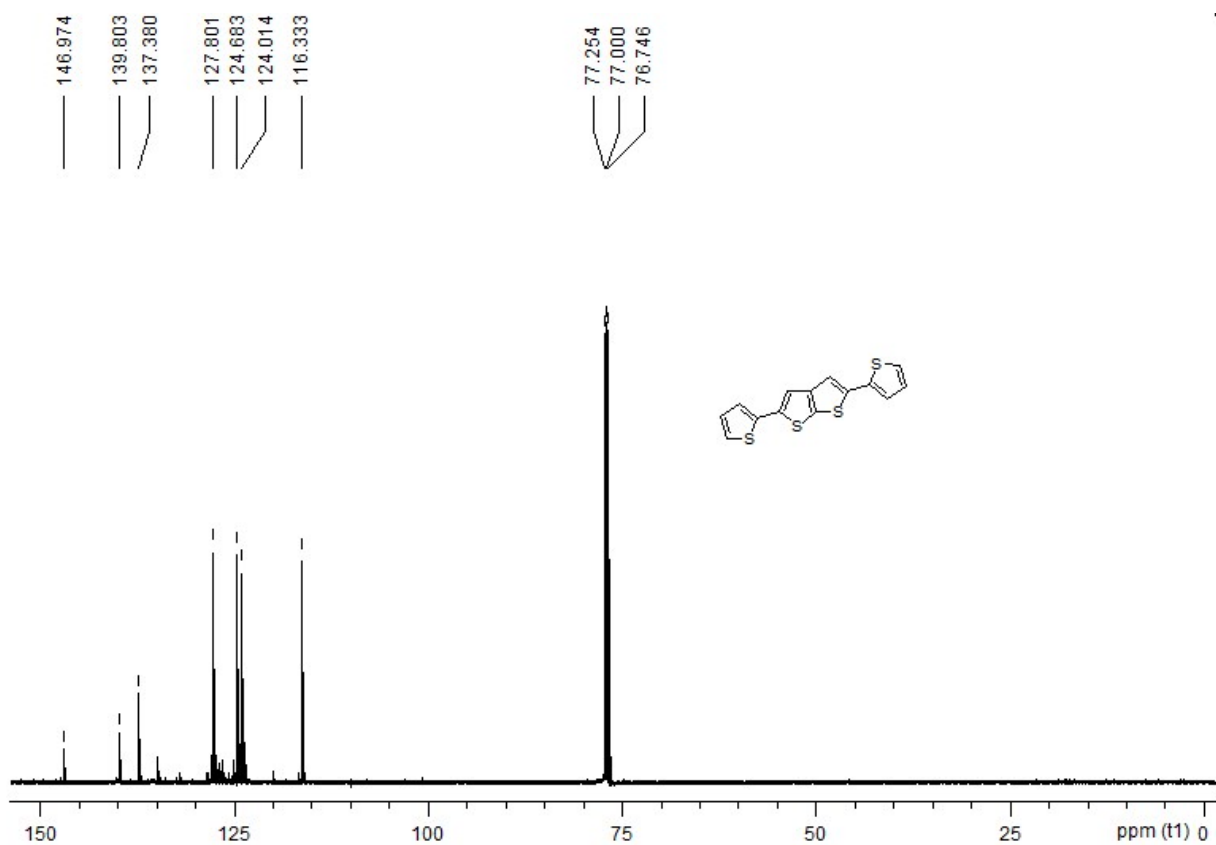
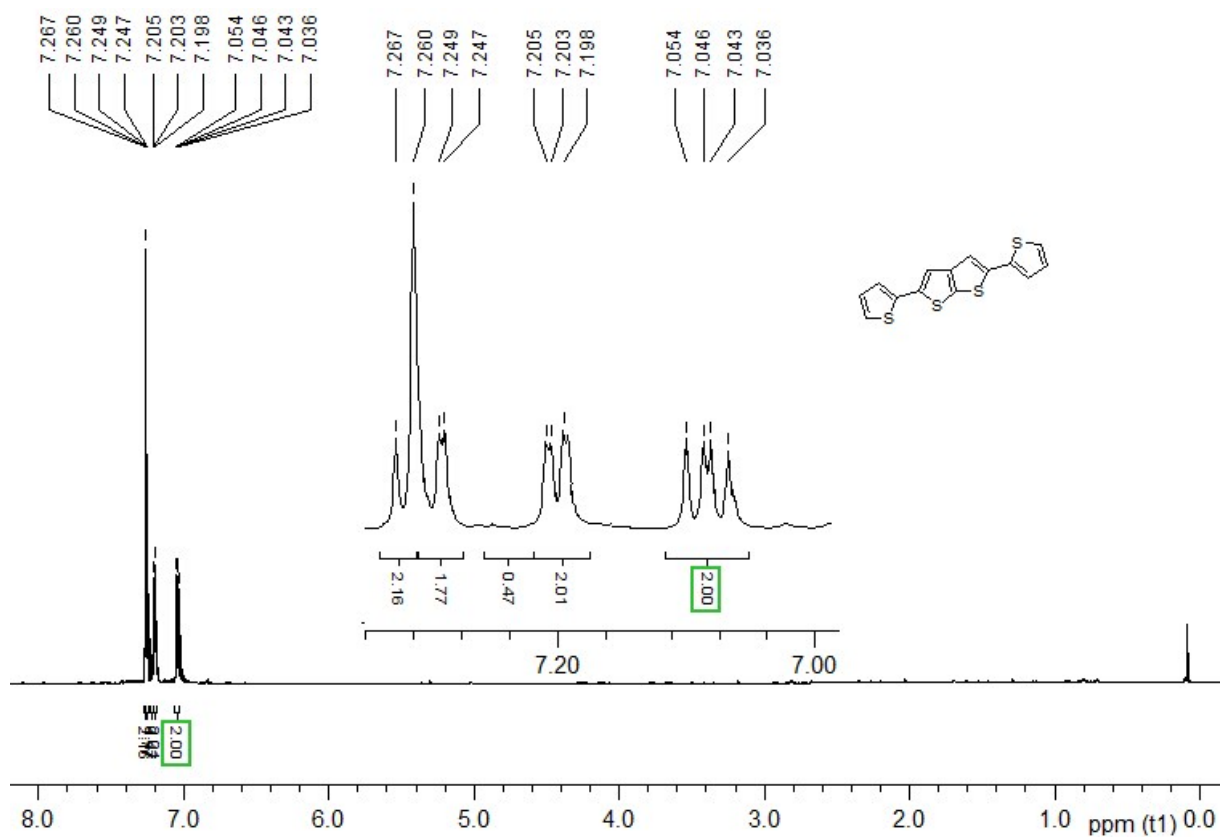


Figure S4. ¹³C-NMR (125 MHz, CDCl₃) spectrum of 6.



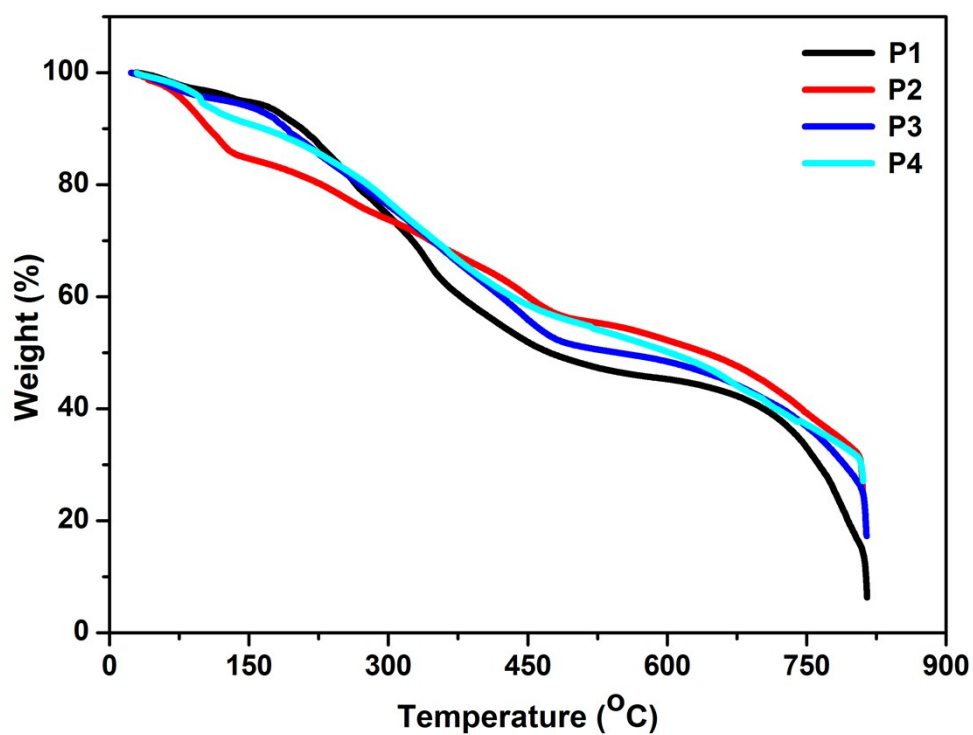


Figure S7. TGA thermograms of polymers **P1-P4**. TGA, thermogravimetric analysis.

Absorption and Emission Spectra in Thin Film

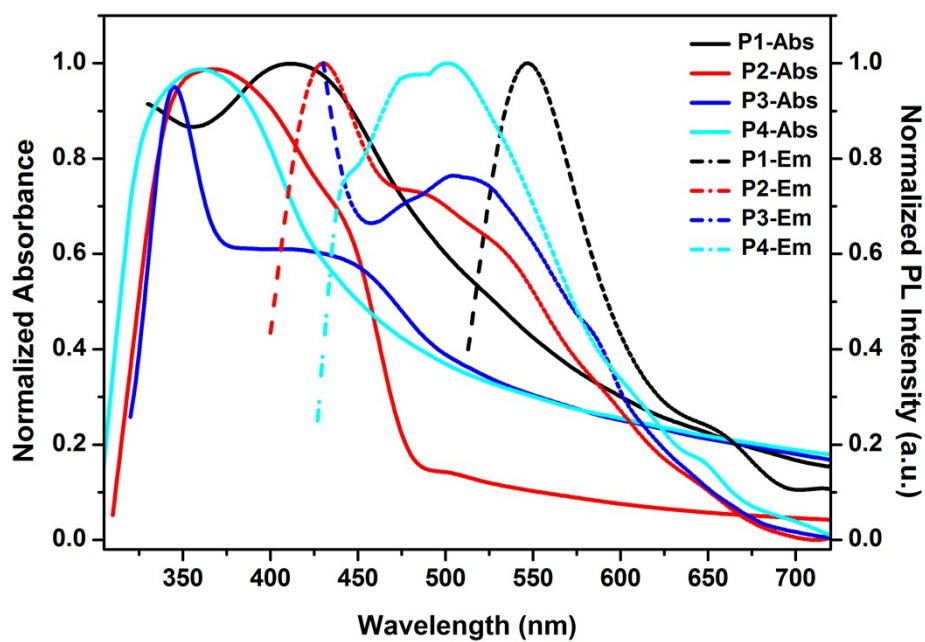


Figure S8. Absorption and emission spectra of **P1-P4** in spin-coated film.

Absorption and Emission Titration Spectra

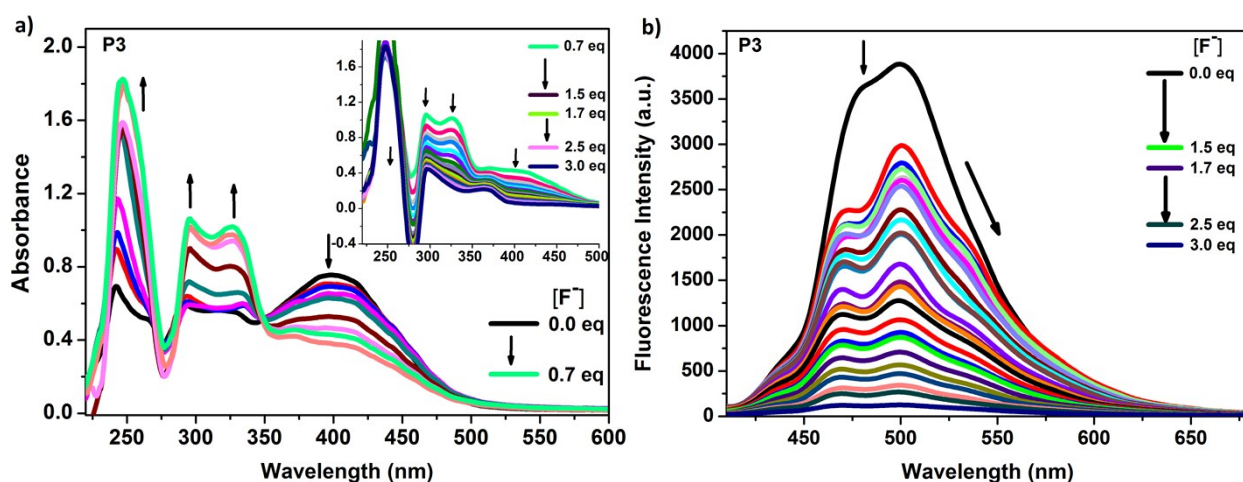


Figure S9. a) Absorption spectra and b) emission spectra ($\lambda_{\text{exc}}=400$ nm) of **P3** (1×10^{-5} M based on boron sites) in THF in the presence of various amounts of TBAF.

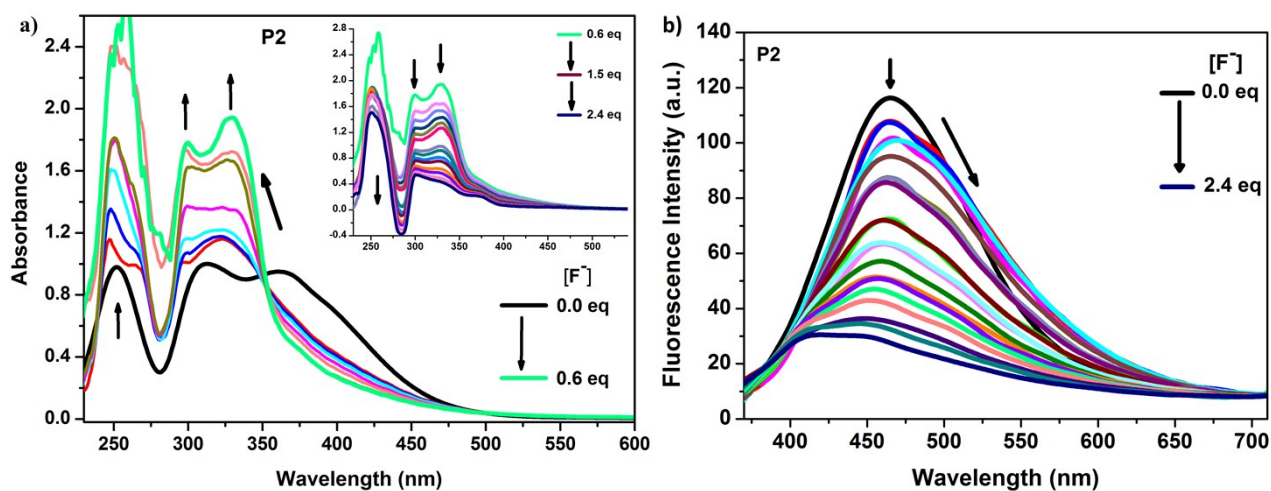


Figure S10. a) Absorption spectra and b) emission spectra ($\lambda_{\text{exc}}=370$ nm) of **P2** (1×10^{-5} M based on boron sites) in THF in the presence of various amounts of TBAF.

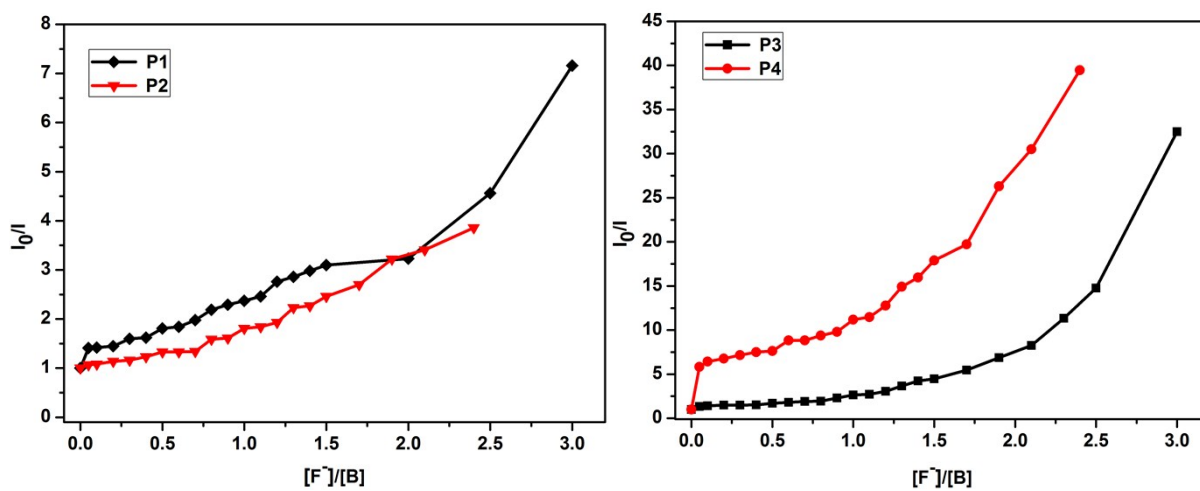


Figure S11. Stern-Volmer plots of the fluorescence intensity change (I_0/I) as a function of $[F^-]$ for polymers **P1-P4**.

Computation

Molecular Orbitals

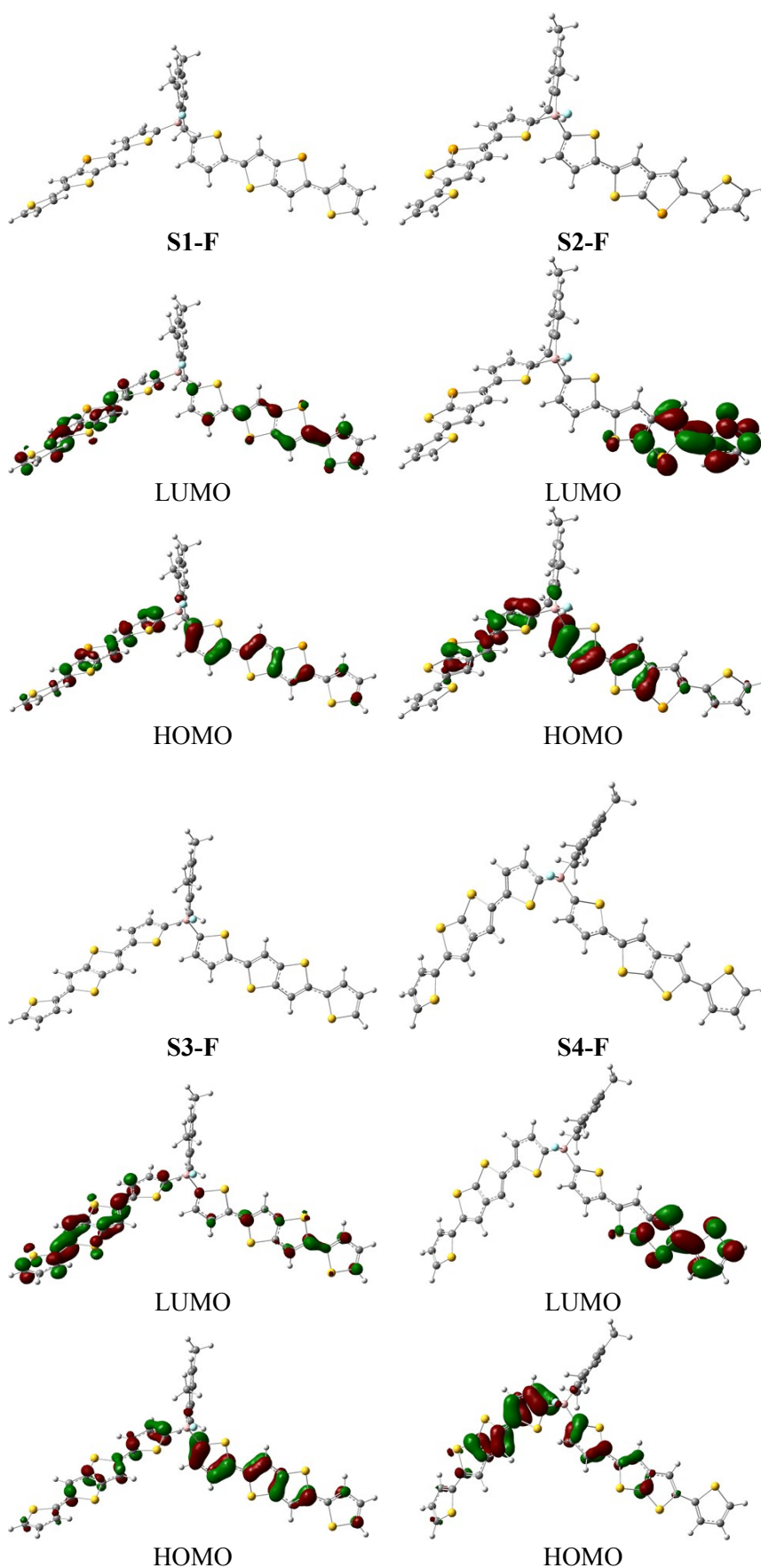


Figure S12. FMOs (isosurface value = 0.04 au) of segments **S1-F** – **S4-F** at (PCM:THF)-B3LYP/6-31G(d) level.

Absorbance and Emission Spectra

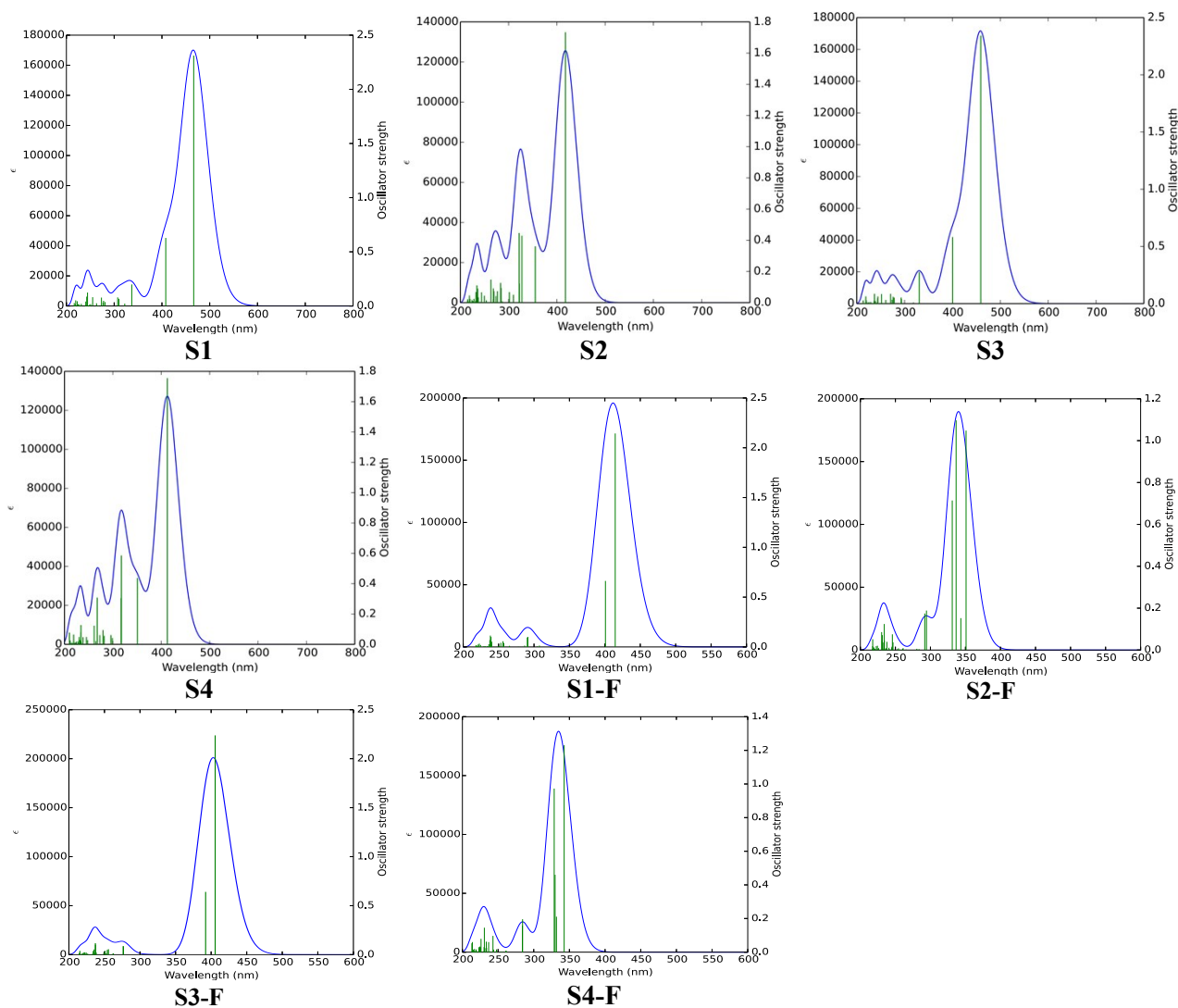


Figure S13. Absorption spectra predicted at the (CPCM:THF)-CAM-TD-B3LYP/6-311++G(d,p) level.

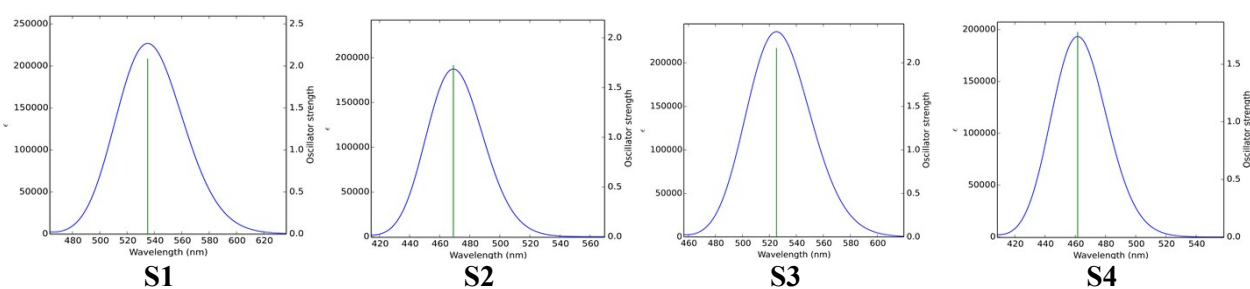


Figure S14. Emission spectra predicted at the (CPCM:THF)-CAM-TD-B3LYP/6-311++G(d,p) level.

Table S1. Computed ((CPCM:THF)-CAM-TD-B3LYP/6-311++G(d,p)) and experimental $\lambda_{\text{emission}}$ values.

Dimer	$\lambda_{\text{emission}}^{\text{calc.}}$ (nm)	$\lambda_{\text{emission}}^{\text{exp.}}$ (nm)
S1	535	542,572(s)
S2	465	464
S3	525	500
S4	461	444

Cartesian Coordinates

M1

C 1.3338090 1.1456970 -0.0252430
C -0.0344720 0.7693600 -0.0183080
H 1.6694460 2.1775160 -0.0375230
C -0.3127550 -0.5936840 -0.0247300
S -1.5141560 1.6992600 -0.0160140
C -1.6920170 -0.9092880 -0.0405340
H -2.0921700 -1.9165280 -0.0653180
C -2.4886100 0.2181290 -0.0416320
C -3.9334630 0.3038800 -0.0532810
C -4.7357090 1.3949670 -0.3178790
S -4.9275960 -1.1012660 0.3105730
C -6.1289450 1.1109300 -0.2390980
H -4.3383320 2.3704840 -0.5779790
C -6.3901170 -0.1924600 0.0836690
H -6.9035910 1.8473370 -0.4226280
H -7.3484490 -0.6796700 0.2033360
C 2.2102030 0.0843840 -0.0313250
C 3.6548880 0.1124490 -0.0381010
C 4.5380050 -0.9225280 -0.2704310
S 4.5428420 1.5990360 0.2805790
C 5.9059630 -0.5344720 -0.2018490
H 4.2121870 -1.9324170 -0.4985210
H 6.7333310 -1.2167930 -0.3627970
Se 1.2790210 -1.5836420 -0.0236990
C 6.0690390 0.7938940 0.0816820
H 6.9884800 1.3538830 0.1873530

M2

C 1.1301080 1.0255910 -0.0214760
C -0.1837380 0.4529610 0.0063770
H 1.3012100 2.0975550 -0.0472500
C -0.1936860 -0.9381570 0.0090260
C 2.1627100 0.1262840 -0.0391420
C 3.5882400 0.3769140 -0.0694270
C 4.6081060 -0.4694290 -0.4503950
S 4.2482860 1.9299420 0.4280480
C 5.9029090 0.1169760 -0.3564650
H 4.4308730 -1.4789370 -0.8076660
H 6.8180800 -0.4005640 -0.6223180
Se 1.5154730 -1.6777010 -0.0051030
S -1.7908330 -1.6024700 0.0179190
C -2.4893790 0.0336700 0.0436980
H -1.5083140 0.9947320 0.0290030
H -1.7239530 2.0576240 0.0523080
C -3.9303620 0.1934840 0.0681350
C -4.8989860 -0.7169100 0.4336240
S -4.6776080 1.7075730 -0.4220030
C -6.2261620 -0.2077080 0.3336490
H -4.6664980 -1.7173680 0.7834570
H -6.2687600 1.0867930 -0.1055330
C -7.1105800 -0.7816610 0.5876510
H -7.1328180 1.7180390 -0.2637700
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H 6.6972720 2.0880940 0.2527310

M3

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S -1.3609900 -1.5801110 0.2003880
C -0.1294900 0.6779340 -0.0903490
H -1.8900680 2.0130960 -0.3123360
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H 1.8900770 -2.0130880 0.3123080
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C 3.7604410 0.1693980 0.0391160
C 4.5727920 1.2743370 0.1913570
S 4.7411520 -1.2777300 -0.1582970
C 5.9633410 0.9682480 0.1593700
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M4

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C -3.7432370 -0.0537120 0.0913740
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C 4.7092780 0.9009320 0.3282320
S 4.4947170 -1.6150980 -0.2040350
C 6.0383960 0.3886080 0.2849520
H 4.4732590 1.9368790 0.5481140
C 6.0843780 -0.9520560 0.0179880
H 6.9216700 0.9942160 0.4557390
H 6.9507140 -1.5948710 -0.0619770
S -1.5959720 1.7013390 -0.2487520
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S1

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H 13.2089240 -3.3740380 -0.9034100
C 12.7393050 -1.4096610 -0.1270890
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S3

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C 8.9193950 -2.1213230 0.0184780
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