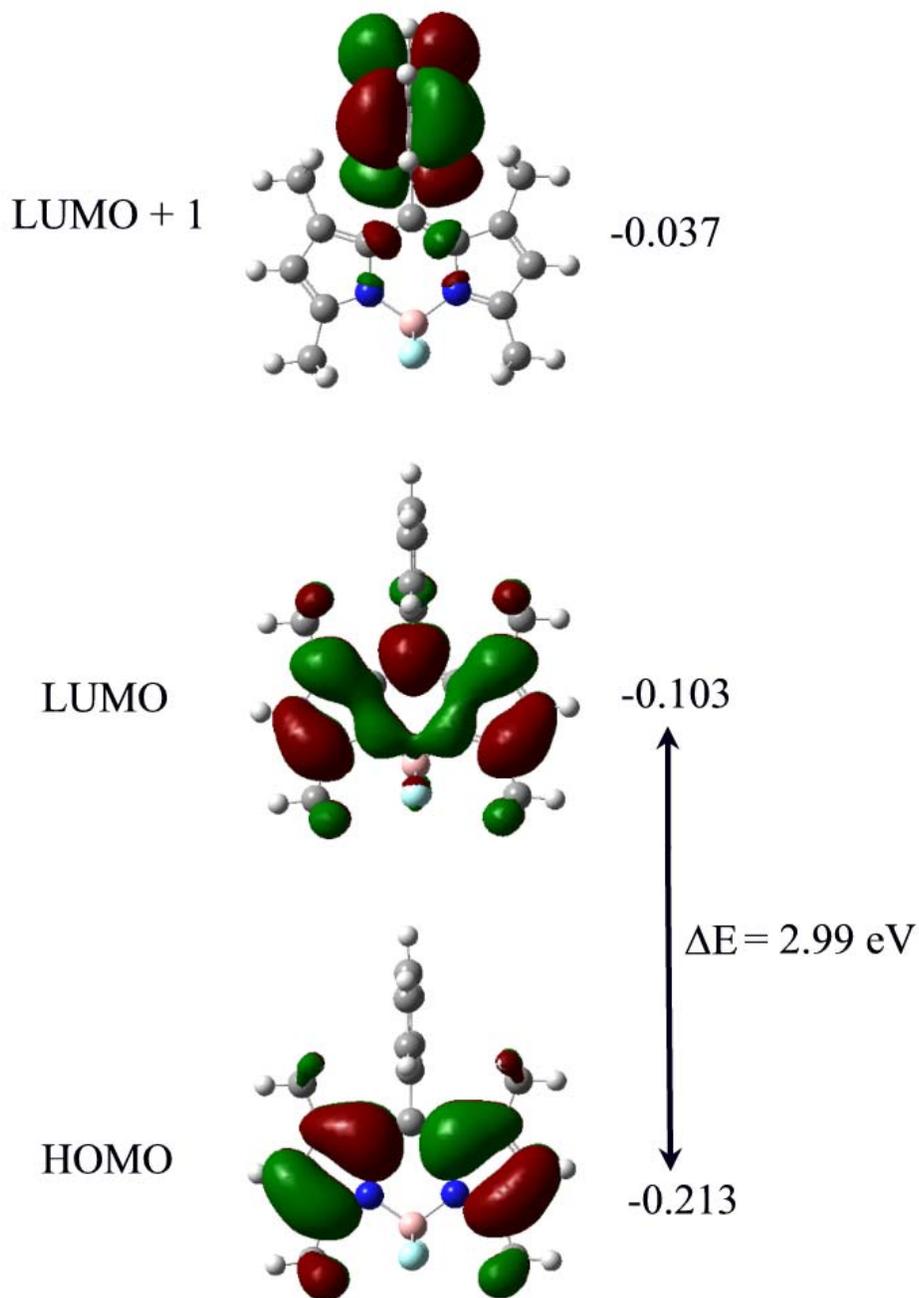


## Supporting Information

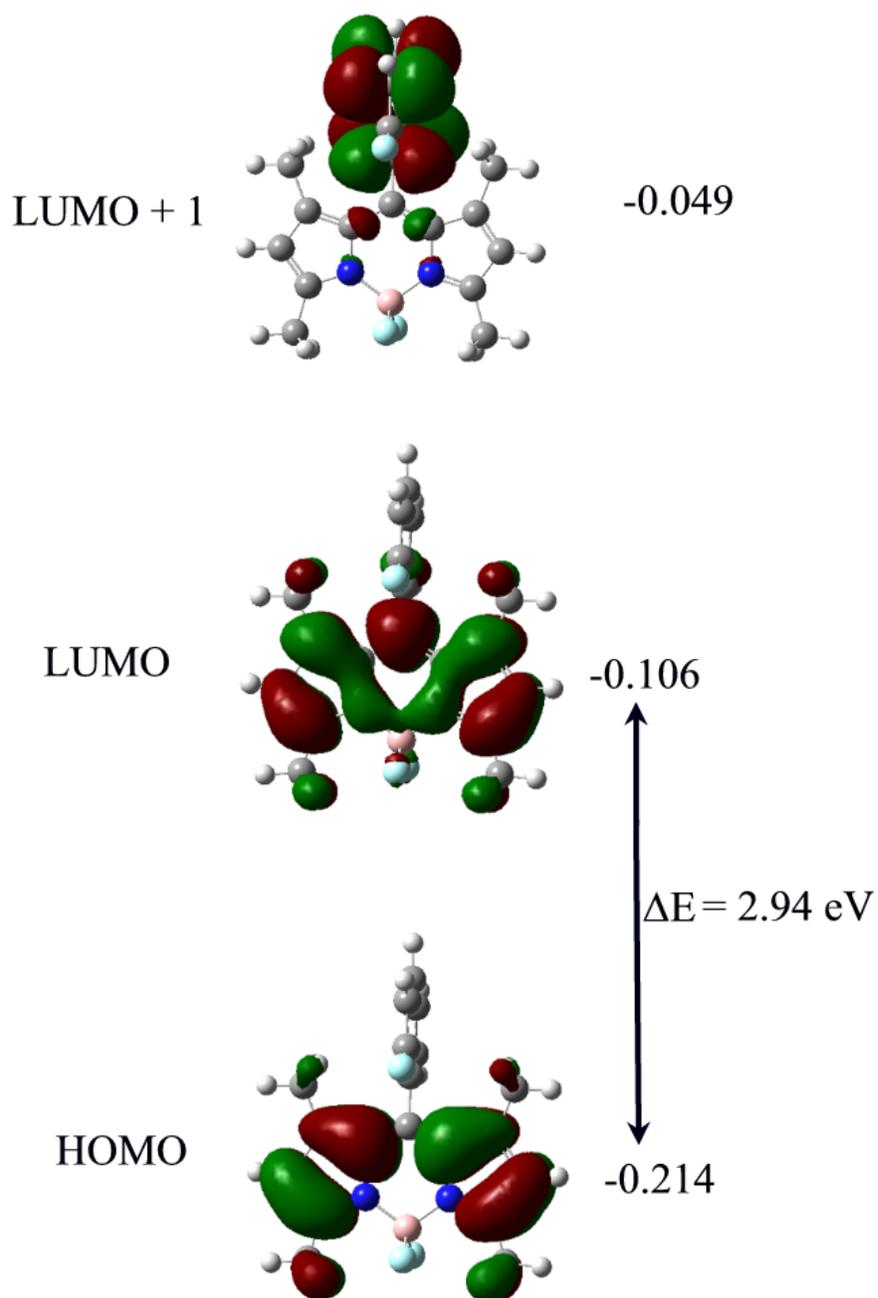
### The fluorine effect: Photophysical properties of borondipyrromethene (Bodipy) dyes appended at the meso position with fluorinated aryl groups

Mohammed A. H. Alamiry,<sup>a</sup> Andrew C. Benniston,<sup>a\*</sup> Jerry Hagon,<sup>a</sup> Thomas P. L. Winstanley,<sup>a</sup> Helge Lemmetyinen<sup>b</sup> and Nikolai V. Tkachenko<sup>b</sup>

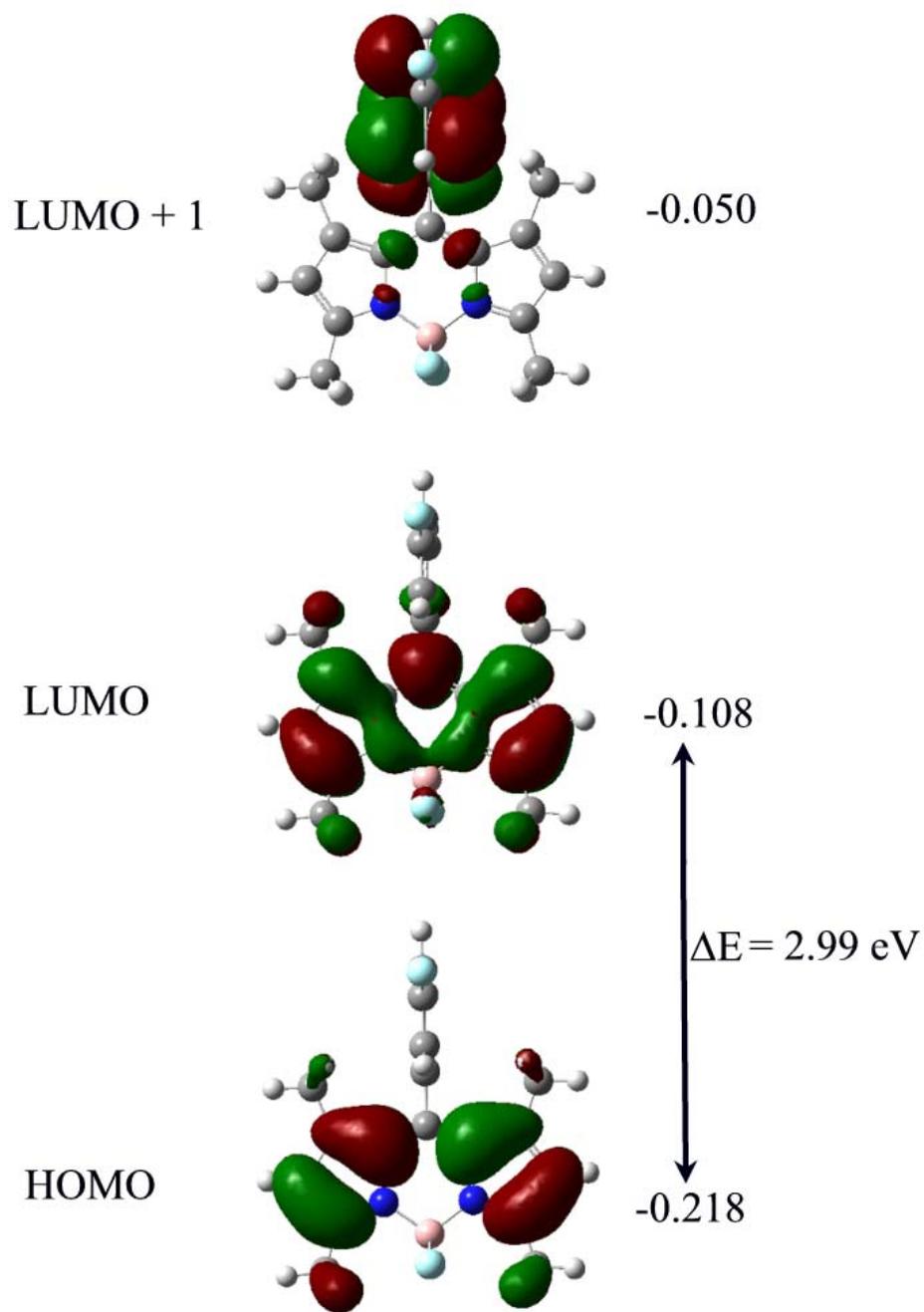
- S1.** Selected molecular orbitals for **BD-Ph** as calculated by DFT and B3LYP and the 6-311G<sup>++</sup> basis set.
- S2.** Selected molecular orbitals for **BD-1Fo** as calculated by DFT and B3LYP and the 6-311G<sup>++</sup> basis set.
- S3.** Selected molecular orbitals for **BD-1Fm** as calculated by DFT and B3LYP and the 6-311G<sup>++</sup> basis set.
- S4.** Selected molecular orbitals for **BD-1Fp** as calculated by DFT and B3LYP and the 6-311G<sup>++</sup> basis set.
- S5.** Selected molecular orbitals for **BD-2F** as calculated by DFT and B3LYP and the 6-311G<sup>++</sup> basis set.
- S6.** Selected molecular orbitals for **BD-3F** as calculated by DFT and B3LYP and the 6-311G<sup>++</sup> basis set.
- S7.** Selected molecular orbitals for **BD-5F** as calculated by DFT and B3LYP and the 6-311G<sup>++</sup> basis set.
- S8.** Comparison of the HOMO-LUMO gap for **BD-Ph** (1), **BD-1Fo** (2), **BD-1Fm** (3), **BD-1Fp** (4), **BD-2F** (5), **BD-3F** (6) and **BD-5F** (7).
- S9.** Effect of applied pressure on the uncorrected fluorescence spectra recorded for **BD-2F** in dilute methylcyclohexane. Insert shows the change in relative peak area with respect to the applied pressure.
- S10.** Effect of applied pressure on the uncorrected fluorescence spectra recorded for **BD-1Fp** in dilute methylcyclohexane. Insert shows the change in relative peak area with respect to the applied pressure.
- S11.** Effect of applied pressure on the uncorrected fluorescence spectra recorded for **BD-3F** in dilute methylcyclohexane. Insert shows the change in relative peak area with respect to the applied pressure.
- S12.** Effect of applied pressure on the uncorrected fluorescence spectra recorded for **BD-1Fm** in dilute methylcyclohexane. Insert shows the change in relative peak area with respect to the applied pressure.



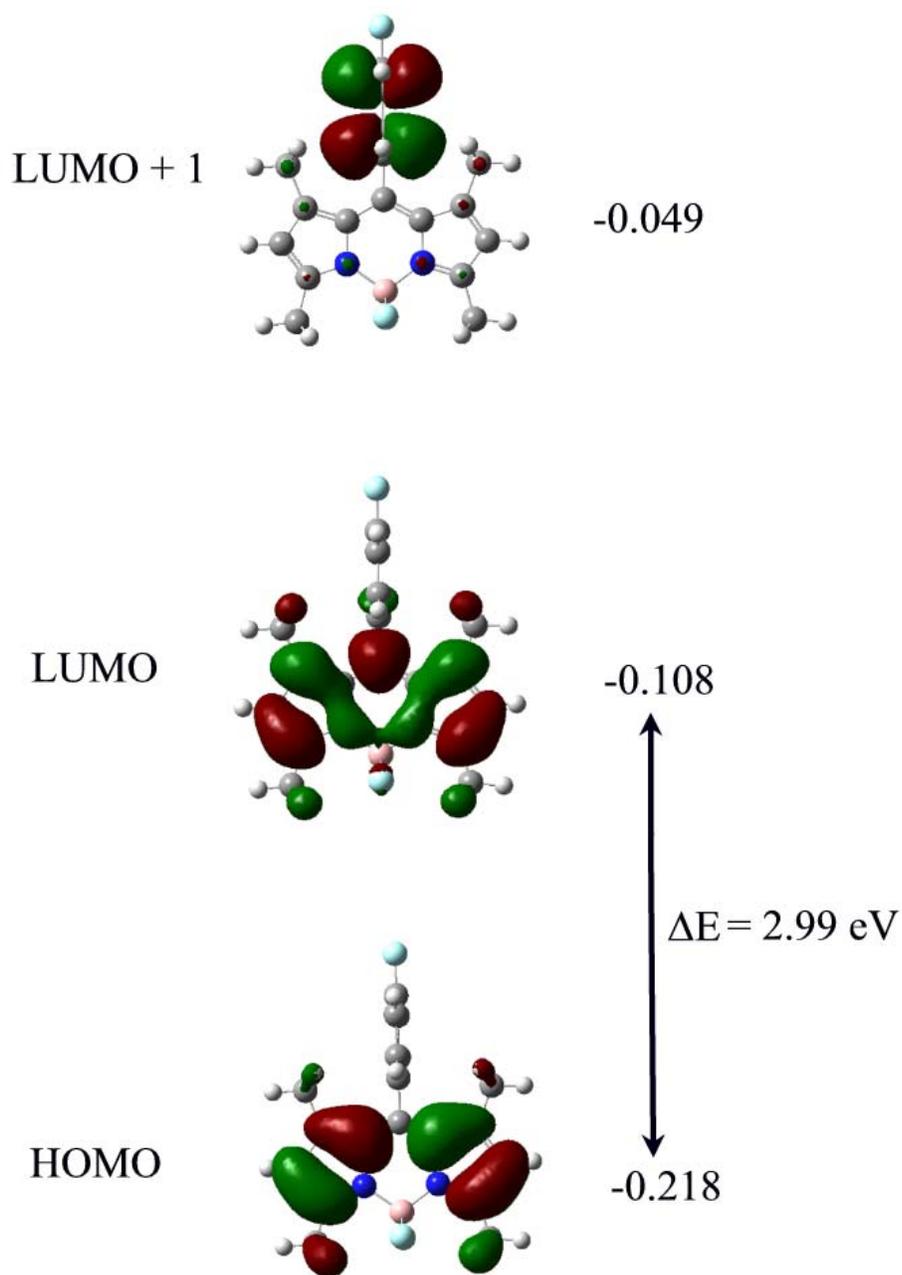
**S1.** Selected molecular orbitals for **BD-Ph** as calculated by DFT and B3LYP and the 6-311G<sup>++</sup> basis set.



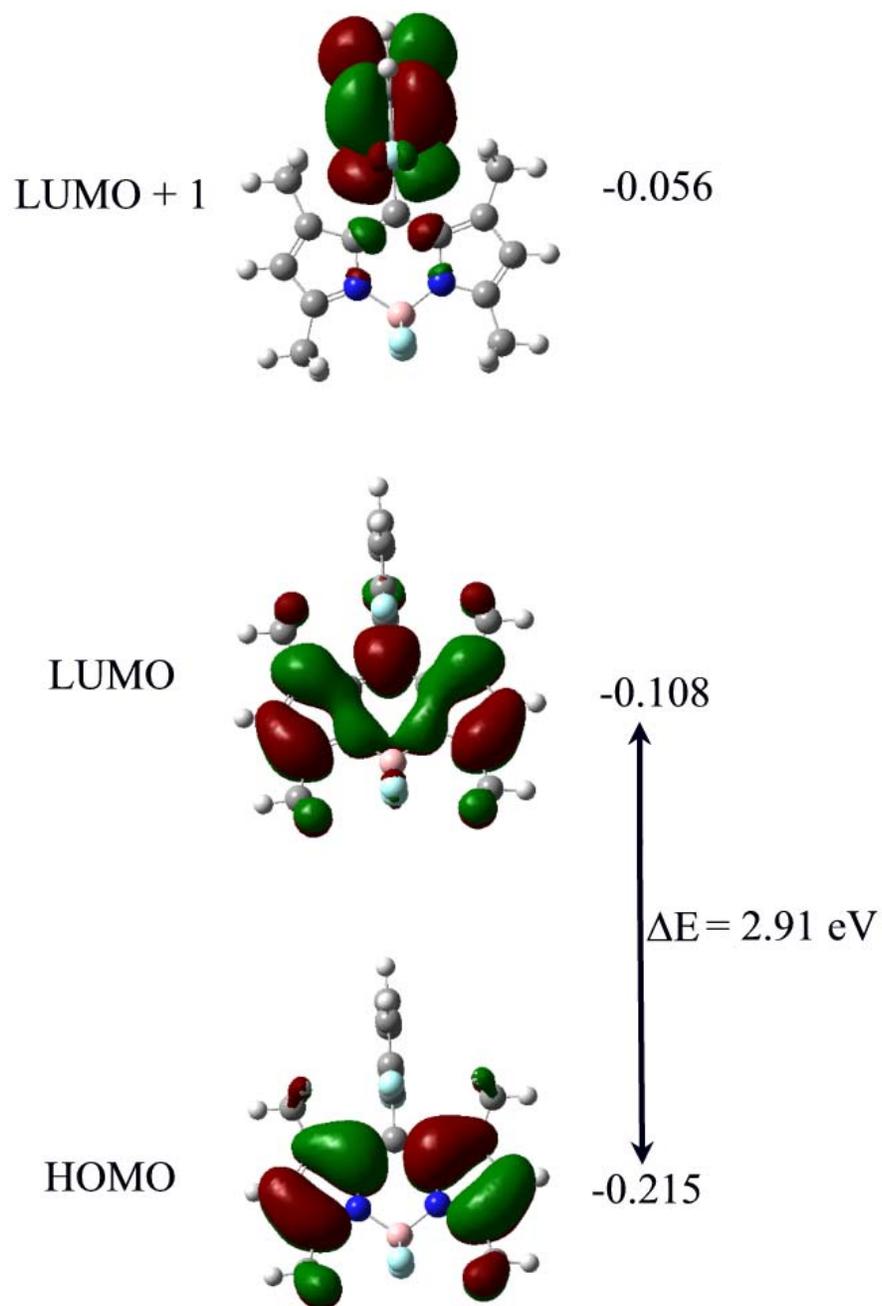
**S2.** Selected molecular orbitals for **BD-1Fo** as calculated by DFT and B3LYP and the 6-311G<sup>++</sup> basis set.



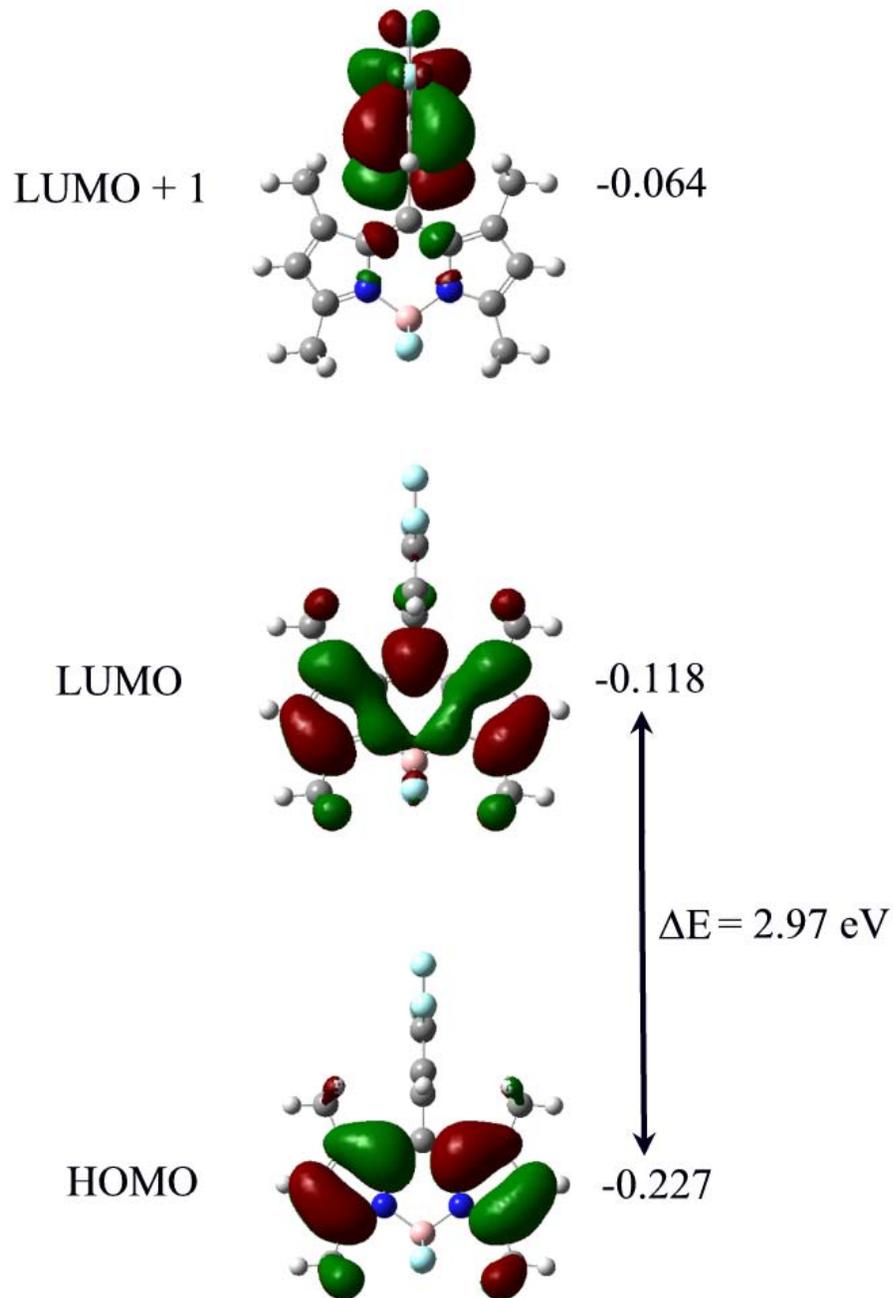
**S3.** Selected molecular orbitals for **BD-1Fm** as calculated by DFT and B3LYP and the 6-311G<sup>++</sup> basis set.



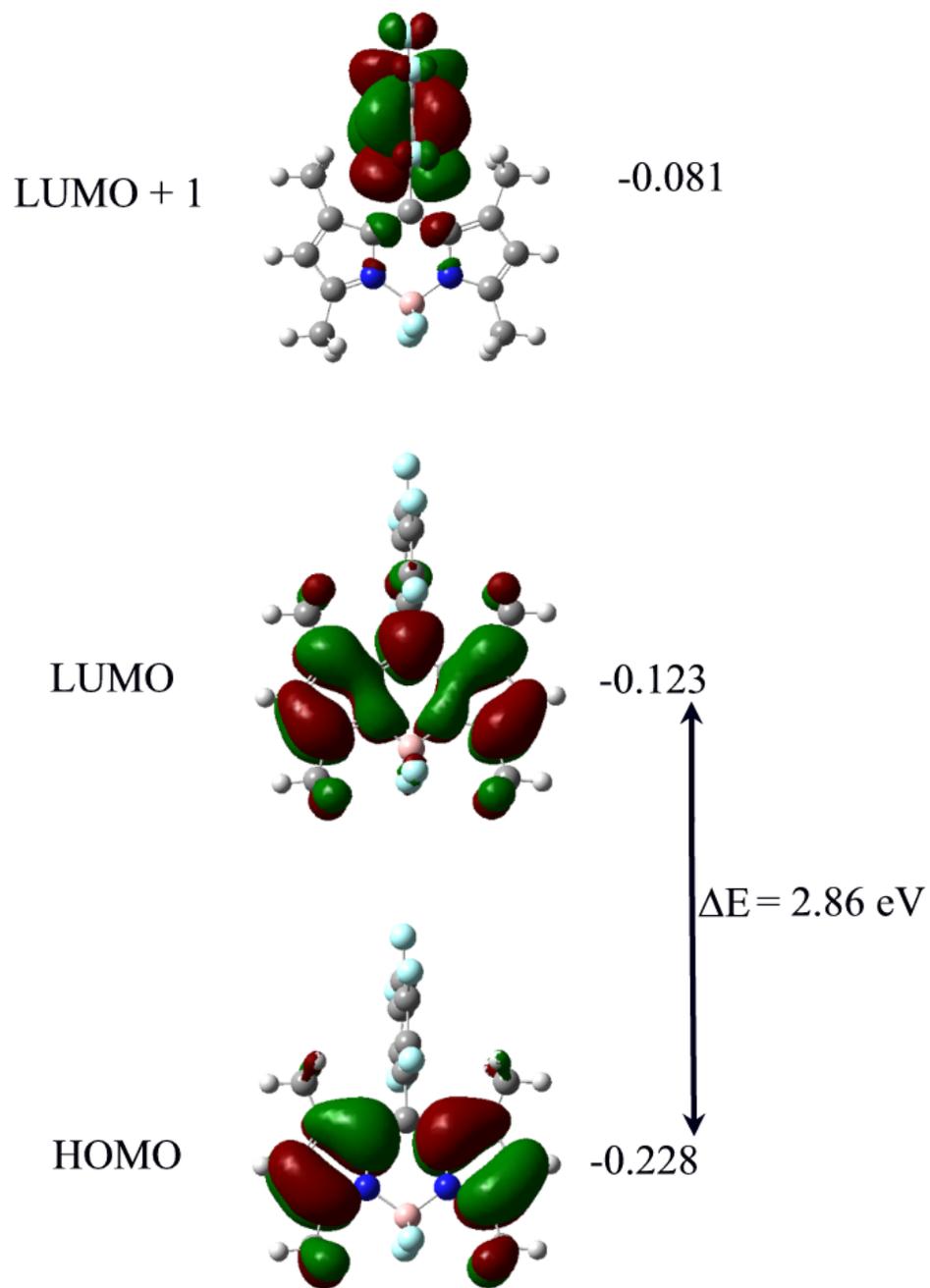
**S4.** Selected molecular orbitals for **BD-1Fp** as calculated by DFT and B3LYP and the 6-311G<sup>++</sup> basis set.



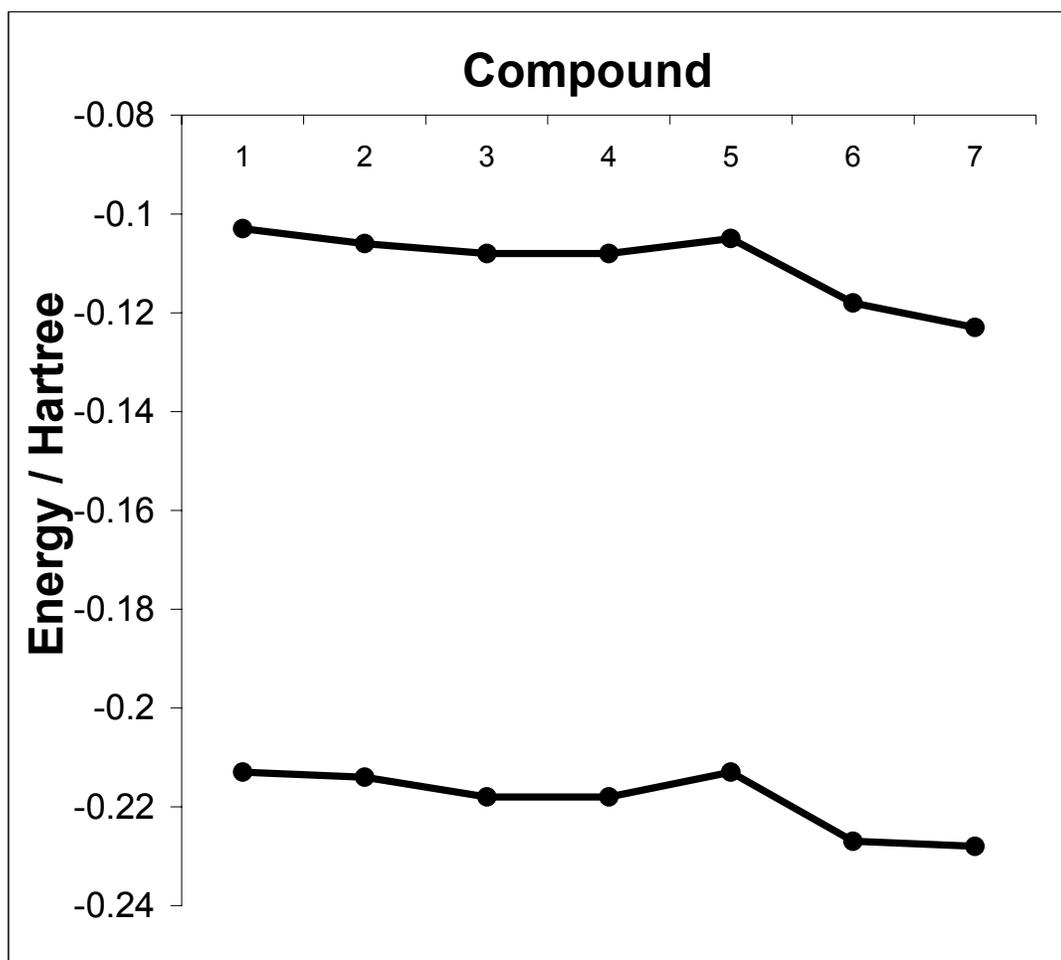
**S5.** Selected molecular orbitals for **BD-2F** as calculated by DFT and B3LYP and the 6-311G<sup>++</sup> basis set.



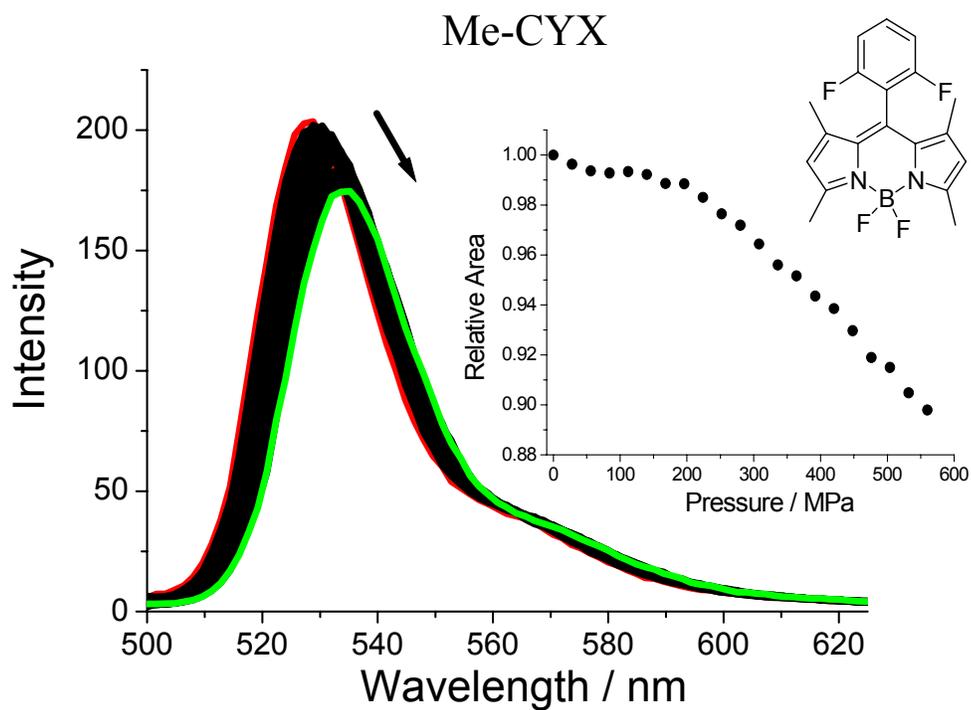
**S6.** Selected molecular orbitals for **BD-3F** as calculated by DFT and B3LYP and the 6-311G<sup>++</sup> basis set.



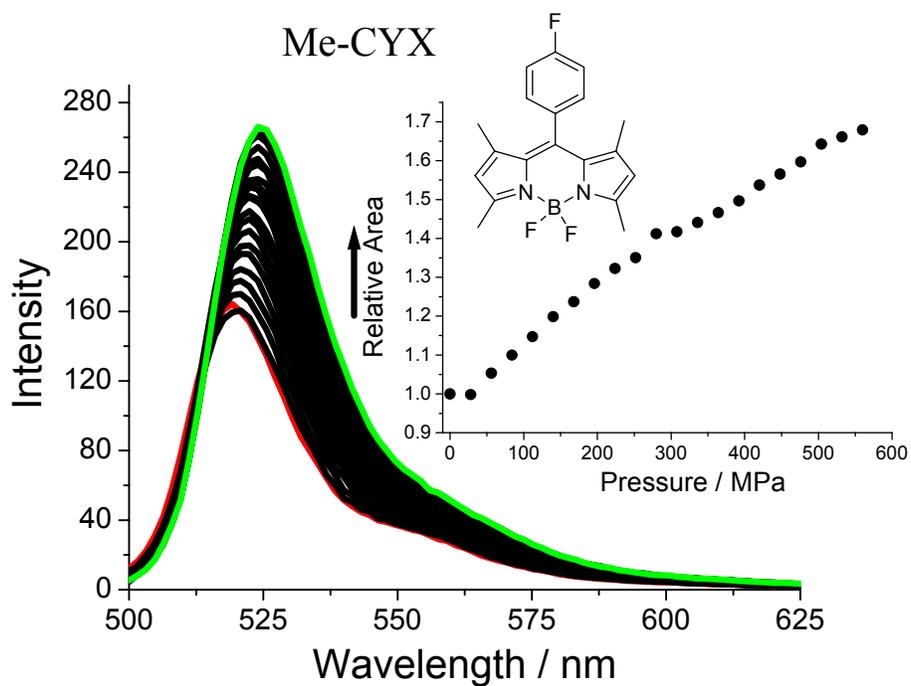
S7. Selected molecular orbitals for **BD-5F** as calculated by DFT and B3LYP and the 6-311G<sup>++</sup> basis set.



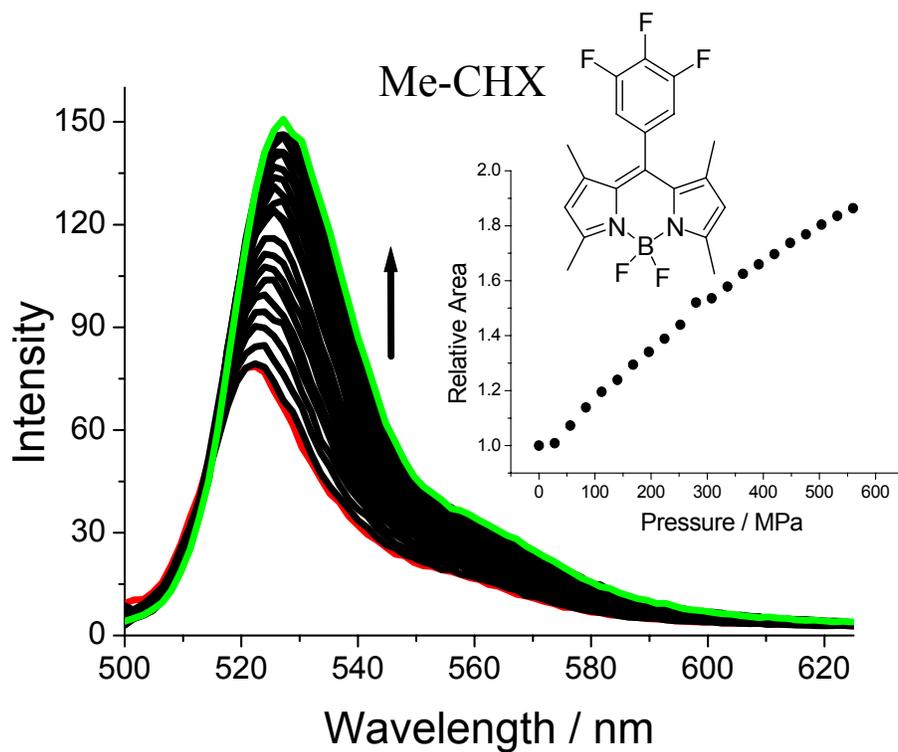
**S8.** Comparison of the HOMO-LUMO gap for **BD-Ph** (1), **BD-1Fo** (2), **BD-1Fm** (3), **BD-1Fp** (4), **BD-2F** (5), **BD-3F** (6) and **BD-5F** (7).



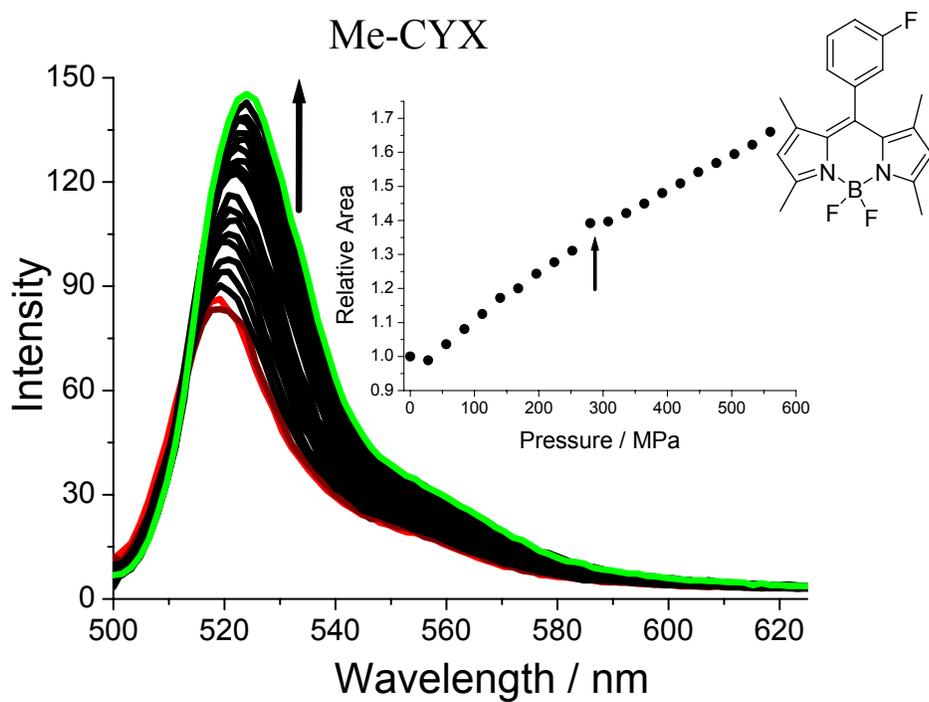
**S9.** Effect of applied pressure on the uncorrected fluorescence spectra recorded for **BD-2F** in dilute methylcyclohexane. Insert shows the change in relative peak area with respect to the applied pressure.



**S10.** Effect of applied pressure on the uncorrected fluorescence spectra recorded for **BD-1Fp** in dilute methylcyclohexane. Insert shows the change in relative peak area with respect to the applied pressure.



**S11.** Effect of applied pressure on the uncorrected fluorescence spectra recorded for **BD-3F** in dilute methylcyclohexane. Insert shows the change in relative peak area with respect to the applied pressure.



**S12.** Effect of applied pressure on the uncorrected fluorescence spectra recorded for **BD-1Fm** in dilute methycyclohexane. Insert shows the change in relative peak area with respect to the applied pressure.