

Bodipy Dyes with Thienylthia-Substituents – Synthesis, Redox and Fluorescent Properties

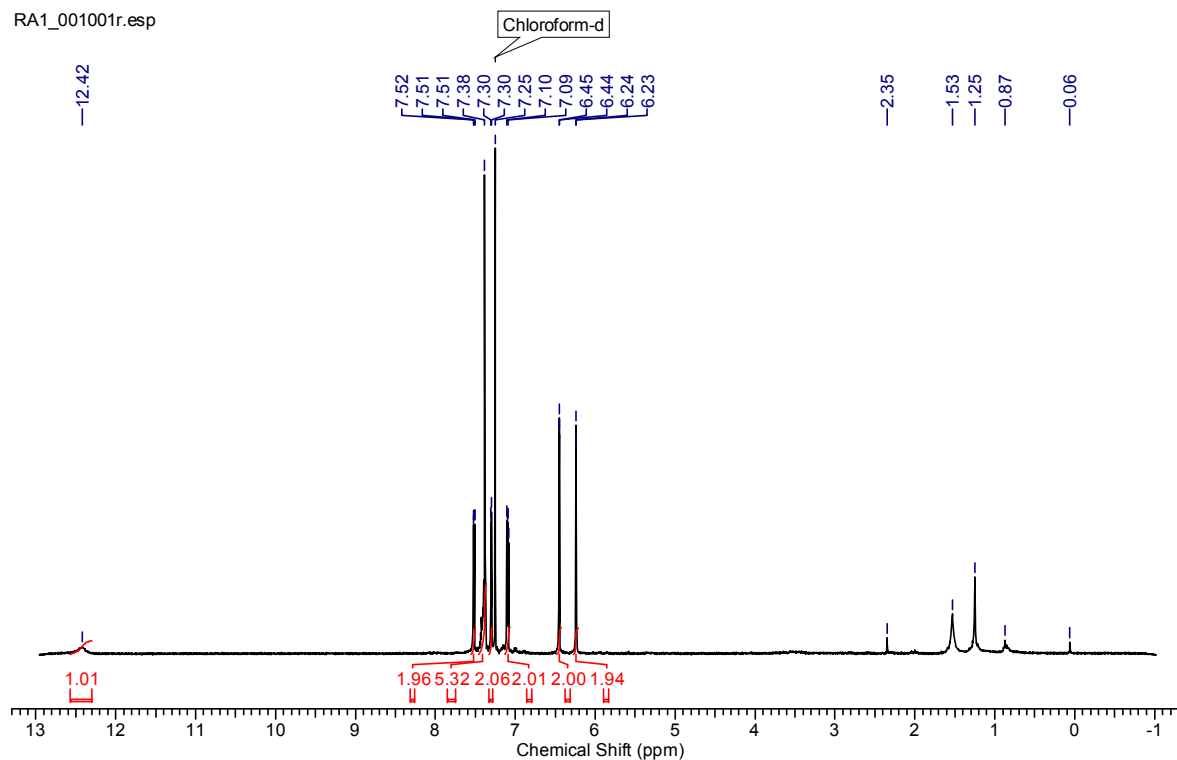
E.A. Leushina, I.A. Usol'tsev, S.I. Bezzubov, A.A. Moiseeva, M.V. Terenina, A.V. Anisimov, I. Taydakov, A. Khoroshutin

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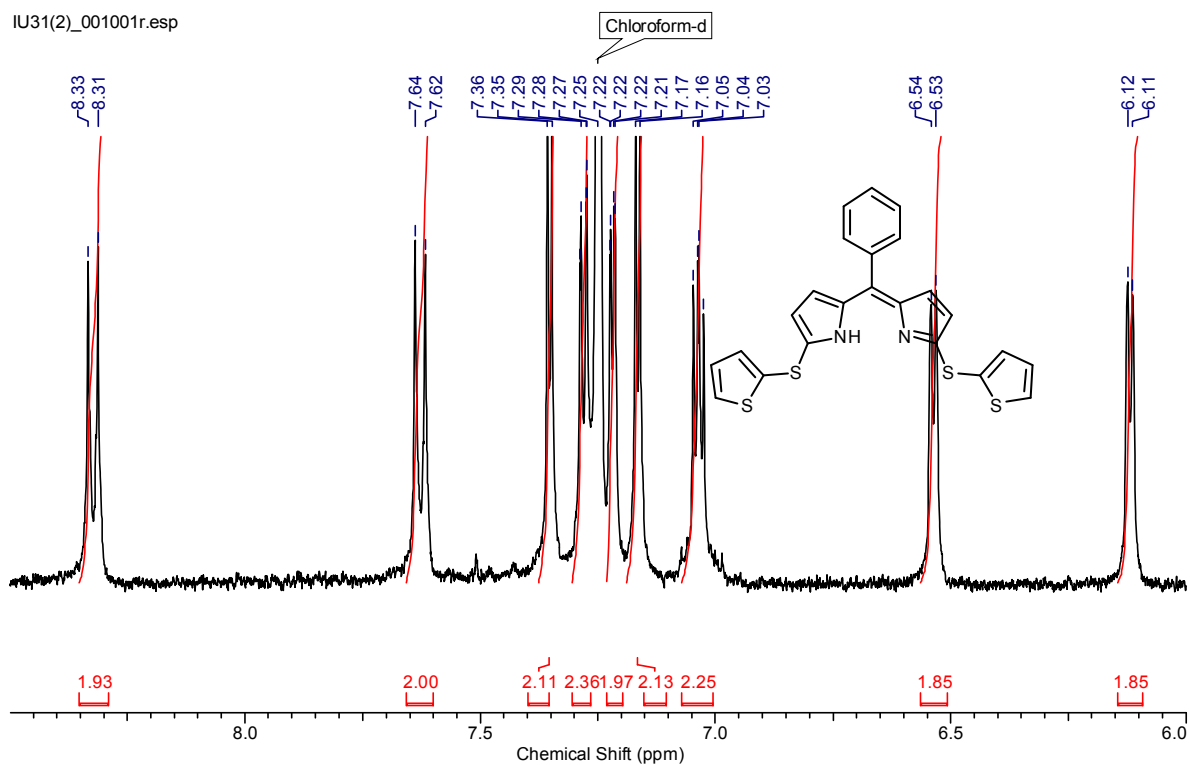
1.NMR spectra of the studied compounds

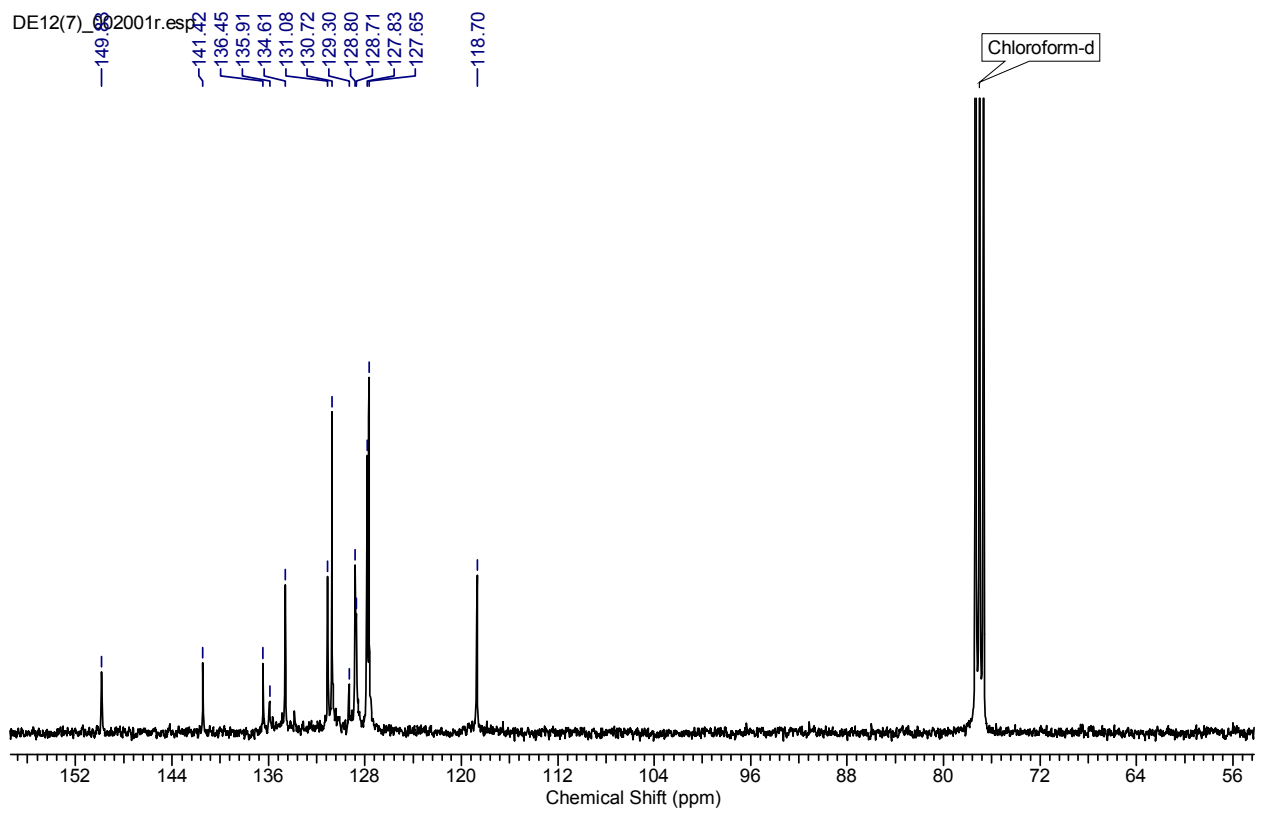
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IU31(2)_001001r.esp

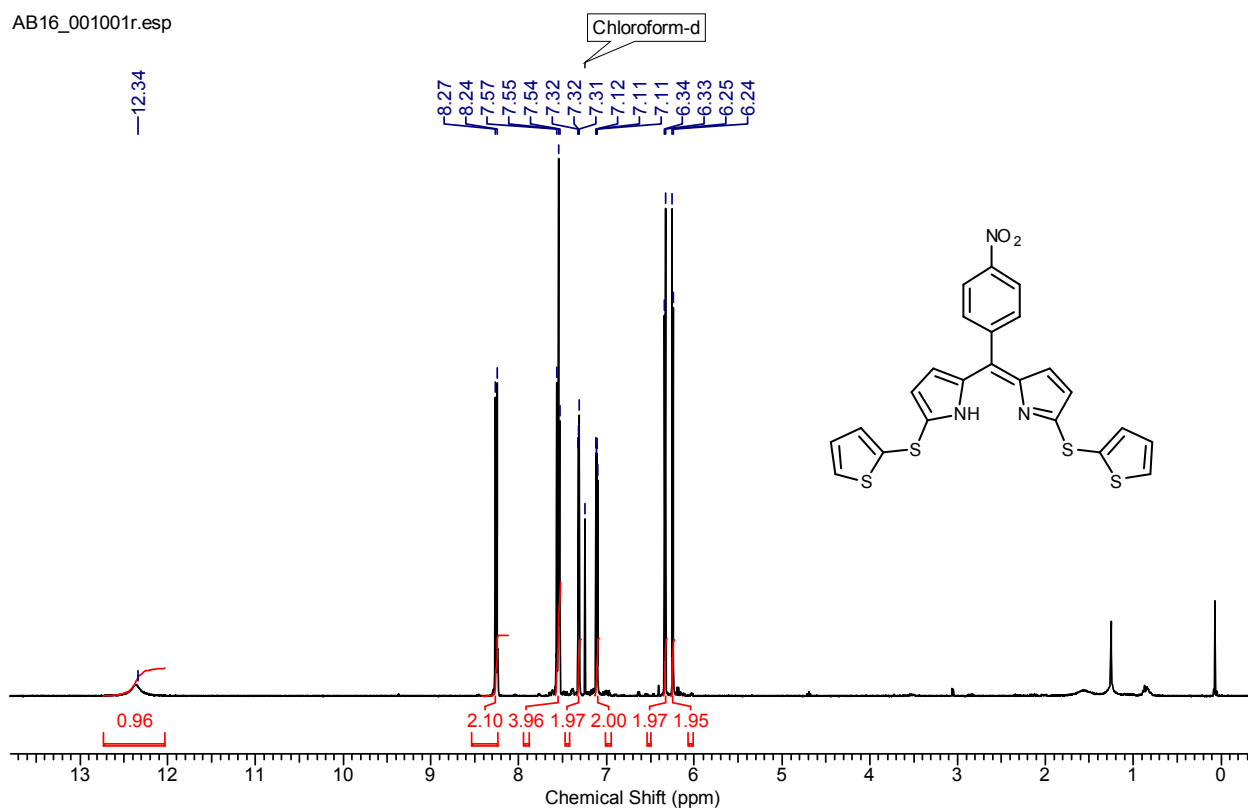




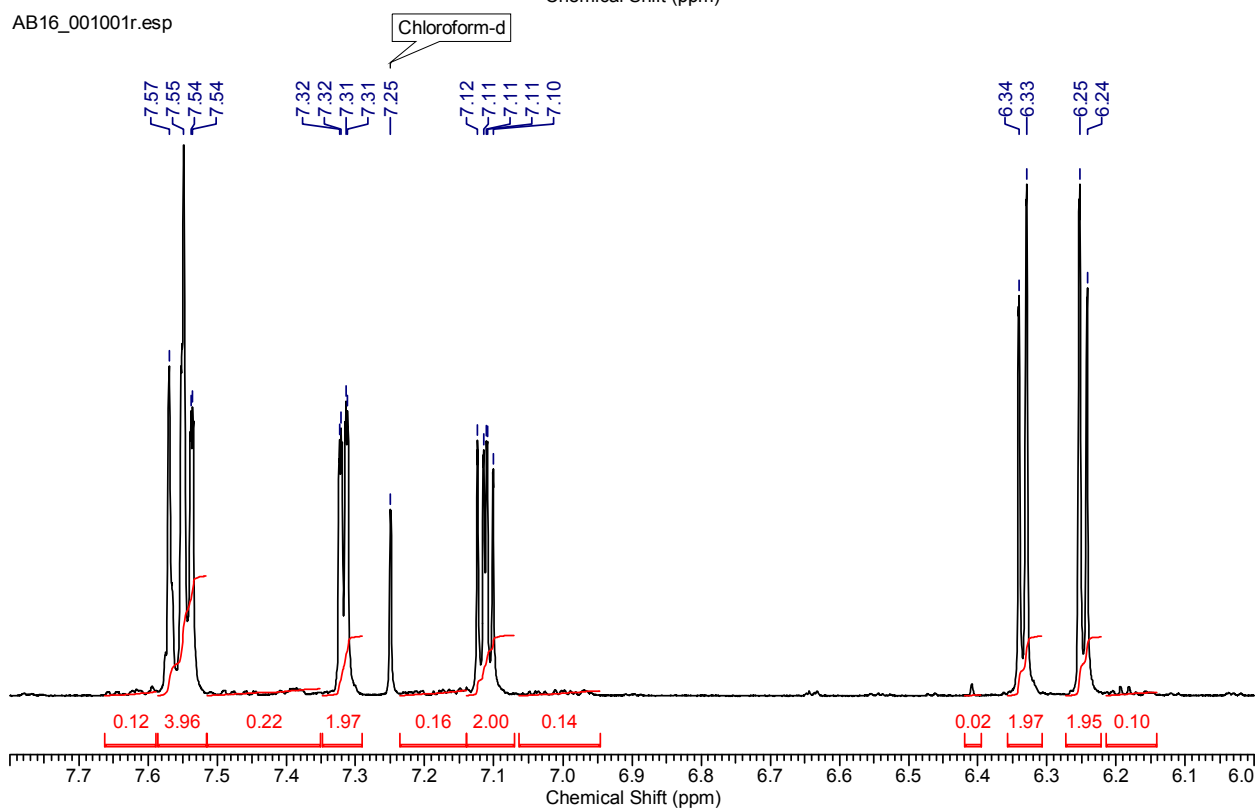
RA1 DE12(7)

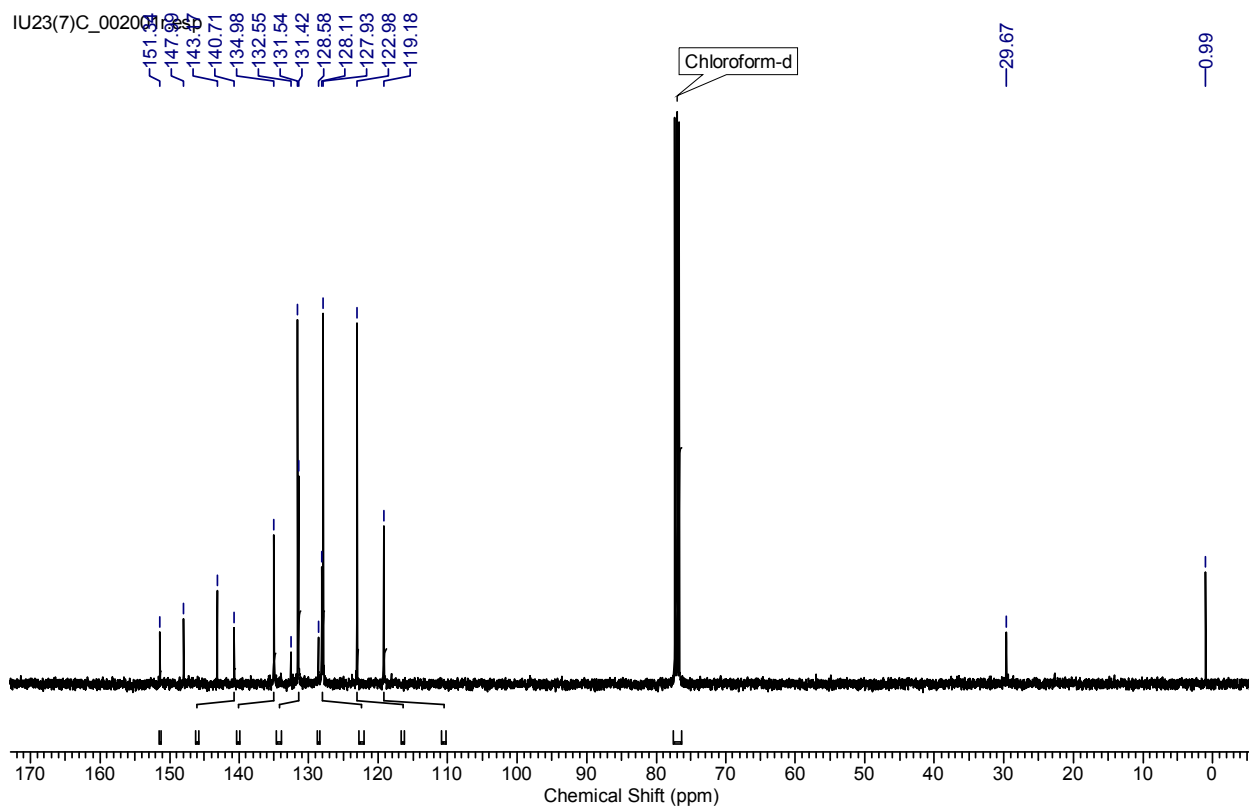
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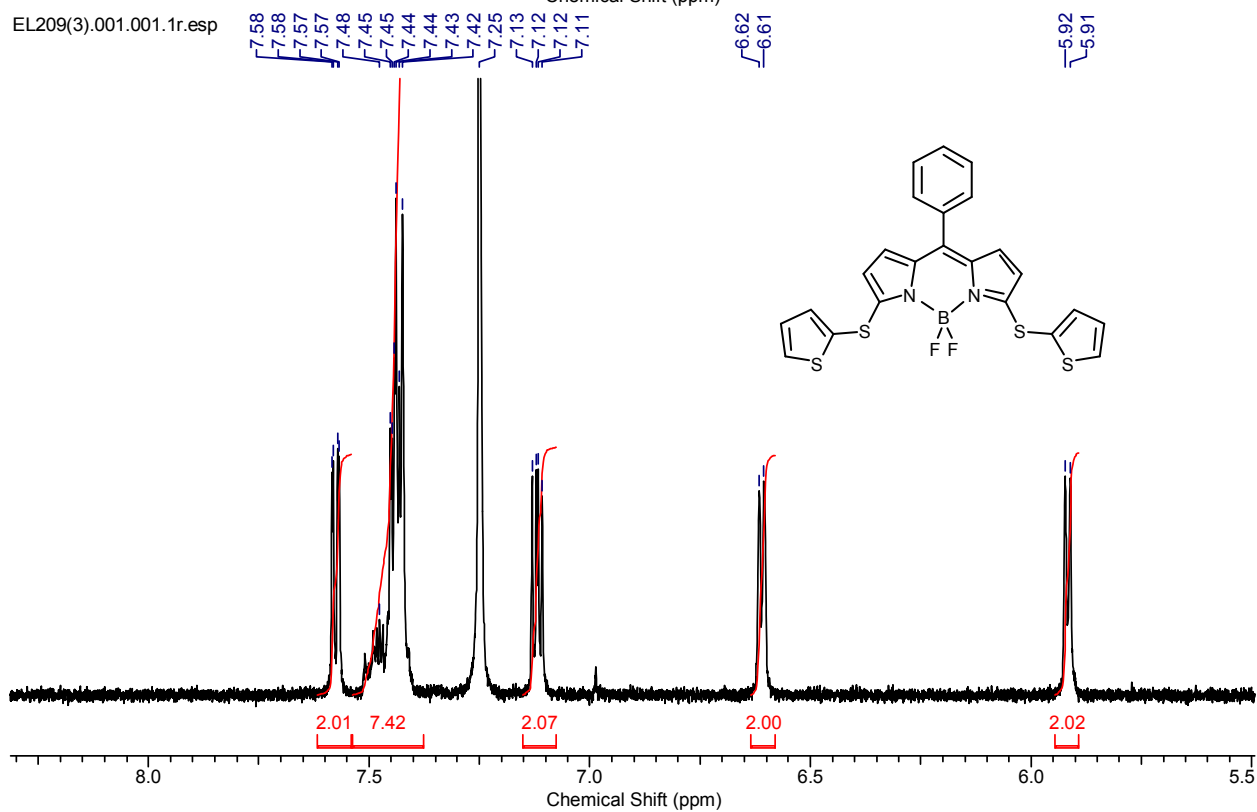
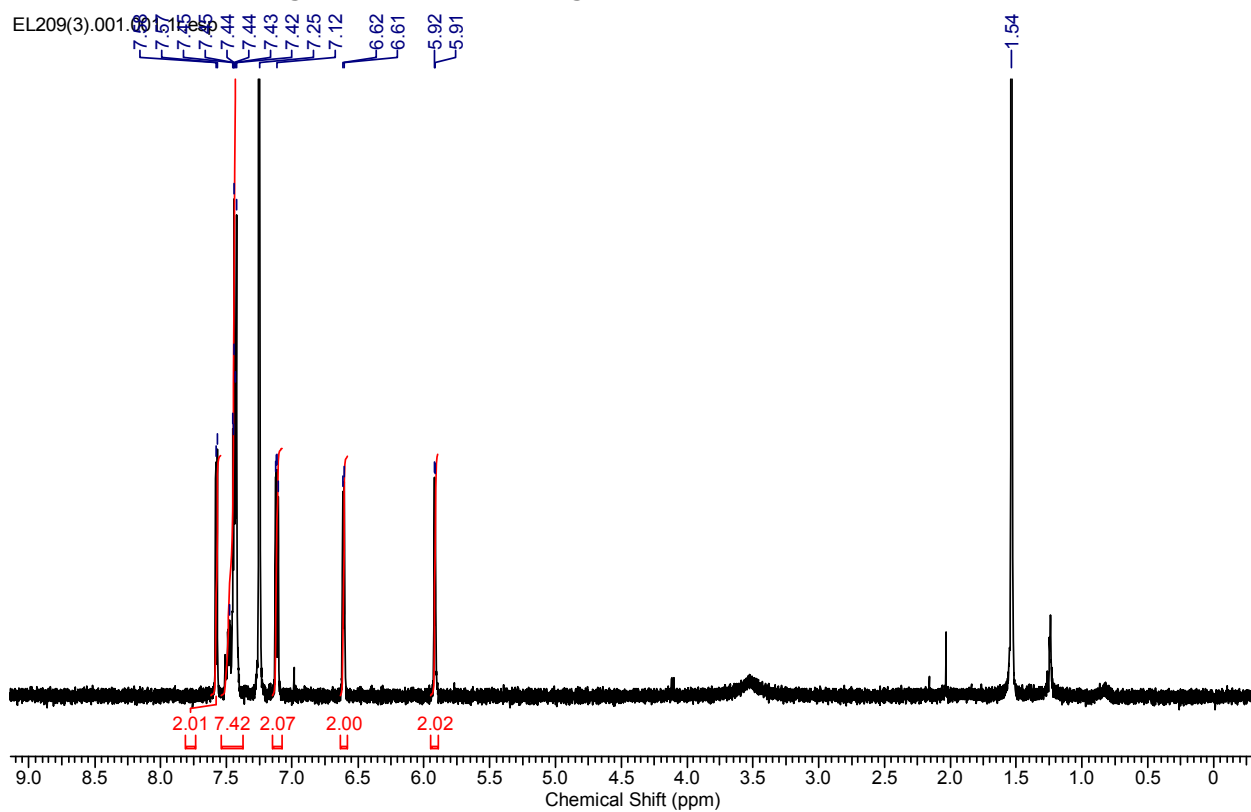
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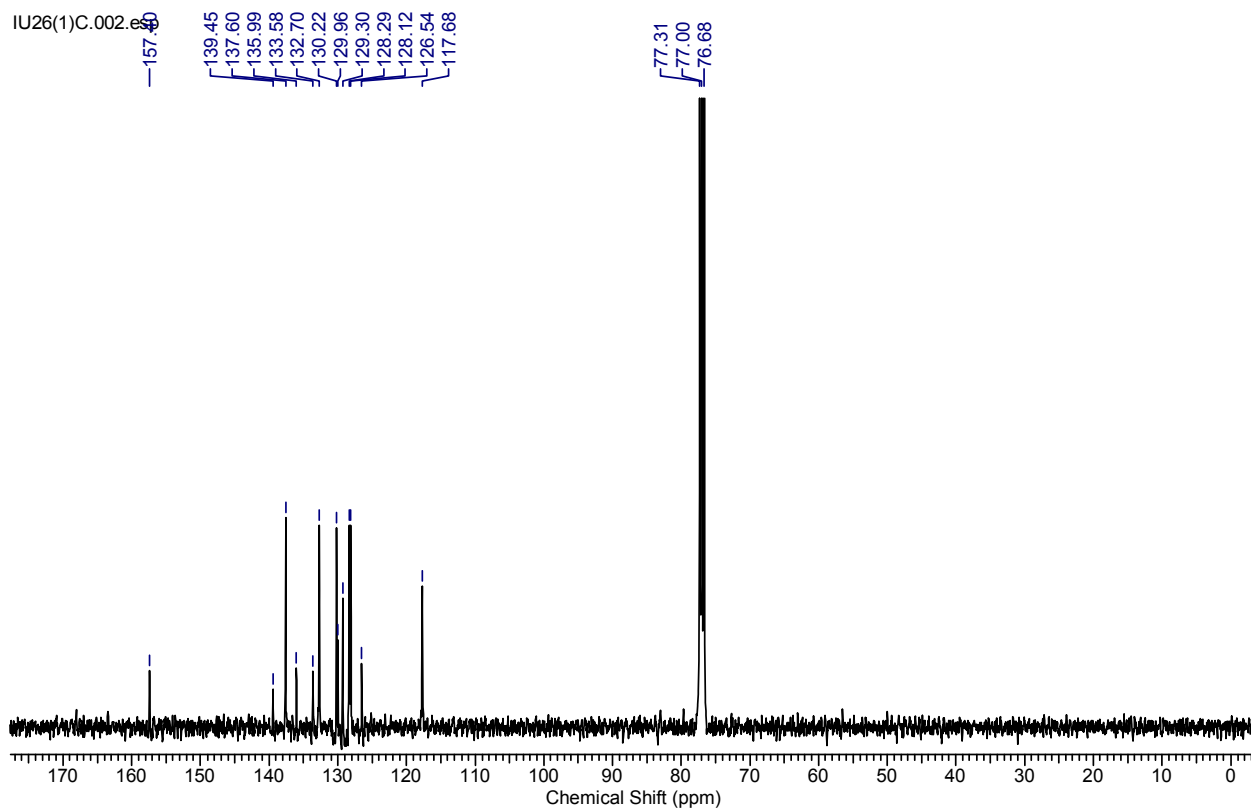




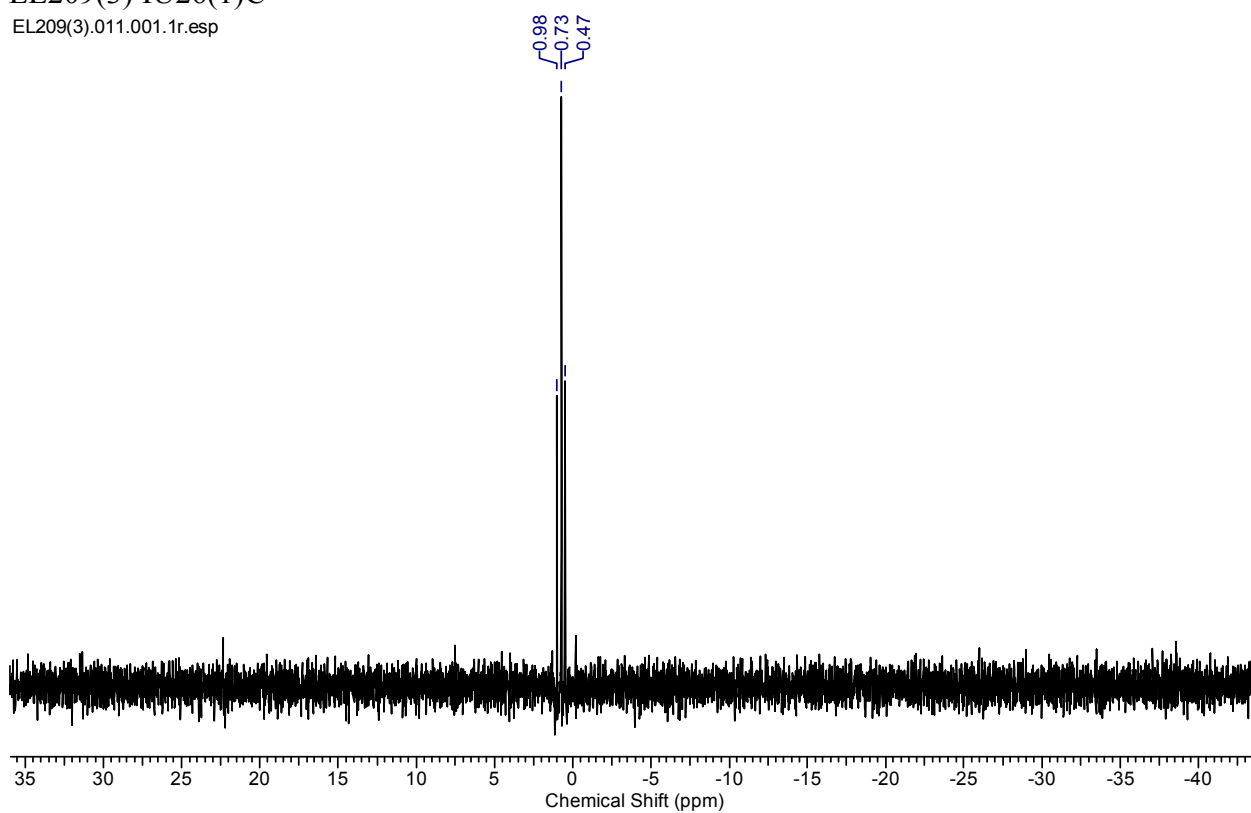
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3,5-di(thien-2-ylthio)-8-phenyl-BODIPY 5



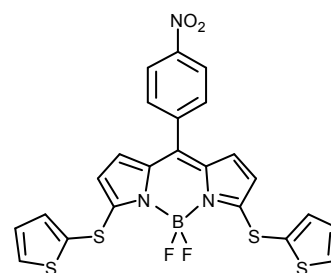
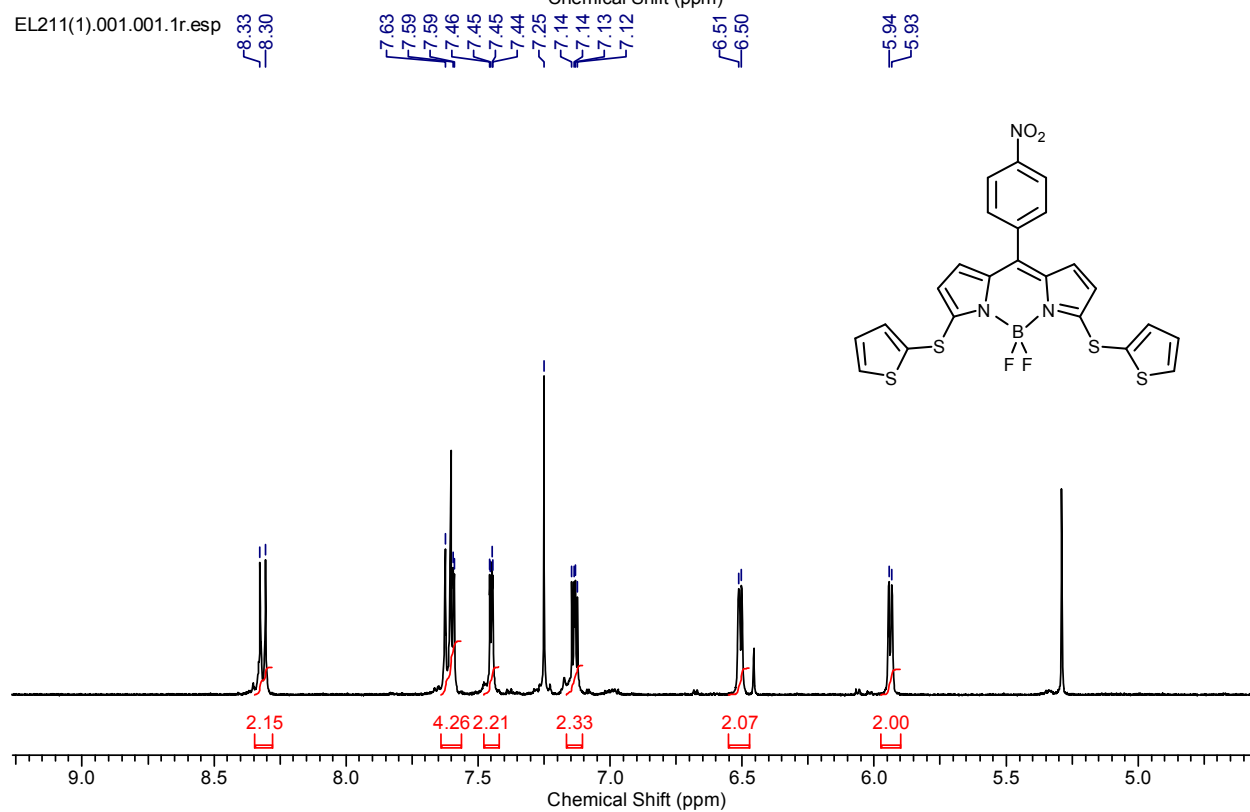
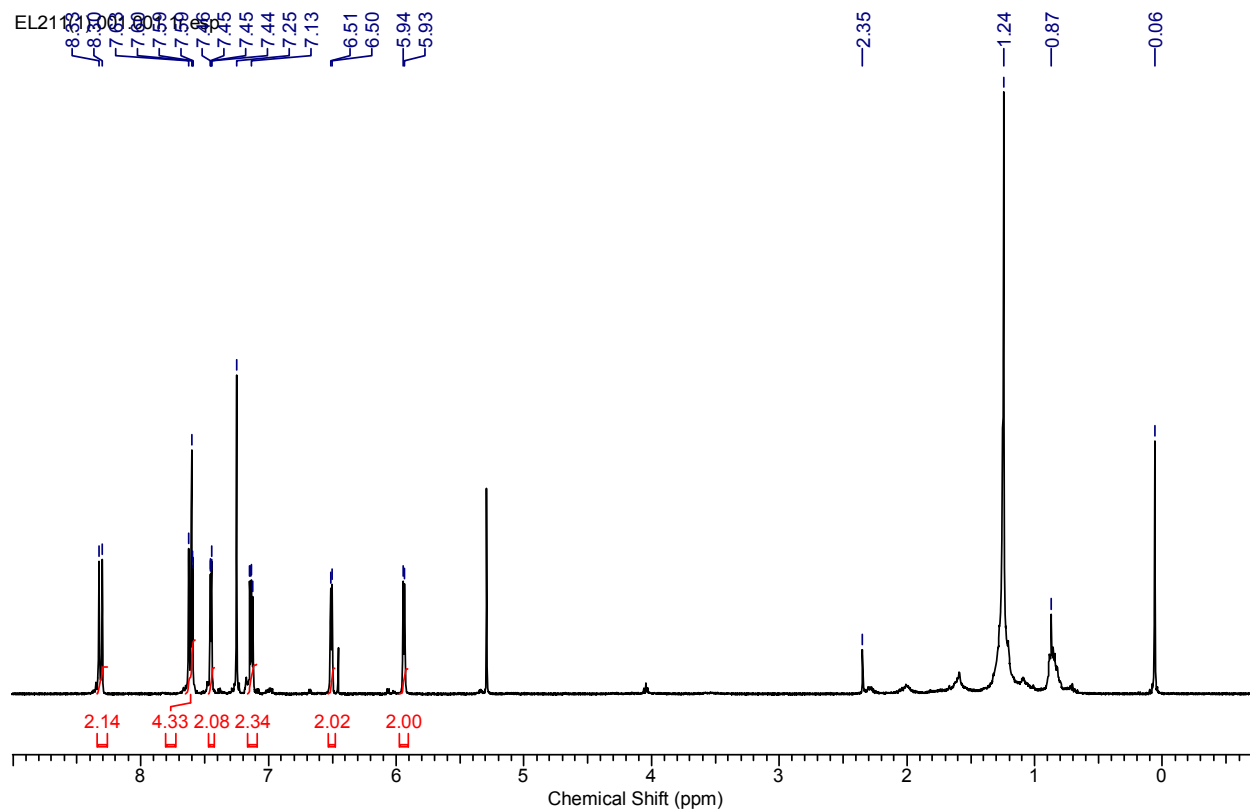


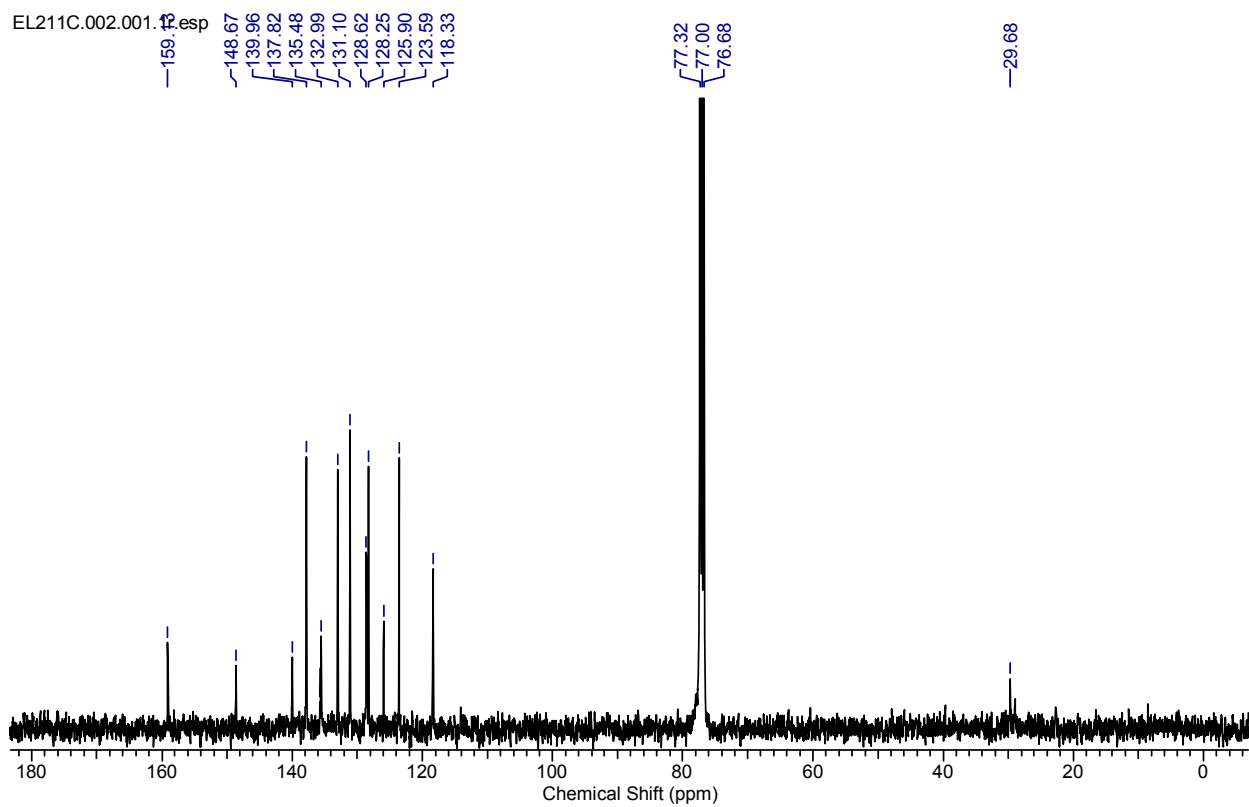
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EL209(3)

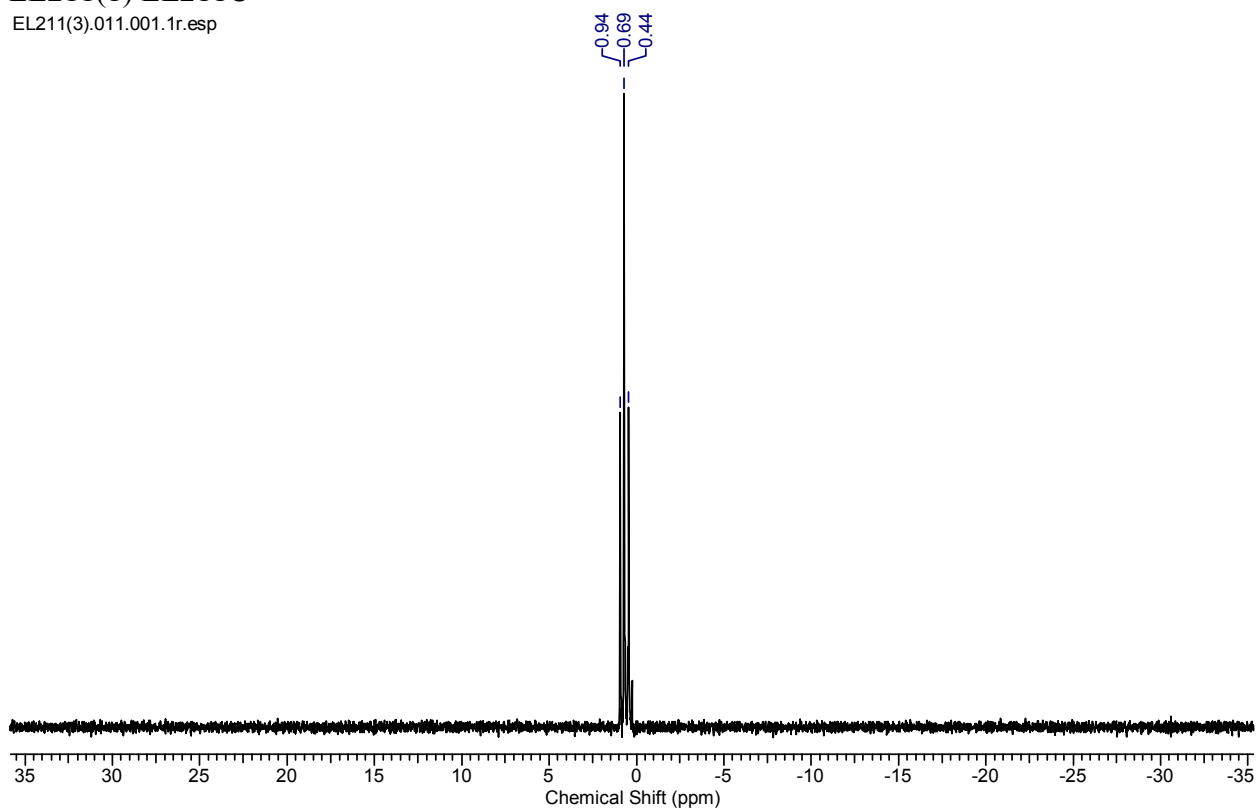
3,5-di(thien-2-ylthio)-8-(4-nitrophenyl)-BODIPY 6





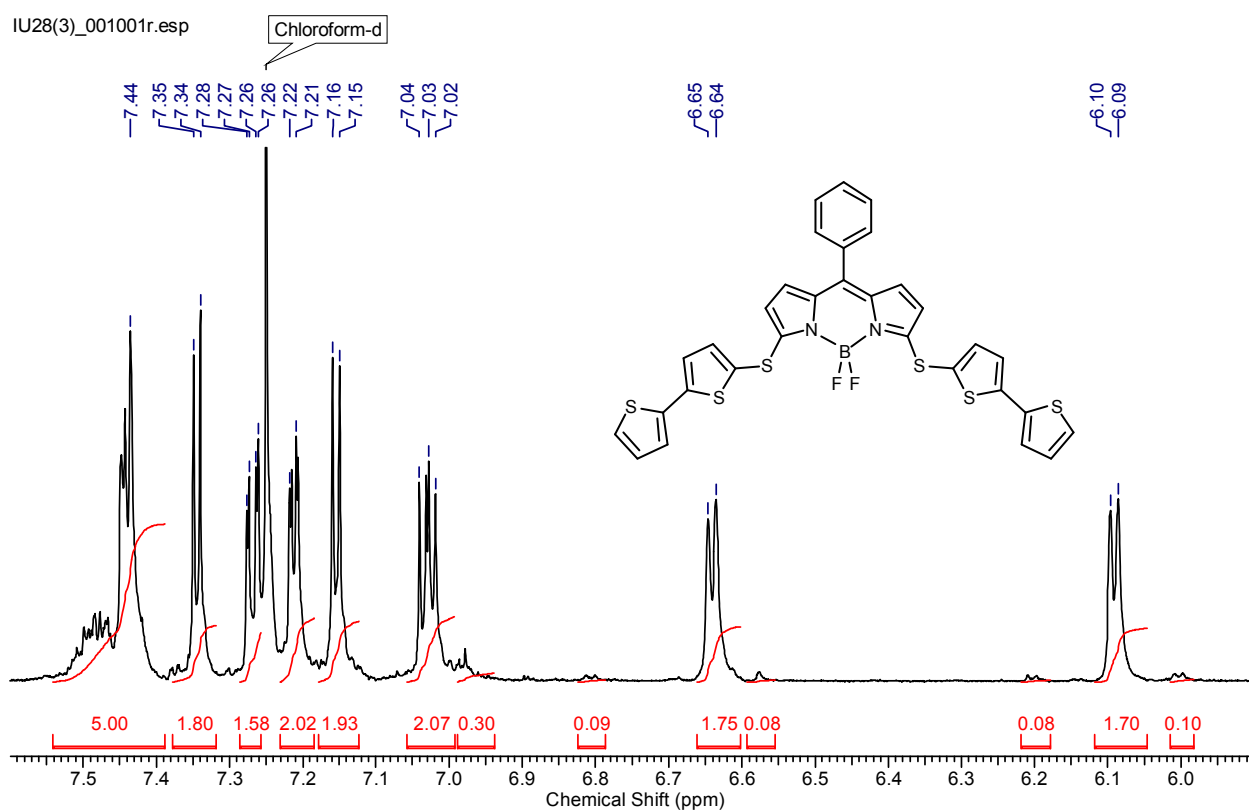
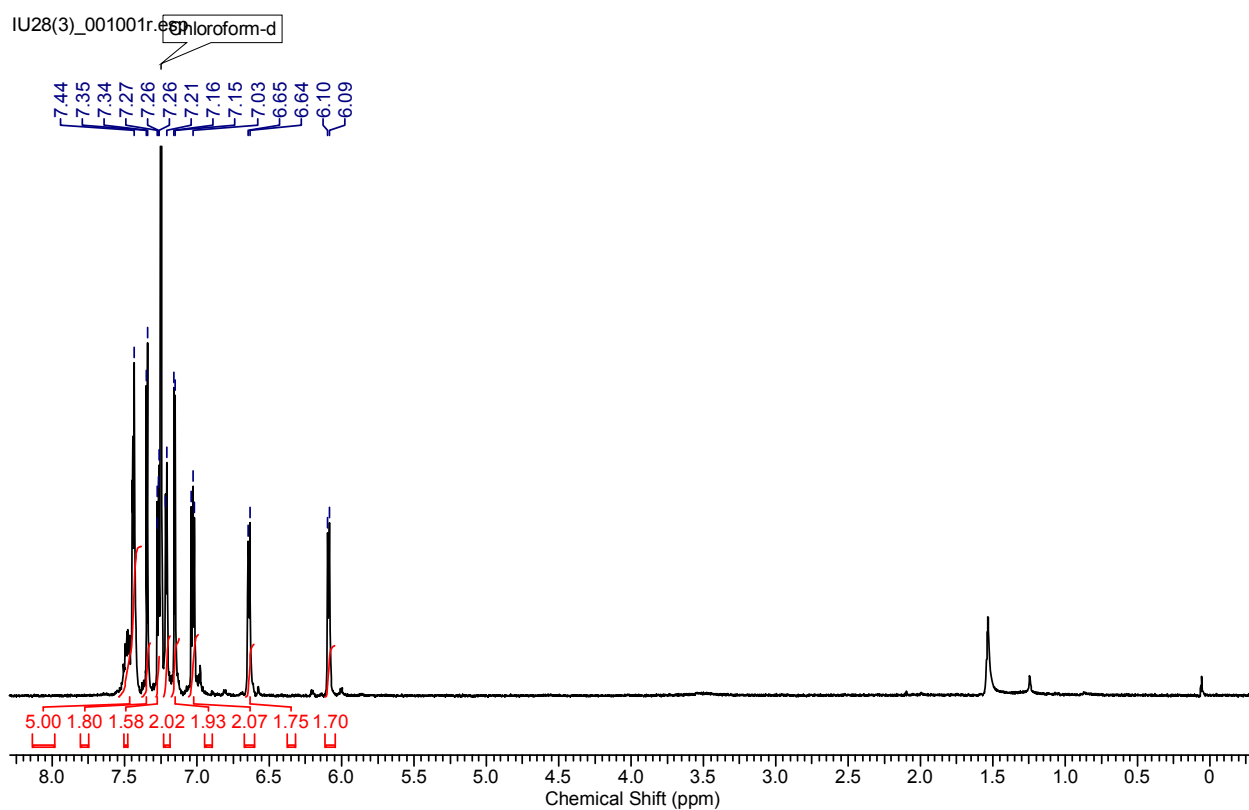
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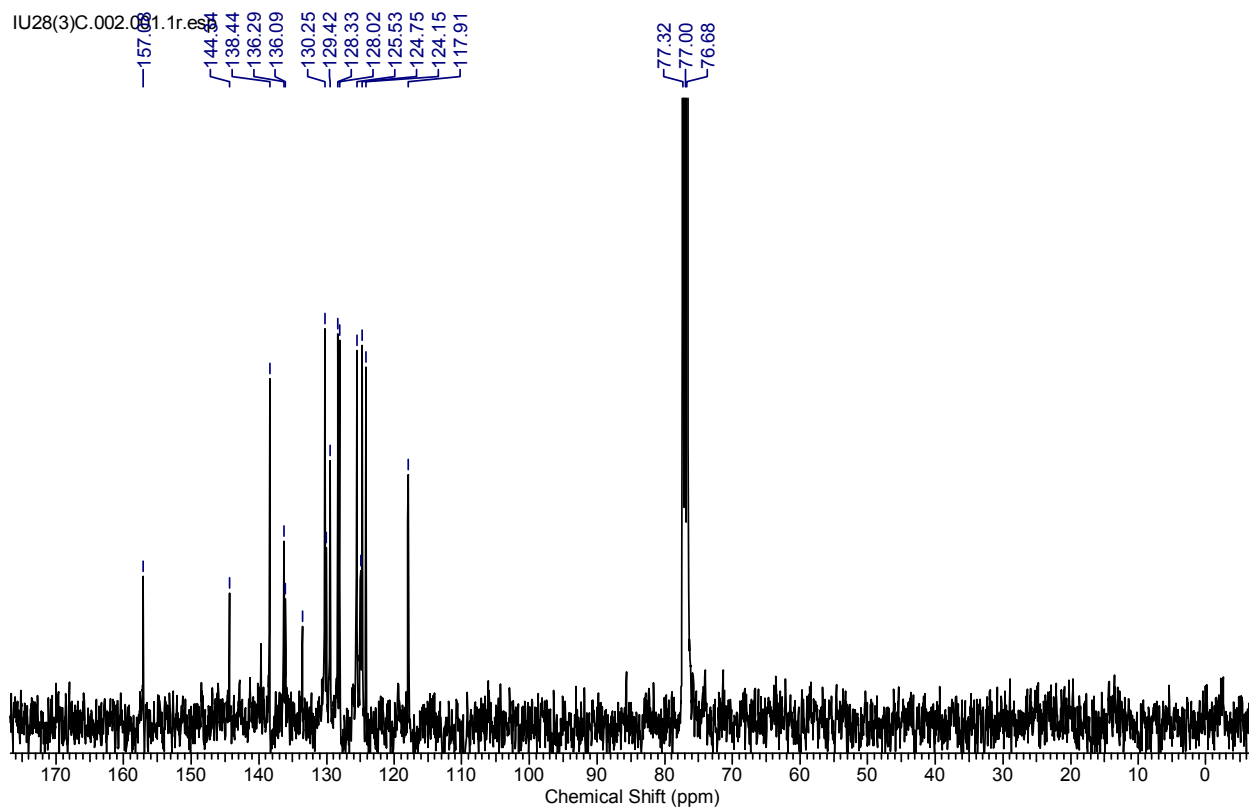
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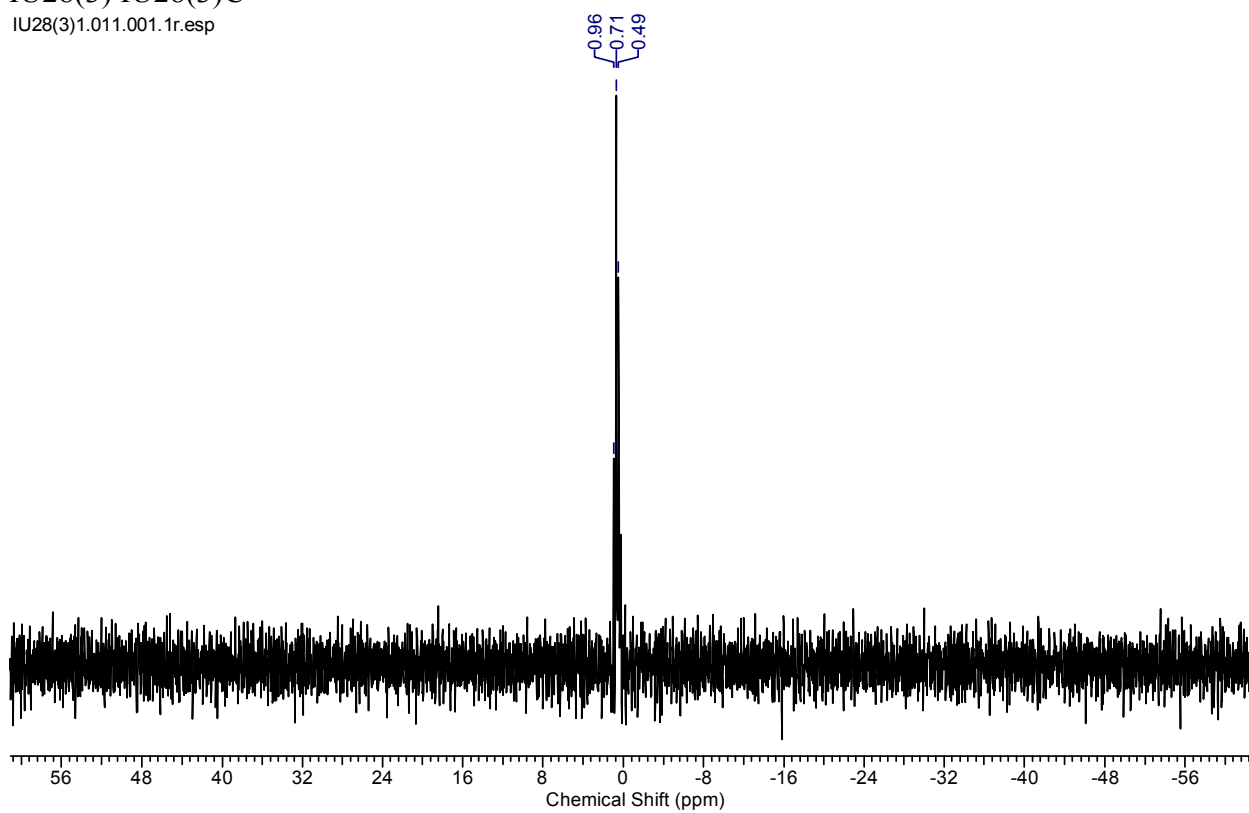
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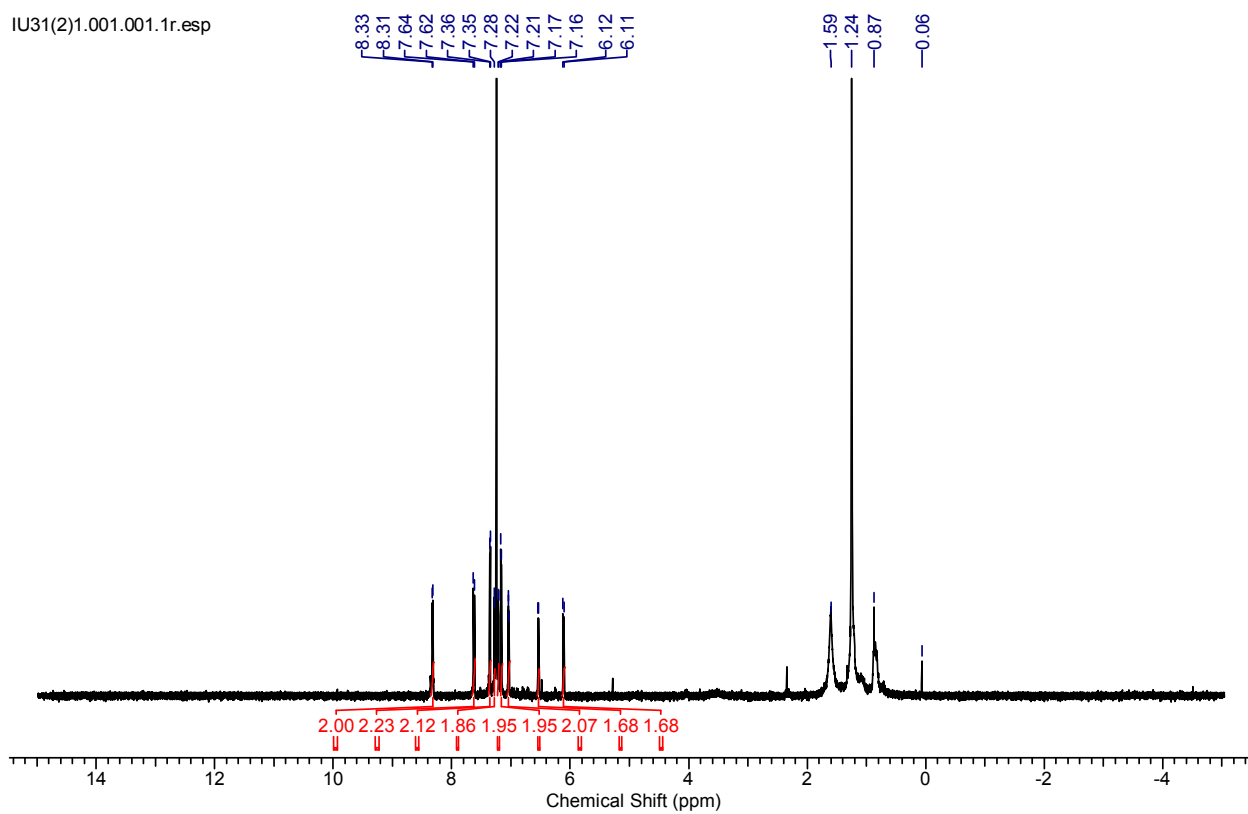




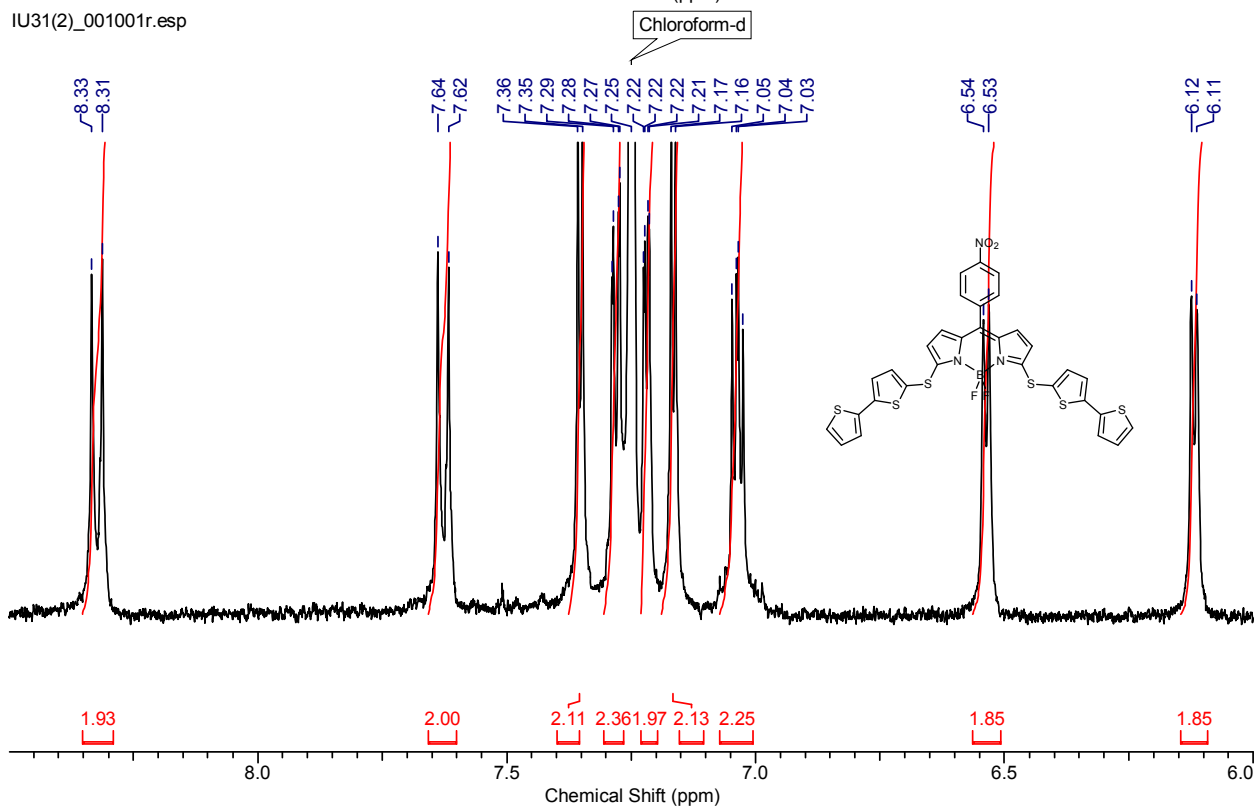
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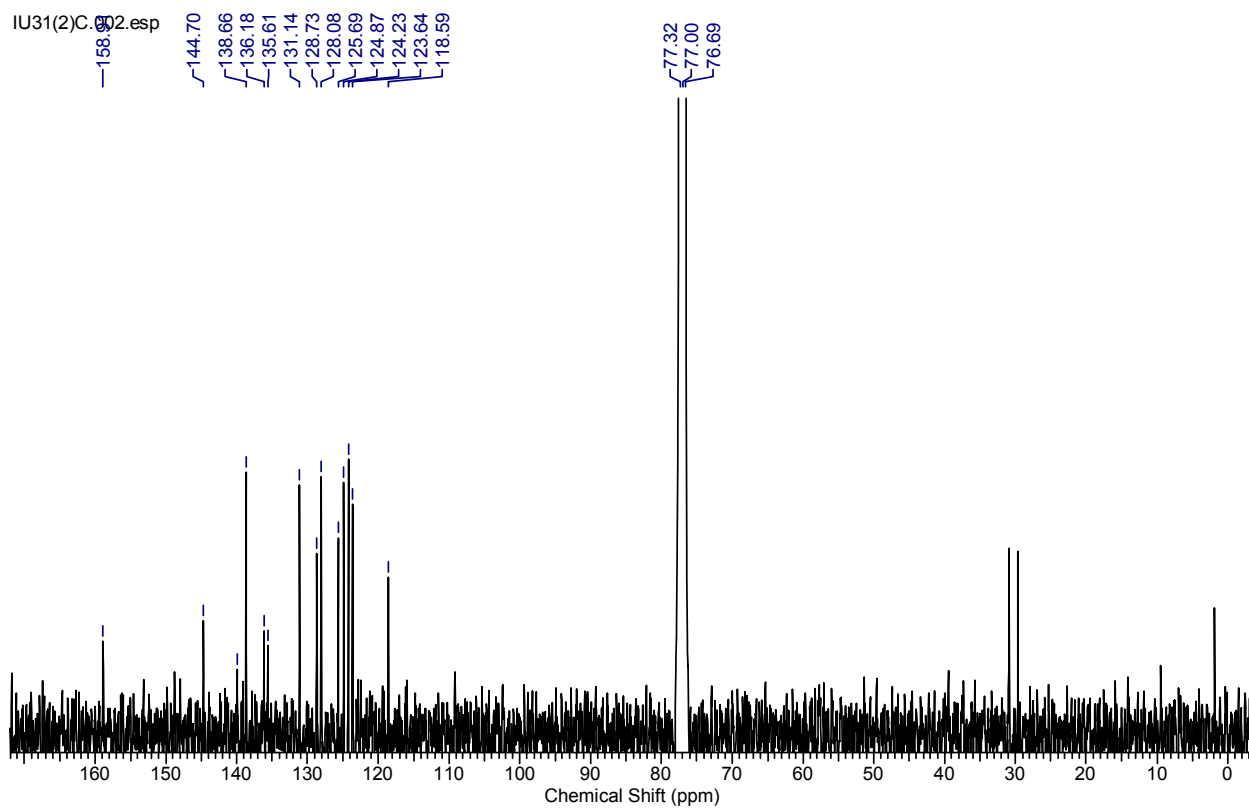


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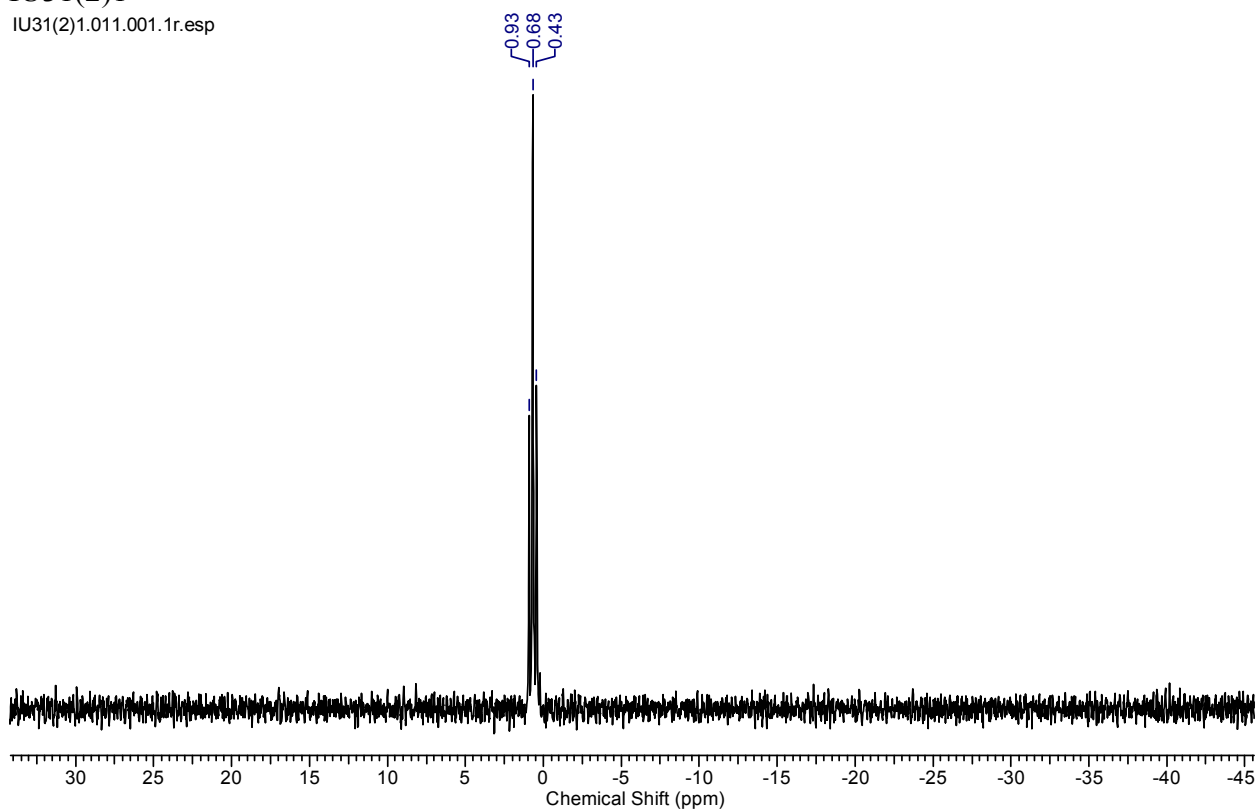
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IU31(2)1

IU31(2)1.011.001.1r.esp



IU31(2)1

2. UV-Vis spectra

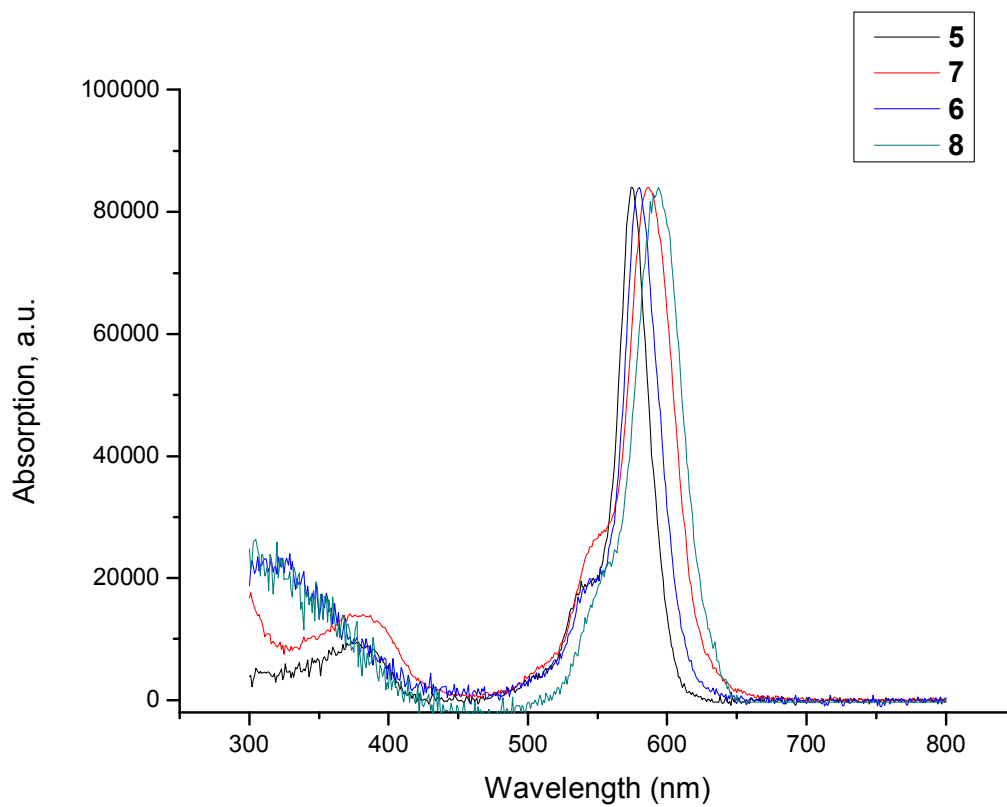


Fig. S1. Normalized absorption spectra of **5-8**, toluene.

3. Solid Fluorescence

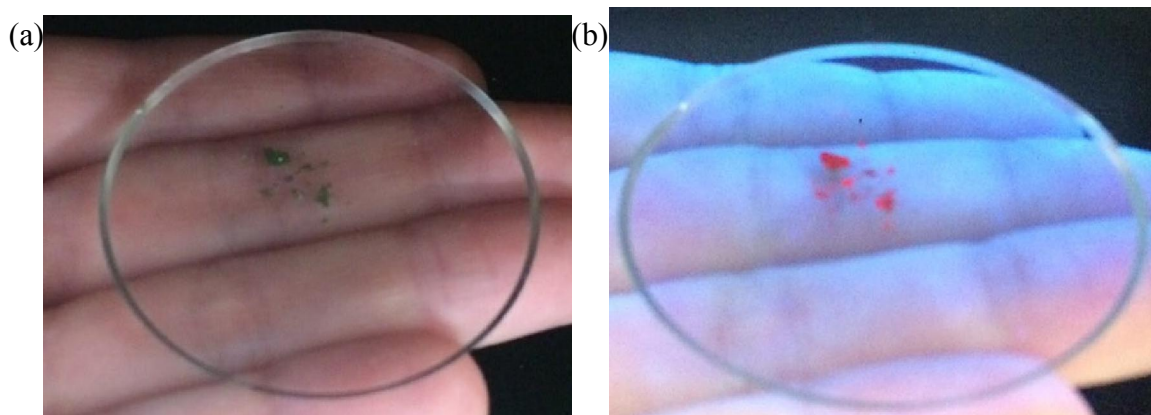


Fig S2. Sample of **5** crystals at (a) ambient and (b) UV ($\lambda = 254$ nm) light.

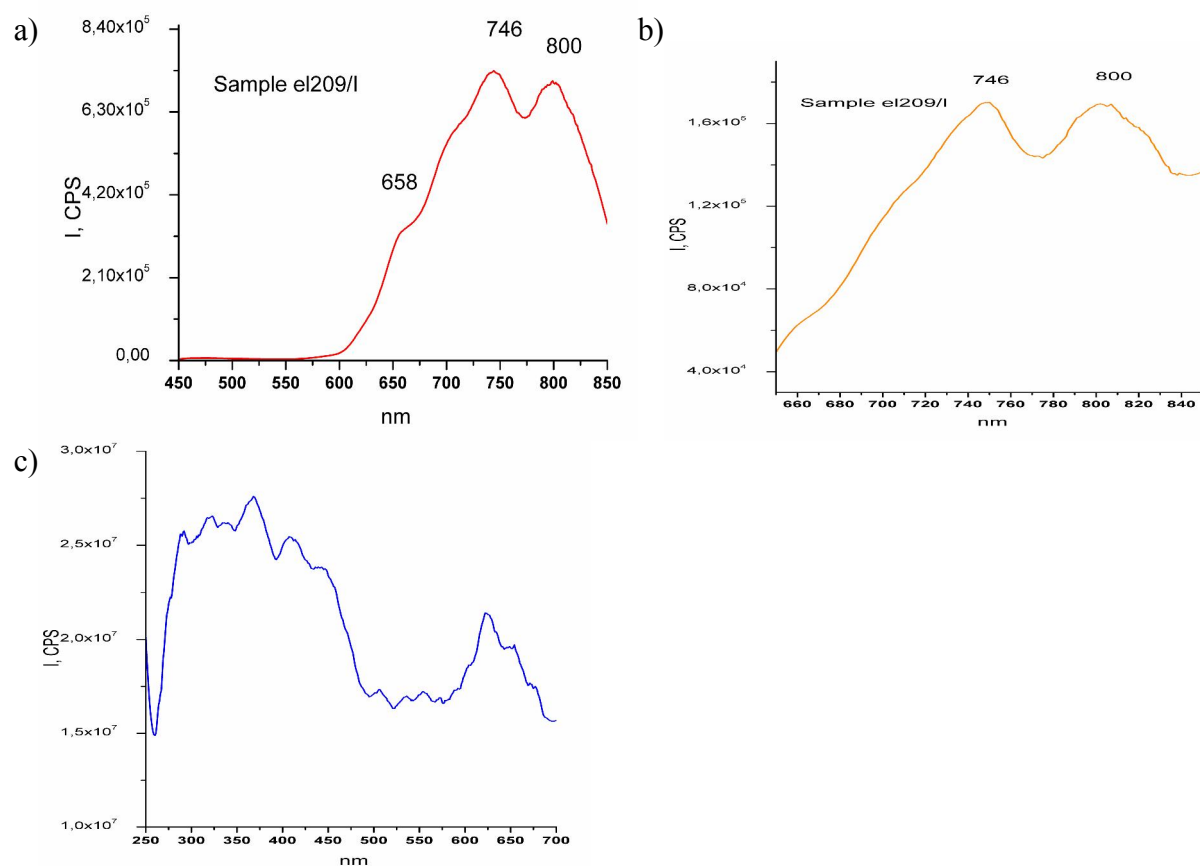


Fig. S3. Solid luminescence measurements of crystals of **5**. a) Emission, excited at 390 nm, filter down to 450 nm; b) emission, excited at 670 nm, non-filtered; c) Fluorescence excitation, registration at 750 nm, filtered down to 450 nm.

4. CVA measurements

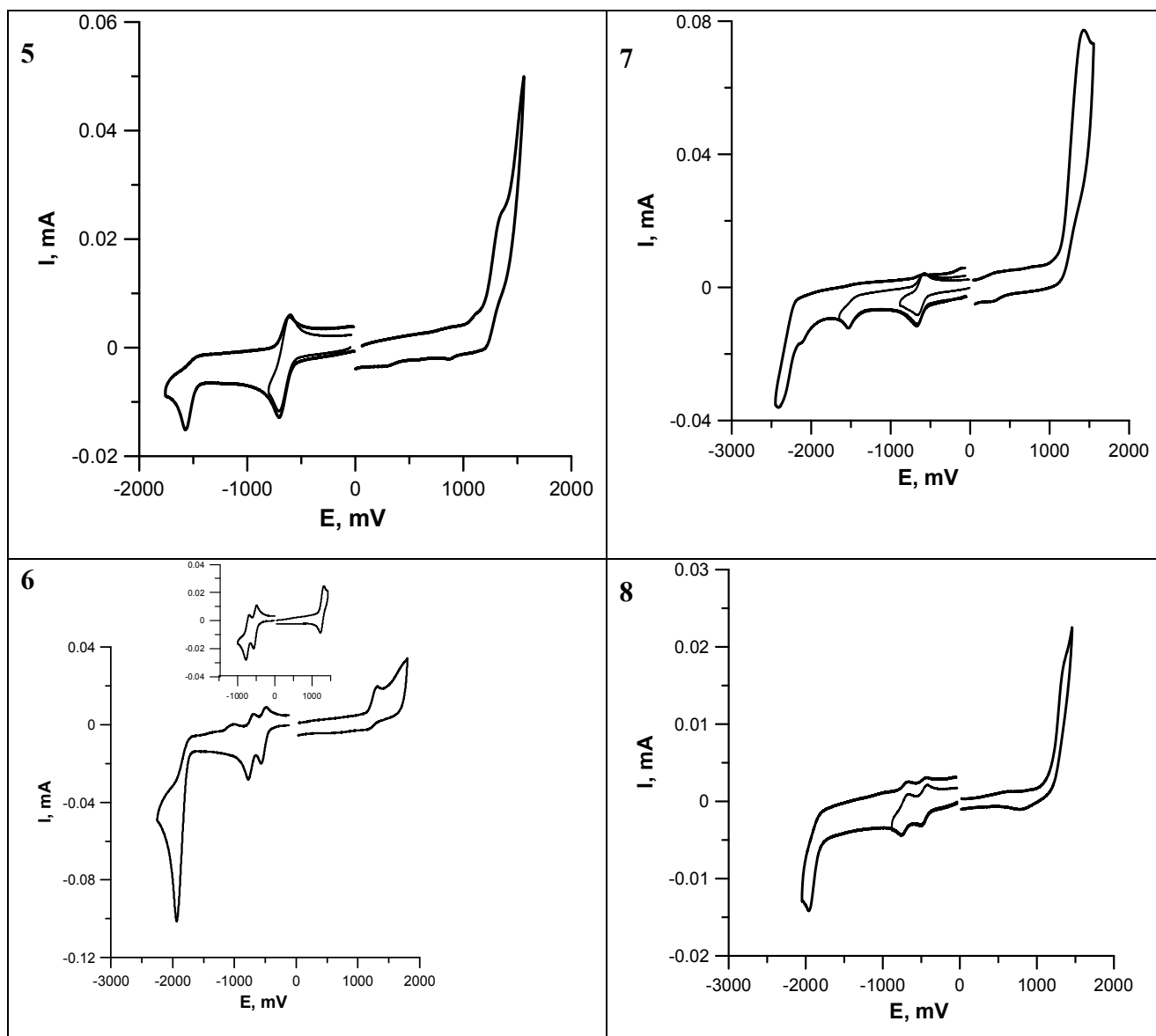


Fig. S4 CVA curves of the compounds **5-8**. CVA was done on glassy carbon electrode for 10^{-3} M solutions in DMF, 0.1M of NBu_4ClO_4 was used as background, potentials were reported vs. Ag/AgCl

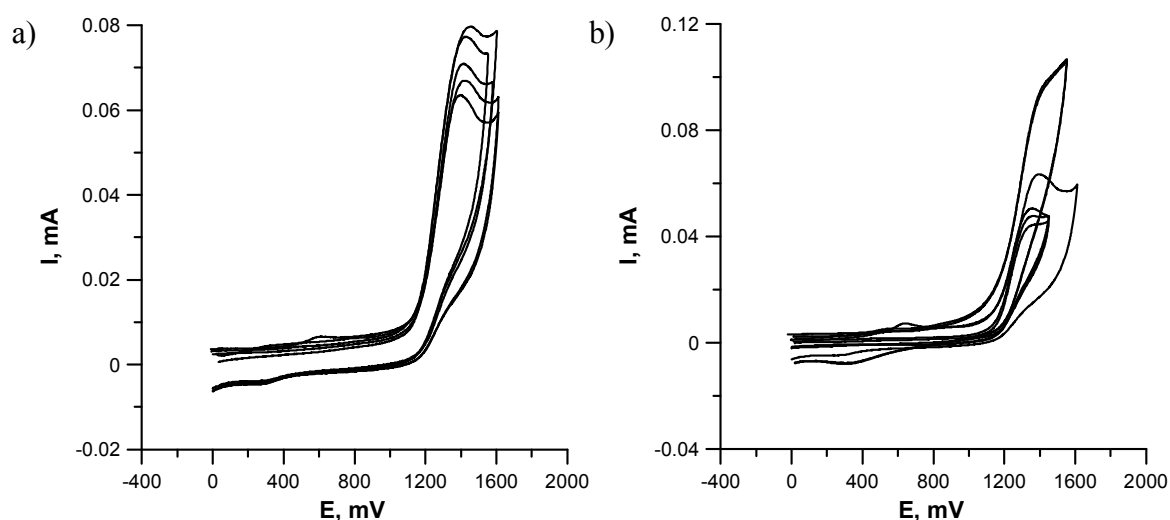


Fig S5. Current increase in CVA experiments of **7** on the repetitive cycling a) glass carbon electrode b) Au electrode

5. Calculations

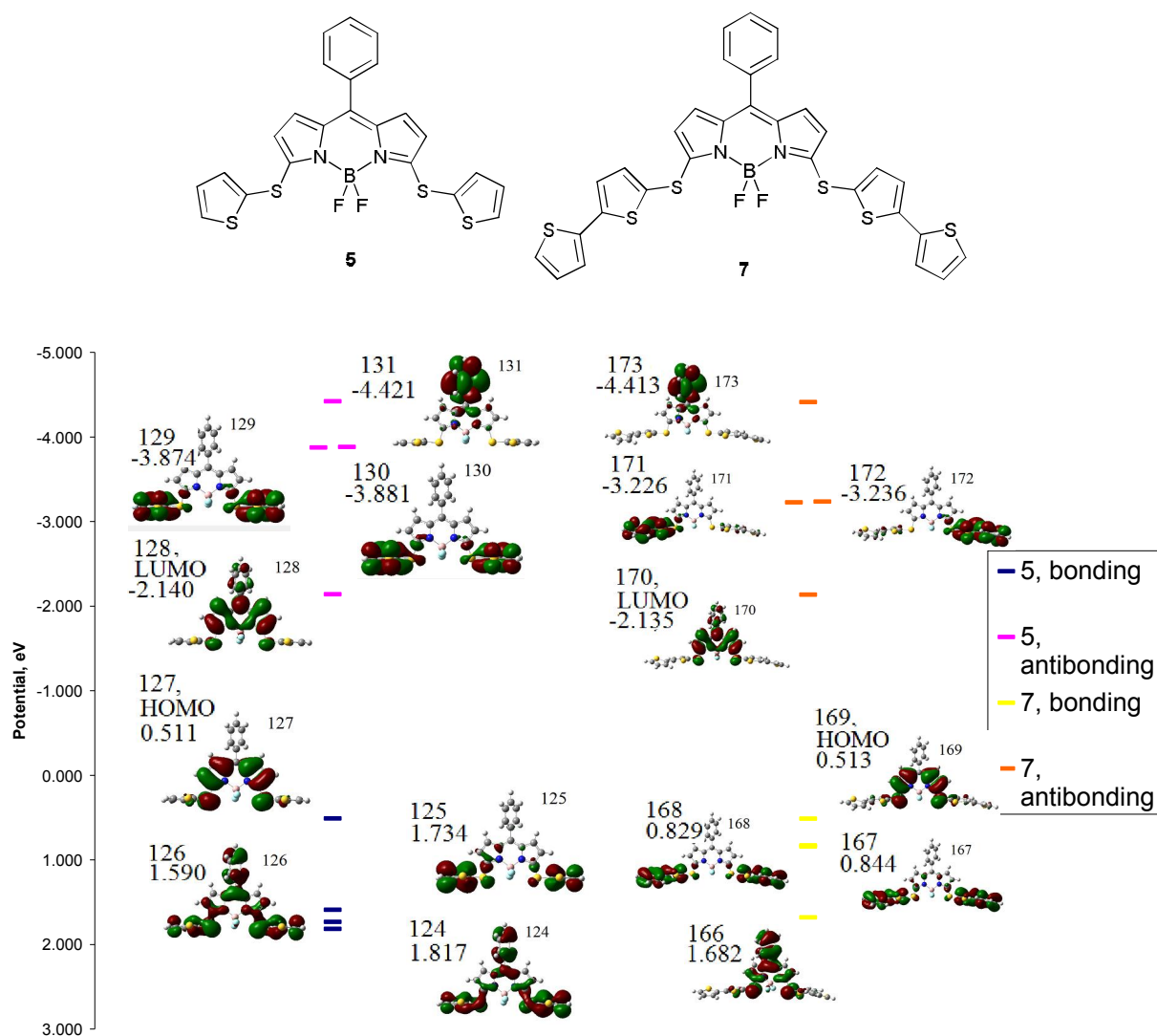


Fig. S6 – MO energies of **5** and **7**, according to B3LYP/6-31+g(d) calculations, corrected to CVA experiments conditions ($E_{\text{DMF, eV}} = -(4.73 + E_{\text{vac, Hartree}} \times 27.1)$), referenced vs Fe/Fe^+ in DMF.

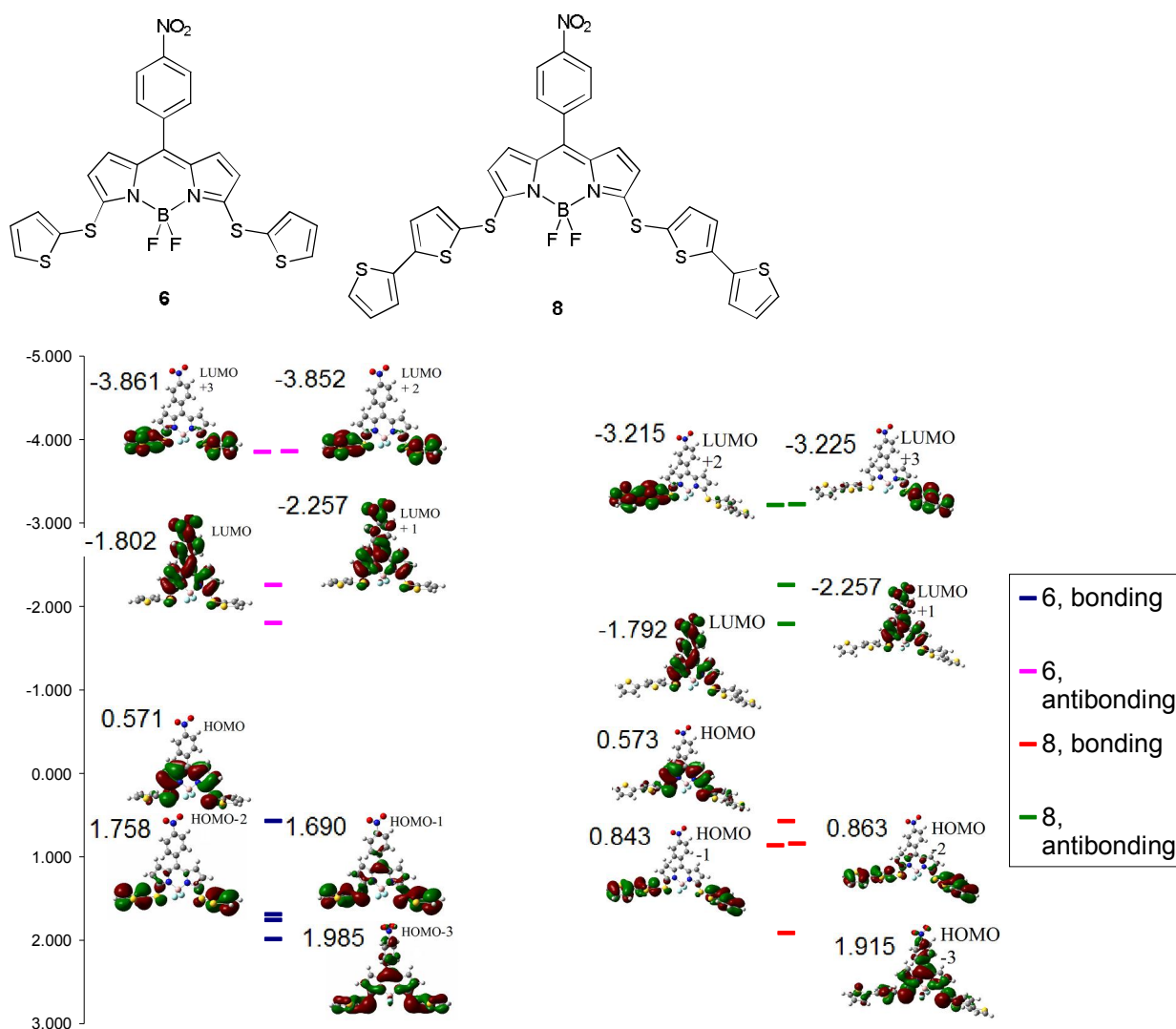


Fig. S7 – MO energies of **6** and **8**, according to B3LYP/6-31+g(d) calculations, corrected to CVA experiments conditions ($E_{\text{DMF, eV}} = -(4.73 + E_{\text{vac, Hartree}} \times 27.1)$), referenced vs Fe/Fe^+ in DMF.

SCE vs vacuum 4.71

NHE vs vacuum 4.6 V