

Supporting Information File 2
for
Structure–property relationships and third-order
nonlinearities in diketopyrrolopyrrole based
D– π –A– π –D molecules

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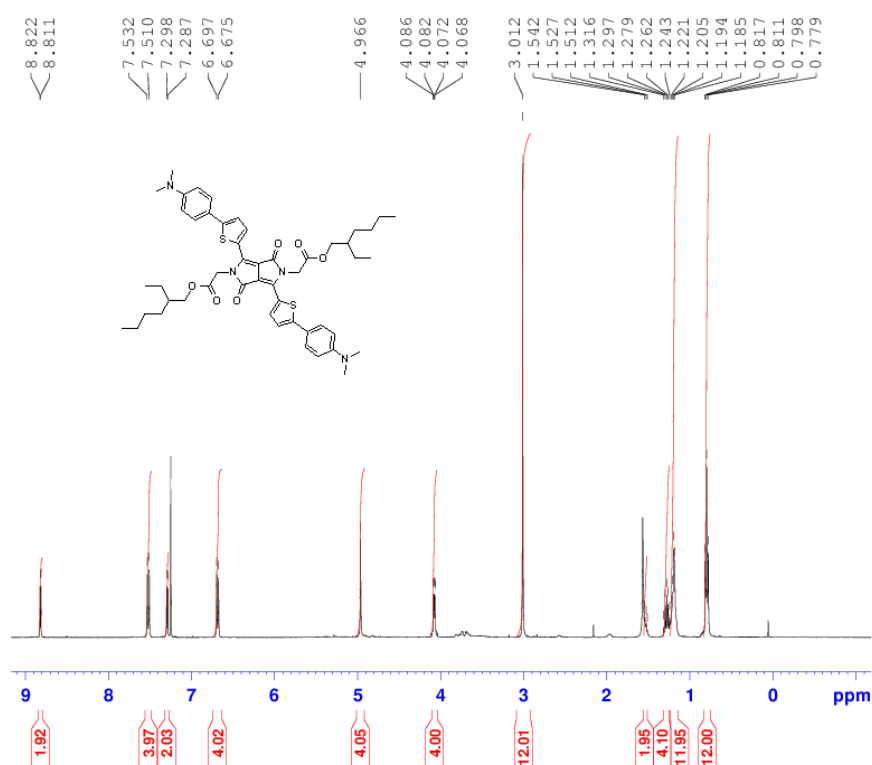
**¹H and ¹³C NMR spectra, HR-MALDI-MS spectra, CV curves, UV–vis
absorption/emission spectra, and HOMO/LUMO localizations**

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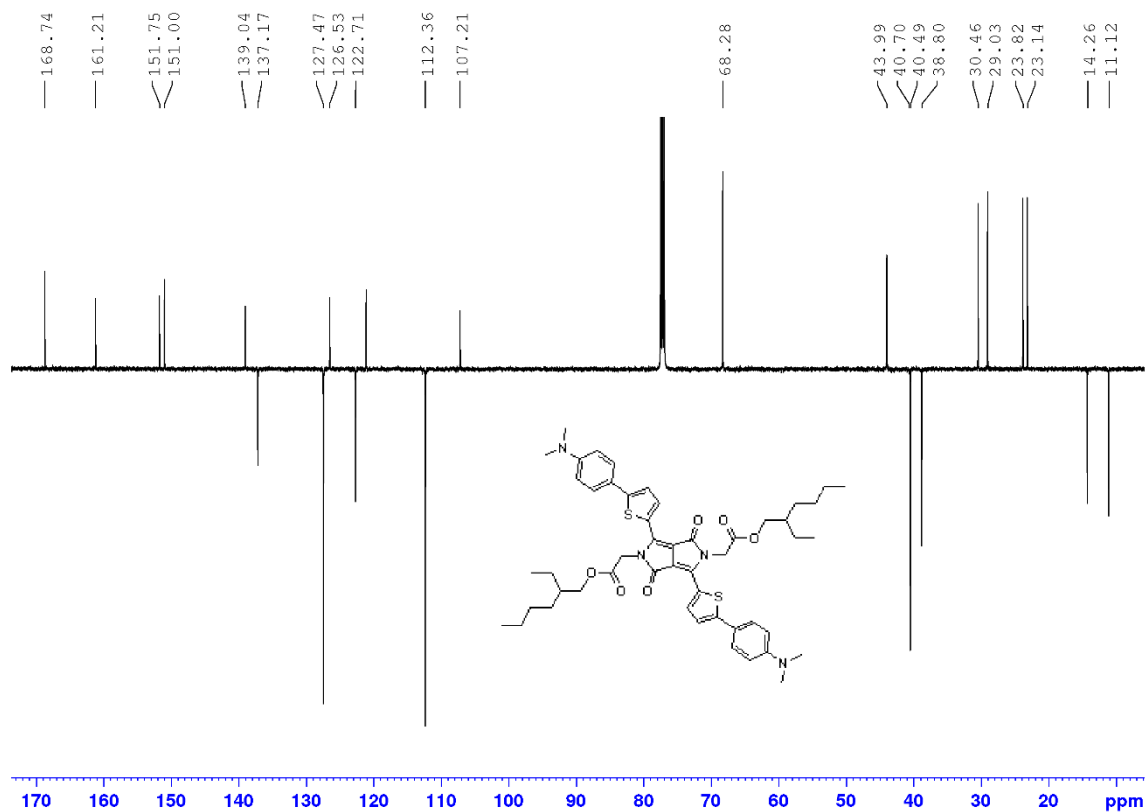
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1. ^1H and ^{13}C NMR and HR-MALDI-MS spectra of chromophore 1a

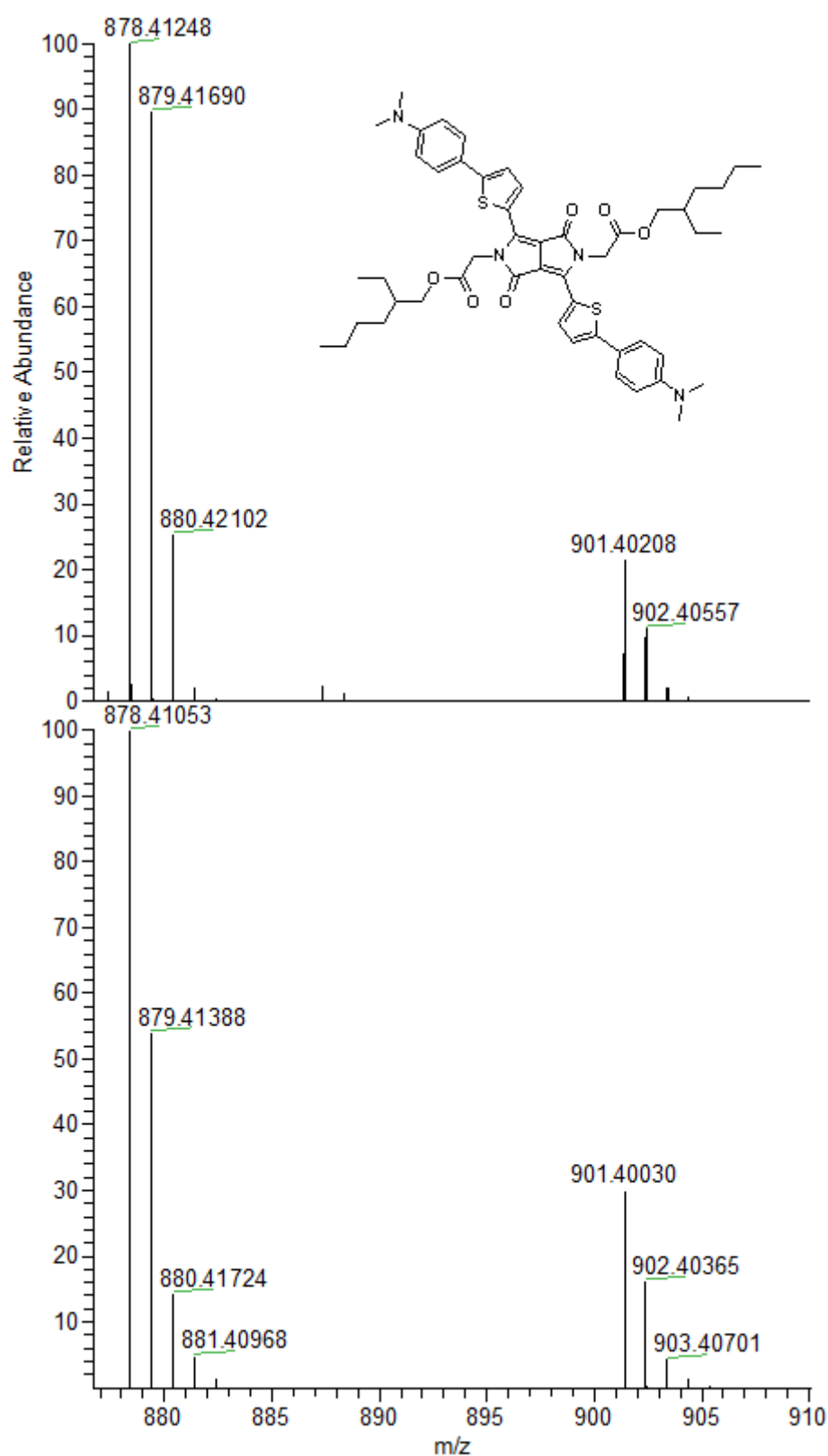
^1H NMR spectrum (400 MHz, CDCl_3 , 25 °C) of **1a**



^{13}C NMR spectrum (125 MHz, CDCl_3 , 25 °C) of **1a**

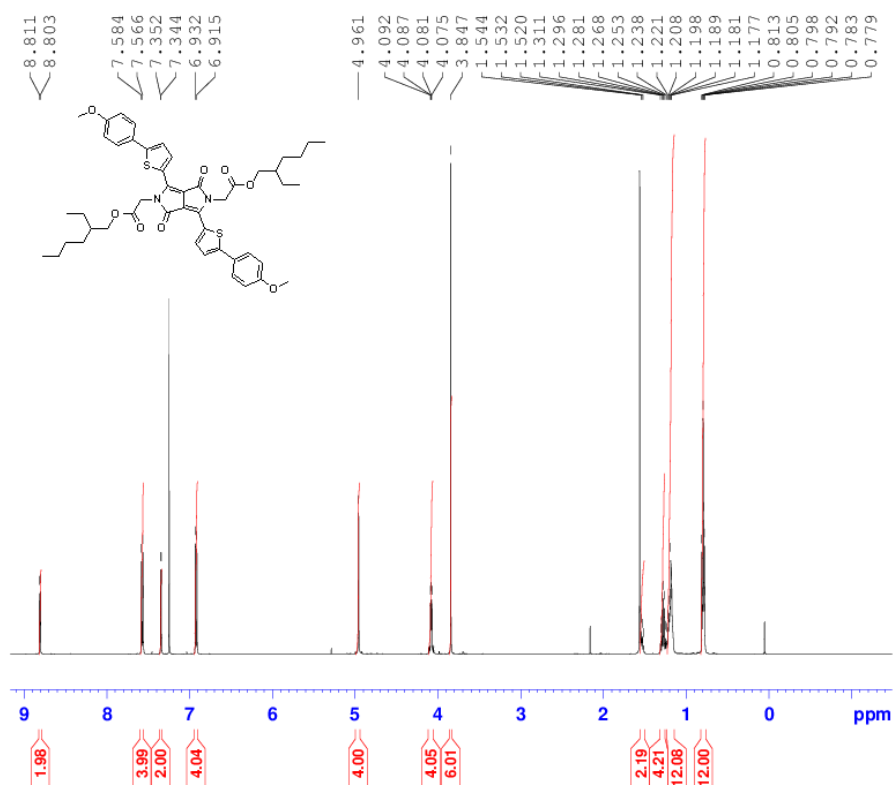


Experimental (up) and calculated (down) MALDI spectra of **1a**

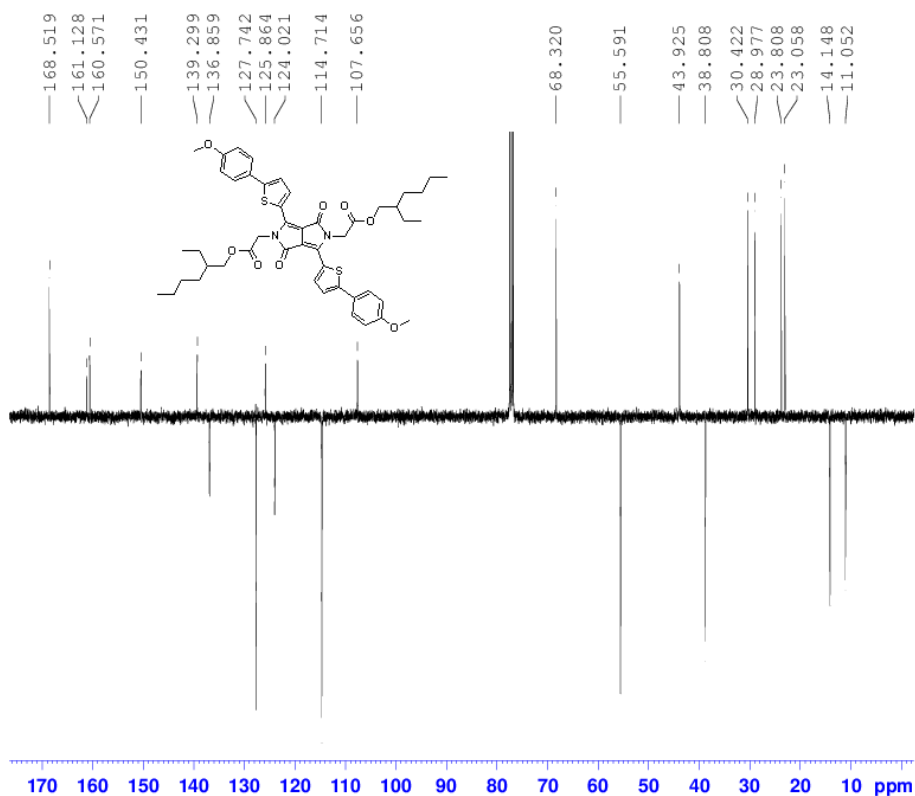


2. ^1H and ^{13}C NMR and HR-MALDI-MS spectra of chromophore 2a

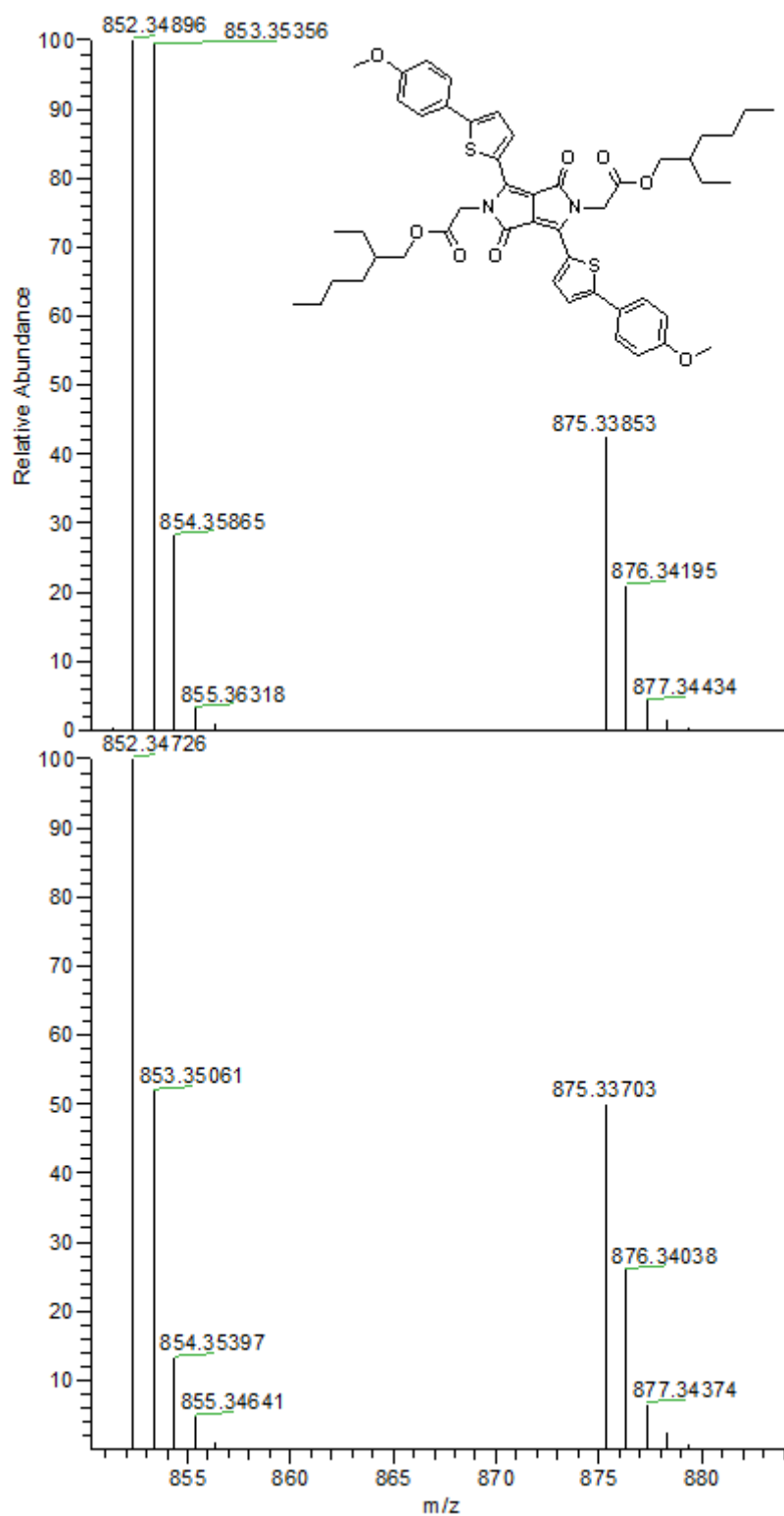
^1H NMR spectrum (500 MHz, CDCl_3 , 25 °C) of **2a**



^{13}C NMR spectrum (100 MHz, CDCl_3 , 25 °C) of **2a**

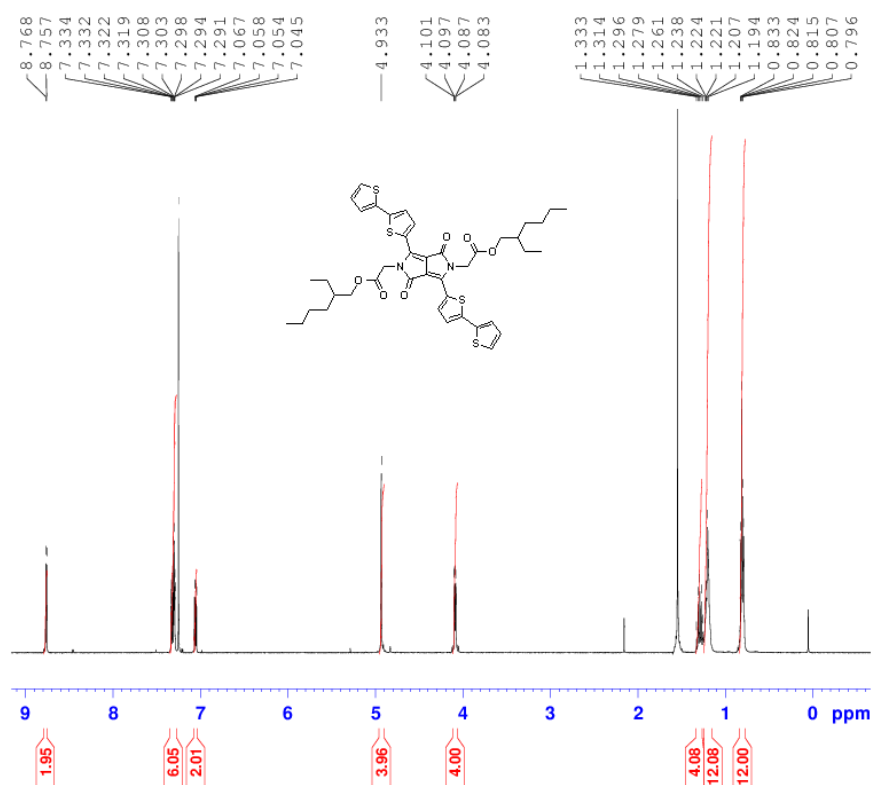


Experimental (up) and calculated (down) MALDI spectra of **2a**

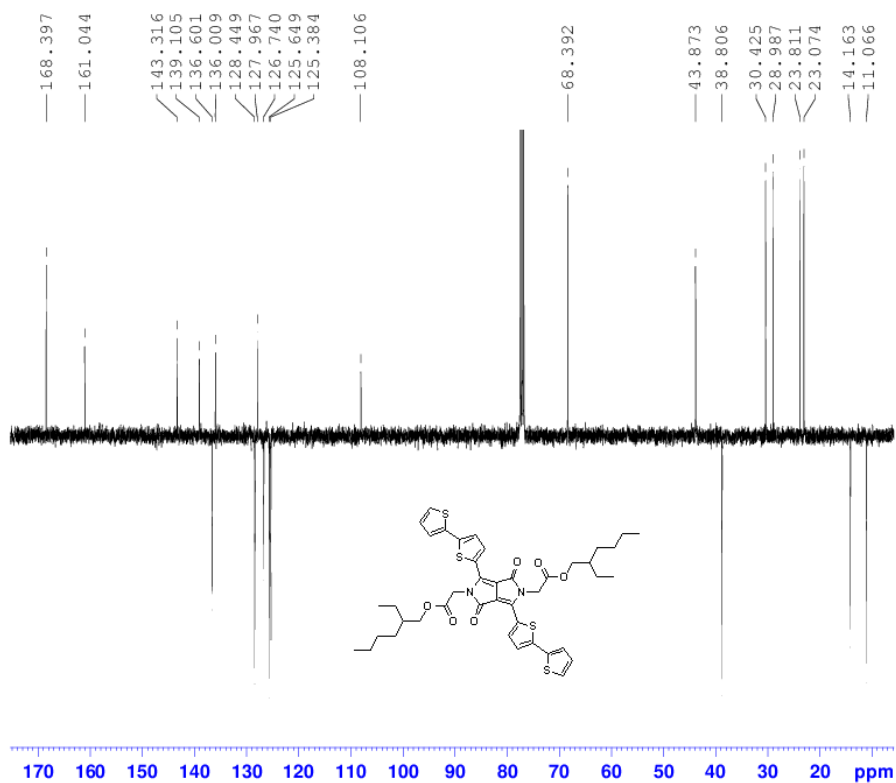


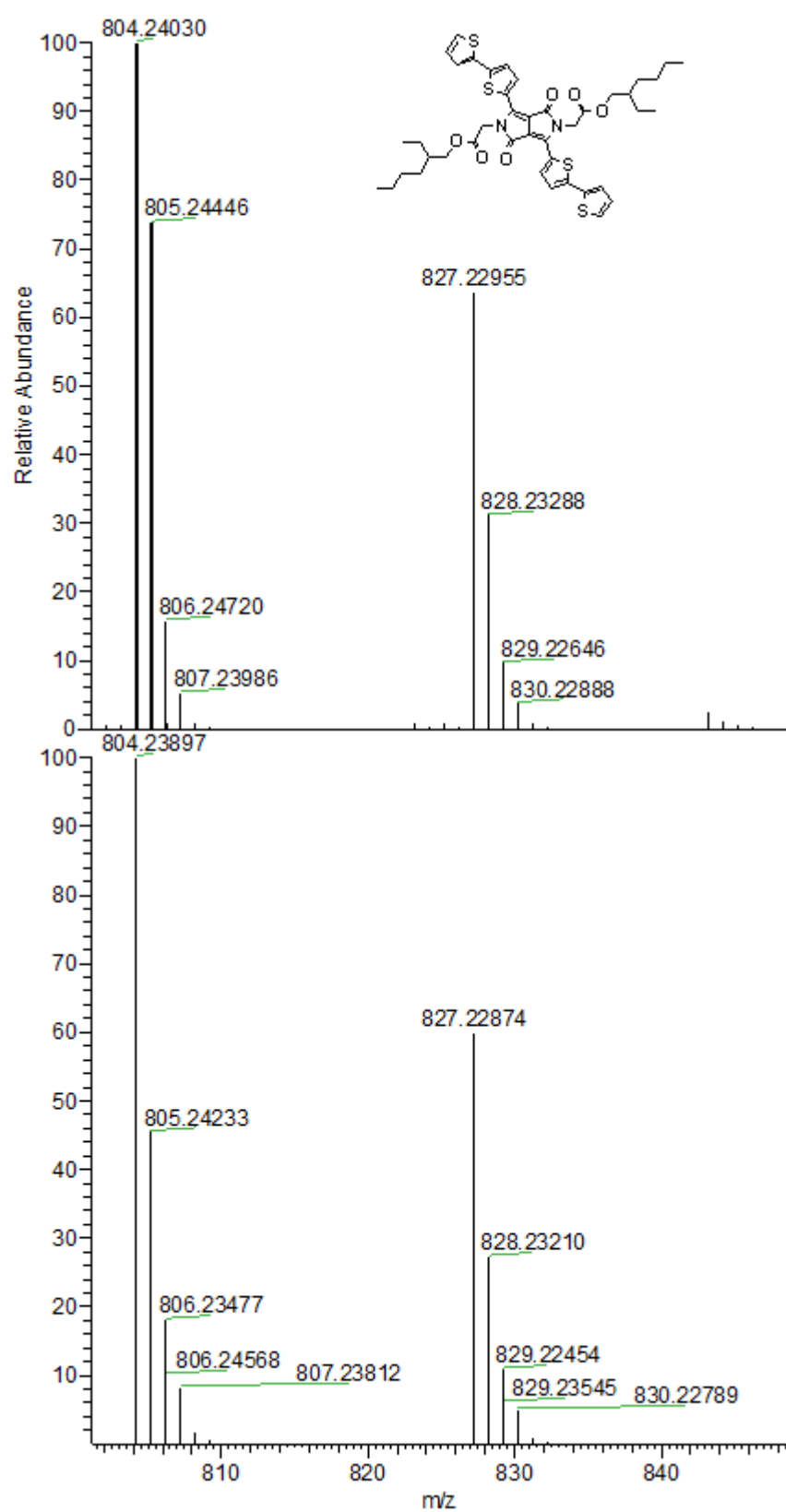
3. ^1H and ^{13}C NMR and HR-MALDI-MS spectra of chromophore 3a

^1H NMR spectrum (400 MHz, CDCl_3 , 25 °C) of 3a



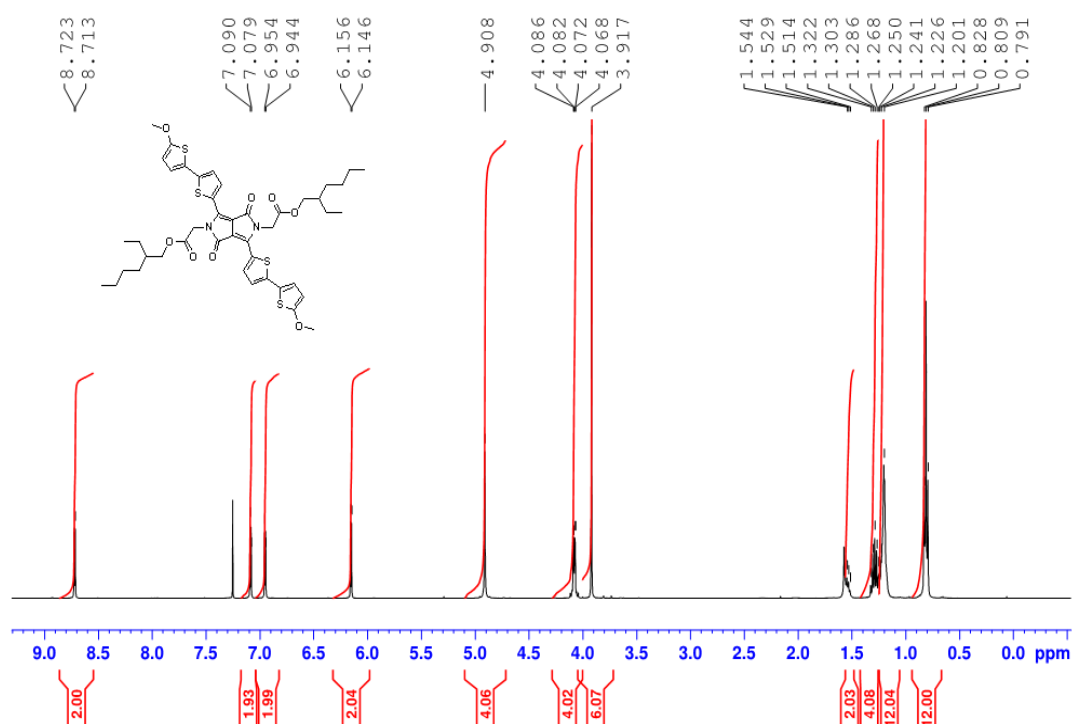
^{13}C NMR spectrum (100 MHz, CDCl_3 , 25 °C) of 3a



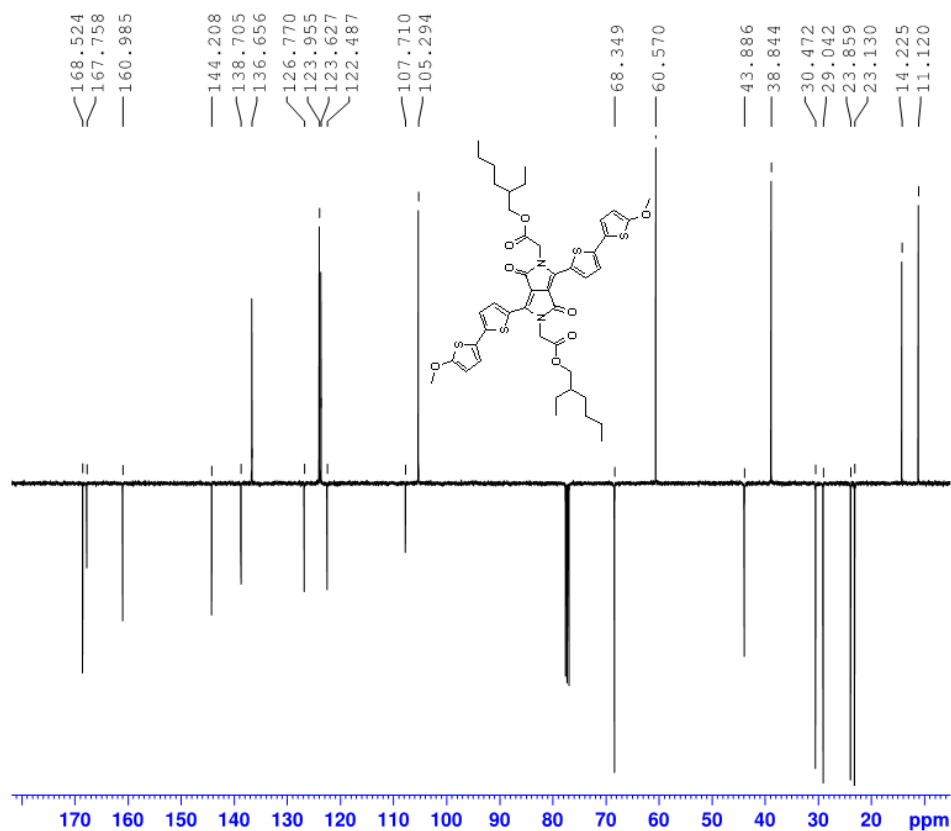
Experimental (up) and calculated (down) MALDI spectra of **3a**

4. ^1H and ^{13}C NMR and HR-MALDI-MS spectra of chromophore 4a

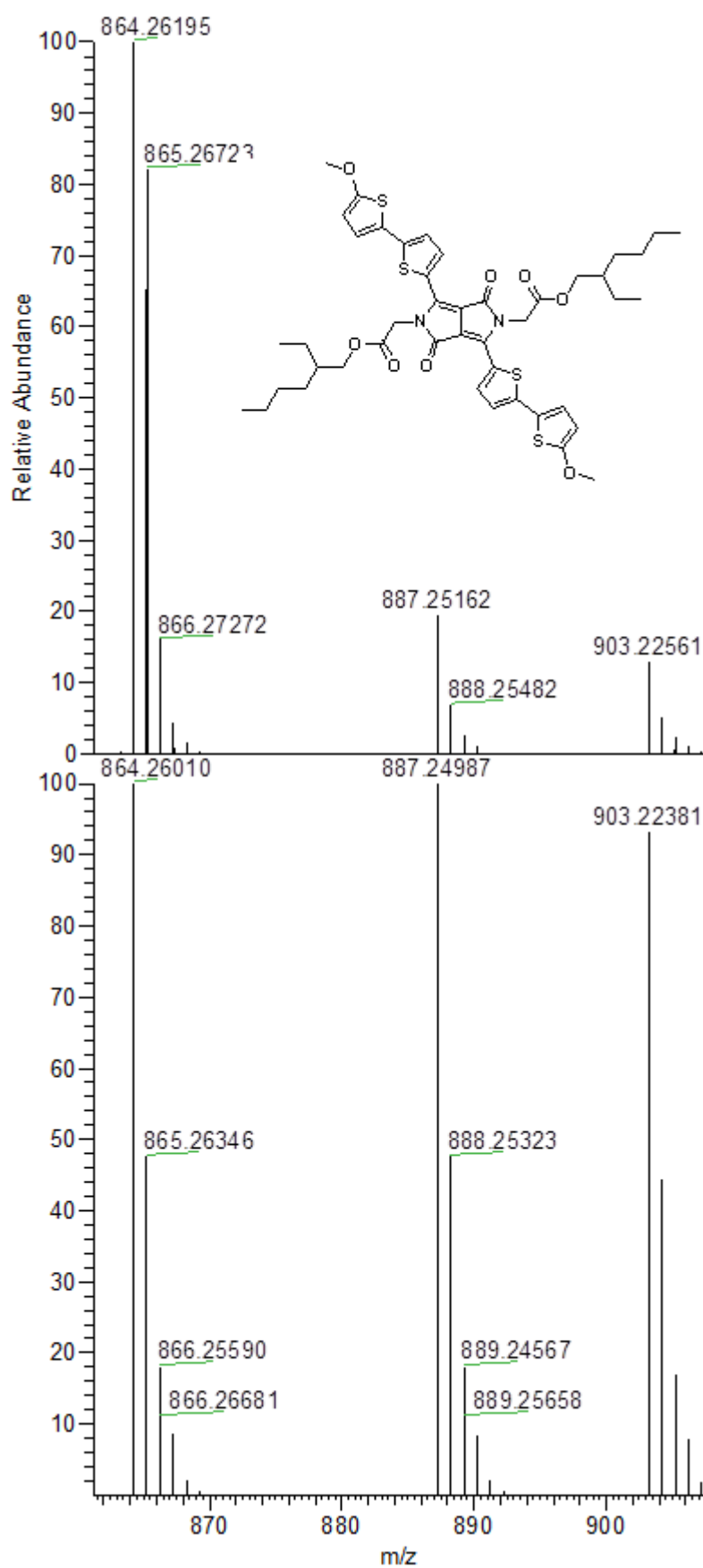
^1H NMR spectrum (400 MHz, CDCl_3 , 25 °C) of 4a



^{13}C NMR spectrum (100 MHz, CDCl_3 , 25 °C) of 4a

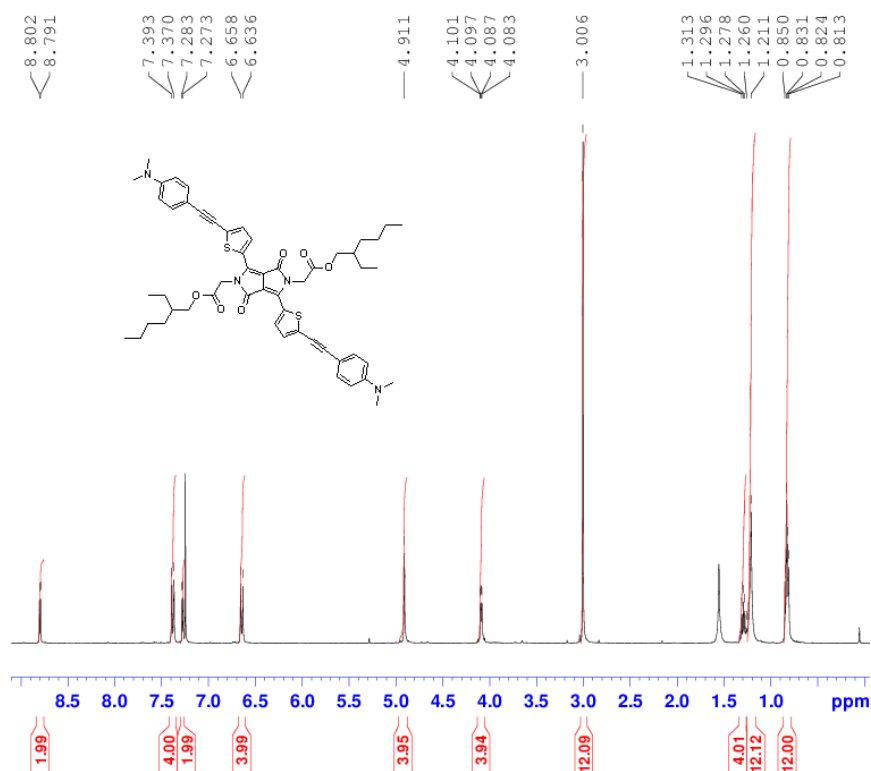


Experimental (up) and calculated (down) MALDI spectra of **4a**

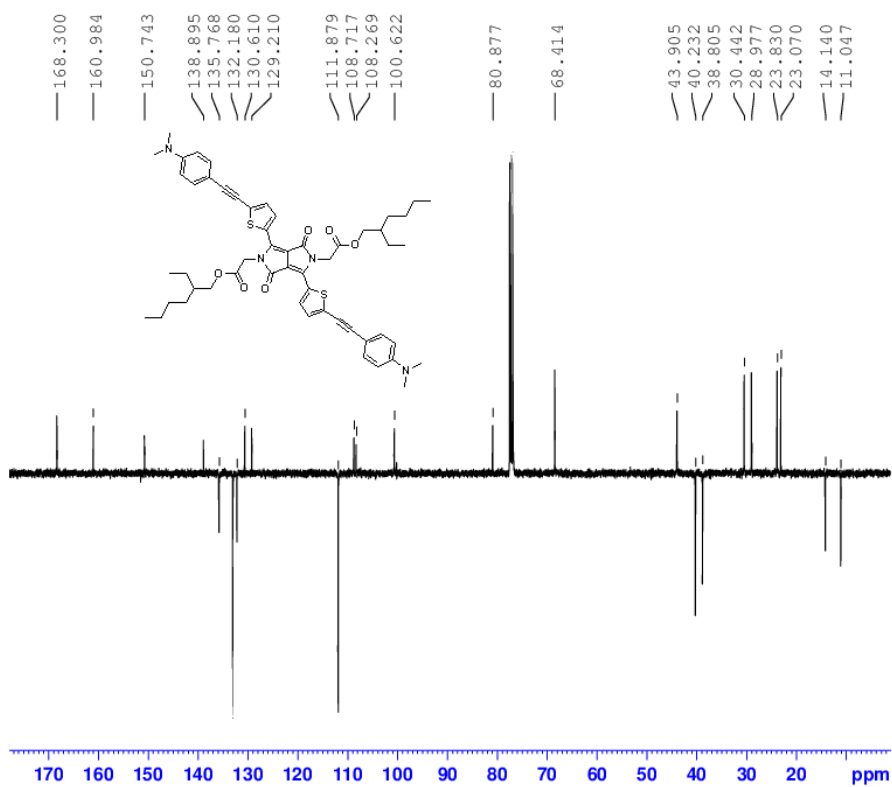


5. ^1H and ^{13}C NMR and HR-MALDI-MS spectra of chromophore **1b**

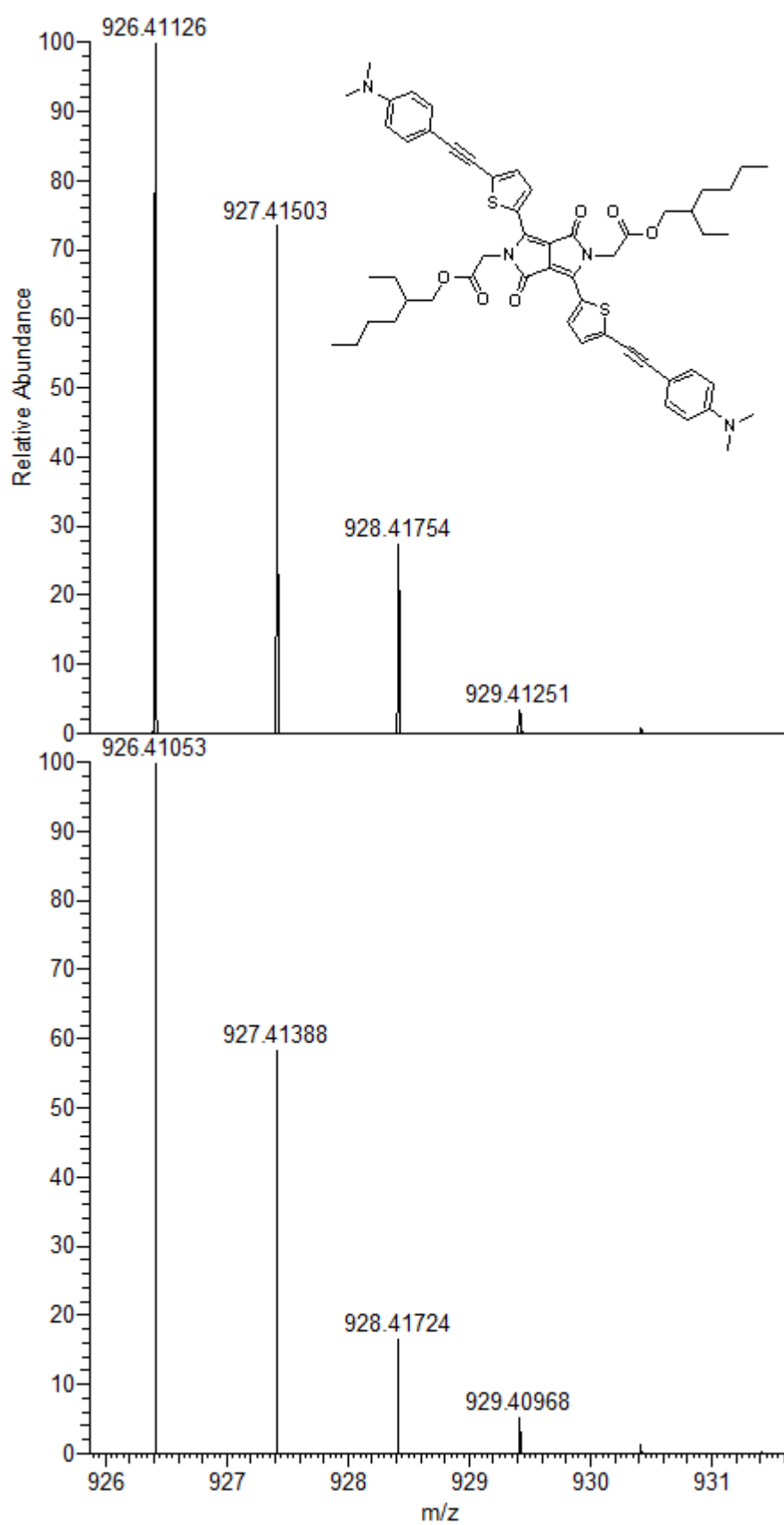
^1H NMR spectrum (400 MHz, CDCl_3 , 25 °C) of **1b**



^{13}C NMR spectrum (100 MHz, CDCl_3 , 25 °C) of **1b**

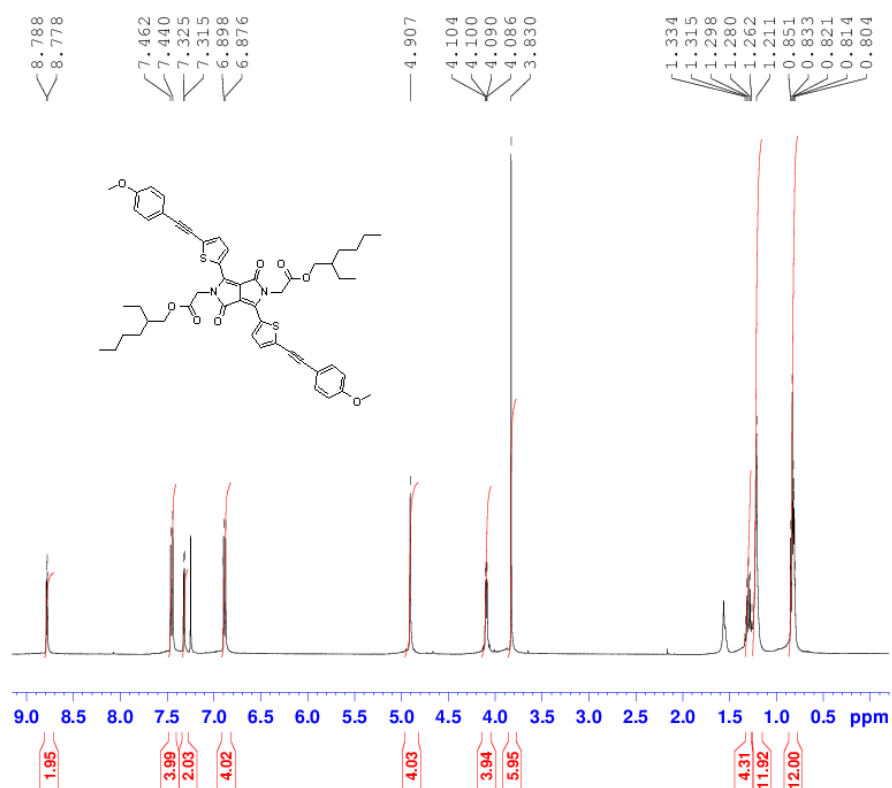


Experimental (up) and calculated (down) MALDI spectra of **1b**

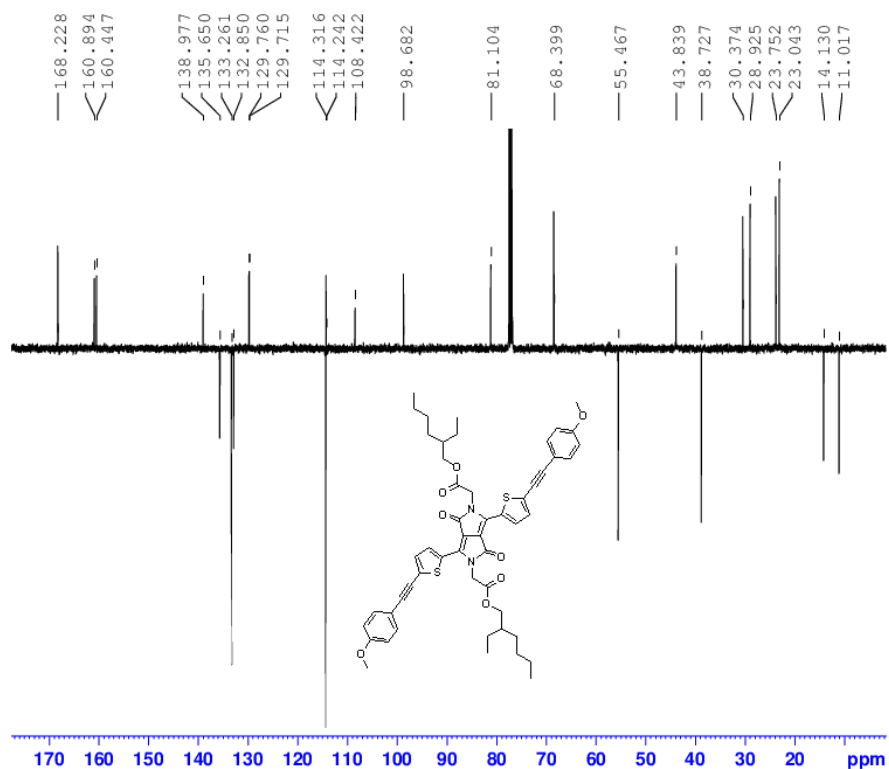


6. ^1H and ^{13}C NMR and HR-MALDI-MS spectra of chromophore 2b

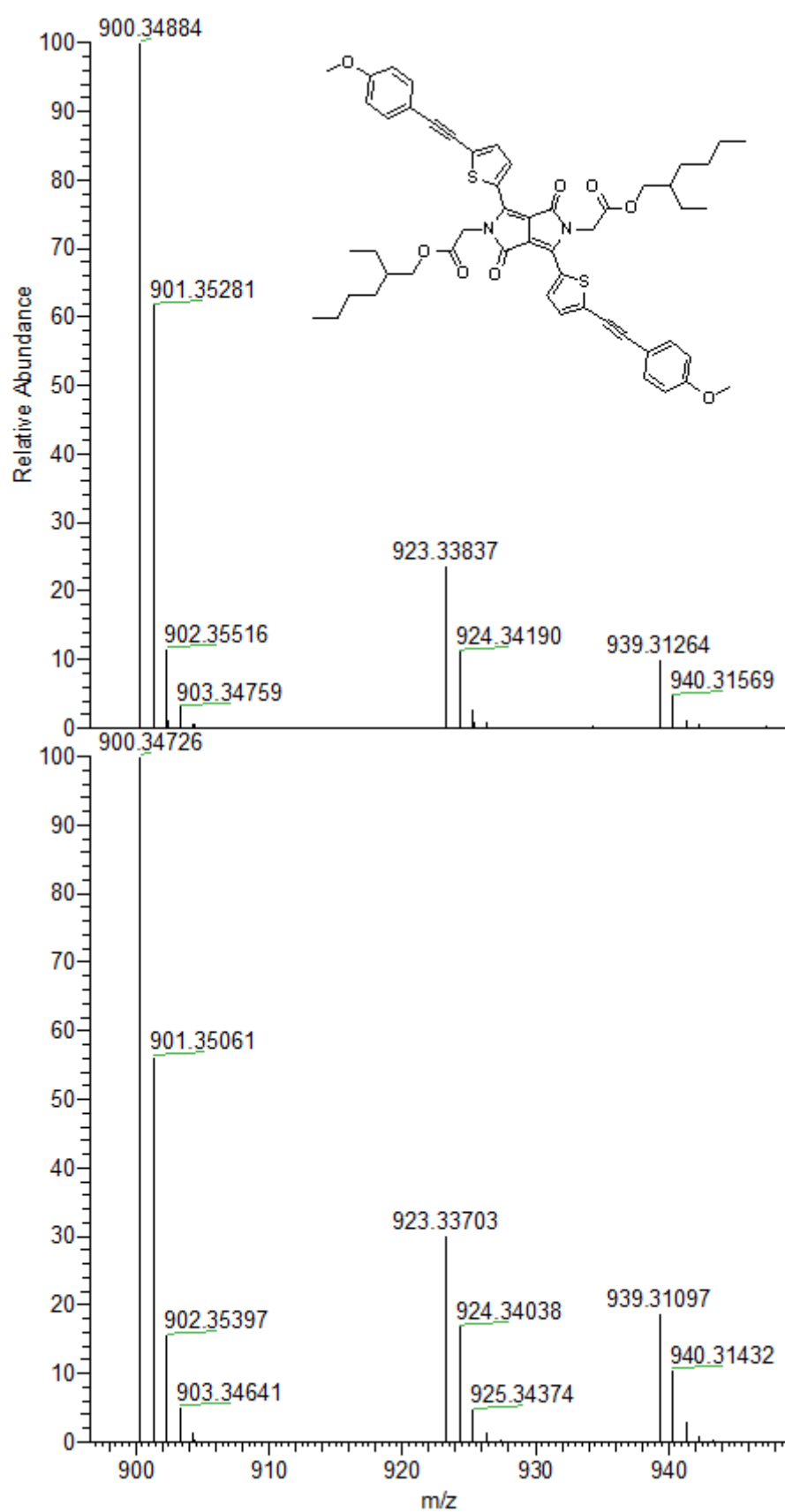
^1H NMR spectrum (400 MHz, CDCl_3 , 25 °C) of **2b**



^{13}C NMR spectrum (100 MHz, CDCl_3 , 25 °C) of **2b**

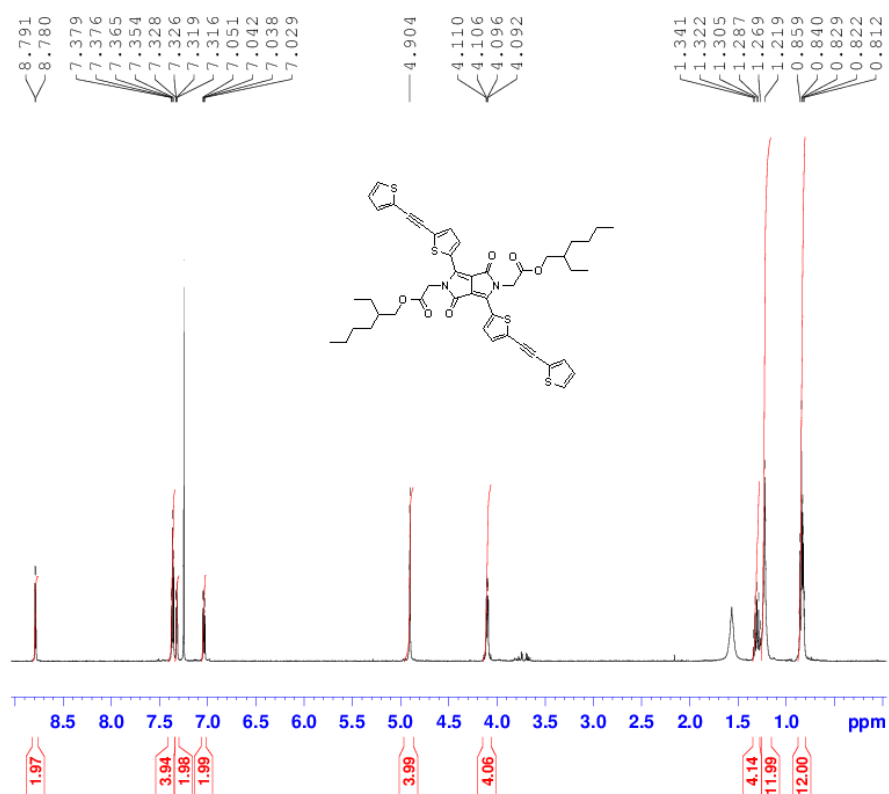


Experimental (up) and calculated (down) MALDI spectra of **2b**

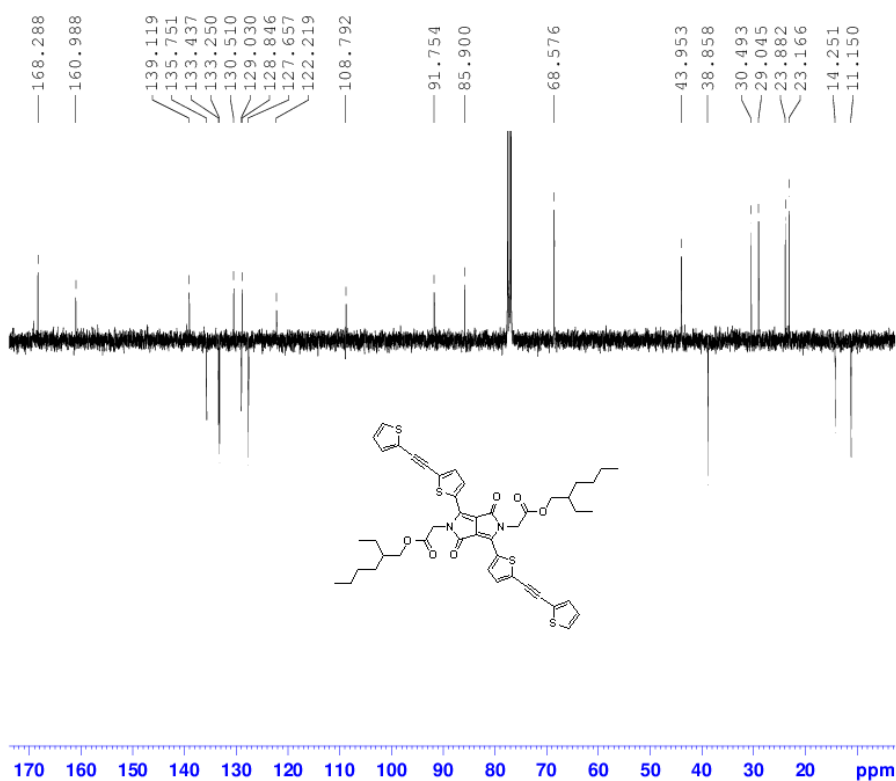


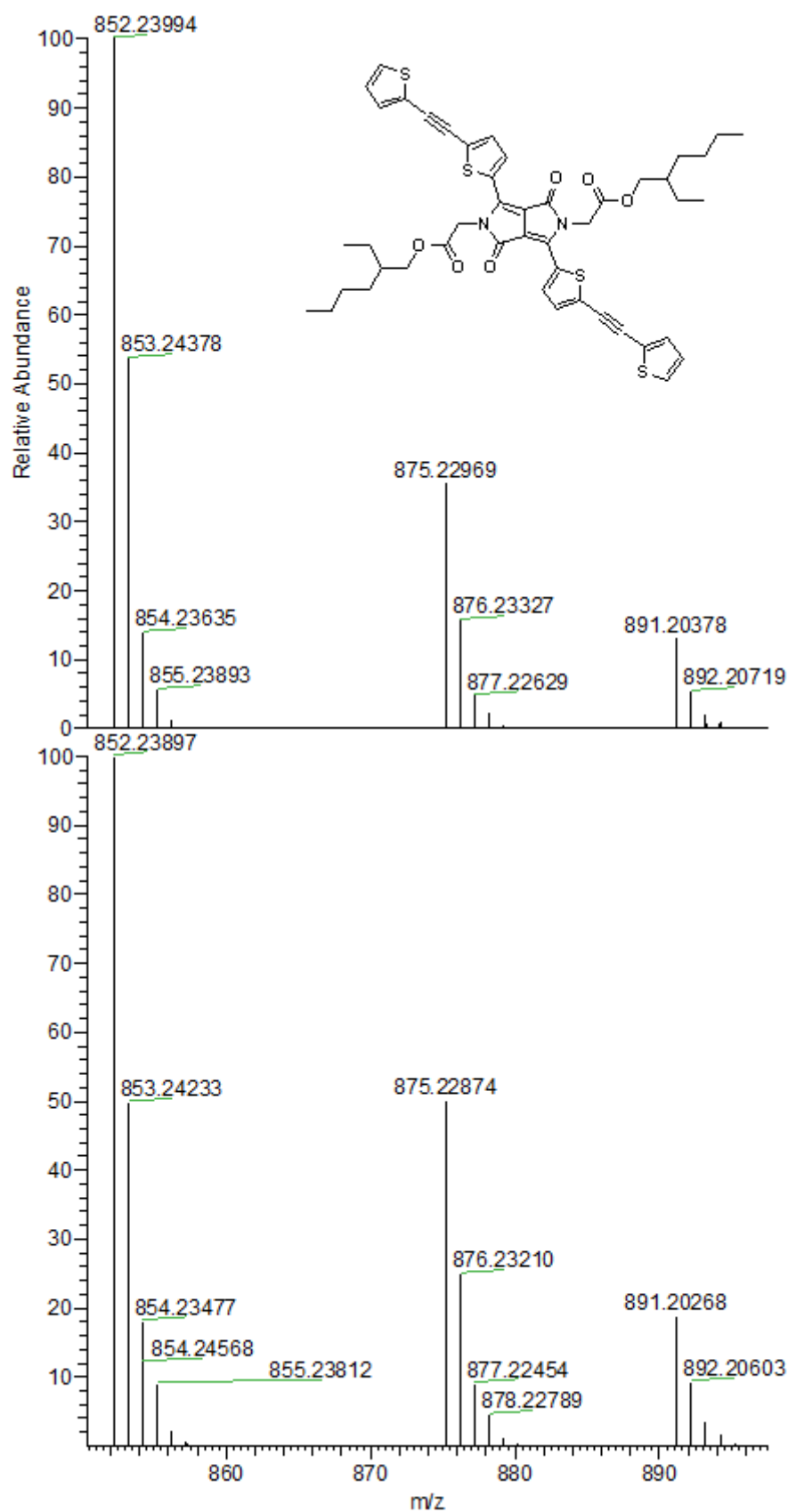
7. ^1H and ^{13}C NMR and HR-MALDI-MS spectra of chromophore **3b**

^1H NMR spectrum (400 MHz, CDCl_3 , 25 °C) of **3b**



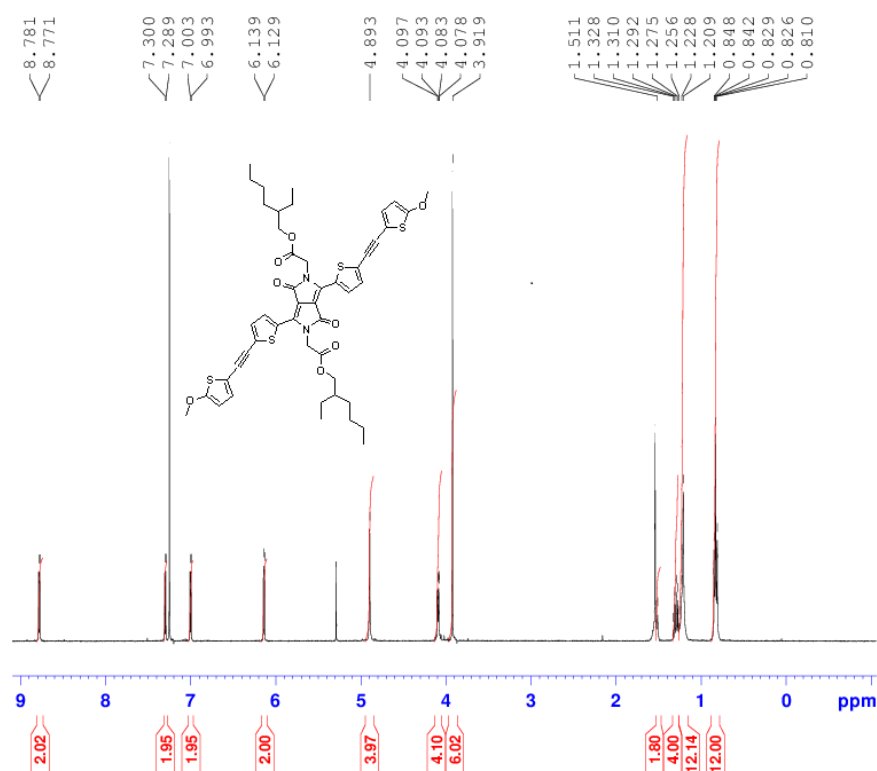
^{13}C NMR spectrum (100 MHz, CDCl_3 , 25 °C) of **3b**



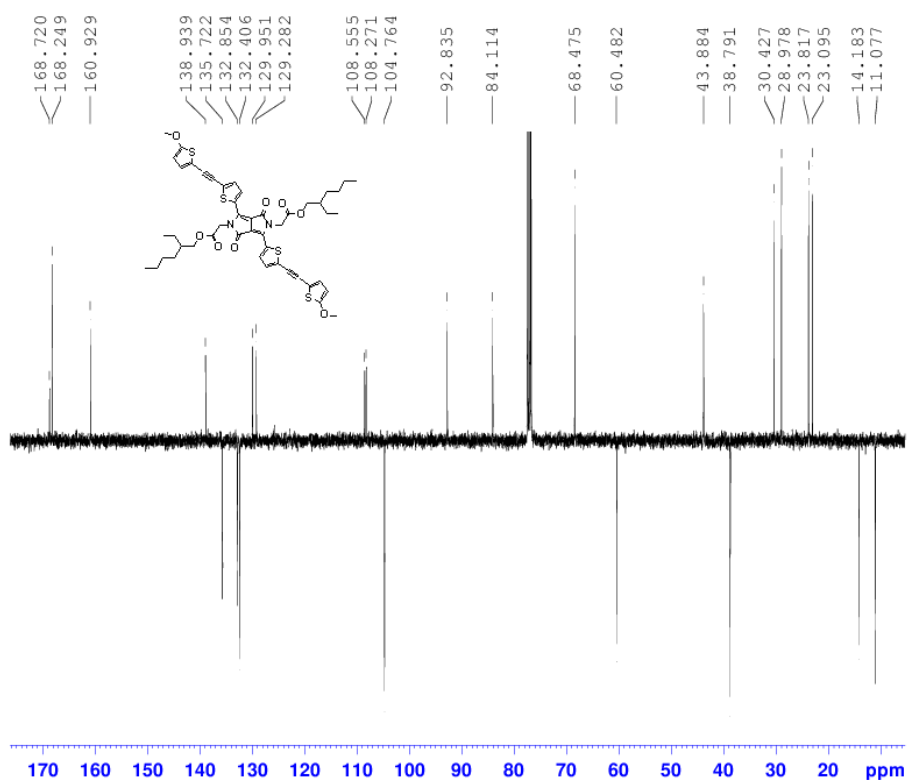
Experimental (up) and calculated (down) MALDI spectra of **3b**

8. ^1H and ^{13}C NMR and HR-MALDI-MS spectra of chromophore 4b

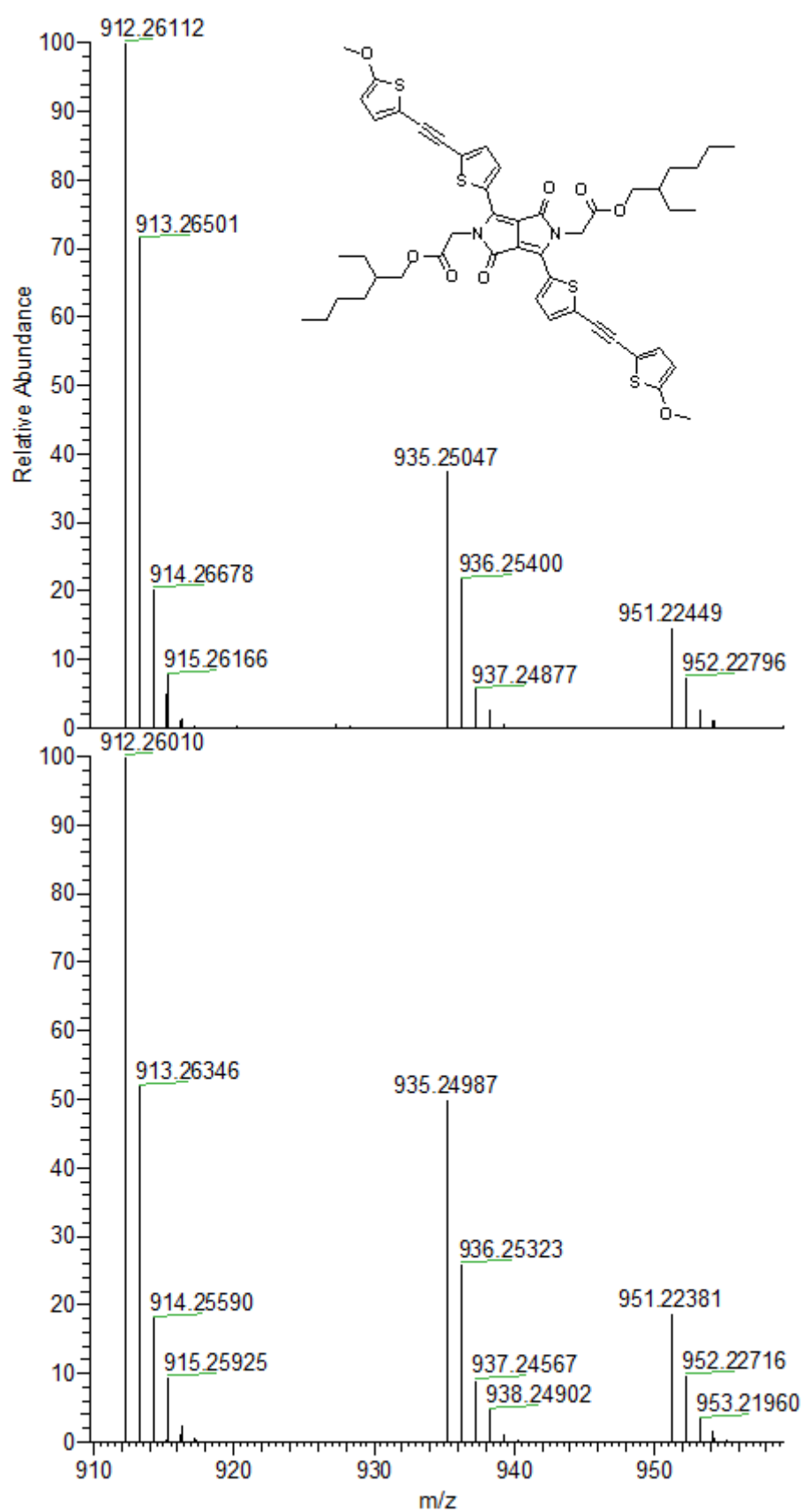
^1H NMR spectrum (400 MHz, CDCl_3 , 25 °C) of **4b**



^{13}C NMR spectrum (100 MHz, CDCl_3 , 25 °C) of **4b**

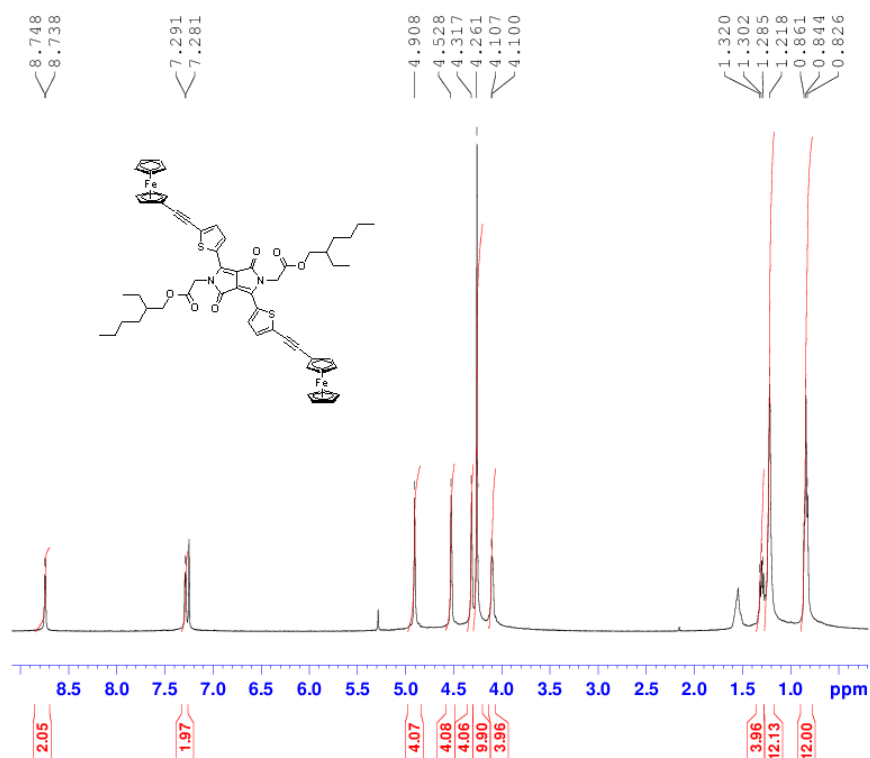


Experimental (up) and calculated (down) MALDI spectra of **4b**

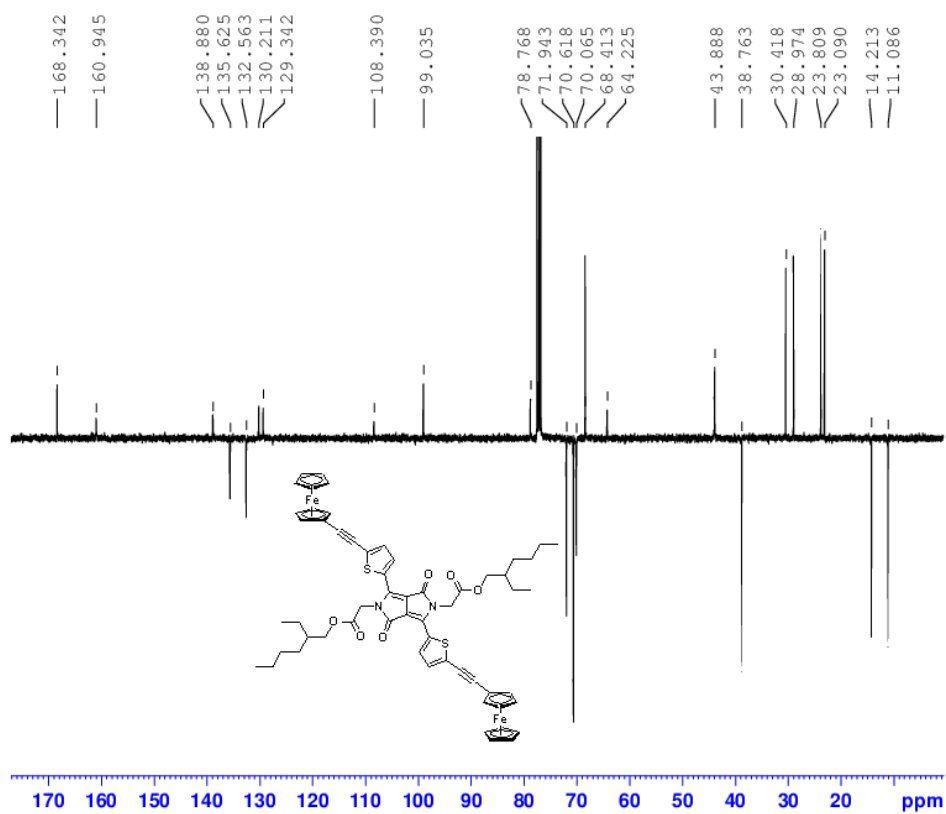


9. ^1H and ^{13}C NMR and HR-MALDI-MS spectra of chromophore **5b**

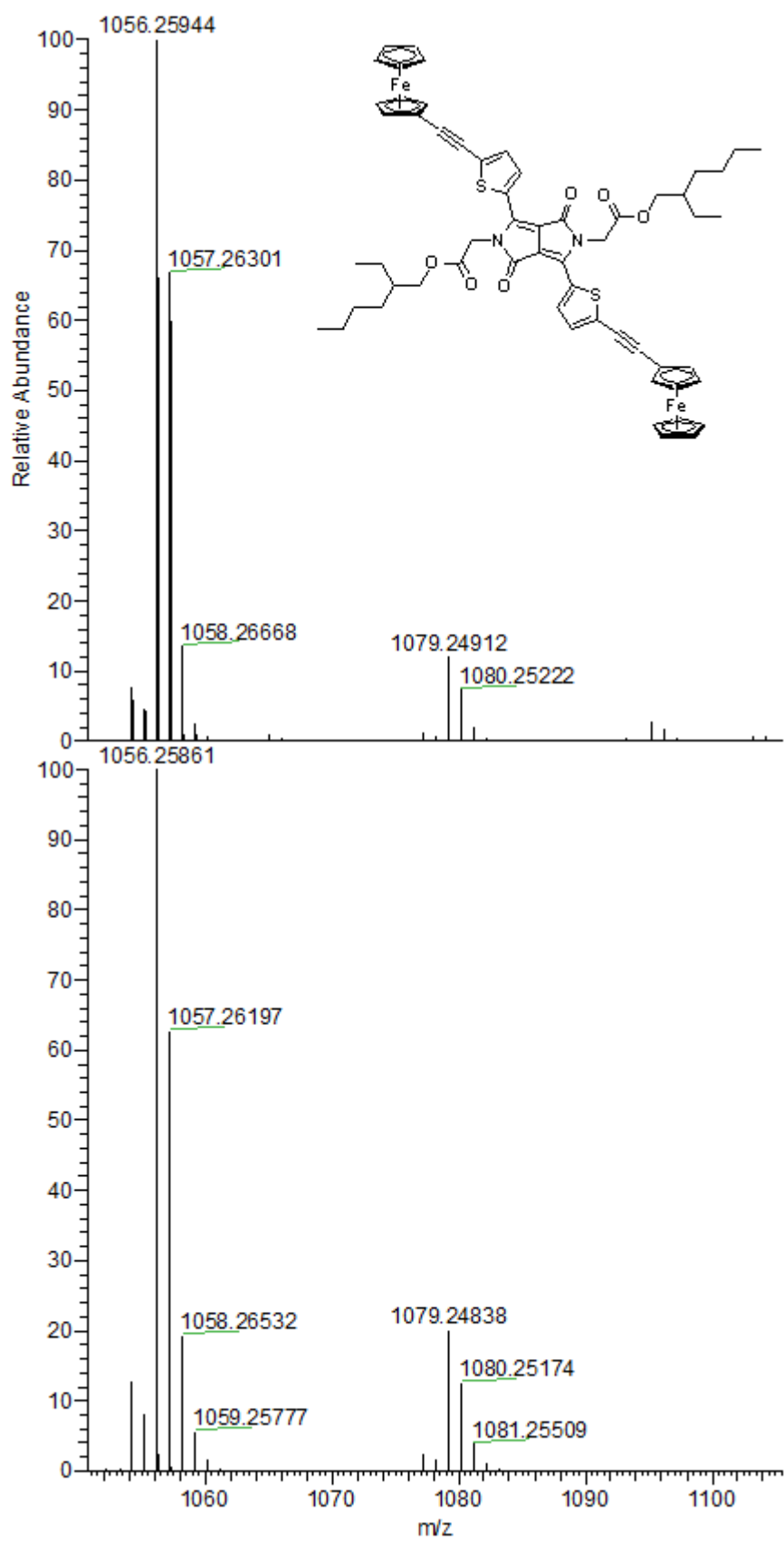
^1H NMR spectrum (400 MHz, CDCl_3 , 25 °C) of **5b**



^{13}C NMR spectrum (100 MHz, CDCl_3 , 25 °C) of **5b**

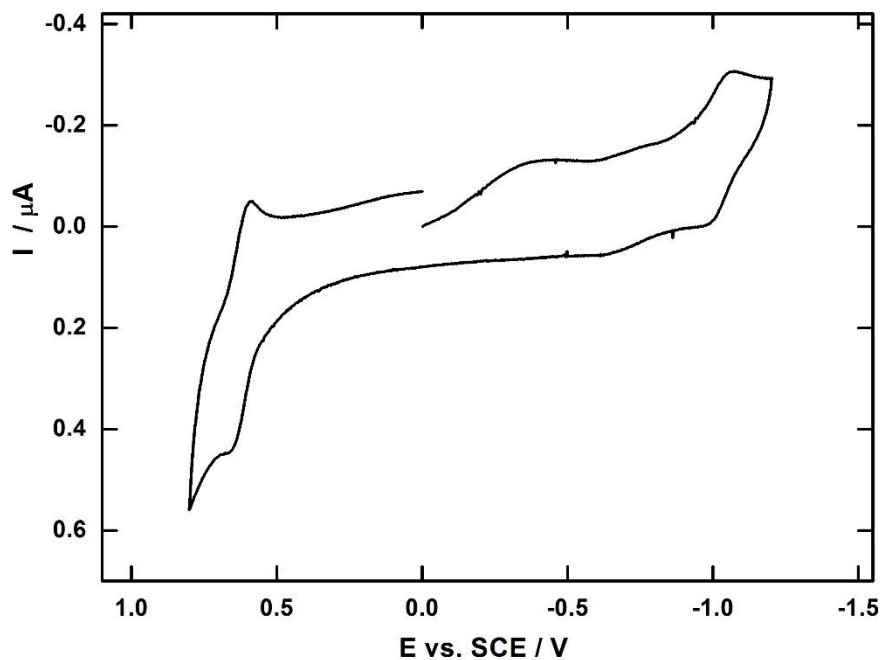


Experimental (up) and calculated (down) MALDI spectra of **5b**

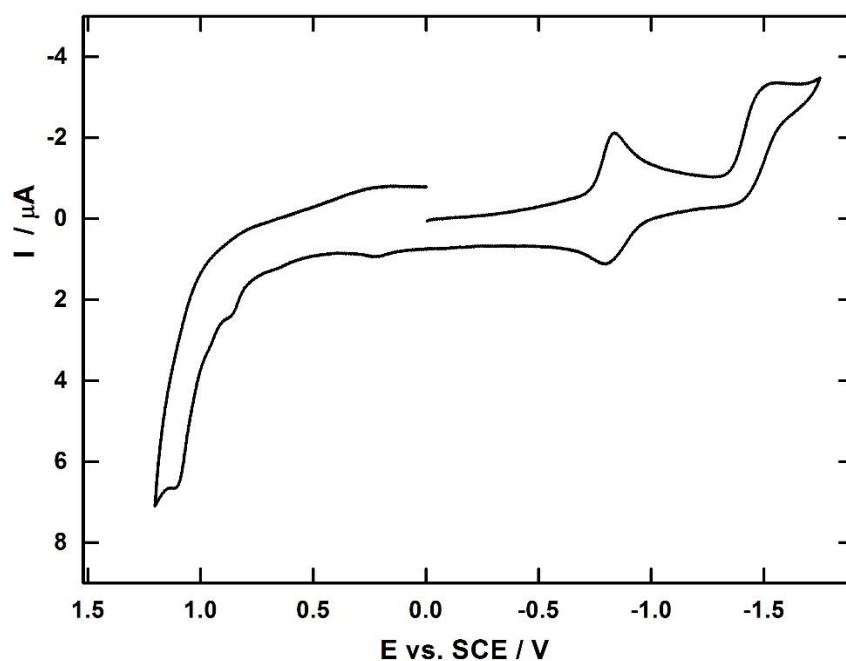


10. Electrochemistry

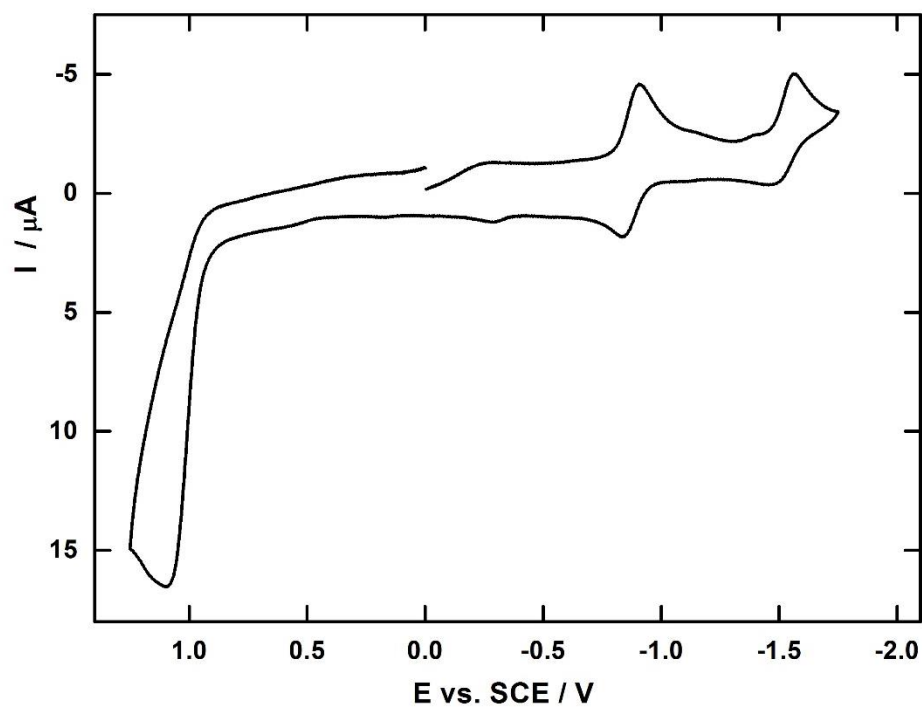
Representative CV curve of the oxidation and reduction of compound **1a** at Pt electrode in *N,N*, -dimethylformamide containing 0.1 M Bu₄NPF₆; scan rate 100mV/s



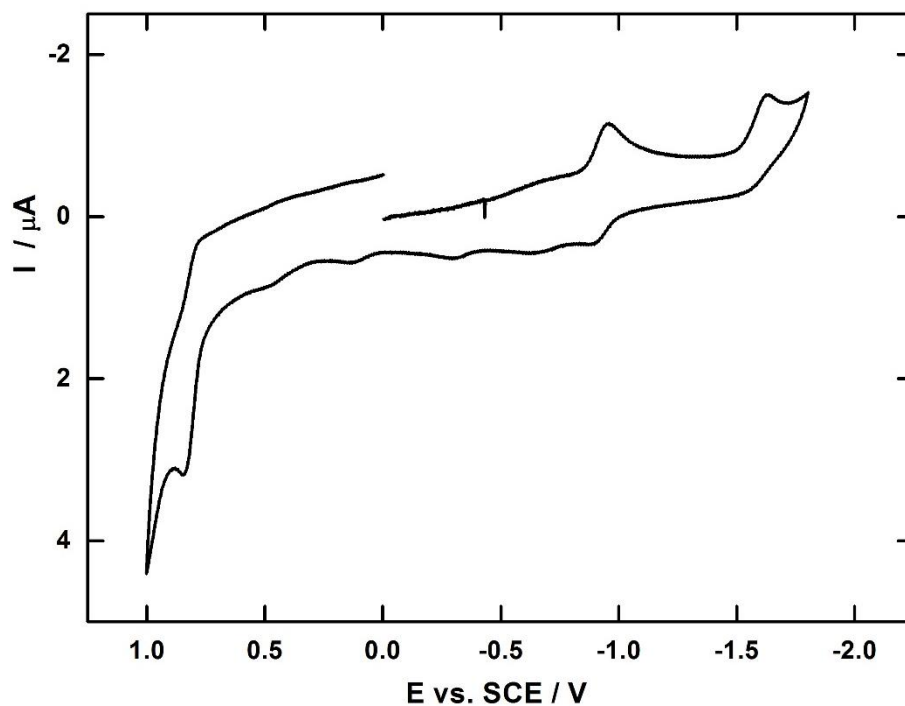
Representative CV curve of the oxidation and reduction of compound **2b** at Pt electrode in *N,N*, -dimethylformamide containing 0.1 M Bu₄NPF₆; scan rate 100mV/s



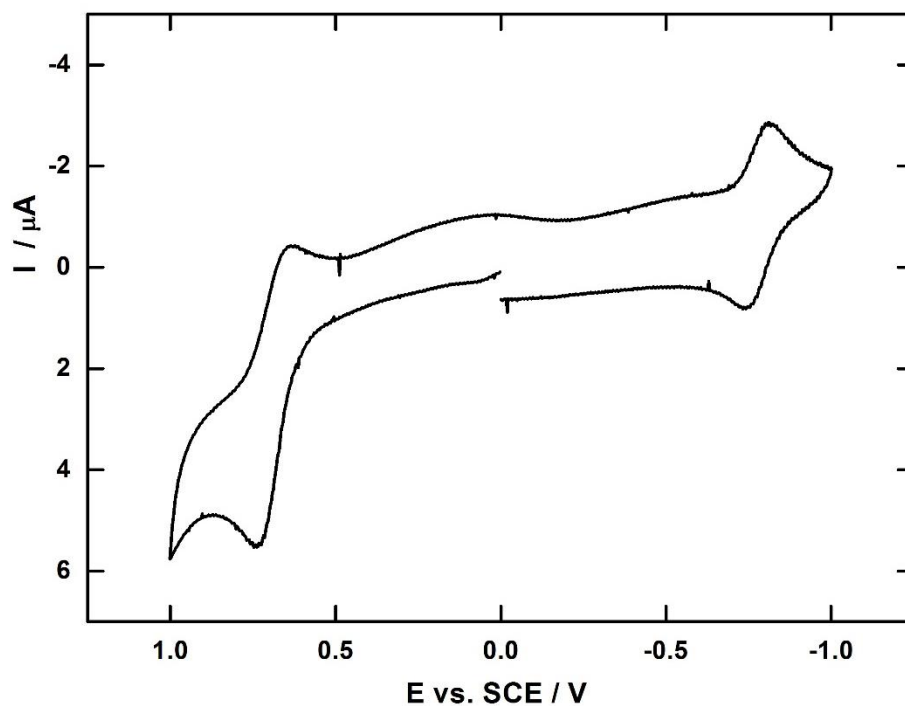
Representative CV curve of the oxidation and reduction of compound **3a** at Pt electrode in *N,N*-dimethylformamide containing 0.1 M Bu₄NPF₆; scan rate 100mV/s



Representative CV curve of the oxidation and reduction of compound **4a** at Pt electrode in *N,N*-dimethylformamide containing 0.1 M Bu₄NPF₆; scan rate 100mV/s

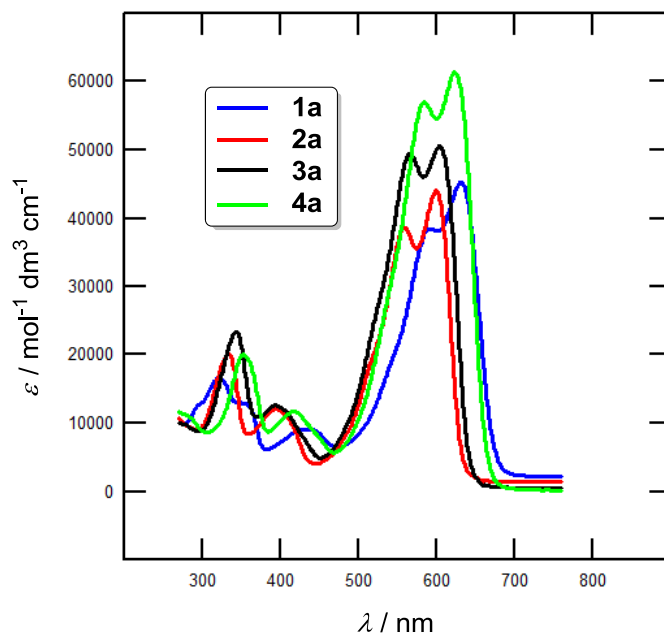


Representative CV curve of the oxidation and reduction of compound **5b** at Pt electrode in *N,N*-dimethylformamide containing 0.1 M Bu₄NPF₆; scan rate 100mV/s

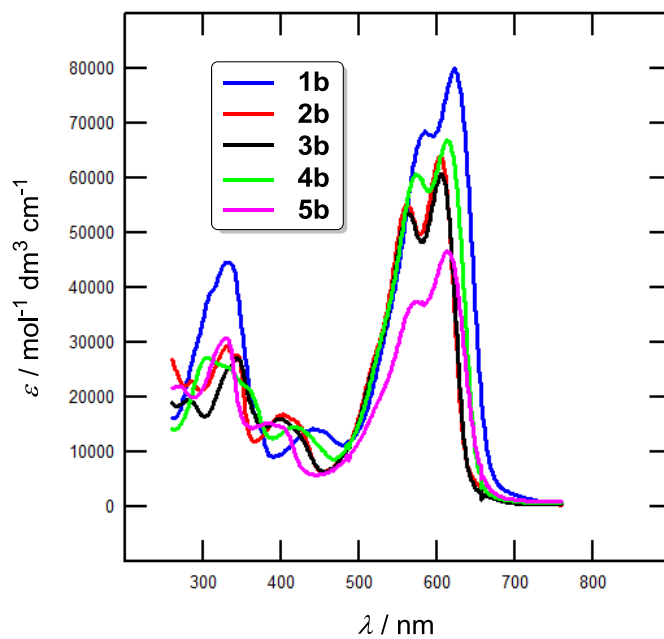


11. Electronic absorption and emission spectra

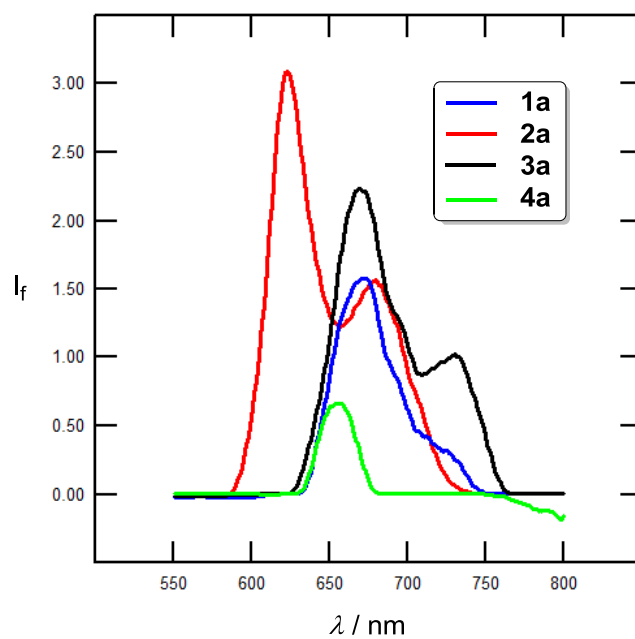
UV/VIS absorption spectra of chromophores **1a-4a** in 1,4-dioxane at concentration 1×10^{-5} M



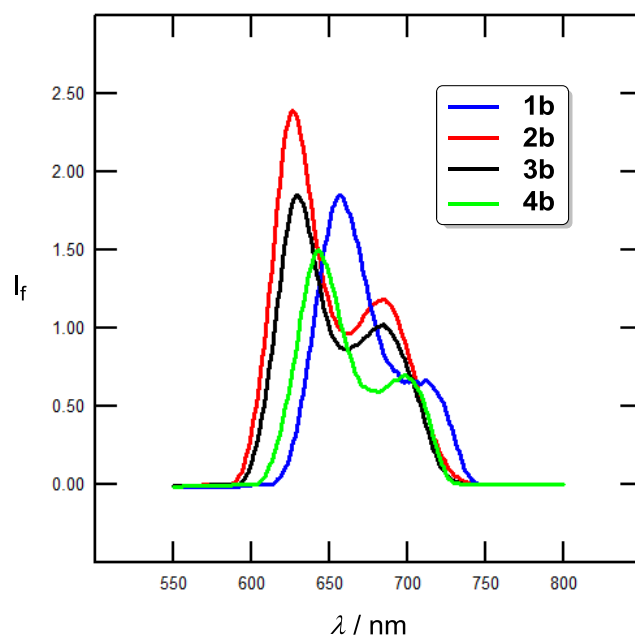
UV/VIS absorption spectra of chromophores **1b-5b** in 1,4-dioxane at concentration 1×10^{-5} M



Emission fluorescent spectra of chromophores **1a-4a** in 1,4-dioxane

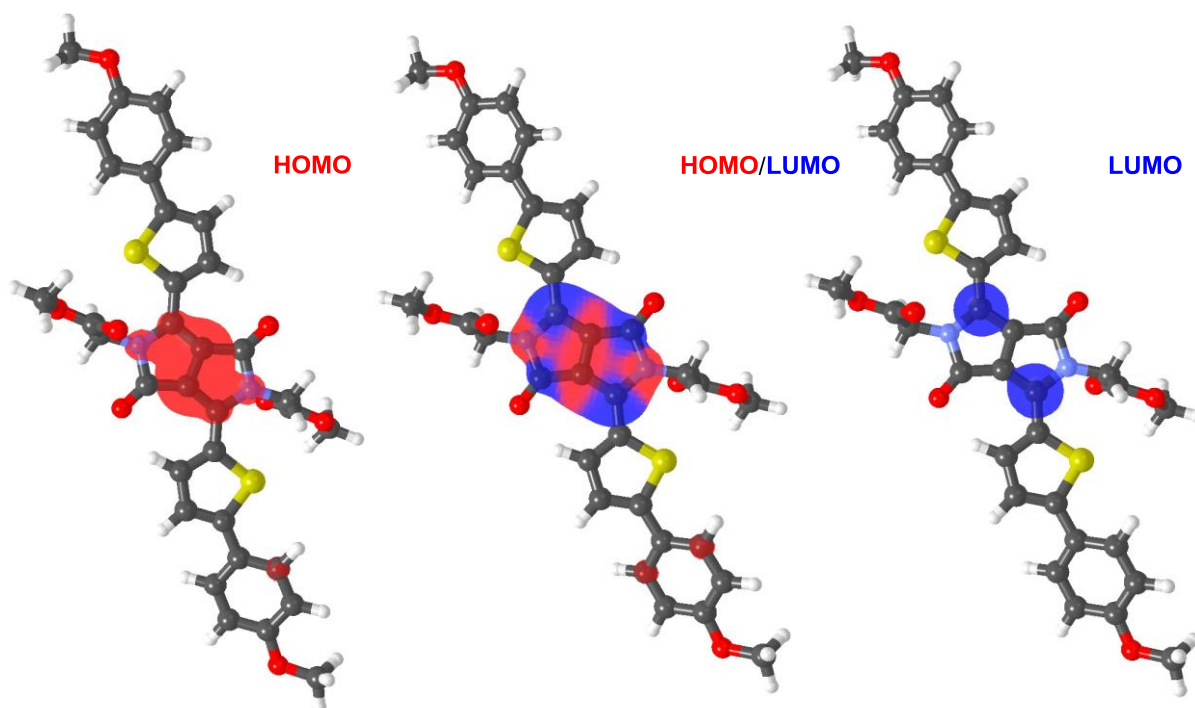


Emission fluorescent spectra of chromophores **1b-4b** in 1,4-dioxane

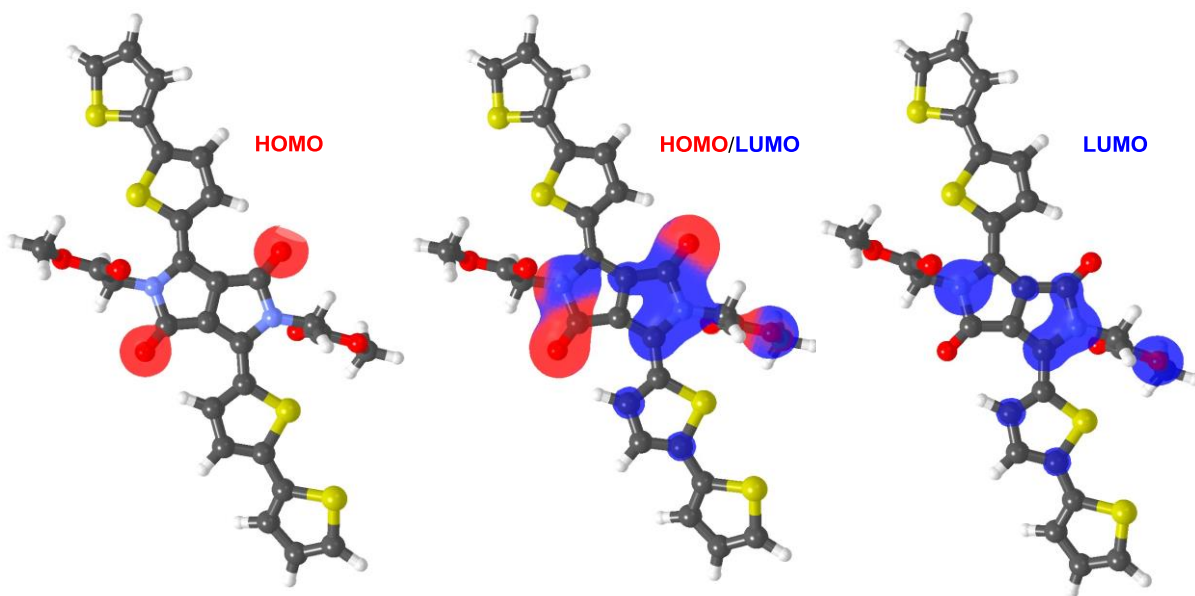


12. HOMO and LUMO visualization

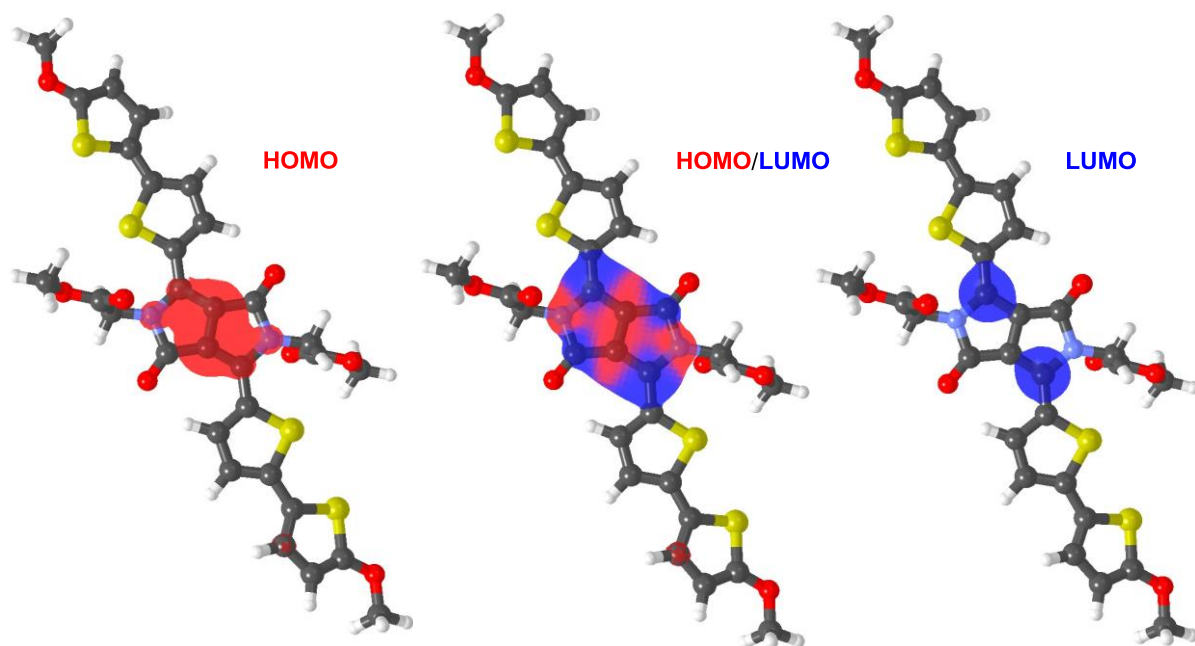
HOMO (red) and LUMO (blue) localizations in **2a**



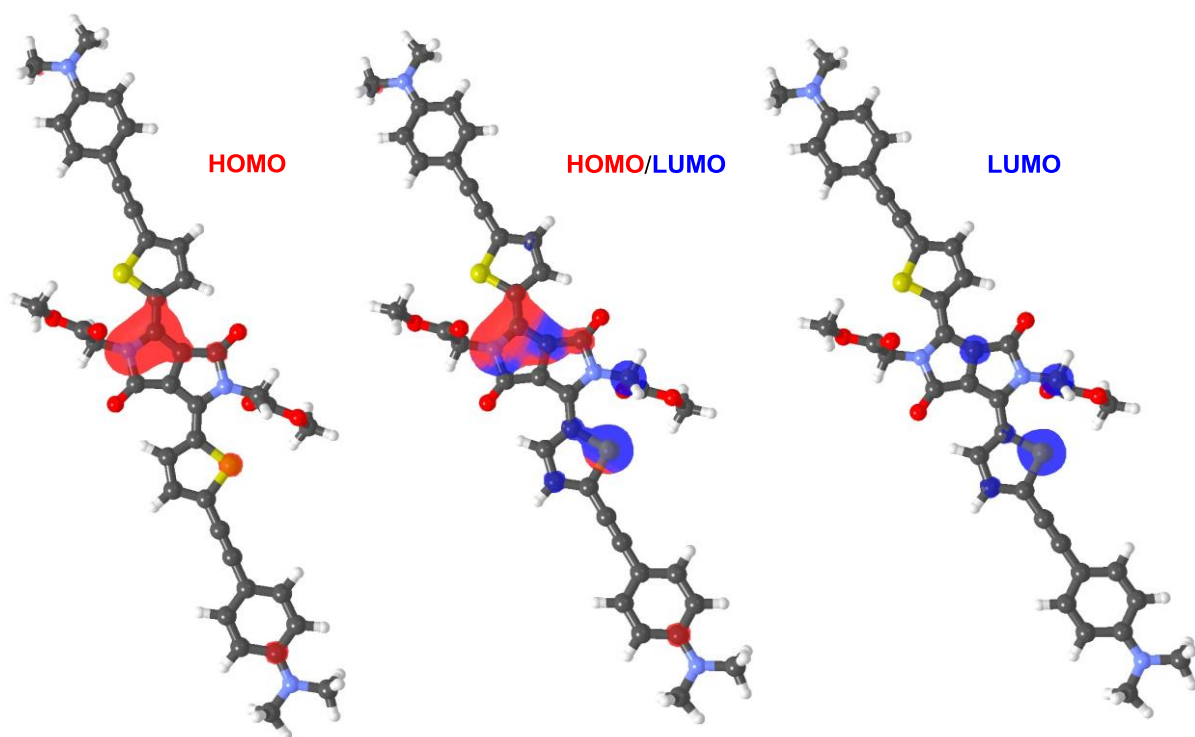
HOMO (red) and LUMO (blue) localizations in **3a**



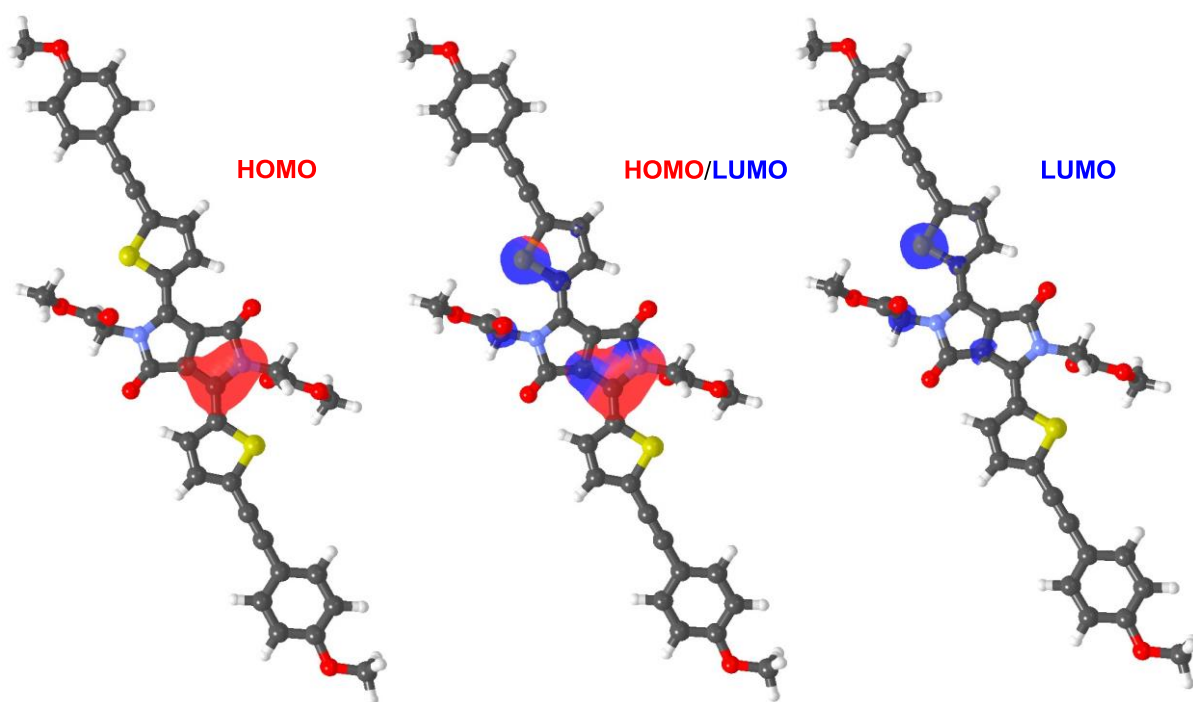
HOMO (red) and LUMO (blue) localizations in **4a**



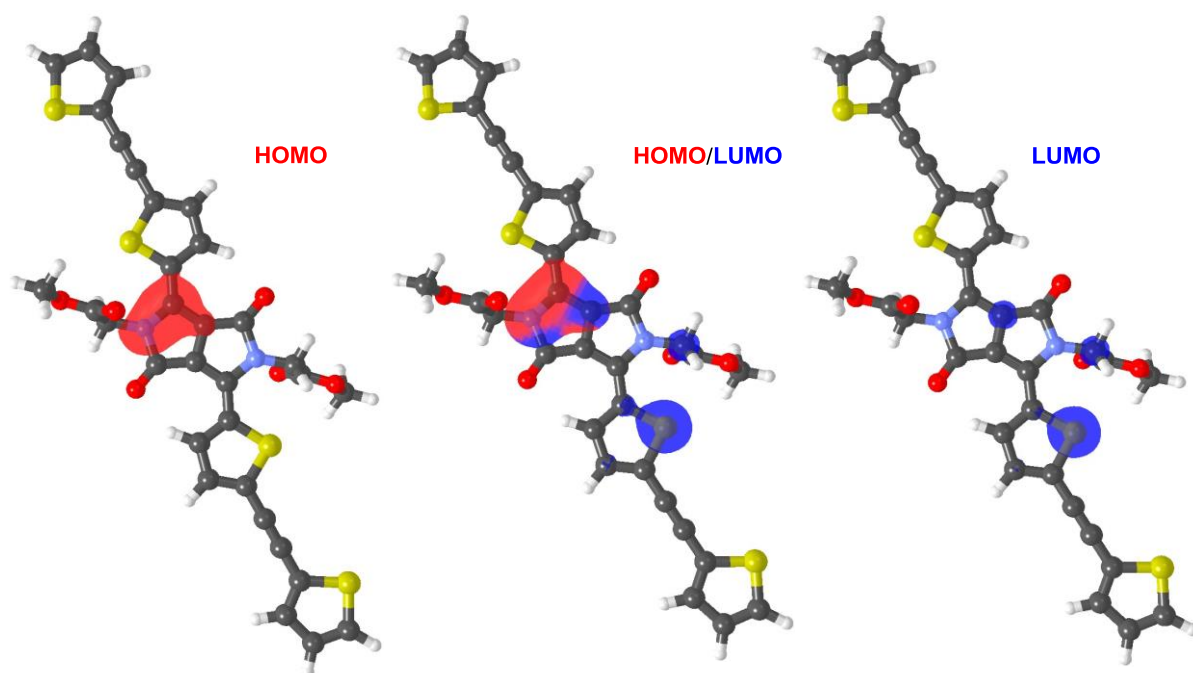
HOMO (red) and LUMO (blue) localizations in **1b**



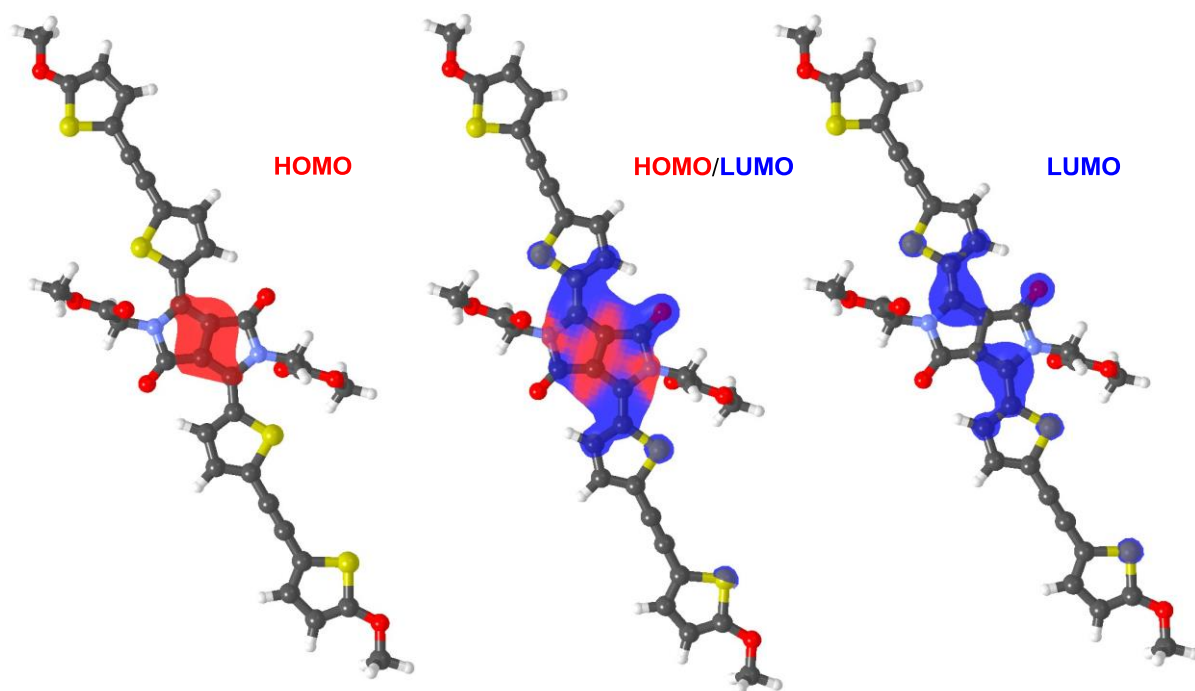
HOMO (red) and LUMO (blue) localizations in **2b**



HOMO (red) and LUMO (blue) localizations in **3b**



HOMO (red) and LUMO (blue) localizations in **4b**



HOMO (red) and LUMO (blue) localizations in **5b**

