

Supporting information

Synthesis of Dipyrrolopyrazine based sensitizer as new π -bridge end-capped with Donor-Acceptor for DSSC: A combined experimental and theoretical investigation

Puttavva Meti ^a, Goli Nagaraju ^b, Jung-Won Yang ^a, Sun Hwa Jung ^a, and Young-Dae Gong ^{a*}

^a Innovative Drug Library Research Center, Department of Chemistry, College of Science, Dongguk University,

26, 3-ga, Pil-dong, Jung-gu, Seoul 04620, Republic of Korea

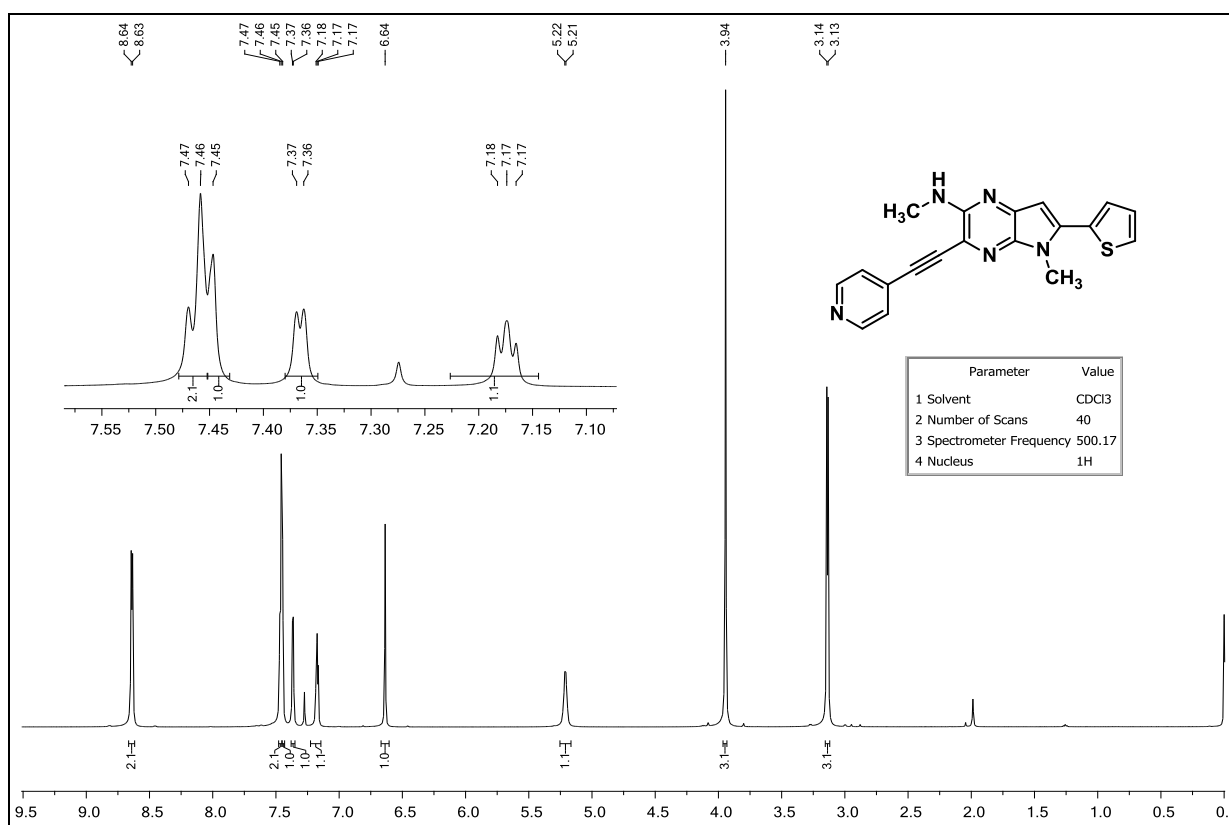
^b Department of Chemical engineering, College of Engineering, Kyung Hee University, 1 Seocheon-dong,

Giheung-gu, Yongin-si, Gyeonggi-do 446-70, Republic of Korea

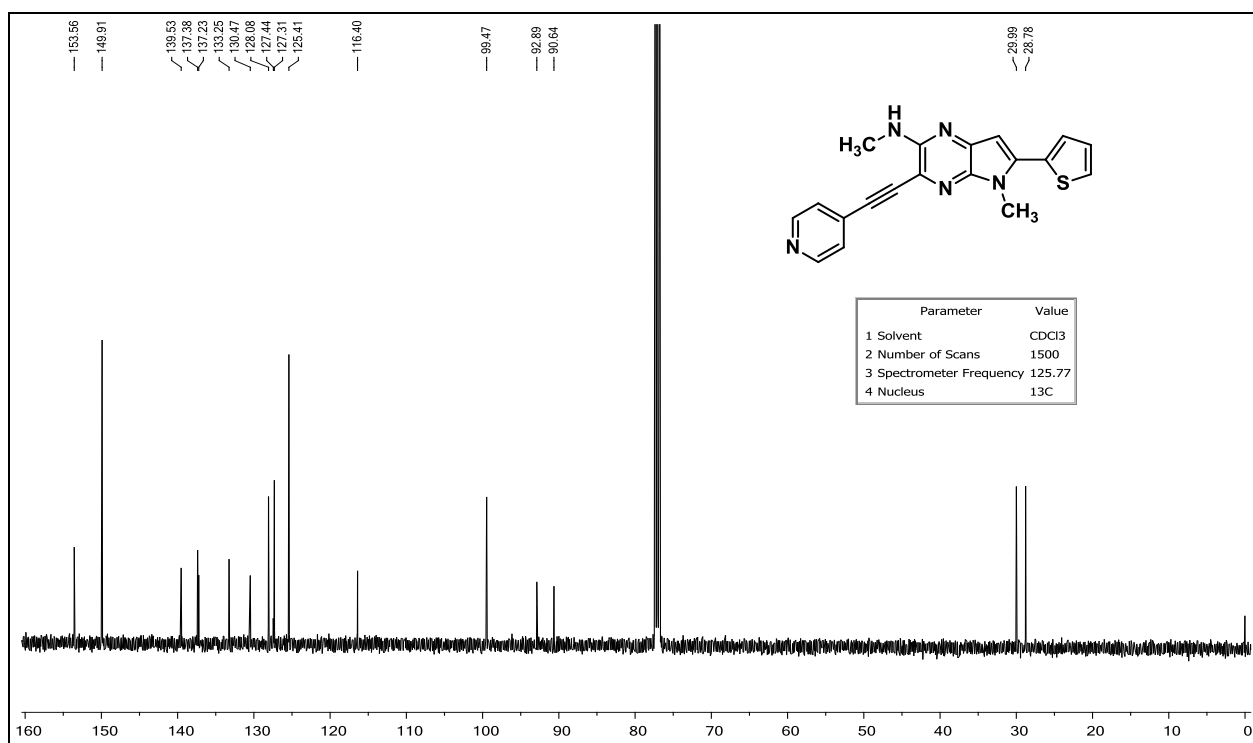
Contents

1. ¹ H NMR and ¹³ C NMR of intermediates 2(a-c)	S2-S3
2. ¹ H NMR and ¹³ C NMR of chromophores 3(a-c)	S4-S6
3. HRMS spectra of intermediates 2(a-c)	S7
4. HRMS spectra of final compounds 3(a-c)	S8
5. Cyclic Voltammograms of dyes 3(b-d)	S9

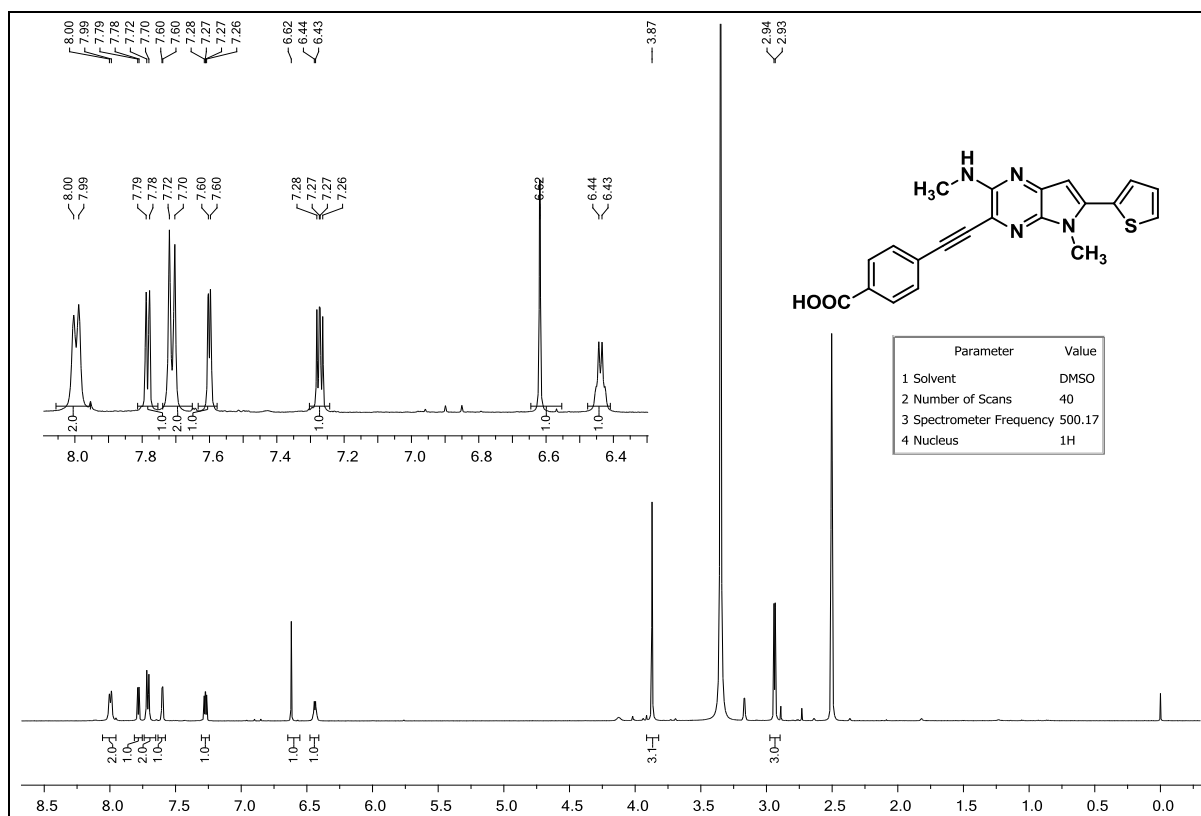
¹H NMR ¹³C NMR spectra of compounds



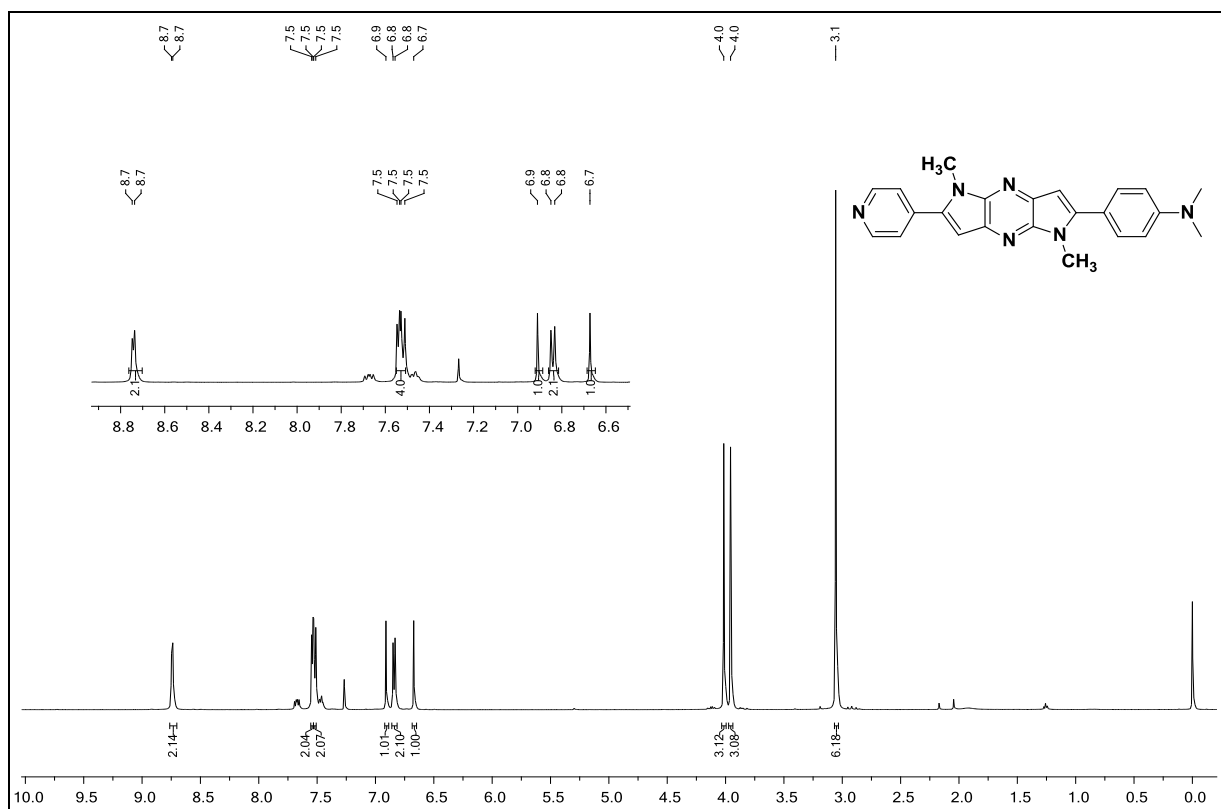
¹H NMR – 2b



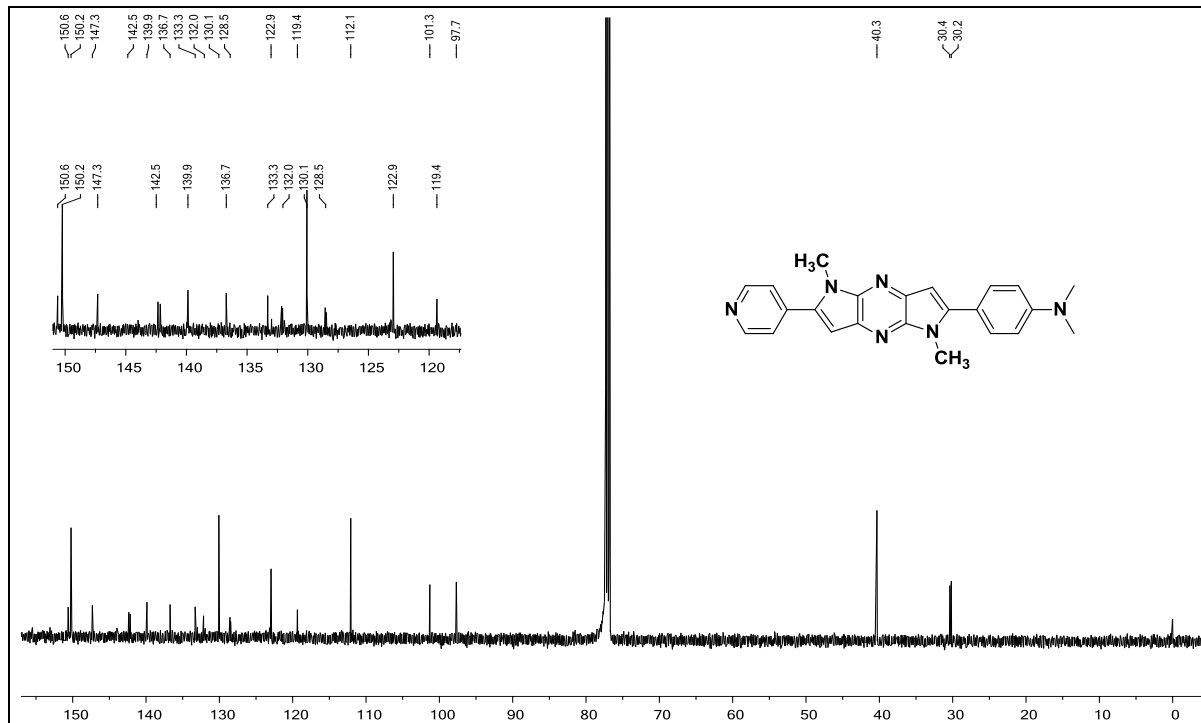
¹³C NMR – 2b



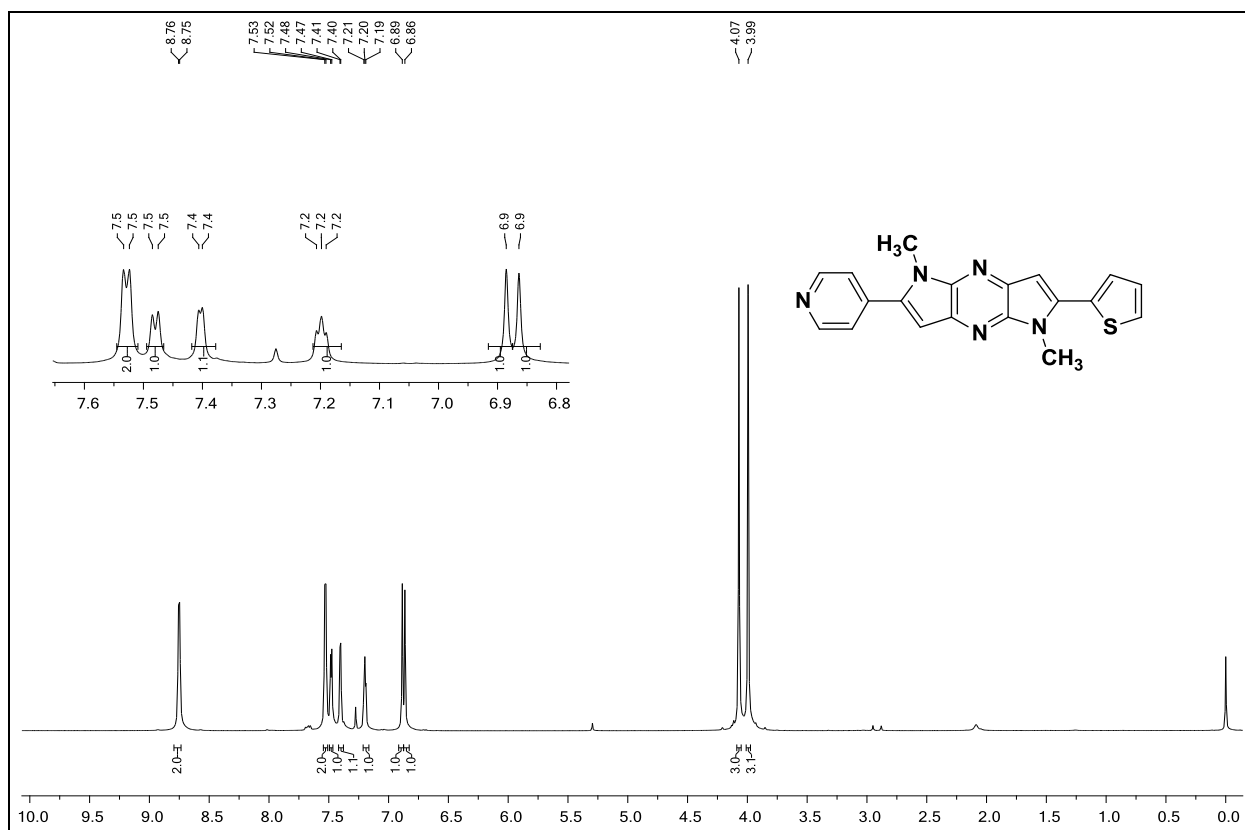
¹H NMR – 2c



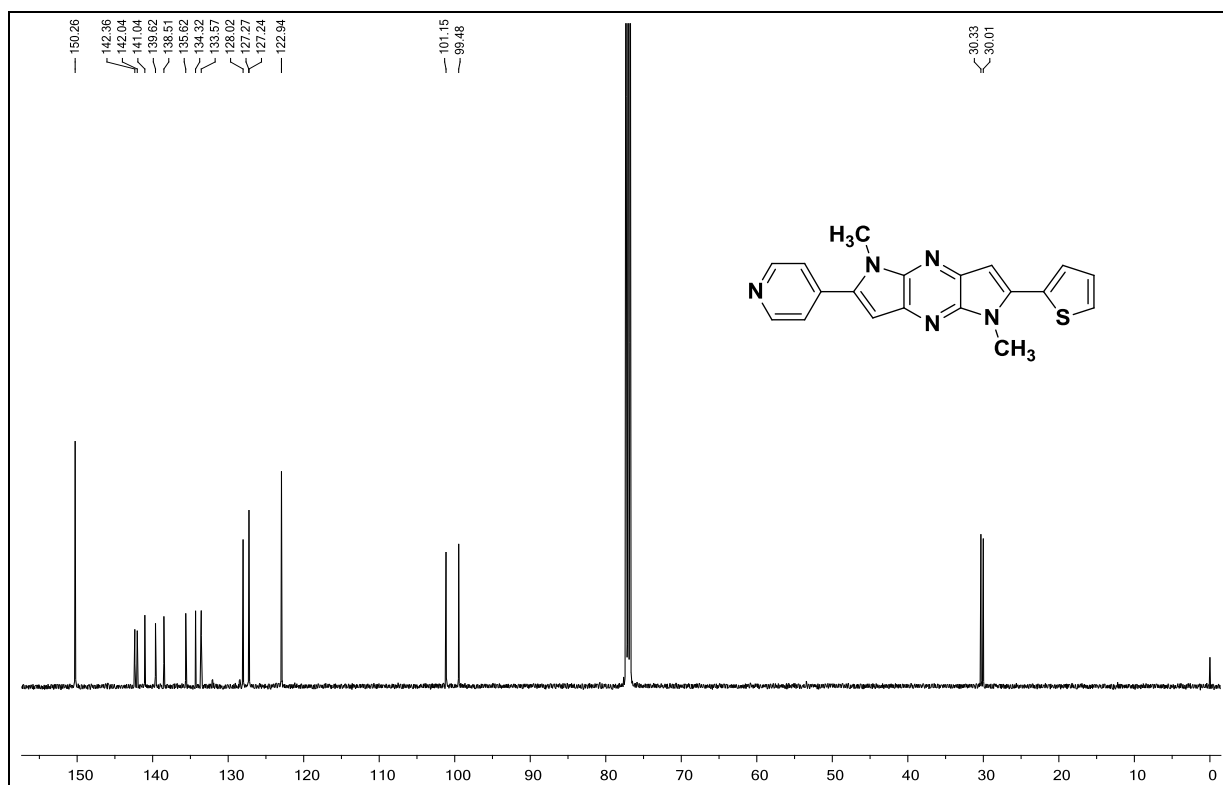
¹H NMR – 3a



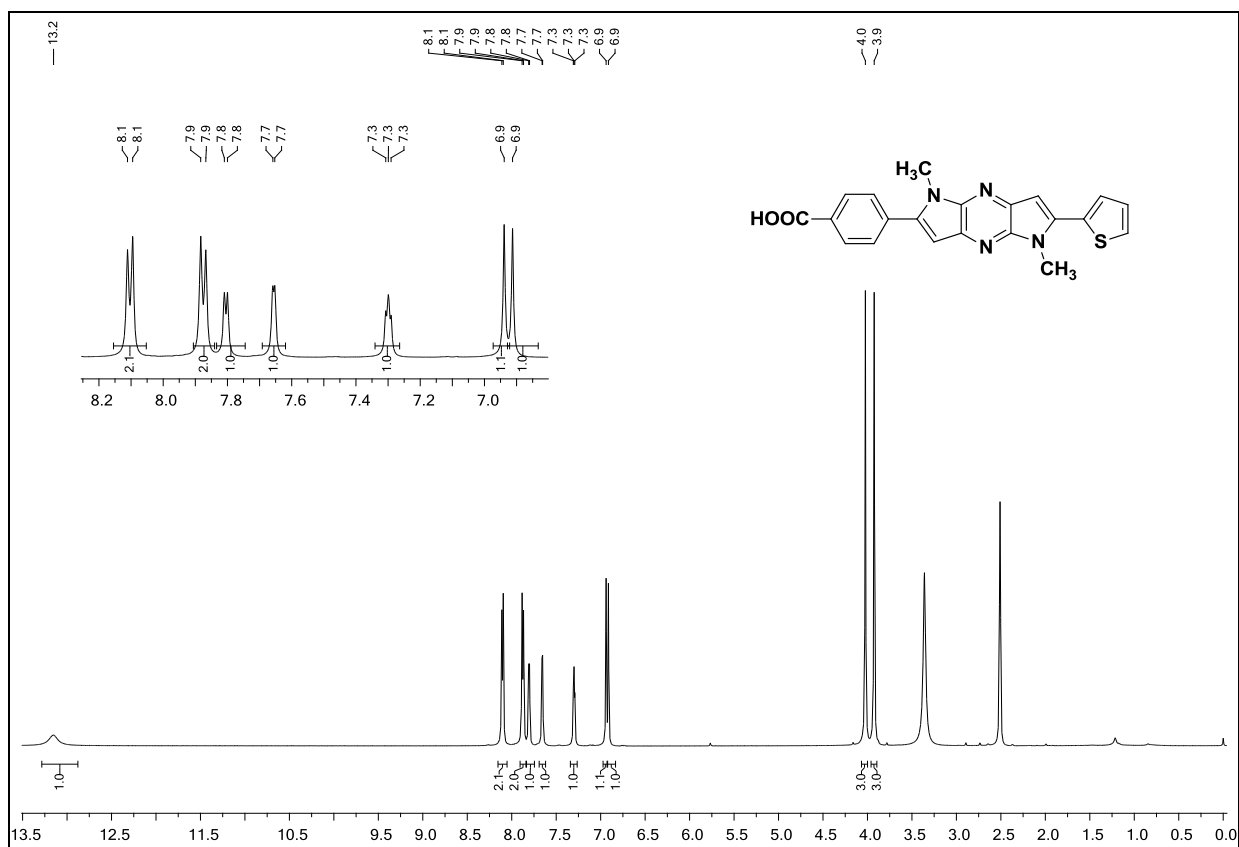
¹³C NMR – 3a



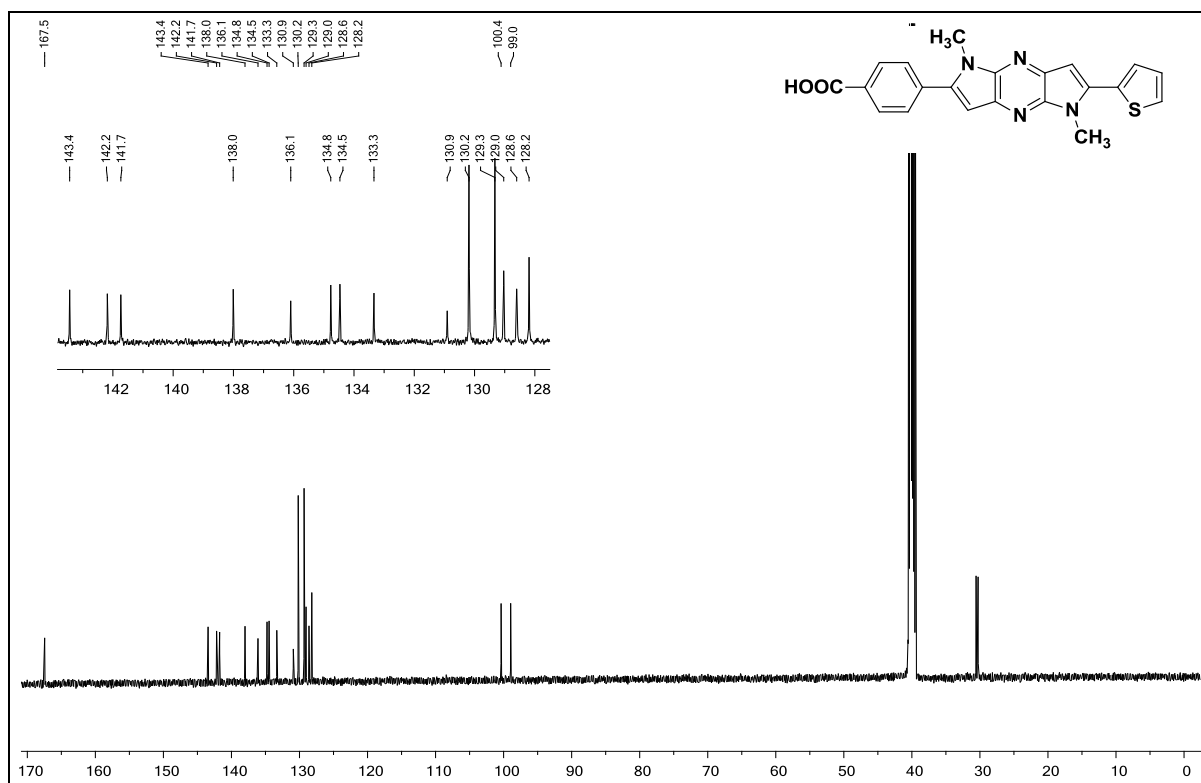
¹H NMR – 3b



¹³C NMR – 3b

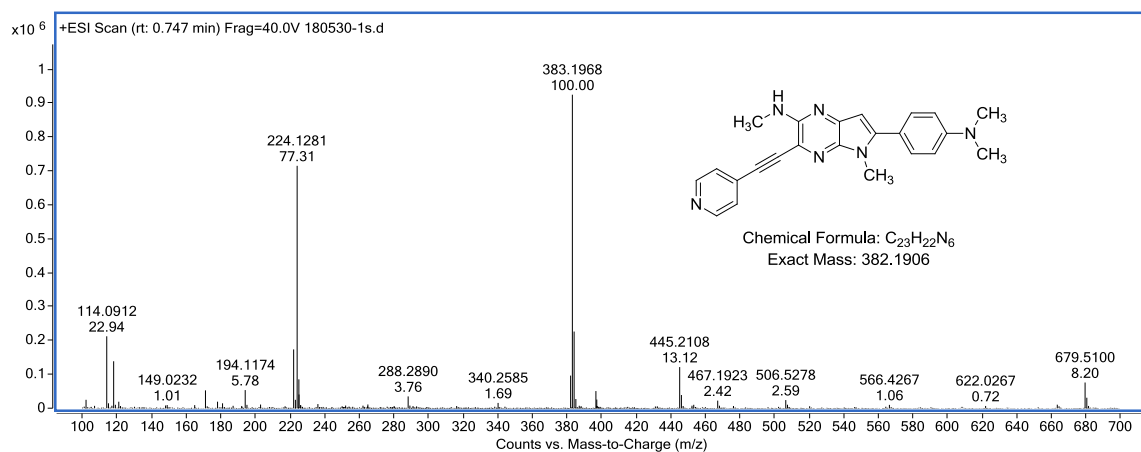


¹H NMR – 3c

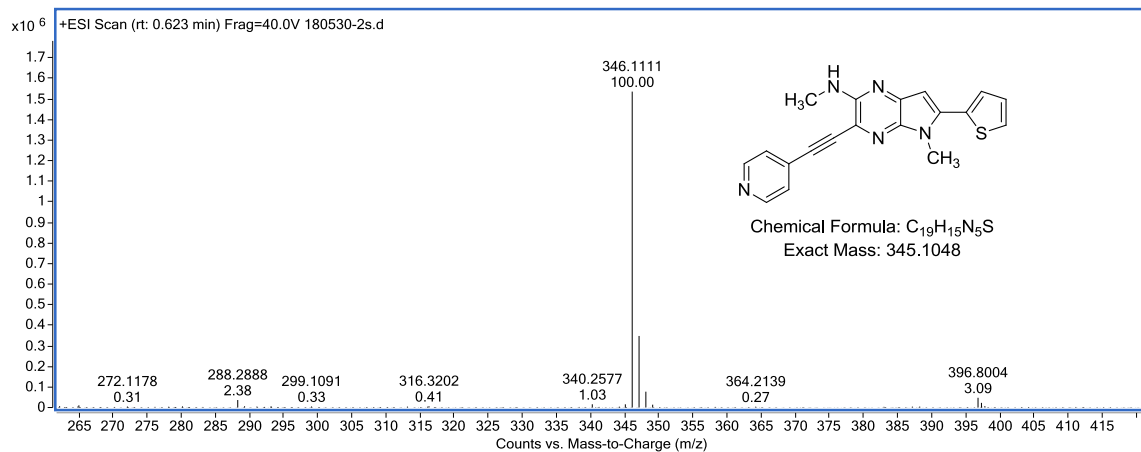


¹³C NMR – 3c

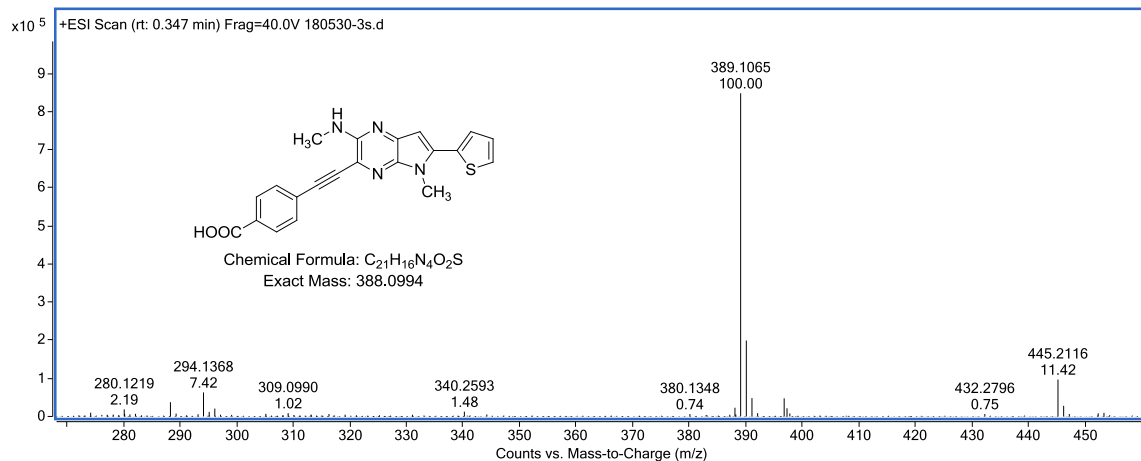
HRMS spectra of intermediates and final compounds



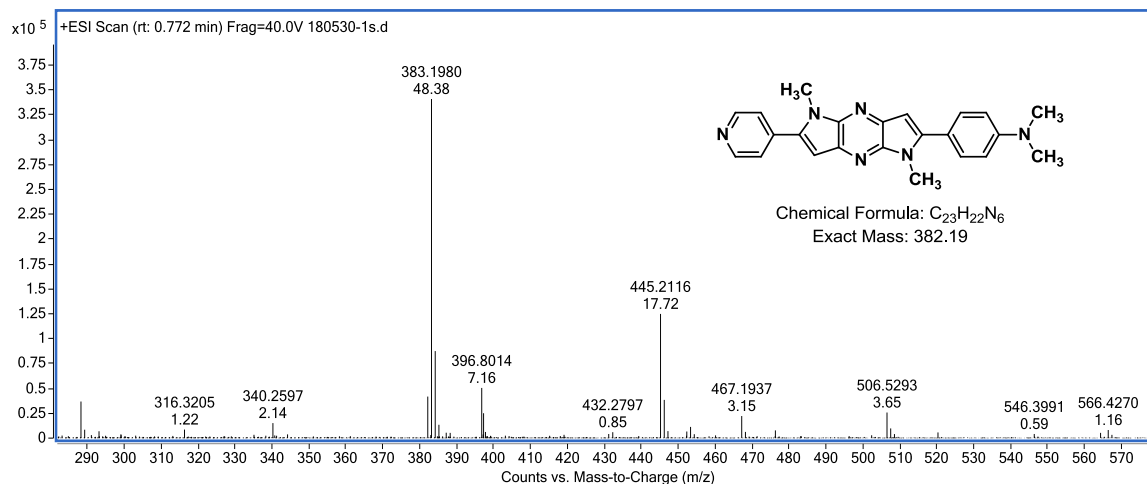
HRMS – 2a



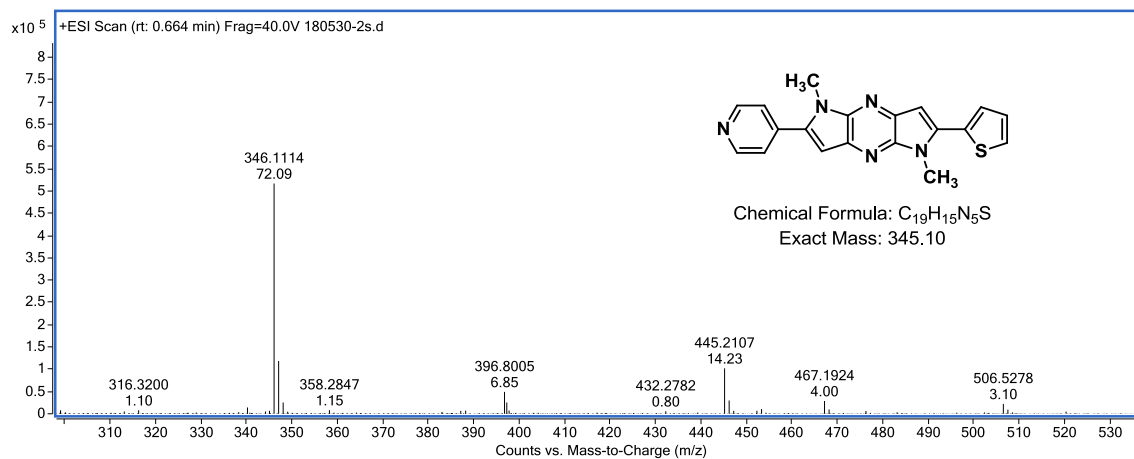
HRMS – 2b



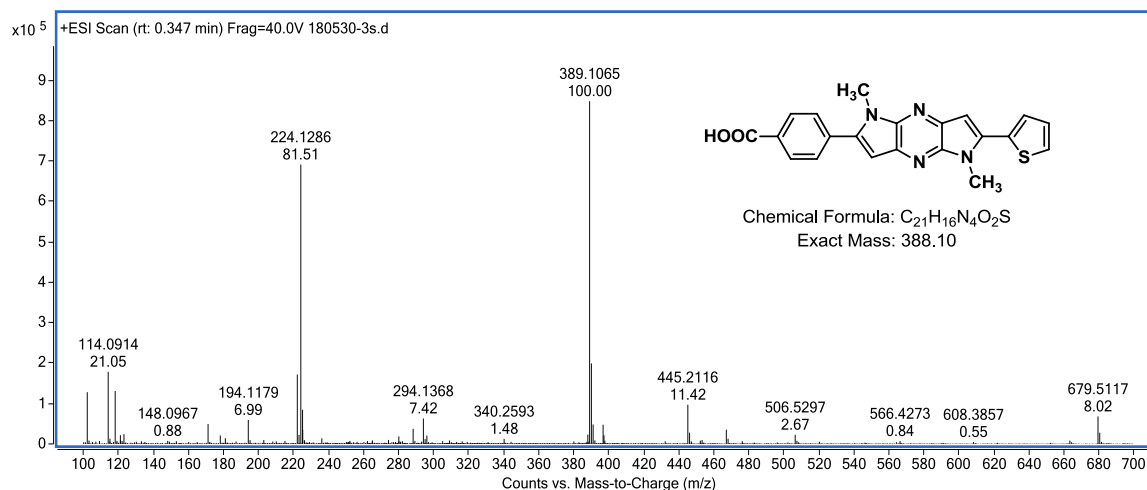
HRMS – 2c



HRMS – 3a



HRMS – 3b



HRMS – 3c

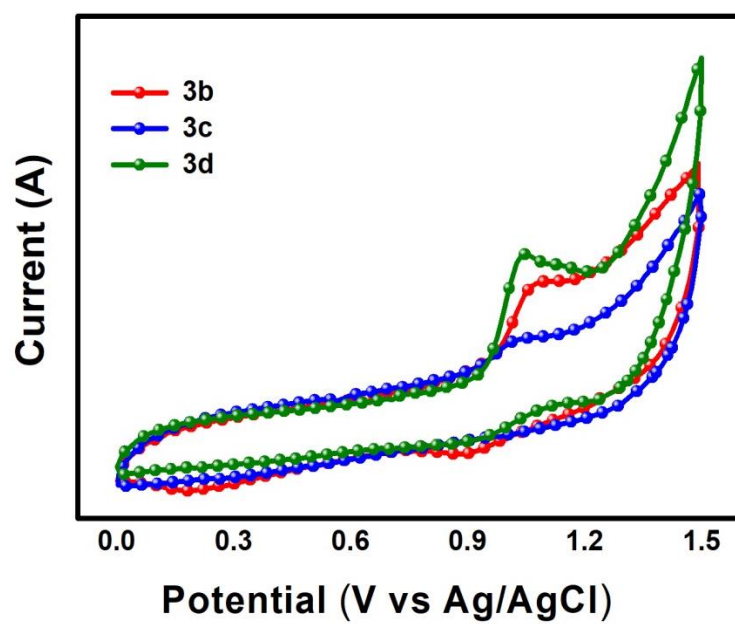


Fig 1. Cyclic Voltammograms of **3(b-d)** in CH_2Cl_2 solution with 0.1M nBu_4NPF_6 used as supporting electrolyte, scan rate 50 m V/s.