

Supporting Information

From Non-Detectable to Decent: Replacement of Oxygen with Sulfur in Naphthalene Diimide Boosts Electron Transport in Organic Thin-Film Transistors (OTFT)

Wangqiao, Chen^{a,b,†}, Jing, Zhang^{a,‡}, Long, Guankui^a, Yi Liu,^c Qichun Zhang^{a,b,d*}

^a School of Materials Science and Engineering, Nanyang Technological University, 50 Nanyang Avenue, Singapore 639798, Singapore

^b Institute for Sports Research, Nanyang Technological University, 50 Nanyang Avenue, Singapore 639798, Singapore

^c The Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, California, 94720, United States

^d Division of Chemistry and Biological Chemistry, School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore 637371 (Singapore)

Content

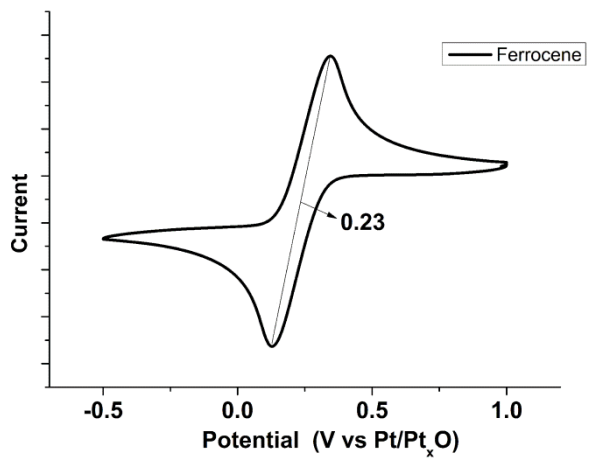
1. Cyclic voltammetry of ferrocene.....	S3
2. X-ray diffraction (XRD) for thionated NDI.....	S4
3. Molecular length for thionated NDI.....	S5
4. NMR spectra for the thionated NDI.....	S6
5. HR-MS spectra for the thionated NDI.....	S10
6. Output characteristics of thin-film OFETs.....	S11

General information

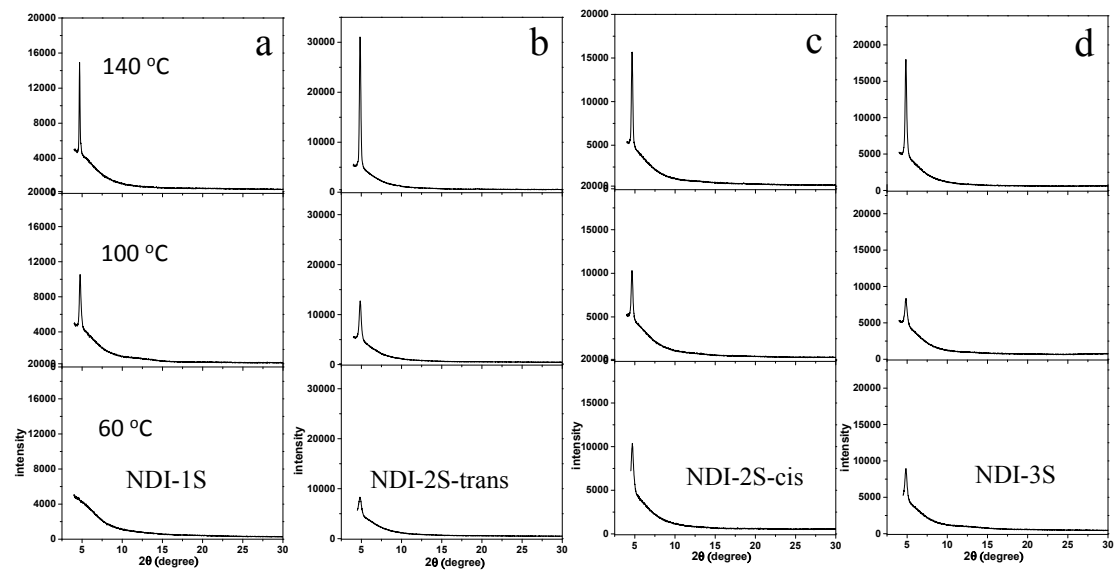
All reactions were performed under Argon protection. The solvents were purified and dried according to standard procedures. The chemicals were purchased from Alfa Aesar, Sigma-Aldrich, Acros Ltd and used as received.

NMR spectra were recorded with a Bruker AV 300 Spectrometer at 300 MHz (^1H NMR) and 75 MHz (^{13}C NMR). High Resolution Mass Spectra (HRMS) were recorded on Waters ACQUITY UPLC® System. The Thermogravimetric analysis (TGA) analysis of thionated NDI derivatives were recorded under a nitrogen atmosphere on a TA Instrument 2950. The differential scanning calorimetry (DSC) analysis of thionated NDI derivatives were recorded under a nitrogen atmosphere on an Instrument TAQ-10 at heating rates of $10^\circ\text{C min}^{-1}$. UV–Vis absorption spectra were taken on a SHIMADZU UV-2501PC. Electrochemical cyclic voltammetry (CV) was analyzed on a CHI 660C Electrochemical Workstation. In the CV measurement, a Pt disk was used as the working electrode, one Pt wire as the counter electrode and another Pt wire as the reference electrode were used in dried solution of methylene chloride with 0.1 M tetrabutylammonium hexafluorophosphate (NBu_4PF_6) at 100 mV s^{-1} . Meanwhile, CV of ferrocene was also taken for comparison.

1. Cyclic voltammetry of ferrocene



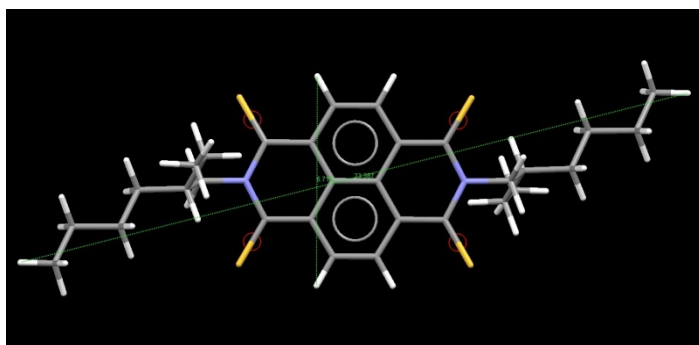
2. X-ray diffraction (XRD) for thionated NDI



3. Molecular length for thionated NDI



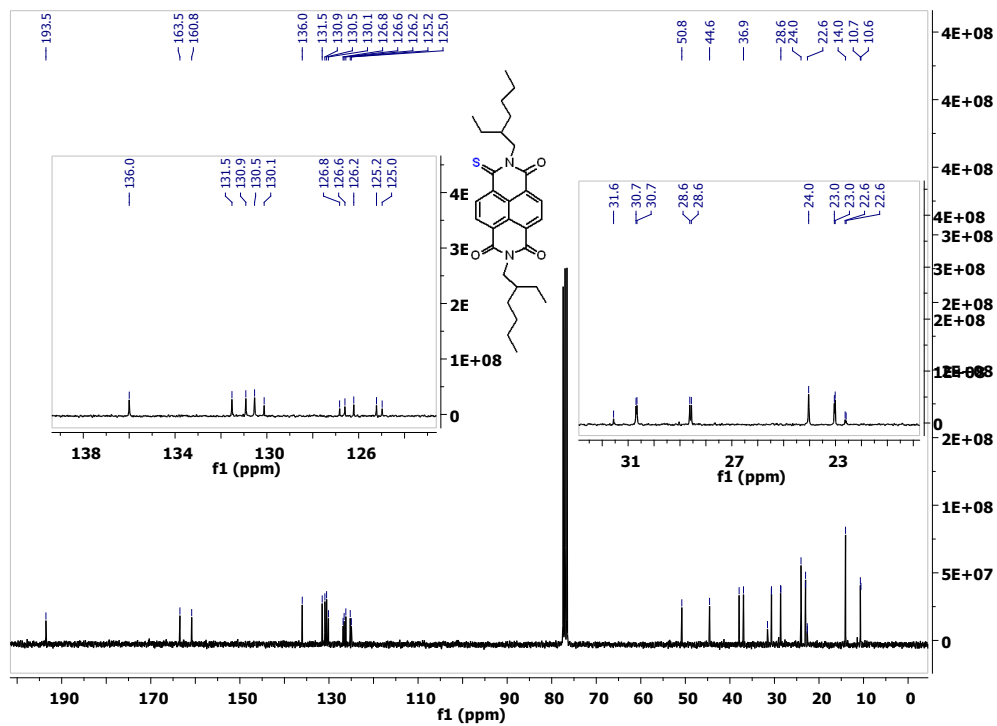
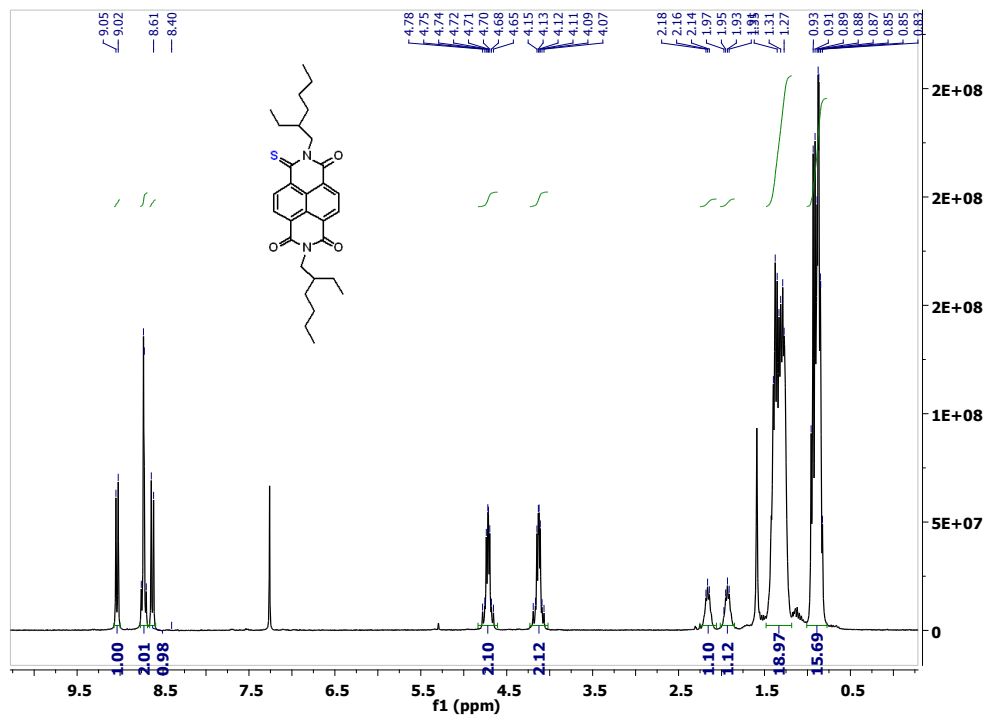
molecular length for EH-NDI:
23.46045 A*6.71465 A



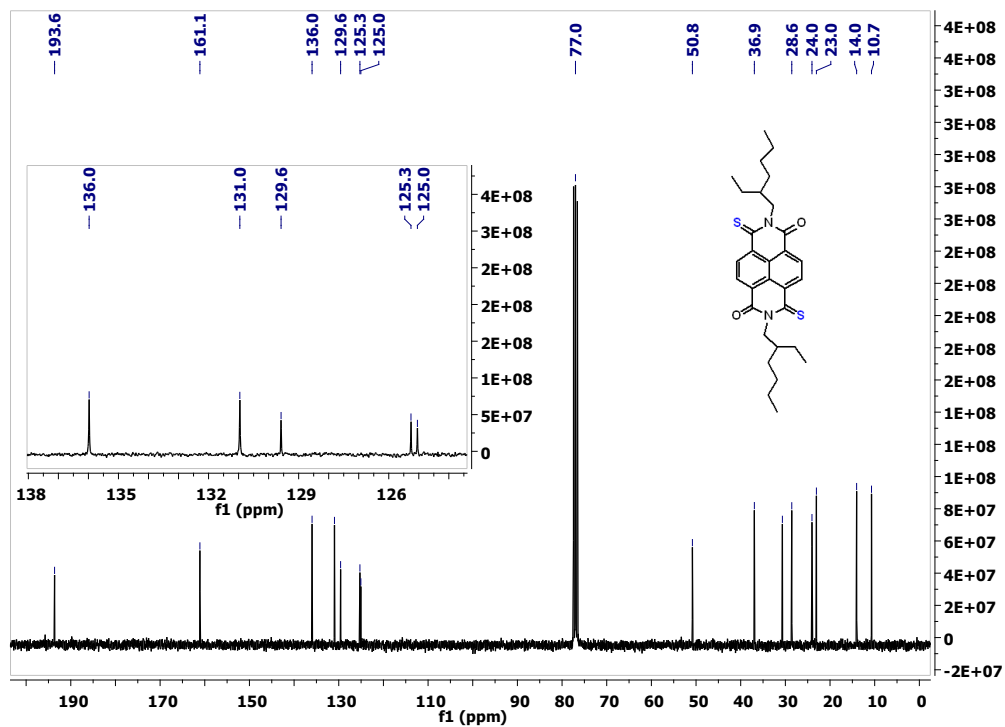
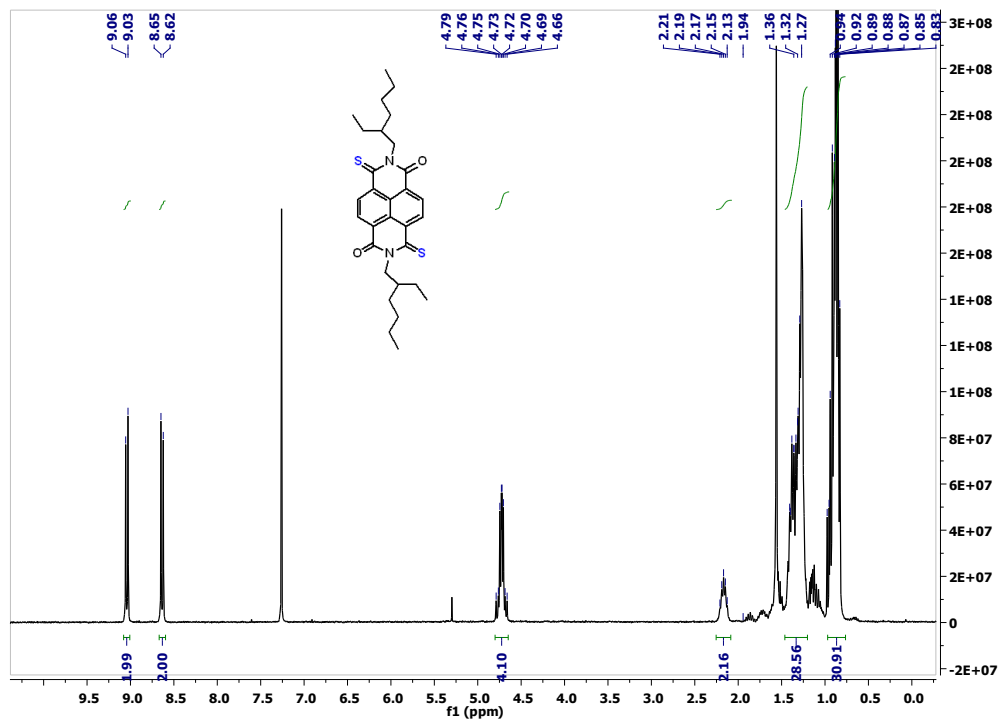
molecular length for EH-NDI-4S:
23.38696 A*6.71489 A

4. NMR spectra for thionated NDI

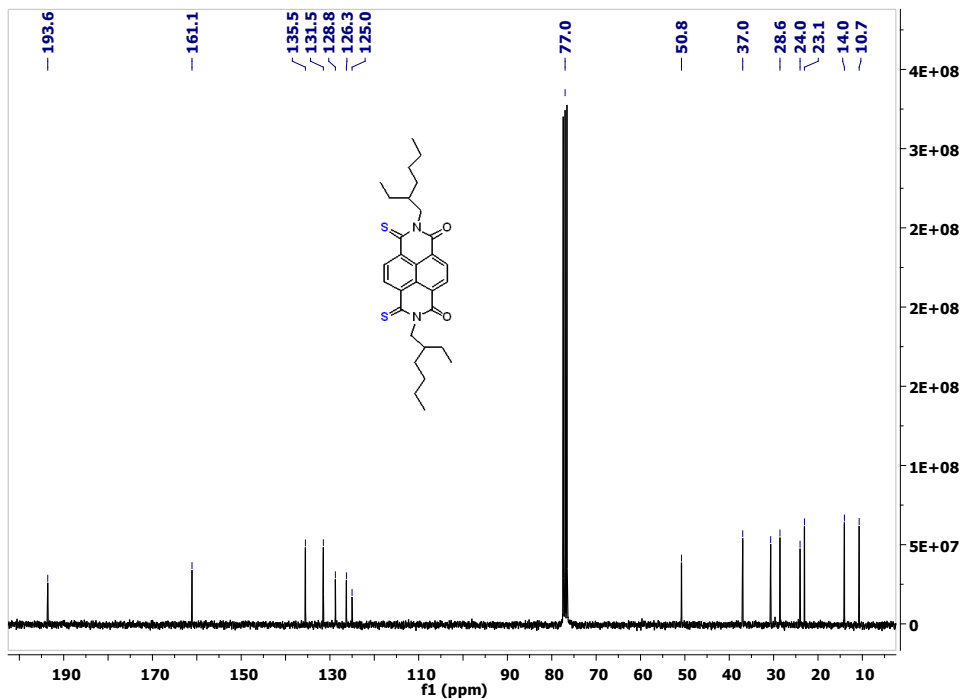
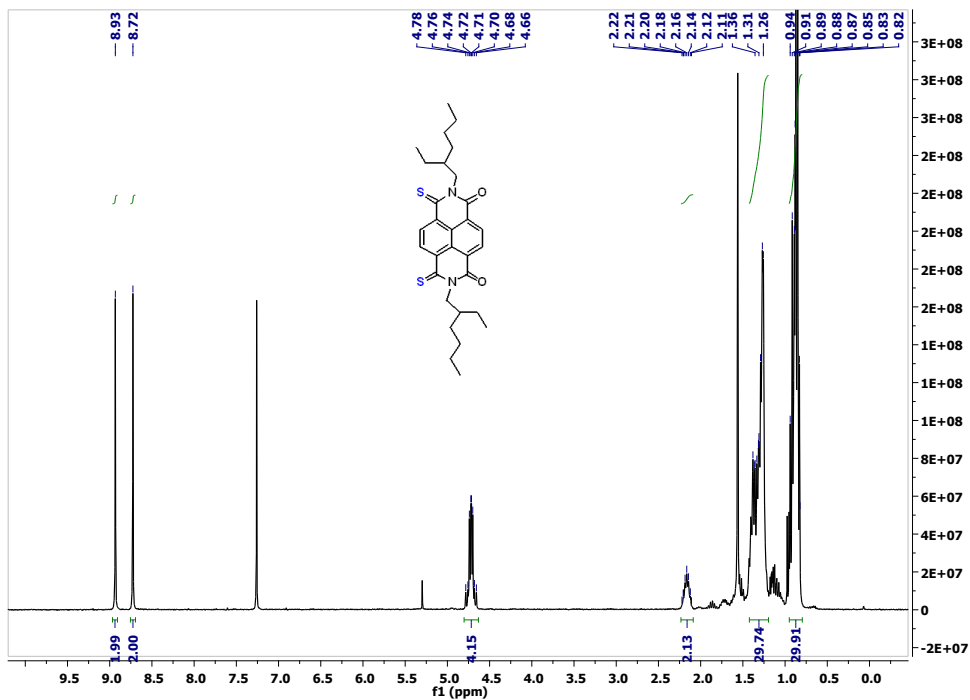
NDI-1S



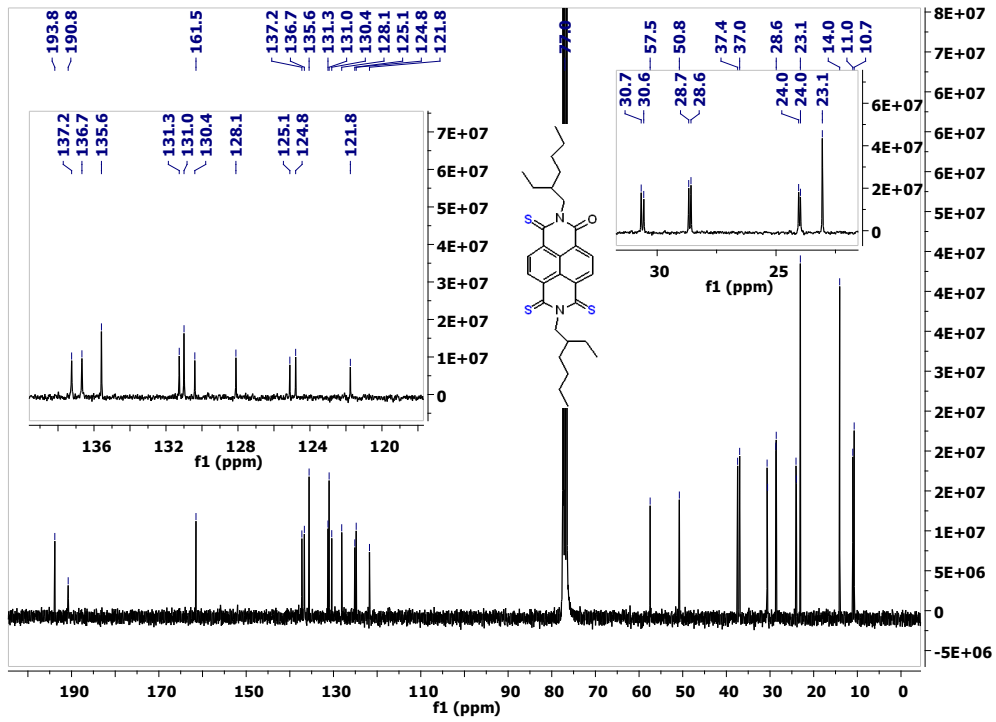
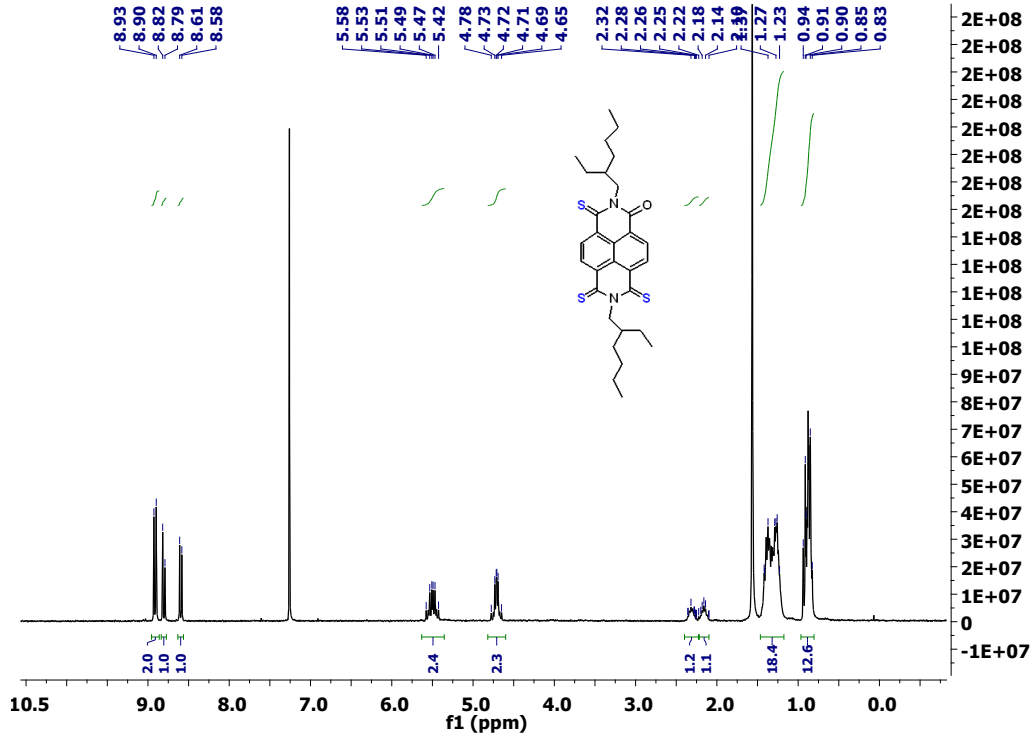
NDI-2S-trans



NDI-2S-cis

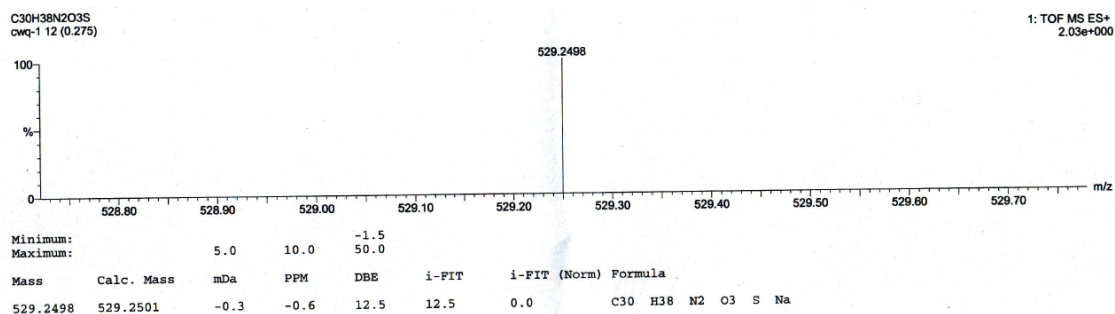


NDI-3S

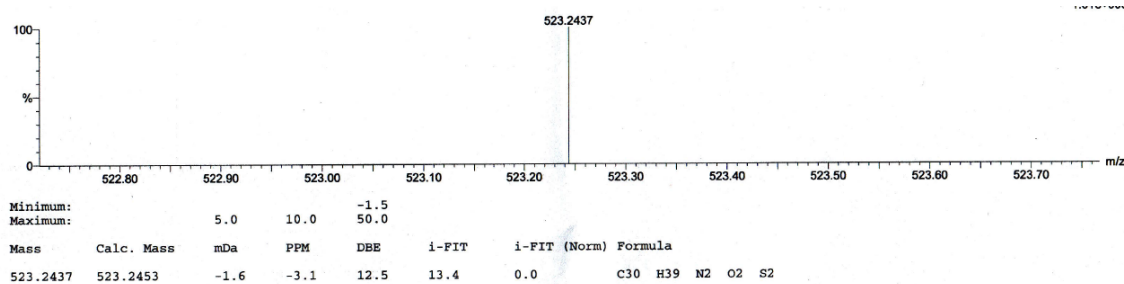


5. HR-MS spectra for thionated NDI

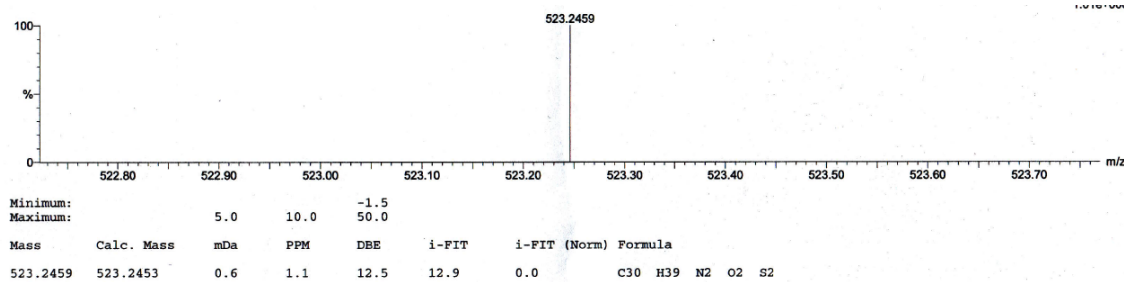
NDI-1S:



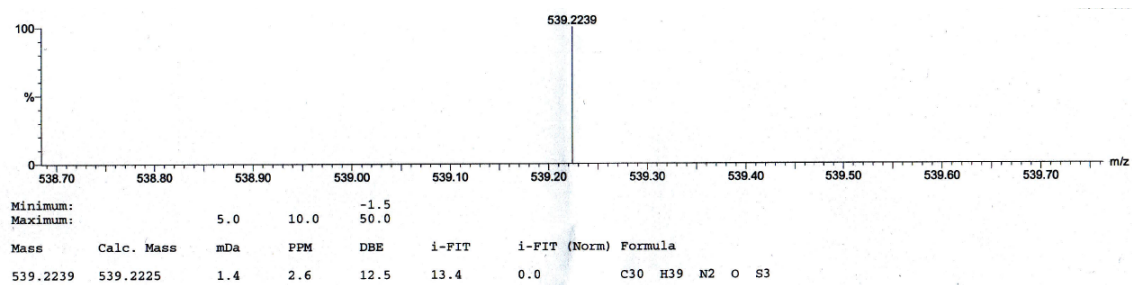
NDI-2S-Trans



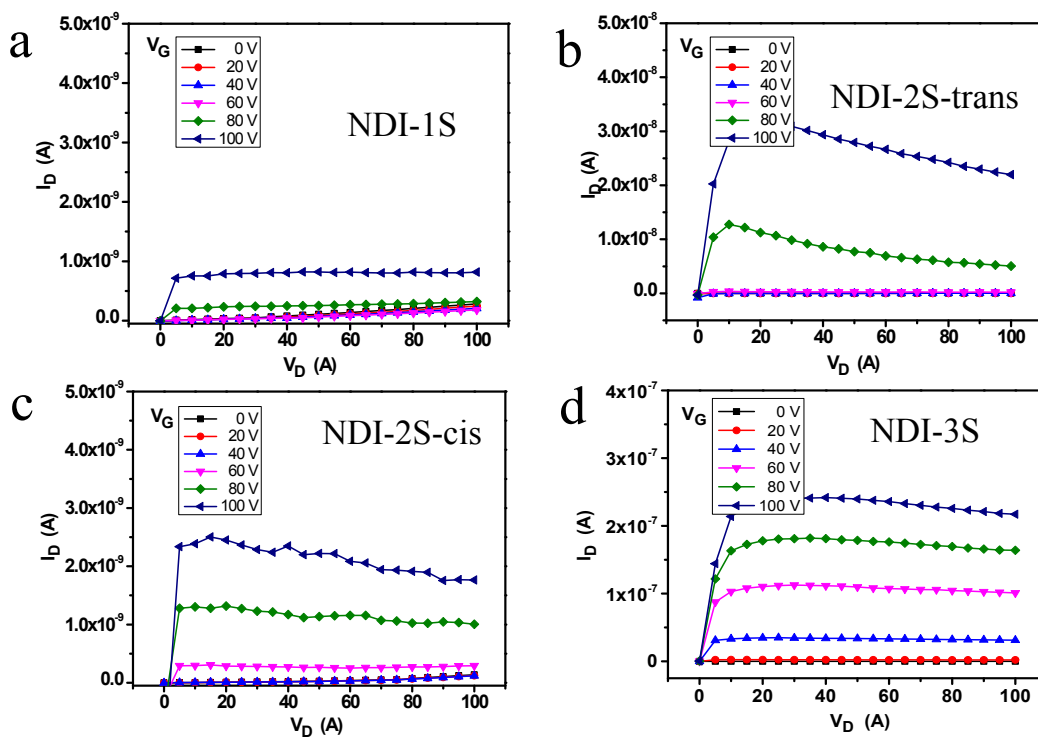
NDI-2S-cis



NDI-3S



6. Output characteristics of thin-film OFETs



Output characteristics of thin-film OFETs of thionated NDIs after annealing at optimized temperature (a: NDI-1S, b: NDI-2S-trans, c: NDI-2S-cis, d: NDI-3S).