

Supporting Information

Naphthalimide End-Capped Diphenylacetylene: A Versatile Organic Semiconductor for Blue Light Emitting Diodes and Donor or Acceptor for Solar Cells

Thu-Trang Do,^a Jegadesan Subbiah,^b Sudam Chavan,^c Tsu-Hao Ou,^c Sergei Manzhos,^d

David Jones, ^b John M. Bell,^a JwoHuei Jou^c and Prashant Sonar^{a}*

^aSchool of Chemistry, Physics and Mechanical Engineering, Queensland University of Technology (QUT), 2 George Street, Brisbane, QLD-4001, Australia.

^bSchool of Chemistry, University of Melbourne, Bio21 Institute, 30 Flemington Road, Parkville, Victoria 3010, Australia

^cDepartment of Materials Science and Engineering, National Tsing-Hua University, 101 Sec-2 Kuang -Fu Road, Hsinchu -30013 Taiwan

^dDepartment of Mechanical Engineering, Faculty of Engineering, National University of Singapore, Block EA #07-08, 9 Engineering Drive 1, Singapore 117576.

*E-mail: sonar.prashant@qut.edu.au.

KEYWORDS: Naphthalimide, Electron Acceptors, Electron Donor, Wide Band-gap Molecules, Organic Solar Cells.

Contents

1. Figure S1. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **1**
2. Figure S2. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **2**
3. Figure S3. ^1H NMR (400 MHz, CDCl_3) spectrum of **3**
4. Figure S4. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **5**
5. Figure S5. ^1H NMR (600 MHz, CDCl_3) spectrum of compound **6**
6. Figure S6. (a) ^1H NMR (600 MHz, CDCl_3) spectrum and (b) ^{13}C NMR (150 MHz, CDCl_3) spectrum of **NAI-PVP-NAI**
7. Figure S7. HRMS spectrum of **NAI-PVP-NAI**
8. Figure S8. Emission spectra of **NAI-PVP-NAI** in various solvents
9. Figure S9. X-ray diffraction spectra of **NAI-PVP-NAI** neat film and CBP doped with 3-wt % **NAI-PVP-NAI** film
10. Figure S10. Current density –voltage curve of electron only device made up using **NAI-PVP-NAI**.

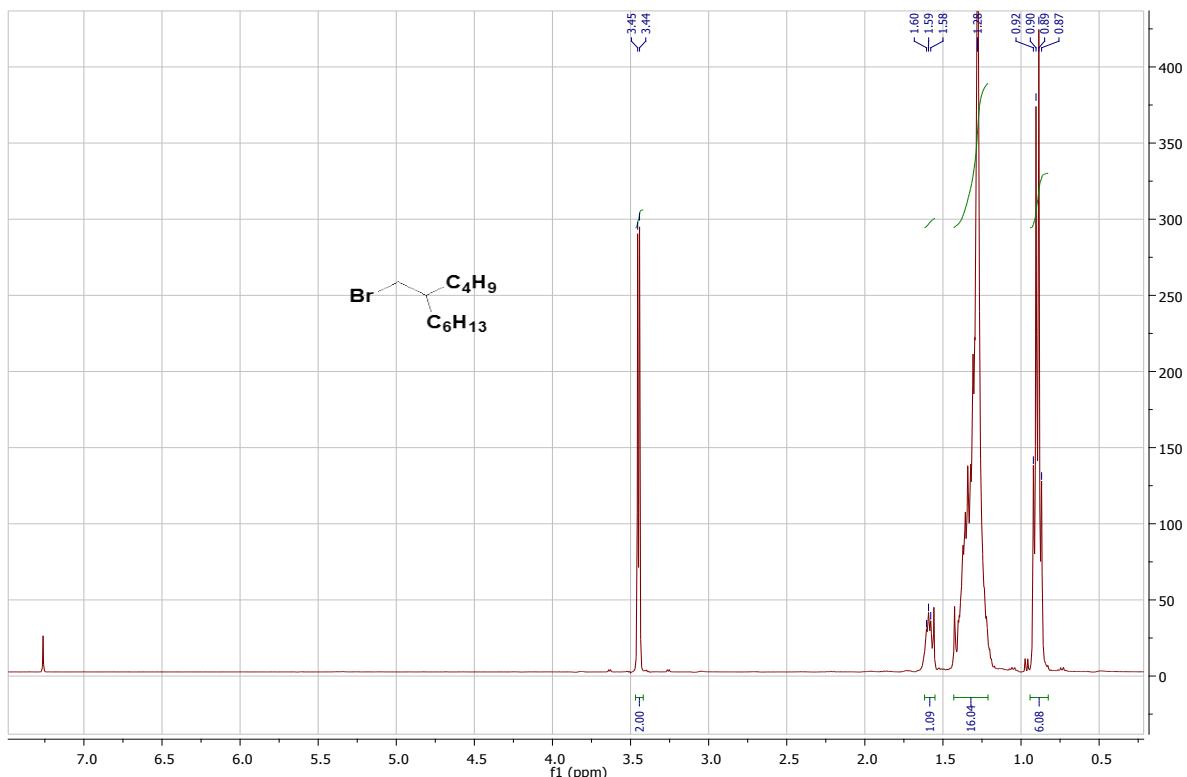


Figure S1. ^1H NMR (400 MHz, CDCl_3) spectrum of compound 1

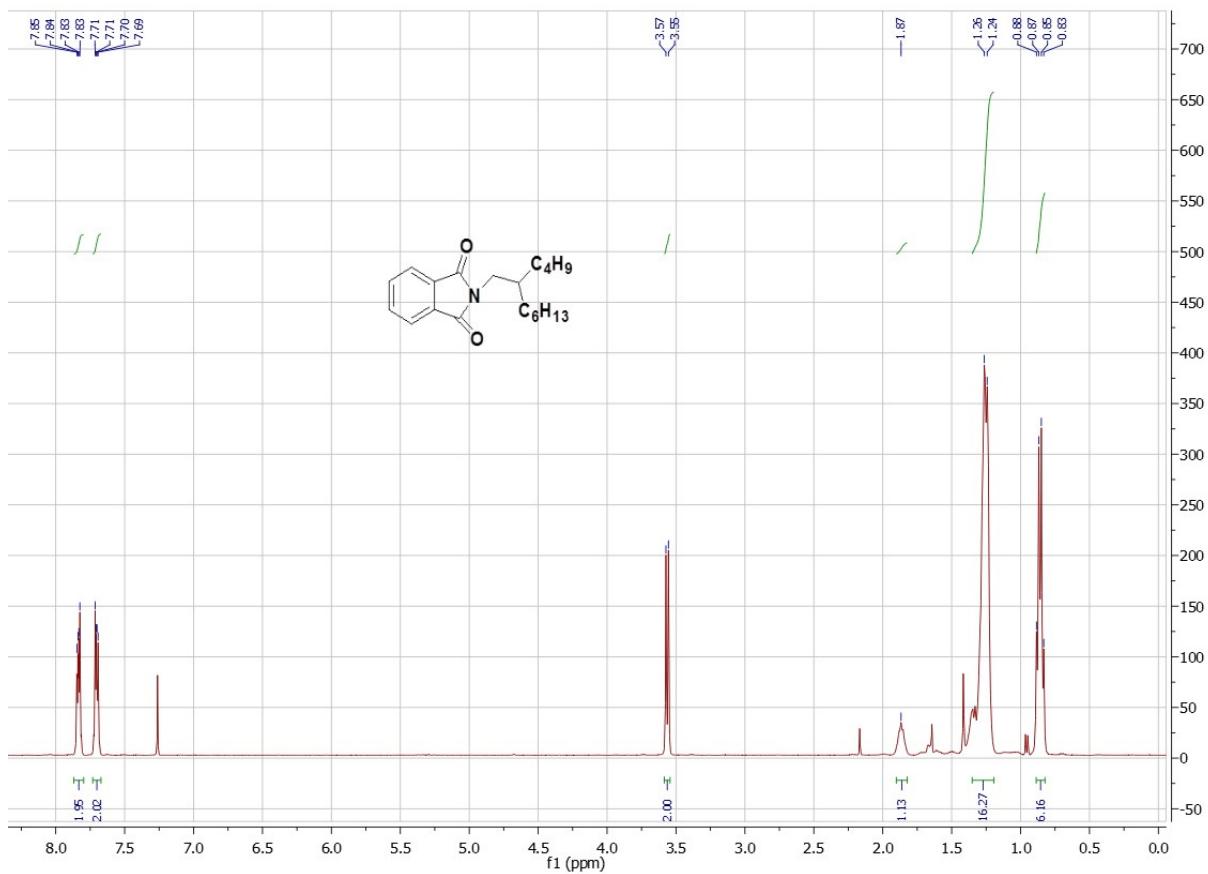


Figure S2. ^1H NMR (400 MHz, CDCl_3) spectrum of compound 2

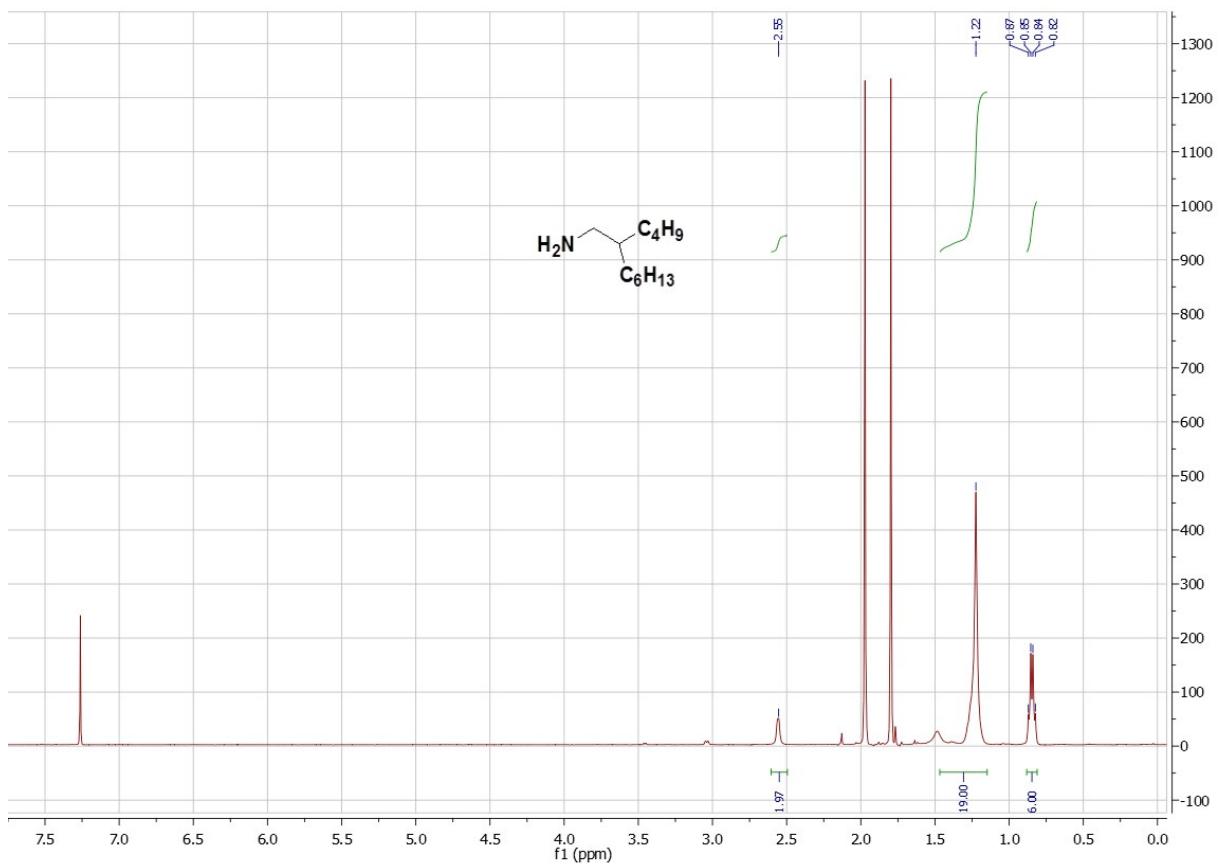


Figure S3. ^1H NMR (400 MHz, CDCl_3) spectrum of **3**

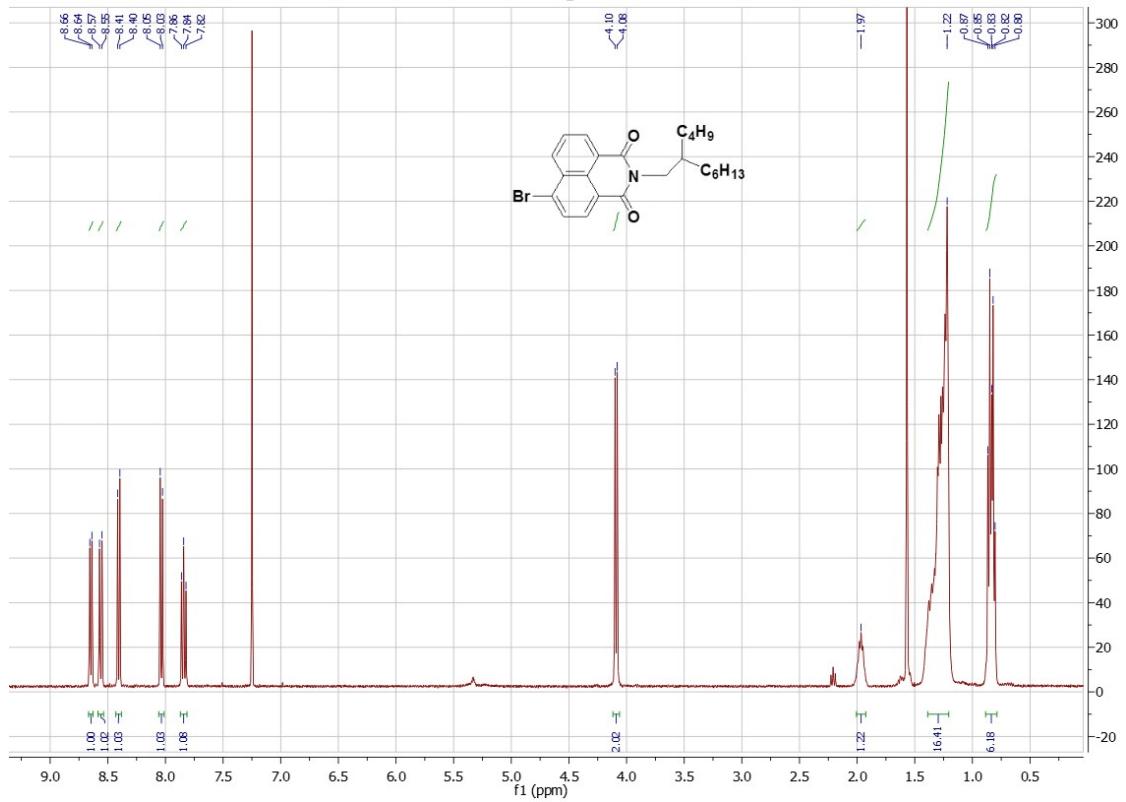


Figure S4. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **5**

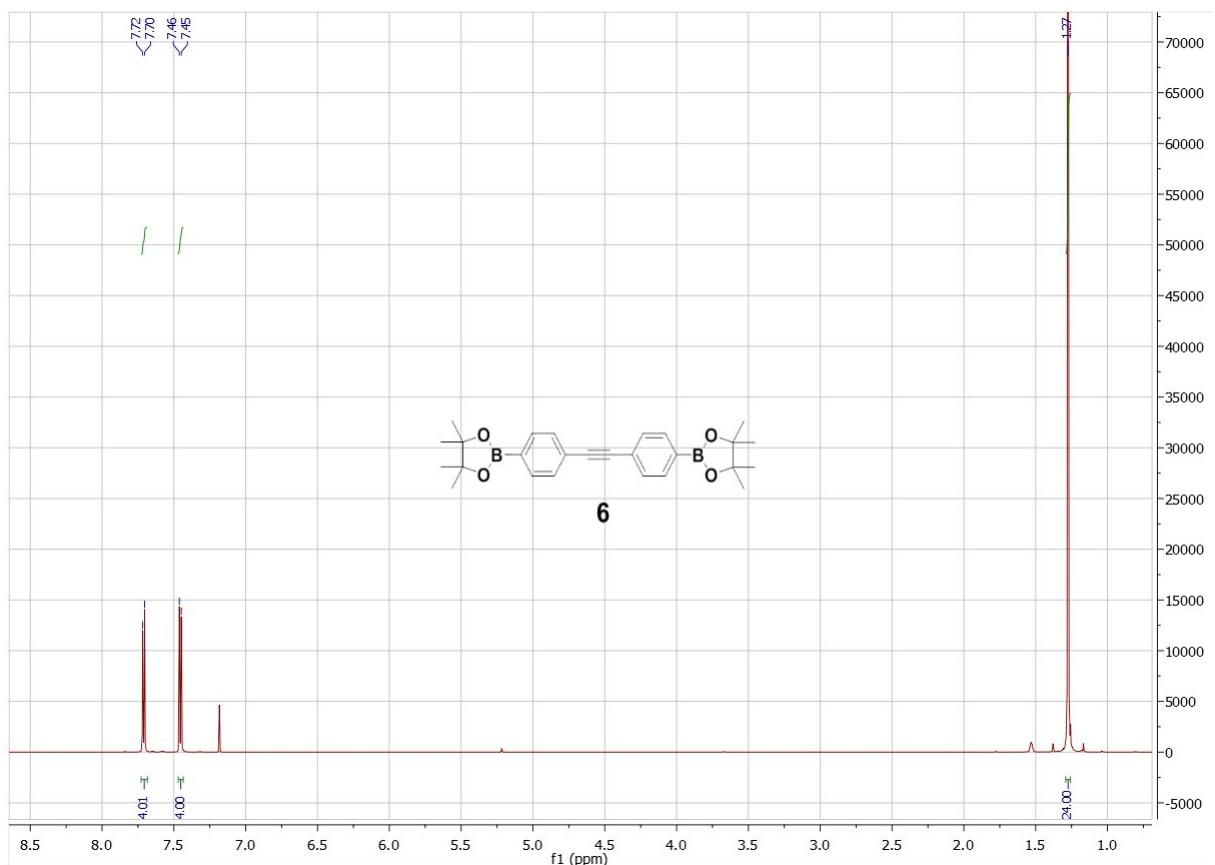


Figure S5. ¹H NMR (600 MHz, CDCl₃) spectrum of compound **6**

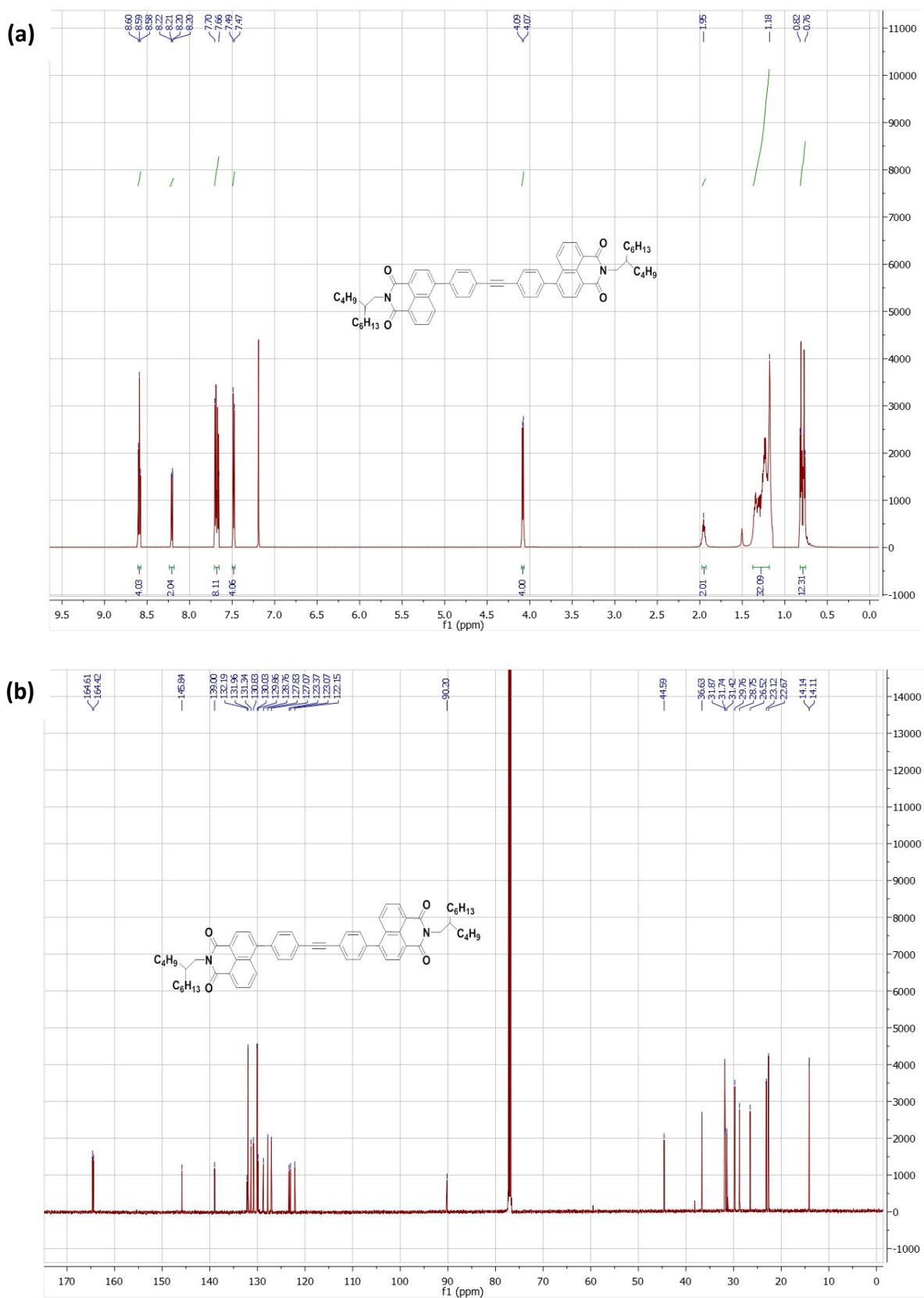


Figure S6. (a) ^1H NMR (600 MHz, CDCl_3) spectrum and (b) ^{13}C NMR (150 MHz, CDCl_3) spectrum of **NAI-PVP-NAI**

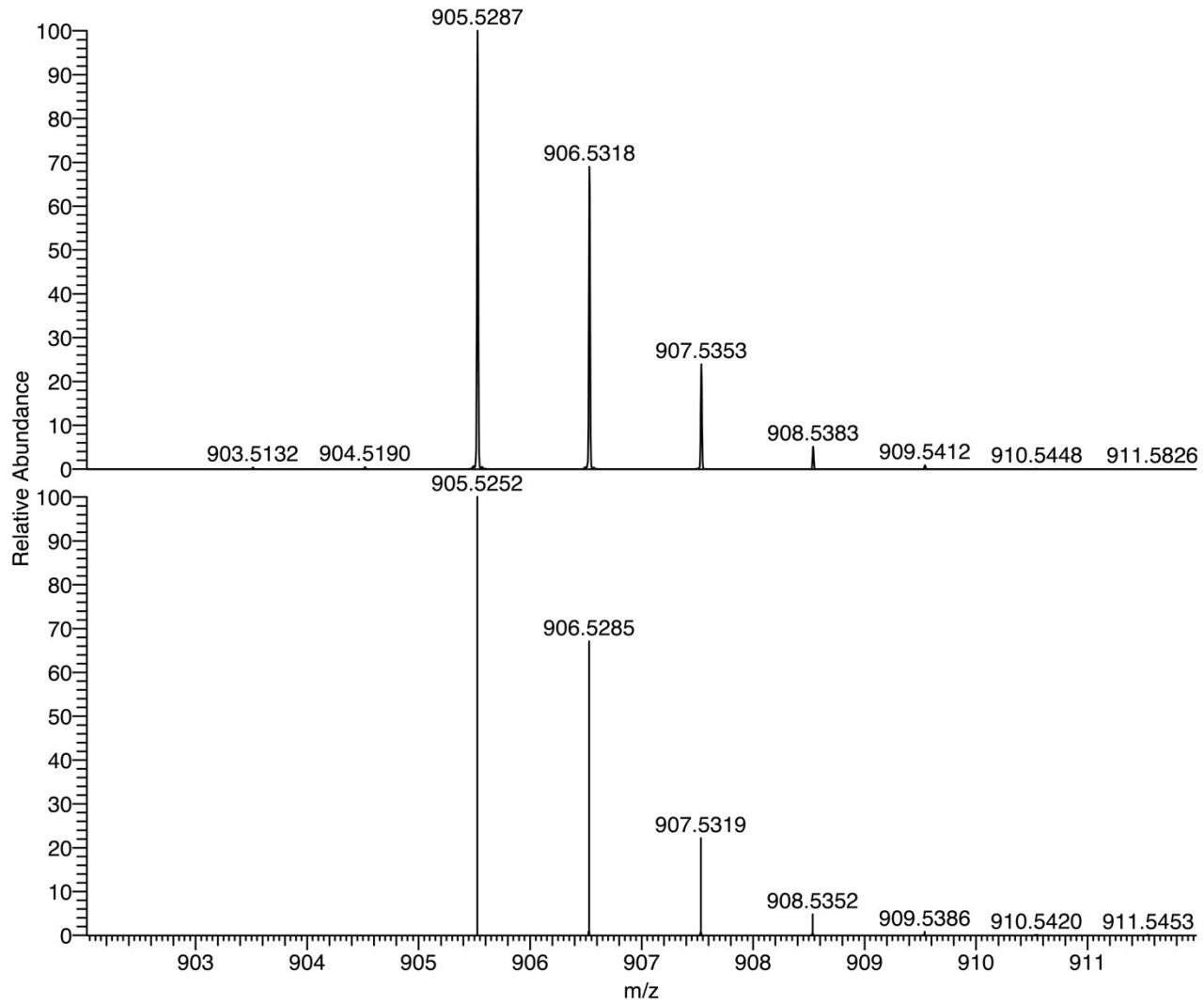


Figure S7. HRMS spectrum of **NAI-PVP-NAI**

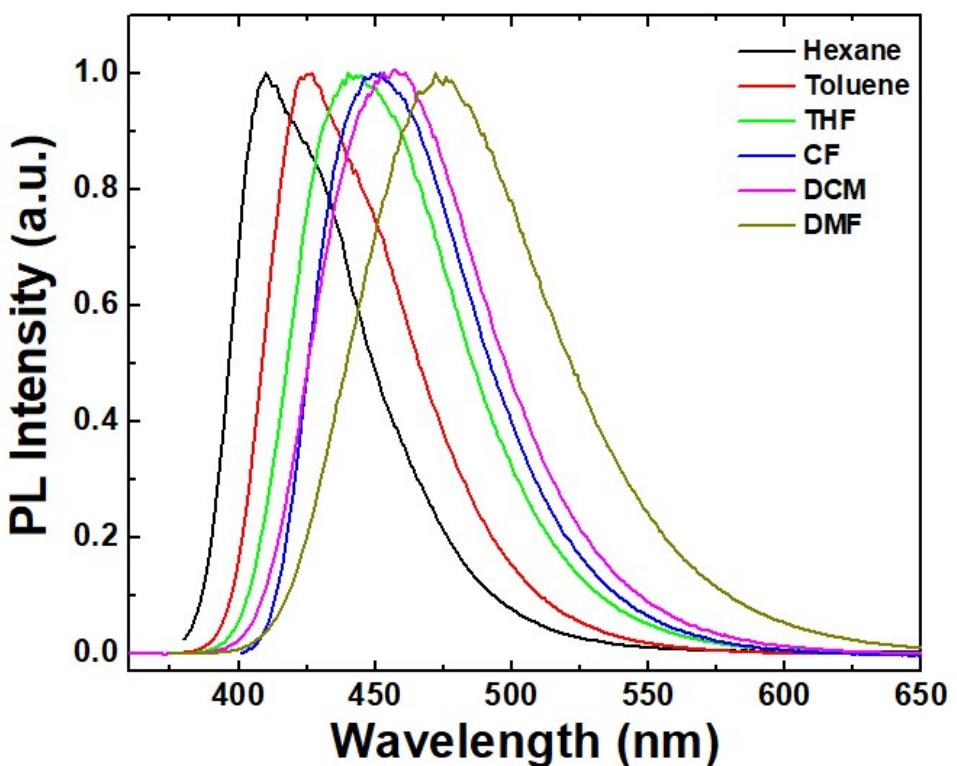


Figure S8. Emission spectra of **NAI-PVP-NAI** in various solvents

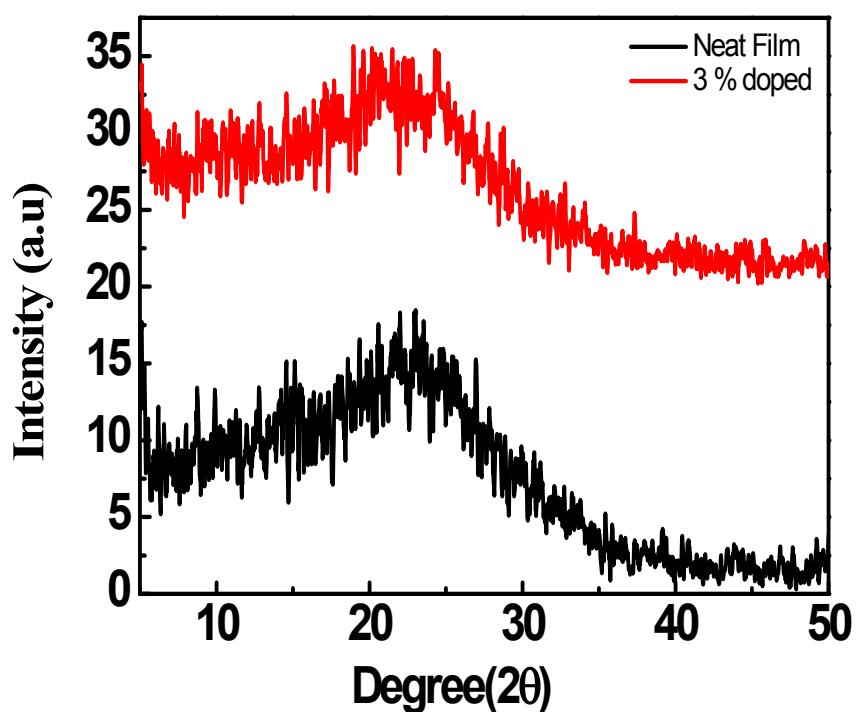


Figure S9: X-ray diffraction spectra of NAI-PVP-NAI neat film and CBP doped with 3-wt % **NAI-PVP-NAI** film.

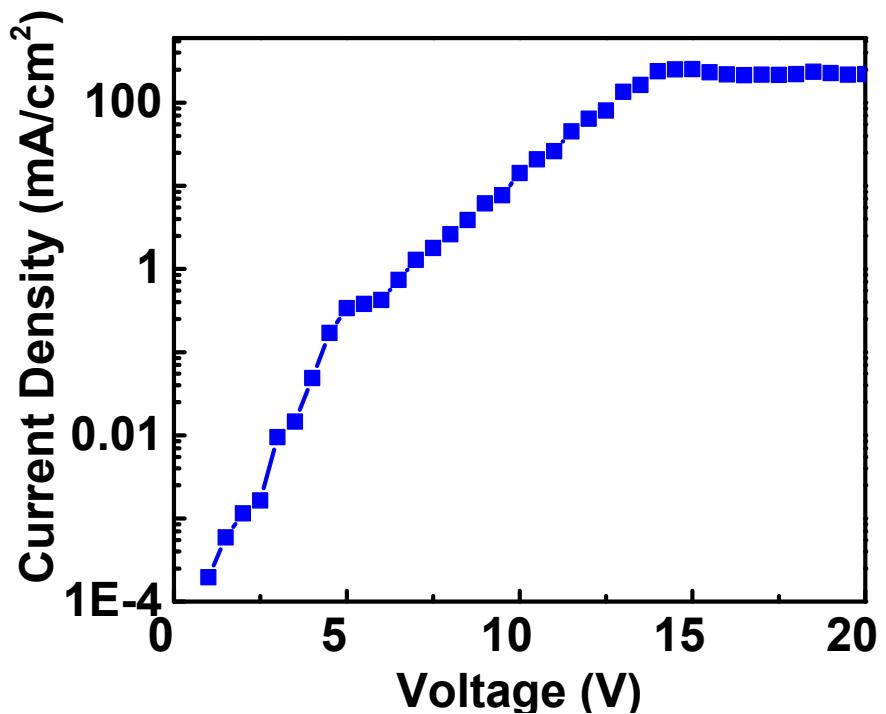


Figure S10. Current density –voltage curve of electron only device made up using **NAl-PVP-NAl**.