Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A

C–H activation: making diketopyrrolopyrrole derivatives easily accessible

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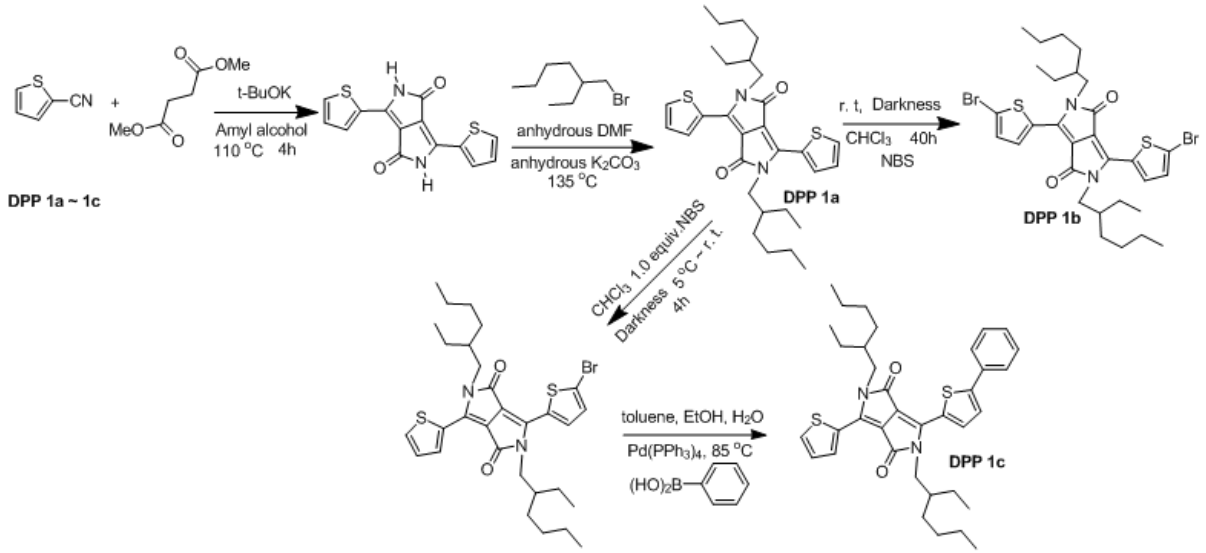
1. Instruments and materials

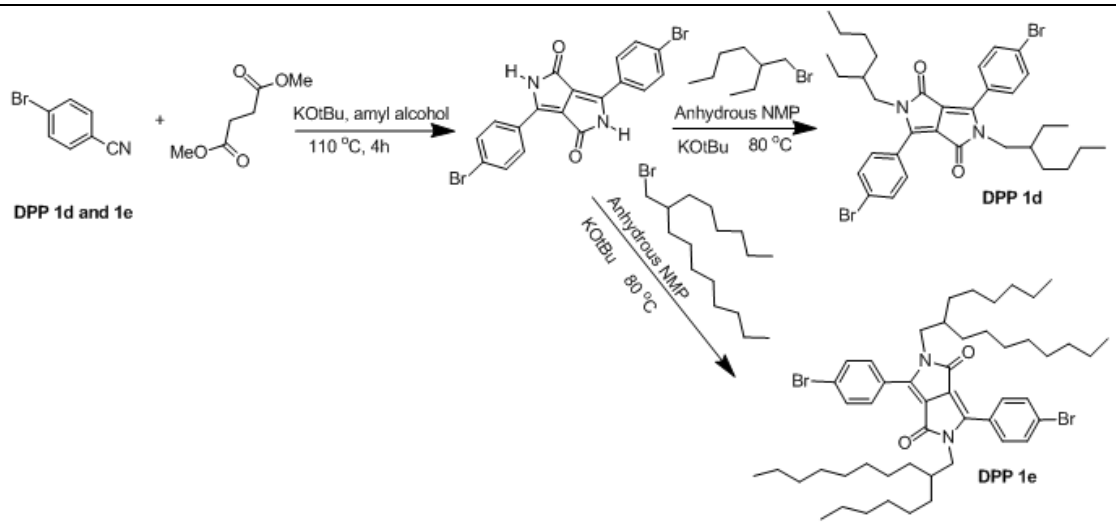
All ^{1}H and ^{13}C NMR spectra were obtained in chloroform-*d*, unless otherwise noted, with Bruker DMX-500 or Bruker DMX-300. ^{13}C NMR (126 MHz or 76 MHz) spectra were measured with a proton-decoupling pulse program. Chemical shifts for ^{1}H and ^{13}C NMR were referenced to residual signals from $CDCl_3$ (^{1}H NMR δ =7.26 ppm and ^{13}C NMR δ =77.23 ppm). Matrix-assisted laser desorption/ionizationtime of flight mass spectrometry (MALDI-TOF MS MS) was performed on a Voyager DE STR using 2,5-Dihydroxybenzoicacid or α-Cyano-4-hydroxycinnamicacid as the matrixes. Samples were prepared by diluting the molecules in chloroform with the matrix. Elemental analyses were conducted on a Flash EA 1112 elemental analyzer. UV-visible absorption spectra were taken on a Shimadzu UV-2450 spectrophotometer. Cyclic voltammetry (CV) was done on a CHI 660C electrochemical workstation with Pt disk, Pt plate, and standard 10 calomel electrode (SCE) as working electrode, counter electrode, and reference electrode, respectively, in a 0.1 mol/L tetrabutylammonium hexafluorophosphate (Bu_4NPF_6) CH_2Cl_2 solution.

All starting organic compounds were purchased from Aldrich, Alfa Aesar, Alladin, Energy chemical, or TCI and used without further purification. The solvent toluene and dimethyl acetamide (DMA) are anhydrous.

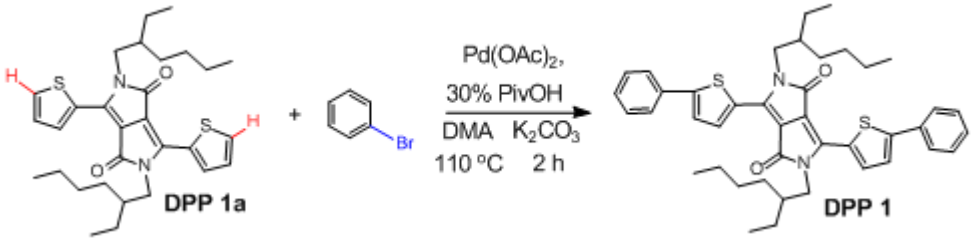
2. Synthetic route for the DPP 1a-1e and DPP 1-17



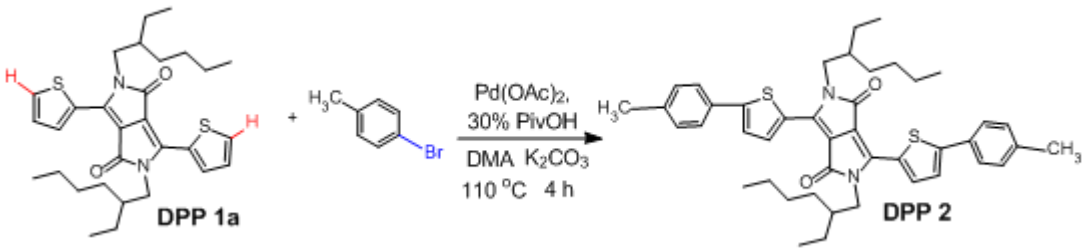
Scheme S1. Synthetic route of parent **DPP 1a-1c**



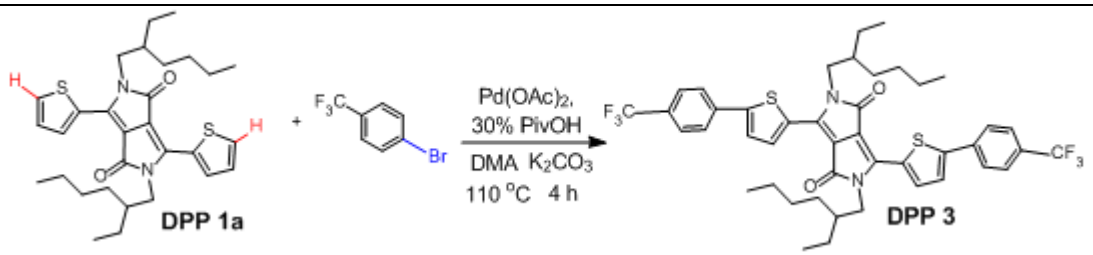
Scheme S2. Synthetic route of parent **DPP 1d** and **1e**



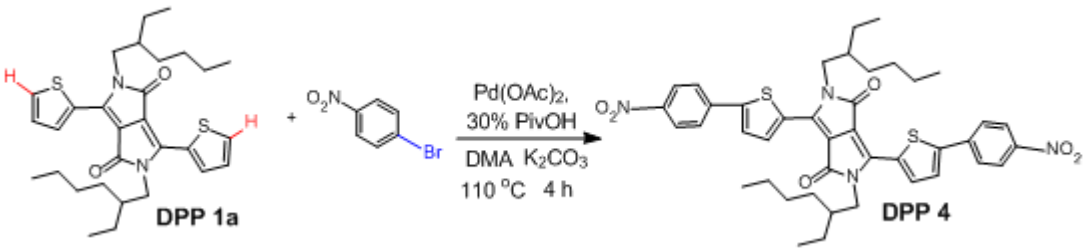
Scheme S3. Synthetic route of **DPP 1**



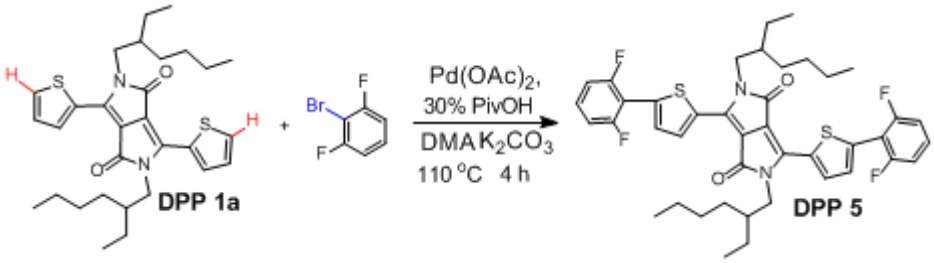
Scheme S4. Synthetic route of **DPP 2**



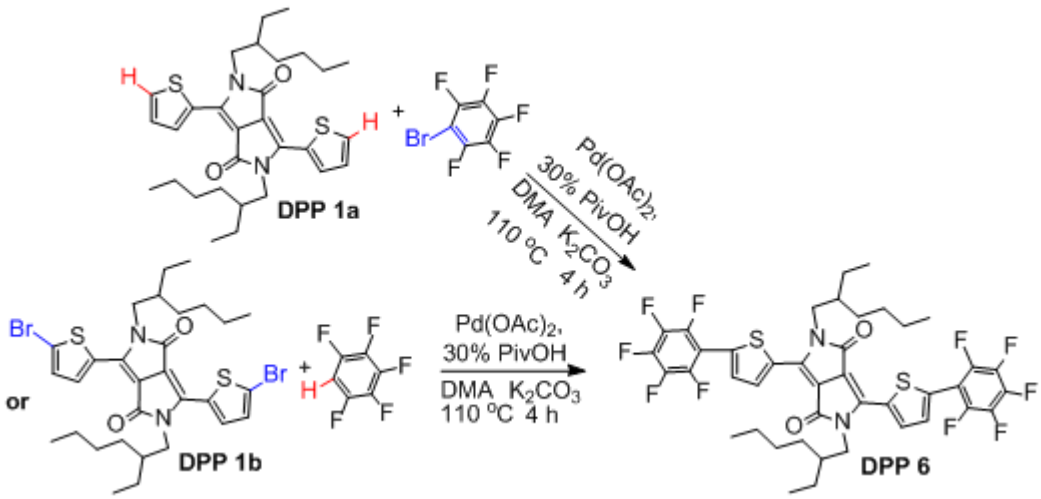
Scheme S5. Synthetic route of **DPP 3**



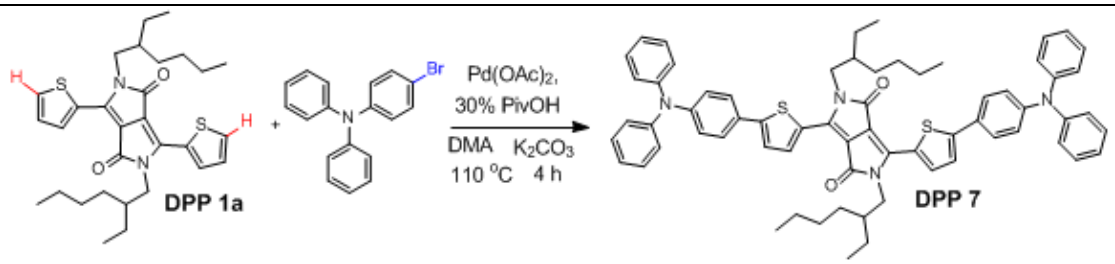
Scheme S6. Synthetic route of **DPP 4**



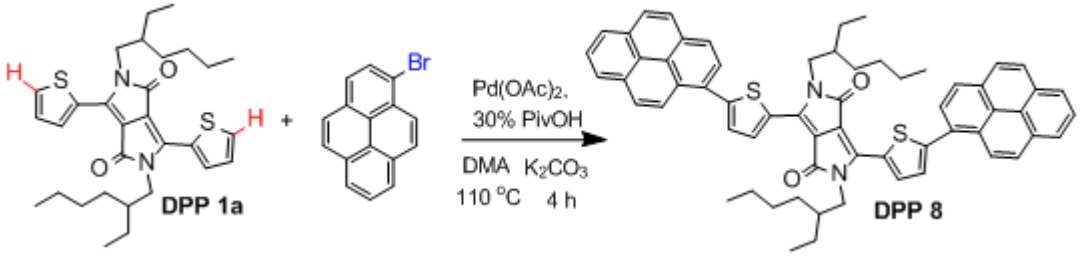
Scheme S7. Synthetic route of **DPP 5**



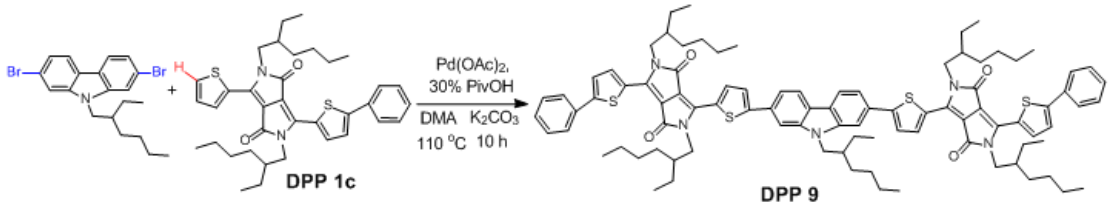
Scheme S8. Synthetic route of **DPP 6**



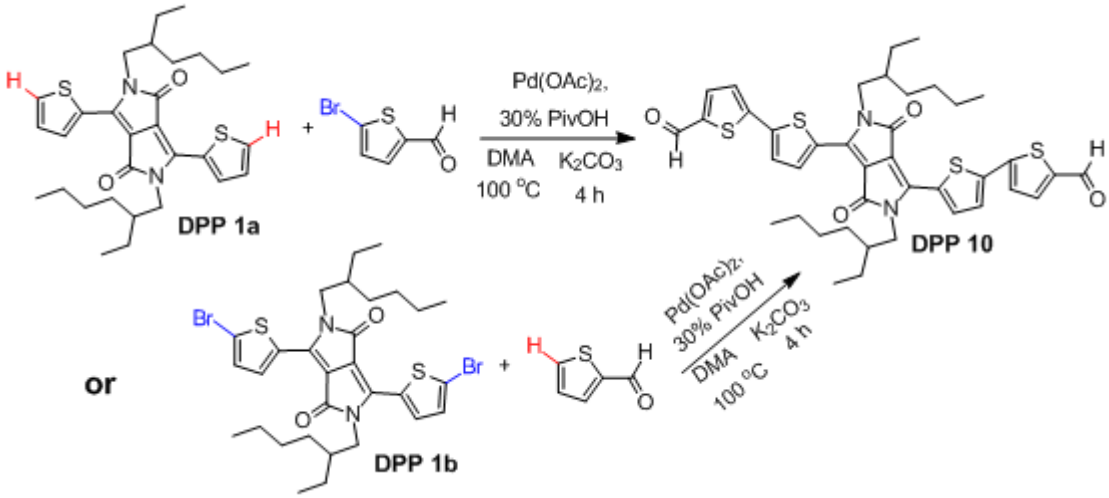
Scheme S9. Synthetic route of **DPP 7**



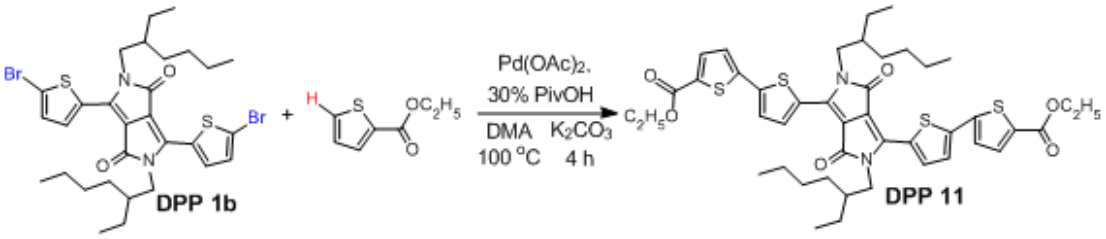
Scheme S10. Synthetic route of **DPP 8**



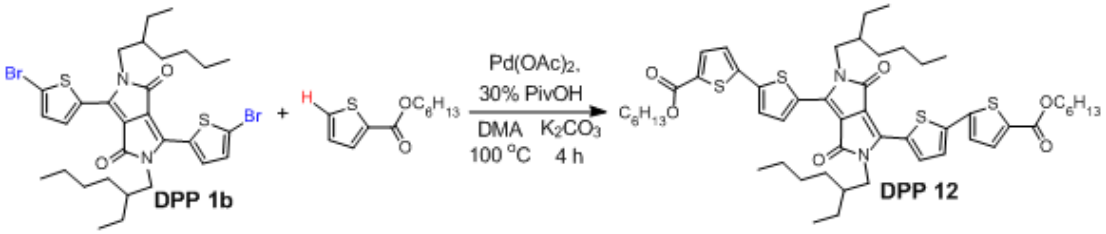
Scheme S11. Synthetic route of **DPP 9**



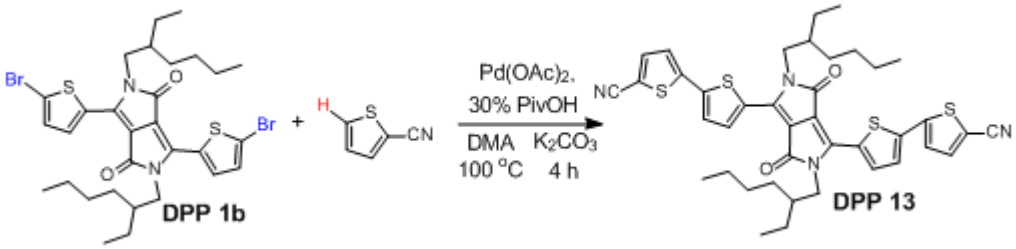
Scheme S12. Synthetic route of **DPP 10**



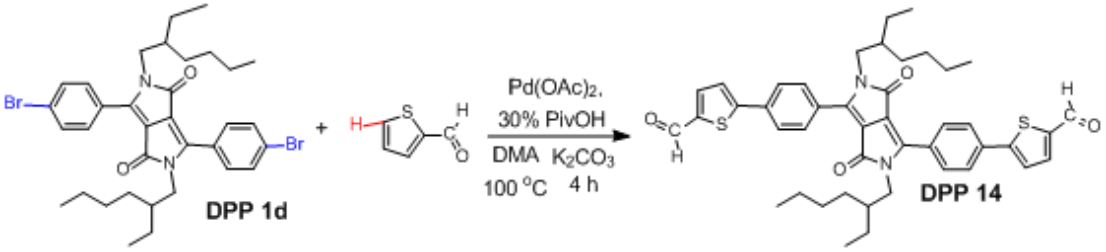
Scheme S13. Synthetic route of **DPP 11**



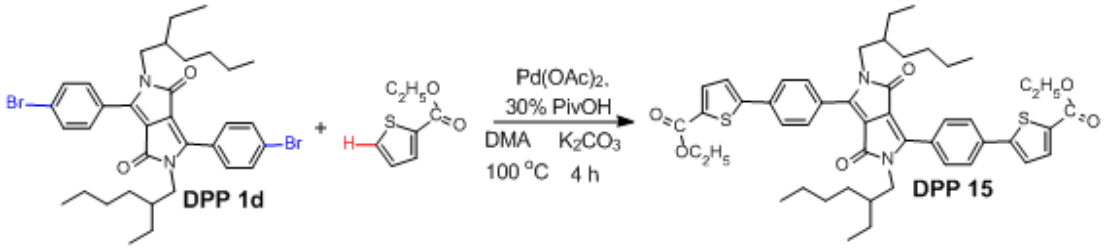
Scheme S14. Synthetic route of **DPP 12**



Scheme S15. Synthetic route of **DPP 13**

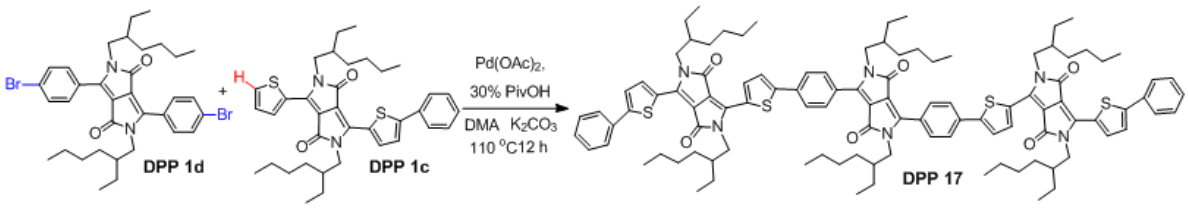


Scheme S16. Synthetic route of **DPP 14**



Scheme S17. Synthetic route of **DPP 15**

Scheme S18. Synthetic route of **DPP 16**

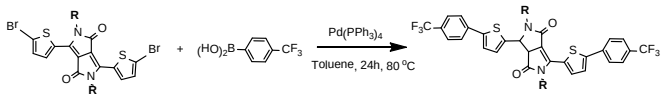


Scheme S19. Synthetic route of **DPP 17**

3. The comparison between our method and the reported methods

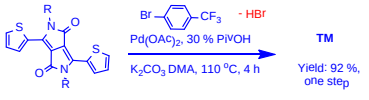
Case 1

Reported method:



J. Mater. Chem. **2010,** 20, 3626, *Energy Environ. Sci.*, **2011**, 4, 3617. 69 %

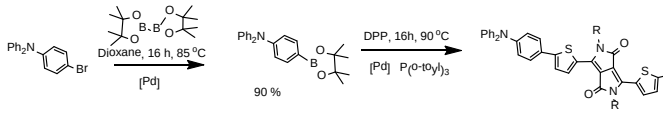
Our method:



DPP 3

Case 2

Reported method:



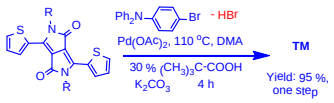
90 %

Adv. Mater. **2011**, 23, 5359.

50 %

Two steps, Total Yield: 45 %

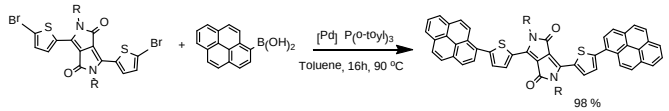
Our method:



DPP 8

Case 3

Reported method:



98 %

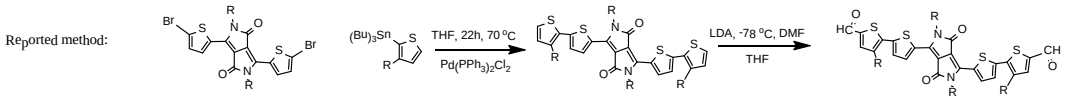
Adv. Mater. **2011**, 23, 5359.

Our method:

DPP 9

Case 4

Reported method:



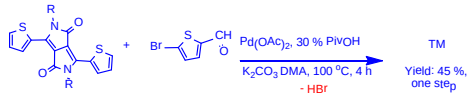
19 %

45 %

Two steps, Total Yield: <10 %

Macromol. Rap. Commun. **2010,** 31, 1554

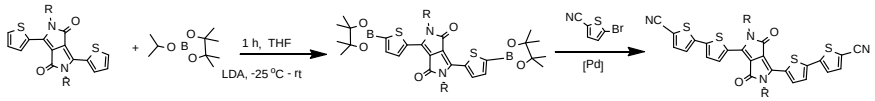
Our method:



DPP 10

Case 5

Reported method:



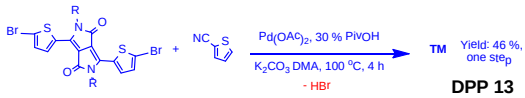
78%

40%

Two steps, Total Yield: 31 %

J. Org. Chem. **2011**, 76, 2426.

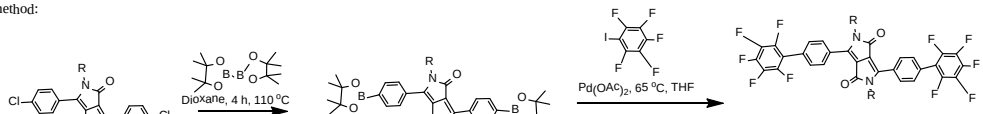
Our method:



DPP 13

Case 6

Reported method:



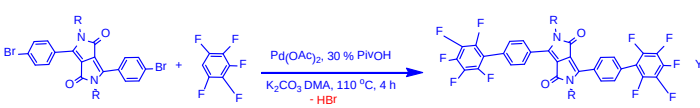
63 %

24 %

Two steps, Total Yield: 13 %

Eur. J. Org. Chem. **2012**, 5282

Our method:



DPP 16

Scheme S20. The comparison between our method and the reported methods

4. Fluorescence spectra of DPP 1-17

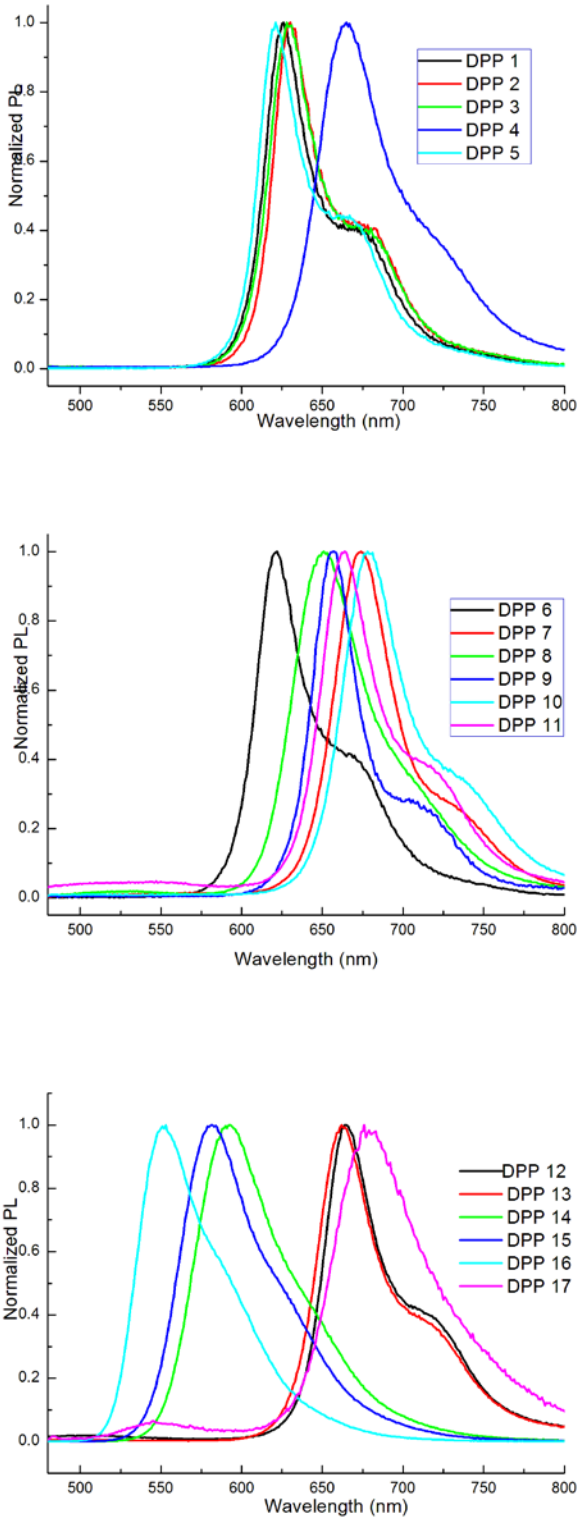


Fig. S1. Fluorescence spectra of **DPP 1-17** in $CHCl_3$ (excitation at 467 nm)

5. ^{1}H & ^{13}C NMR and MALDI-TOF MS spectra

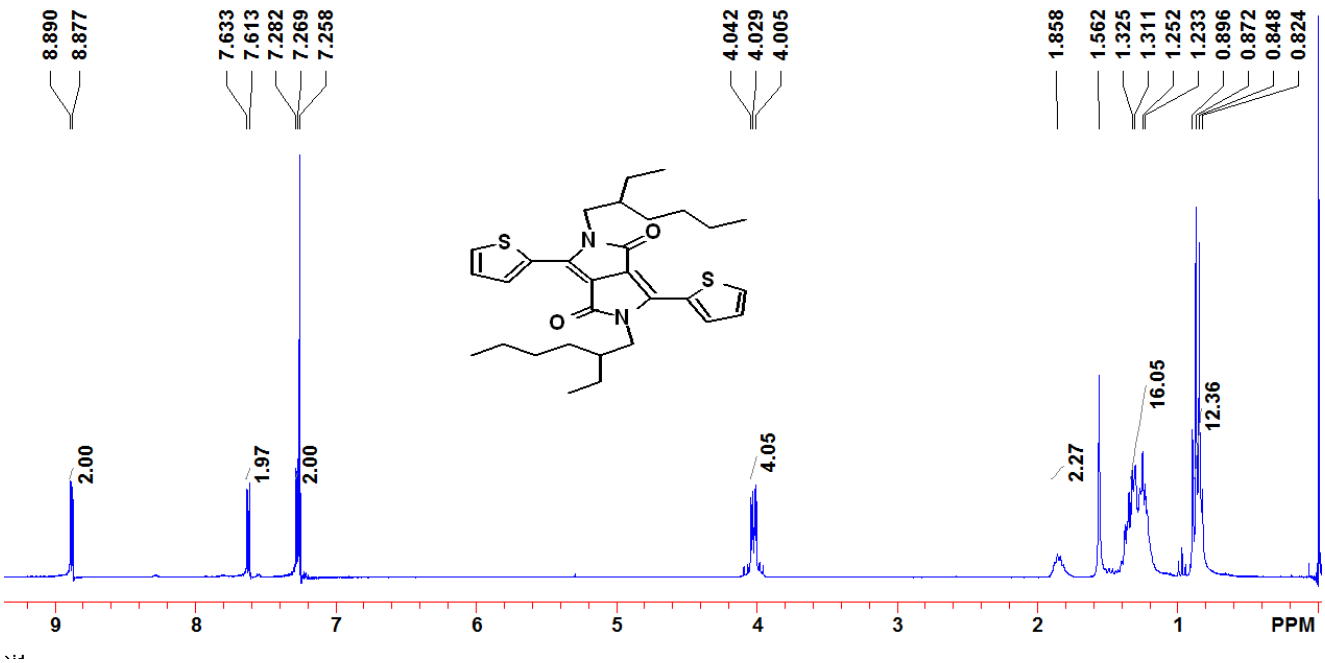


Fig. S2. ^{1}H NMR for **DPP 1a**

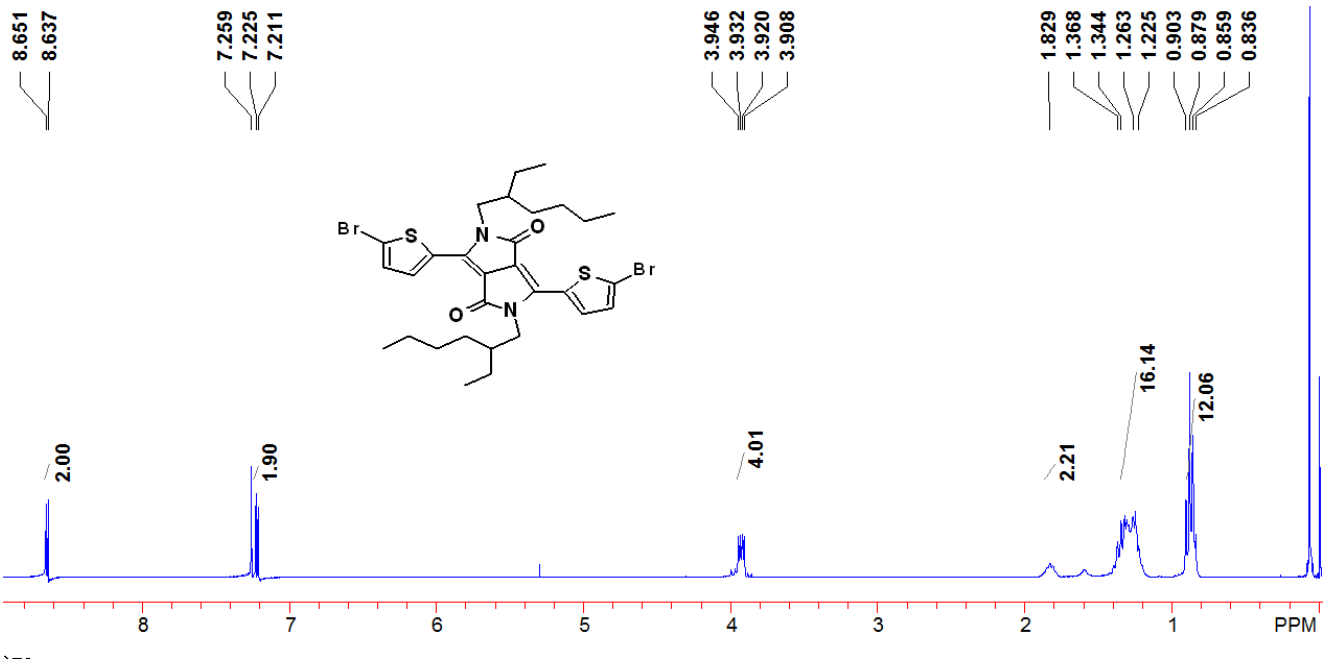


Fig. S3. ^{1}H NMR for **DPP 1b**

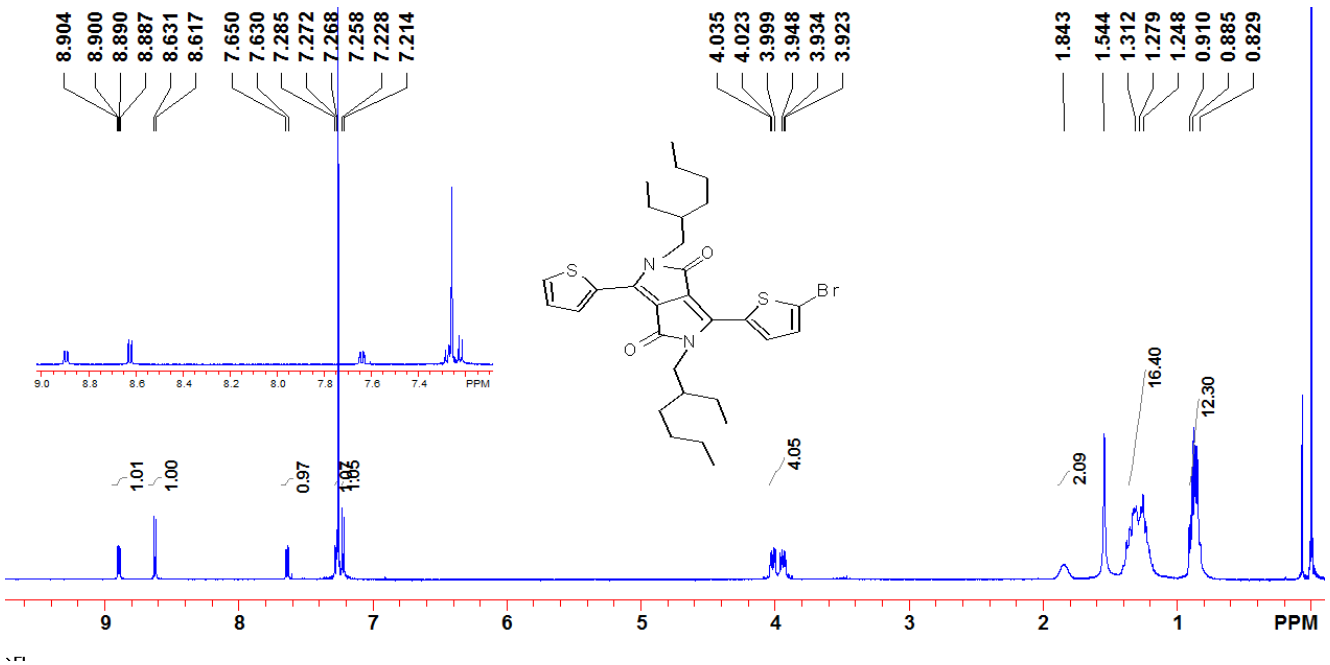


Fig. S4. ^{1}H NMR for mono-bromo-**DPP**

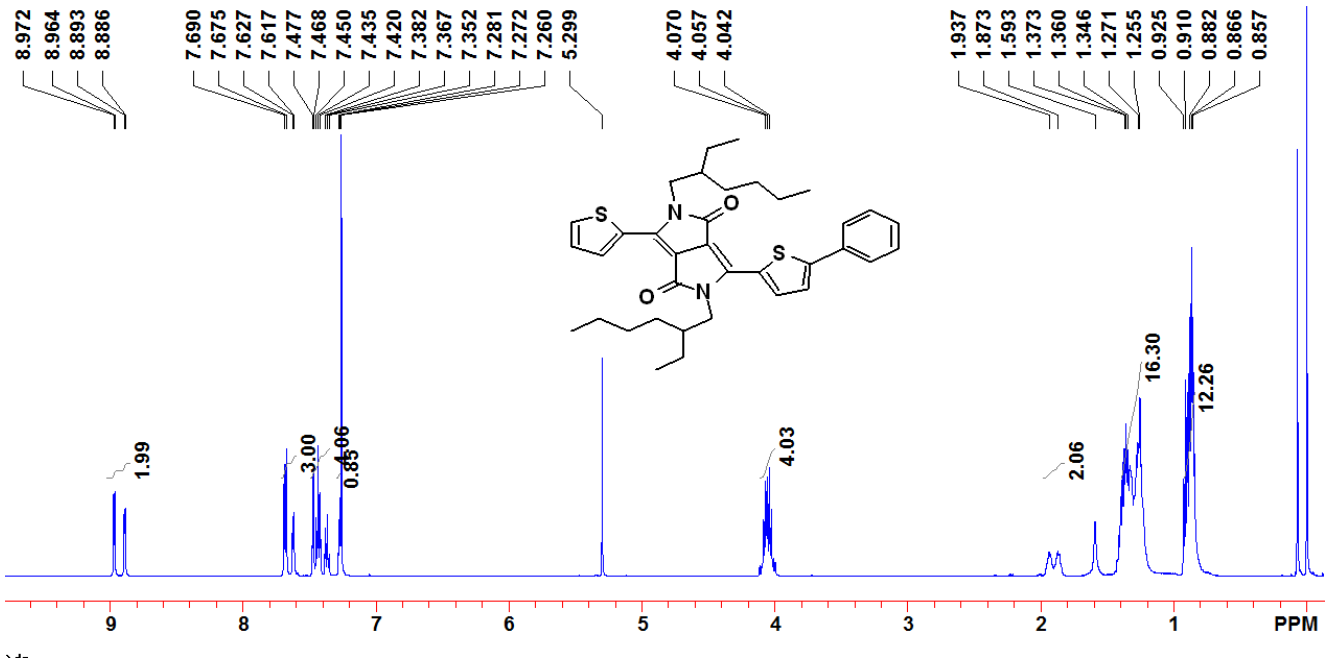


Fig. S5. ^{1}H NMR for **DPP 1c**

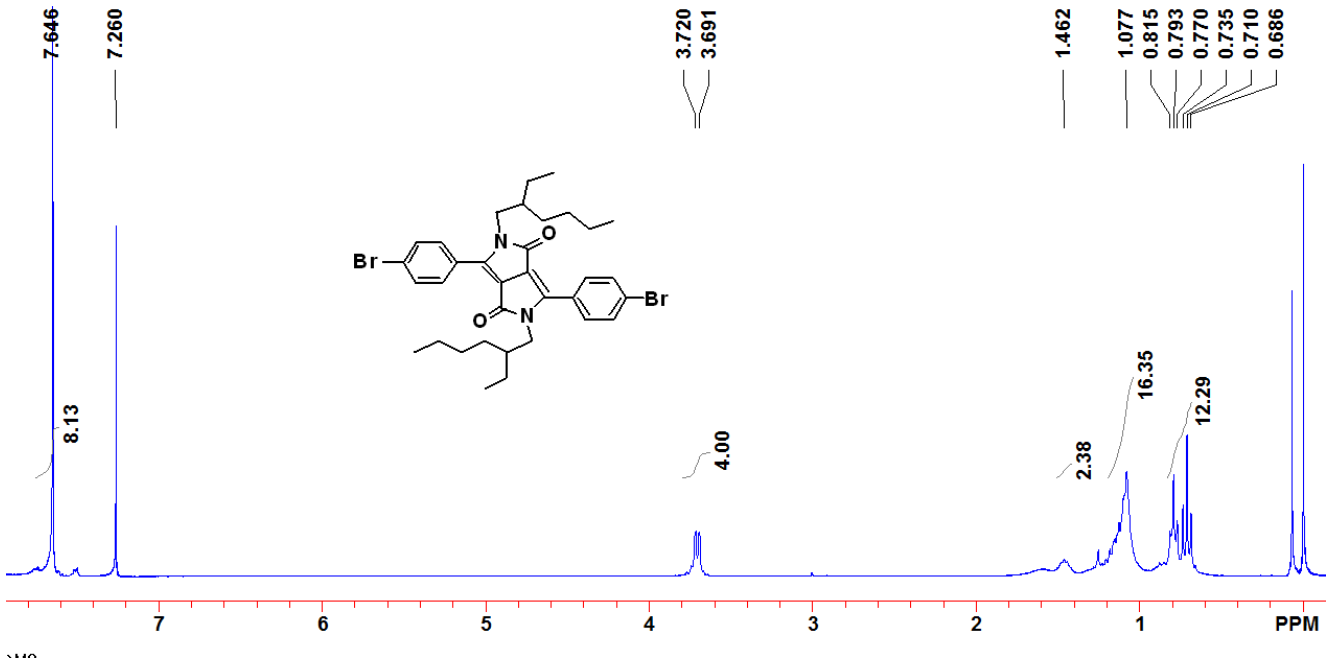


Fig. S6. ^{1}H NMR for **DPP 1d**

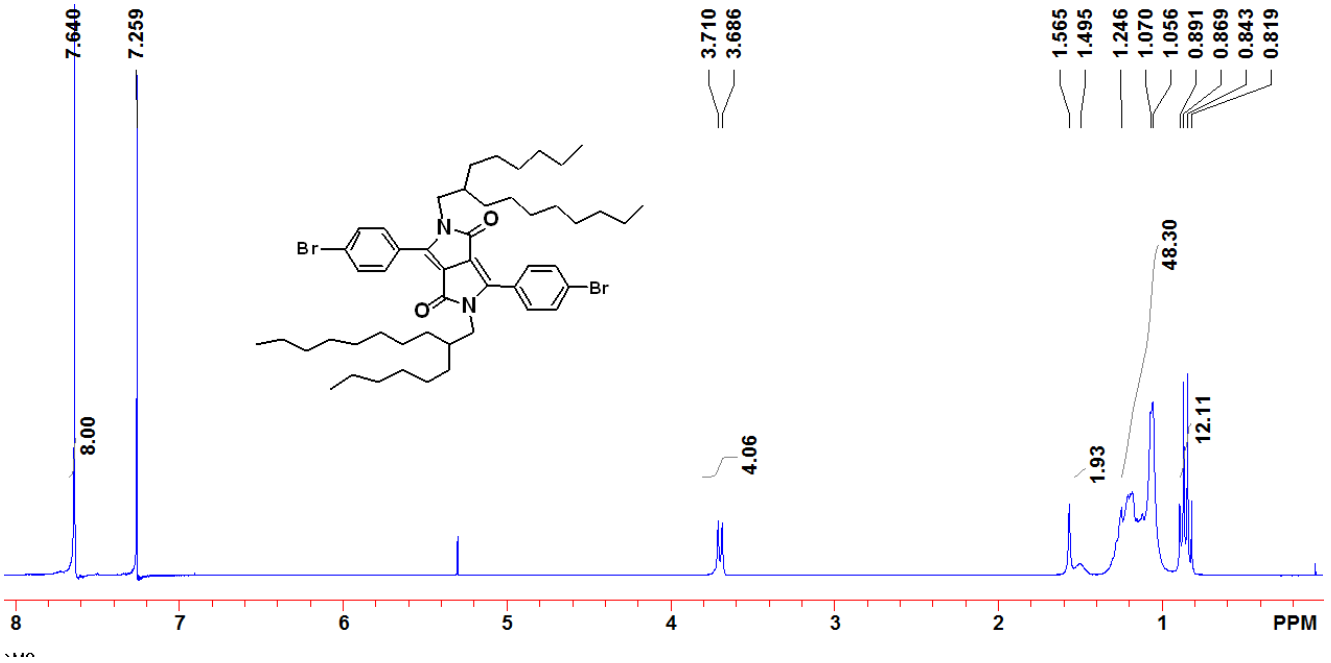


Fig. S7. ^{1}H NMR for **DPP 1e**

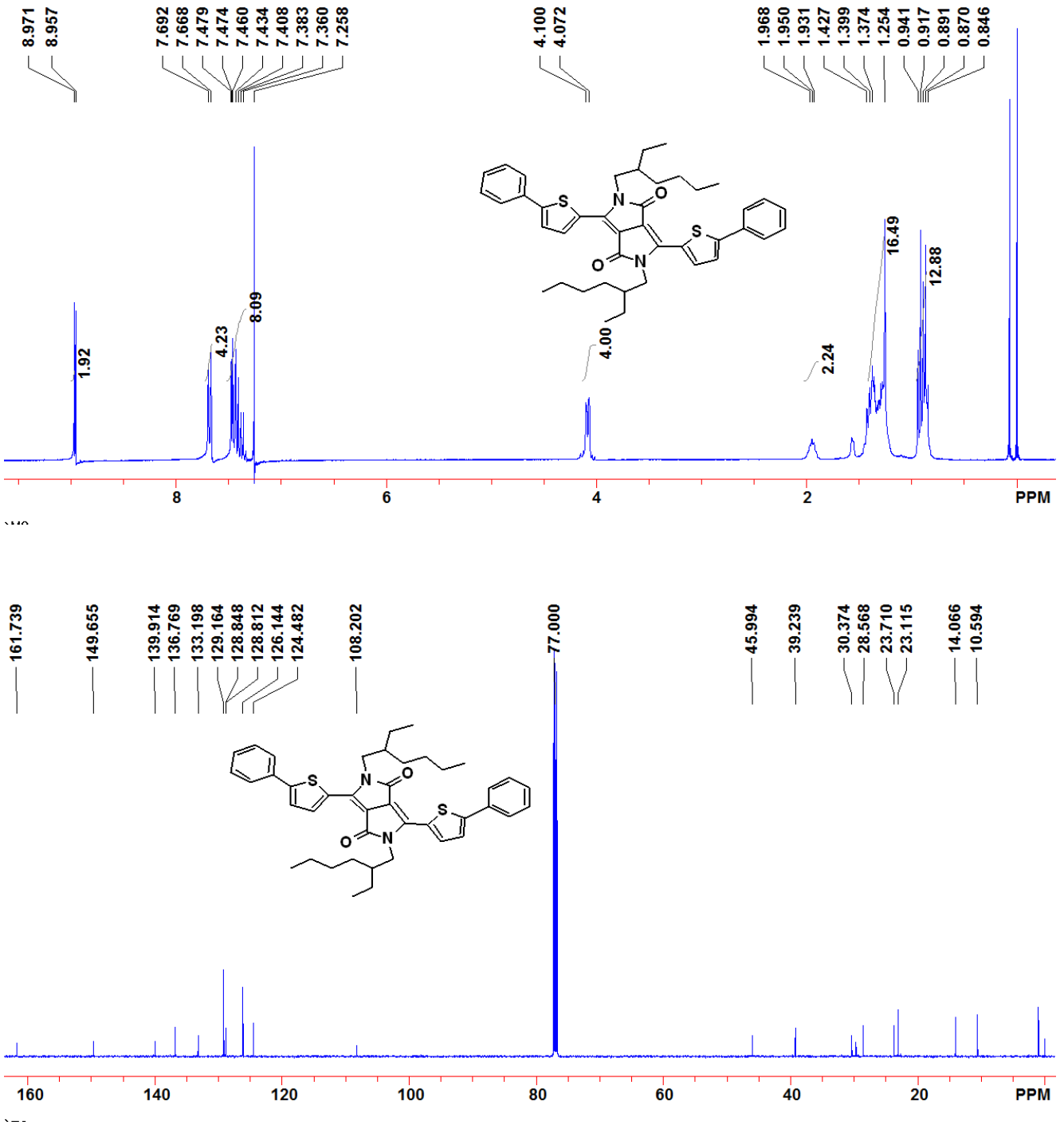


Fig. S8. ^{1}H &^{13}C NMR for **DPP 1**

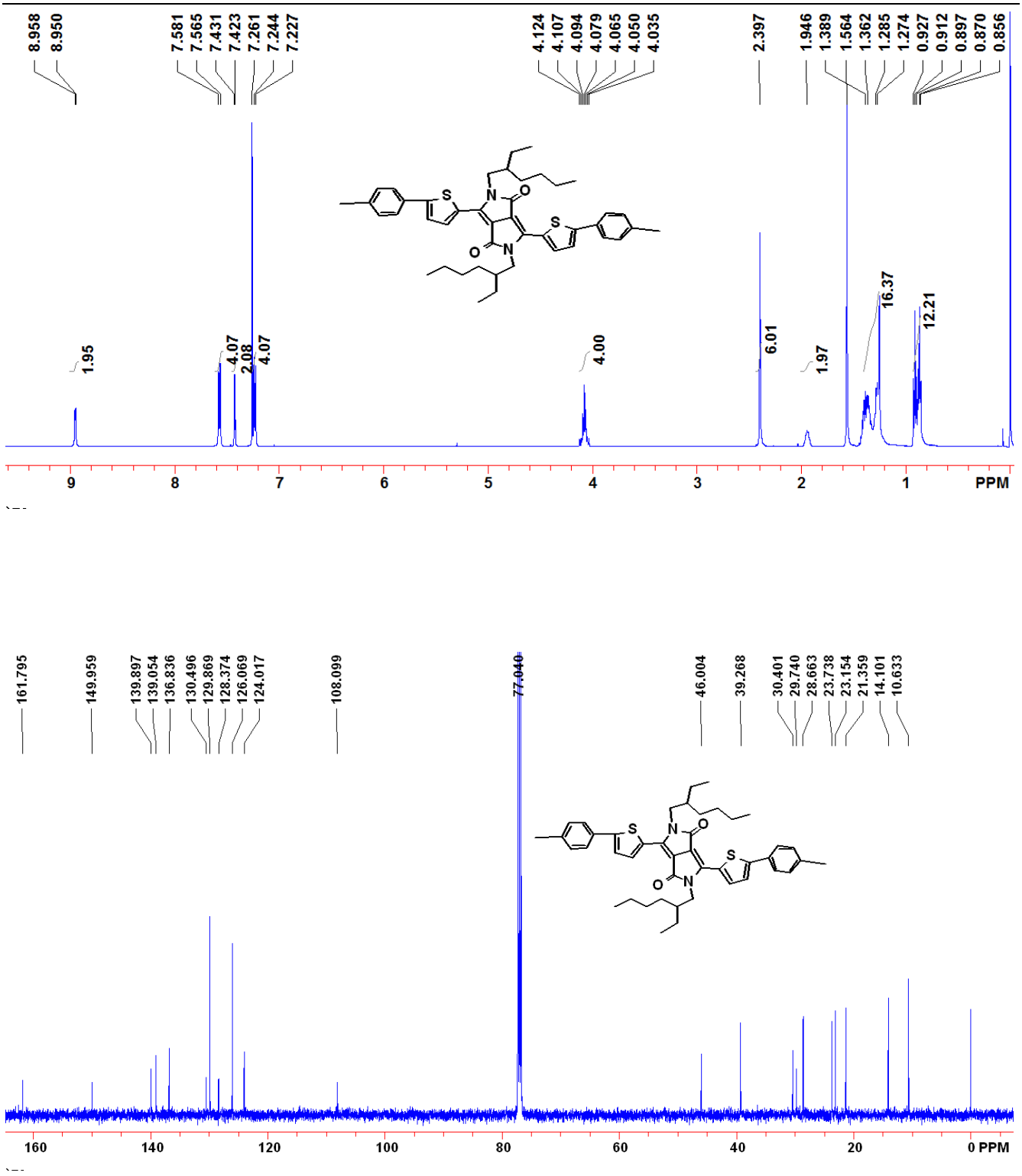


Fig. S9. ^{1}H &^{13}C NMR for **DPP 2**

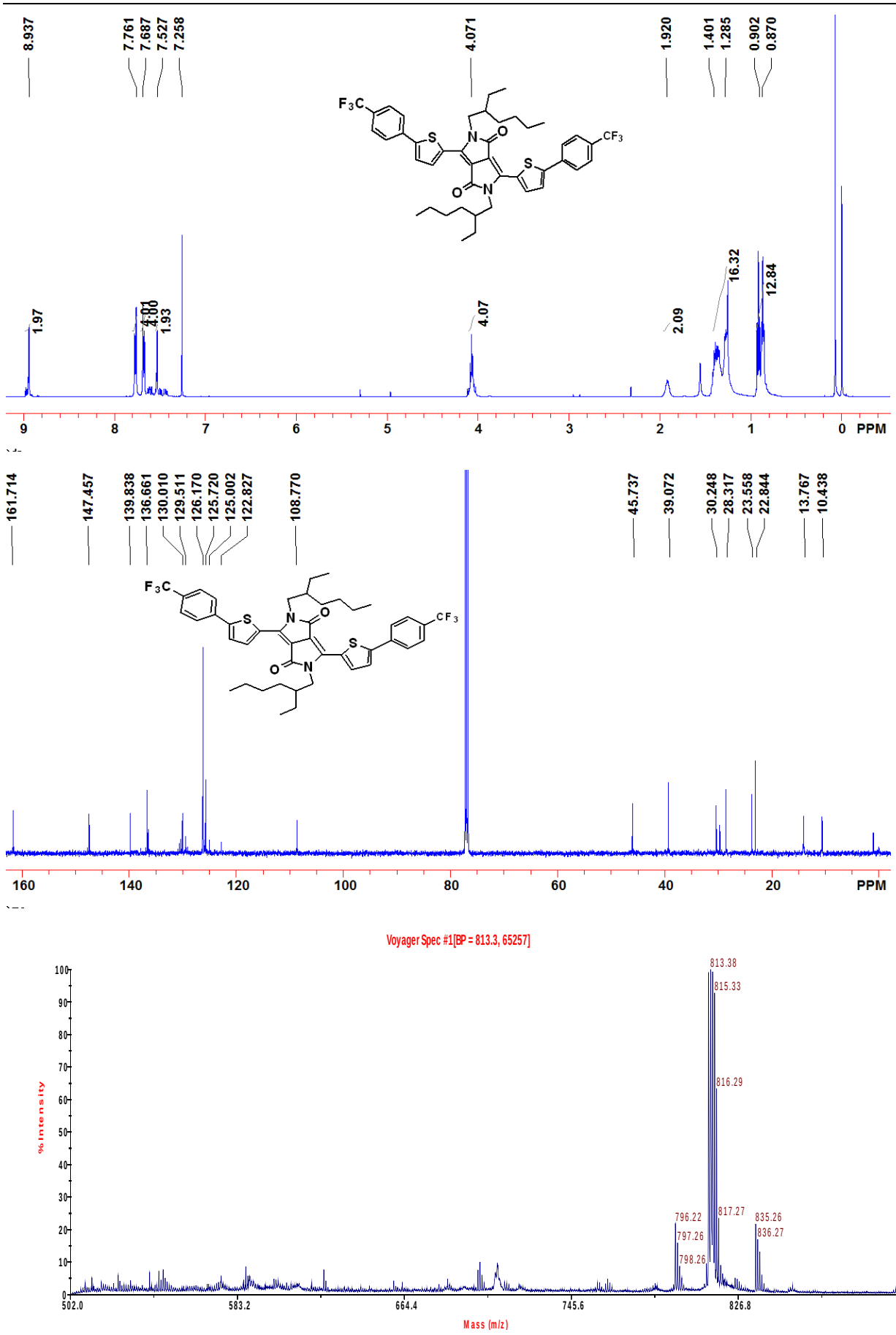


Fig. S10. ^{1}H &^{13}C NMR and MALDI-TOF MS for **DPP 3**

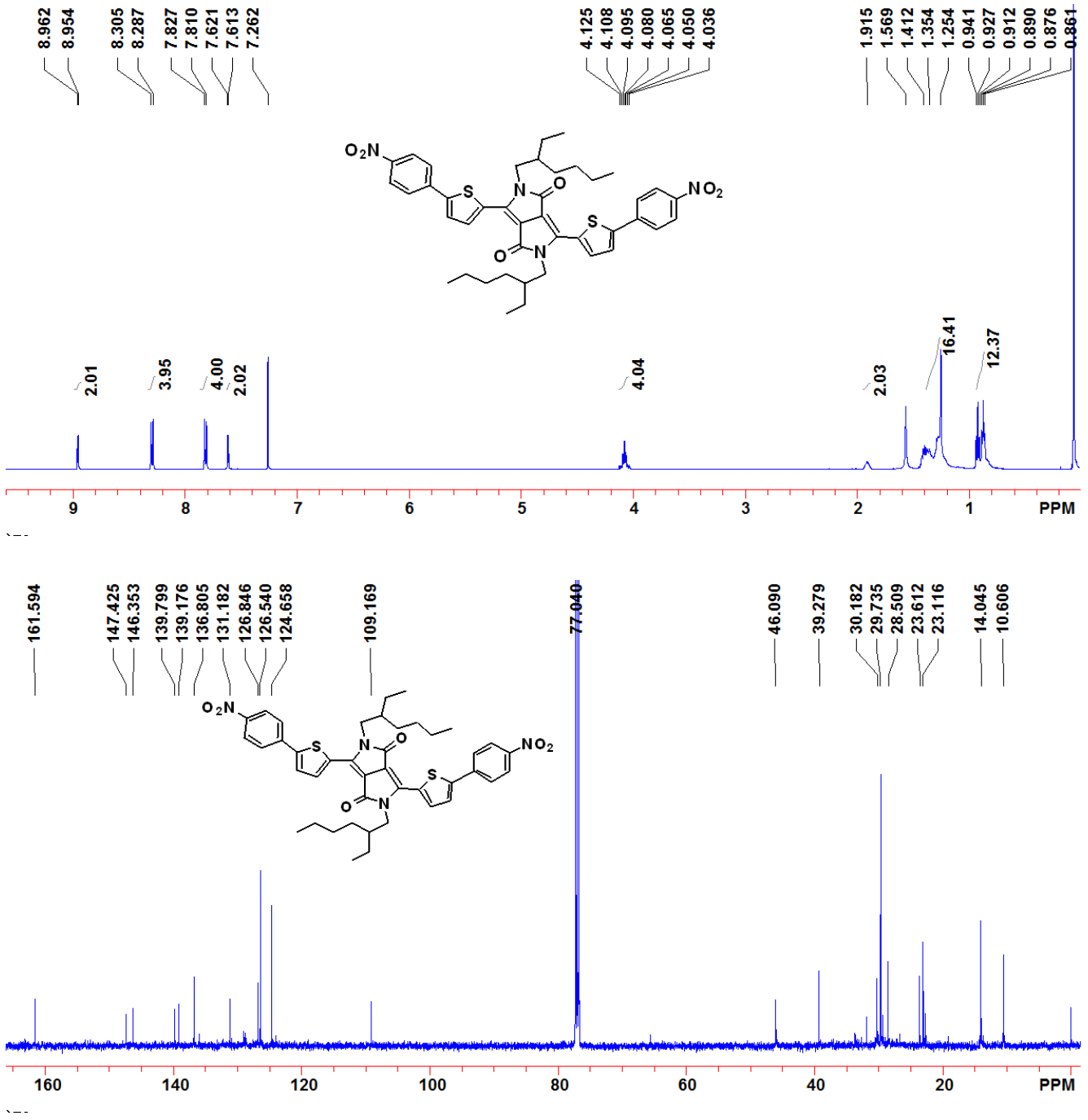


Fig. S11. ^{1}H &^{13}C NMR for **DPP 4**

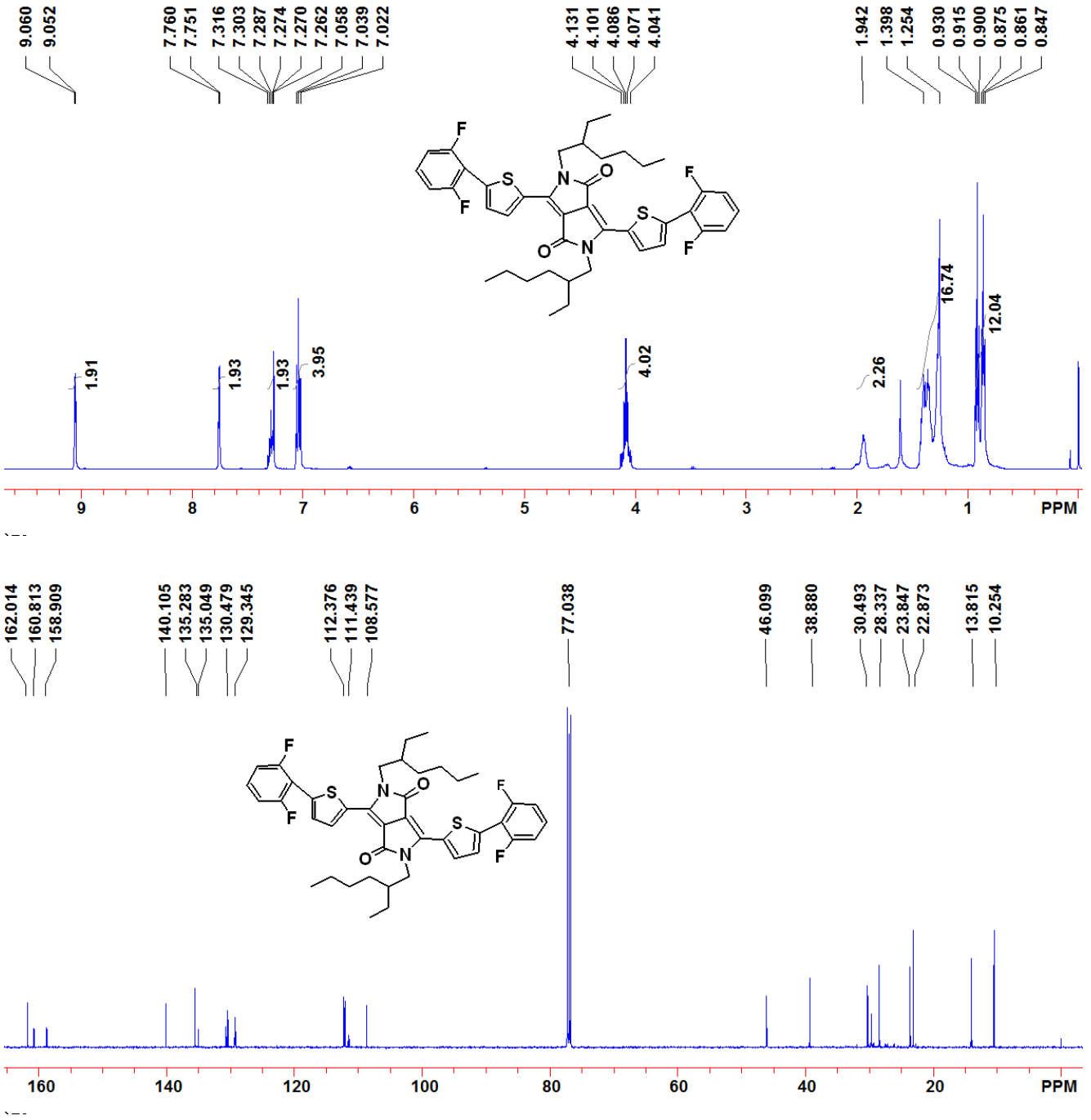


Fig. S12. ^{1}H &^{13}C NMR for **DPP 5**

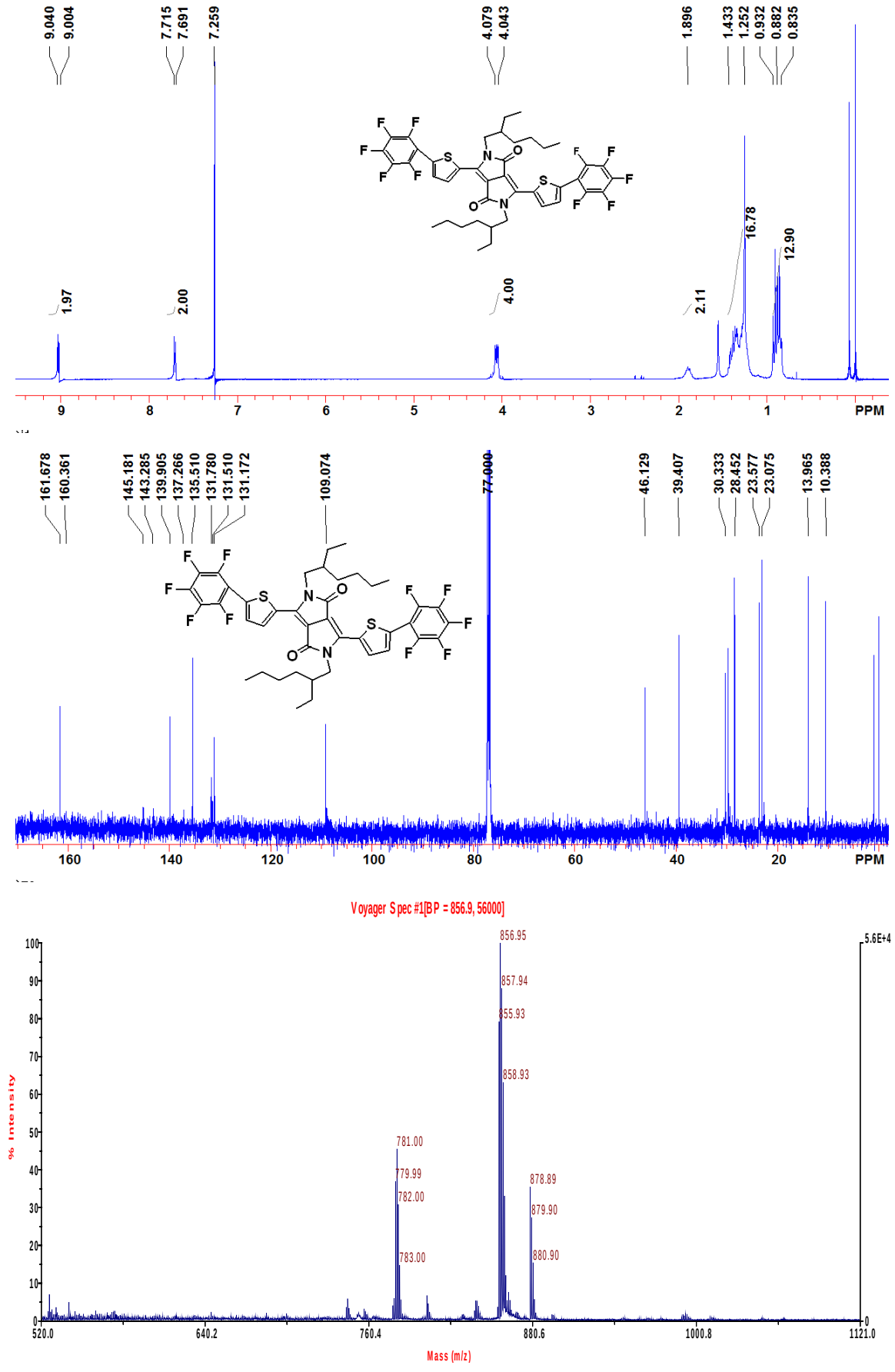


Fig. S13. ^{1}H &^{13}C NMR and MALDI-TOF MS for **DPP 6**

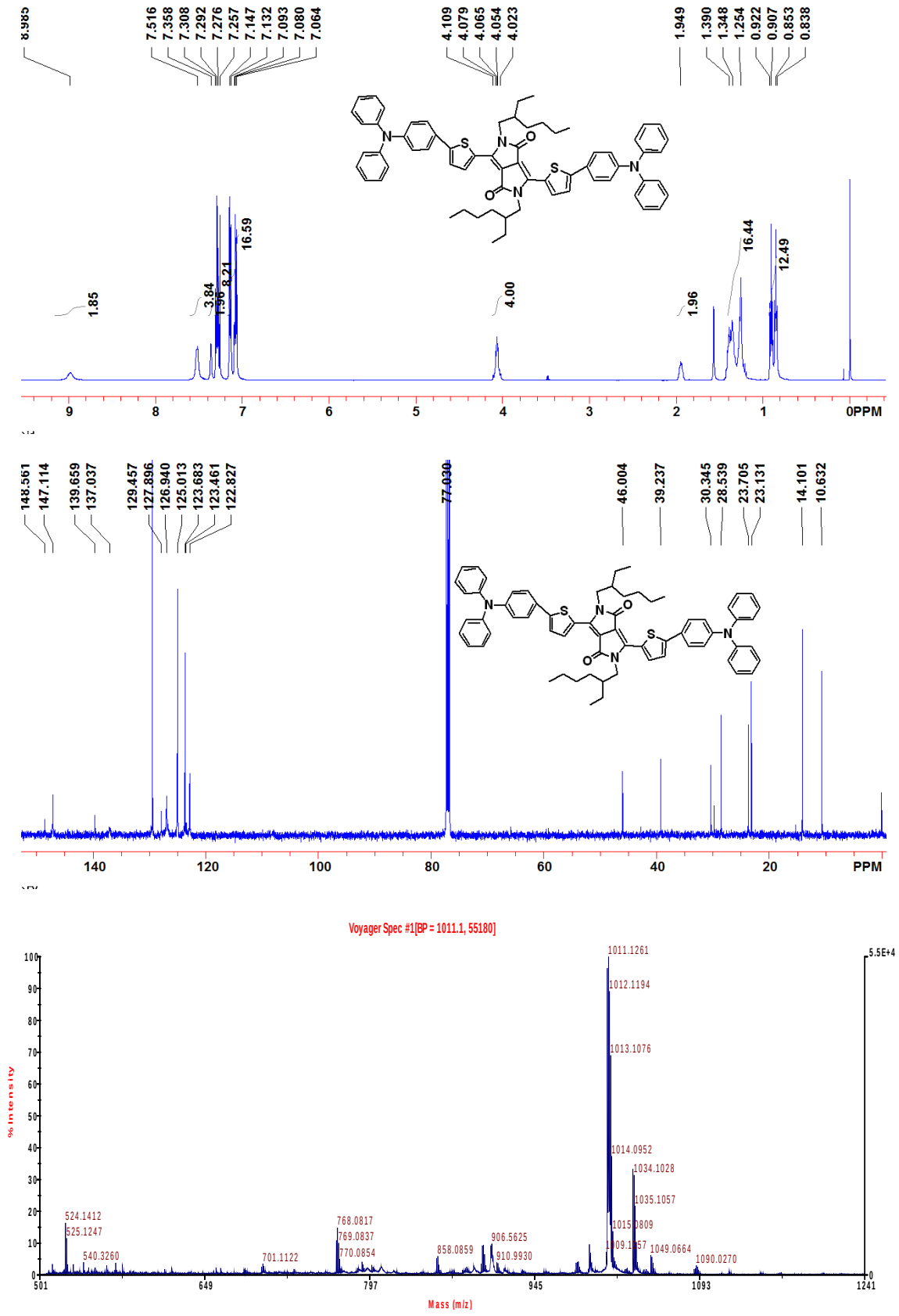


Fig. S14. ^{1}H &^{13}C NMR and MALDI-TOF MS for **DPP 7**

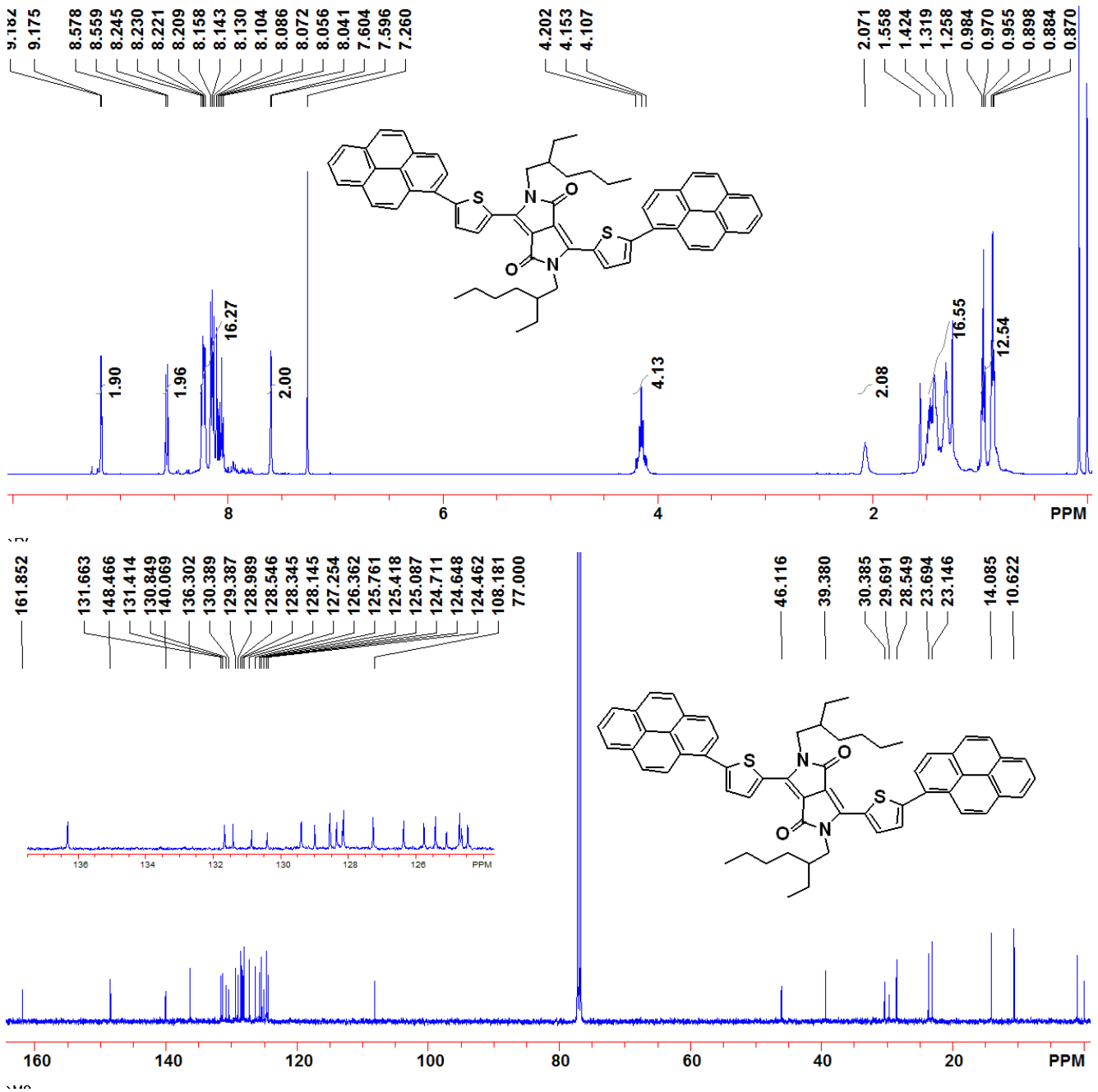


Fig. S15. ^{1}H &^{13}C NMR for **DPP 8**

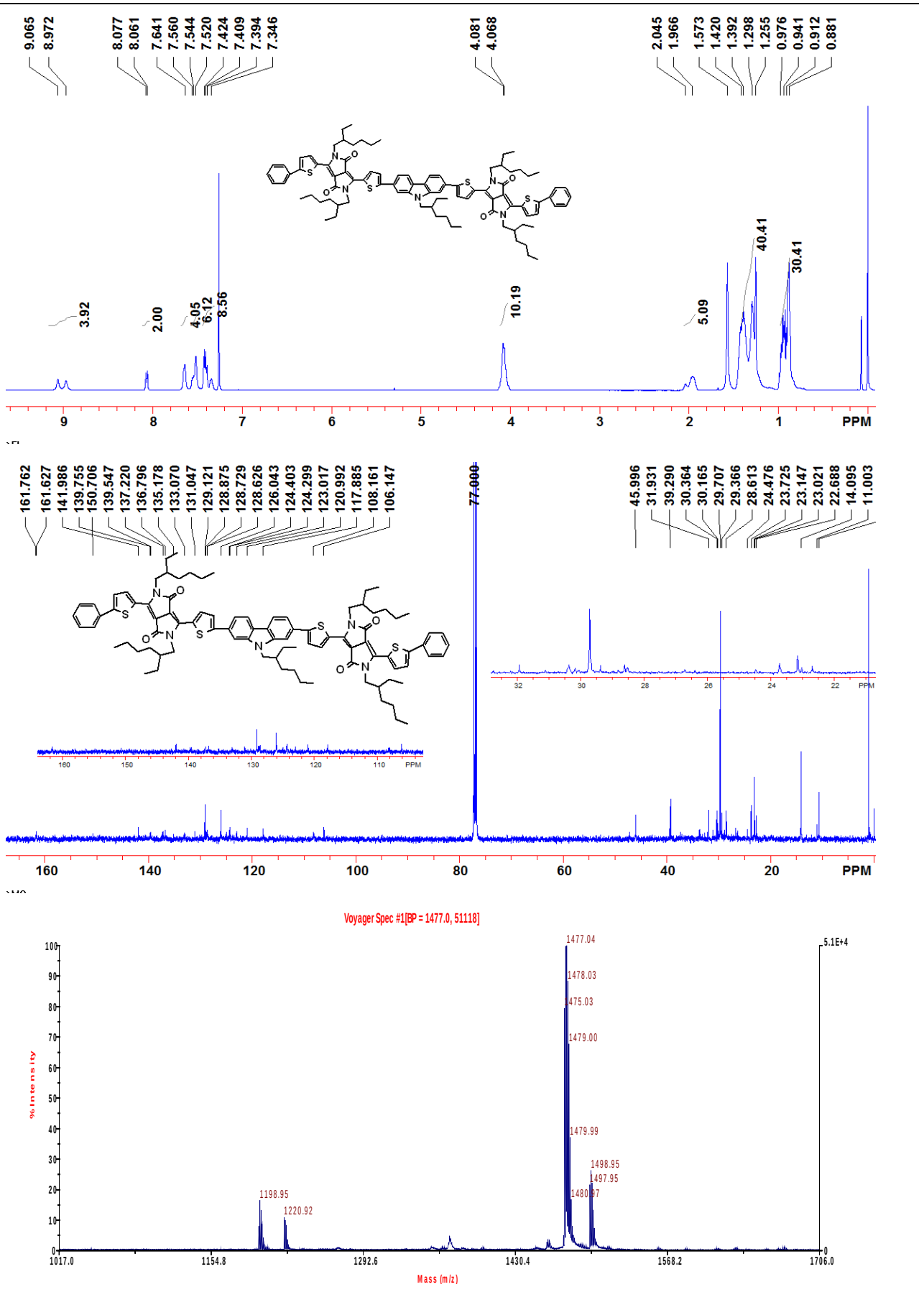


Fig. S16. ^{1}H &^{13}C NMR and MALDI-TOF MS for **DPP 9**

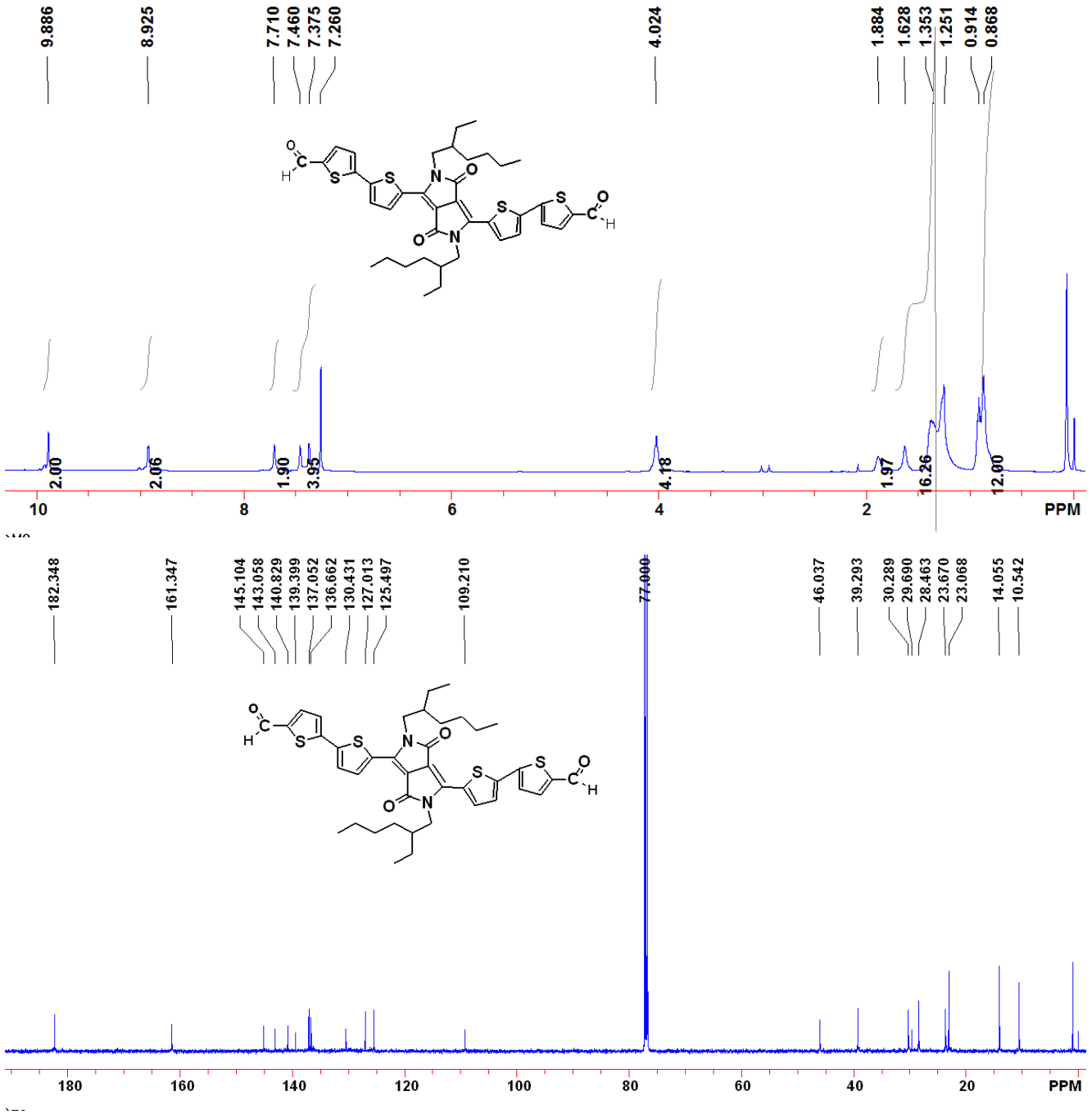


Fig. S17. ^{1}H &^{13}C NMR for **DPP 10**

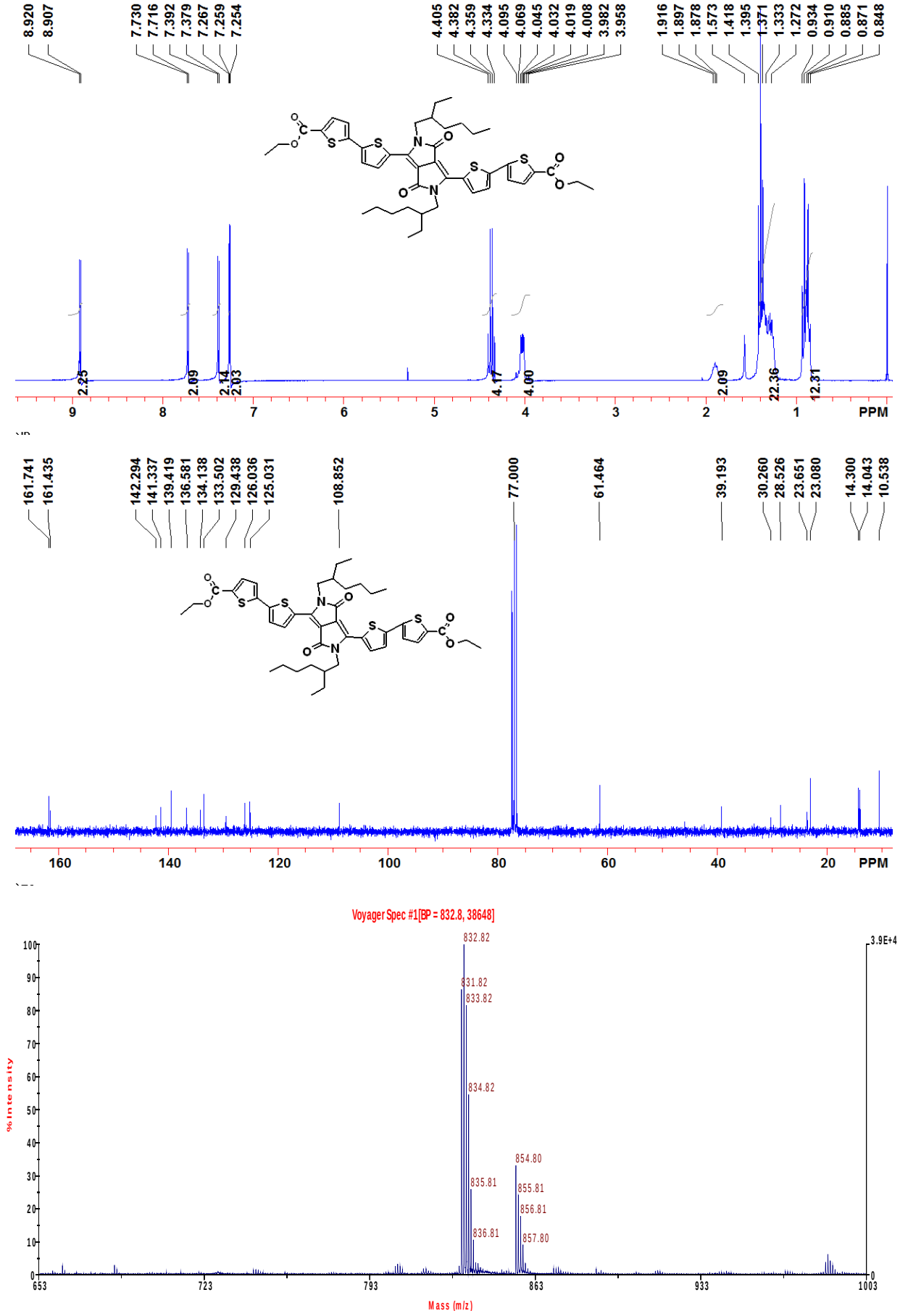


Fig. S18. ^{1}H &^{13}C NMR and MALDI-TOF MS for **DPP 11**

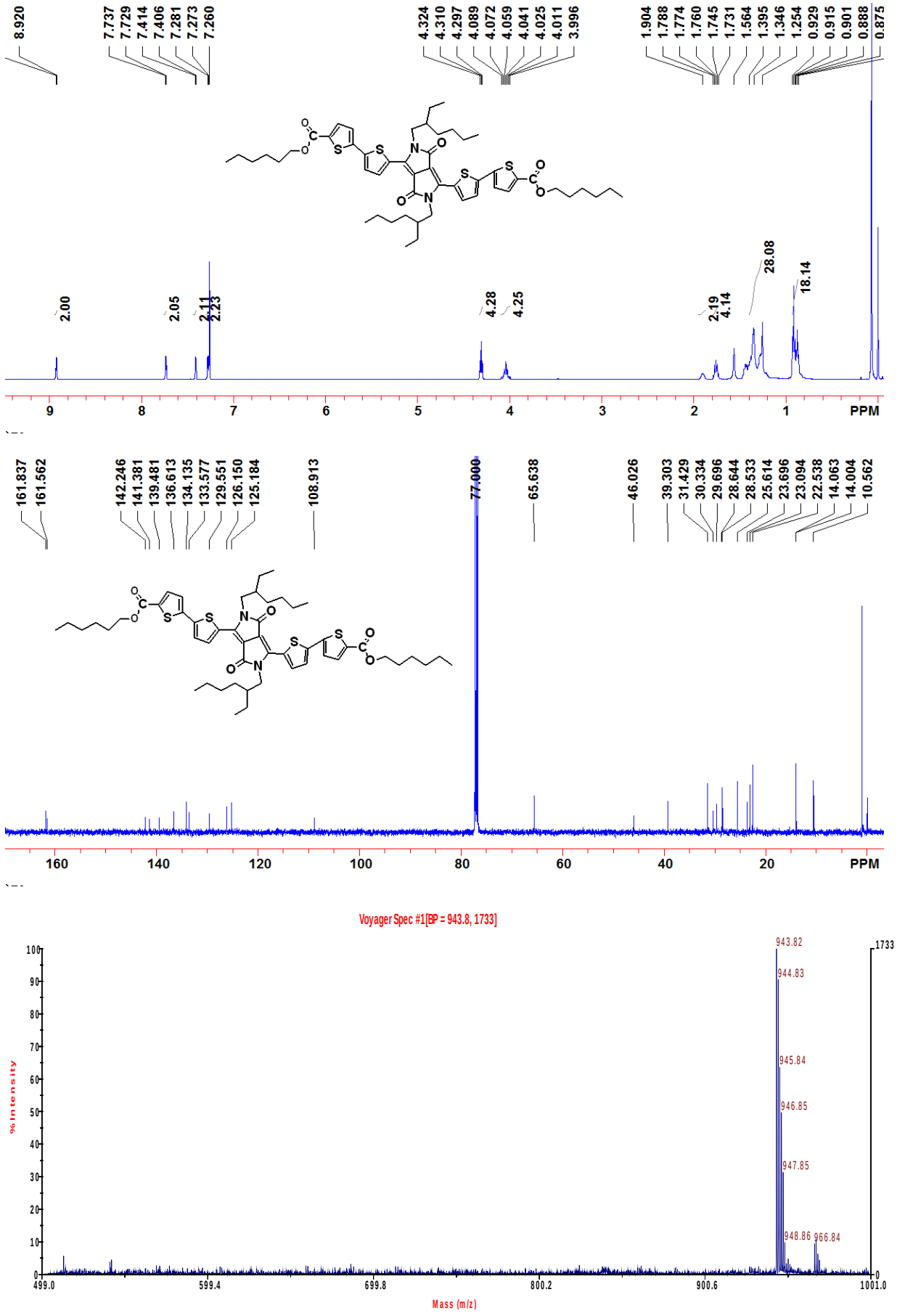


Fig. S19. ^{1}H &^{13}C NMR and MALDI-TOF MS for **DPP 12**

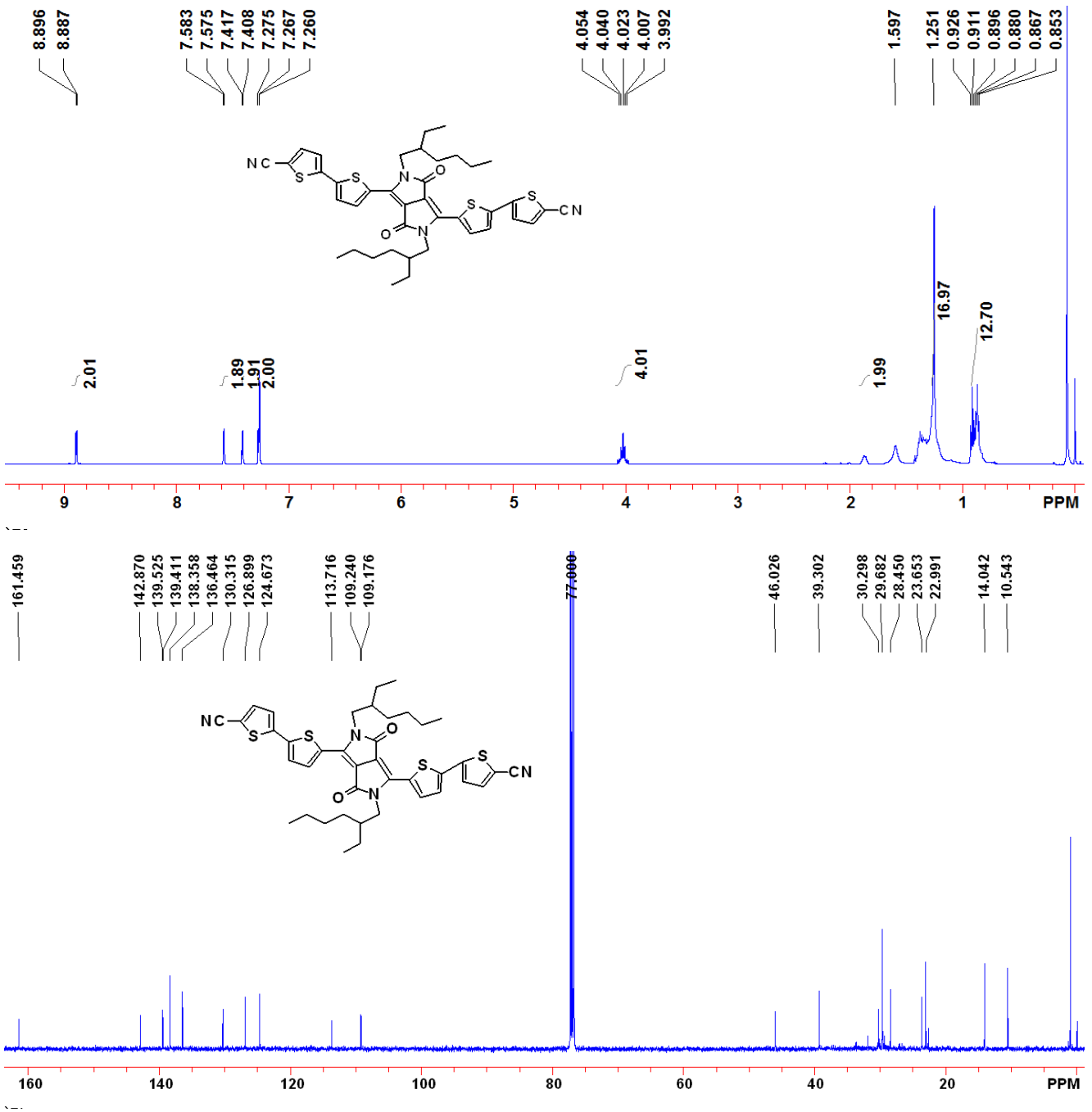


Fig. S20. ^{1}H &^{13}C NMR for **DPP 13**

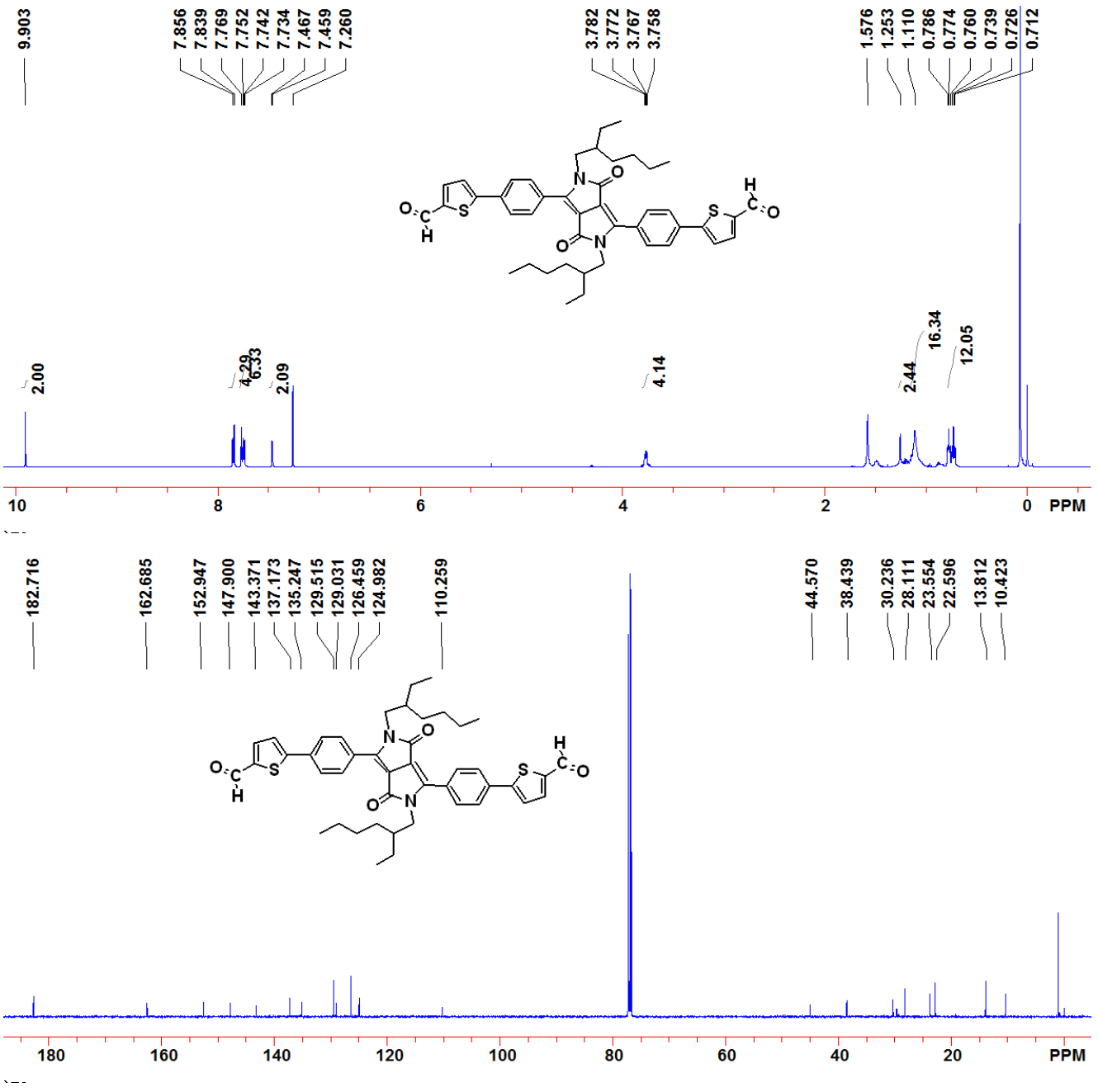


Fig. S21. ^{1}H &^{13}C NMR for **DPP 14**

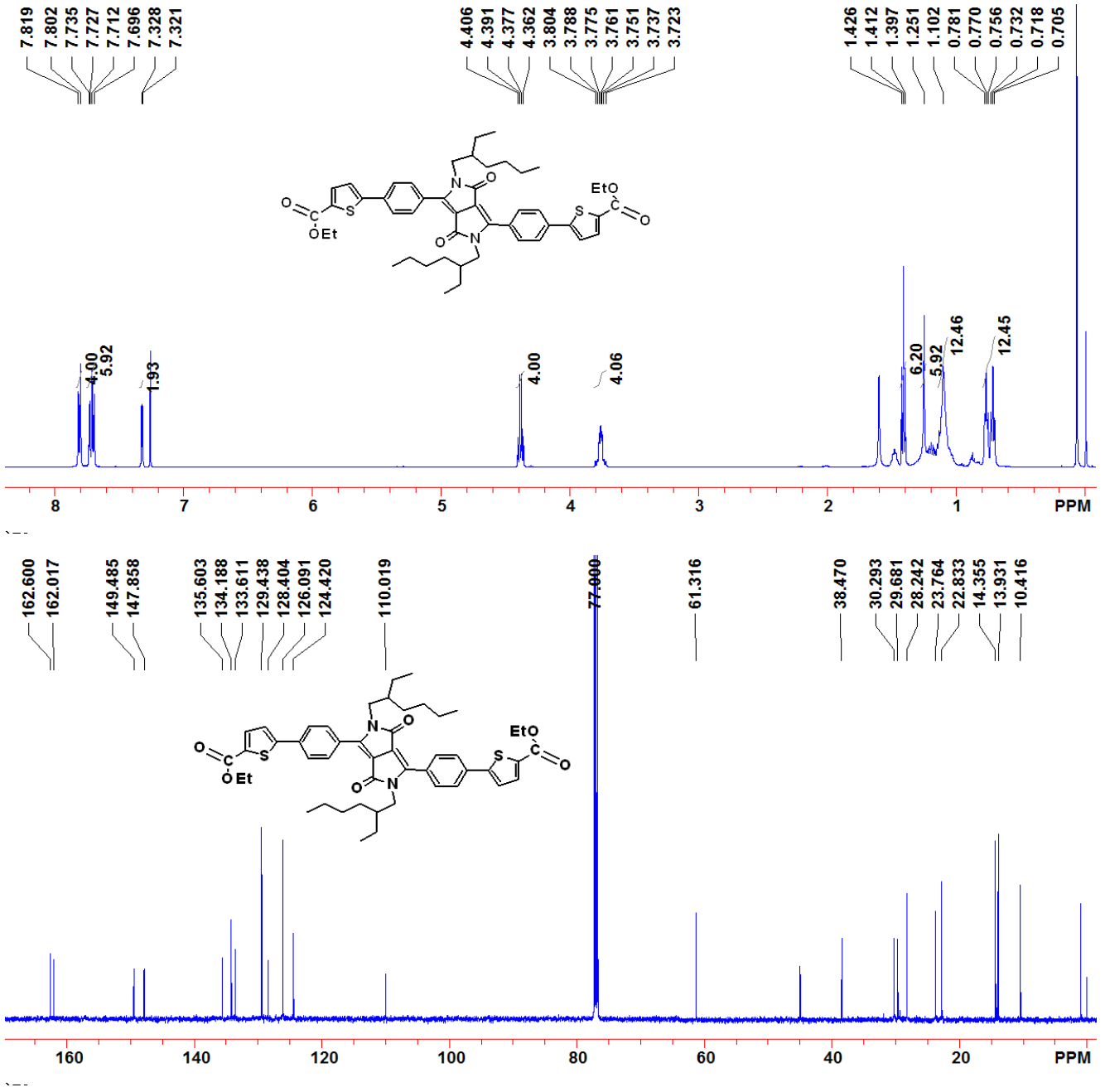


Fig. S22. ^{1}H &^{13}C NMR for **DPP 15**

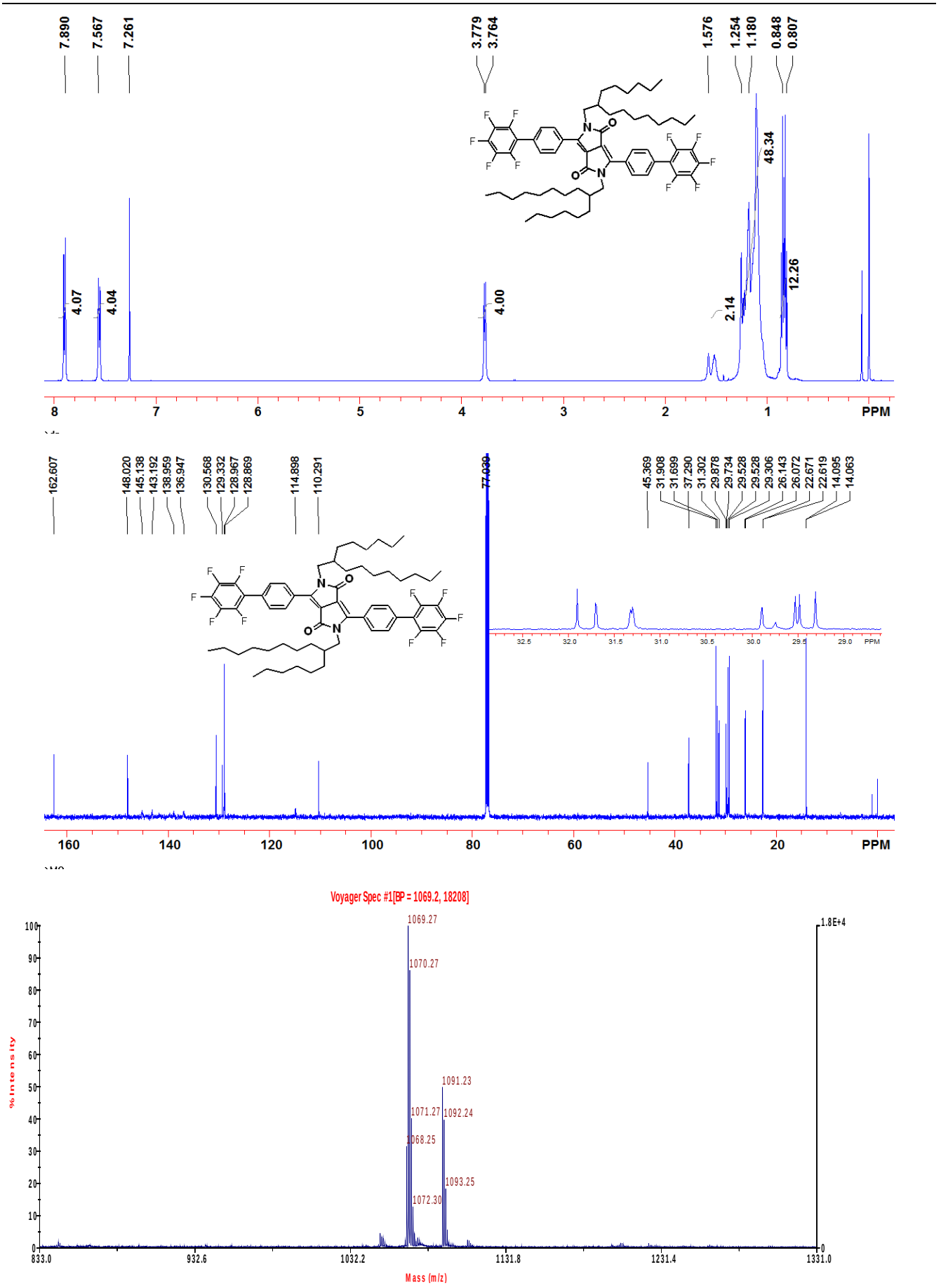


Fig. S23. ^{1}H &^{13}C NMR and MALDI-TOF MS for **DPP 16**

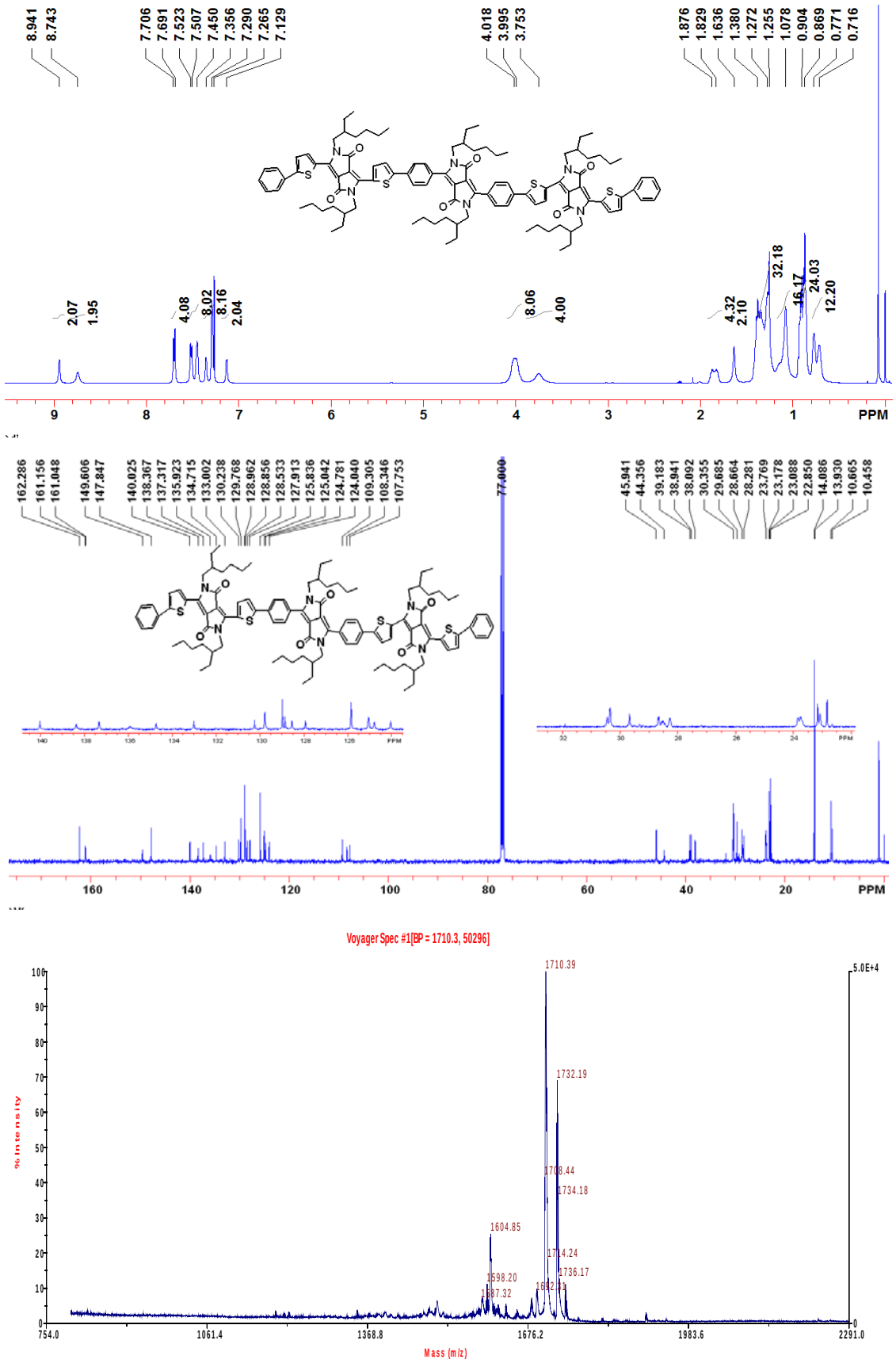


Fig. S24. ^{1}H &^{13}C NMR and MALDI-TOF MS for **DPP 17**