

Supporting Information

Development of Strongly Absorbing S,N-Heterohexacene-Based Donor Materials for Efficient Vacuum-Processed Organic Solar Cells

Christoph Wetzel,^a Amaresh Mishra,^a Elena Mena-Osteritz,^a Karsten Walzer,^b Martin Pfeiffer,^b Peter Bäuerle^{a*}

^aInstitute of Organic Chemistry II and Advanced Materials

University of Ulm, Albert-Einstein-Allee 11, 89081 Ulm, Germany

E-mail: peter.baeuerle@uni-ulm.de

^bHeliatek GmbH, Treidlerstrasse 3, 01139 Dresden, Germany

Content

¹ H- and ¹³ C-NMR spectra of SN6 derivatives 7-11:.....	2
¹ H- and ¹³ C-NMR spectra of dialdehydes 12-16:	7
¹ H-NMR spectra of DCV end-capped SN6 derivatives 1-5:	12

¹H- and ¹³C-NMR spectra of SN6 derivatives 7-11:

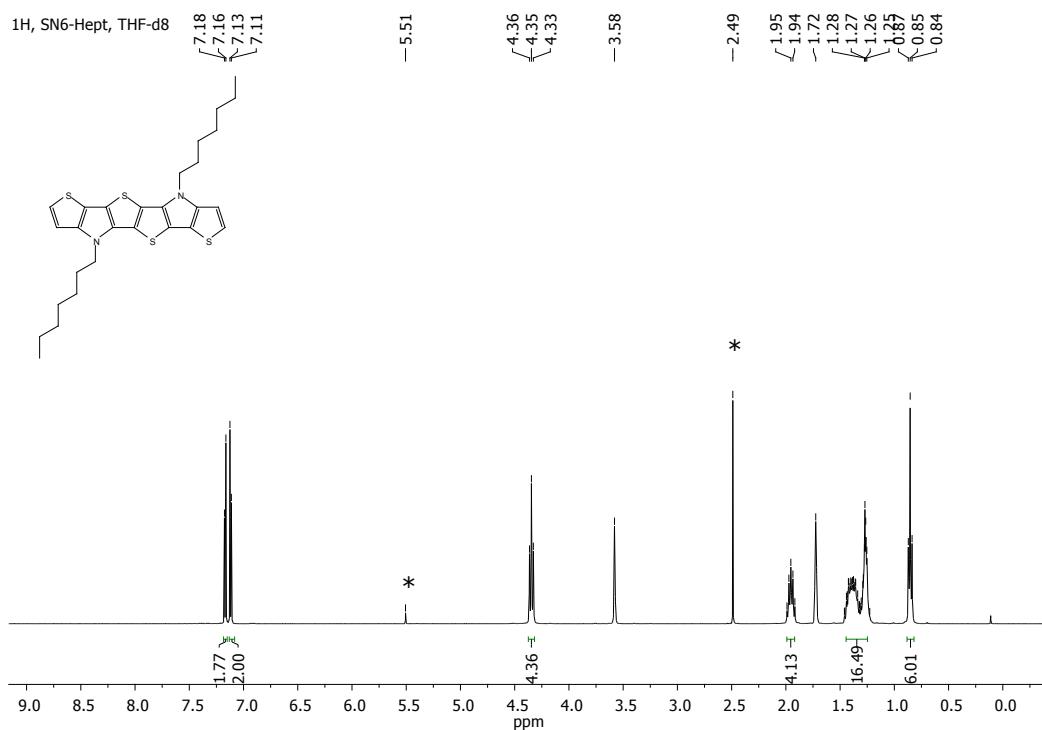


Figure 1. ¹H-NMR spectrum of SN6-Hept 11 in [D8]THF (400 MHz); *solvent impurities.

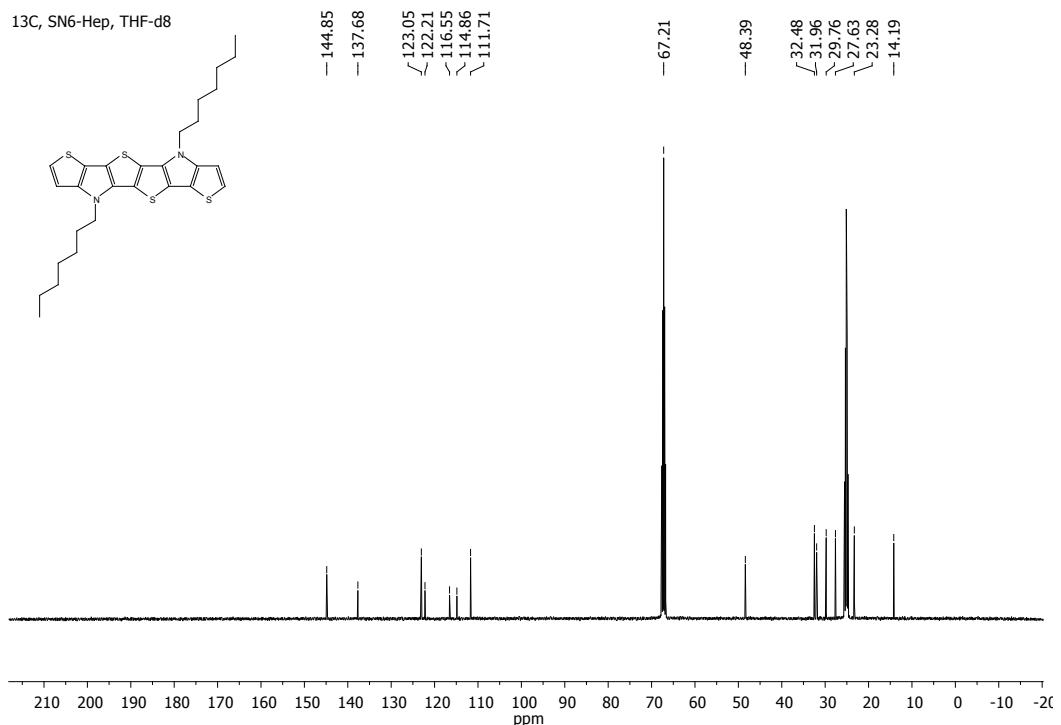


Figure 2. ¹³C-NMR spectrum of SN6-Hept 11 in [D8]THF (100 MHz).

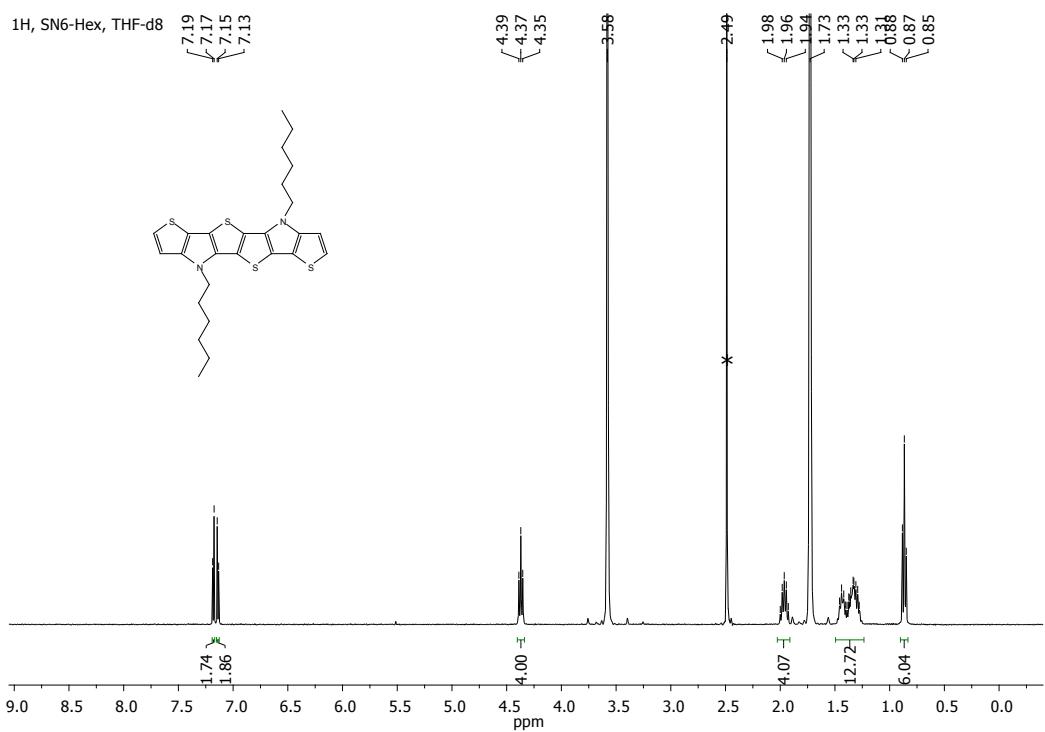


Figure 3. ^1H -NMR spectrum of SN6-Hex 10 in [D8]THF (400 MHz); *solvent impurities.

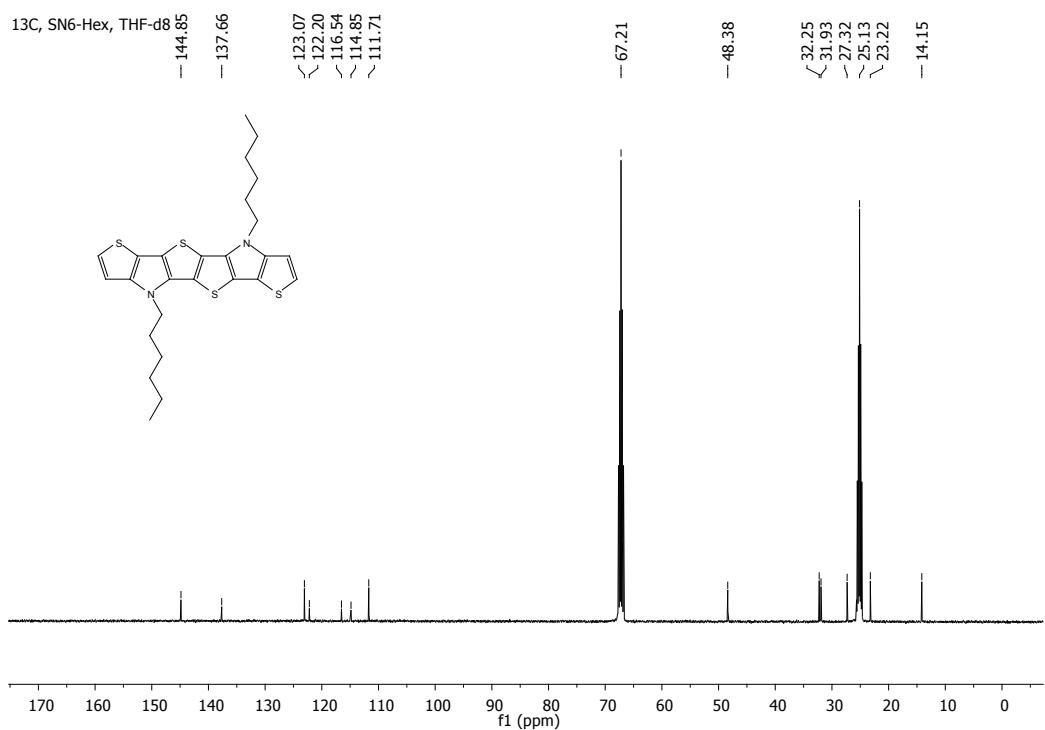


Figure 4. ^{13}C -NMR spectrum of SN6-Hex 10 in [D8]THF (100 MHz).

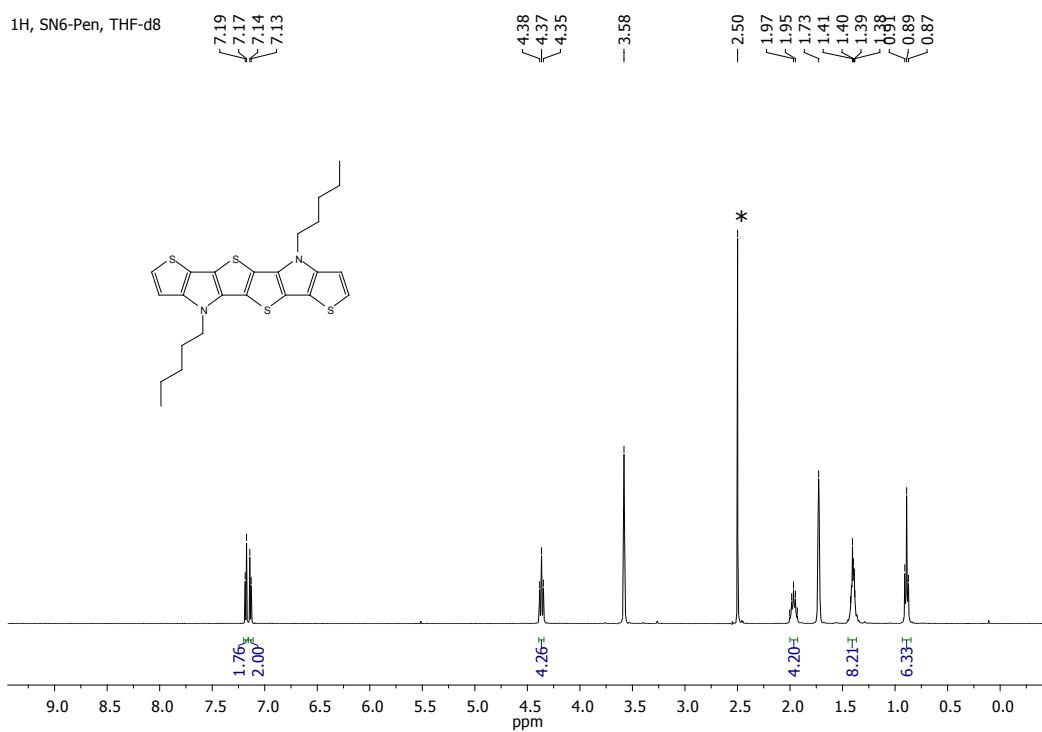


Figure 5. ^1H -NMR spectrum of SN6-Pen 9 in [D8]THF (400 MHz); *solvent impurities.

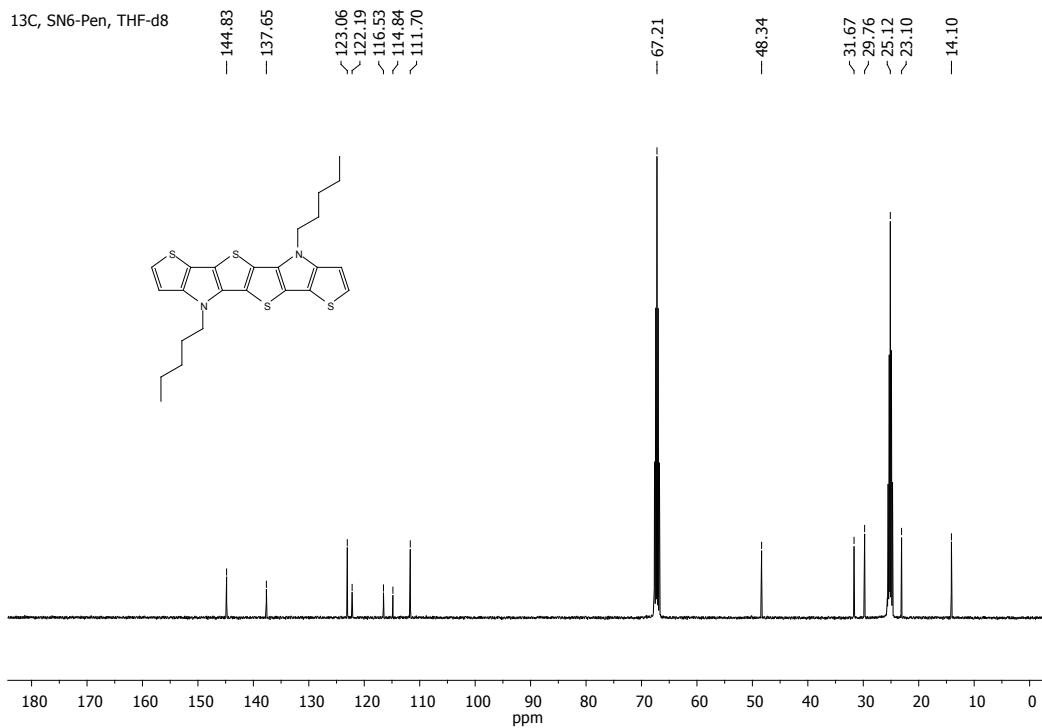


Figure 6. ^{13}C -NMR spectrum of SN6-Pen 9 in [D8]THF (100 MHz).

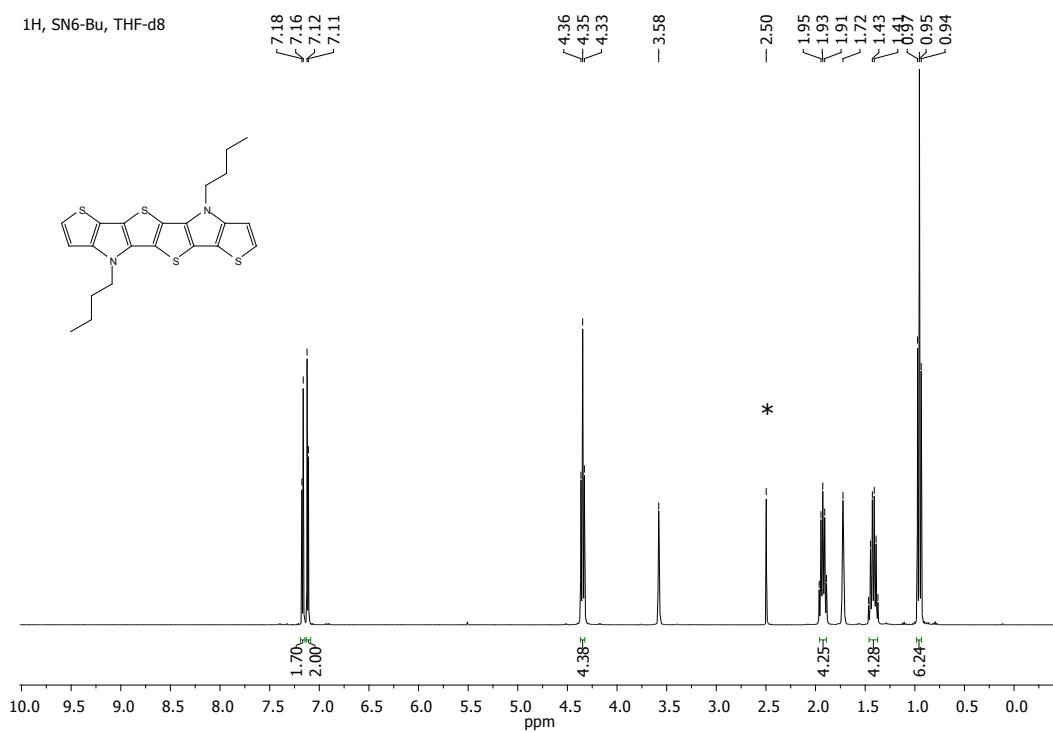


Figure 7. ^1H -NMR spectrum of SN6-Bu 8 in [D8]THF (400 MHz); *solvent impurities.

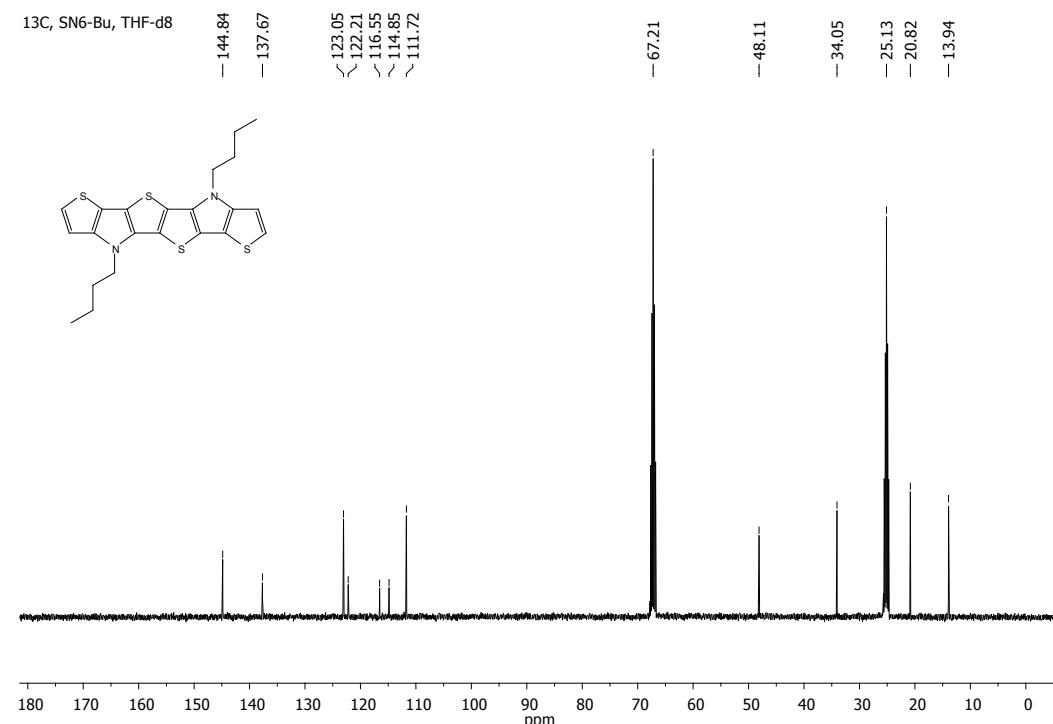


Figure 8. ^1H -NMR spectrum of SN6-Bu 8 in [D8]THF (100 MHz).

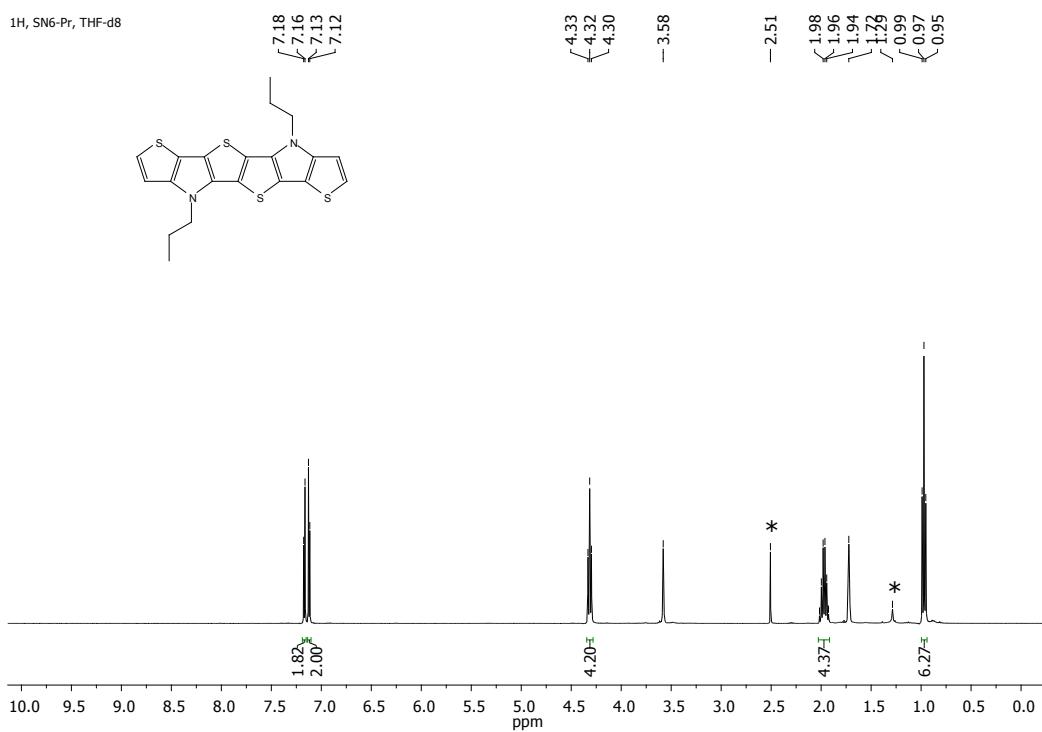


Figure 9. ^1H -NMR spectrum of SN6-Pr 7 in [D8]THF (400 MHz); *solvent imurities.

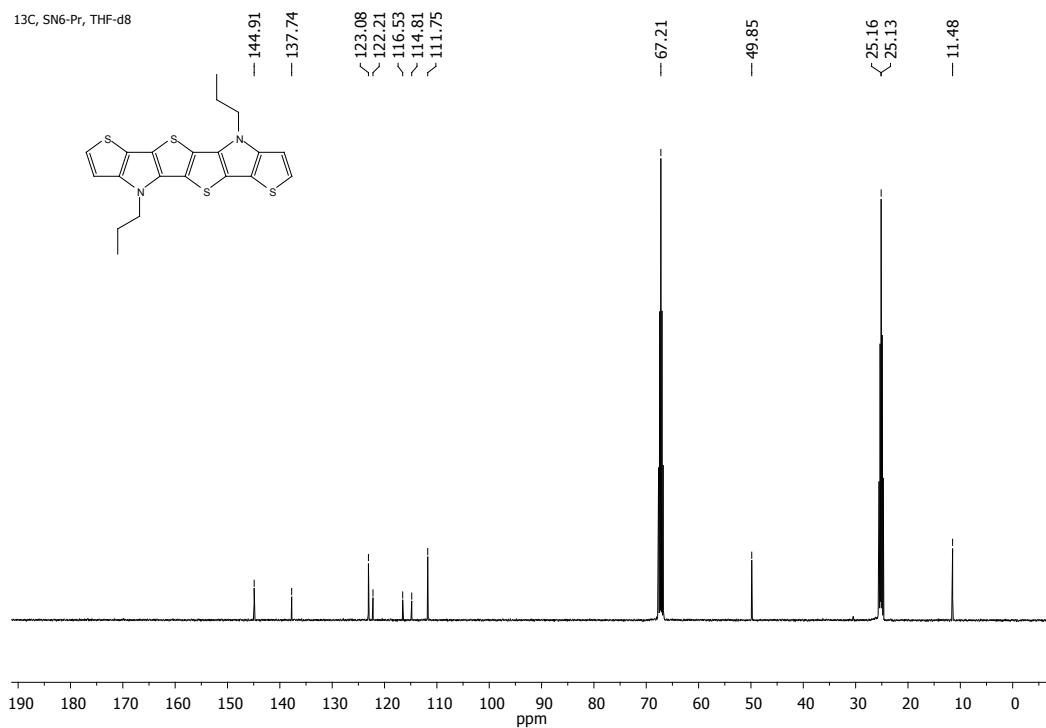


Figure 10. ^{13}C -NMR spectrum of SN6-Pr 7 in [D8]THF (100 MHz).

¹H- and ¹³C-NMR spectra of dialdehydes 12-16:

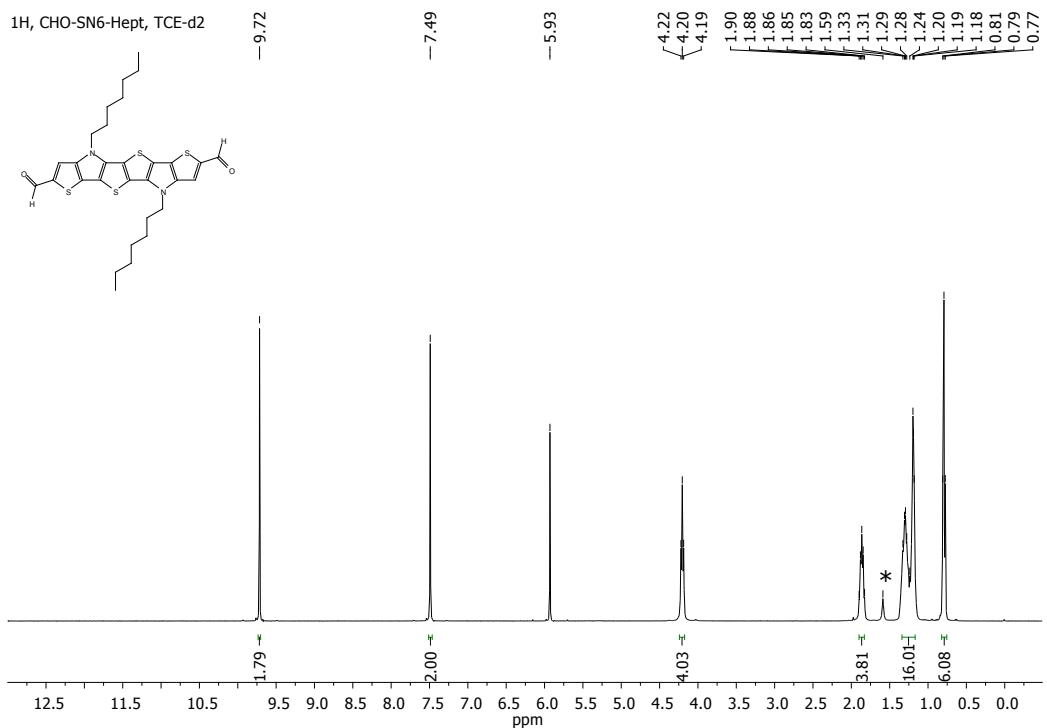


Figure 11. ¹H-NMR spectrum of CHO-SN6-Hept 16 in [D2]TCE (400 MHz); *solvent impurities.

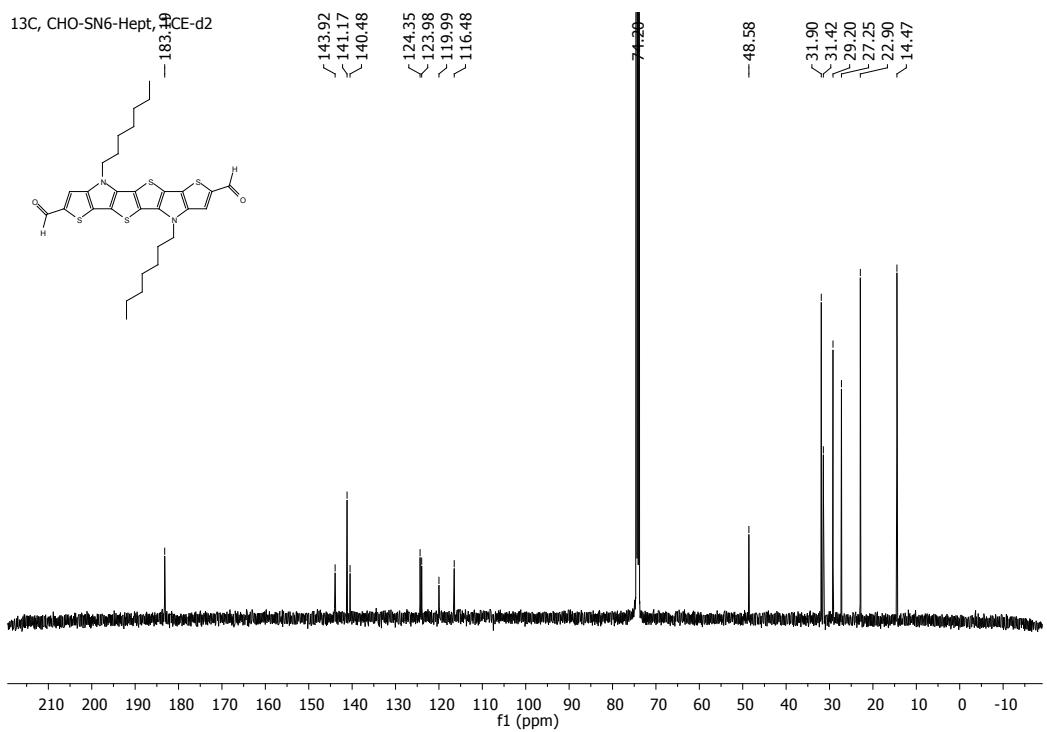


Figure 12. ¹³C-NMR spectrum of CHO-SN6-Hept 16 in [D2]TCE (100 MHz).

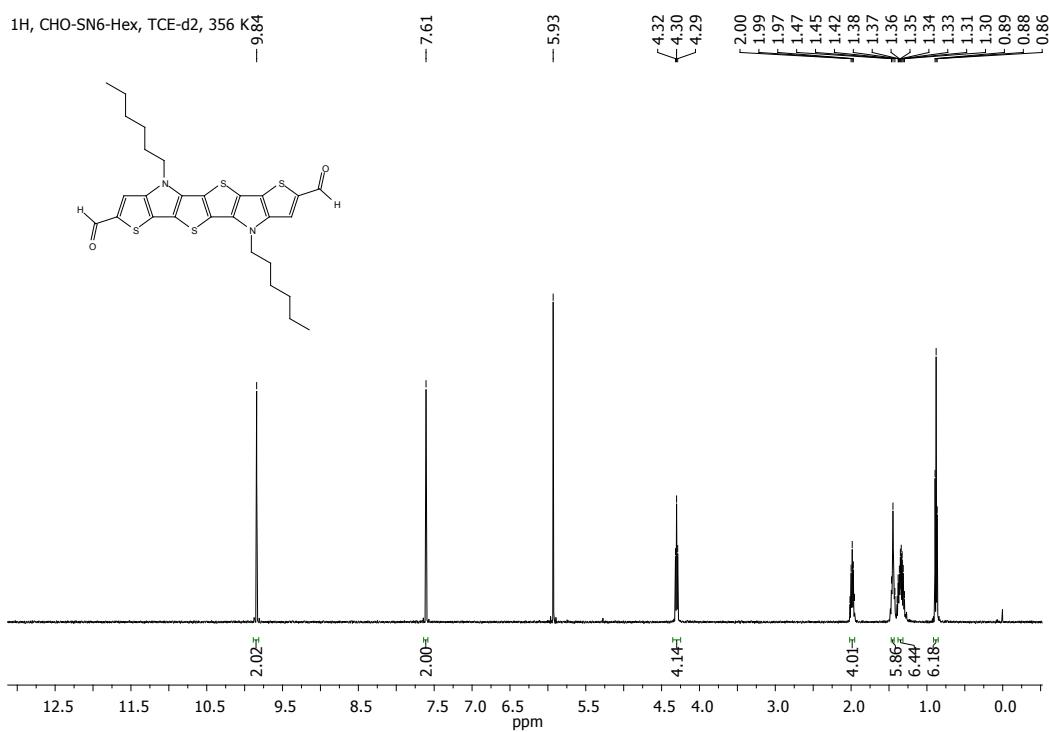


Figure 13. ¹H-NMR spectrum of CHO-SN6-Hex 15 in [D₂]TCE (500 MHz).

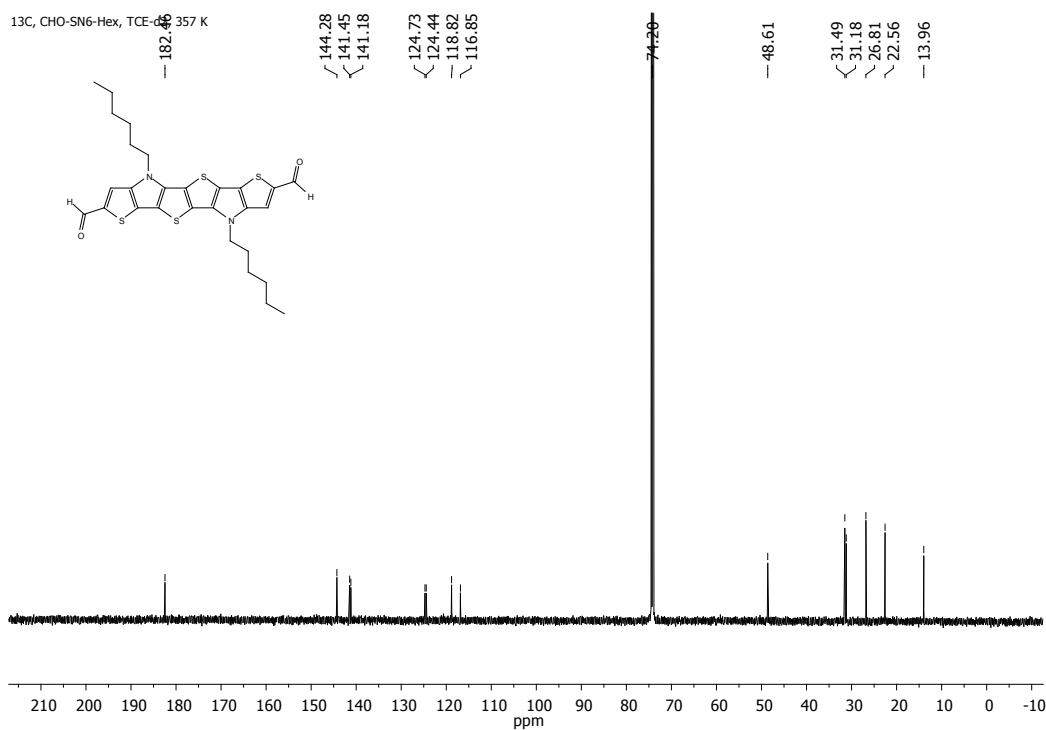


Figure 14. ¹³C-NMR spectrum of CHO-SN6-Hex 15 in [D₂]TCE (125 MHz).

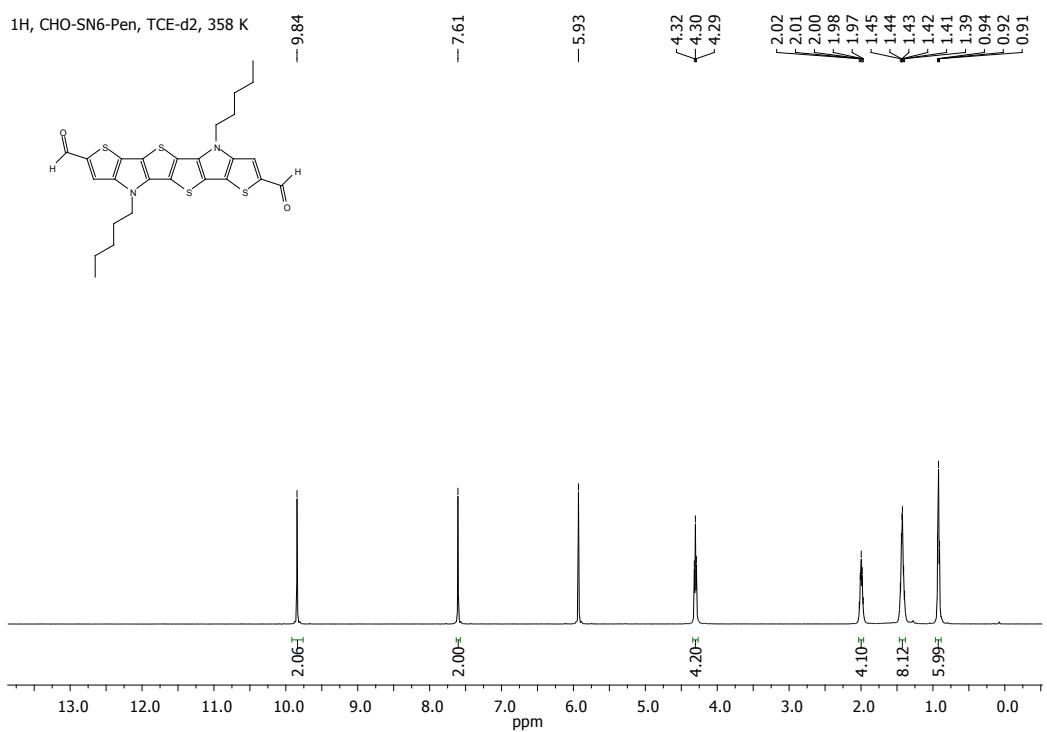


Figure 15. ^1H -NMR spectrum of CHO-SN6-Pen 14 in $[\text{D}2]\text{TCE}$ (500 MHz).

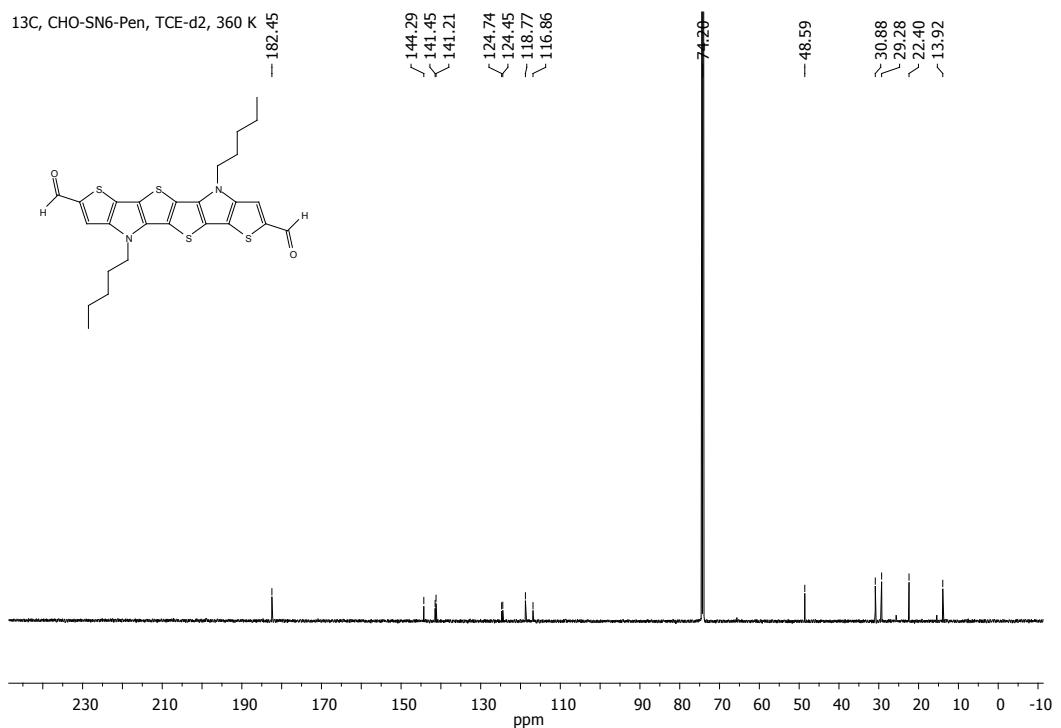


Figure 16. ^{13}C -NMR spectrum of CHO-SN6-Pen 14 in $[\text{D}2]\text{TCE}$ (125 MHz).

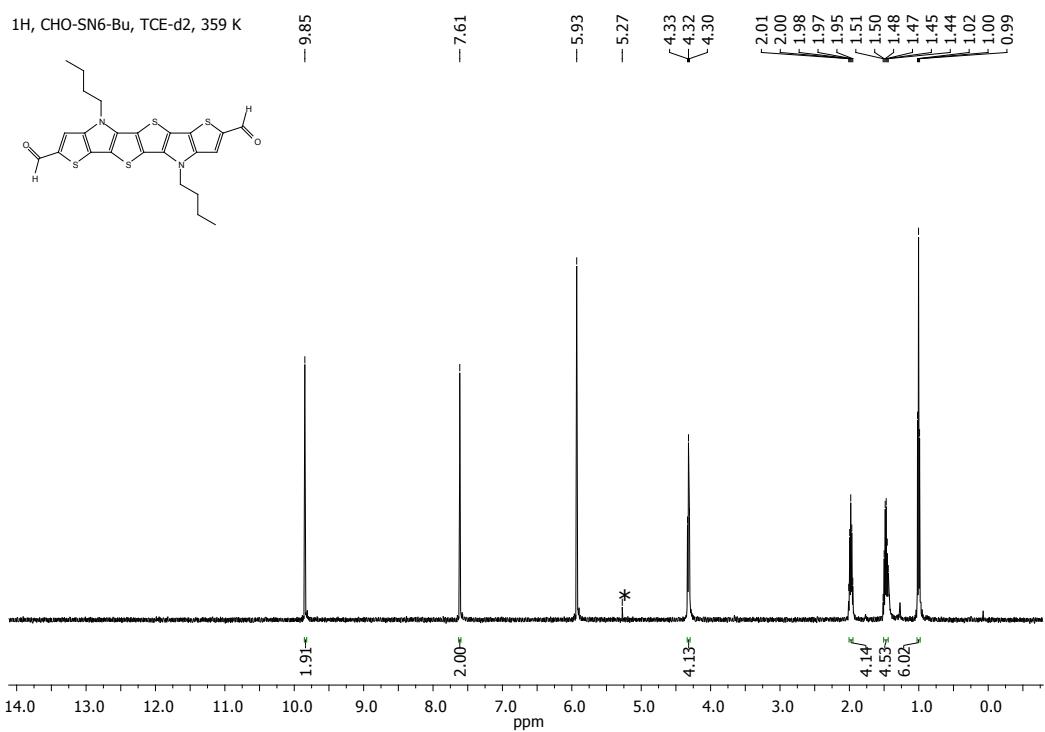


Figure 17. ^1H -NMR spectrum of CHO-SN6-Bu 13 in $[\text{D}2]\text{TCE}$ (500 MHz); *solvent impurities.

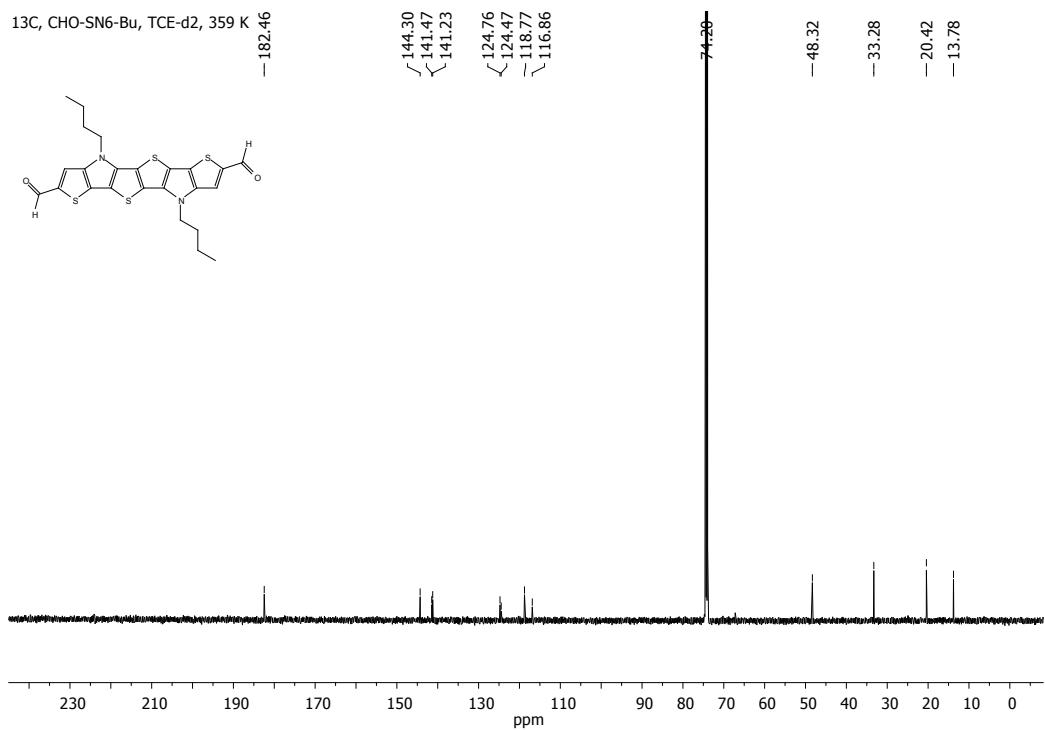


Figure 18. ^{13}C -NMR spectrum of CHO-SN6-Bu 13 in $[\text{D}2]\text{TCE}$ (125 MHz).

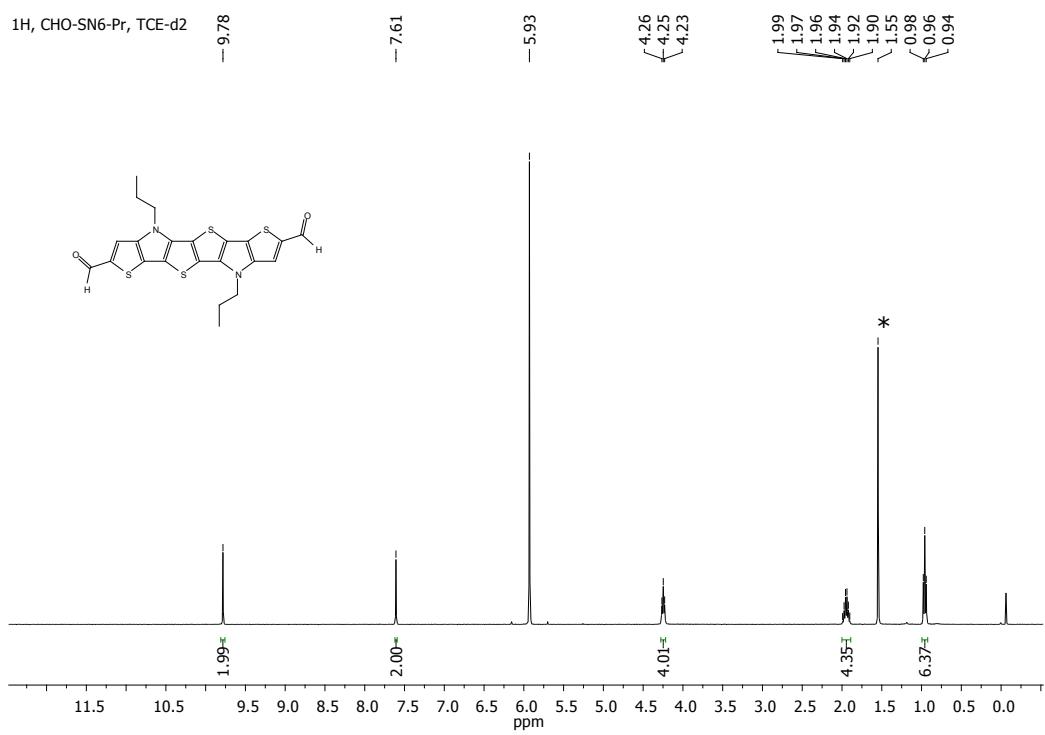


Figure 19. ^1H -NMR spectrum of CHO-SN6-Pr 12 in [D₂]TCE (400 MHz); *solvent impurities.

¹H-NMR spectra of DCV end-capped SN6 derivatives 1-5:

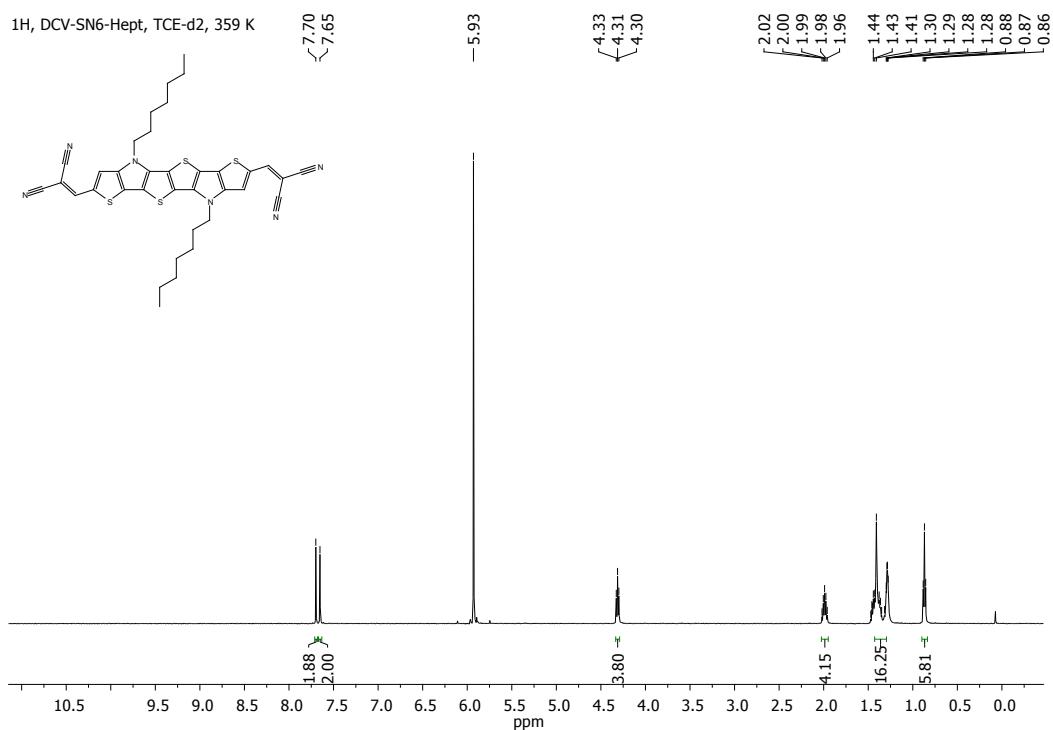


Figure 20. ¹H-NMR spectrum of DCV-SN6-Hept 5 in [D2]TCE (500 MHz).

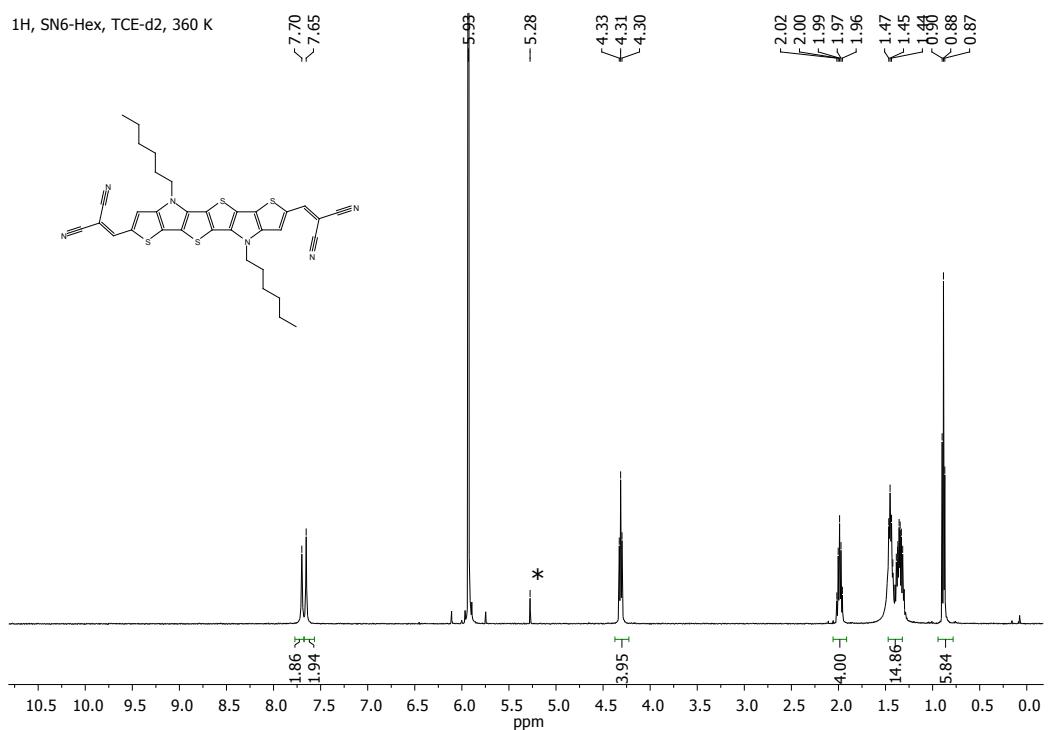


Figure 21. ¹H-NMR spectrum of DCV-SN6-Hex 4 in [D2]TCE (500 MHz); *solvent impurities.

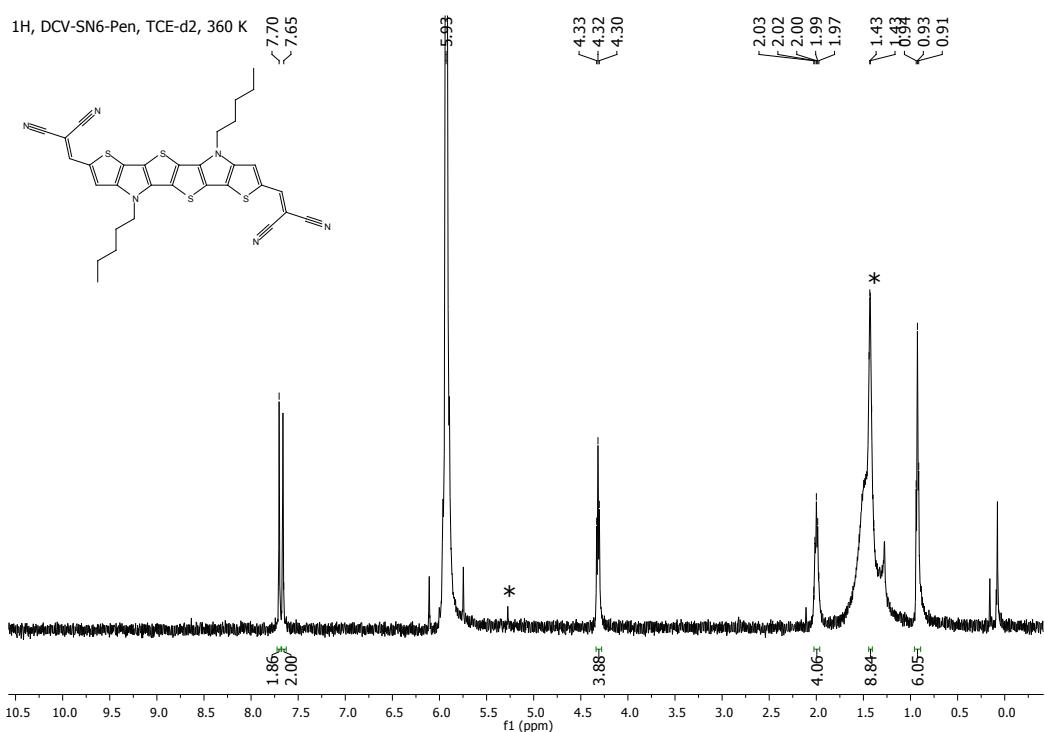


Figure 22. ^1H -NMR spectrum of DCV-SN6-Pen 3 in $[\text{D}2]\text{TCE}$ (500 MHz); *solvent impurities.

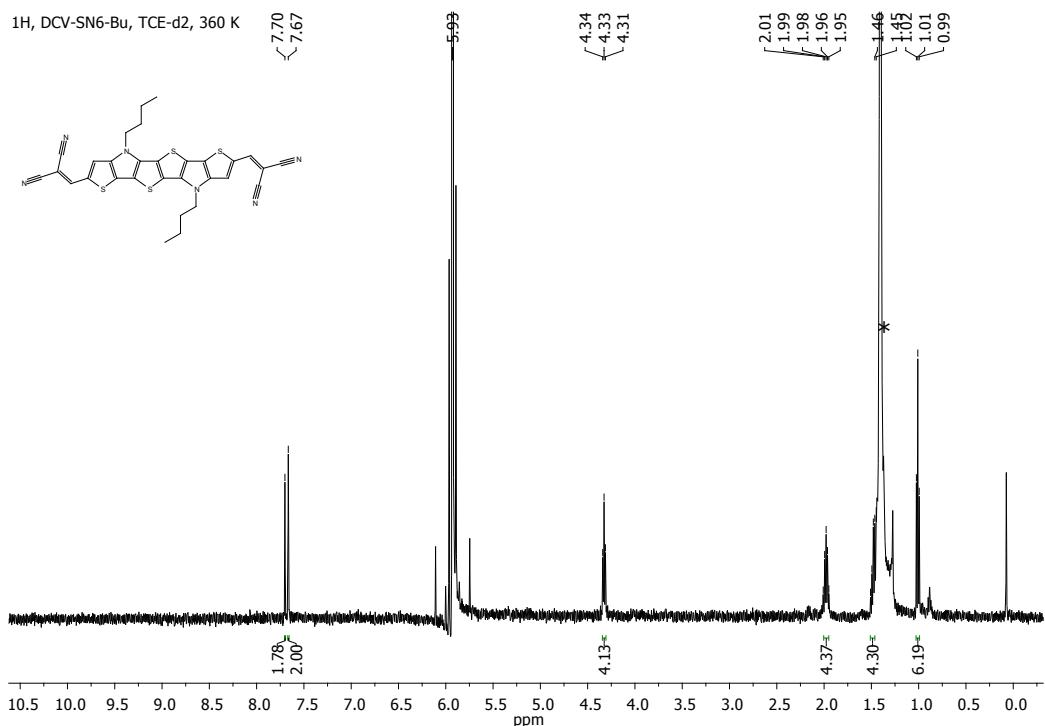


Figure 23. ^1H -NMR spectrum of DCV-SN6-Bu 2 in $[\text{D}2]\text{TCE}$ (500 MHz); *solvent impurities.