Supporting Information

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Optimization of Kumada cross-coupling reactions of tri- and tetra- bromothiophenes and symmetrical di-bromo-2, 2' bithiophene with cyclohexylmagnesium bromide: Synthesis, DFT studies and nonlinear optical analysis

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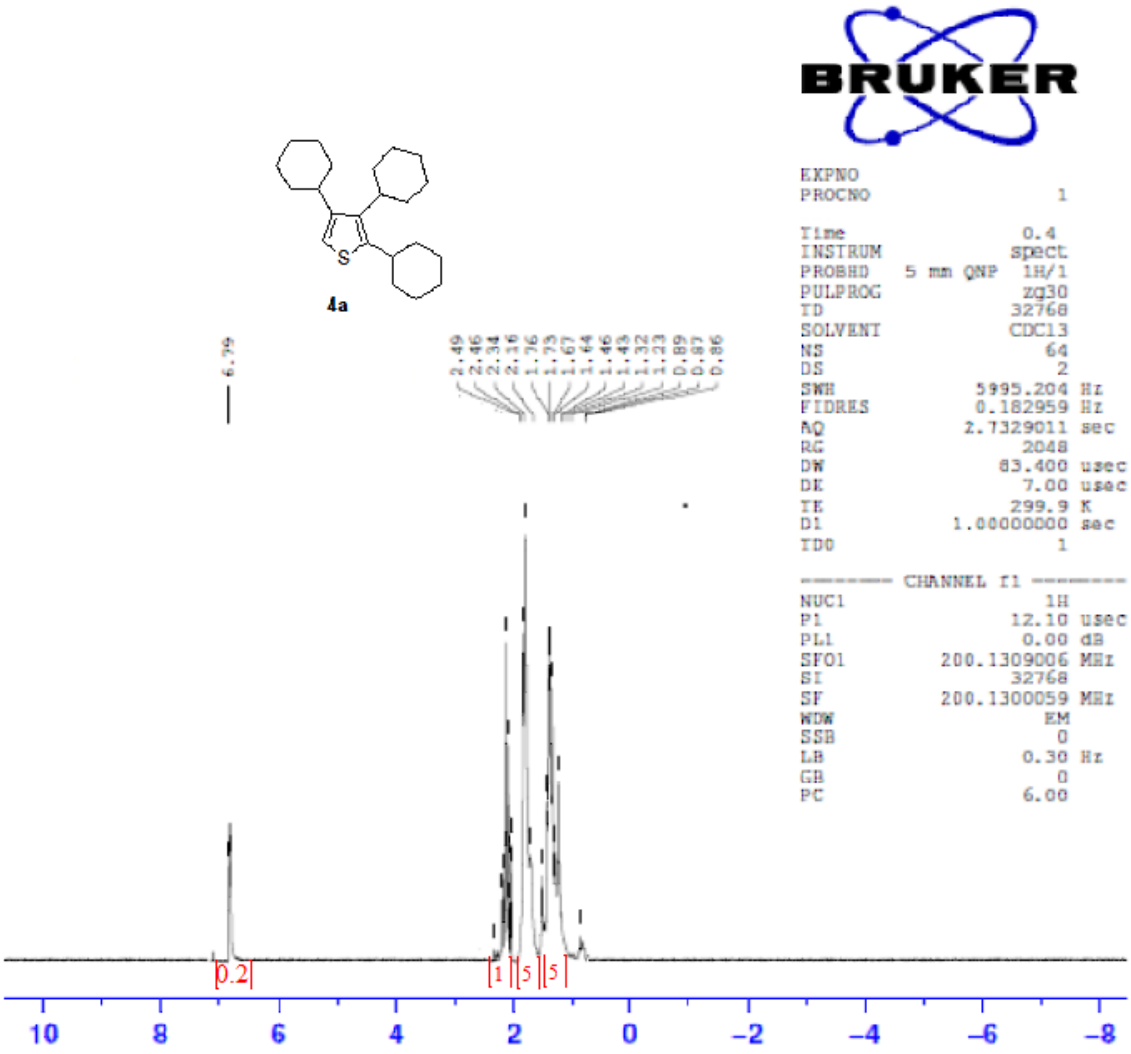

Figure S1: ^{1}H-NMR ($CDCl_3$, 200.13 MHz) Spectrum of **4a**

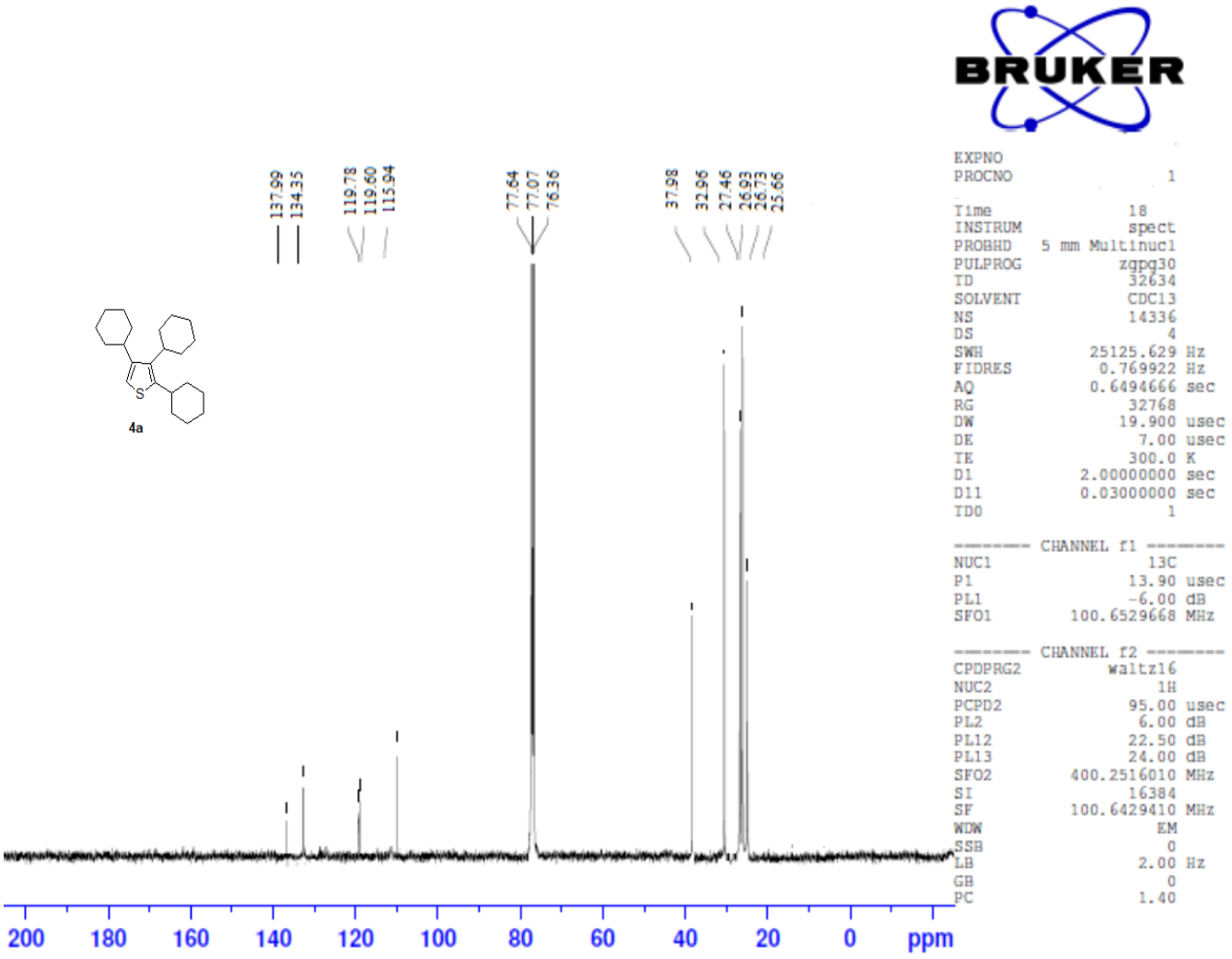

Figure S2: ^{13}C-NMR (CDCl3, 50.32 MHz) Spectrum of **4a**

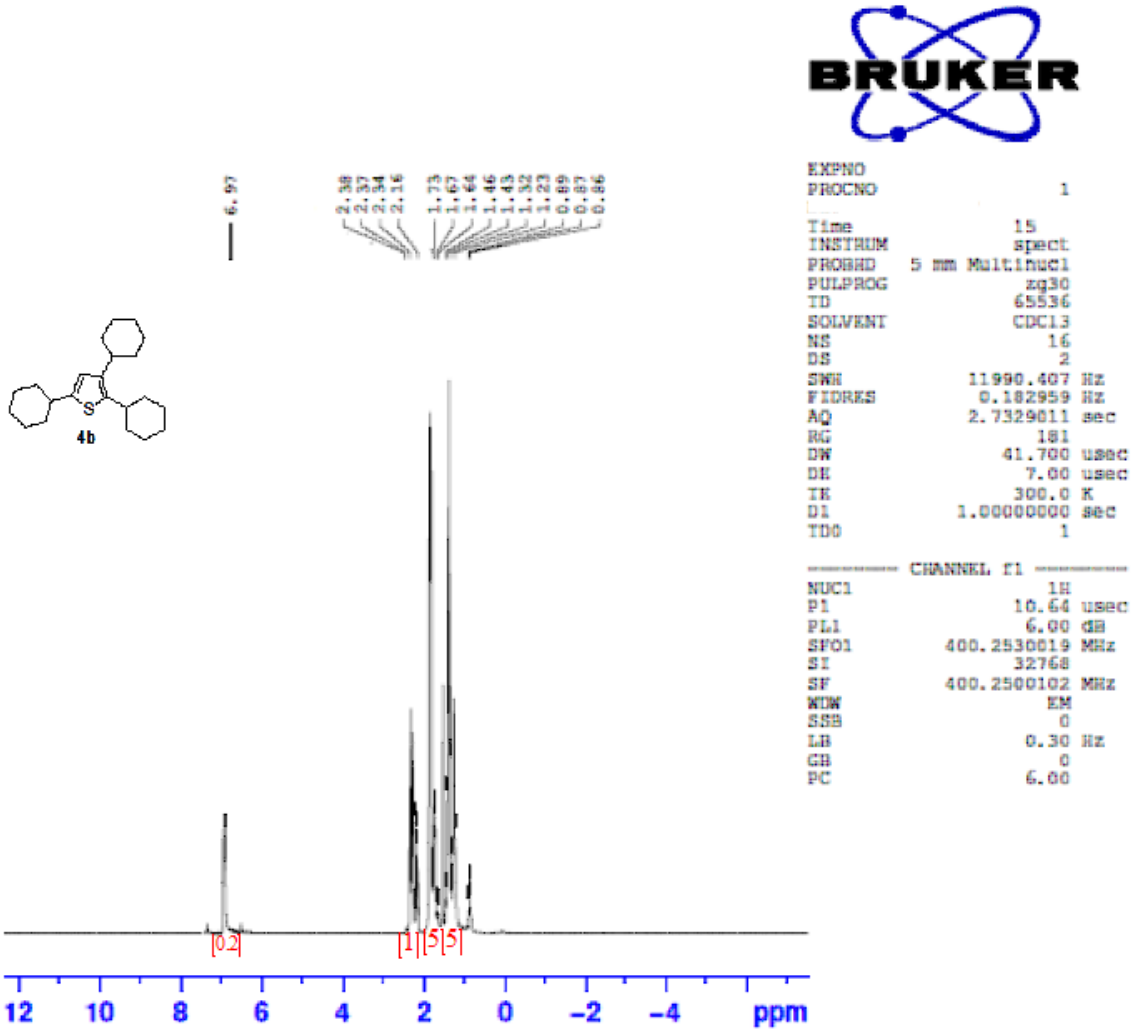

Figure S3: ^{1}H-NMR ($CDCl_3$, 200.13 MHz) Spectrum of **4b**

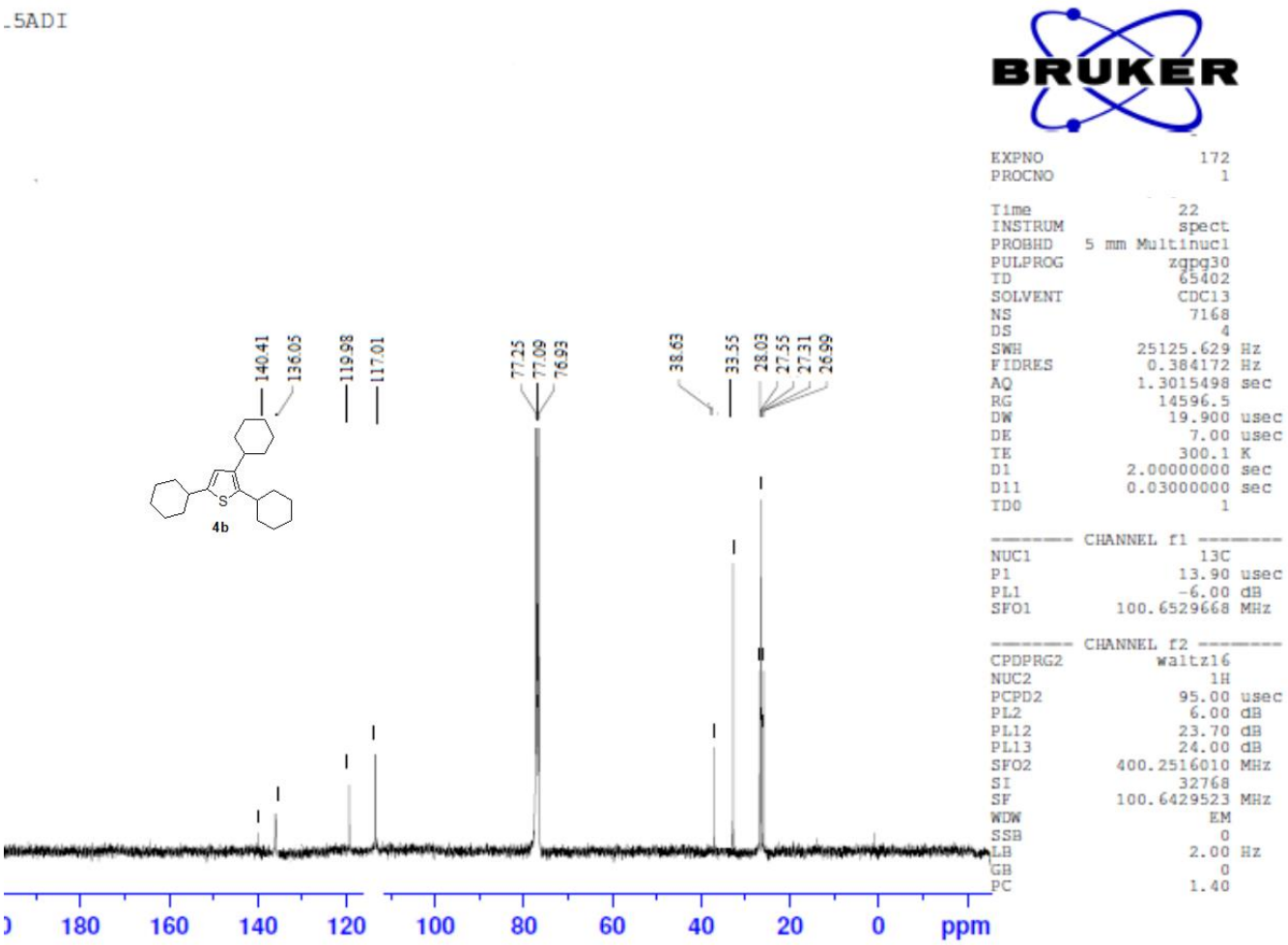

Figure S4: ^{13}C-NMR (CDCl3, 50.32 MHz) Spectrum of **4b**

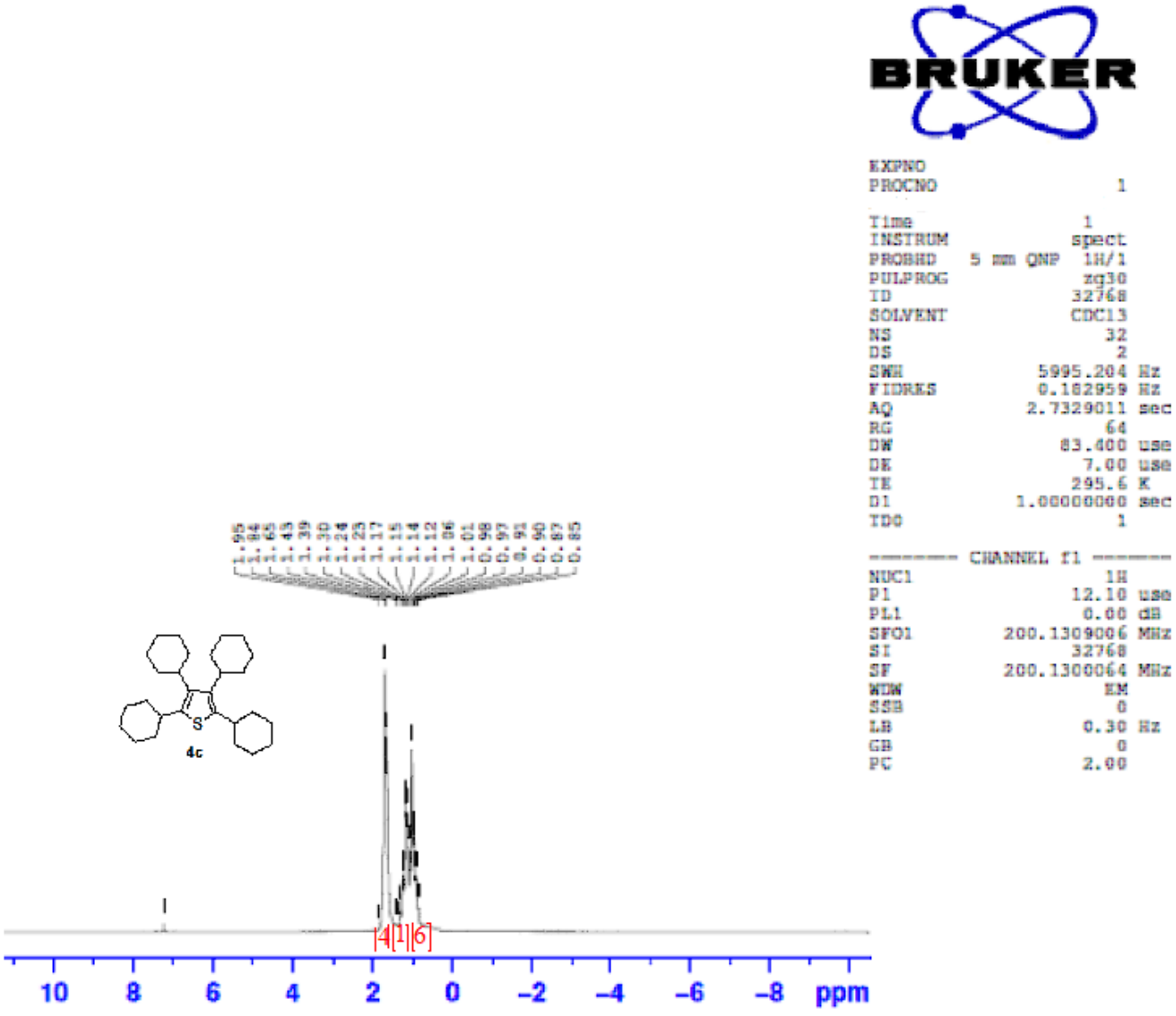

Figure S5: ^{1}H-NMR ($CDCl_3$, 200.13 MHz) Spectrum of **4c**

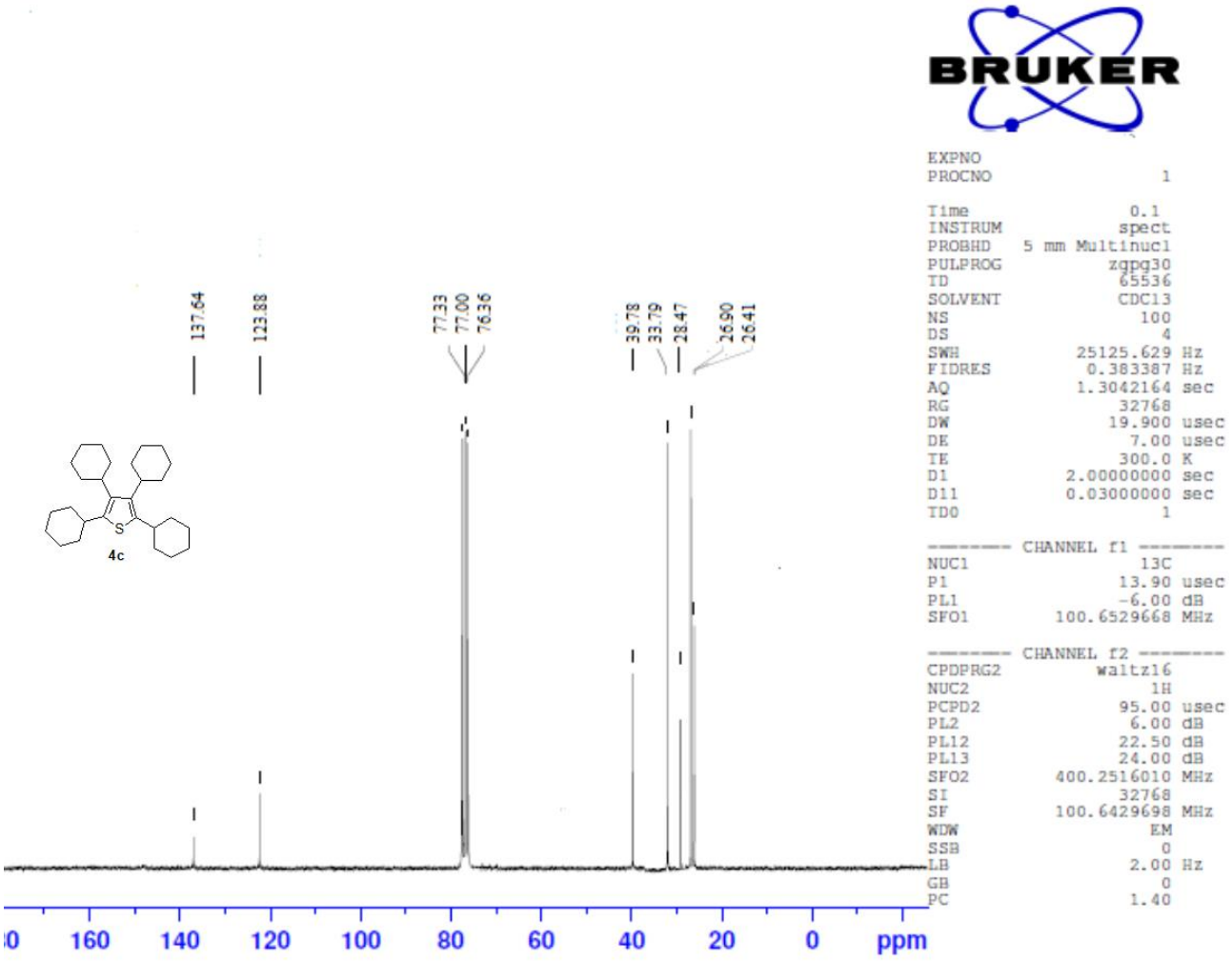

Figure S6: ^{13}C-NMR (CDCl3, 50.32 MHz) Spectrum of **4c**

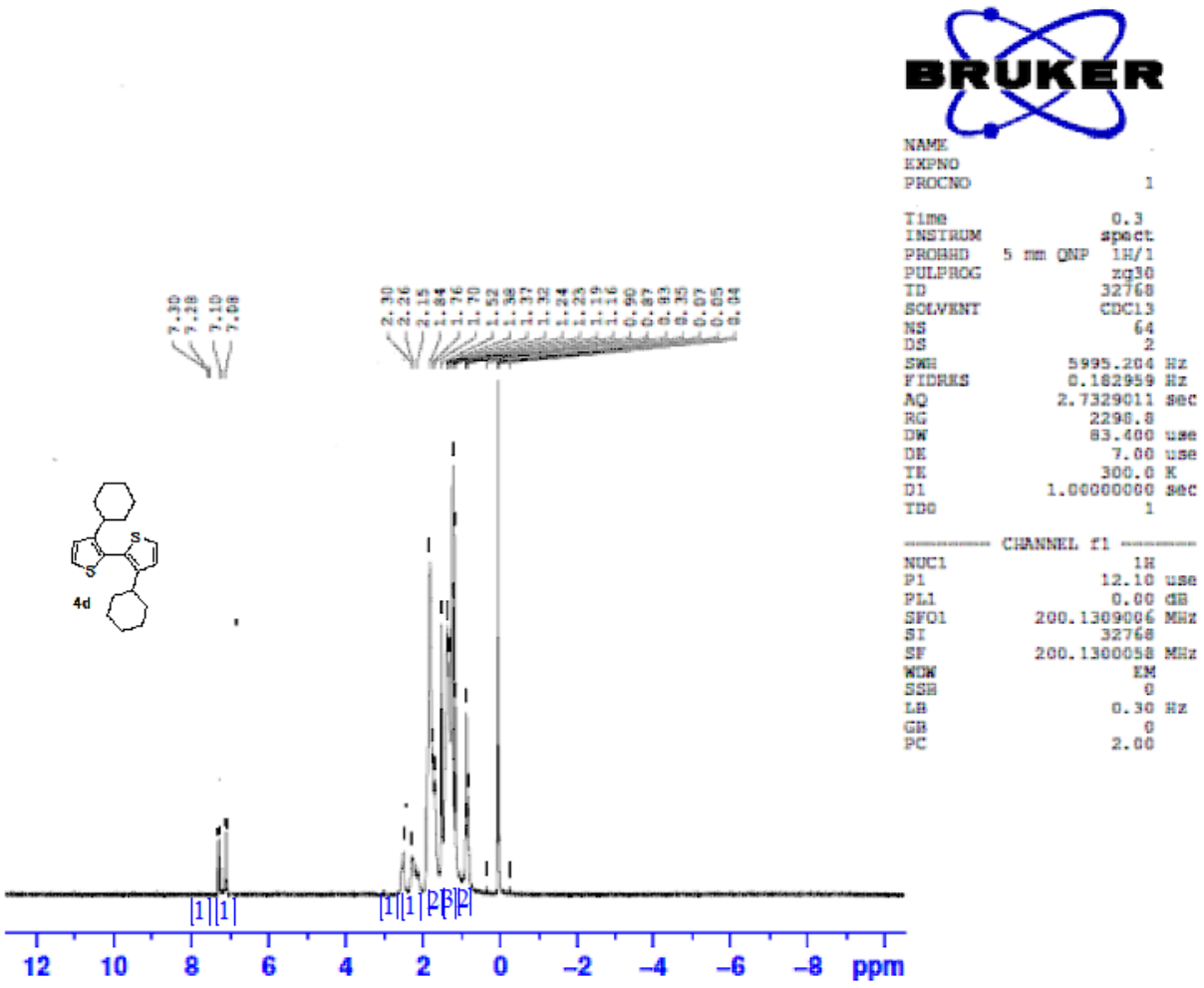

Figure S7: ^{1}H-NMR ($CDCl_3$, 200.13 MHz) Spectrum of **4d**

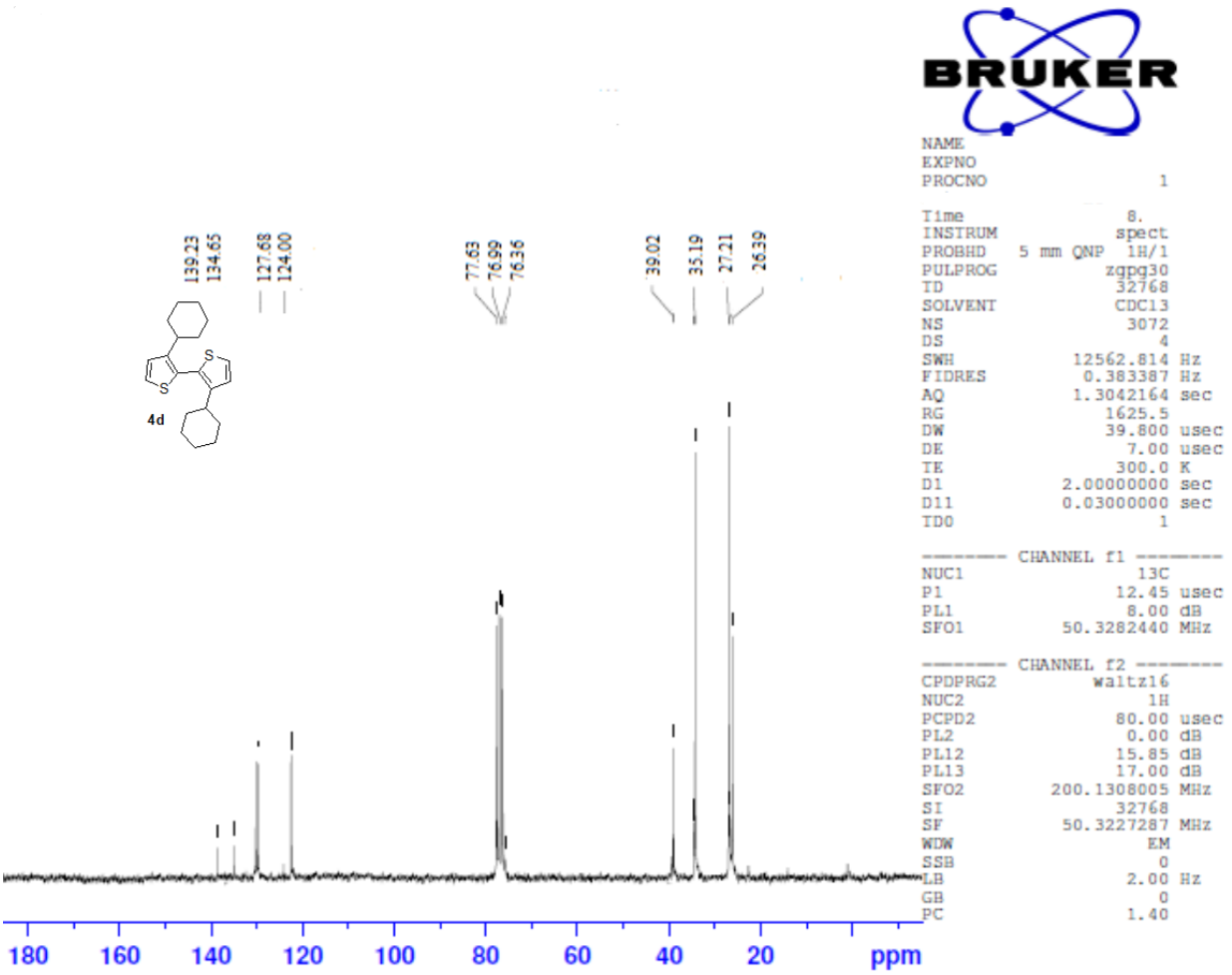

Figure S8: ^{13}C-NMR ($CDCl_3$, 50.32 MHz) Spectrum of **4d**

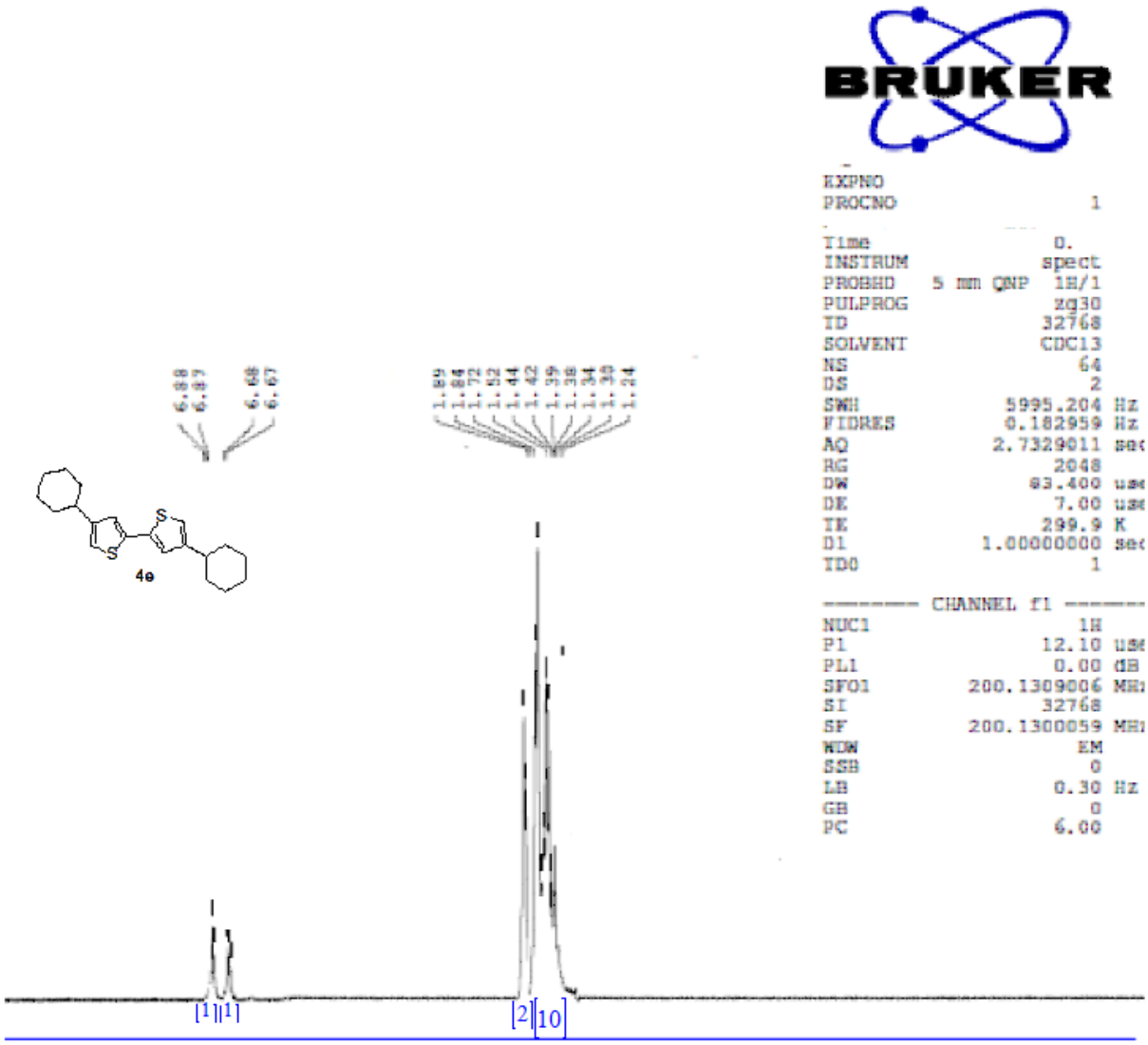

Figure S9: ^{1}H-NMR ($CDCl_3$, 200.13 MHz) Spectrum of **4e**

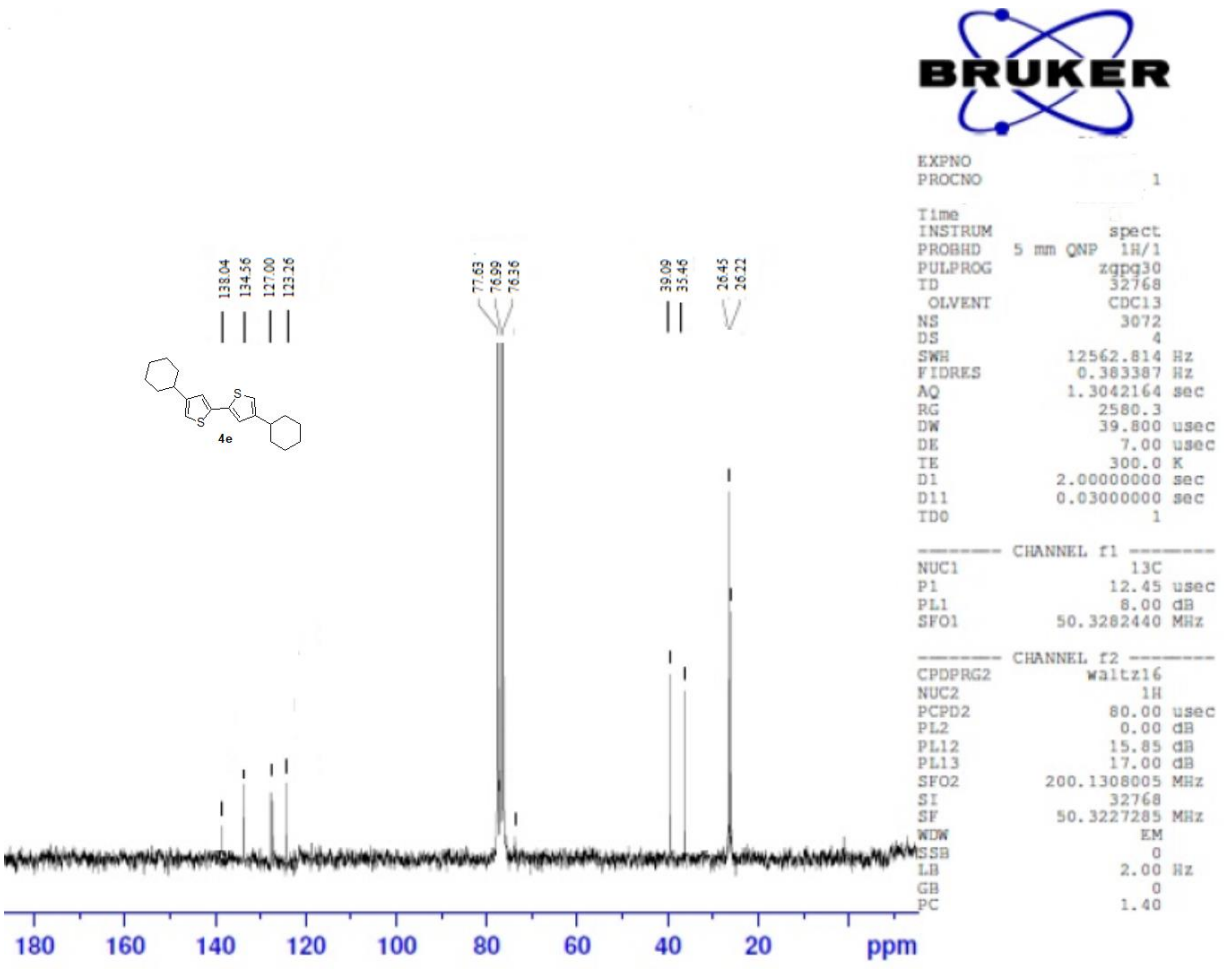

Figure S10: ^{13}C-NMR ($CDCl_3$, 50.32 MHz) Spectrum of **4e**

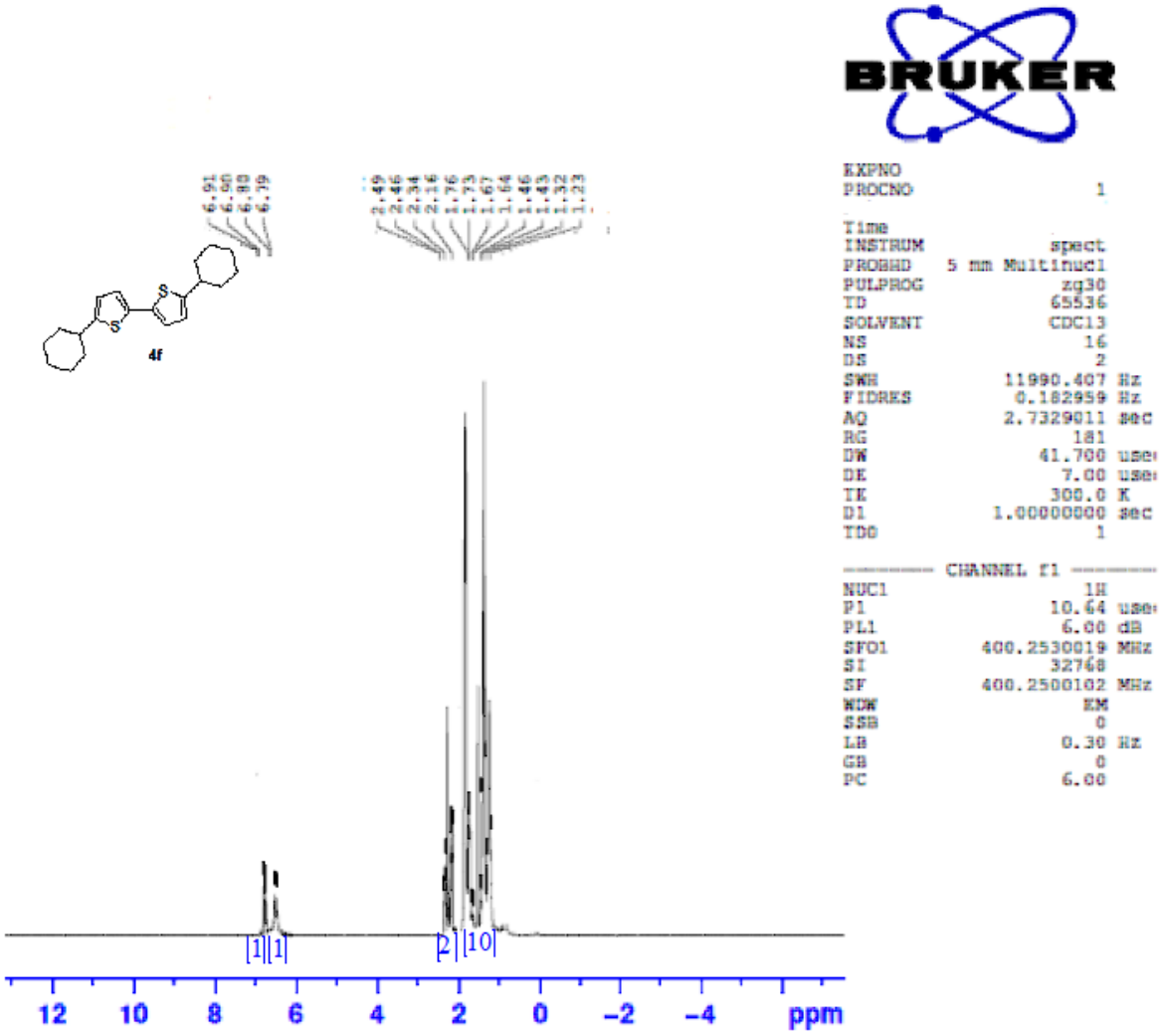

Figure S11: ^{1}H-NMR ($CDCl_3$, 200.13 MHz) Spectrum of **4f**

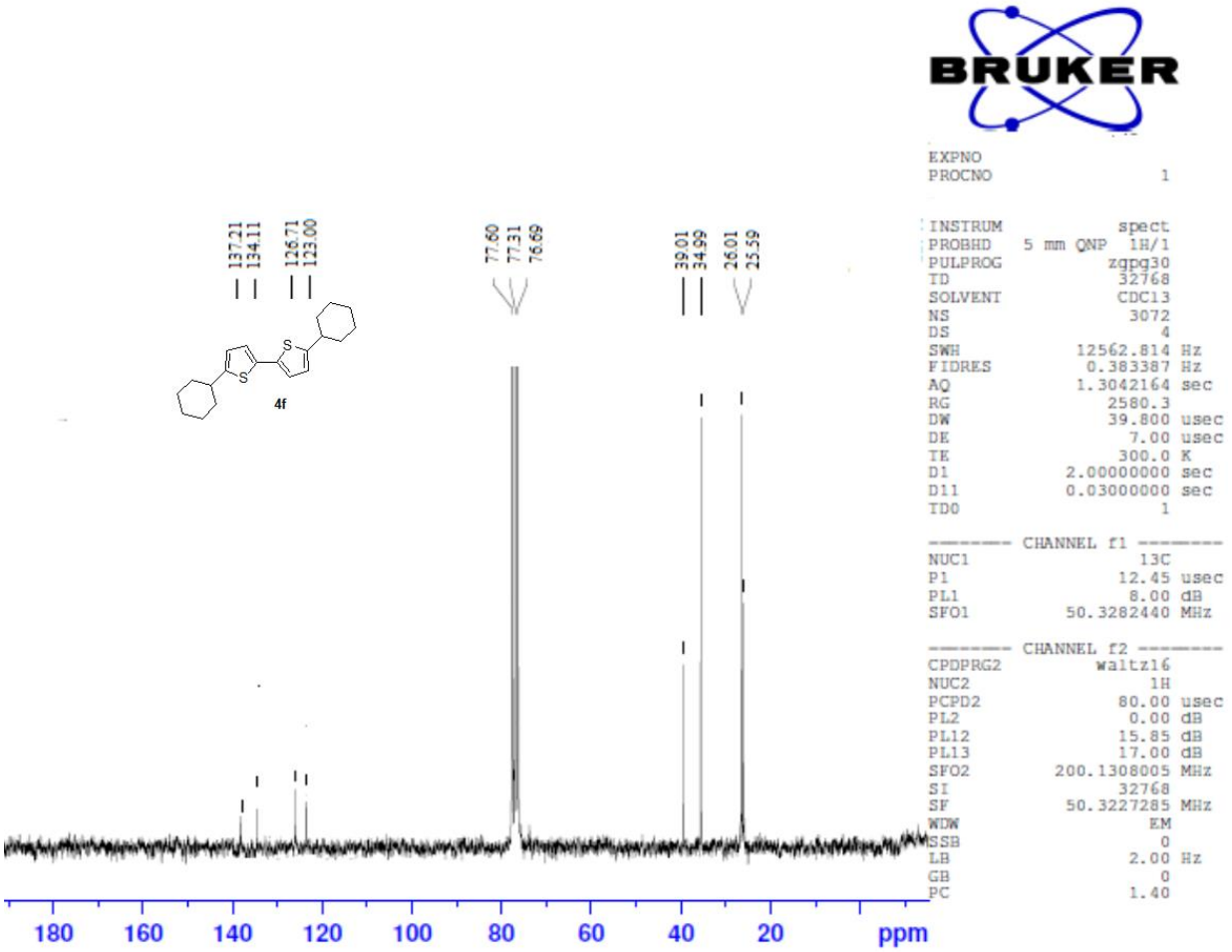

Figure S12: ^{13}C-NMR ($CDCl_3$, 50.32 MHz) Spectrum of **4f**

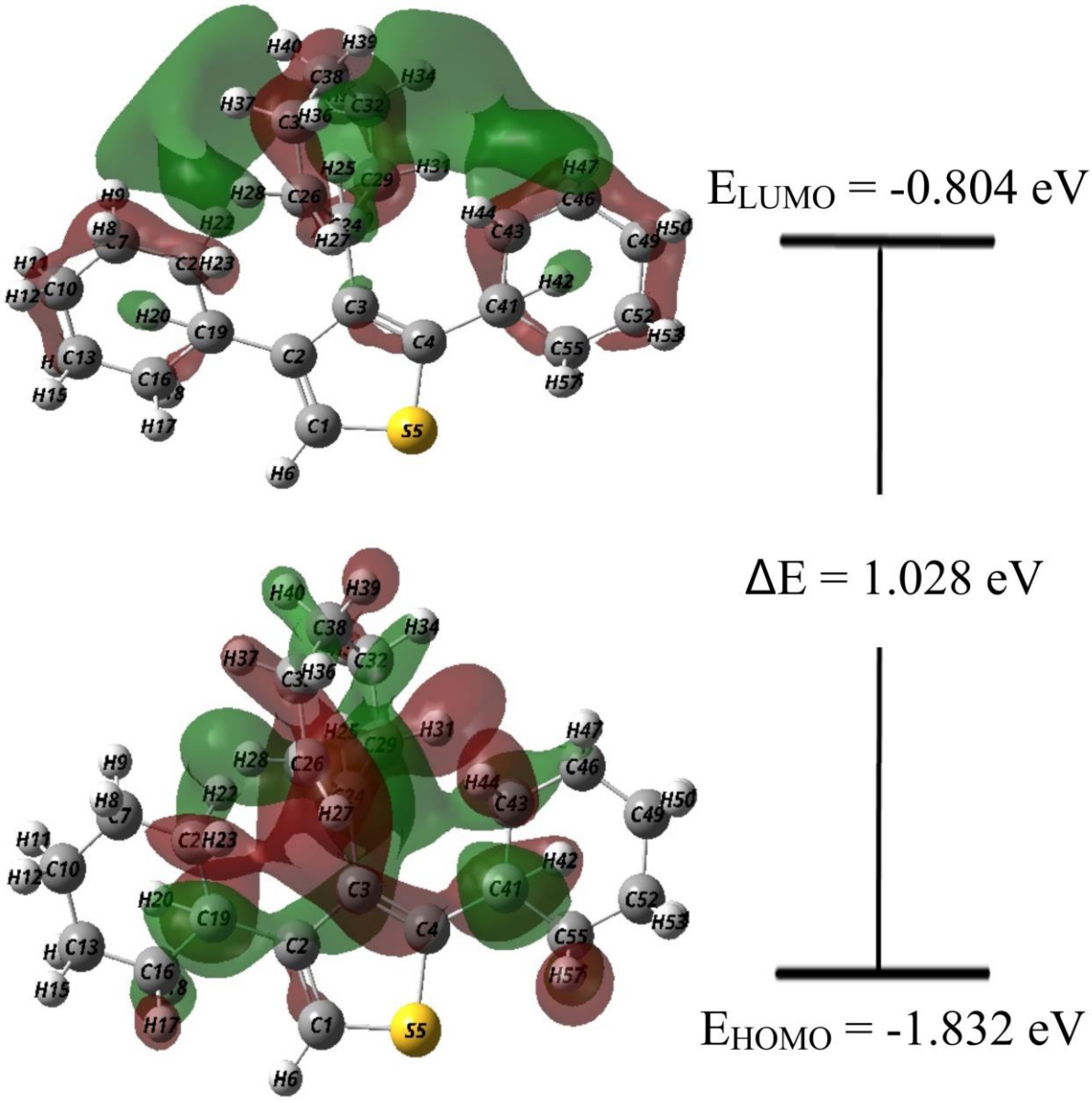

Figure S13 : HOMO-LUMO plot of 2,3,4-tricyclohexylthiophene **4a (isovalue = 0.02**

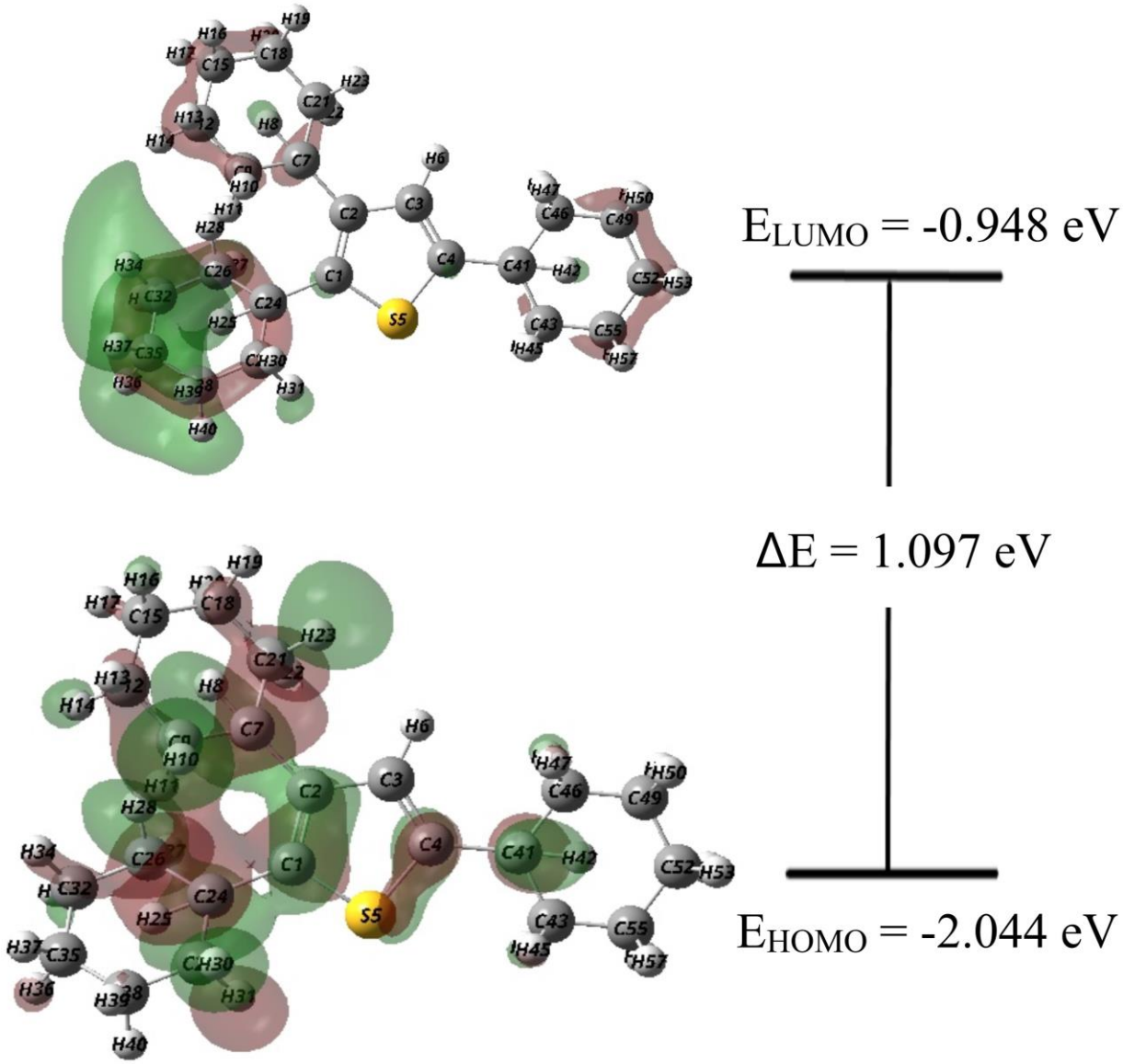

Figure S14 : HOMO-LUMO plot of 2,3,5-tricyclohexylthiophene **4b (isovalue = 0.02)**

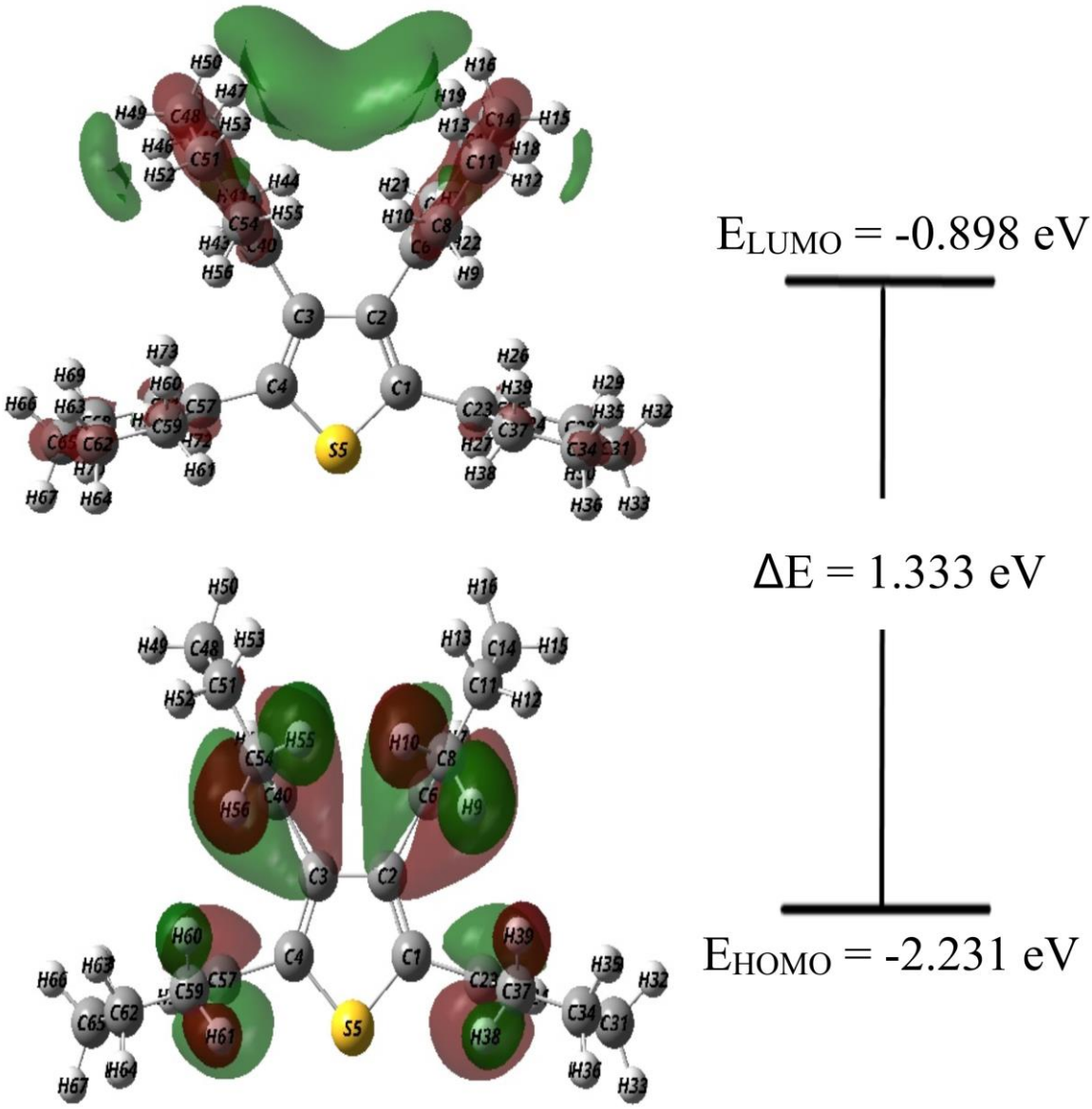

Figure S15 : HOMO-LUMO plot of 2,3,4,5-tetracyclohexylthiophene **4c (isovalue = 0.02)**

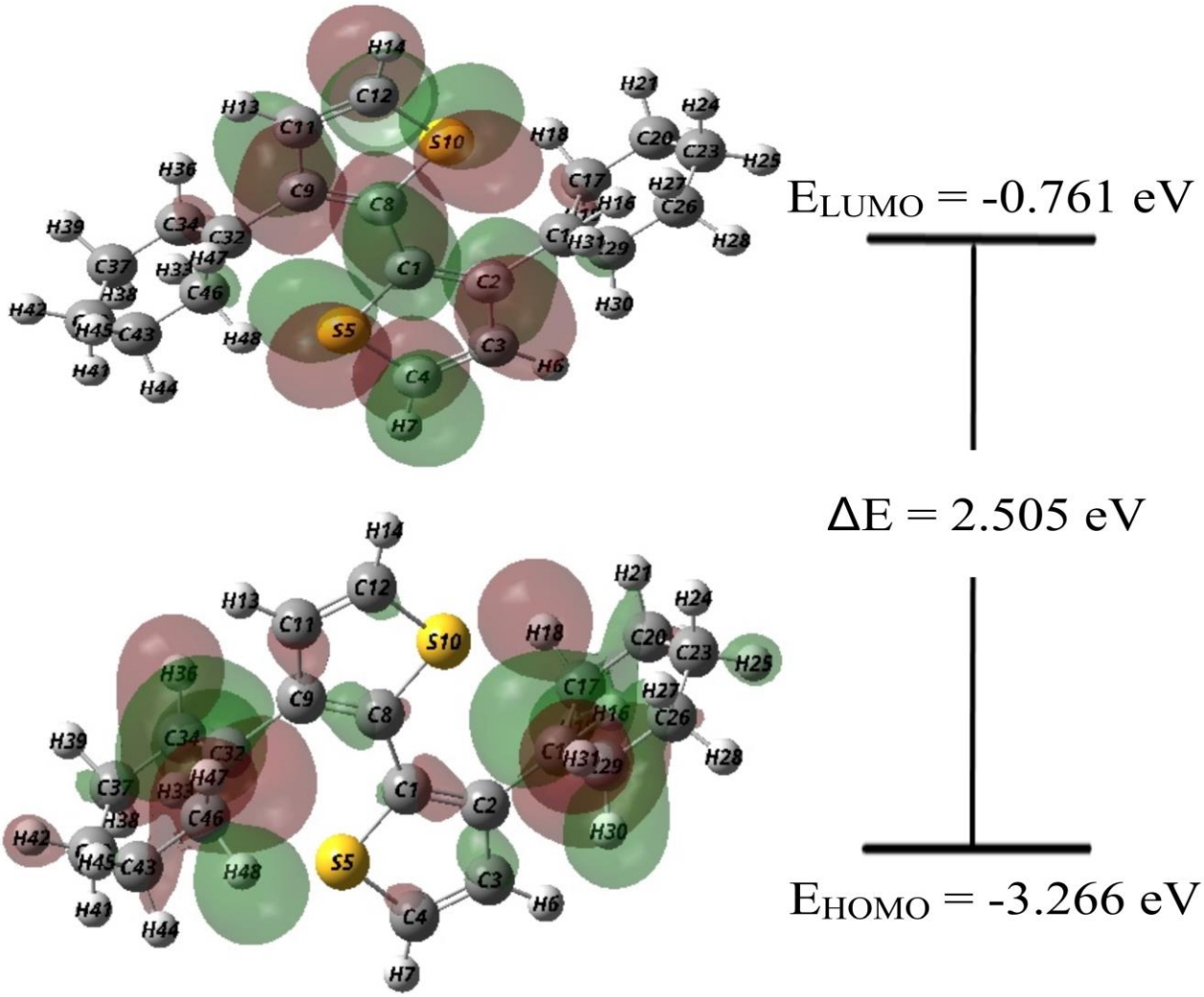

Figure S16 : HOMO-LUMO plot of 3,3'-dicyclohexyl-2,2'-bithiophene **4d (isovalue = 0.02)**

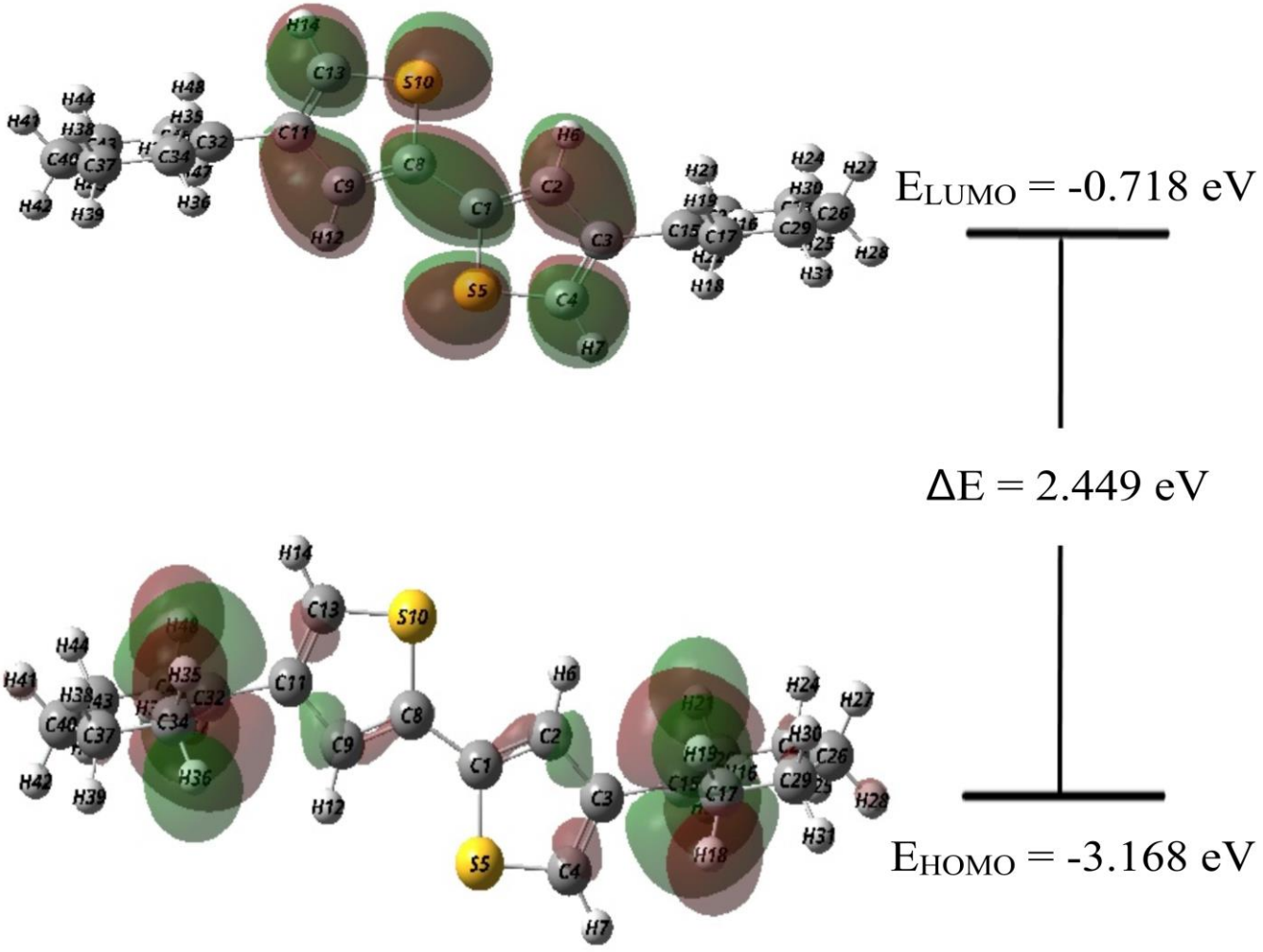

Figure S17 : HOMO-LUMO plot of 4,4'-dicyclohexyl-2,2'-bithiophene **4e (isovalue = 0.02**

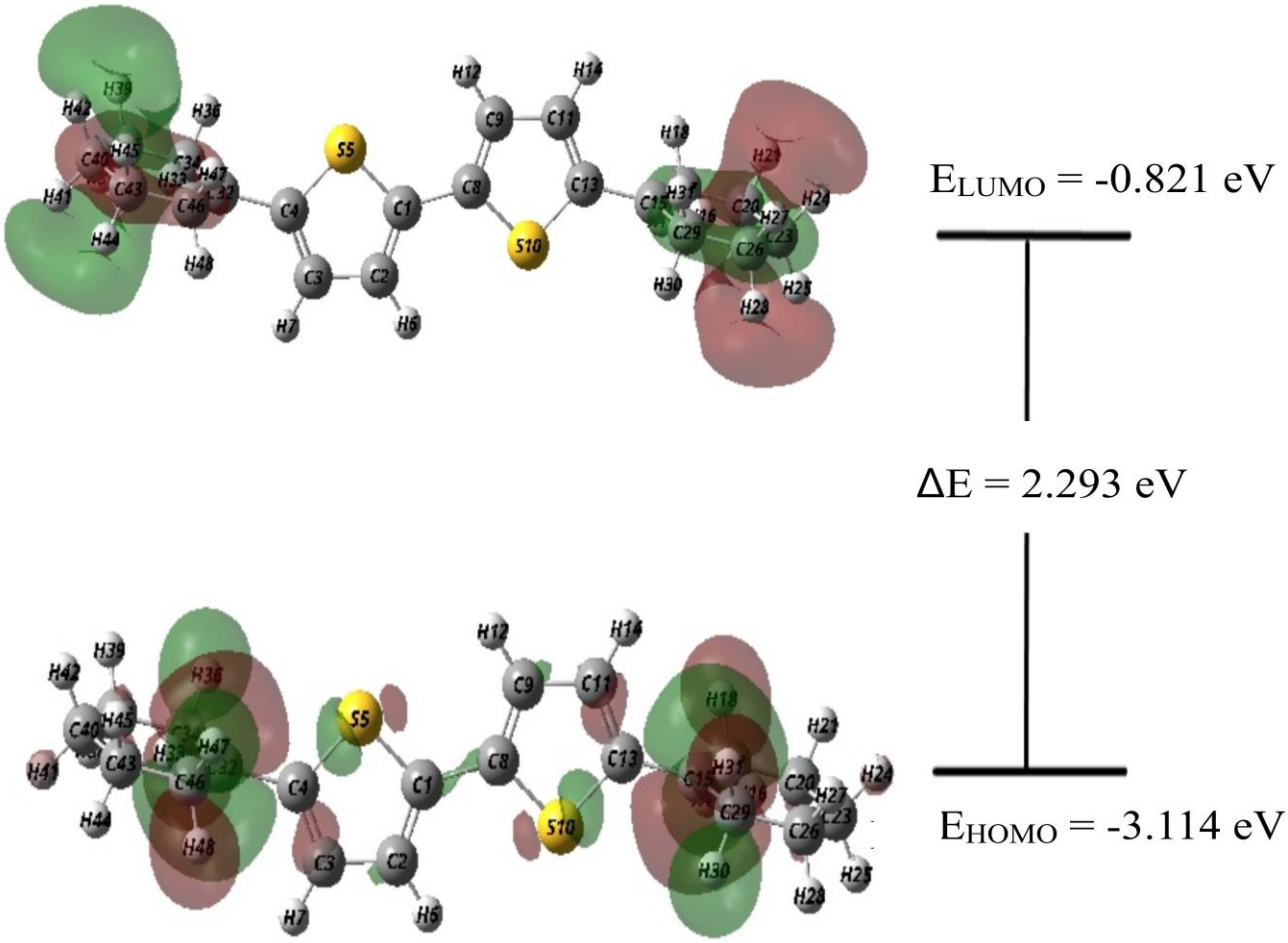

Figure S18 : HOMO-LUMO plot of 5,5'-dicyclohexyl-2,2'-bithiophene **4f (isovalue = 0.02)**

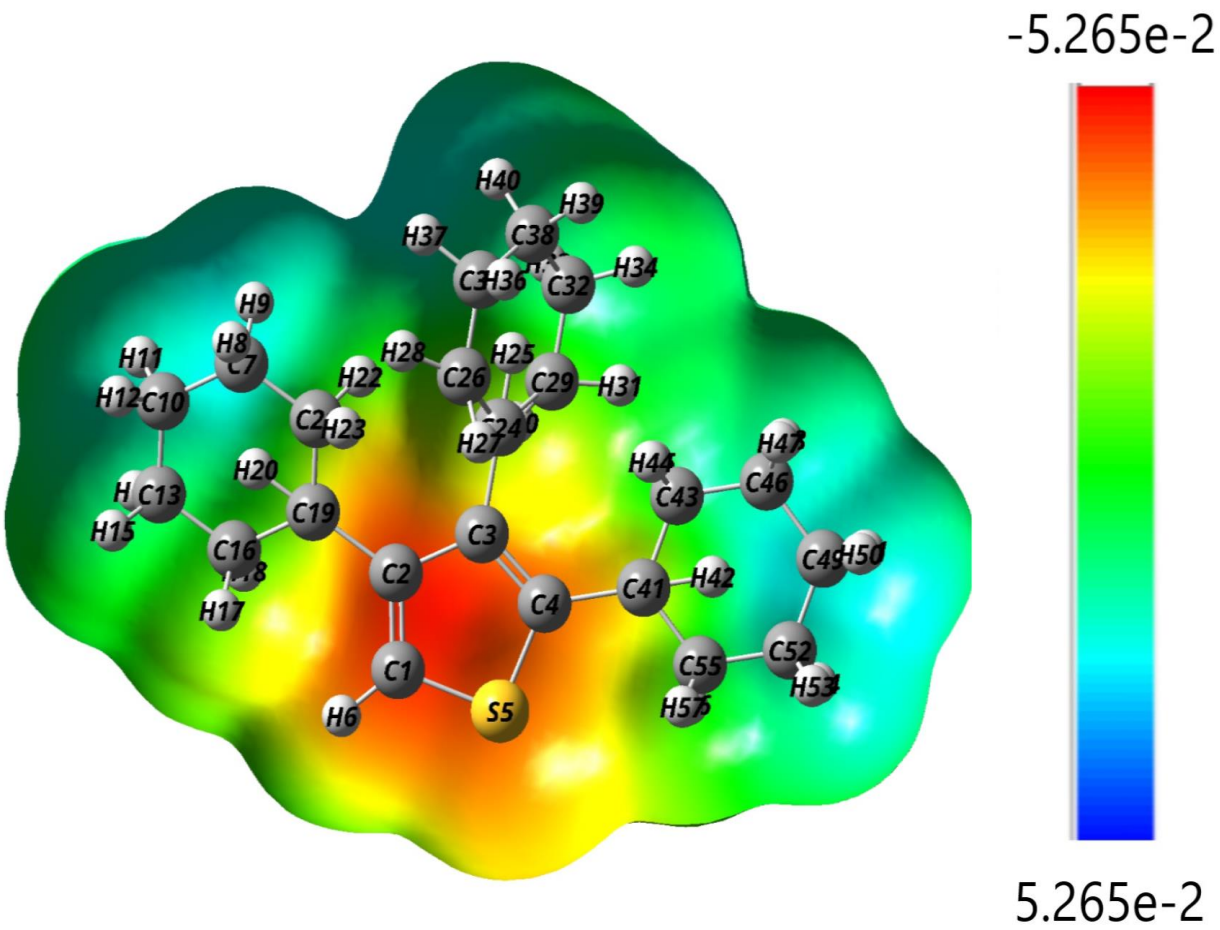

Figure S19 : MEP map of 2,3,4-tricyclohexylthiophene **4a (isovalue = 0.02)**

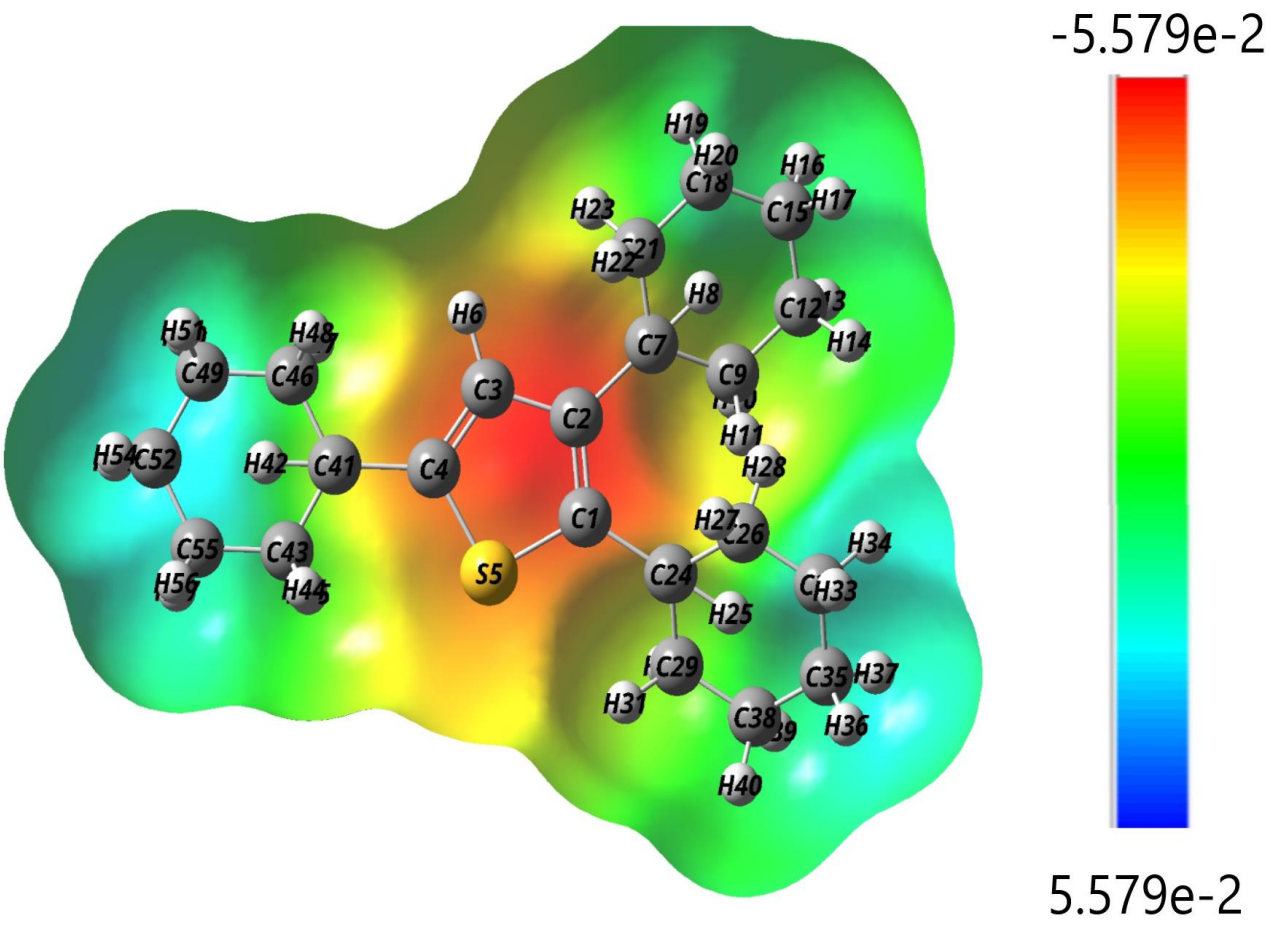

Figure S20 : MEP map of 2,3,5-tricyclohexylthiophene **4b (isovalue = 0.02)**

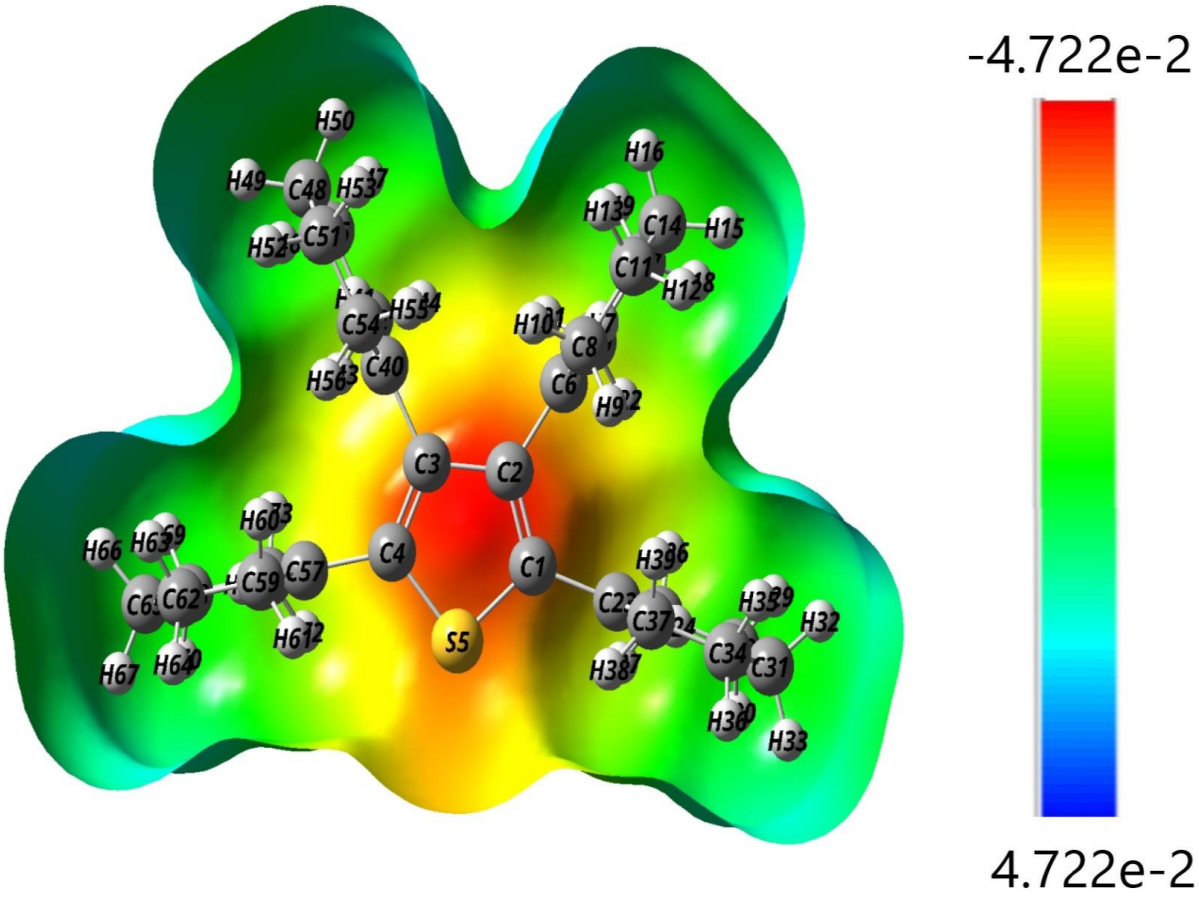

Figure S21 : MEP map of 2,3,4,5-tetracyclohexylthiophene **4c (isovalue = 0.02)**

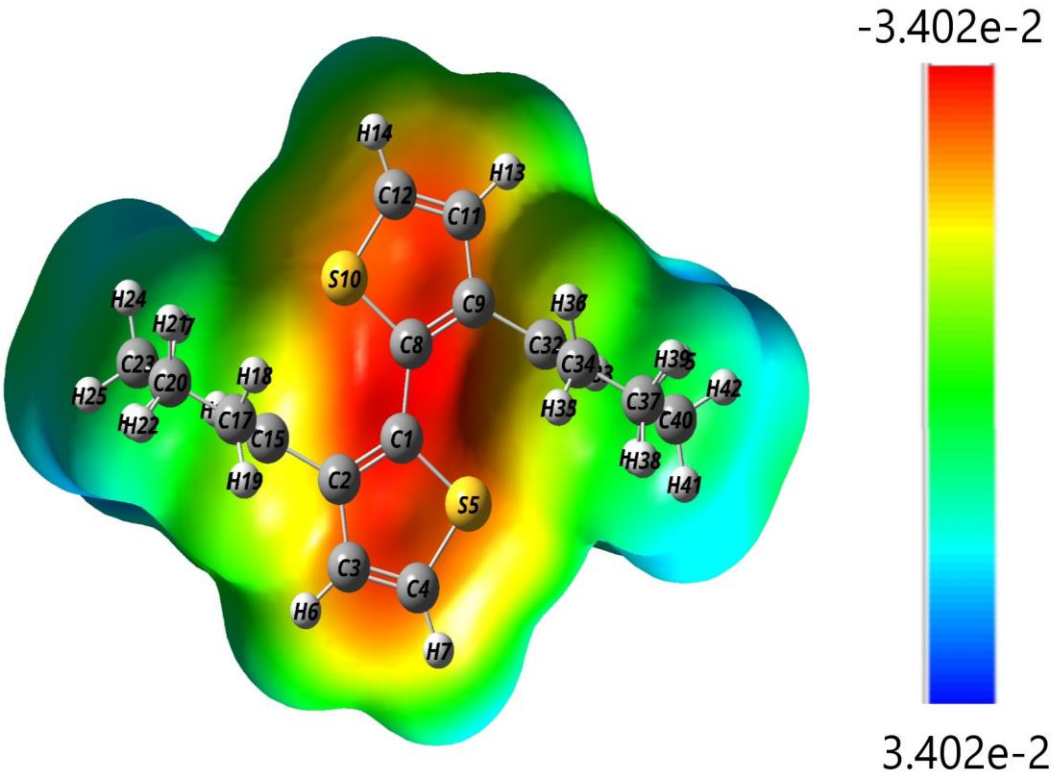

Figure S22 : MEP map of 3,3'-dicyclohexyl-2,2'-bithiophene **4d (isovalue = 0.02)**

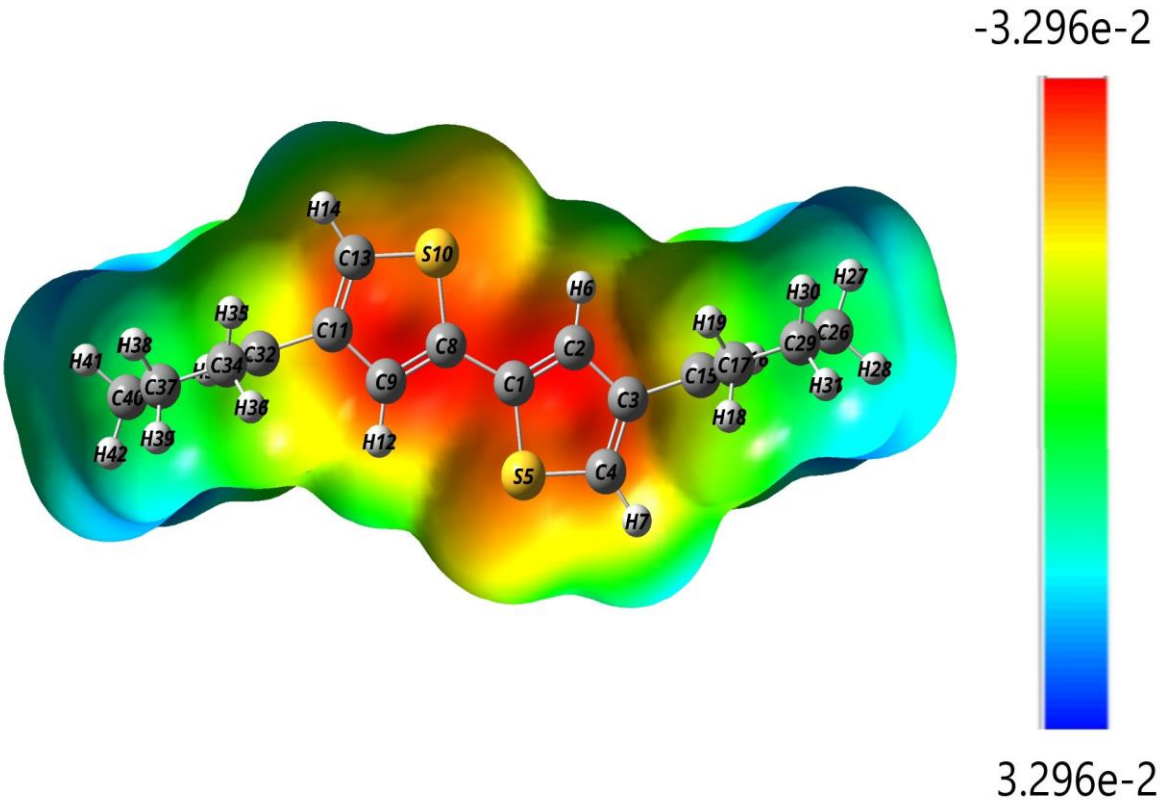

Figure S23 : MEP map of 4,4'-dicyclohexyl-2,2'-bithiophene **4e (isovalue = 0.02)**

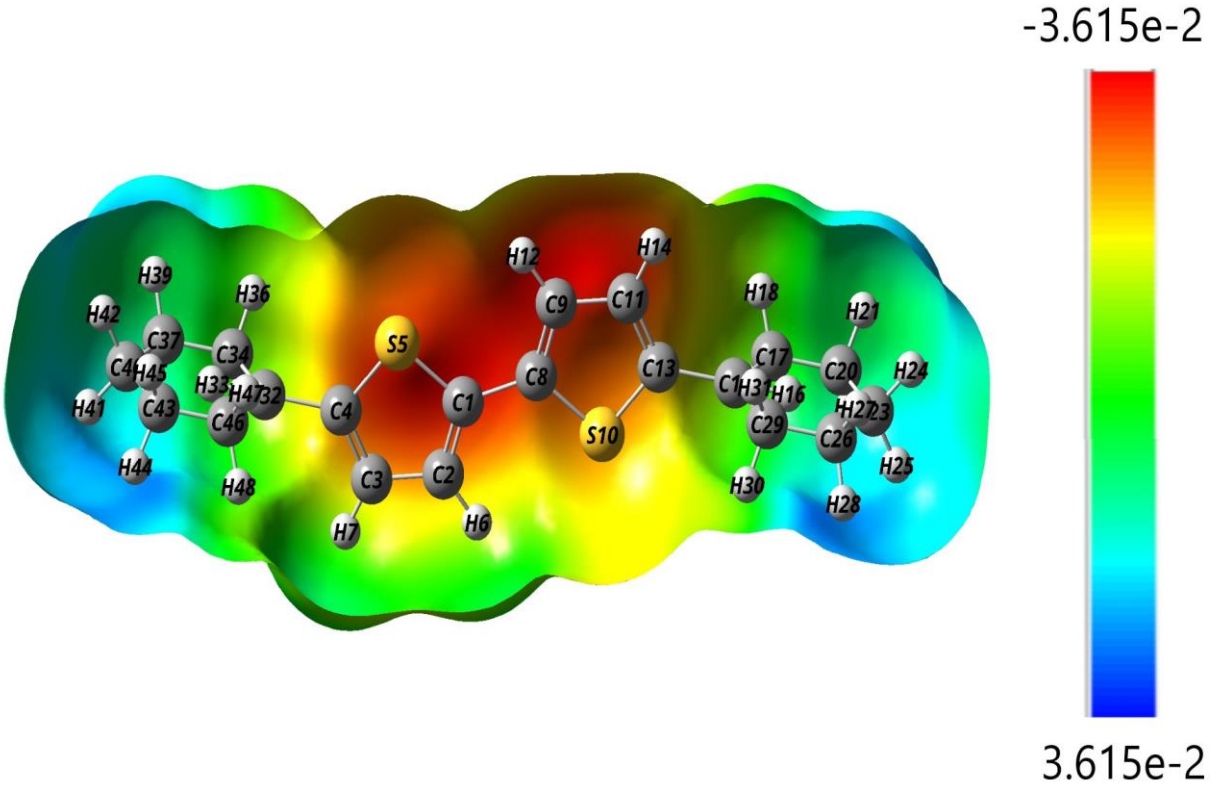

Figure S24 : MEP map of 5,5'-dicyclohexyl-2,2'-bithiophene **4f (isovalue = 0.02)**

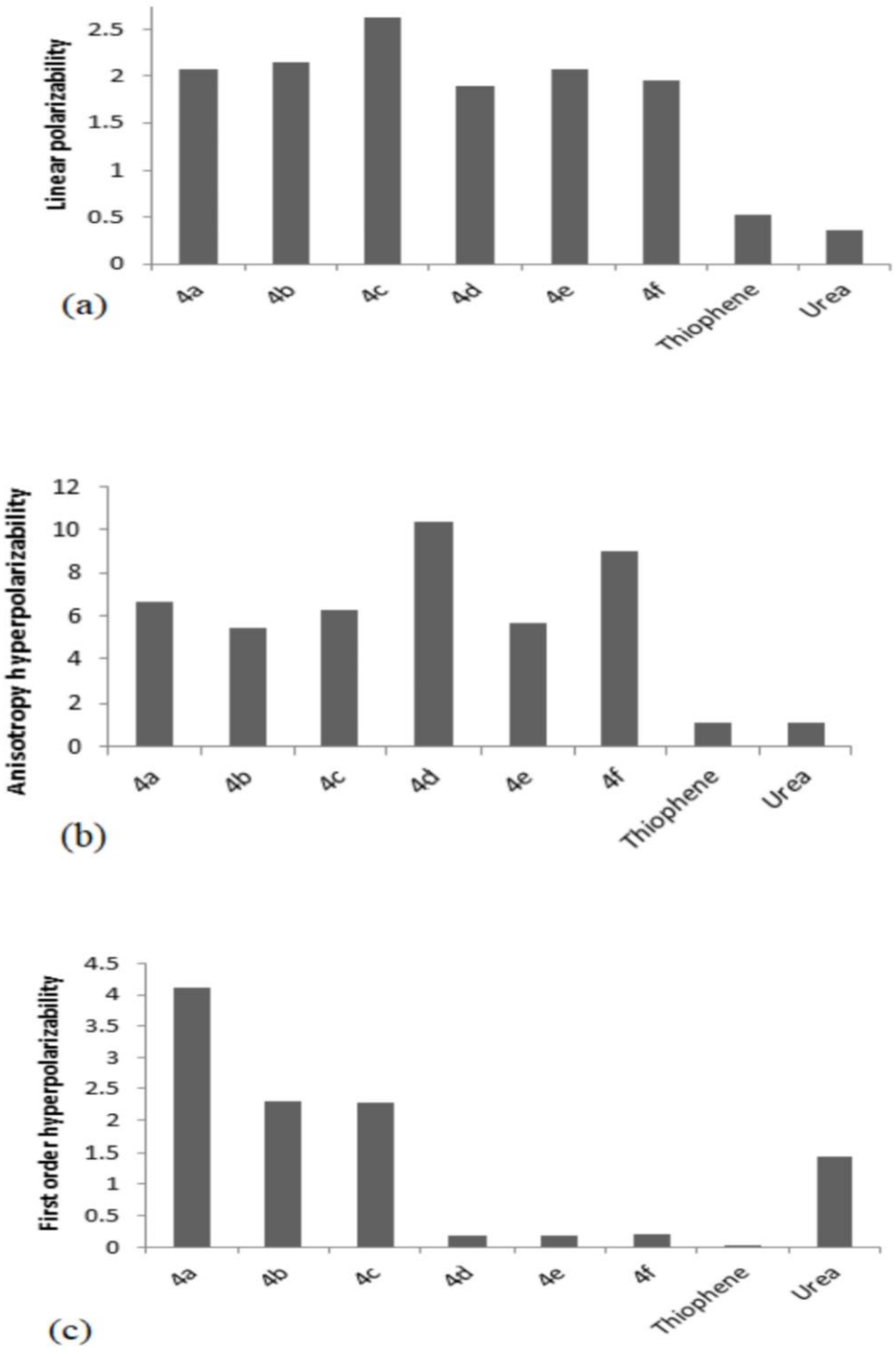

Figure S25: The polarizability α (esu), (a), the anisotropy of the hyperpolarizability Δα (esu), (b), the first order hyperpolarizability β (esu), (c), for the titled compounds 4a-f, thiophene and standard urea.