

Supporting Information

Thienopyrrolo[3,2,1-*jk*]carbazoles: Building Blocks for Functional Organic Materials.

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1. ^1H and ^{13}C NMR Spectra of the Products

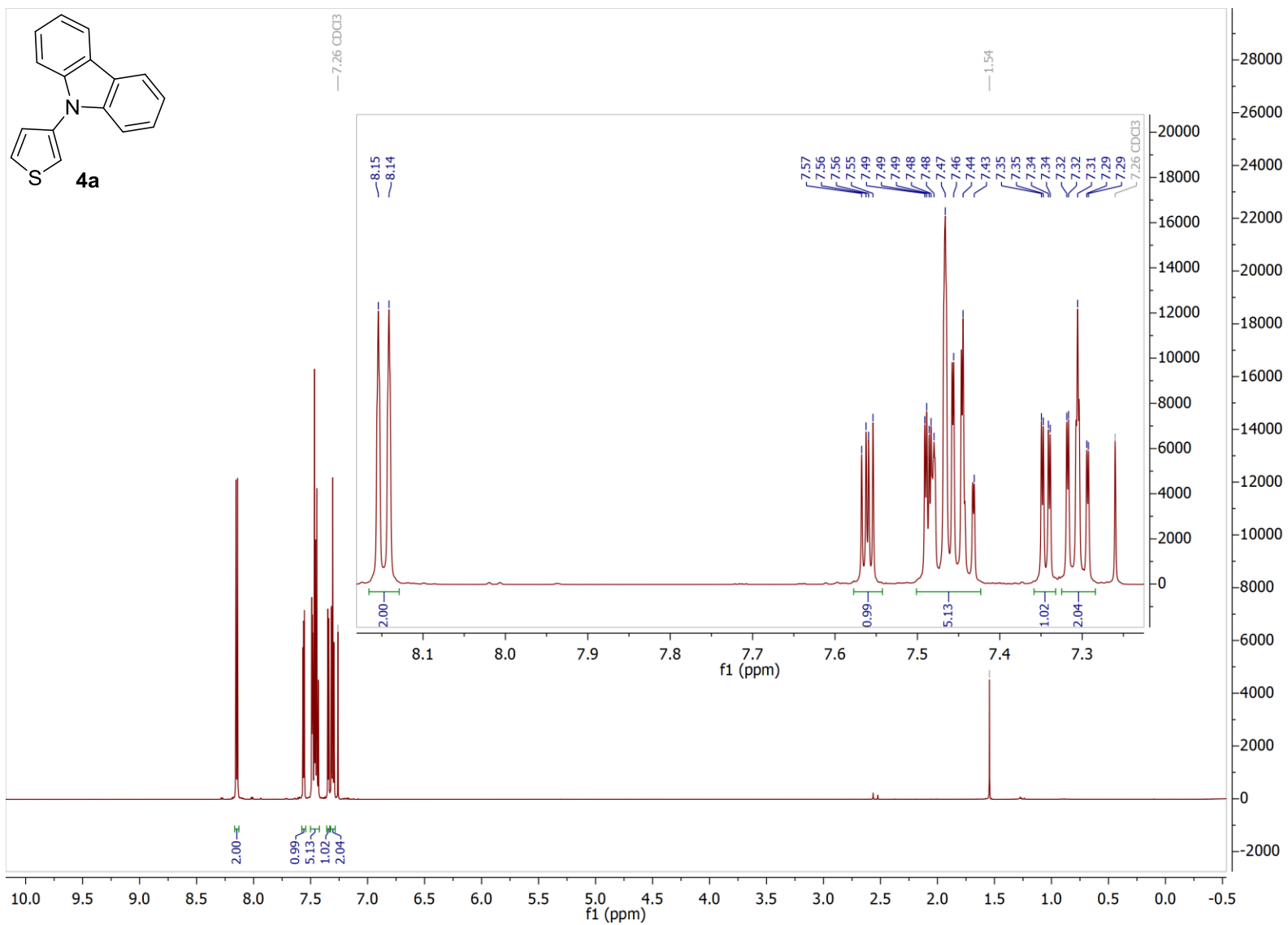


Figure S 1: ¹H NMR spectrum of 4a

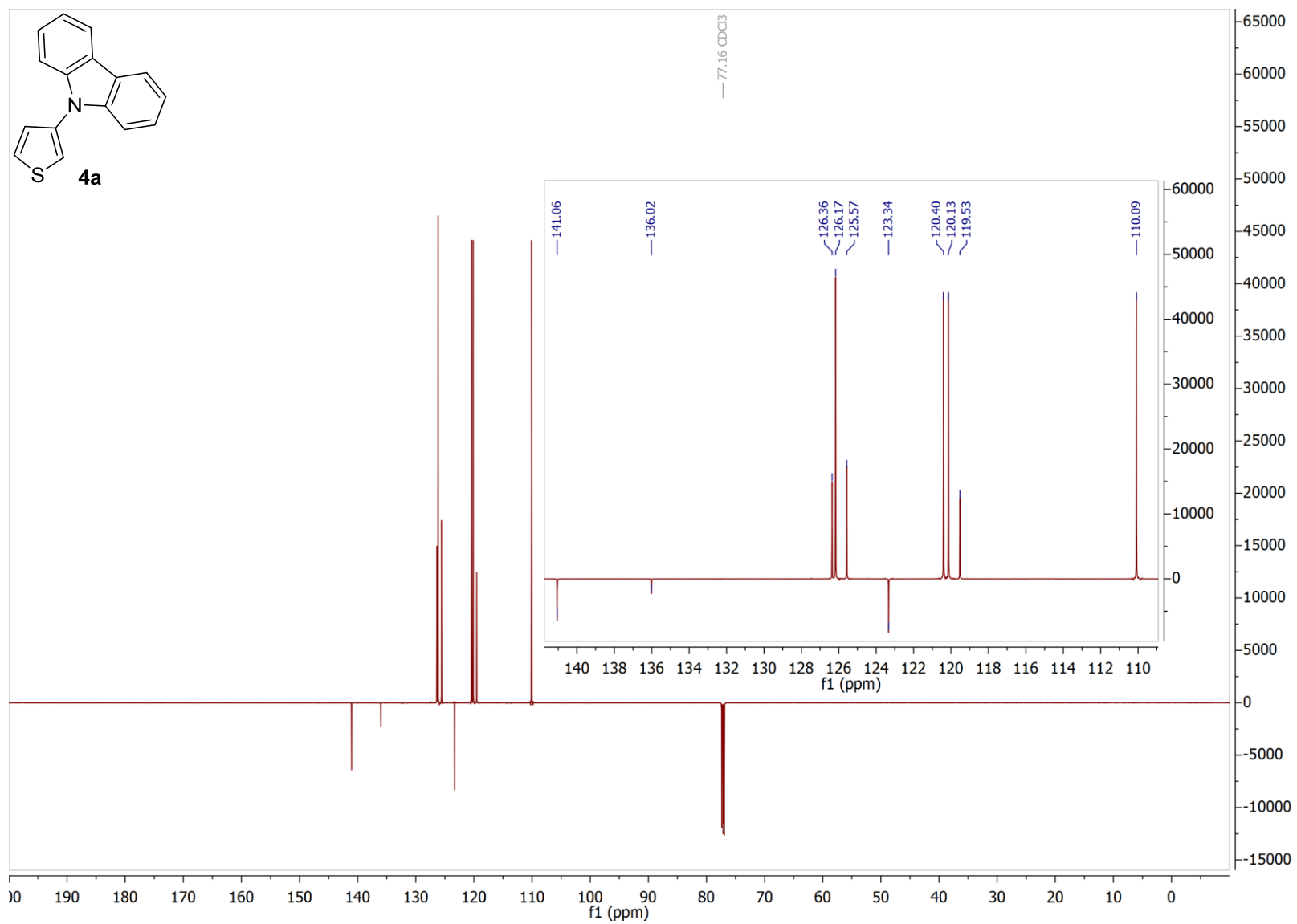


Figure S 2: ^{13}C NMR spectrum of **4a**

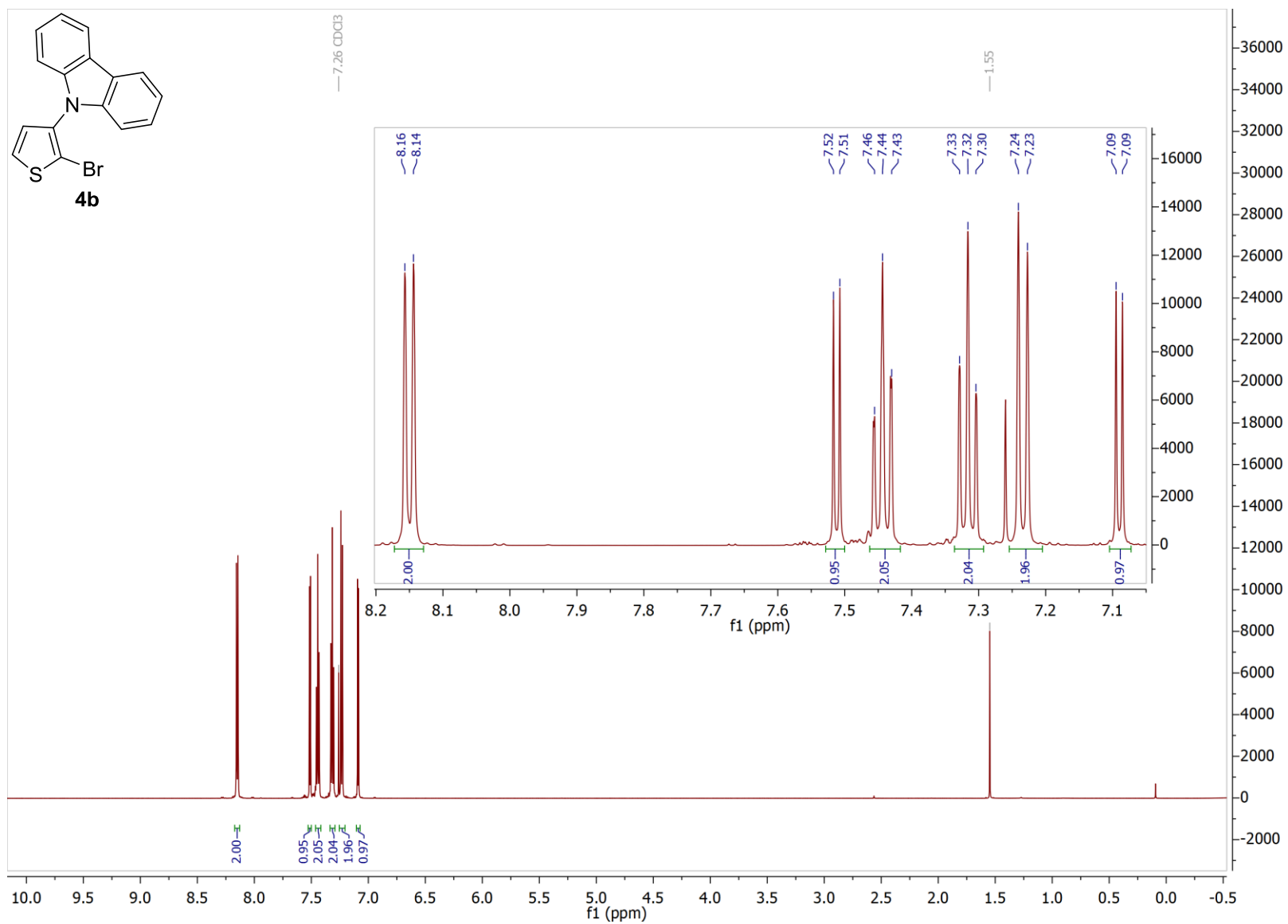


Figure S 3: ¹H NMR spectrum of **4b**

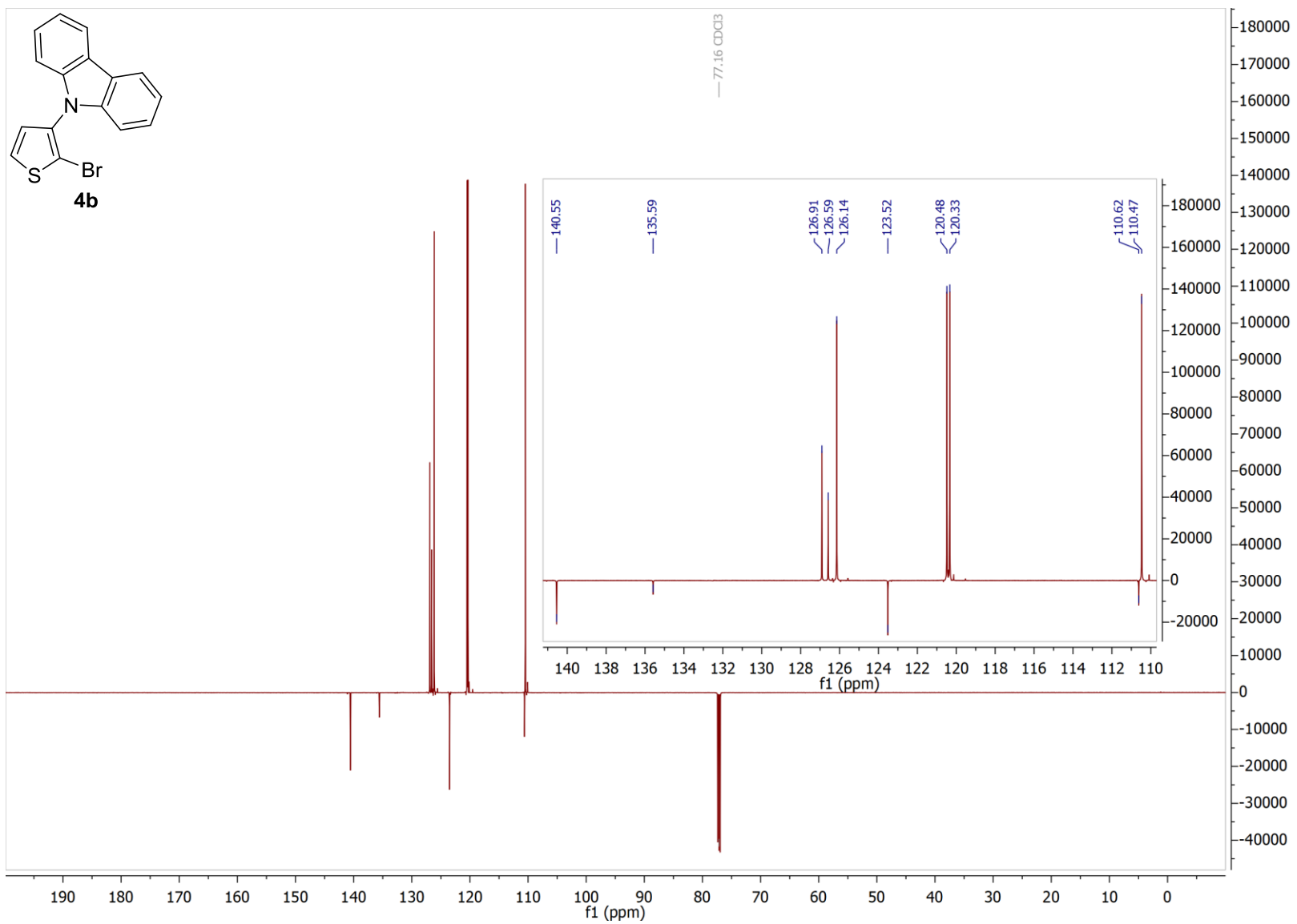


Figure S 4: ^{13}C NMR spectrum of **4b**

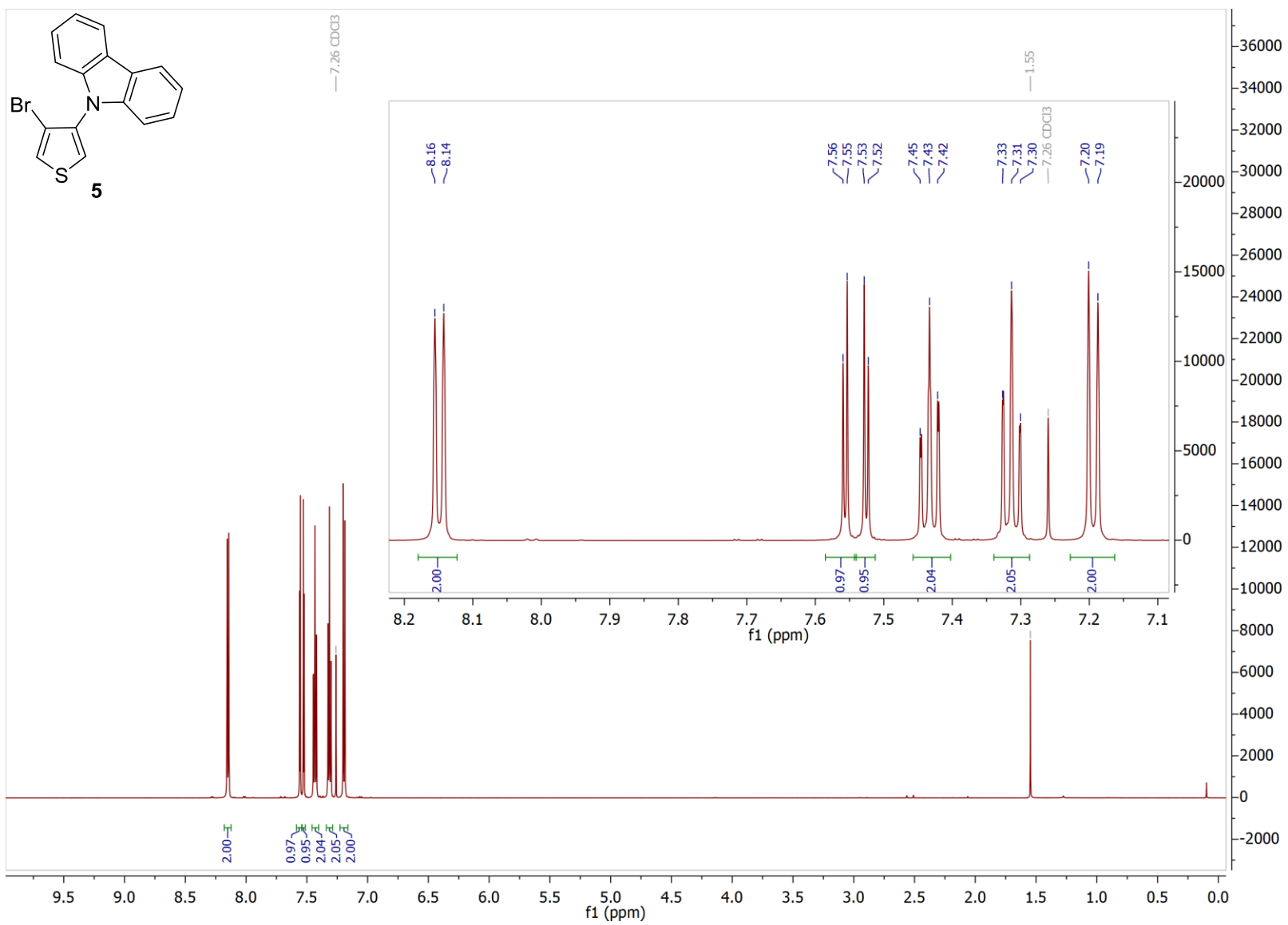


Figure S 5: ¹H NMR spectrum of **5**

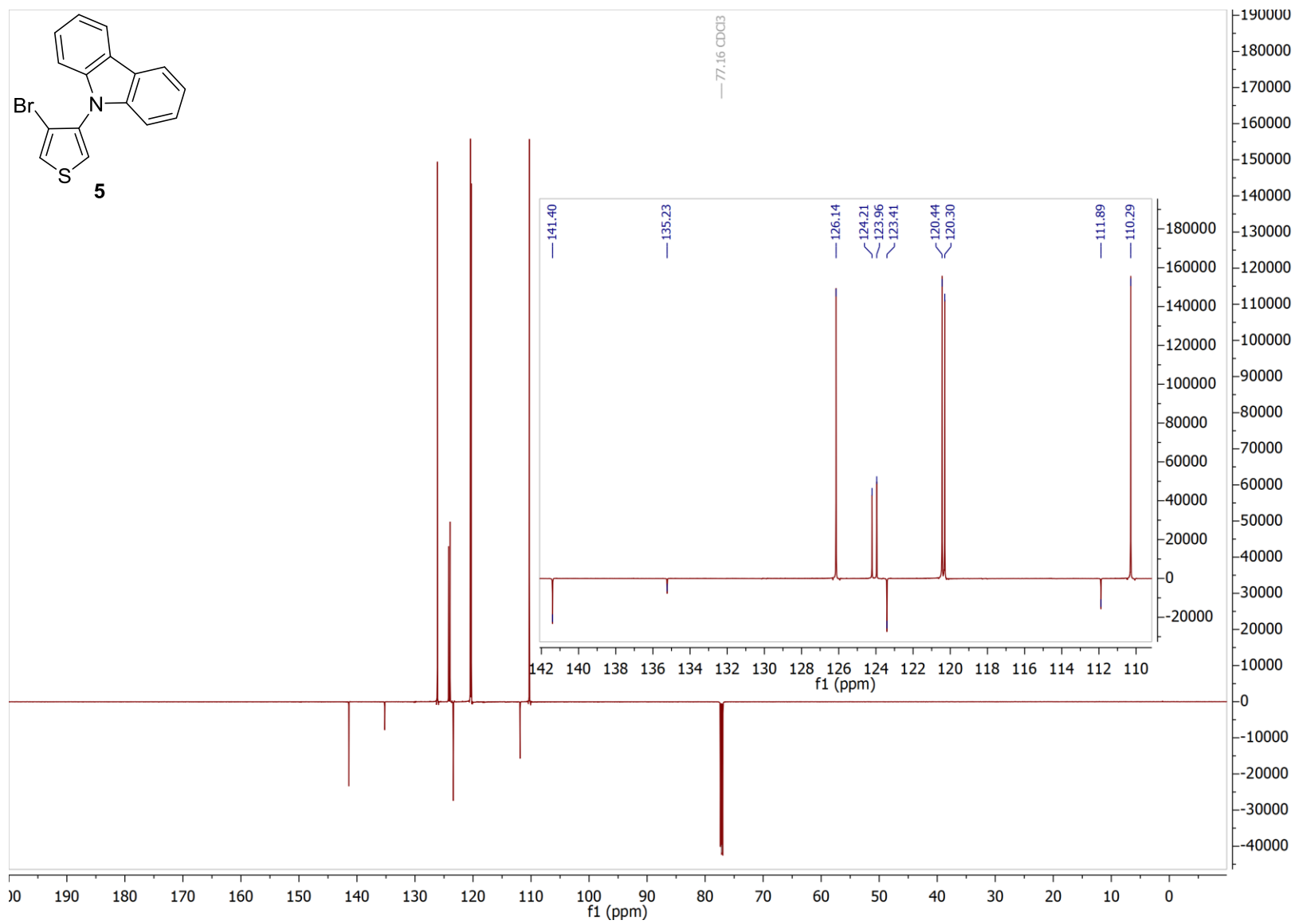


Figure S 6: ^{13}C NMR spectrum of **5**

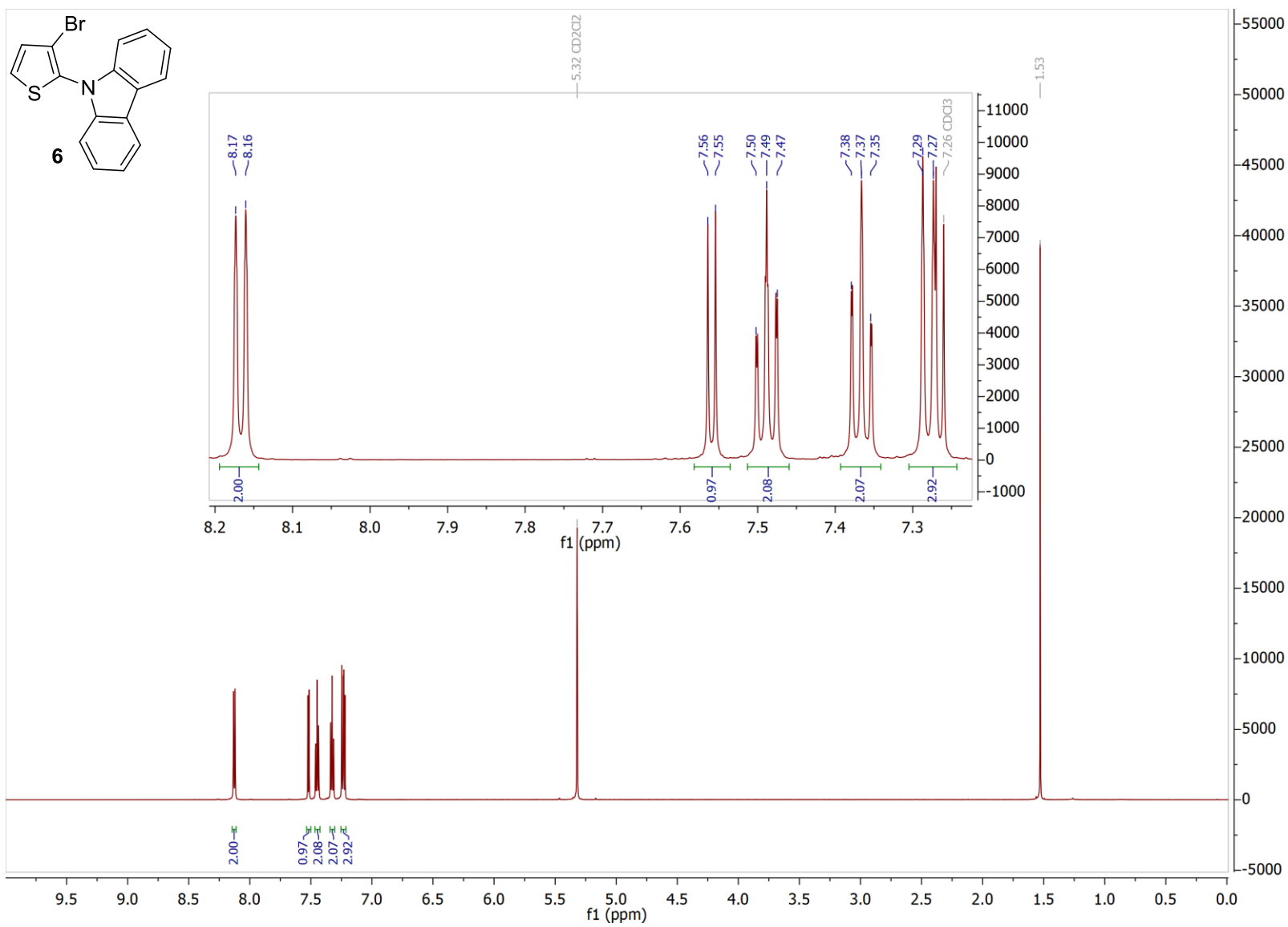


Figure S 7: ^1H NMR spectrum of **6**

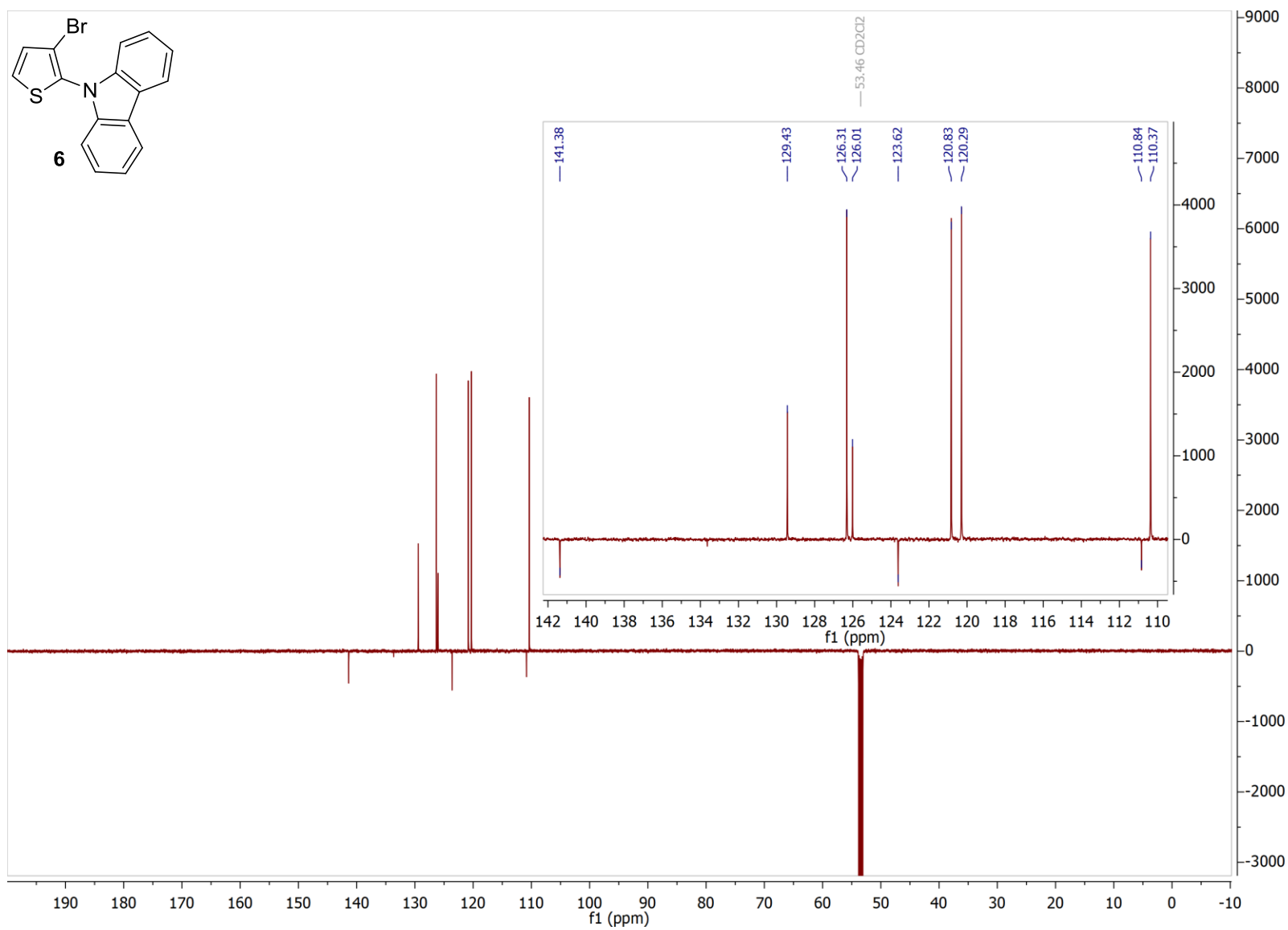


Figure S 8: ^{13}C NMR spectrum of **6**

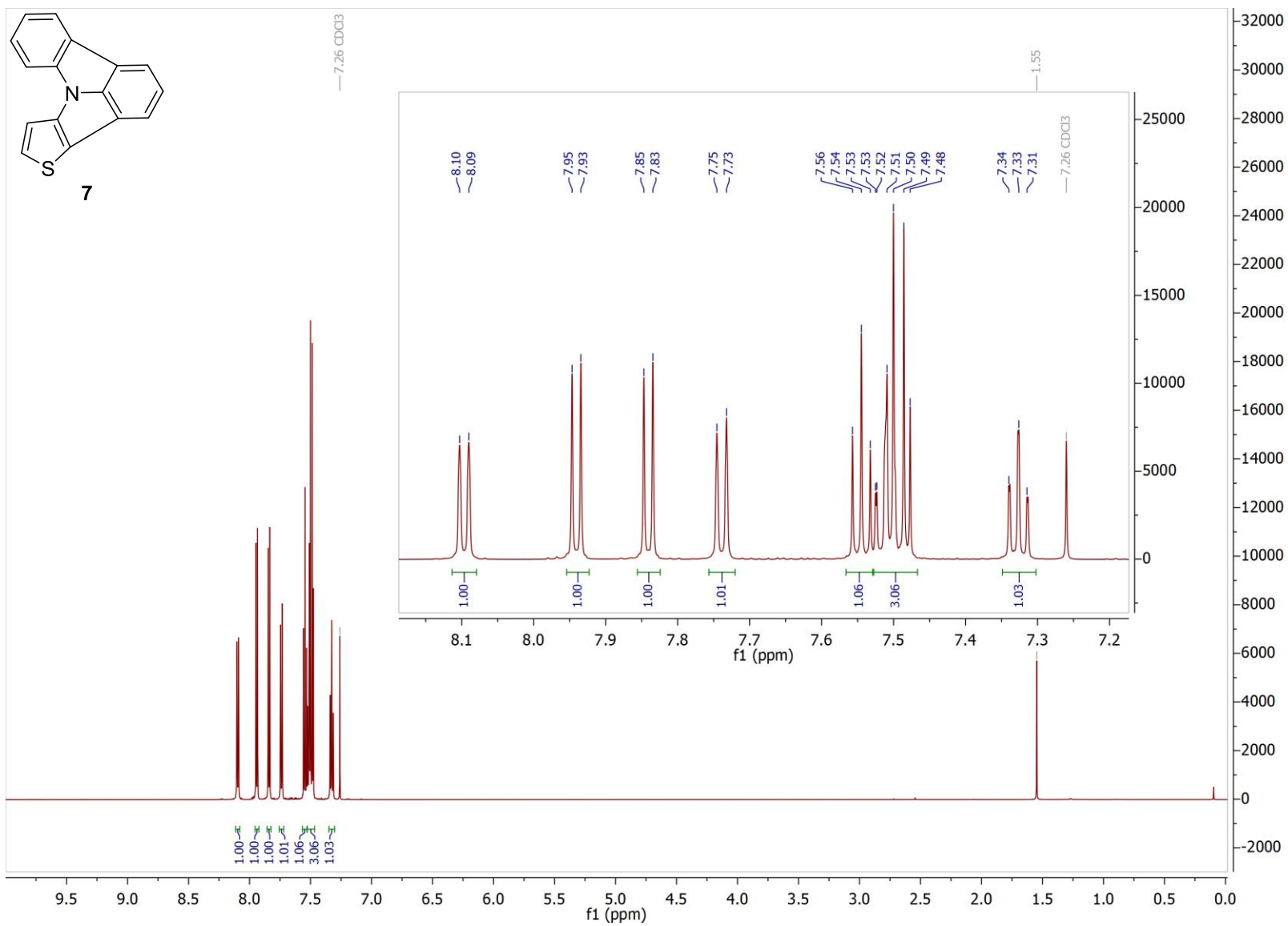


Figure S 9: ¹H NMR spectrum of **7**

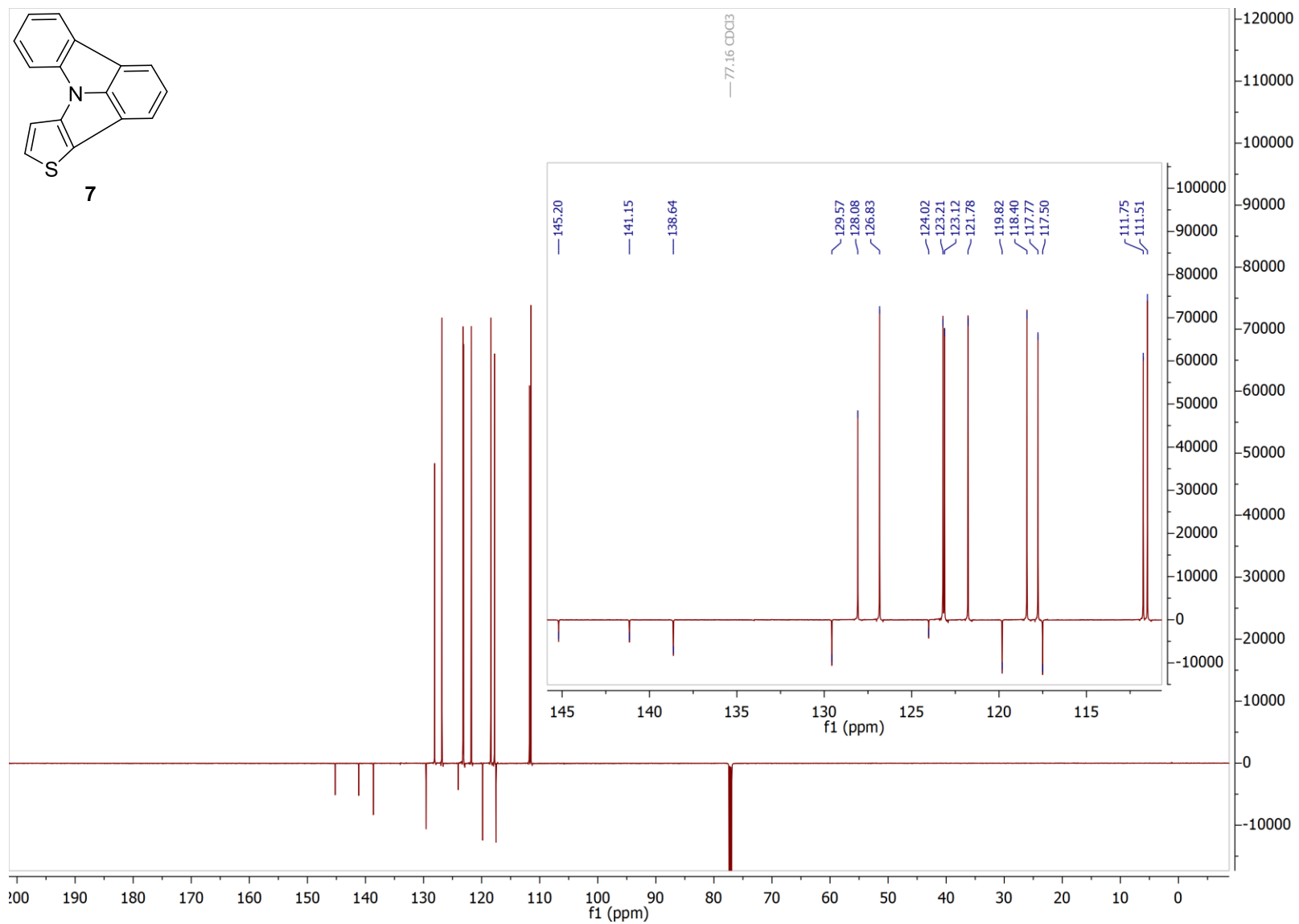


Figure S 10: ^{13}C NMR spectrum of 7

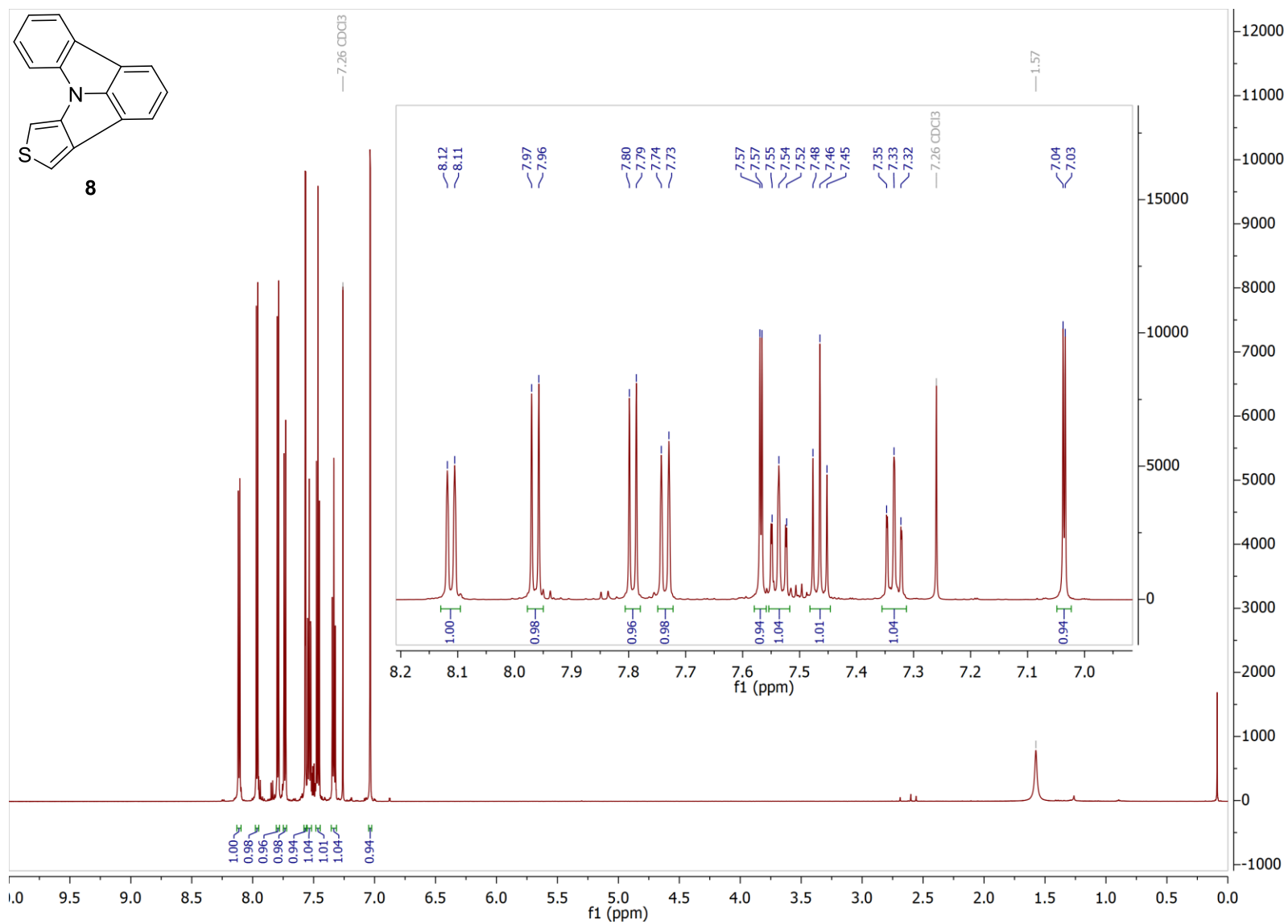


Figure S 11: ¹H NMR spectrum of 8

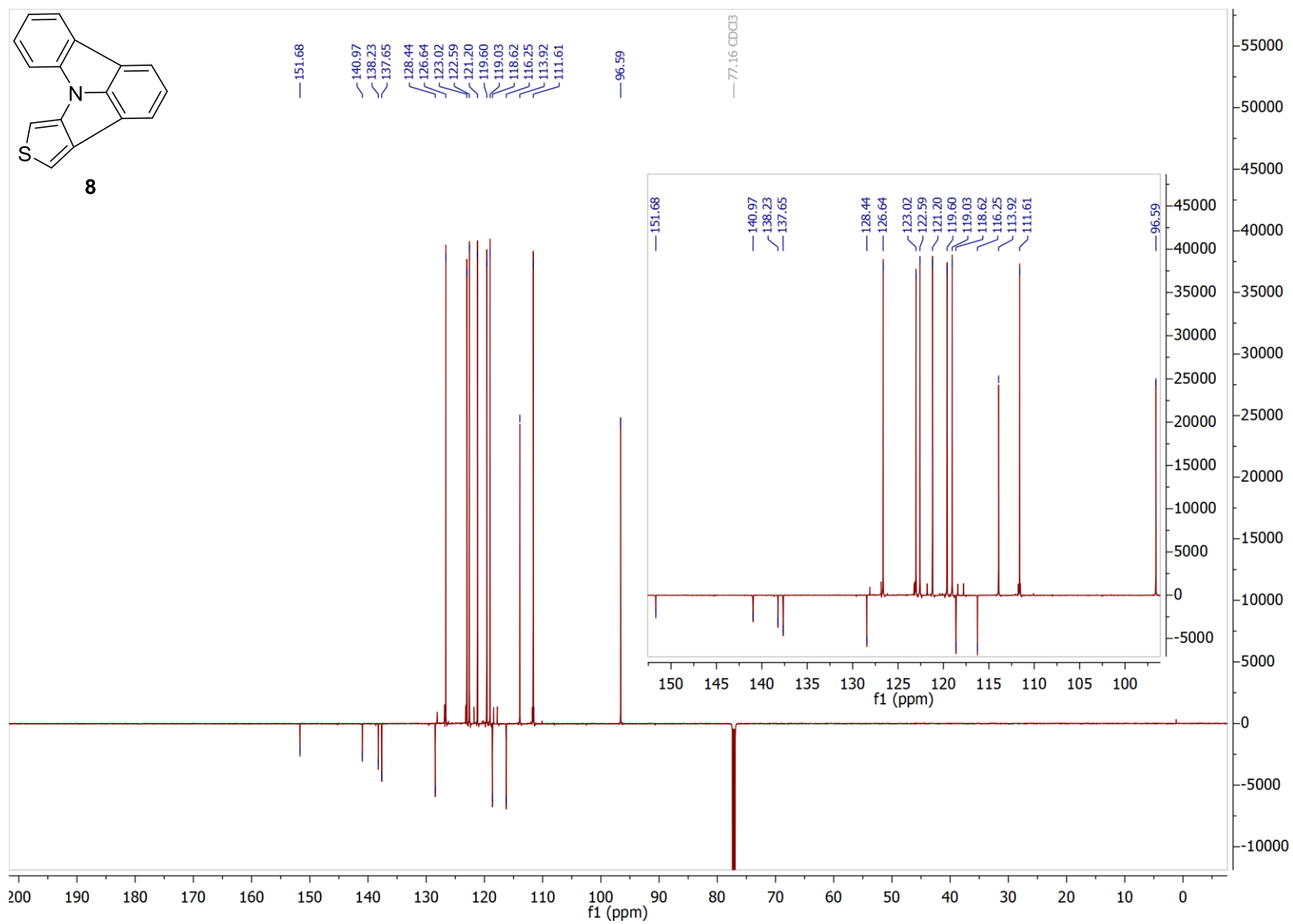


Figure S 12: ^{13}C NMR spectrum of **8**

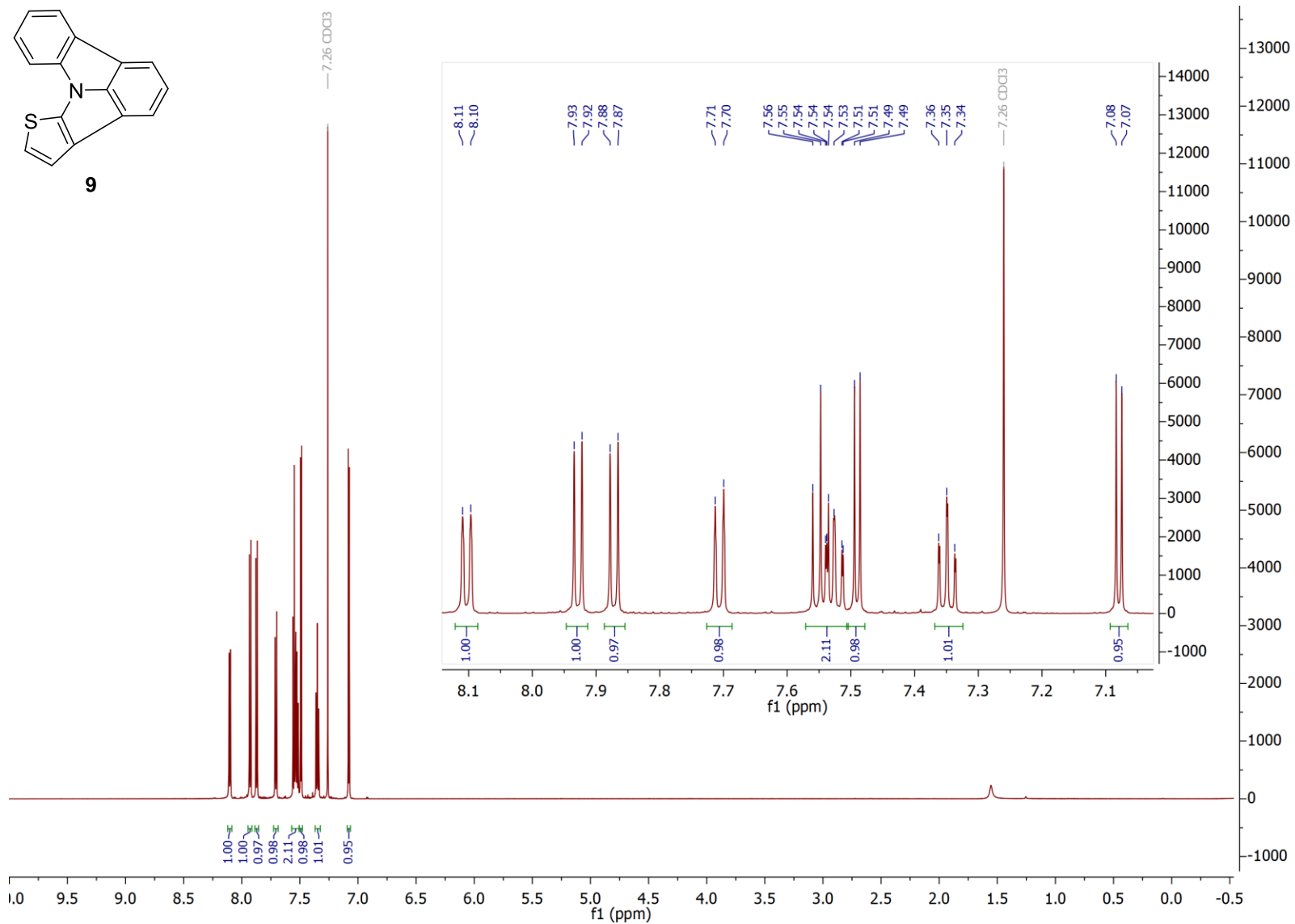


Figure S 13: ^1H NMR spectrum of **9**

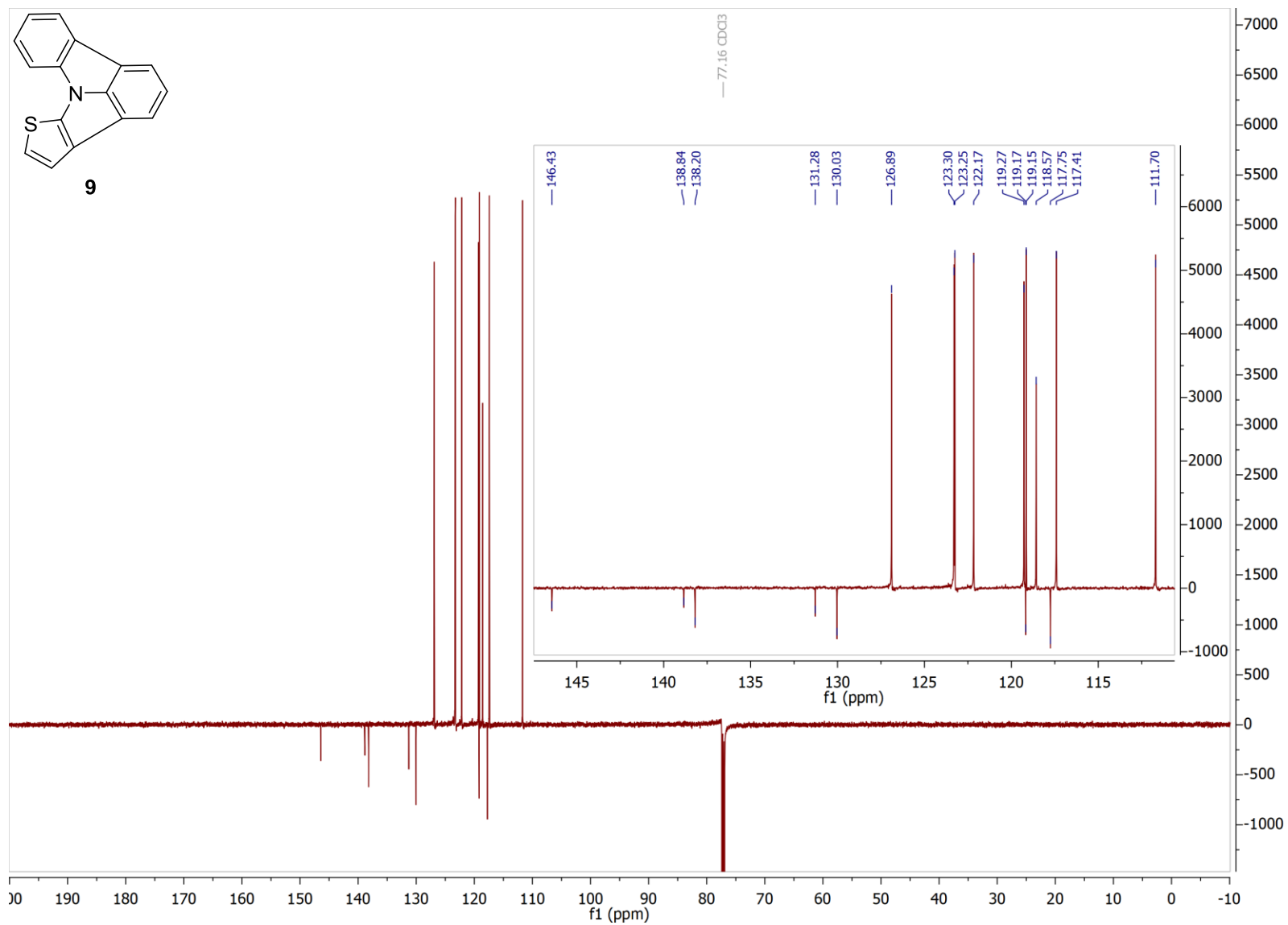


Figure S 14: ^{13}C NMR spectrum of **9**

2. Cyclic Voltammetry

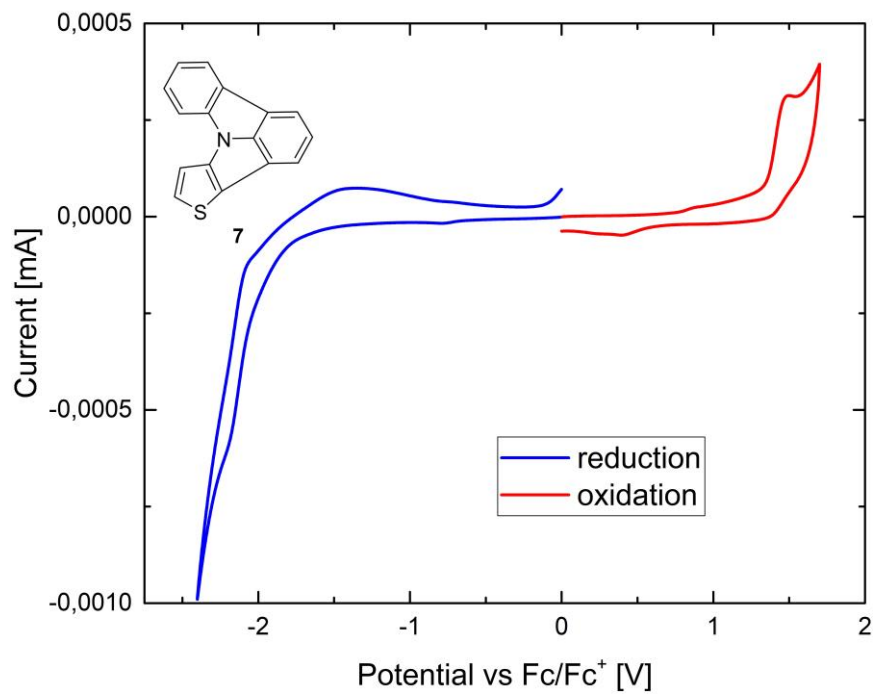


Figure S 15: Cyclovoltamogram of 7

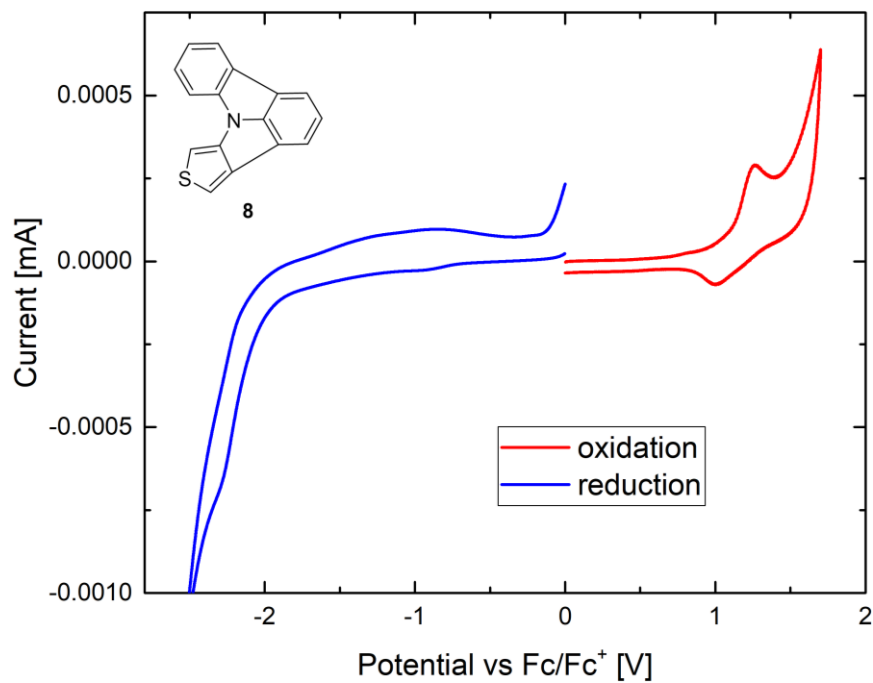


Figure S 16: Cyclovoltamogram of 8

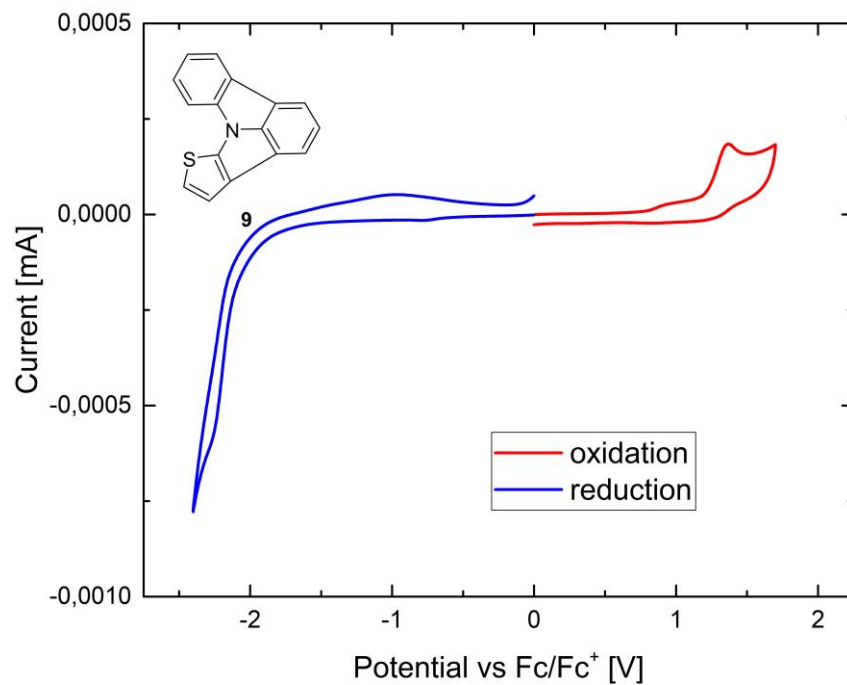


Figure S 17: Cyclic voltammogram of **9**

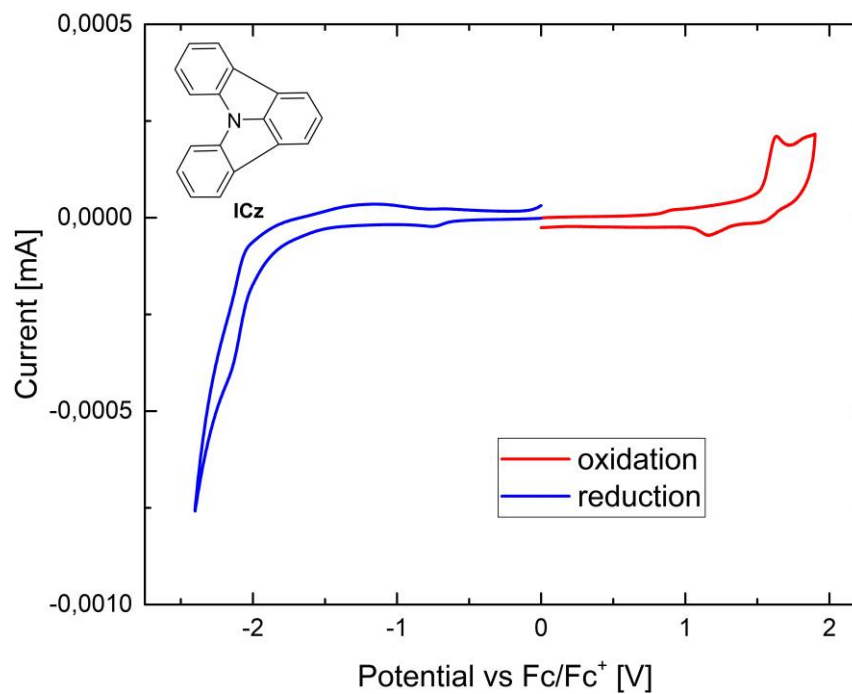


Figure S 18: Cyclic voltammogram of **ICz**

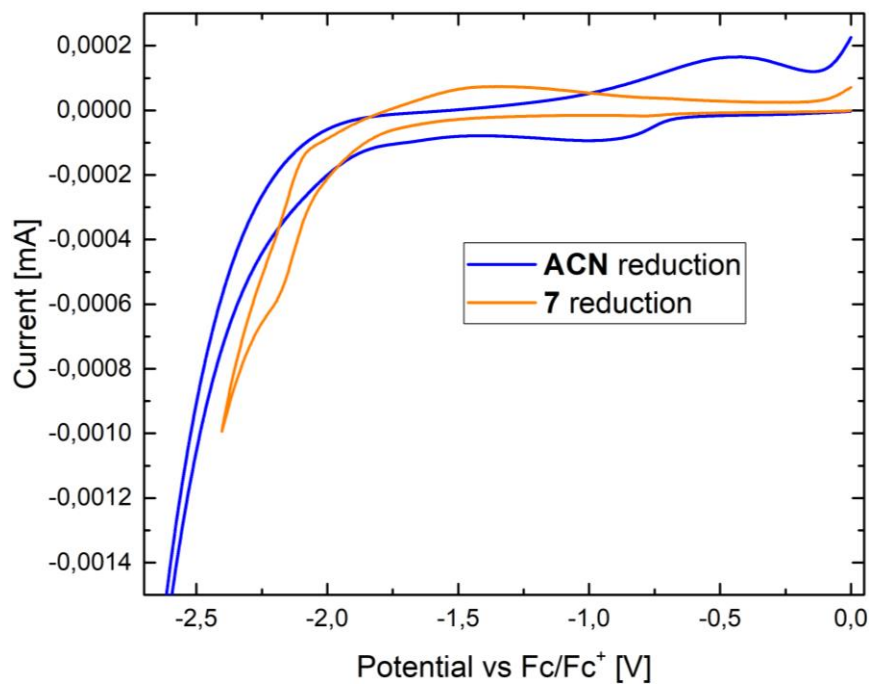


Figure S 19: Cyclic voltammogram of ACN reduction compared to **7**

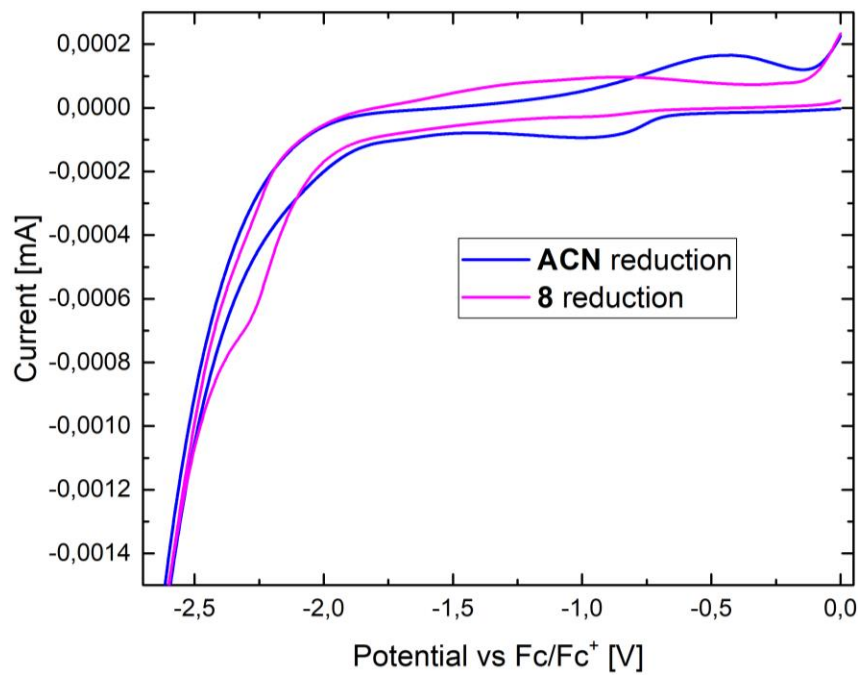


Figure S 20: Cyclic voltammogram of ACN reduction compared to **8**

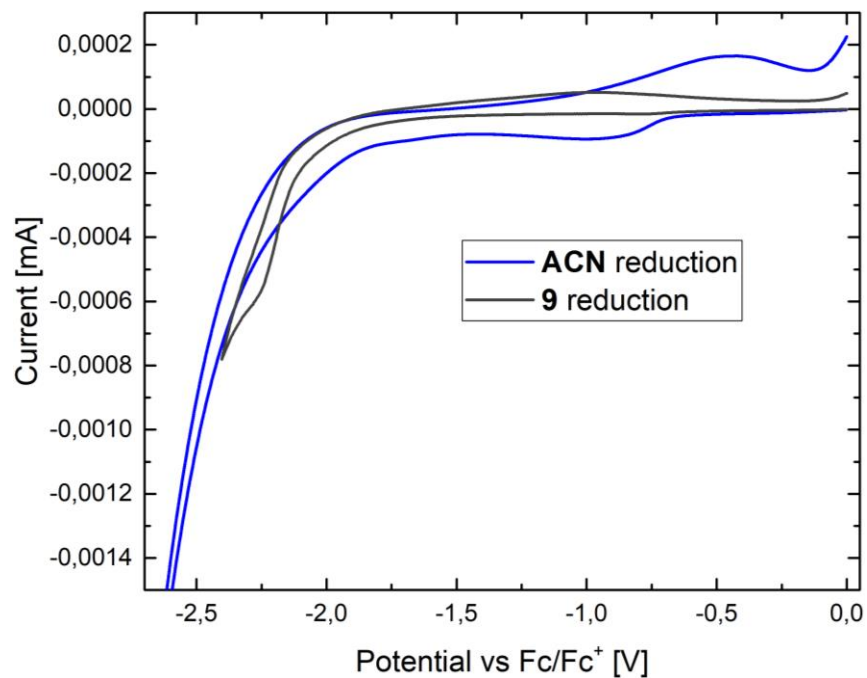


Figure S 21: Cyclic voltammogram of ACN reduction compared to **9**

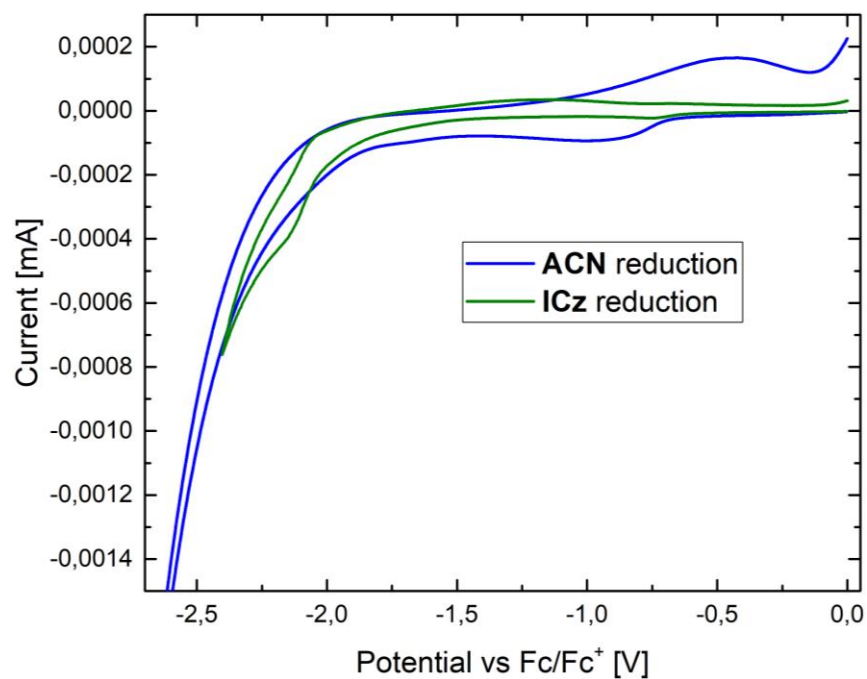


Figure S 22: Cyclic voltammogram of ACN reduction compared to **ICz**

3. HRMS – Spectra

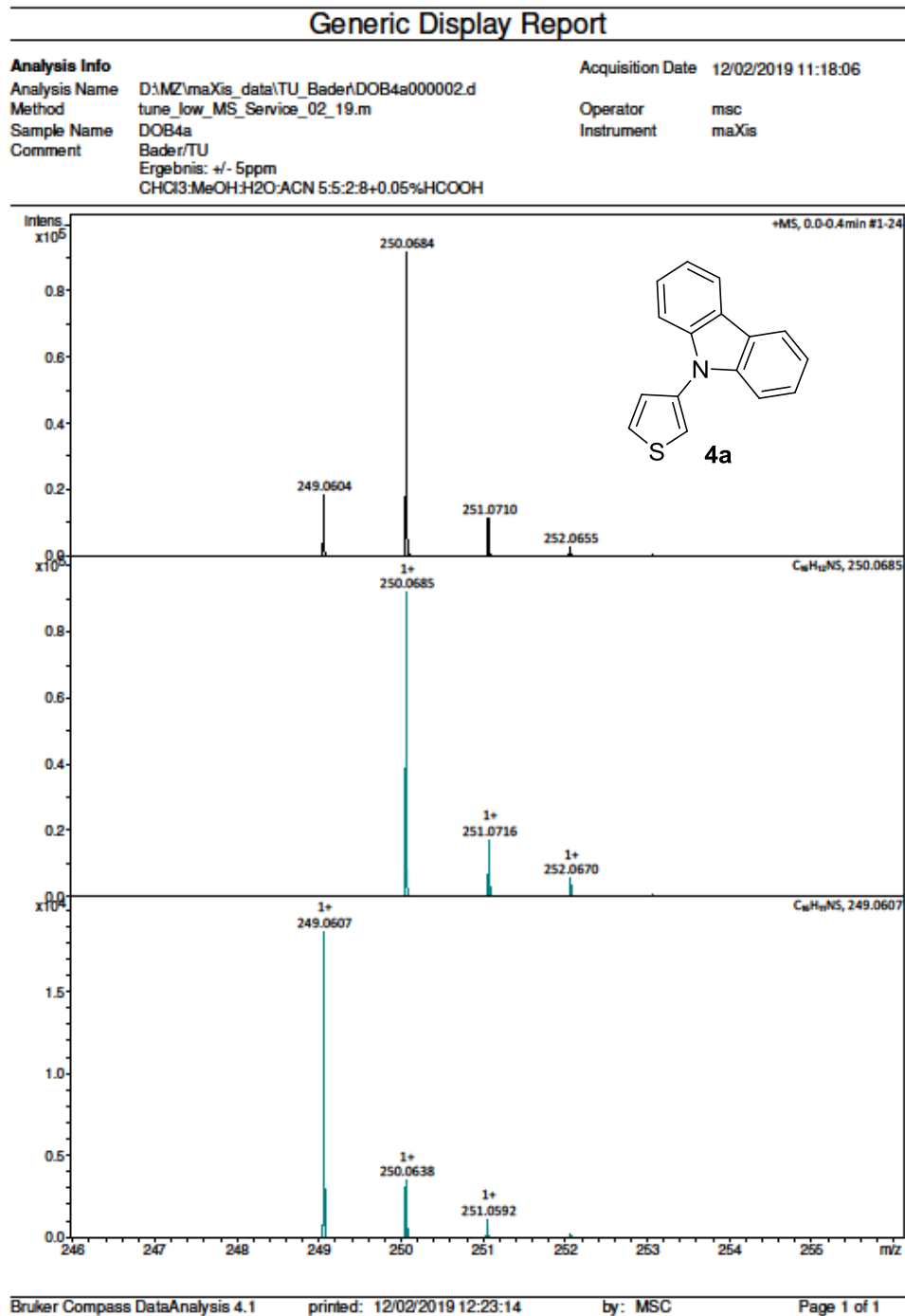


Figure S 23: HRMS spectrum of 4a

Generic Display Report

Analysis Info

Analysis Name D:\MZ\maXis_data\TU_Bader\DOB4b.d
Method tune_low_MS_Service_02_19.m
Sample Name DOB4b
Comment Bader/TU
Ergebnis: +/- 5ppm
2-Propanol/ACN/H2O 1:4:1 + 0.1%HCOOH

Acquisition Date 08/02/2019 15:30:50

Operator msc
Instrument maXis

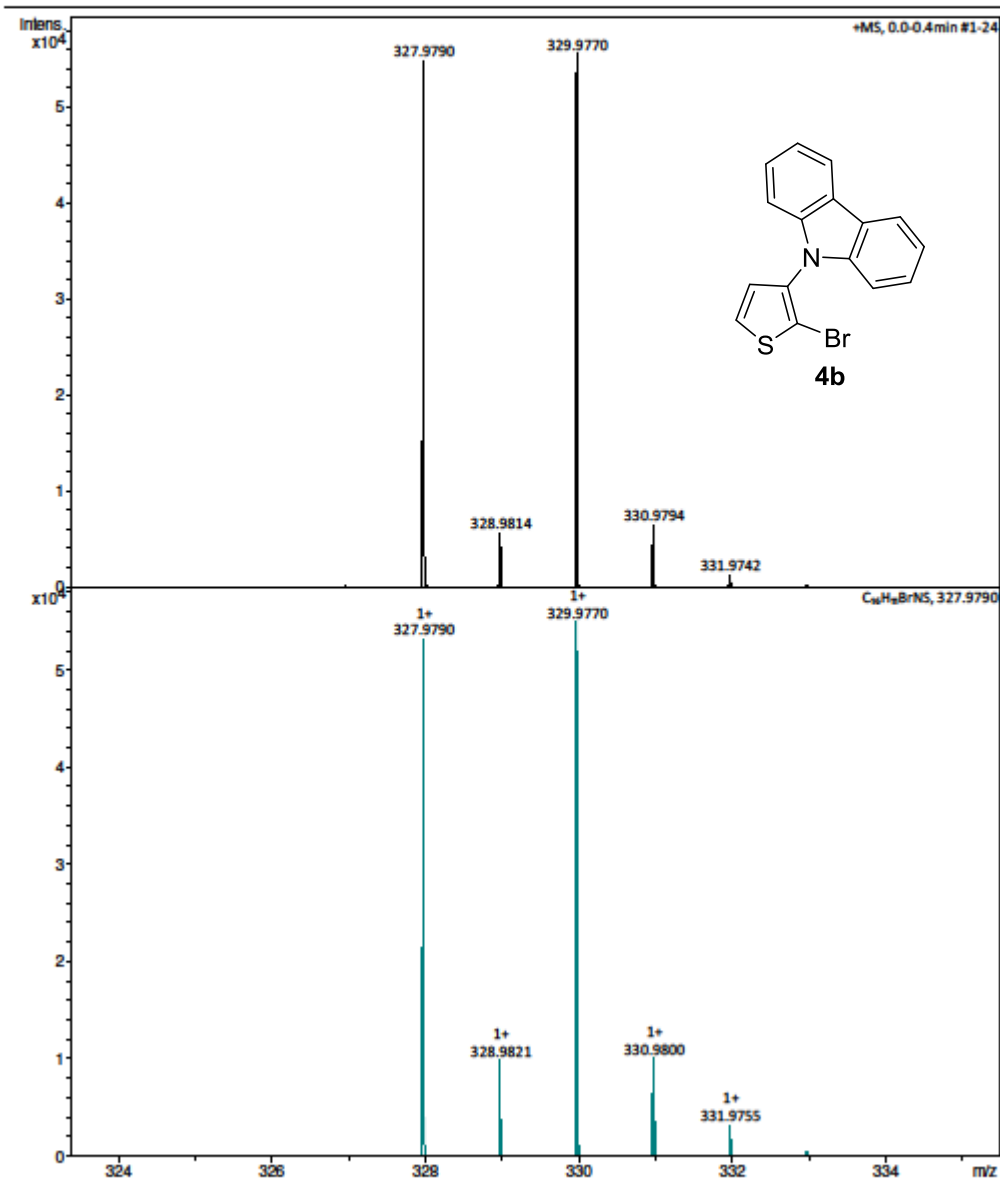


Figure S 24: HRMS spectrum of 4b

Generic Display Report

Analysis Info

Analysis Name D:\MZ\maXis_data\TU_Bader\DOB5.d
Method tune_low_MS_Service_02_19.m
Sample Name DOB5
Comment Bader/TU
Ergebnis: +/- 5ppm
2-Propanol/ACN/H2O 1:4:1 + 0.1%HCOOH

Acquisition Date 08/02/2019 15:14:37

Operator msc
Instrument maXis

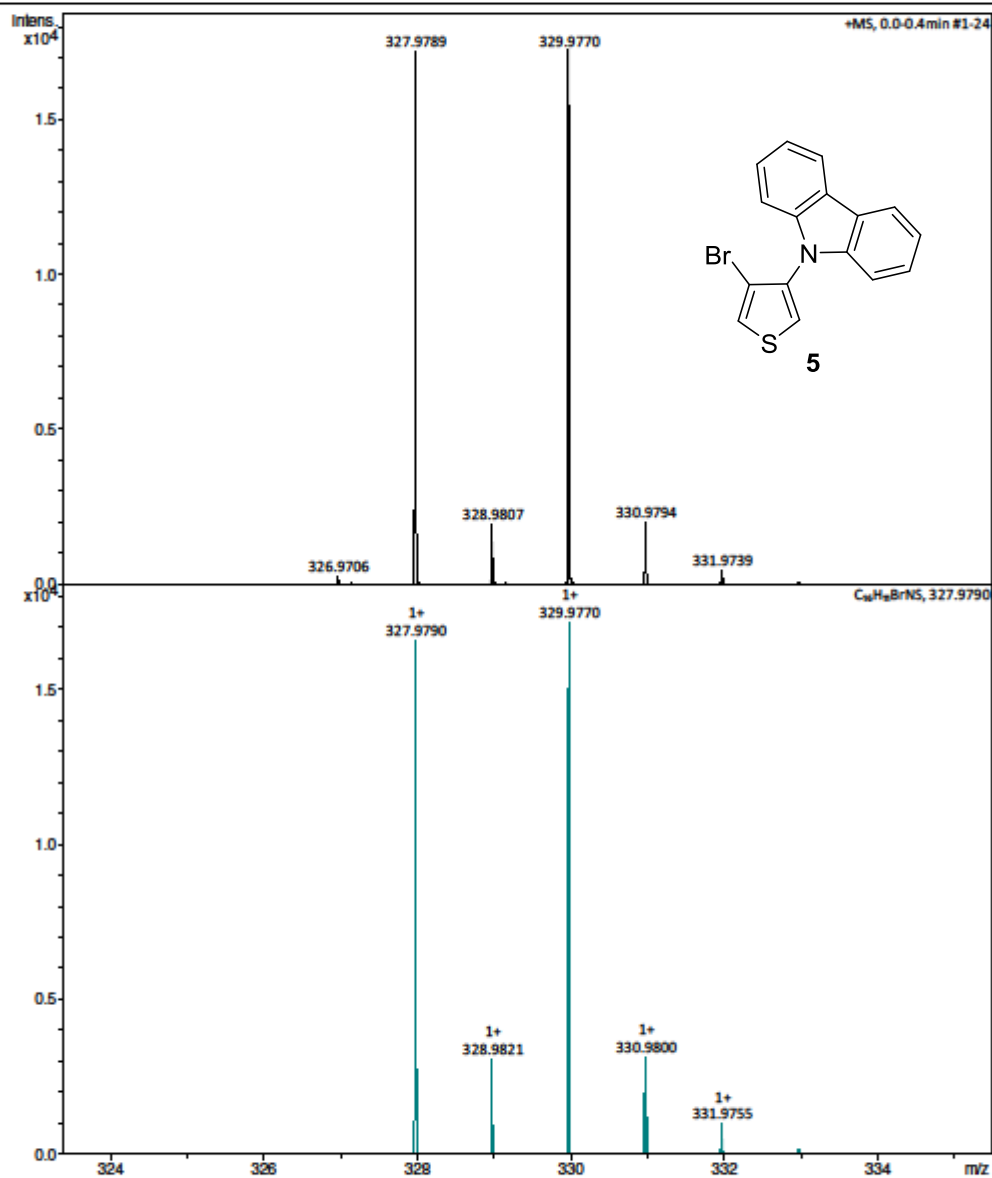


Figure S 25: HRMS spectrum of 5

Generic Display Report

Analysis Info

Analysis Name D:\MZ\maXis_data\TU_Bader\DOB6.d
Method tune_low_MS_Service_02_19.m
Sample Name DOB6
Comment Bader/TU
Ergebnis: +/- 5ppm
2-Propanol/ACN/H2O 1:4:1 + 0.1%HCOOH

Acquisition Date 08/02/2019 15:24:09

Operator msc
Instrument maXis

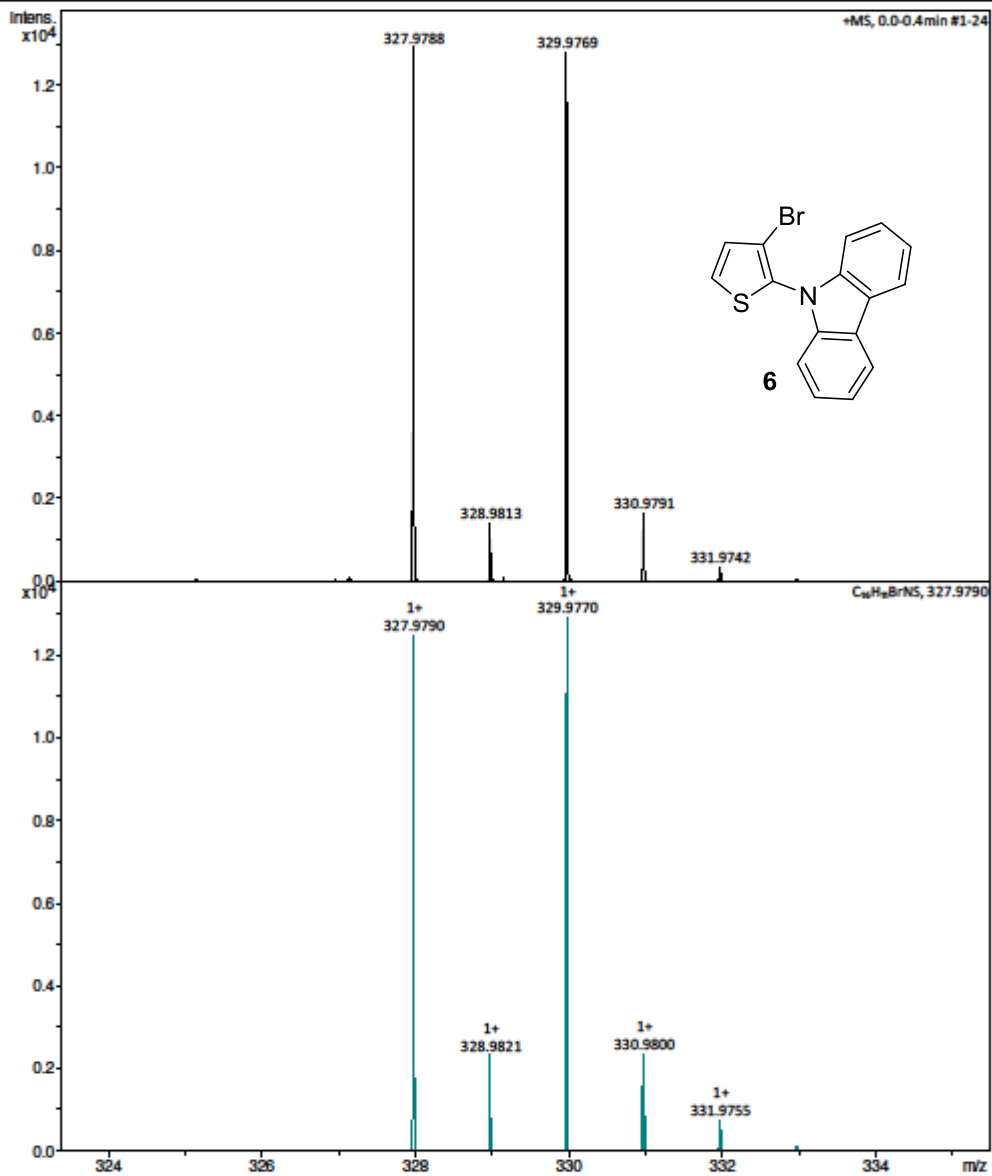


Figure S 26: HRMS spectrum of 6

Generic Display Report

Analysis Info

Analysis Name D:\MZ\maXis_data\TU_Bader\DOB7.d
Method tune_low_MS_Service_02_19.m
Sample Name DOB7
Comment Bader/TU
Ergebnis: +/- 5ppm
2-Propanol/ACN/H2O 1:8:2 + 0.1%HCOOH

Acquisition Date 08/02/2019 15:49:17

Operator msc
Instrument maXis

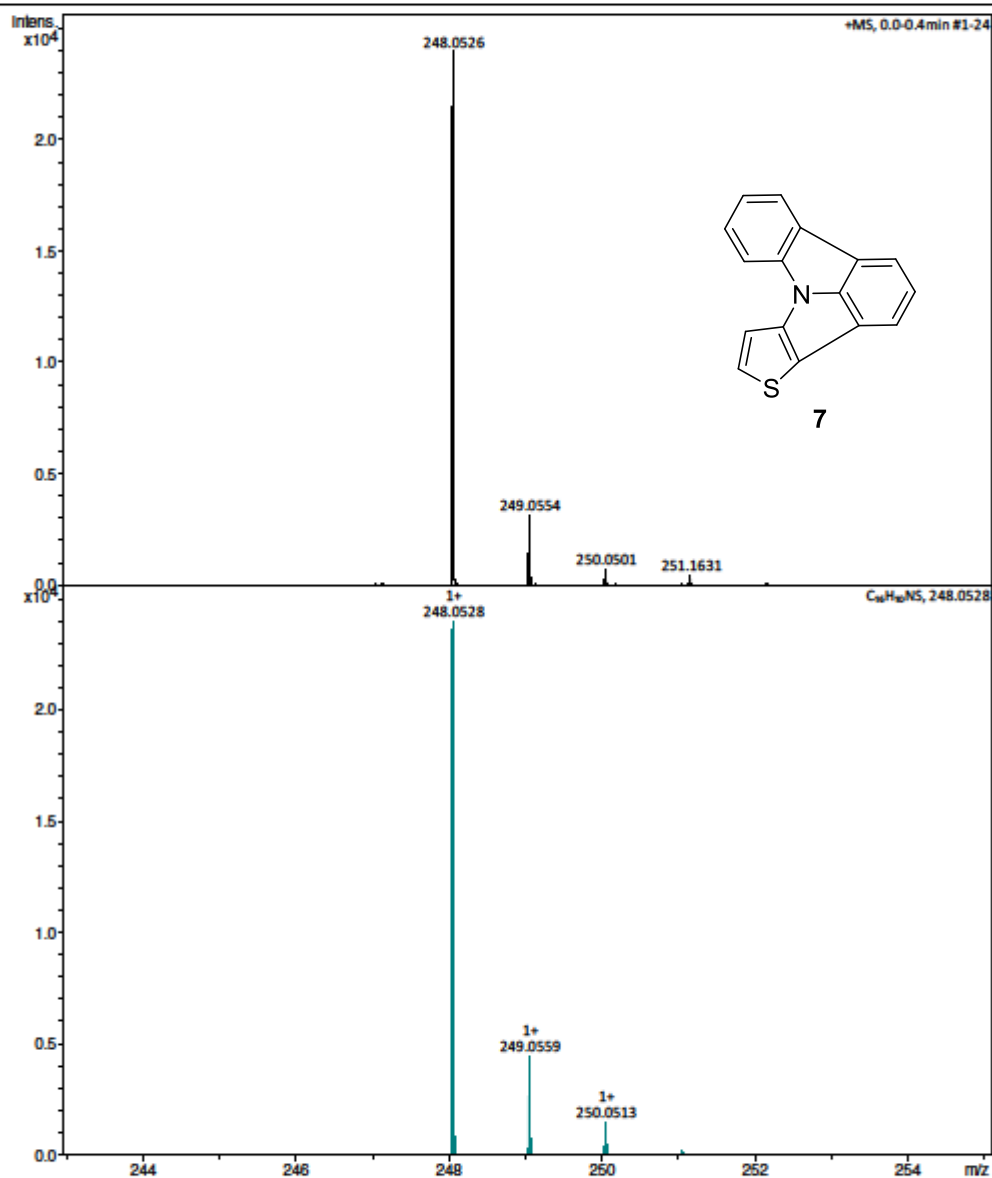


Figure S 27: HRMS spectrum of 7

Generic Display Report

Analysis Info

Analysis Name D:\MZ\maXis_data\TU_Bader\DOB8.d
Method tune_low_MS_Service_02_19.m
Sample Name DOB8
Comment Bader/TU
Ergebnis: +/- 5ppm
2-Propanol/ACN/H2O 1:8:2 + 0.1%HCOOH

Acquisition Date 08/02/2019 15:52:22

Operator msc
Instrument maXis

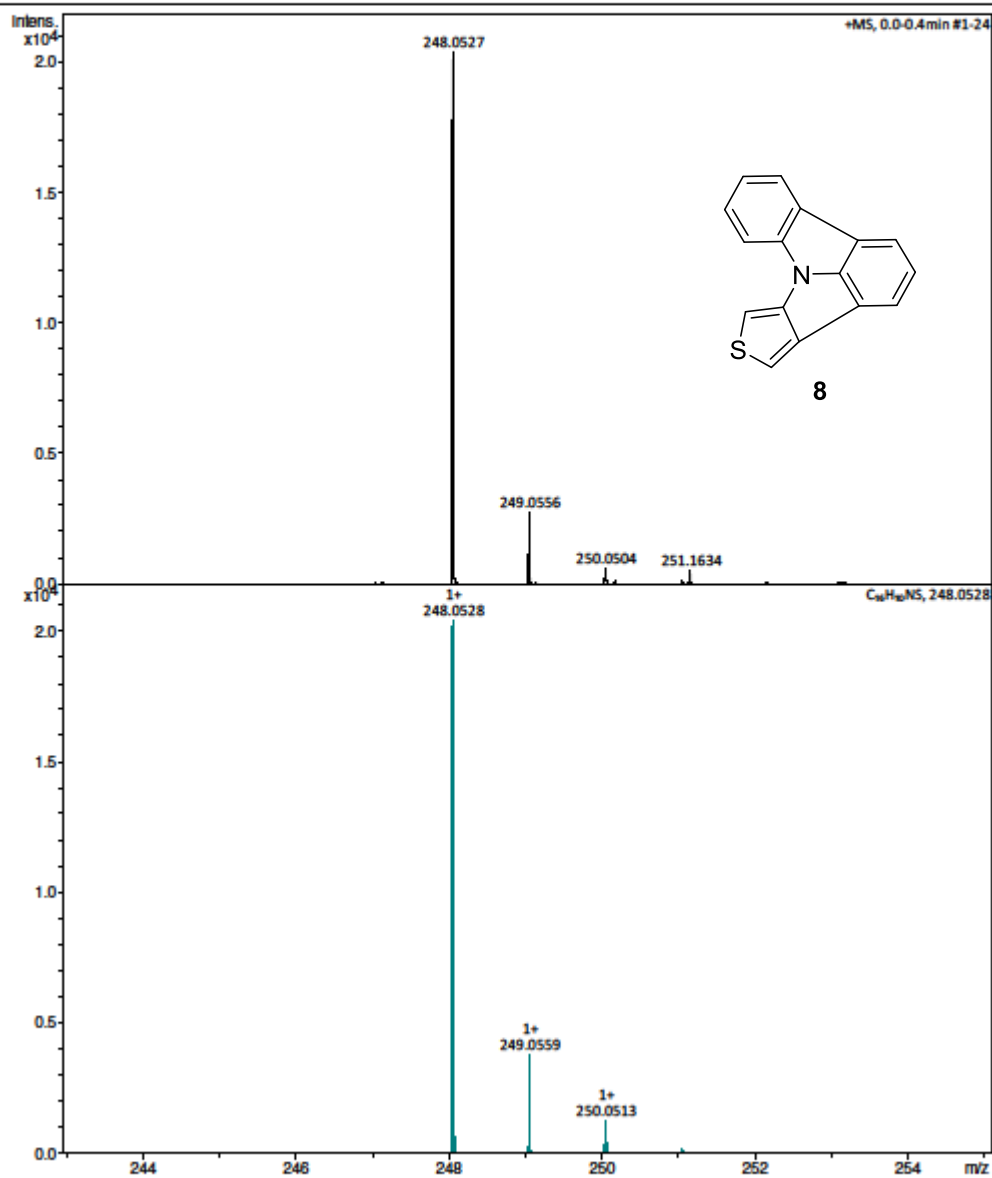


Figure S 28: HRMS spectrum of 8

Generic Display Report

Analysis Info

Analysis Name D:\MZ\maXis_data\TU_Bader\DOB9.d
Method tune_low_MS_Service_02_19.m
Sample Name DOB9
Comment Bader/TU
Ergebnis: +/- 5ppm
2-Propanol/ACN/H2O 1:8:2 + 0.1%HOAc

Acquisition Date 08/02/2019 15:59:27

Operator msc
Instrument maXis

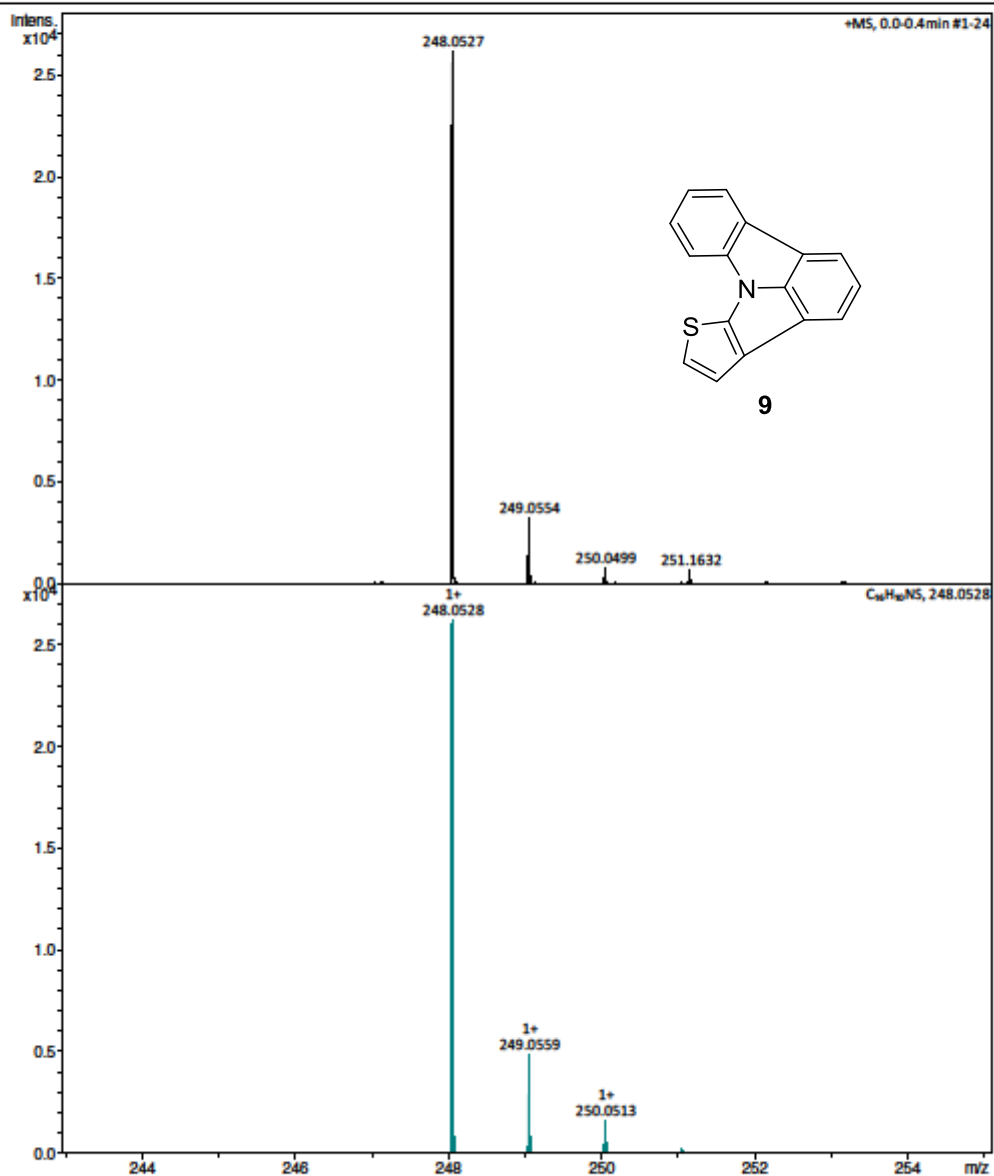


Figure S 29: HRMS spectrum of 9

4. Electrochemical and photophysical data

Table S1. Electrochemical and photophysical data of ICz and the developed thienopyrrolo[3,2,1-*jk*]carbazoles 7-9.

	opt. BG ^{a,b}	λ_{max} ^{b,c}	E_T ^d	HOMO ^e	LUMO ^e	λ_{max} ^{b,f}	ϵ_{max} ^{f,h}	λ_{low} ^{b,g}	ϵ_{low} ^{g,h}
	[eV]	[nm]	[eV]	[eV]	[eV]	[nm]	[L*mol ⁻¹ *cm ⁻¹]	[nm]	[L*mol ⁻¹ *cm ⁻¹]
ICz	3.30	375	2.84	-5.78	-2.27	285	37720	363	11100
7	3.25	390	2.57	-5.68	-2.38	280	29500	347	15140
8	3.30	380	2.71	-5.56	-2.28	284	27760	369	5880
9	3.22	410	2.79	-5.53	-2.30	283	42900	345	4720

^a HOMO-LUMO energy gaps, determined from the absorption onset. ^b measured in DCM solutions (5 μ M) at room temperature; ^c emission maximum; ^d determined from the highest vibronic transition in solid solutions of toluene/iPrOH (10:1; 1 mg/ml) at 77 K; ^e calculated from the onset of the oxidation and reduction peak observed during cyclic voltammetry relative to ferrocene/ferrocene⁺ (4.8 eV); ^f absorption maximum (only peaks > 270 nm considered due to possible solvent interference); ^g lowest energy absorption peak; ^h molar attenuation coefficient, calculated from absorption.