Direct Amination of Antiaromatic Ni^{II} Norcorrole

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NMR spectra

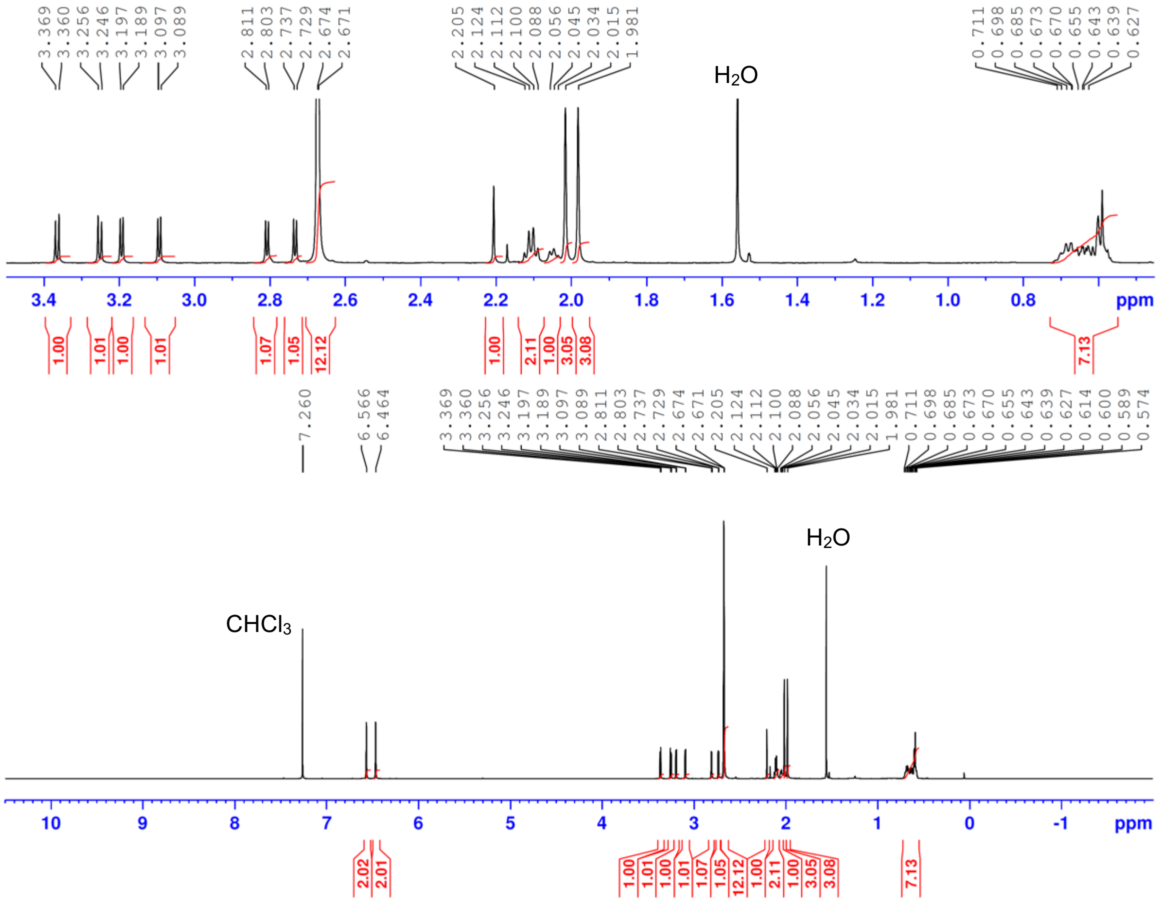

Fig S1. ^{1}H NMR (500 MHz) spectrum of **2a** in $CDCl_3$.

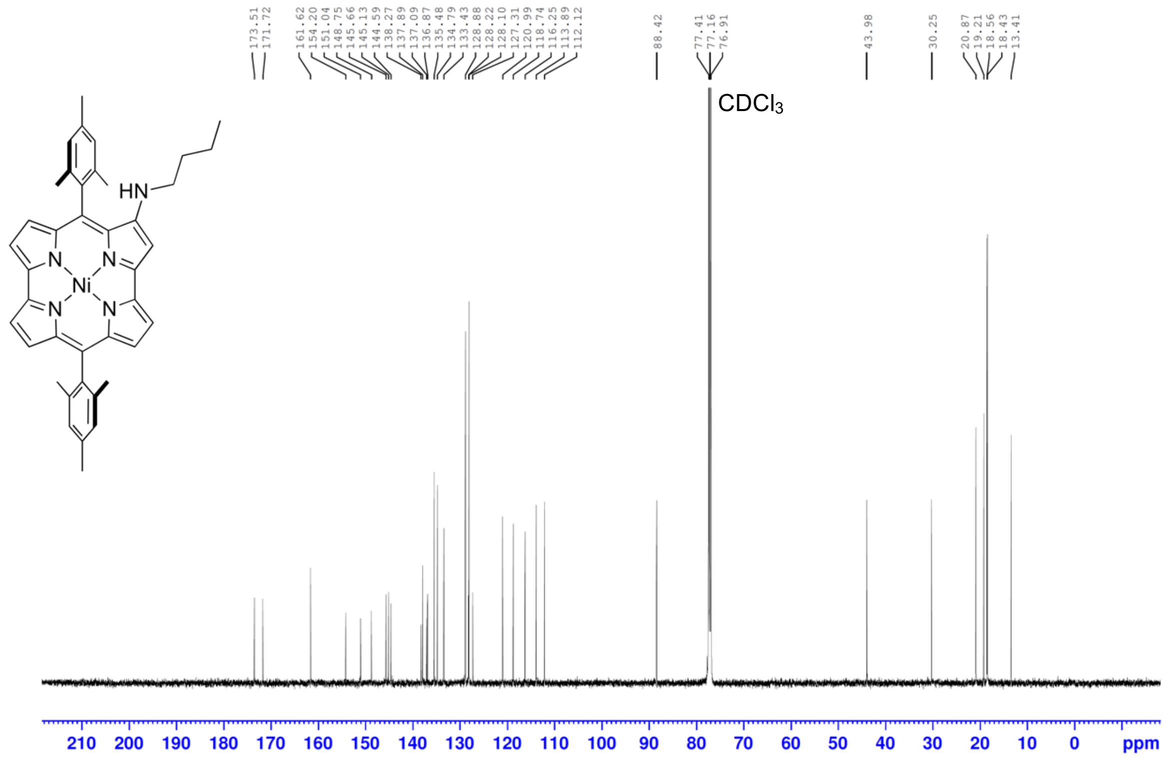

Fig S2. ^{13}C NMR (126 MHz) spectrum of **2a** in $CDCl_3$.

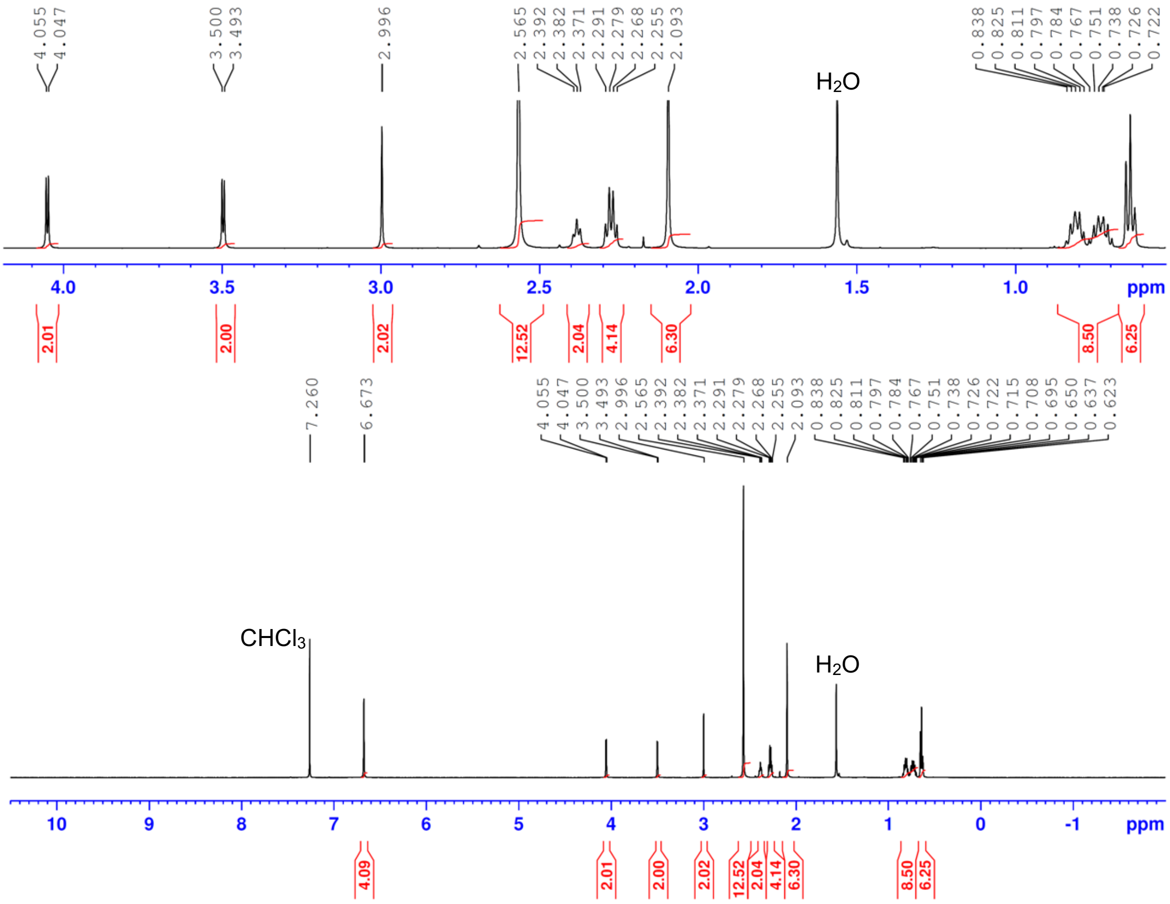

Fig S3. ^{1}H NMR (500 MHz) spectrum of **2b** in $CDCl_3$.

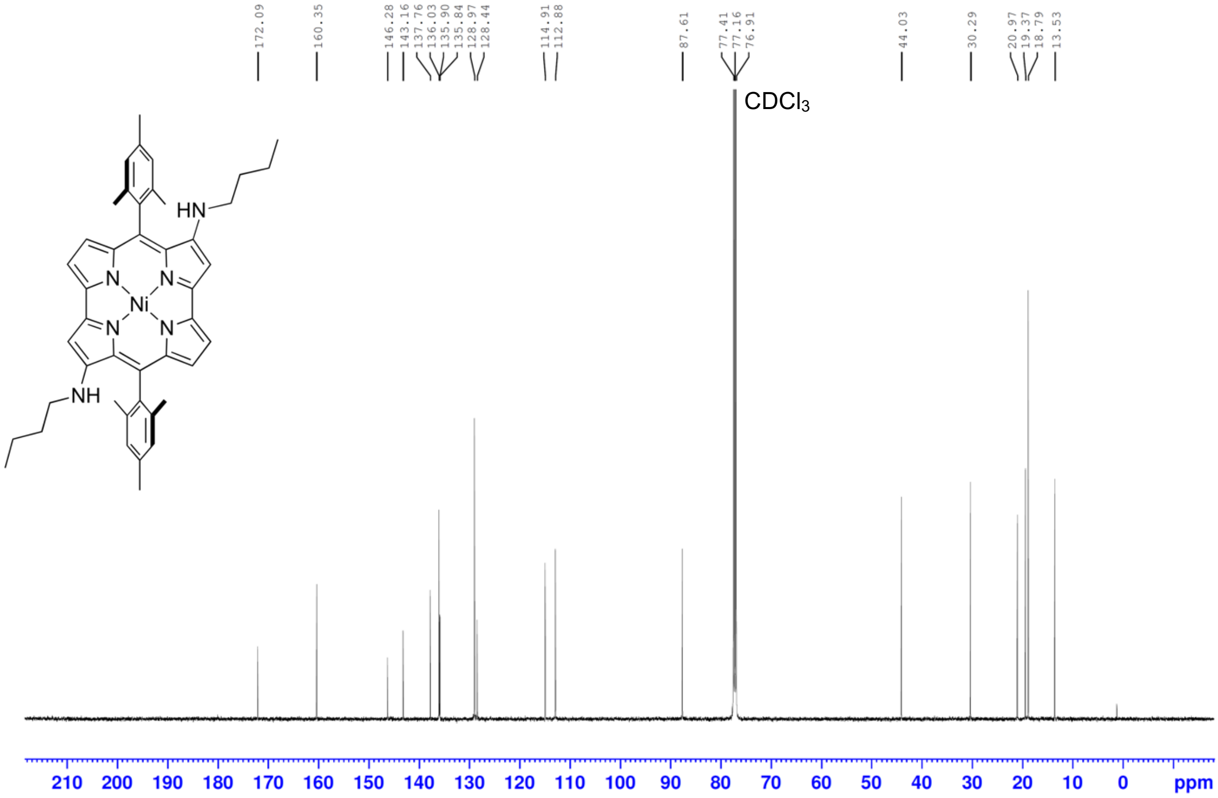

Fig S4. ^{13}C NMR (126 MHz) spectrum of **2b** in $CDCl_3$.

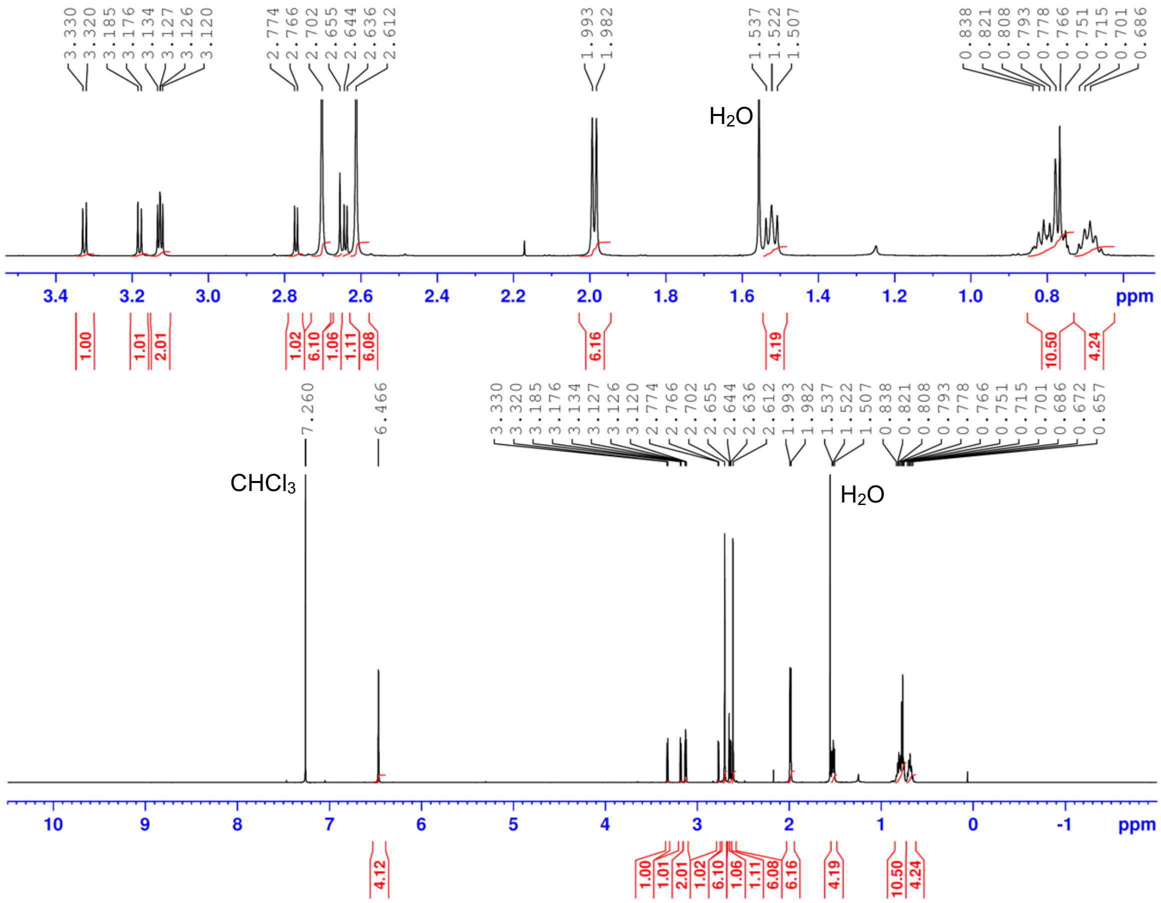

Fig S5. ^{1}H NMR (500 MHz) spectrum of **3a** in $CDCl_3$.

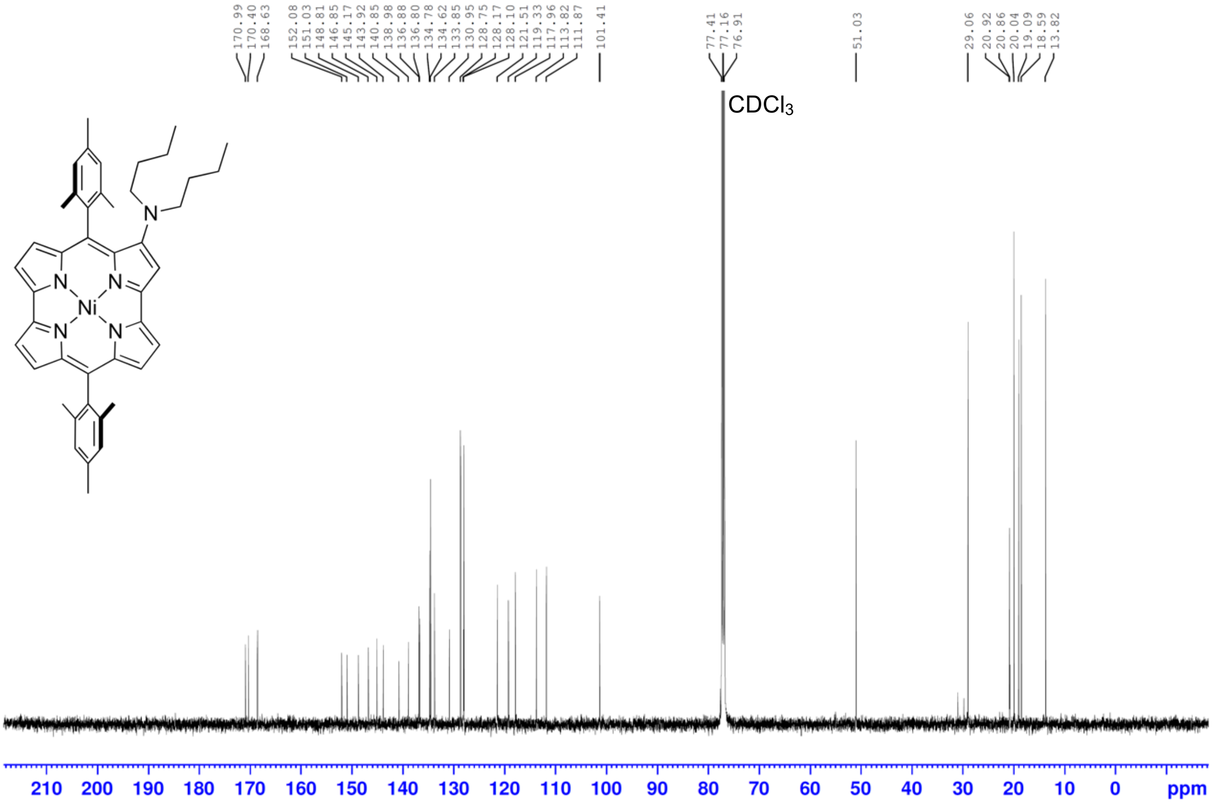

Fig S6. ^{13}C NMR (126 MHz) spectrum of **3a** in $CDCl_3$.

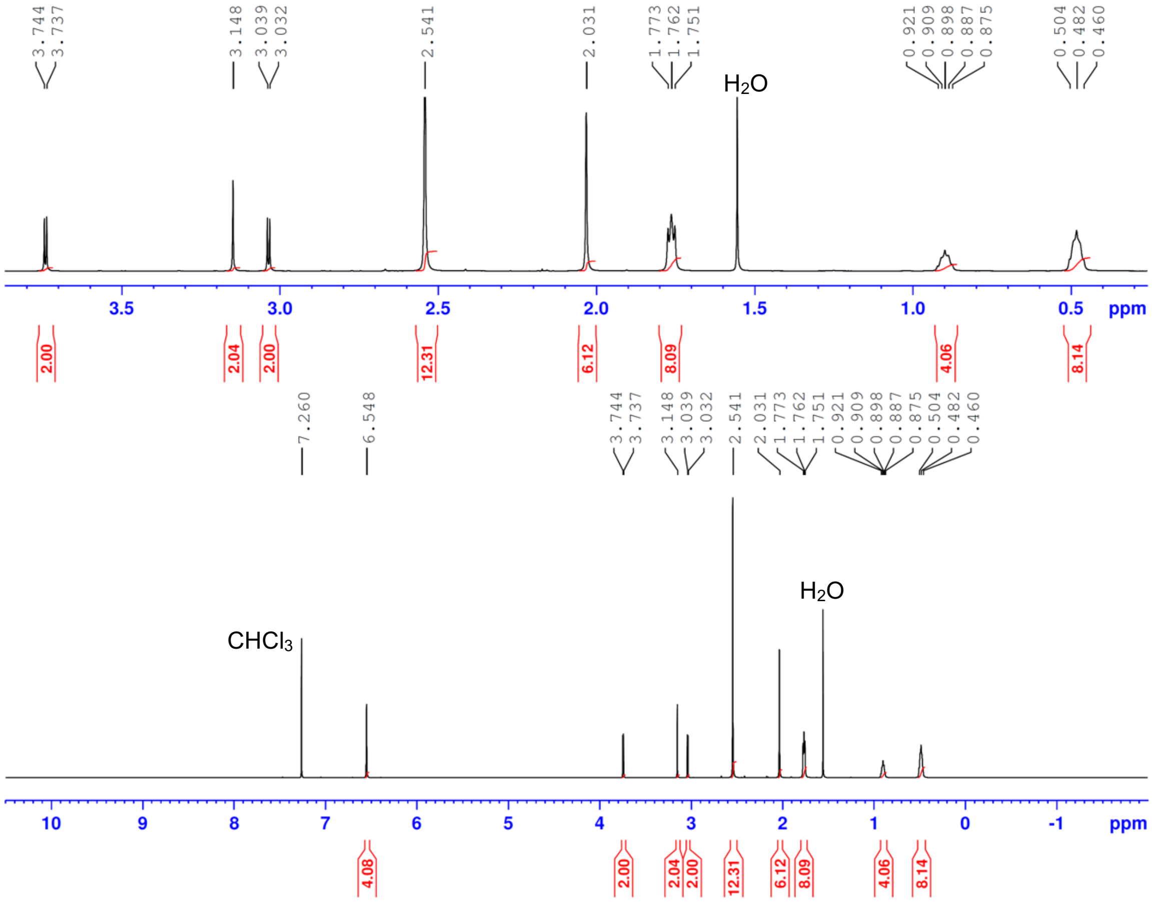

Fig S7. ^{1}H NMR (500 MHz) spectrum of **4b** in $CDCl_3$.

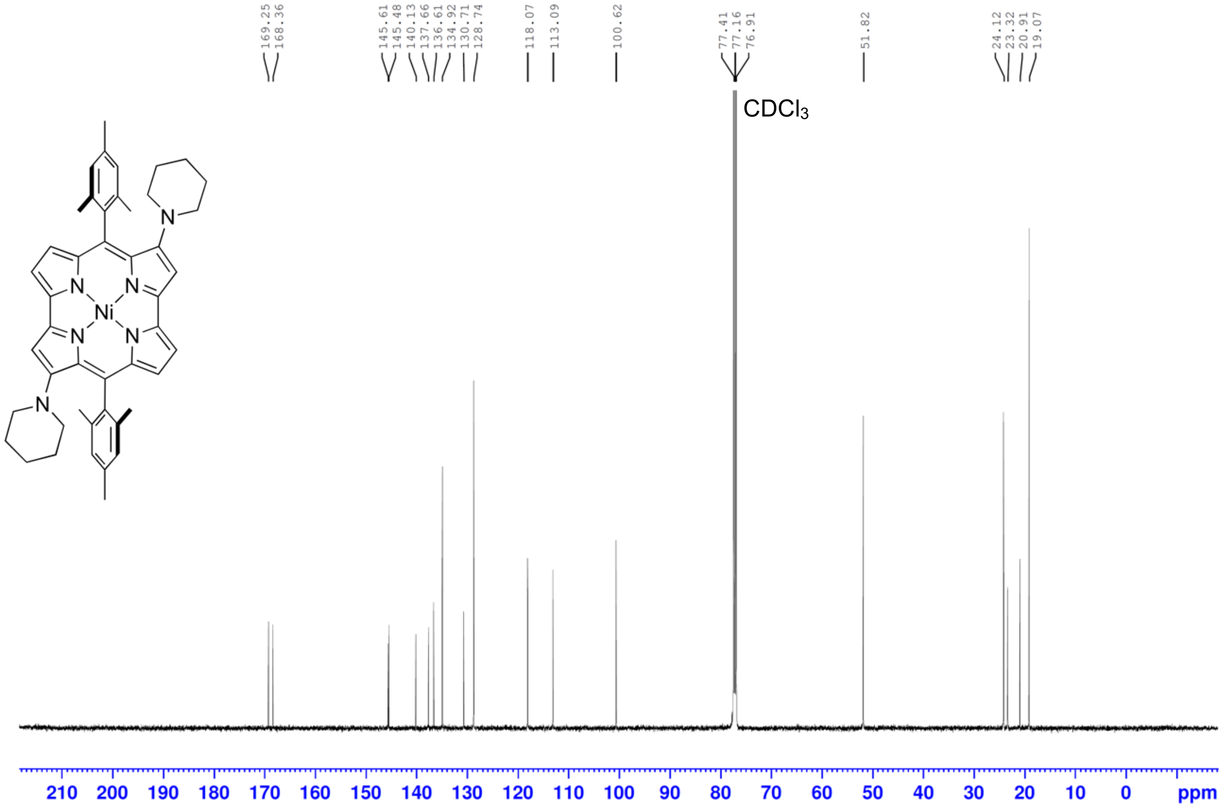

Fig S8. ^{13}C NMR (126 MHz) spectrum of **4b** in $CDCl_3$.

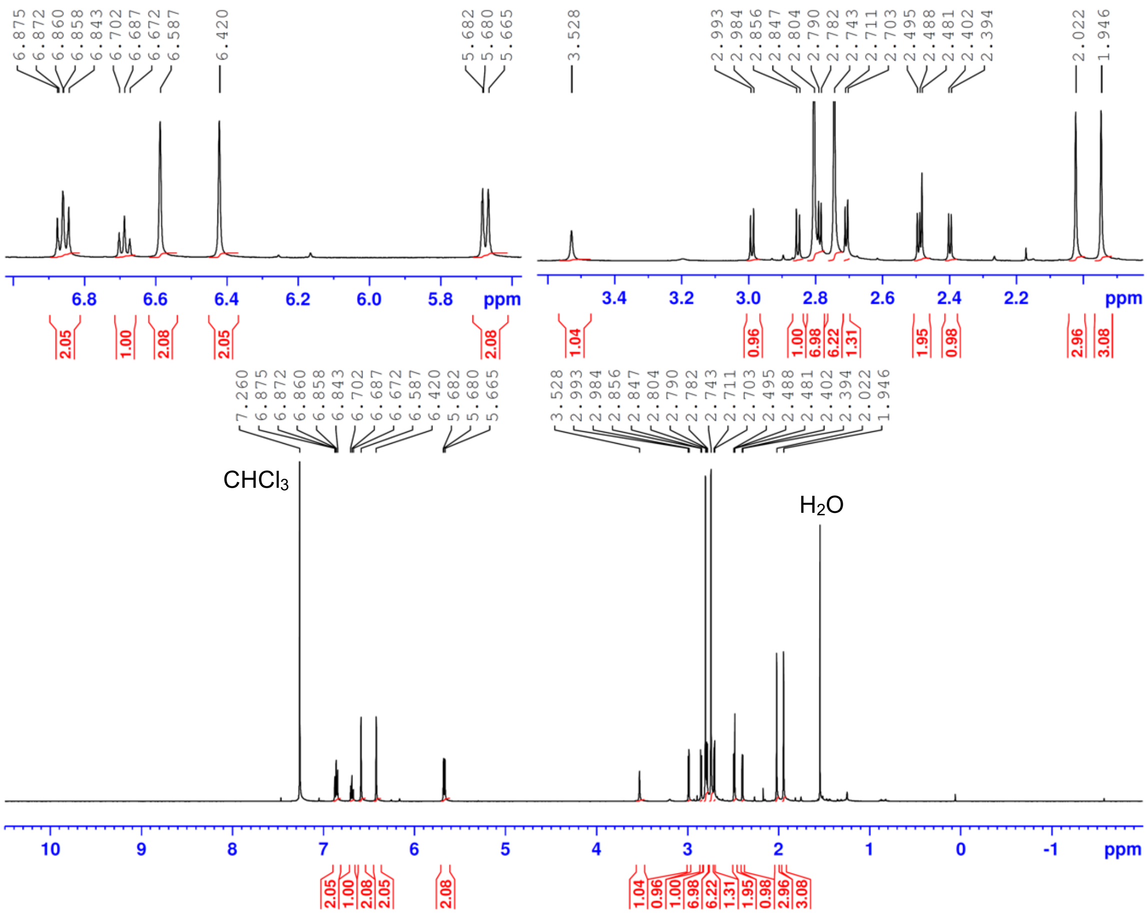

Fig S9. ^{1}H NMR (500 MHz) spectrum of **5a** in $CDCl_3$.

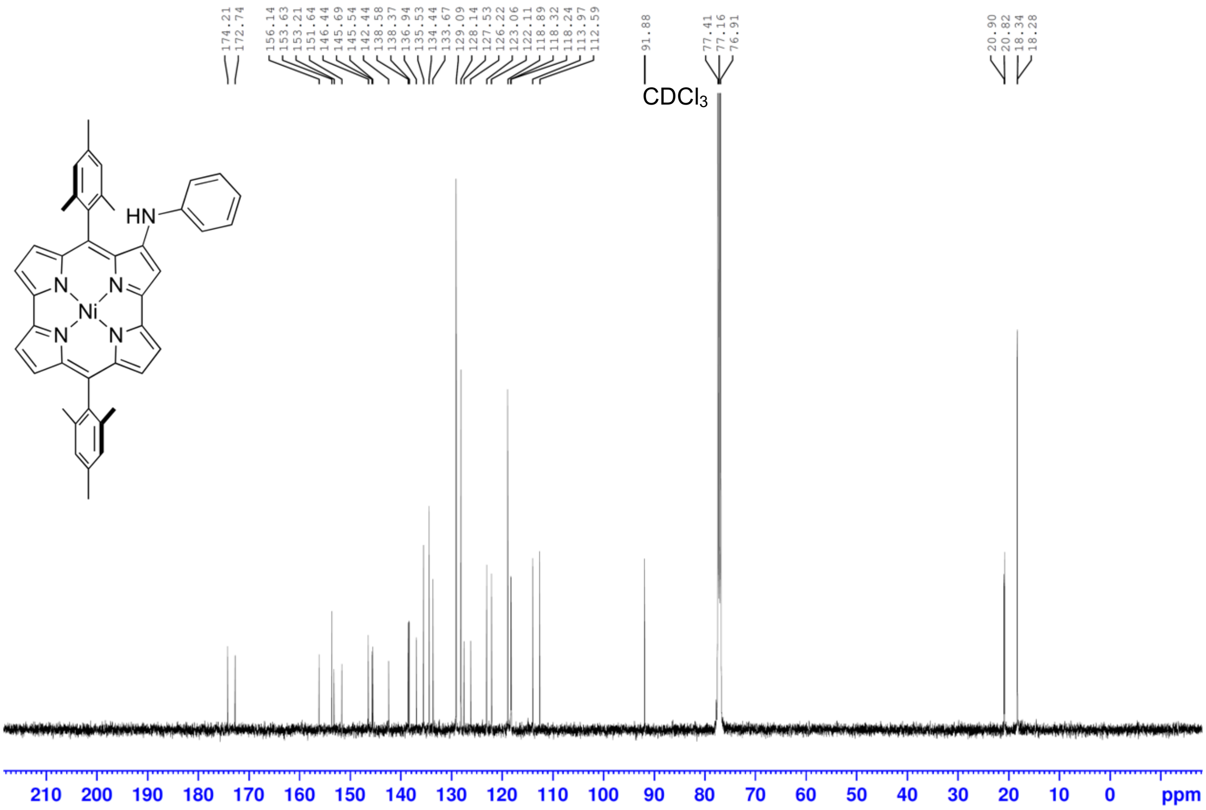

Fig S10. ^{13}C NMR (126 MHz) spectrum of **5a** in $CDCl_3$.

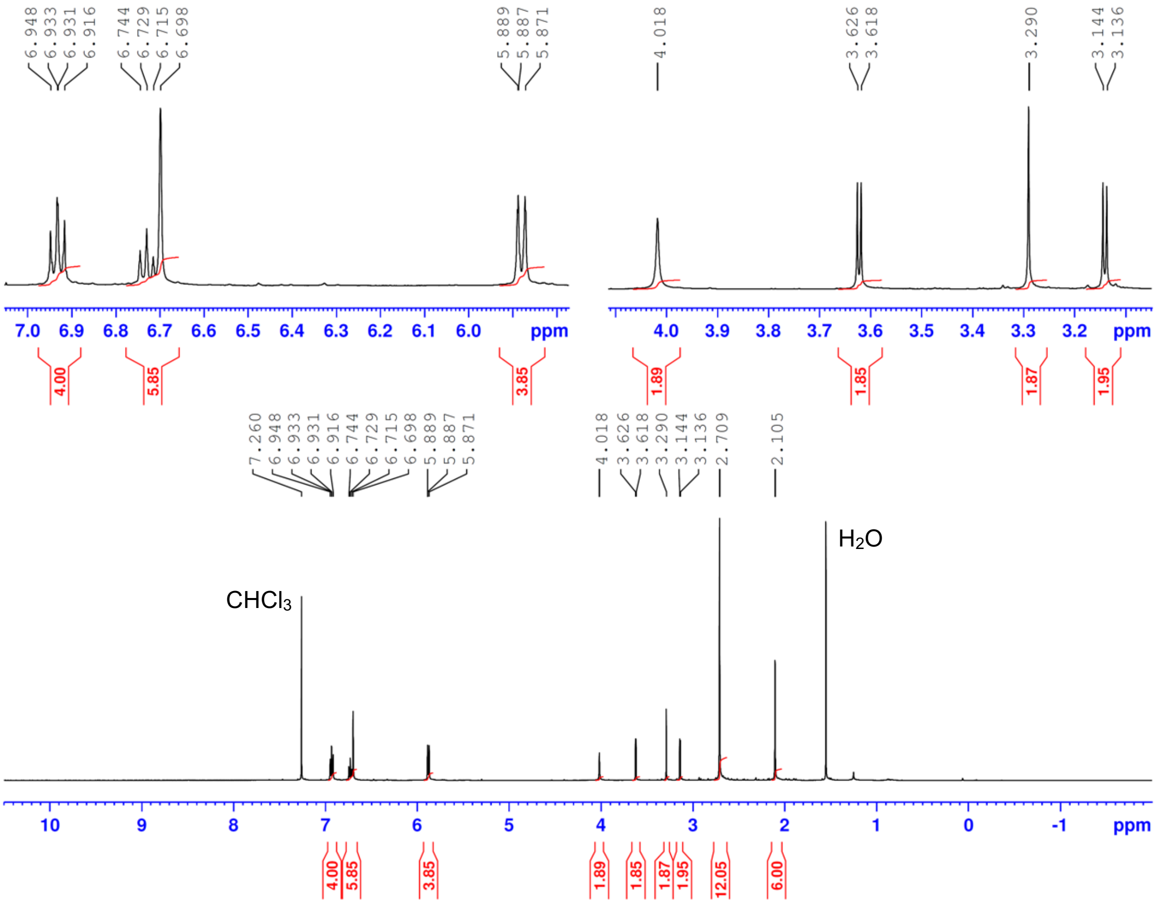

Fig S11. ^{1}H NMR (500 MHz) spectrum of **5b** in $CDCl_3$.

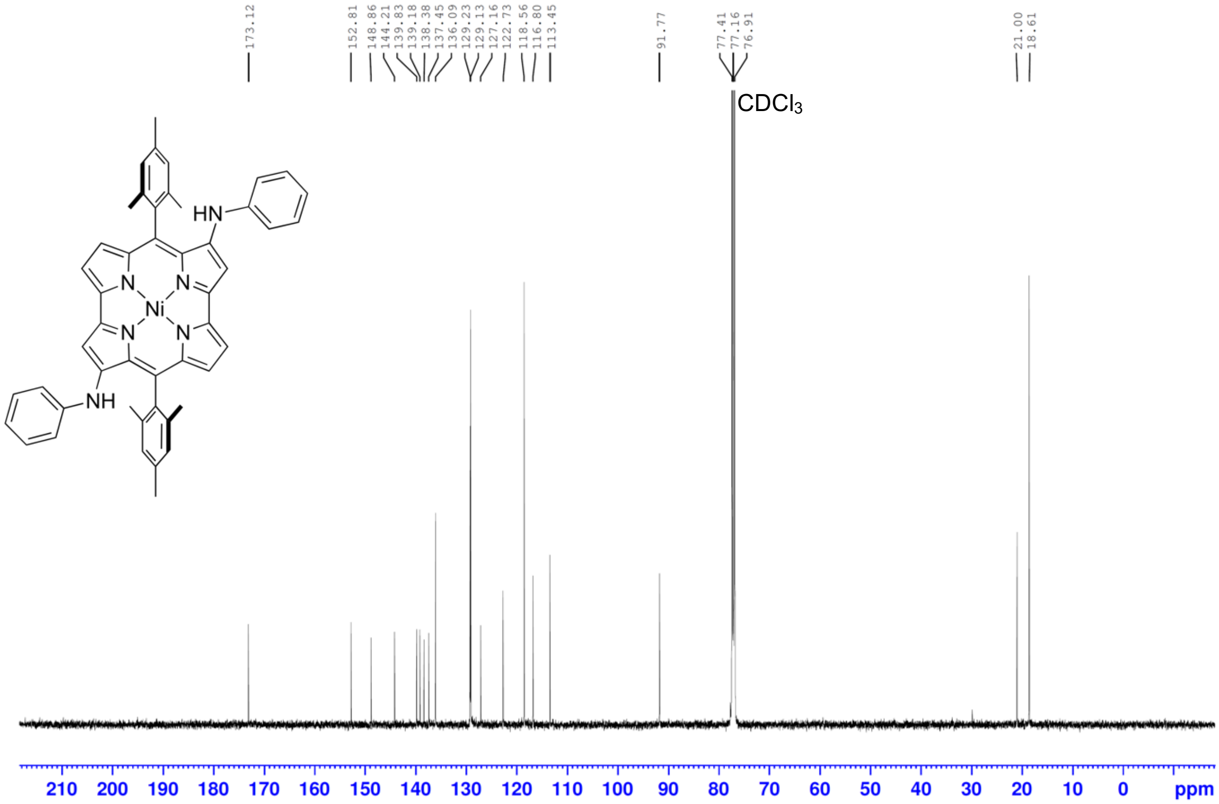

Fig S12. ^{13}C NMR (126 MHz) spectrum of **5b** in $CDCl_3$.

Cyclic Voltammograms

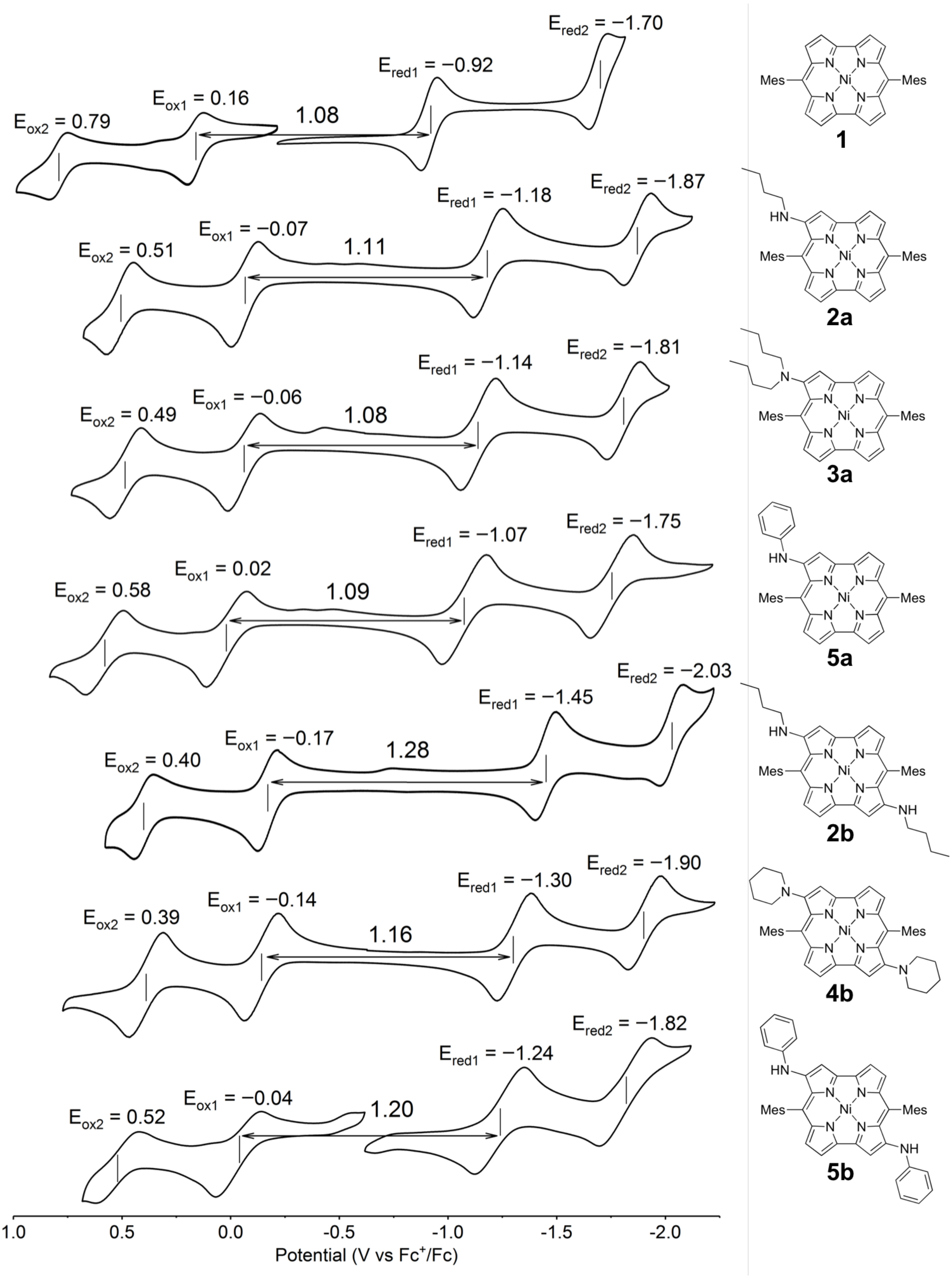

Fig S13. Cyclic voltammograms (0.1 V•s^{-1}) of **1** and **2**–**5** in CH_2Cl_2 (0.1 M $TBAPF_6$). Working electrode: grass carbon, counter electrode: Pt, reference electrode: Ag/$AgClO_4$. The data for **1** was taken from our previous paper.[1]

Theoretical Calculations

All calculations were carried out using the *Gaussian 09* program.[2] Part of the X-ray Structure of **2b** was used as initial geometries of **2a'** and **2b'**. Full optimizations were performed with Becke's three-parameter hybrid exchange functional and the Lee–Yang–Parr correlation functional (B3LYP)[3] and a basis set consisting of SDD[4] for Ni and 6-31G(d) for the rest (denoted as 6-31G(d)+SDD). The calculated absorption wavelengths and oscillator strengths were obtained with the TD-DFT method at the B3LYP/6-31G(d)+SDD level.

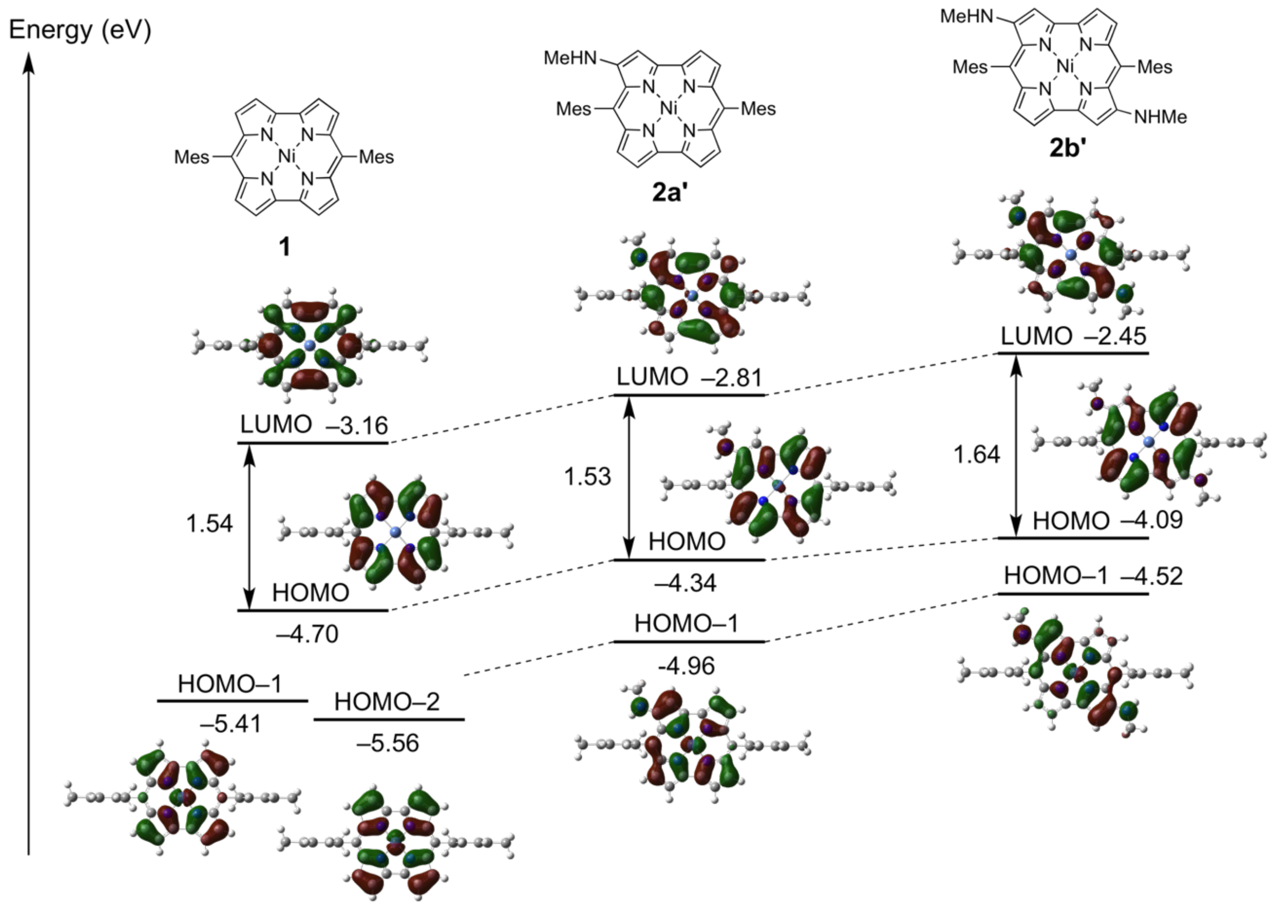

Fig S14. MO diagrams for norcorroles **1**, **2a'** and **2b'** calculated at the B3LYP/6-31G(d)+SDD level.

Table S1. Calculated exited wavelengths (λ) and oscillator strengths (*f*) of selected transitions of **2a'** and **2b'**.

Compound	λ (nm)	*f*	Composition (%)
2a'	1448	0.0022	HOMO→LUMO (100%)
	872	0.0060	HOMO→LUMO (100%)
2b'	1315	0.0000	HOMO→LUMO (100%)
	880	0.0244	HOMO→LUMO (97%)

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