Supporting Information for

A Synthesis of Novel Expanded Porphyrinoids: Ni^{II}-Induced Nitrile Cyclization of Dicyanovinylene-Bis(*meso*-Aryl)Dipyrrin

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Contents

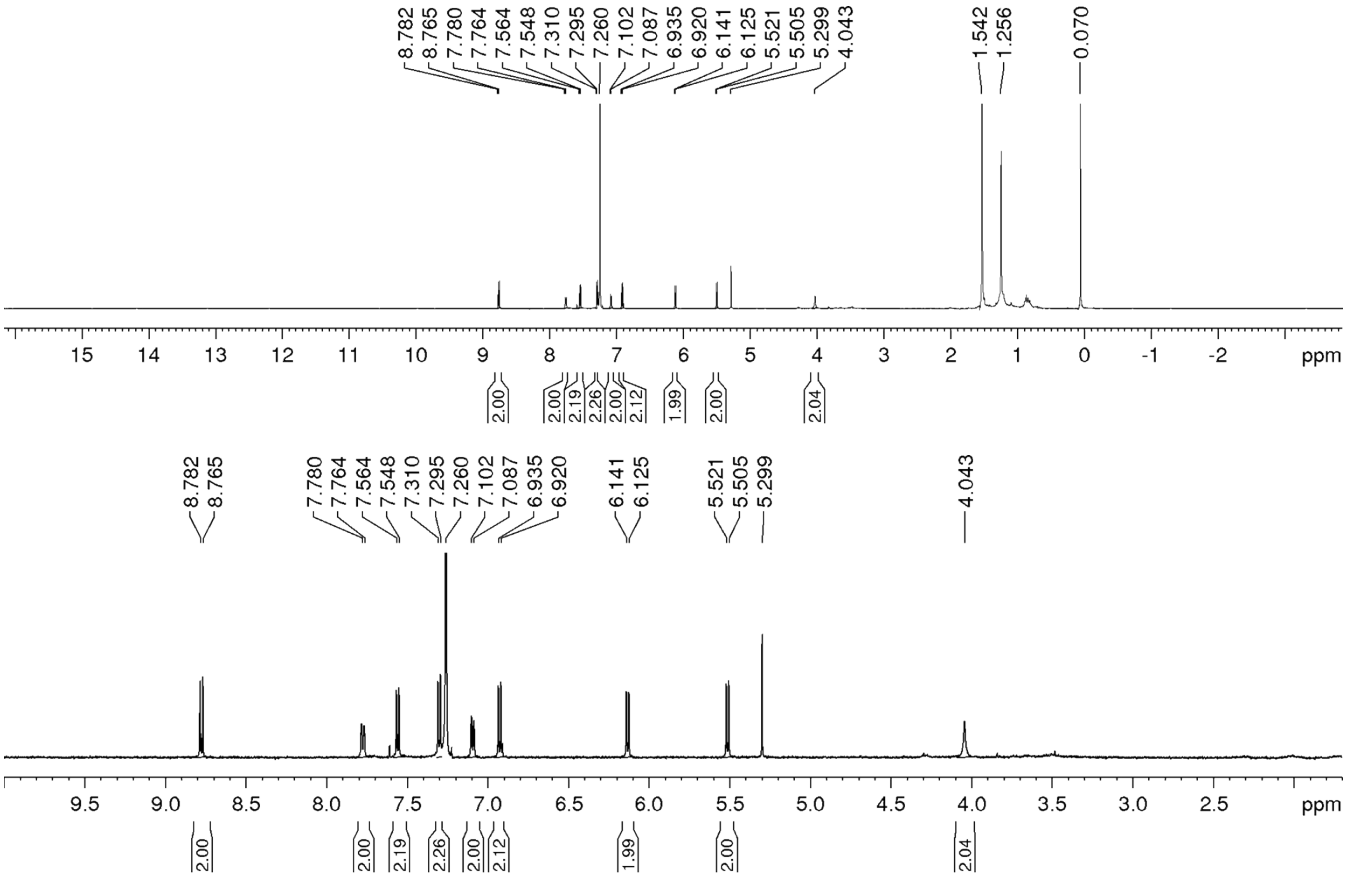

Fig. S1 ^{1}H NMR (300 MHz) spectrum of **2a** in $CDCl_3$.

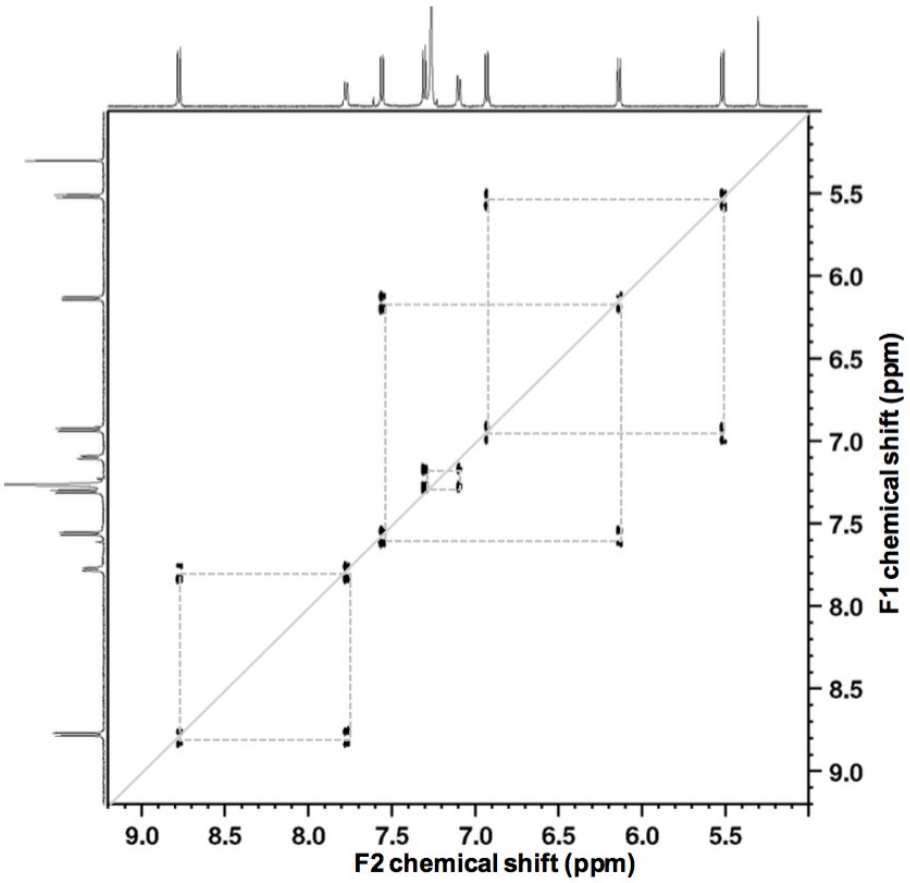

Fig. S2 HH COSY NMR (F1 = F2 = 300 MHz) spectrum of **2a** in $CDCl_3$.

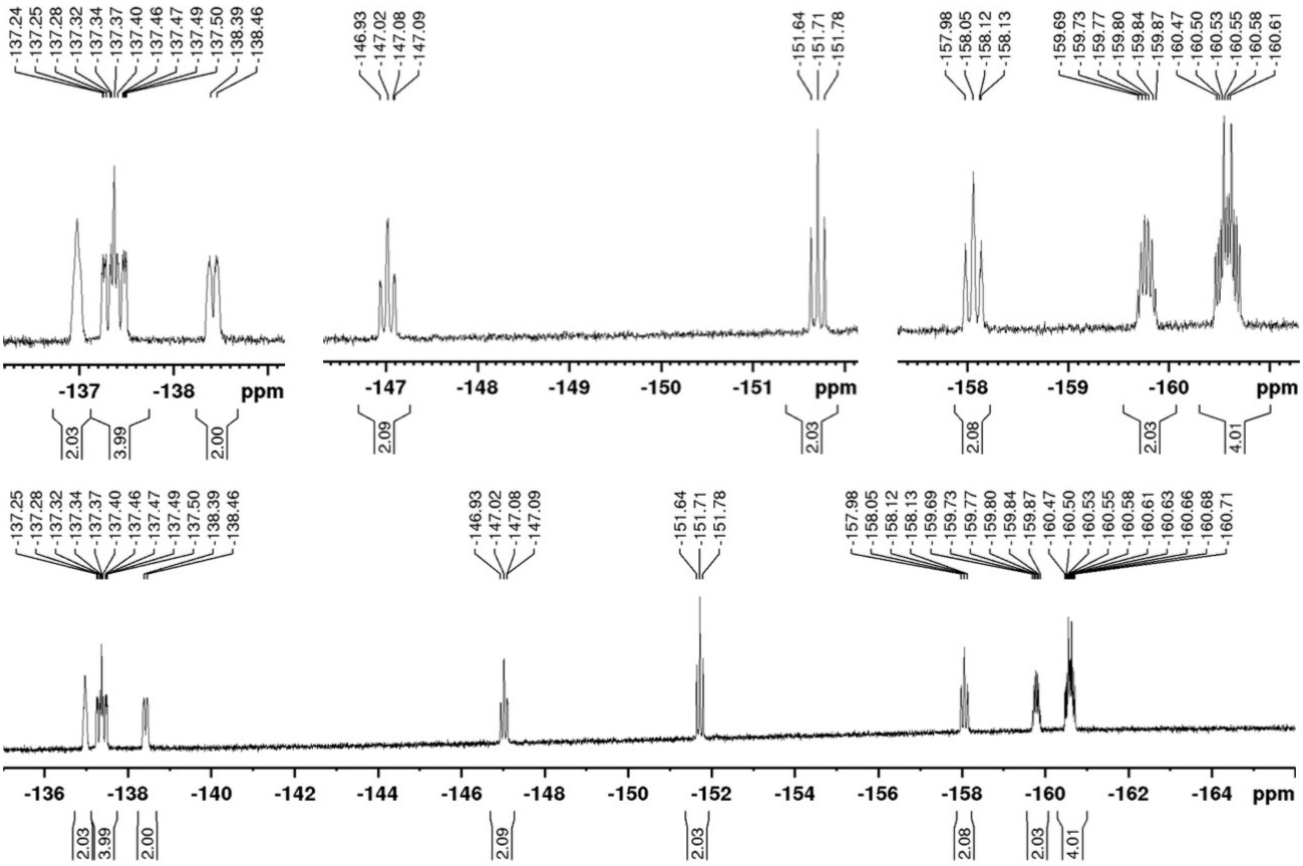

Fig. S3 ^{19}F NMR (282.4 MHz) spectrum of **2a** in $CDCl_3$.

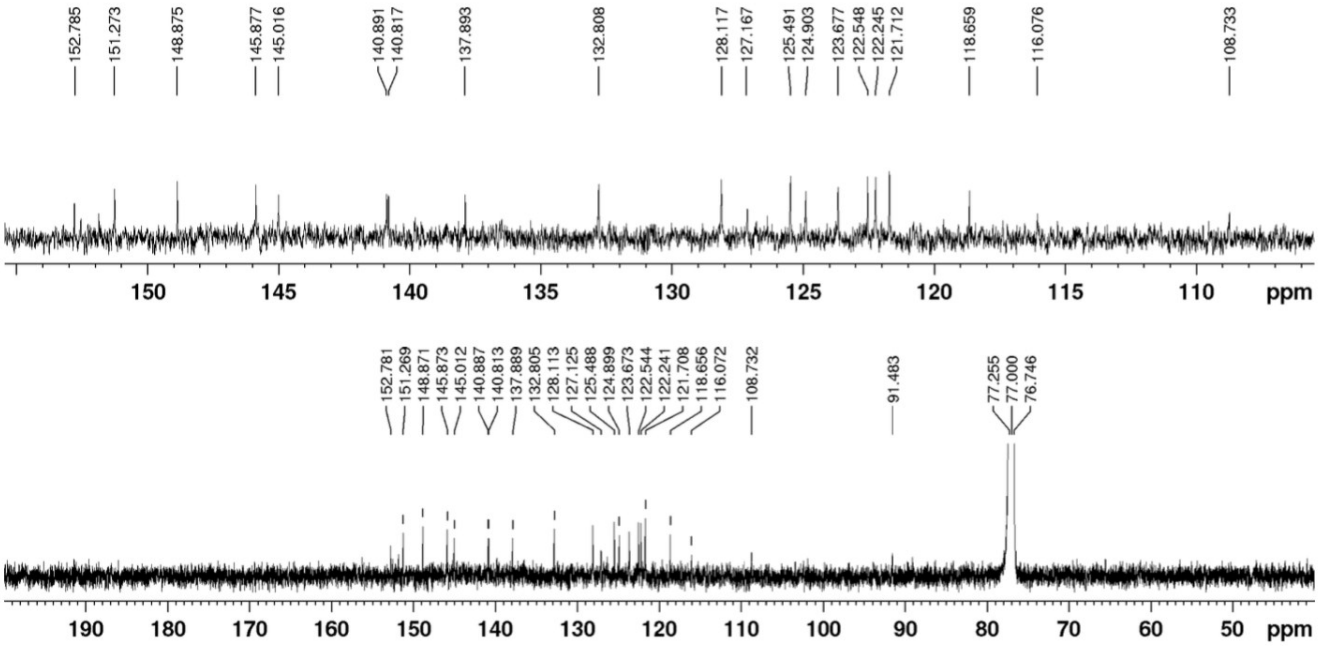

Fig. S4 ^{13}C NMR (125.8 MHz) spectrum of **2a** in $CDCl_3$.

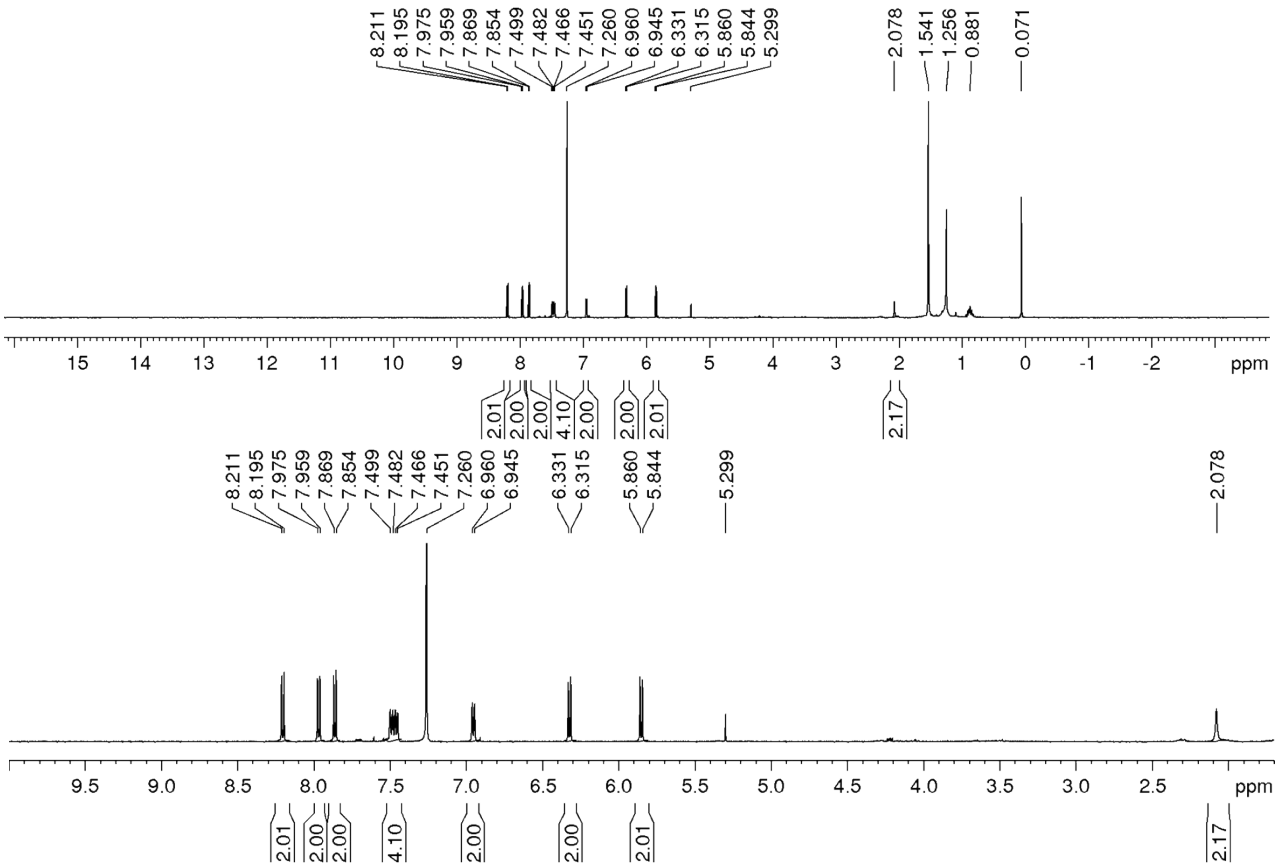

Fig. S5 ^{1}H NMR (300 MHz) spectrum of **2b** in $CDCl_3$.

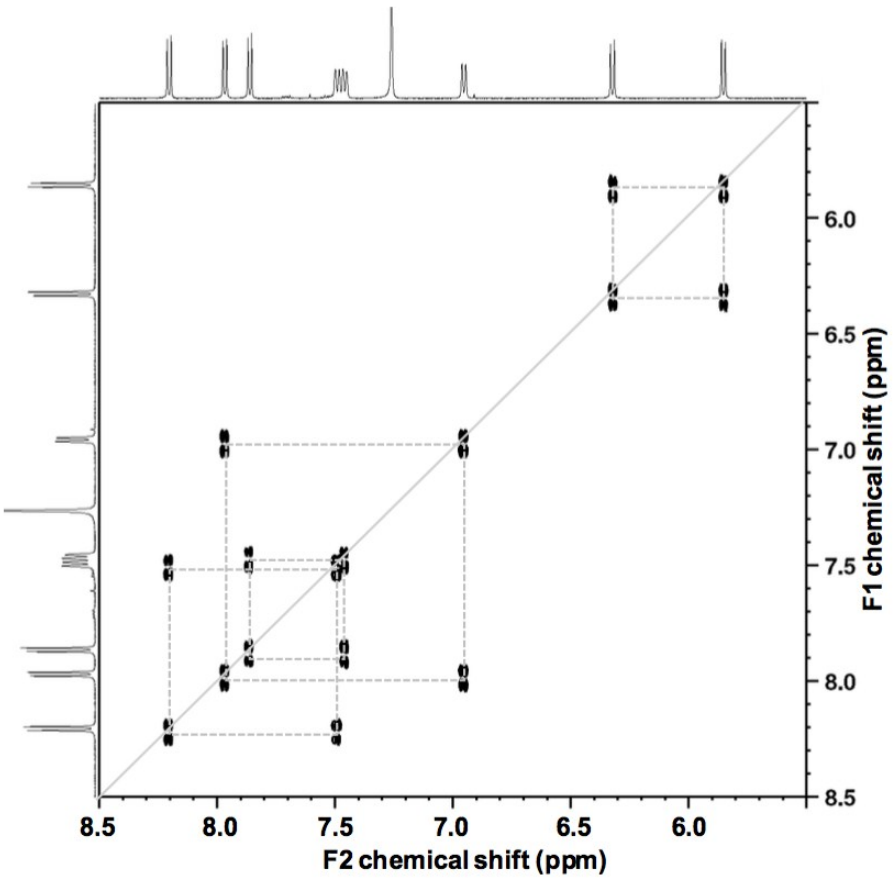

Fig. S6 HH COSY NMR (F1 = F2 = 300 MHz) spectrum of **2b** in $CDCl_3$.

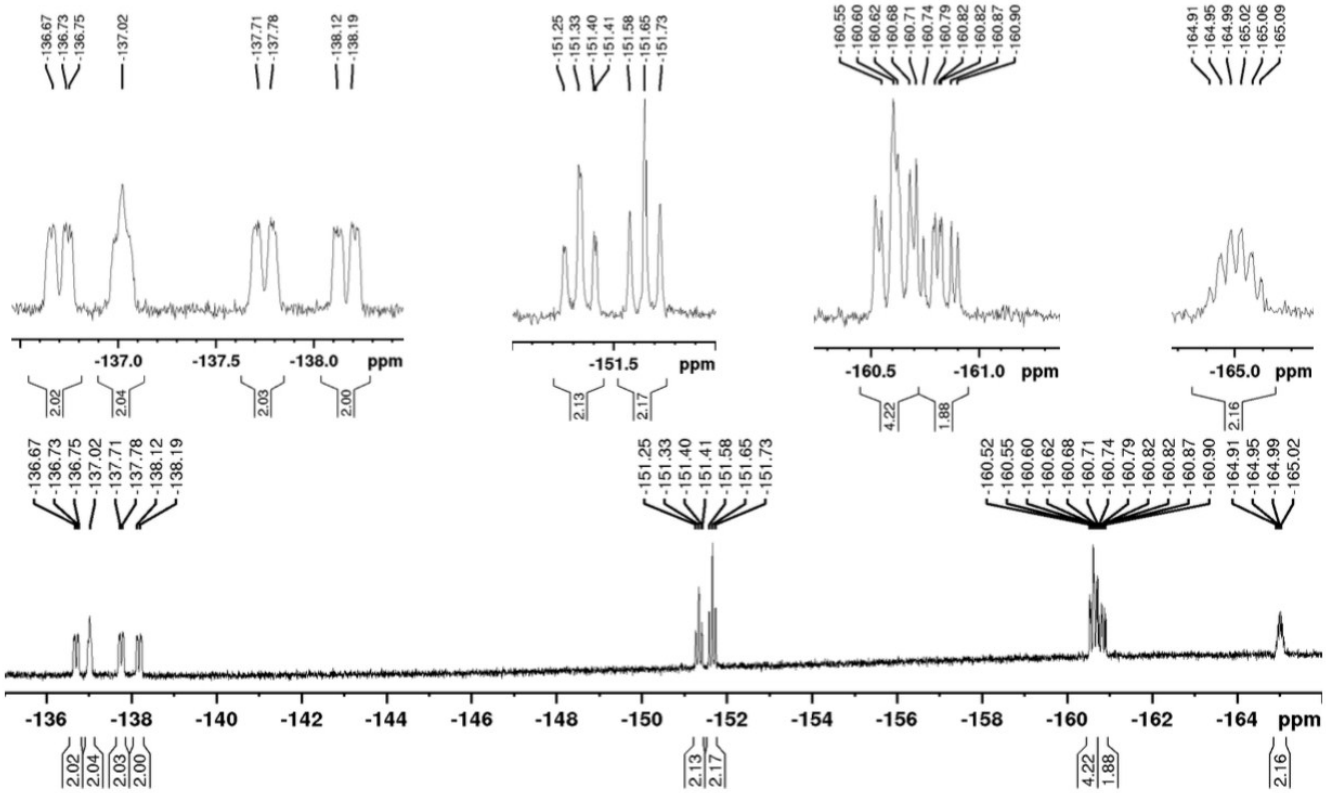

Fig. S7 ^{19}F NMR (282.4 MHz) spectrum of **2b** in $CDCl_3$.

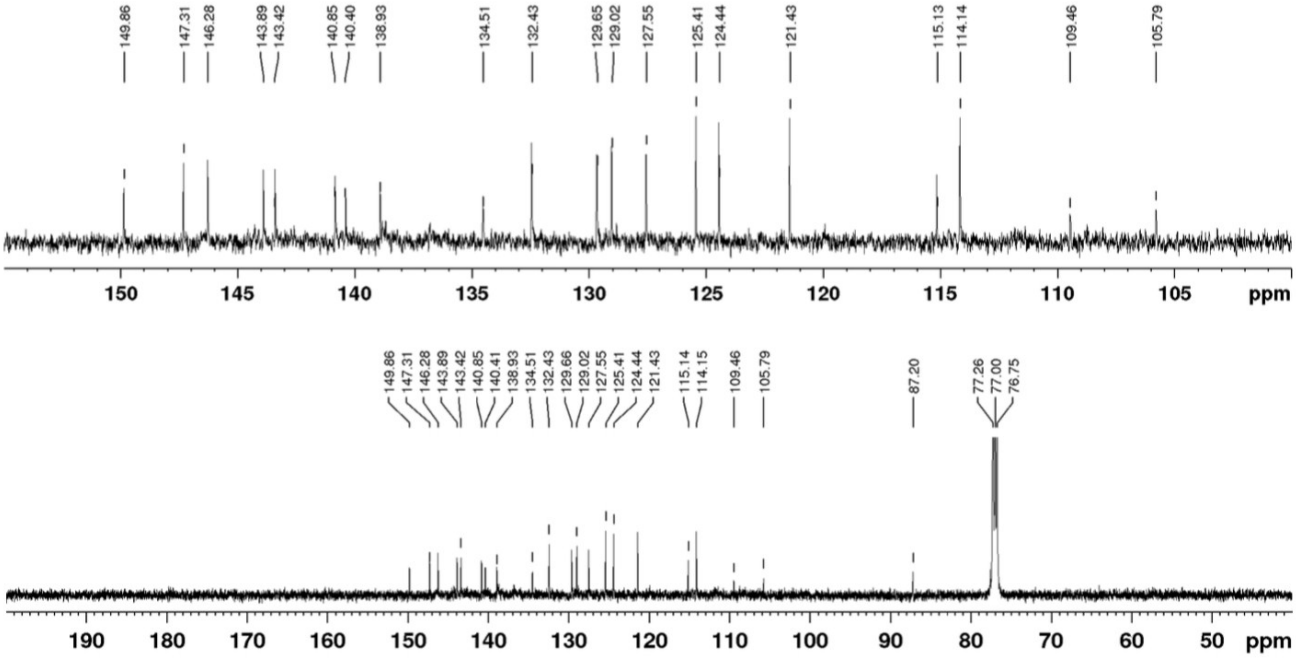

Fig. S8 ^{13}C NMR (125.8 MHz) spectrum of **2b** in $CDCl_3$.

Fig. S9 ^{1}H NMR (300 MHz) spectrum of **3** in $CDCl_3$.

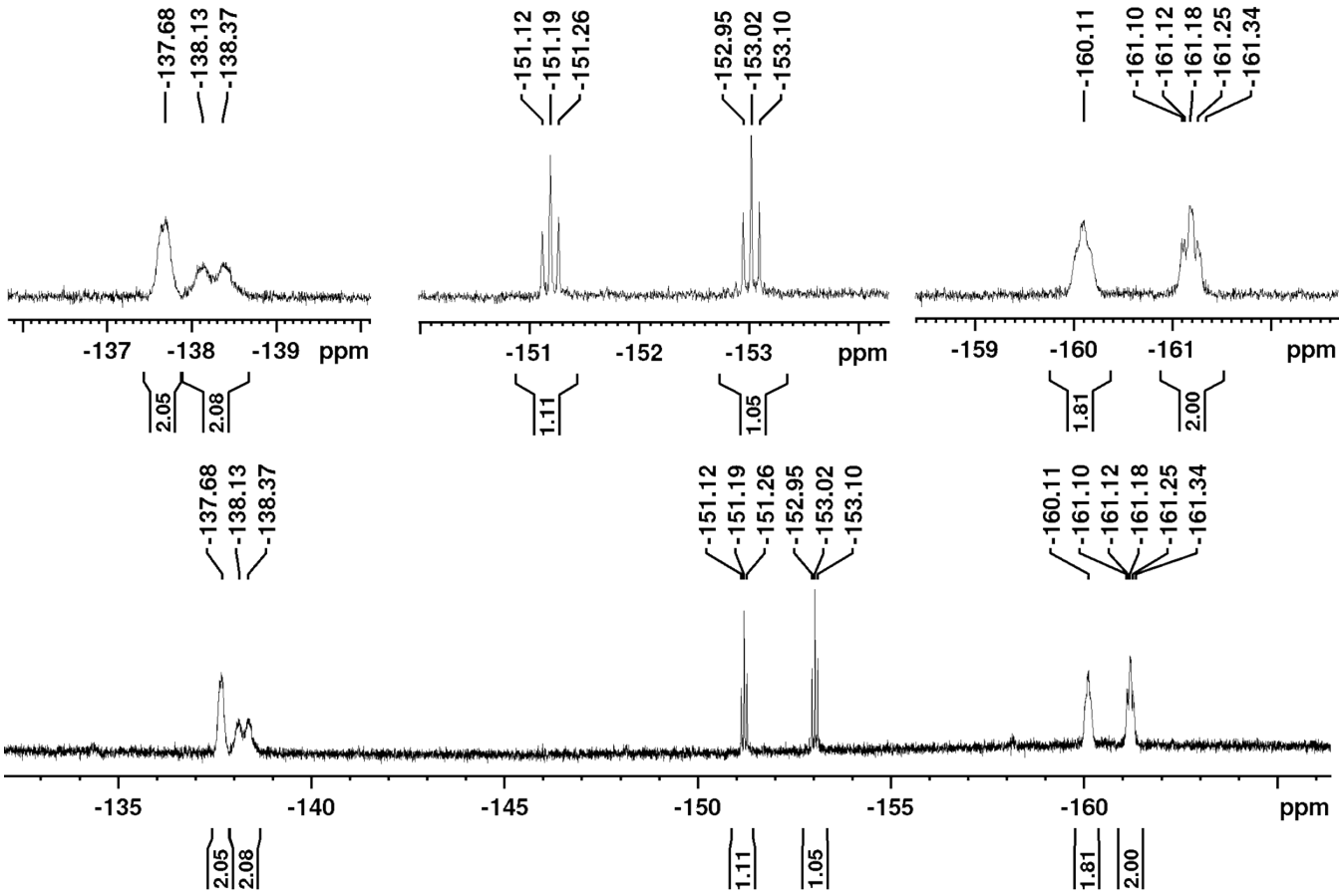

Fig. S10 ^{19}F NMR (282.4 MHz) spectrum of **3** in $CDCl_3$.

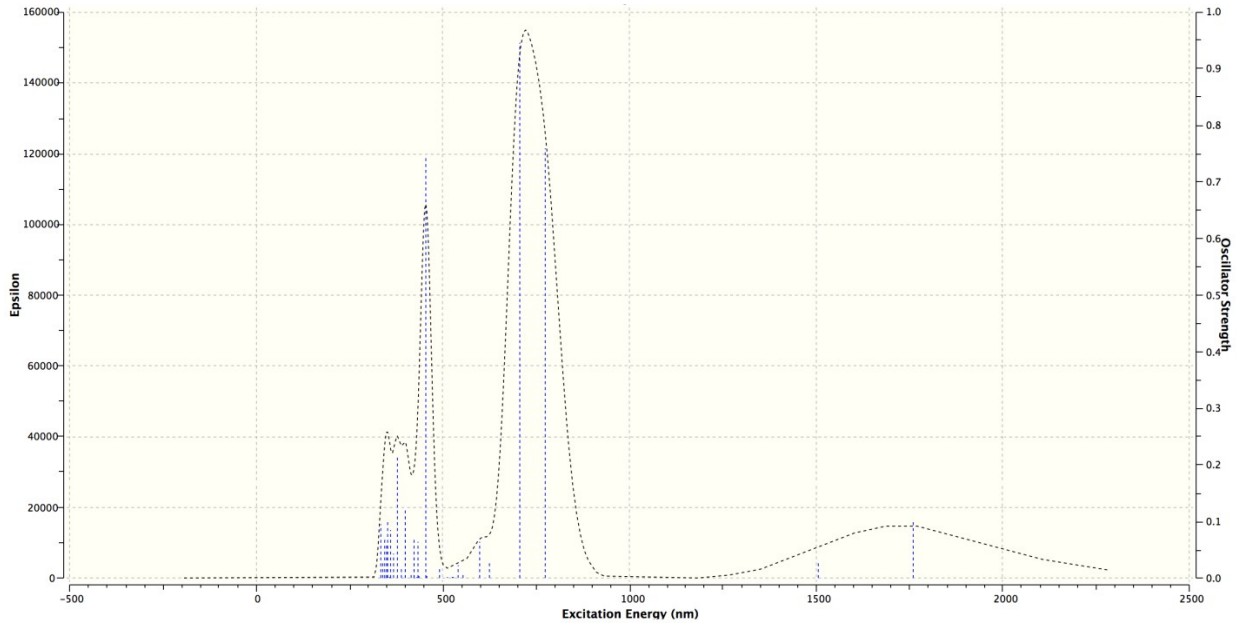

Fig. S11 Absorption spectrum obtained with TD-DFT calculation for **2a** (camB3LYP-631SDD set with CH_2Cl_2 solvent).

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 0.7046 eV 1759.72 nm f = 0.0980 <S**2> = 0.000
362 → 365 0.32120
363 → 364 0.63913
362 ← 365 0.17132

This state for optimization and/or second-order correction.
Total Energy, E (TD-HF / TD-KS) = –5595.30579814
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 0.8238 eV 1505.08 nm f = 0.0273 <S**2> = 0.000
362 → 364 0.64198
363 → 365 –0.29679
363 ← 365 –0.14402

Excited State 3: Singlet-A 1.6015 eV 774.16 nm f = 0.7597 <S**2> = 0.000
362 → 364 0.30891
362 → 365 0.11234
363 → 365 0.64045
362 ← 364 –0.15041

Excited State 4: Singlet-A 1.7578 eV 705.34 nm f = 0.9472 <S**2> = 0.000
362 → 365 0.62565
363 → 364 –0.33436
363 → 365 –0.10457
363 ← 364 0.16375

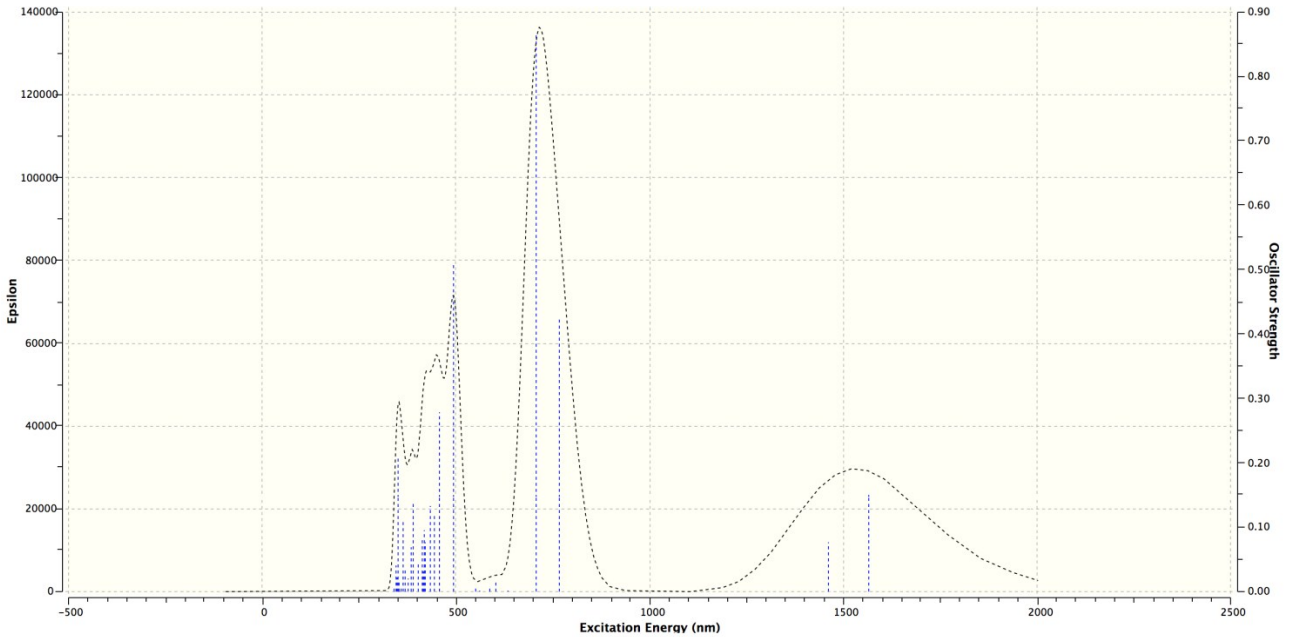

Fig. S14 Absorption spectrum obtained with TD-DFT calculation for **2b** (camB3LYP-631SDD set with CH_2Cl_2 solvent).

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 0.7919 eV 1565.58 nm f = 0.1529 <S**2> = 0.000
362 → 364 –0.34259
362 → 365 0.21181
363 → 364 0.56113
363 → 365 0.17674
362 ← 365 0.11595
This state for optimization and/or second-order correction.
Total Energy, E (TD-HF / TD-KS) = –5595.31143993
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 0.8489 eV 1460.55 nm f = 0.0766 <S**2> = 0.000
362 → 364 0.50311
362 → 365 0.11311
363 → 364 0.36256
363 → 365 –0.32931
363 <- 365 -0.11547

Excited State 3: Singlet-A 1.6145 eV 767.94 nm f = 0.4268 <S**2> = 0.000
362 → 364 0.36033
362 → 365 –0.18059
363 → 365 0.58230
362 ← 364 –0.13951

Excited State 4: Singlet-A 1.7531 eV 707.23 nm f = 0.8677 <S**2> = 0.000
362 → 364 0.12777
362 → 365 0.64365
363 → 364 –0.22731
363 → 365 0.16575
363 ← 364 0.14310