Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

SUPPORTING INFORMATION

Corrole isomers: intrinsic gas-phase shapes *via* travelling wave ion mobility mass spectrometry and dissociation chemistries *via* tandem mass spectrometry

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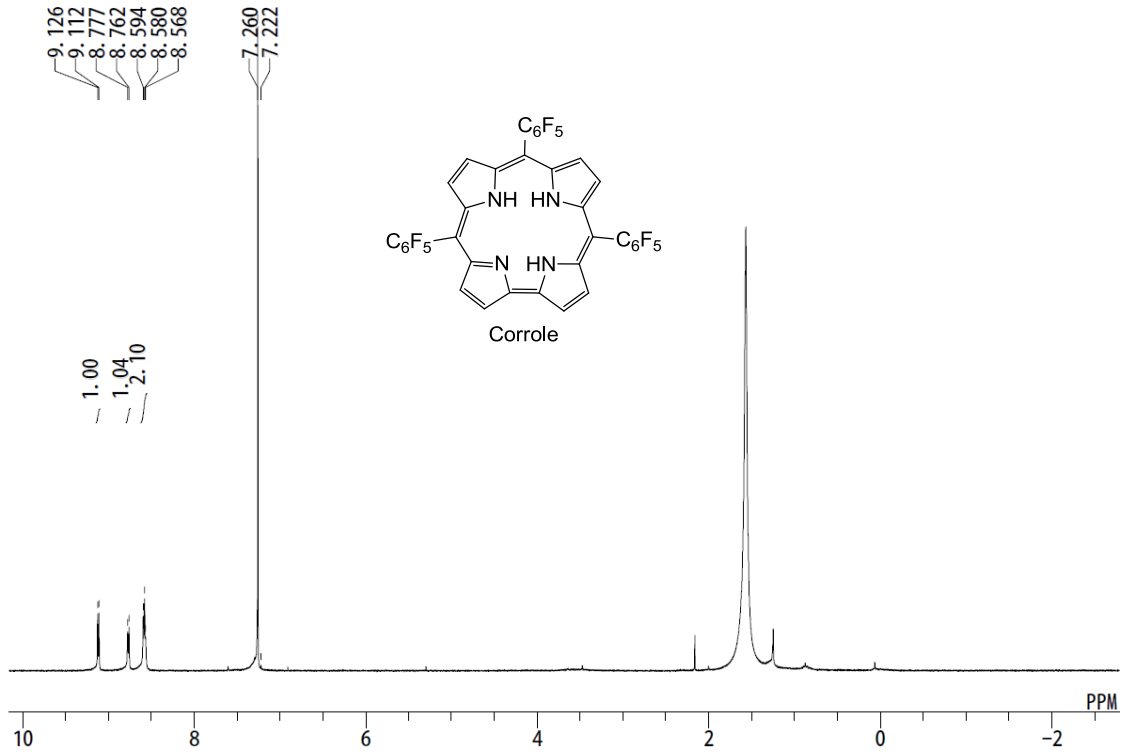
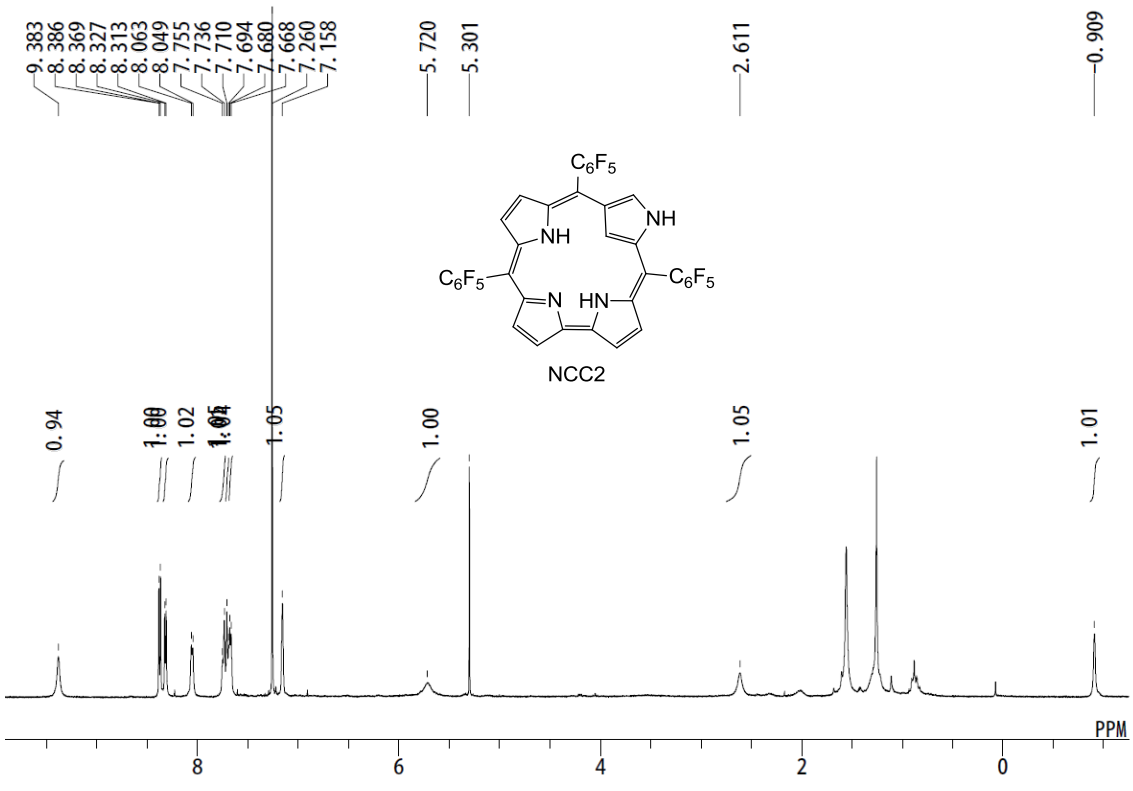
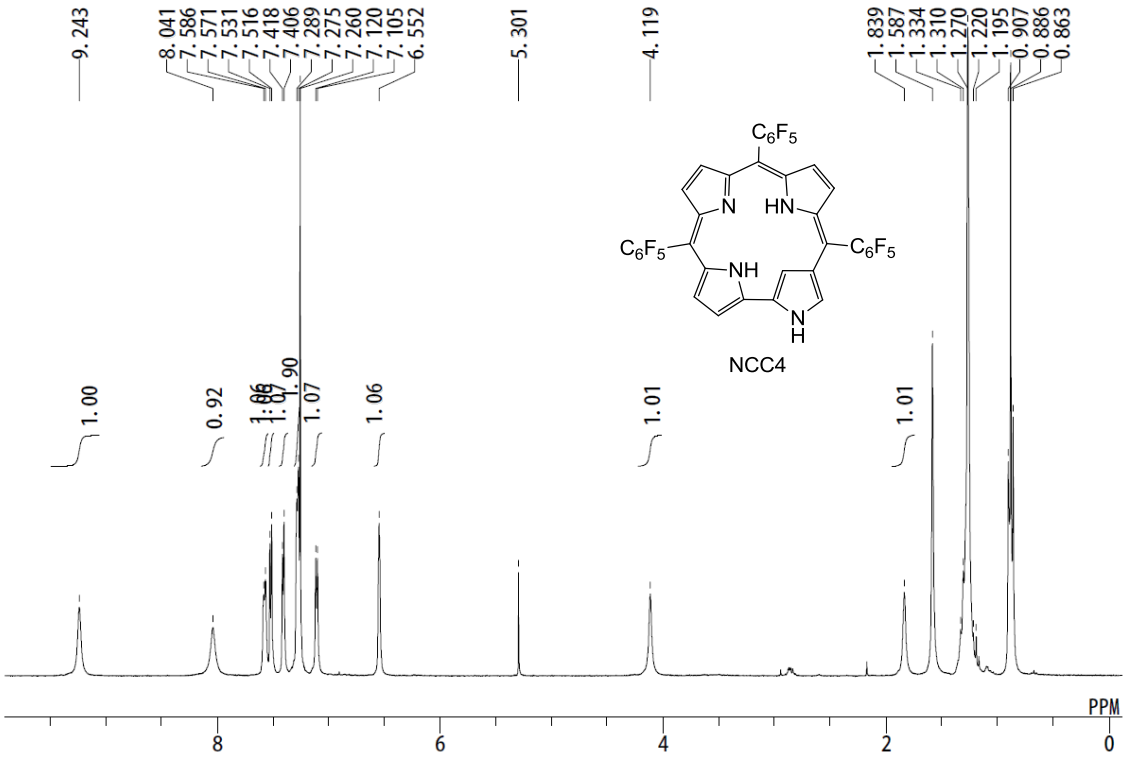
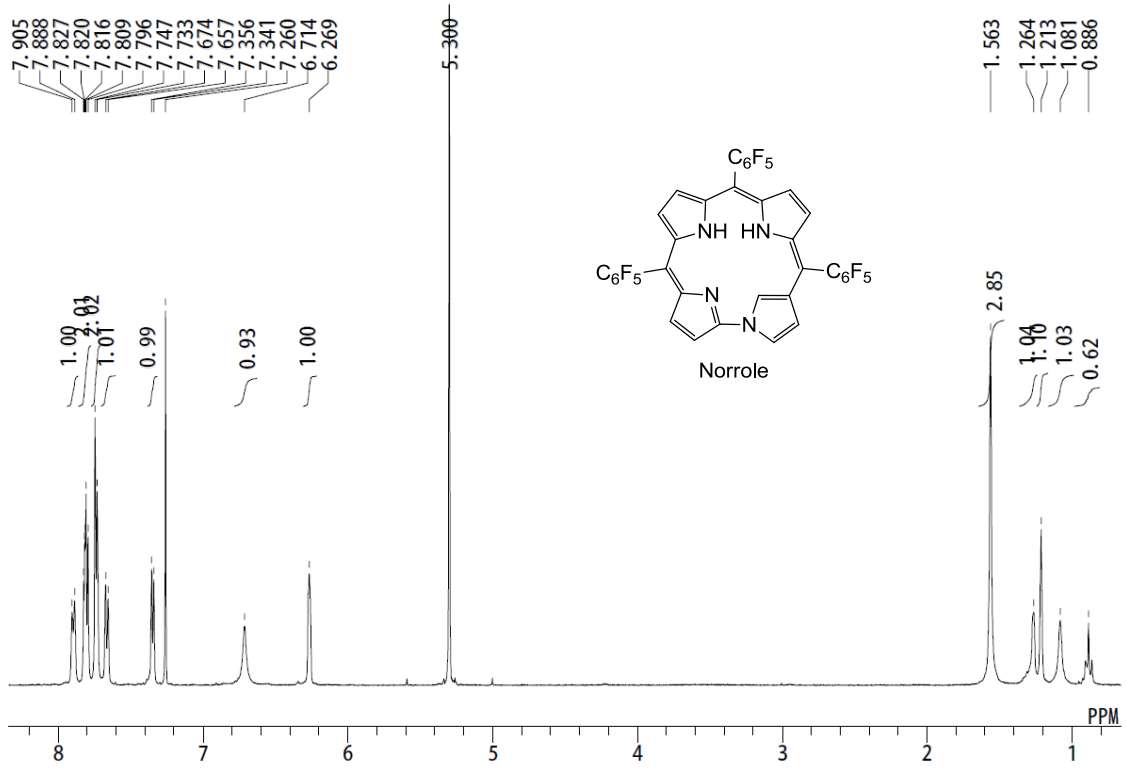
Contents

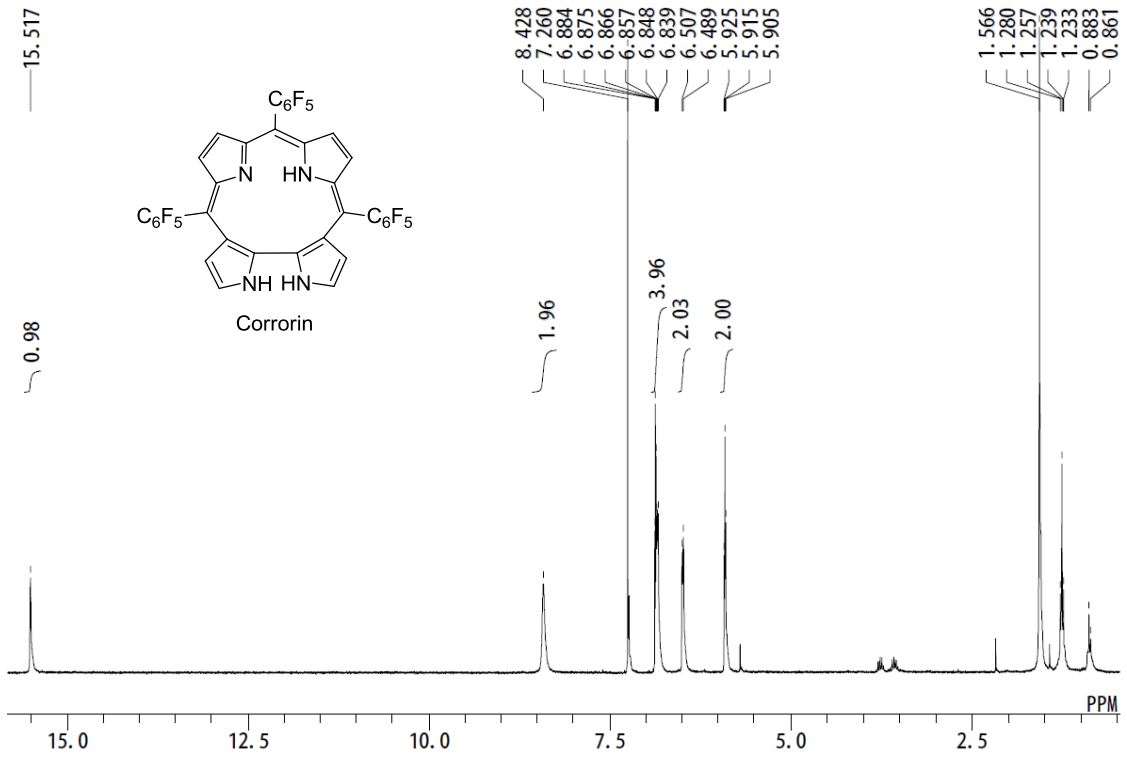
^{1}H NMR spectra of all compounds.





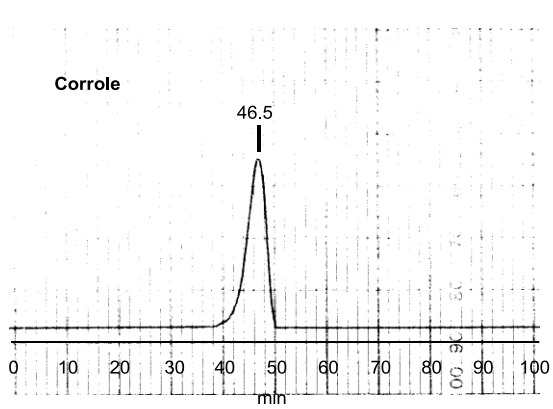


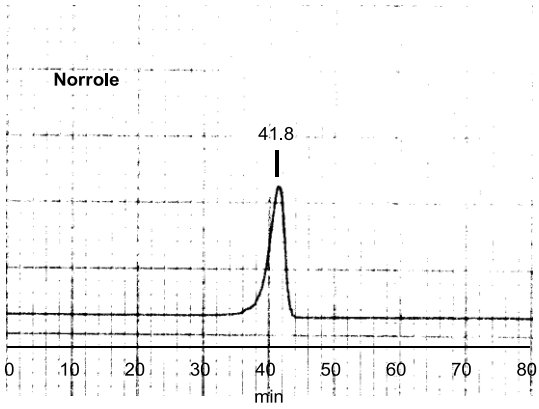


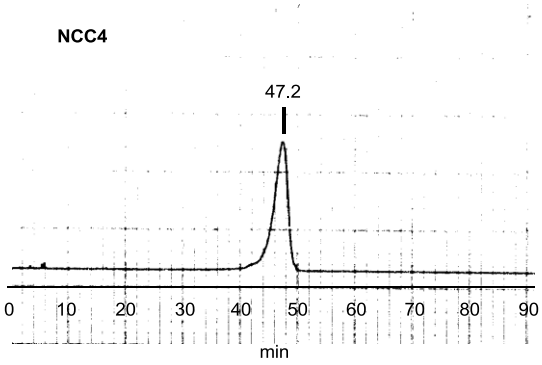


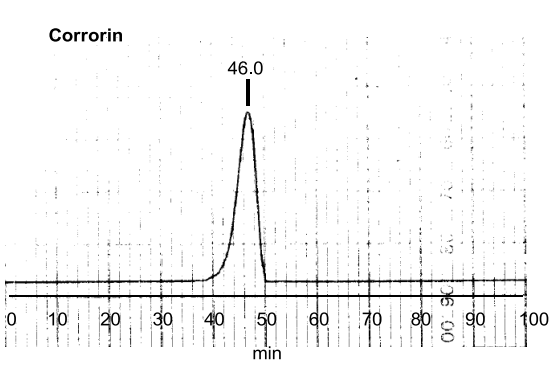
^{1}H NMR spectra were recorded in CDCl3 solution on a JNM-AL SERIES FT-NMR spectrometer (JEOL) at 300 MHz, and chemical shifts were reported relative to a residual proton of a deuterated solvent, CHCl3 (δ = 7.26) in ppm.

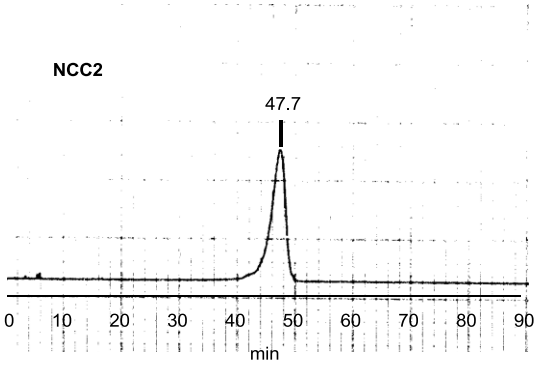
HPLC traces of all compounds with their retention time.





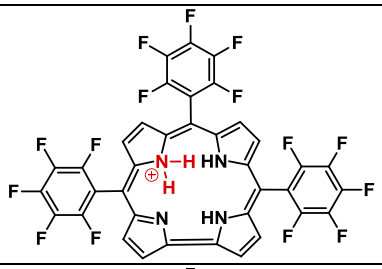
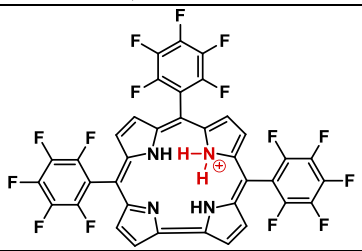
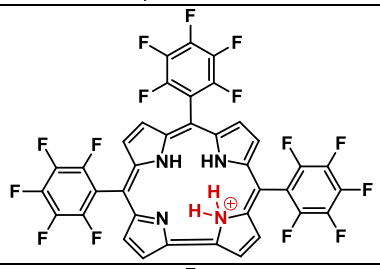
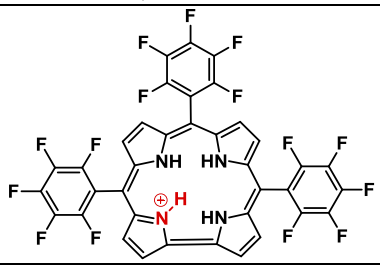




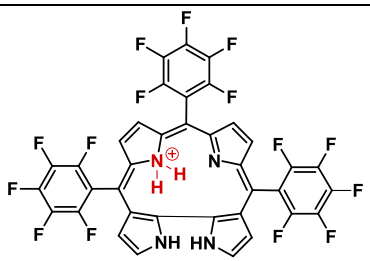
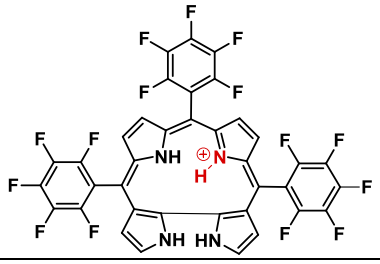
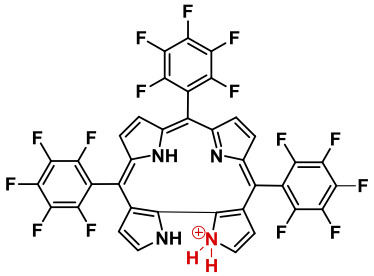
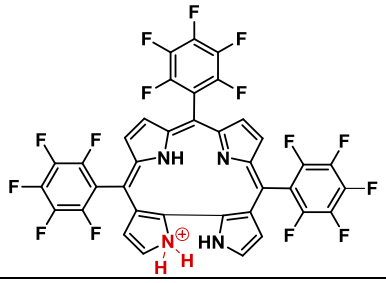


HPLC experiments were performed on a LC-9201R unit composed of a PI-50 pump 3702 UV-detector and JAIGEL-SH-043-15 column filled with silica gel (Japan Analytical Industry Co., Ltd). Eluent was CH_2Cl_2/CH_3OH = 99/1, and flow rate was 3.5 ml/min for all experiments.

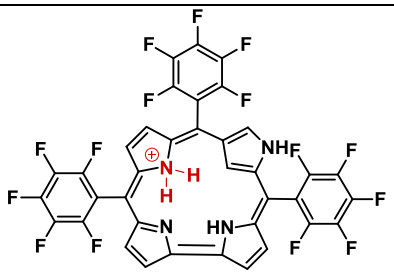
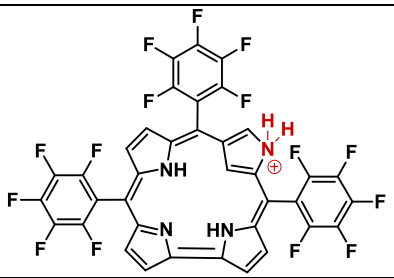
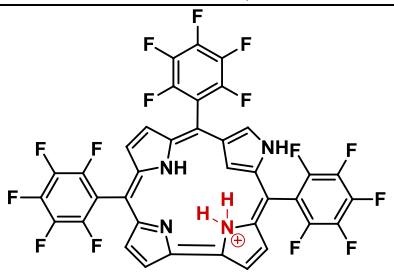
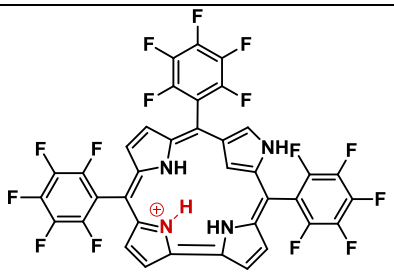
Table S1. Energy optimization (equilibrium geometry) estimated by the Gaussian03 program, for ions representing all possible protonation sites of each isomer.

Species	Structure	E (hartree)	$E_{NORMALIZED}$ (kcal mol^{-1})
Corrole_A*		–	–
Corrole_B		-3133.3353351	**+37.82**
Corrole_C		-3133.3444112	**+32.12**
Corrole_D		-3133.3956063	**0.00**

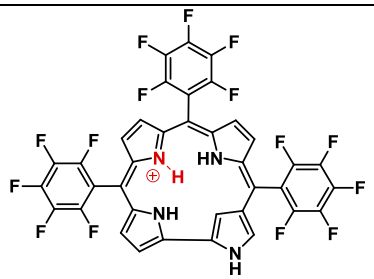
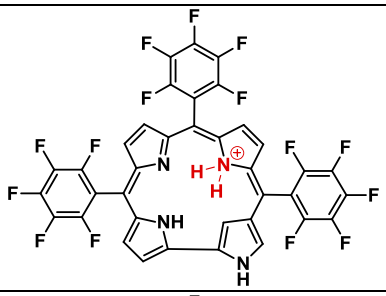
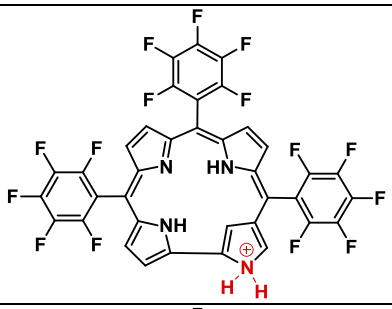
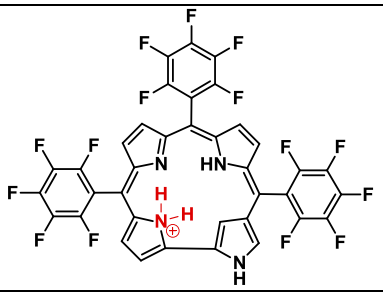
***Species **Corrole_A** is unstable and isomerizes to **Corrole_D** during geometry optimization.

Species	Structure	E (hartree)	$E_{NORMALIZED}$ (kcal mol^{-1})
Corrorin_A*		–	–
Corrorin_B		-3133.3780051	**0.00**
Corrorin_C		-3133.3004419	**+48.67**
Corrorin_D		-3133.3005566	**+48.60**

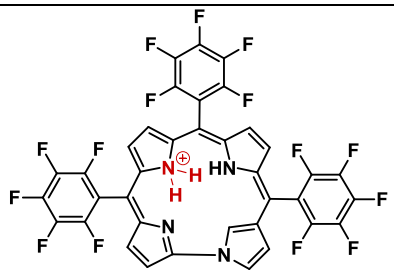
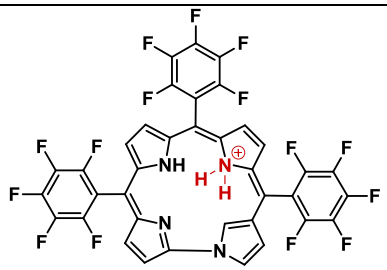
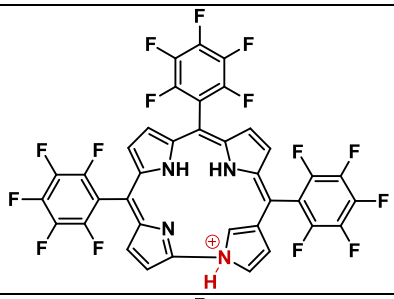
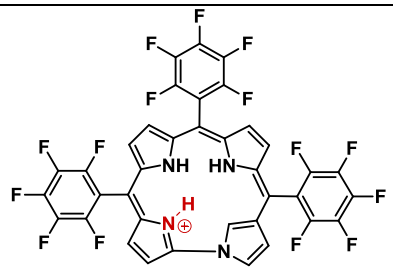
***Species **Corrorin_A** is unstable and isomerizes to **Corrorin_B** during geometry optimization.

Species	Structure	E (hartree)	$E_{NORMALIZED}$ (kcal mol^{-1})
NCC2_A*		-3133.3407083	**+25.01**
NCC2_B		-3133.3084771	**+45.24**
NCC2_C		-3133.3330736	**+29.81**
NCC2_D		-3133.3805720	**0.00**

***Species **NCC2_A** is unstable and isomerizes to **NCC2_D** during geometry optimization.

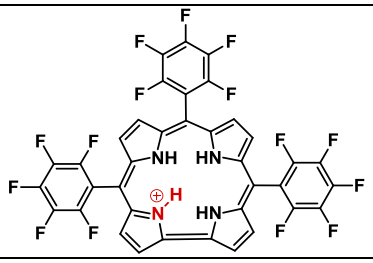
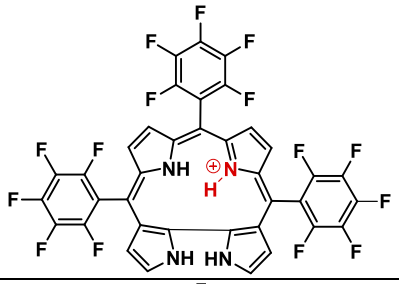
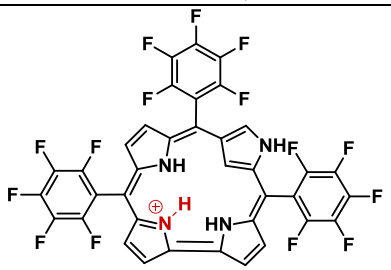
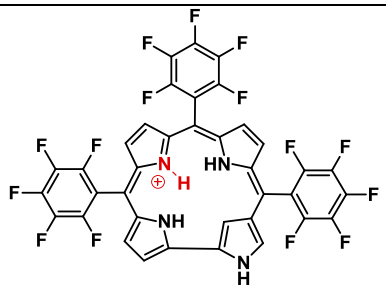
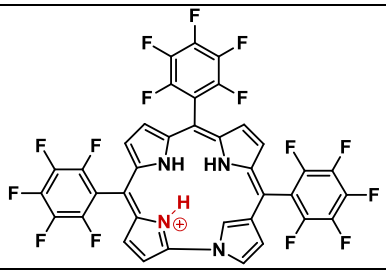
Species	Structure	E (hartree)	$E_{NORMALIZED}$ (kcal mol^{-1})
NCC4_A		-3133.3769576	**0.00**
NCC4_B		-3133.3309288	**+28.88**
NCC4_C		-3133.3039268	**+45.83**
NCC4_D*		–	–

***Species NCC4_D** is unstable and isomerizes to **NCC4_A** during geometry optimization.

Species	Structure	E (hartree)	$E_{NORMALIZED}$ (kcal mol^{-1})
Norrole_A*		–	–
Norrole_B		-3133.3156630	**+30.94**
Norrole_C		-3133.3092324	**+34.98**
Norrole_D		-3133.3649717	**0.00**

***Species **Norrole_A** is unstable and isomerizes to **Norrole_D** during geometry optimization.

Table S2. Collision cross sections (CCS) in $Å^2$ estimated by the MOBCAL program with the Trajectory Method (TM), for the ions of each isomer representing sites of protonation of lowest energy.

Species	Structure	CCS ($Å^2$)
CORROLE		**210.77**
CORRORIN		**209.78**
NCC2		**212.23**
NCC4		**210.11**
NORROLE		**209.27**