SUPPORTING INFORMATION

to:

meso-Arylporpholactones and their Reduction Products

Christian Brückner[†,*], Junichi Ogikubo[†], Jason R. McCarthy[†,‡],
Joshua Akhigbe[†], Michael A. Hyland[†], Pedro Daddario[†], Jill L. Worlinsky[†],
Matthias Zeller[§], James T. Engle,[%] Christopher J. Ziegler,[%]
Matthew J. Ranaghan[&], Megan N. Sandberg[†], and Robert R. Birge[†,&]

Department of Chemistry, University of Connecticut, Storrs, CT 06269-3060, United States. Department of Molecular and Cell Biology, University of Connecticut, Storrs, CT 06269-3125, United States. Department of Chemistry, Youngstown State University, One University Plaza, Youngstown, OH 44555-3663, United States. Department of Chemistry, University of Akron, Akron, OH 44325-3601, United States.

* Author to whom correspondence should be addressed: Fax: (+1) 860 486-2981; Tel: (+1) 860 486-2743; e-mail: c.bruckner@uconn.edu

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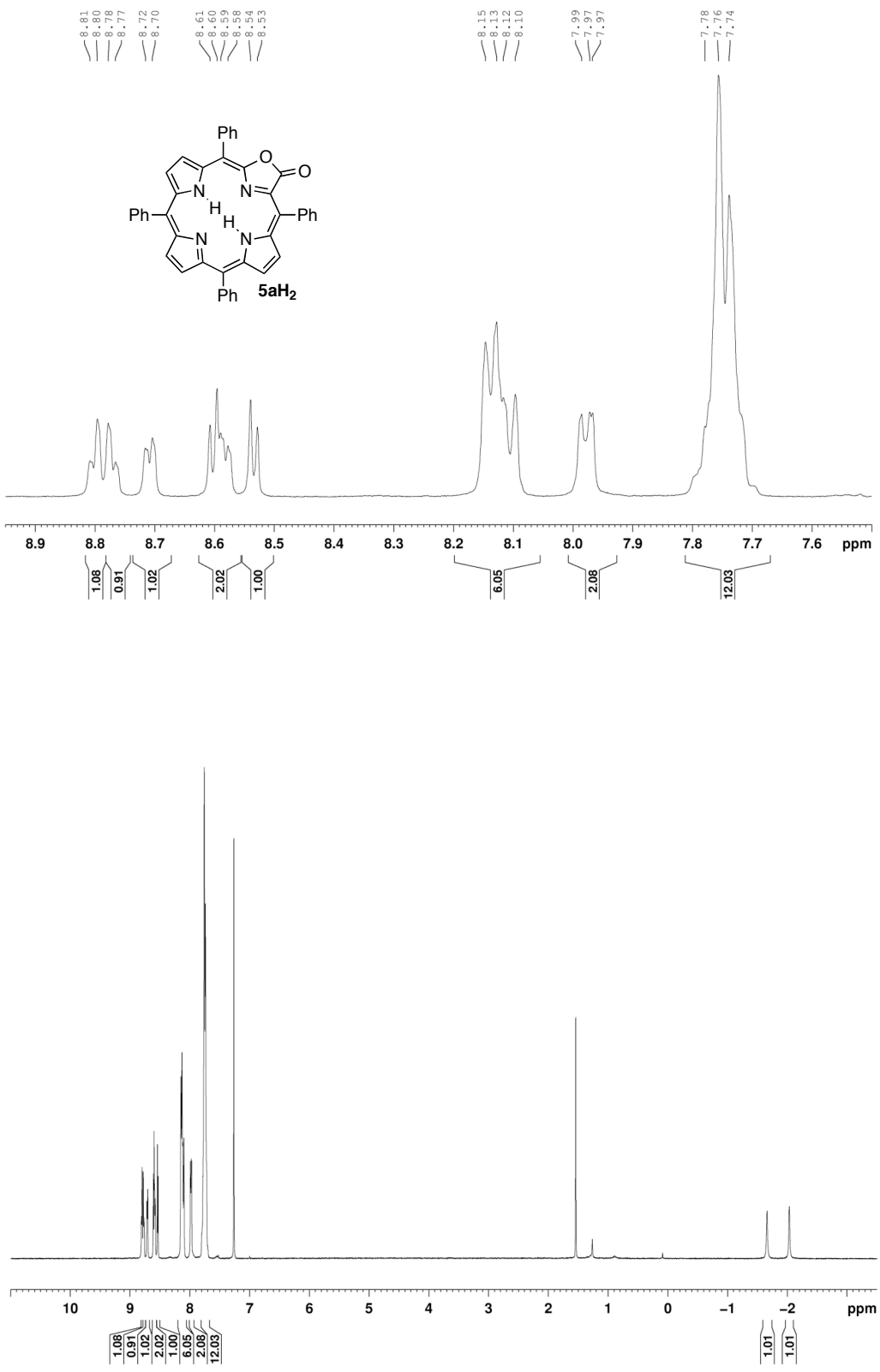

Figure S1. ^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of **$5aH_2$**

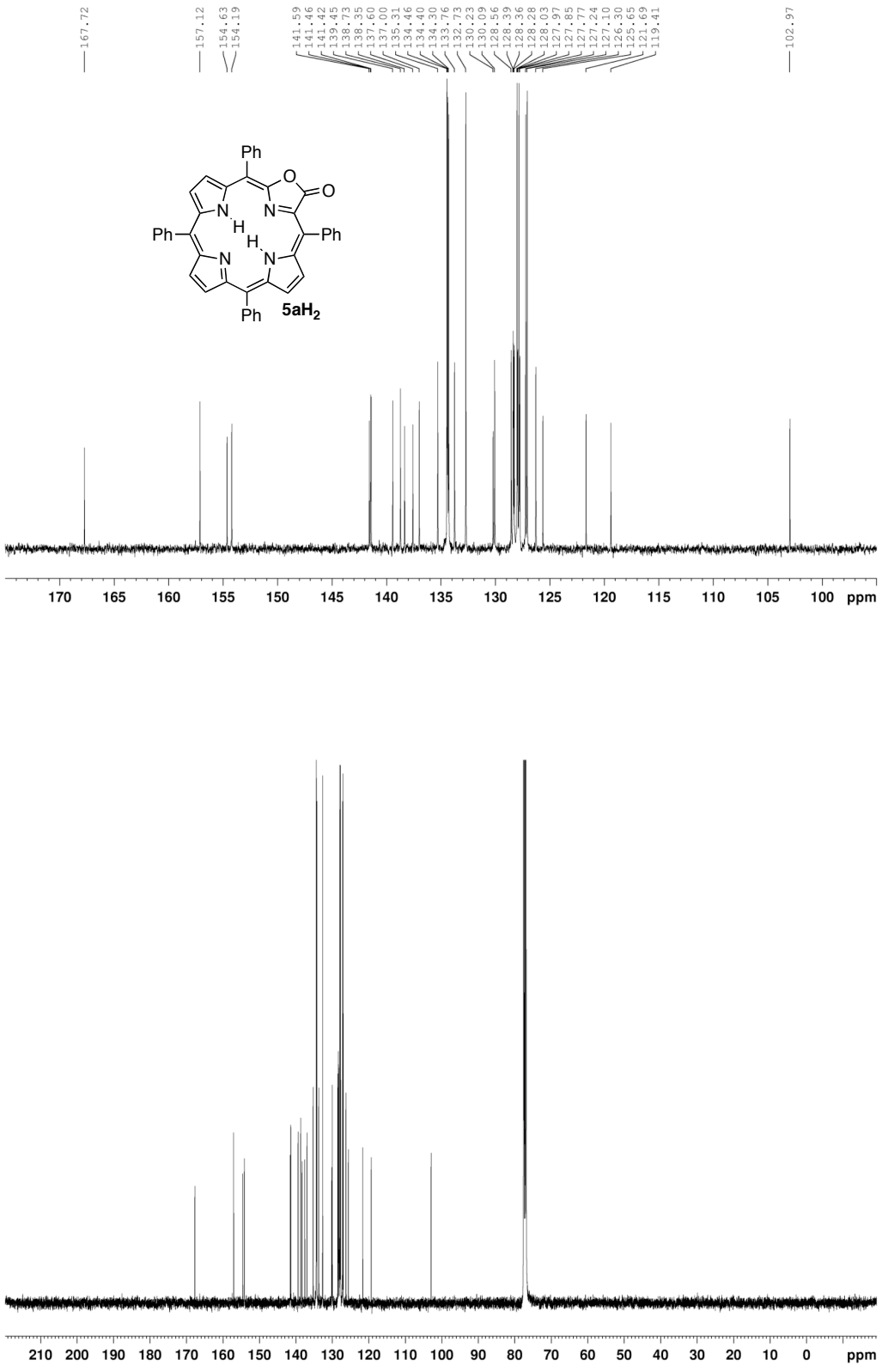

Figure S2. ^{13}C NMR Spectrum (100 MHz, $CDCl_3$) of **5aH$_2$**

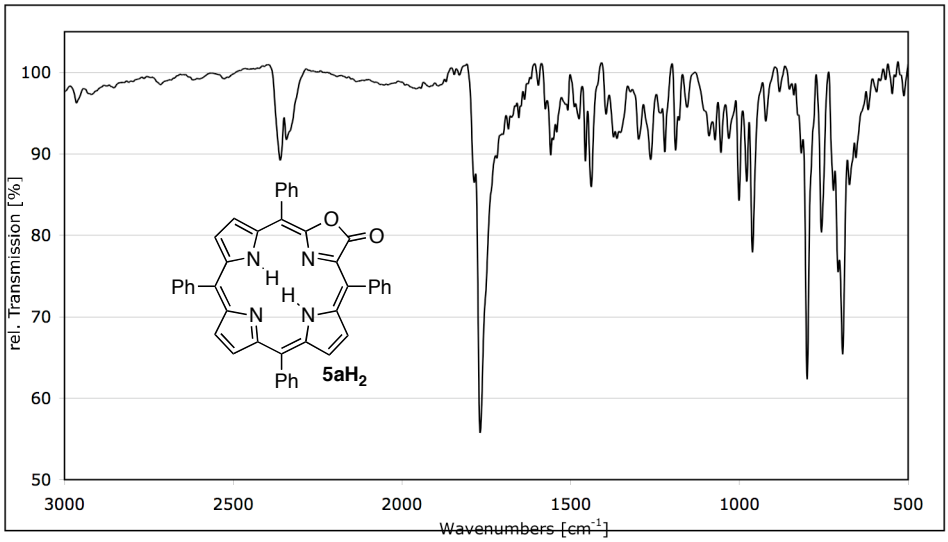

Figure S3. FT-IR Spectrum (KBr) of **5aH$_2$**

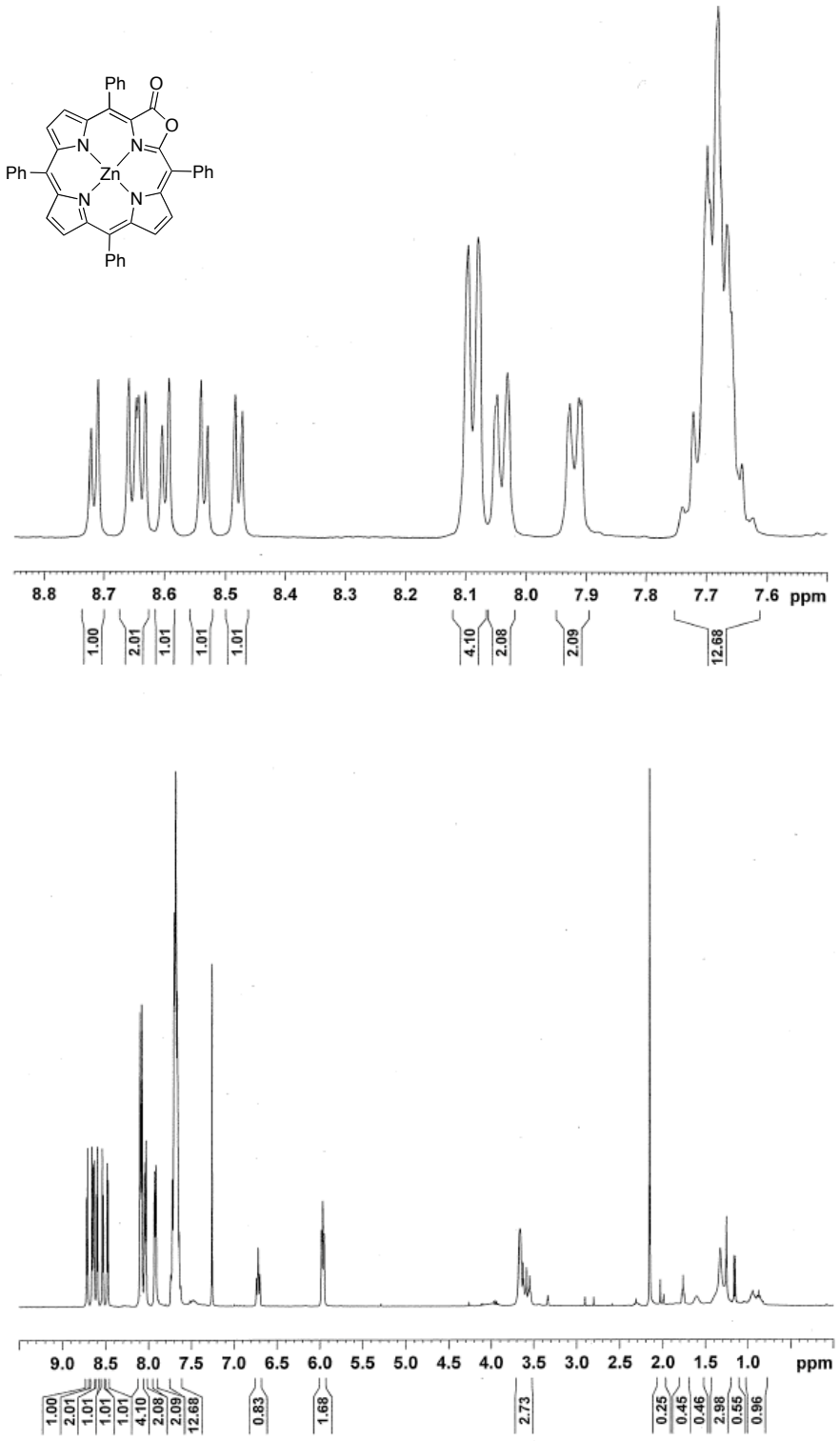

Figure S4. ^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of **5aZn**

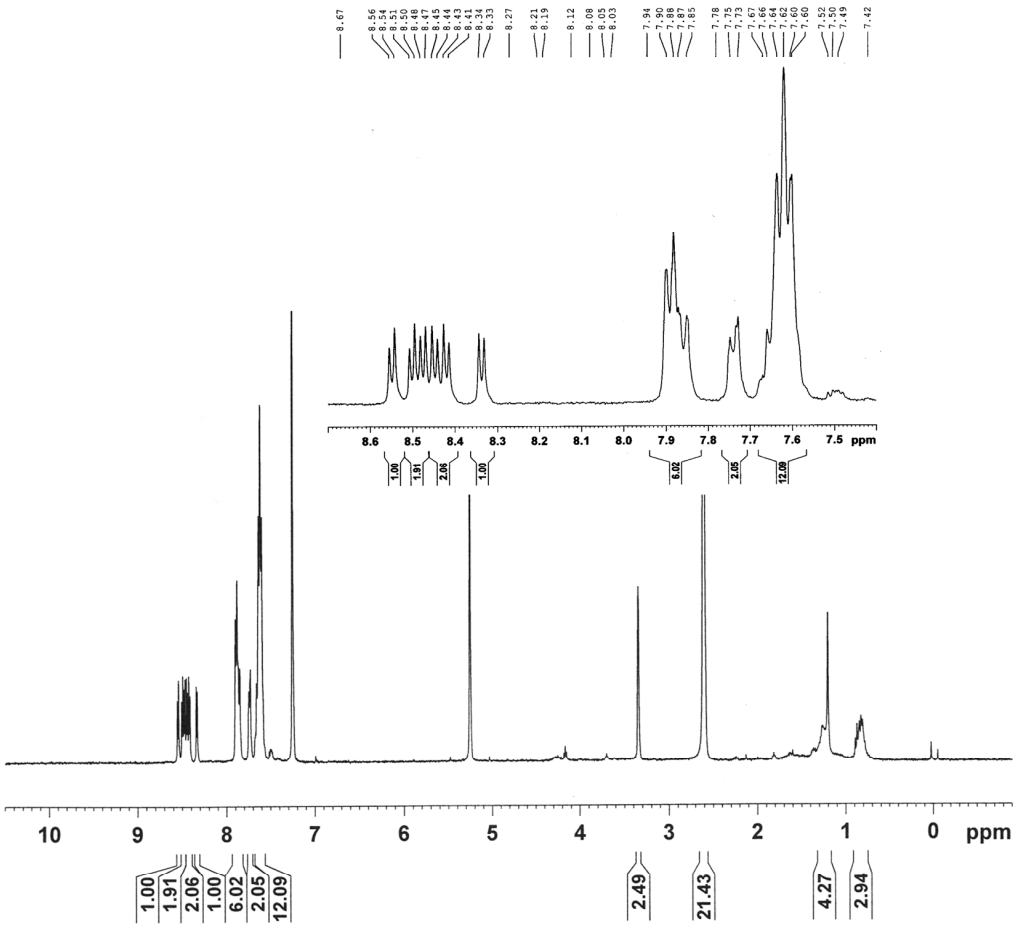

Figure S5. ^{1}H NMR (400 MHz, $CDCl_3$ + 10% MeOH-d_4, 25 °C) of **5aNi.** The compound possesses limited solubility.

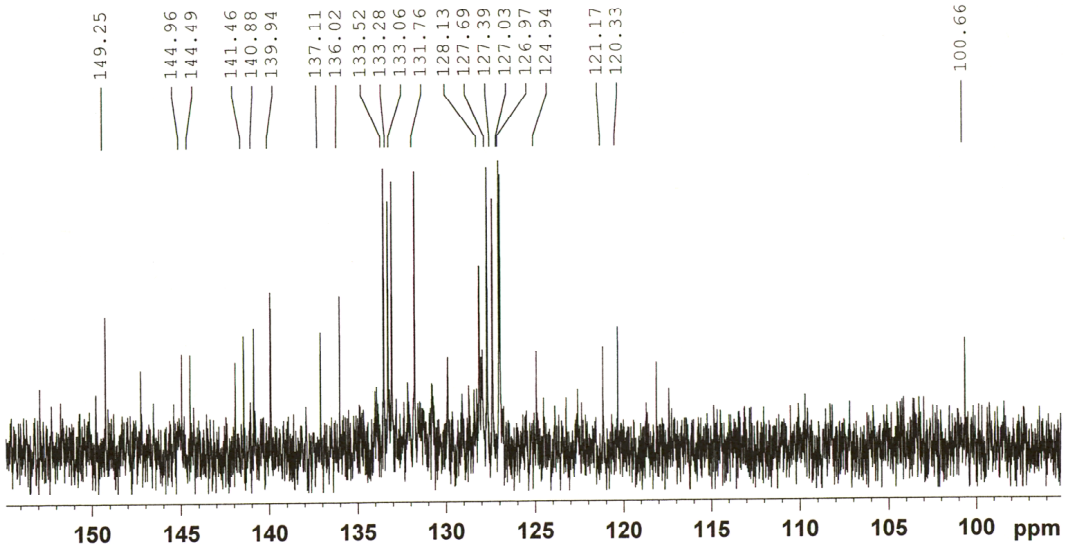

Figure S6. ^{13}C NMR (100 MHz, $CDCl_3$ + 10% MeOH-d_4, 25 °C, D1 = 3s) of **5aNi**. The compound possesses limited solubility.

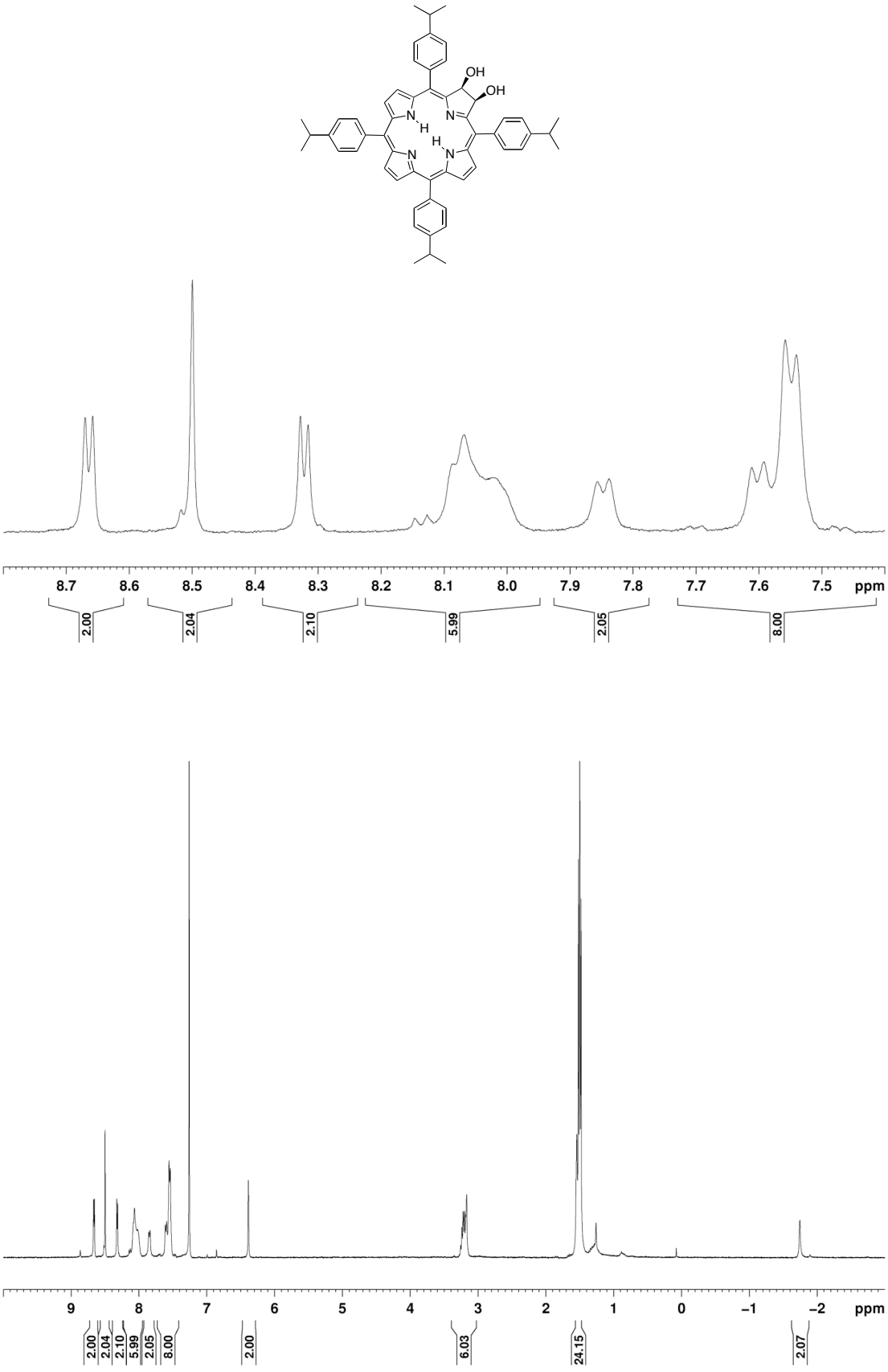

Figure S7. ^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of **7bH_2**

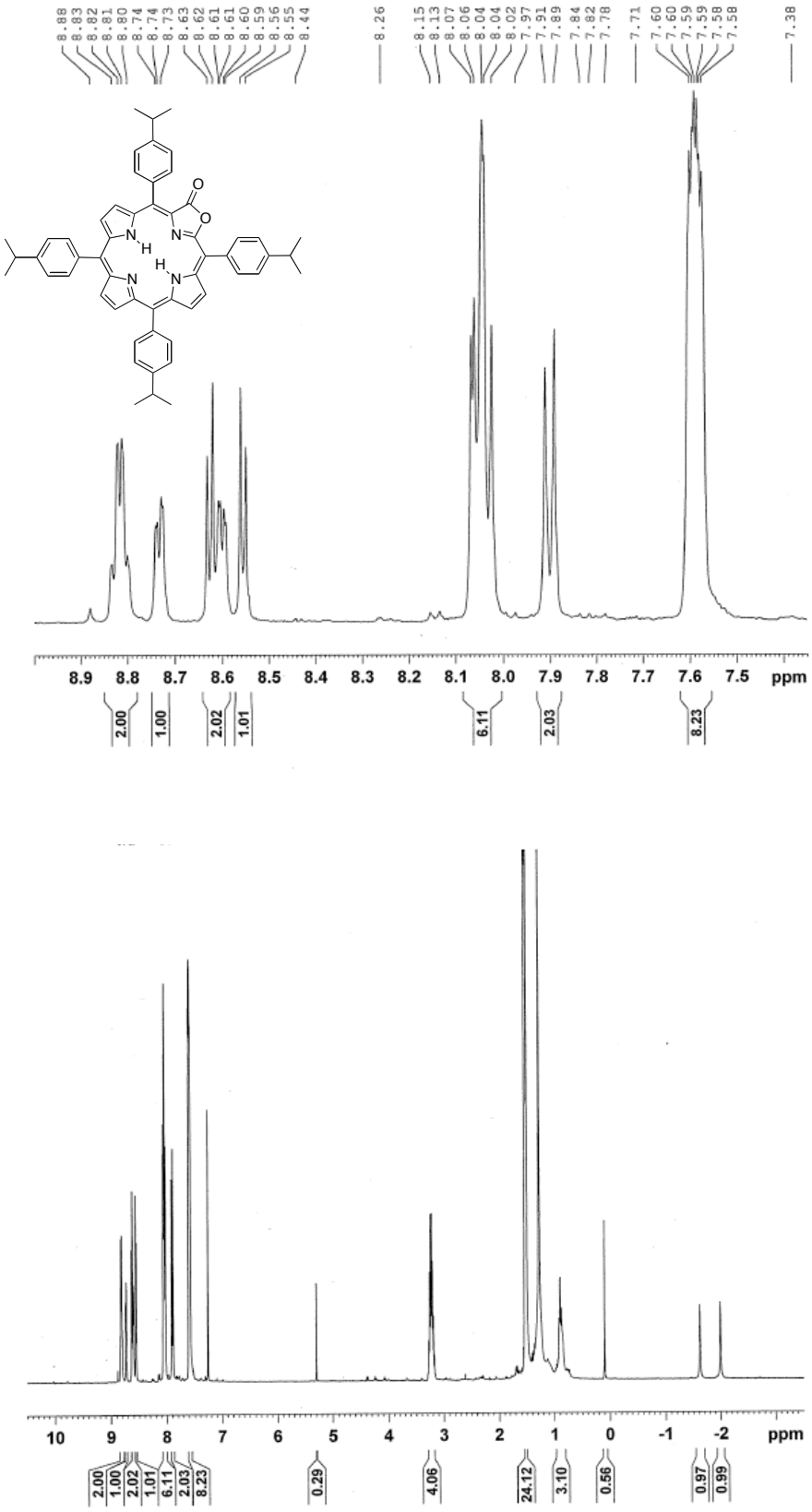

Figure S8. ^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of **5bH$_2$**

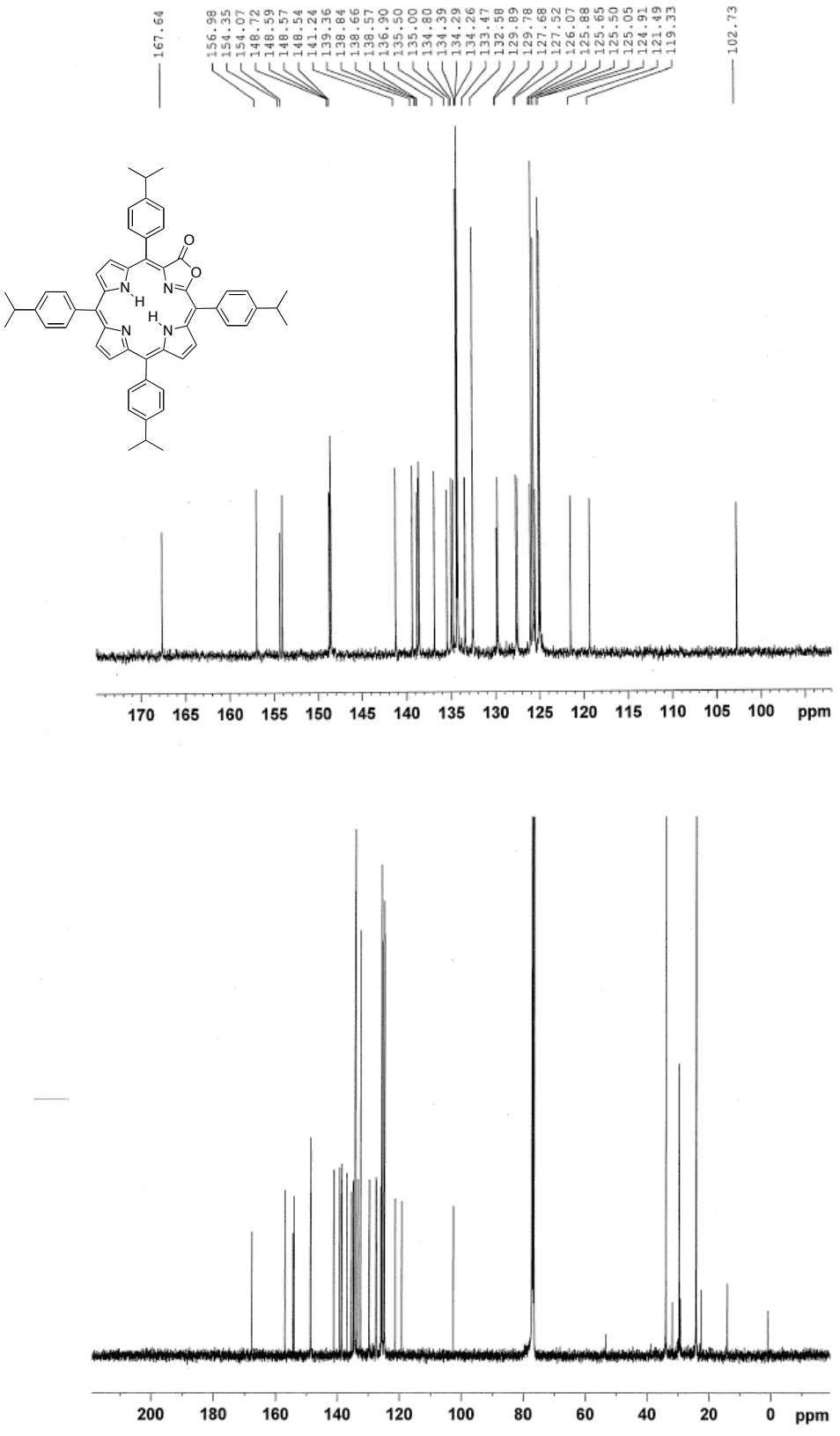

Figure S9. ^{13}C NMR Spectrum (100 MHz, $CDCl_3$, D1 = 3s) of **5bH$_2$**

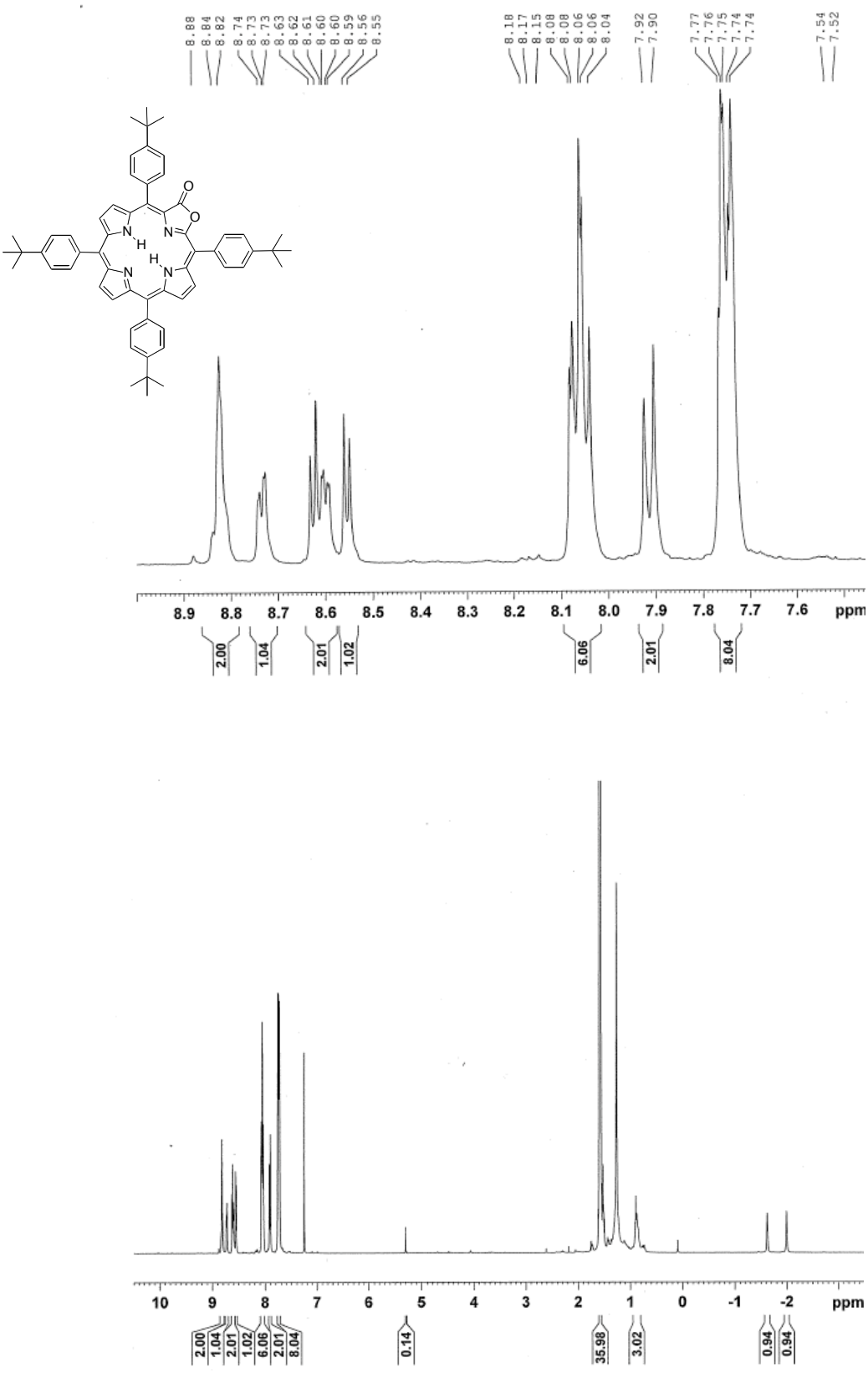

Figure S10. ^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of **5cH$_2$**

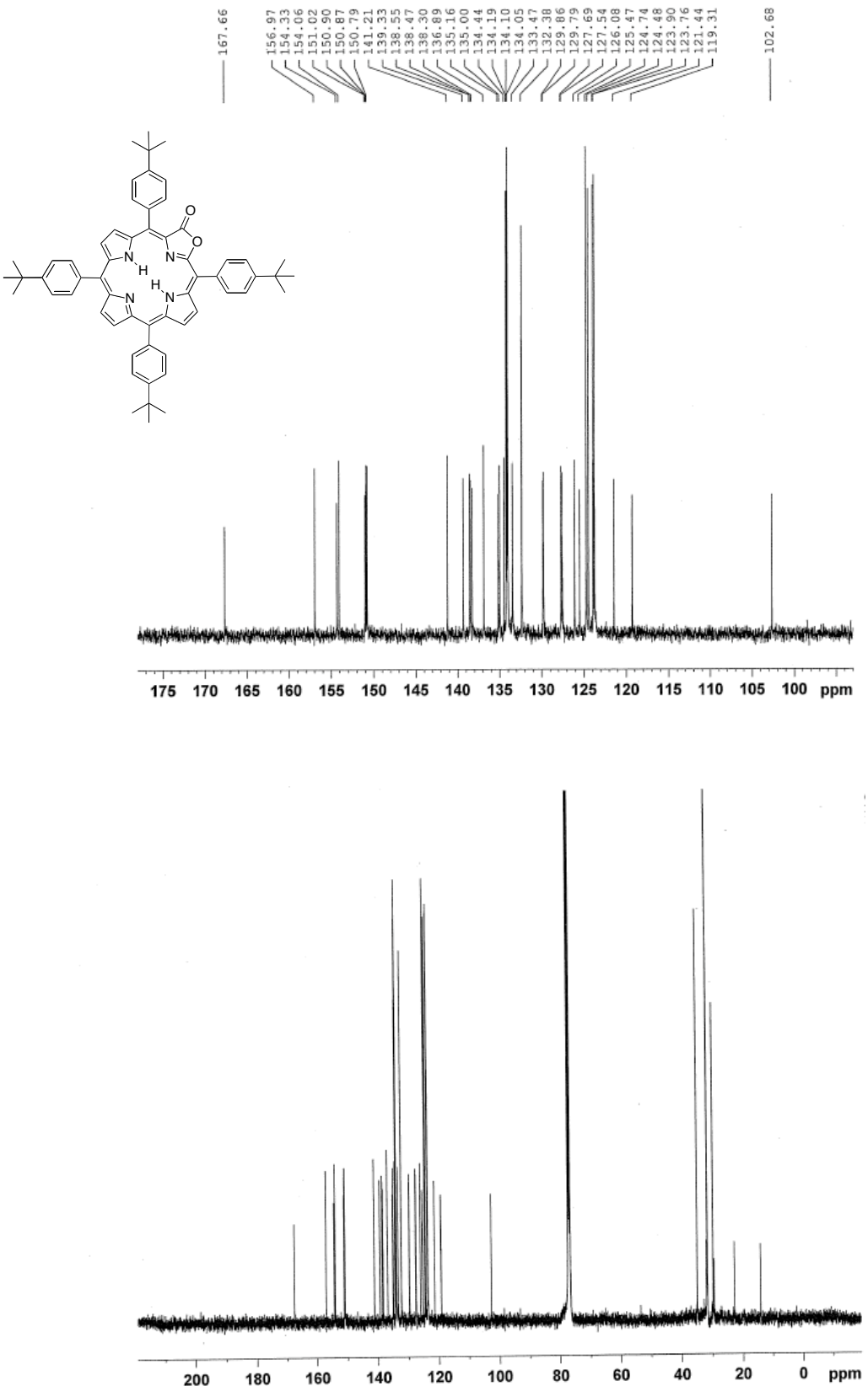

Figure S11. ^{13}C NMR Spectrum (100 MHz, $CDCl_3$, D1 = 3s) of **5cH_2**

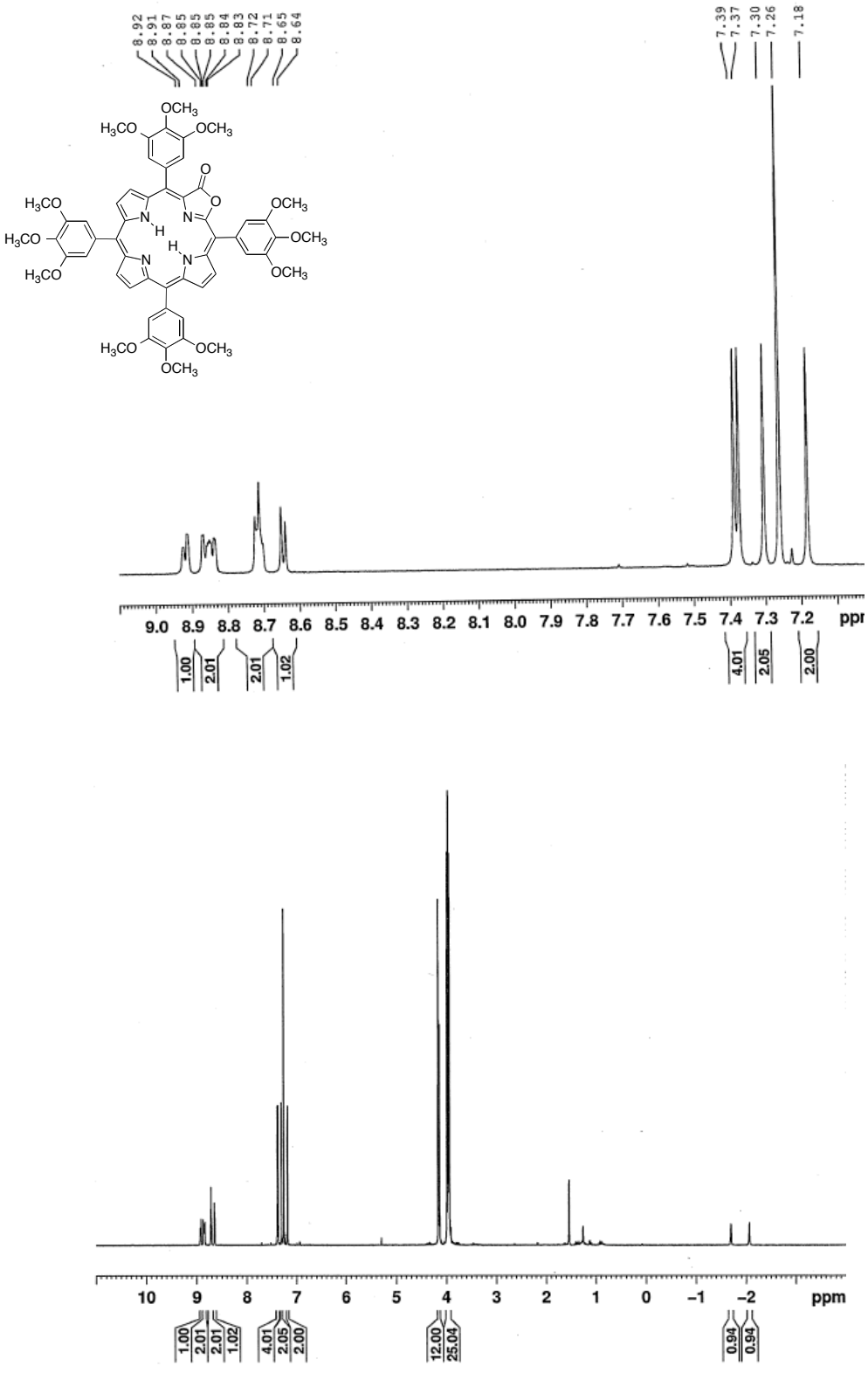

Figure S12. ^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of **5dH$_2$**

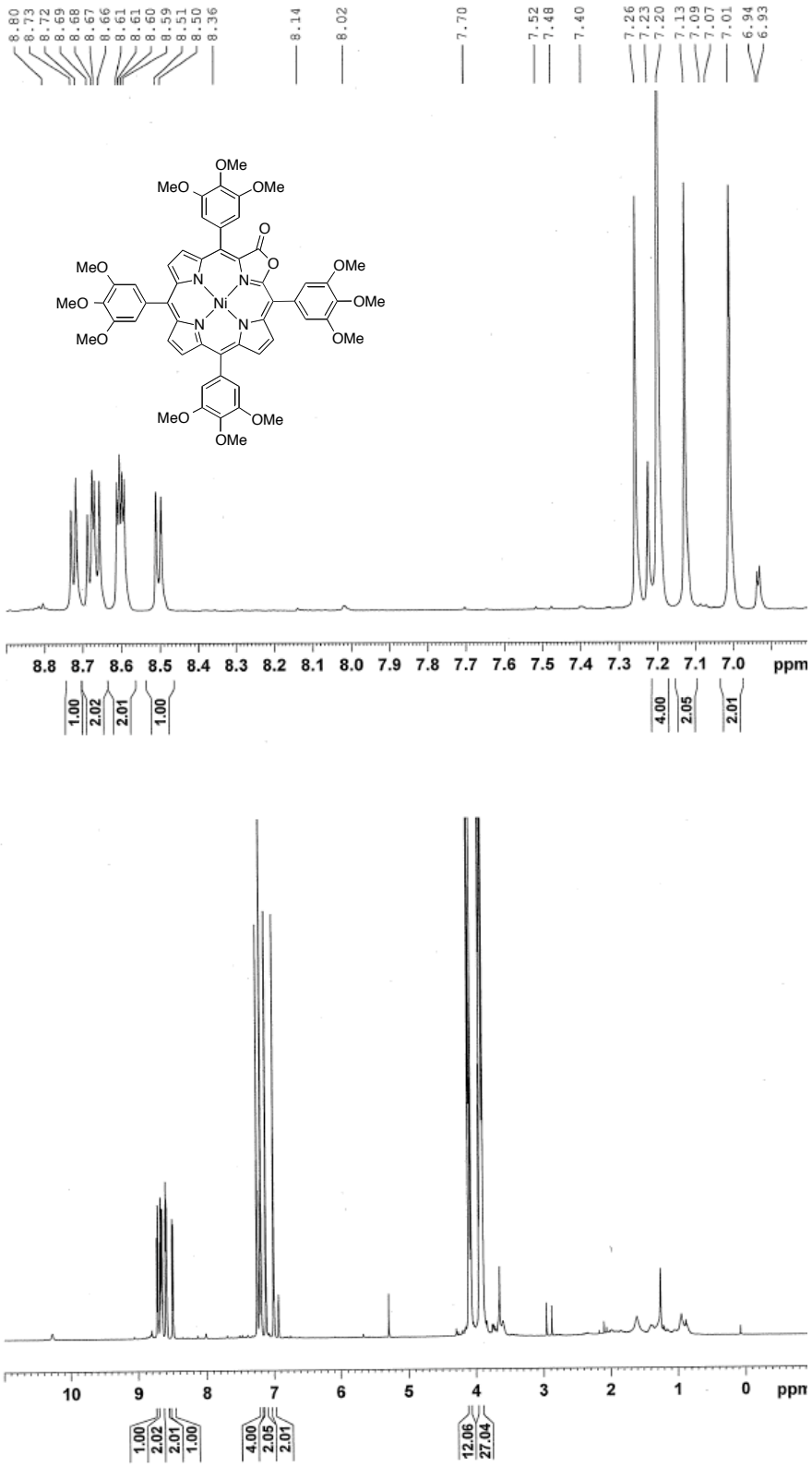

Figure S13. ^{1}H NMR (400 MHz, $CDCl_3$) of **5dNi**

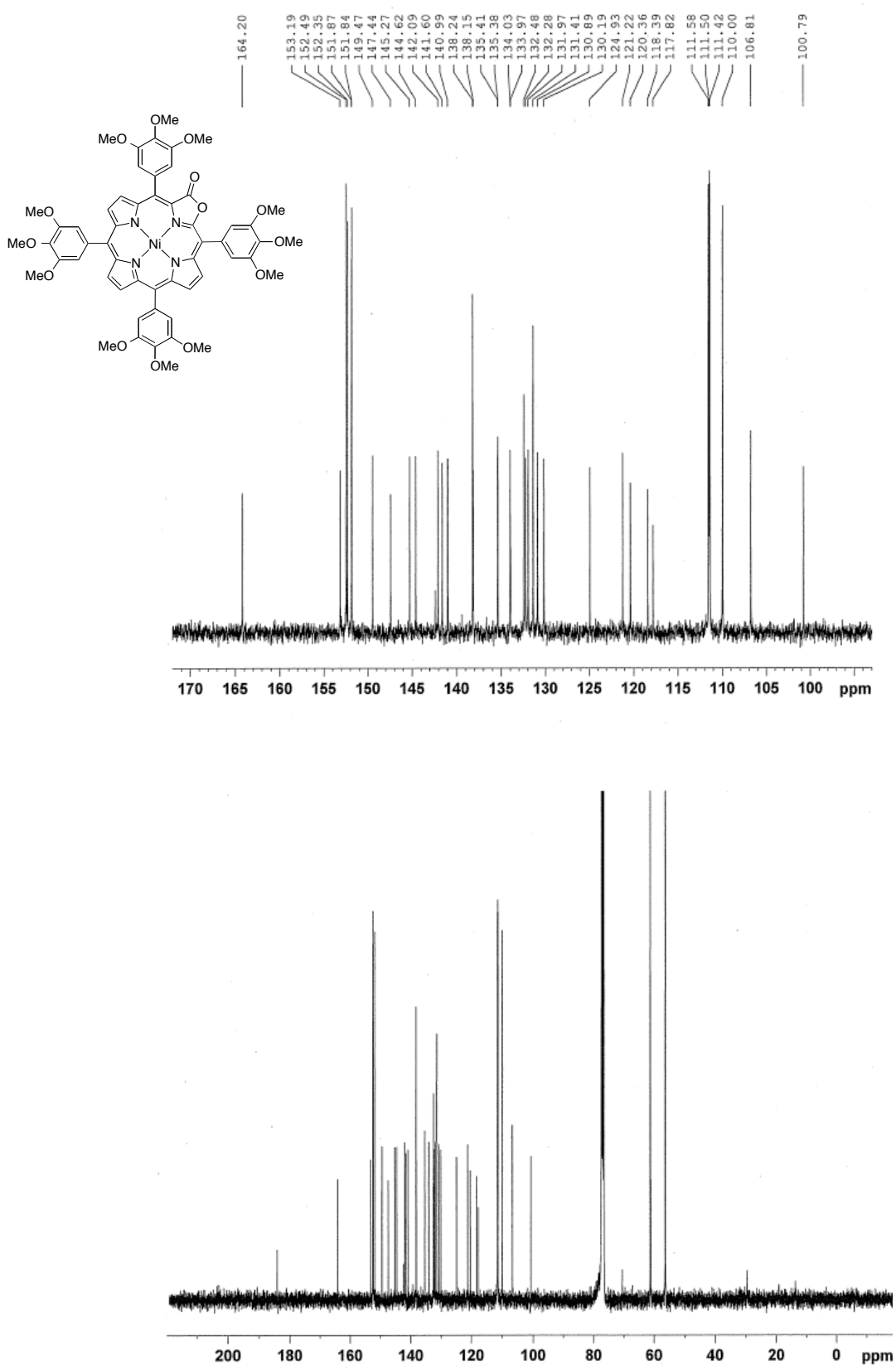

Figure S14. ^{13}C NMR Spectrum (100 MHz, $CDCl_3$, D1 = 3s) of **5dNi**

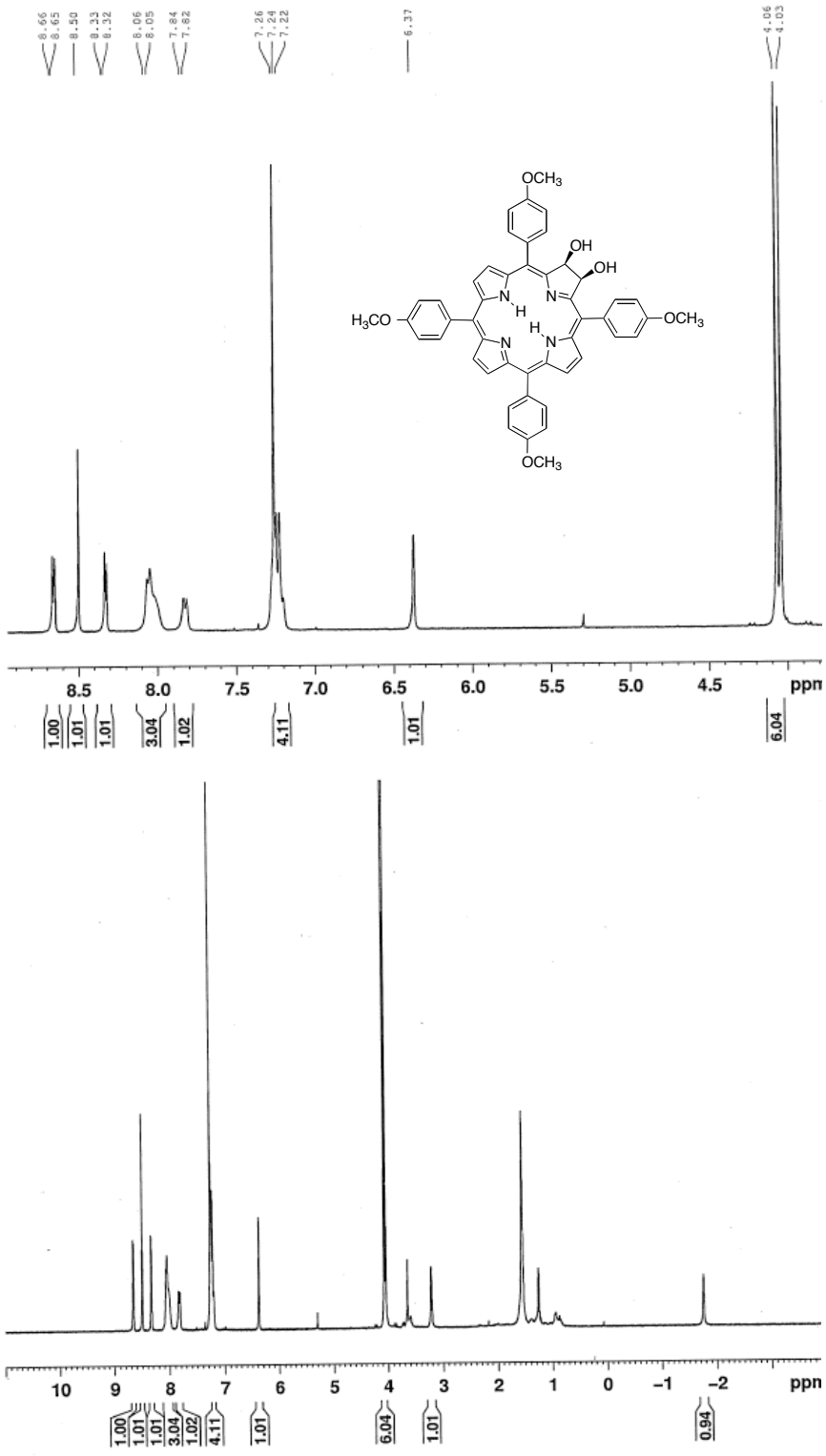

Figure S15. ^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of **7eH_2**

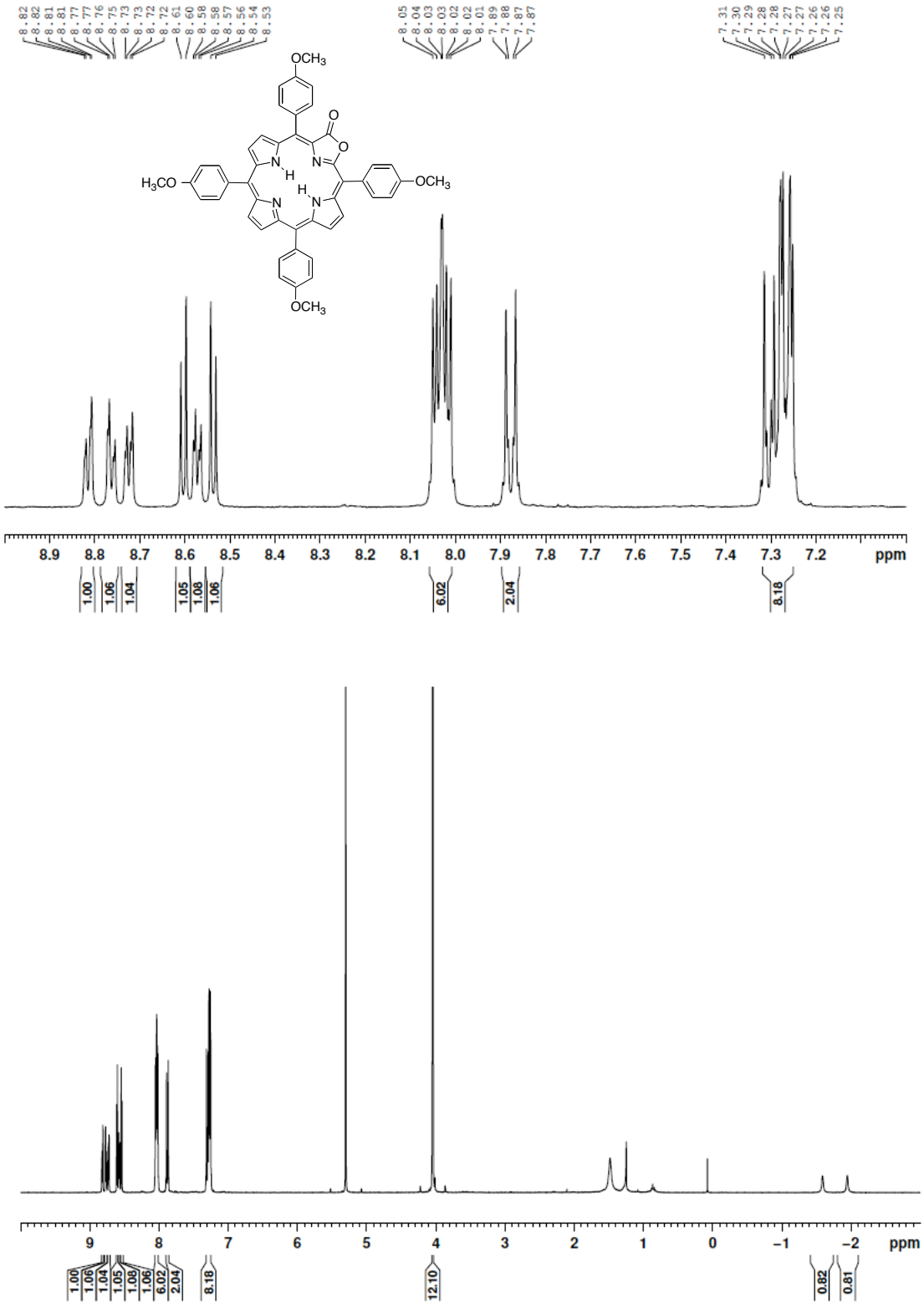

Figure S16. ^{1}H NMR Spectrum (400 MHz, CD_2Cl_2) of **5eH$_2$**

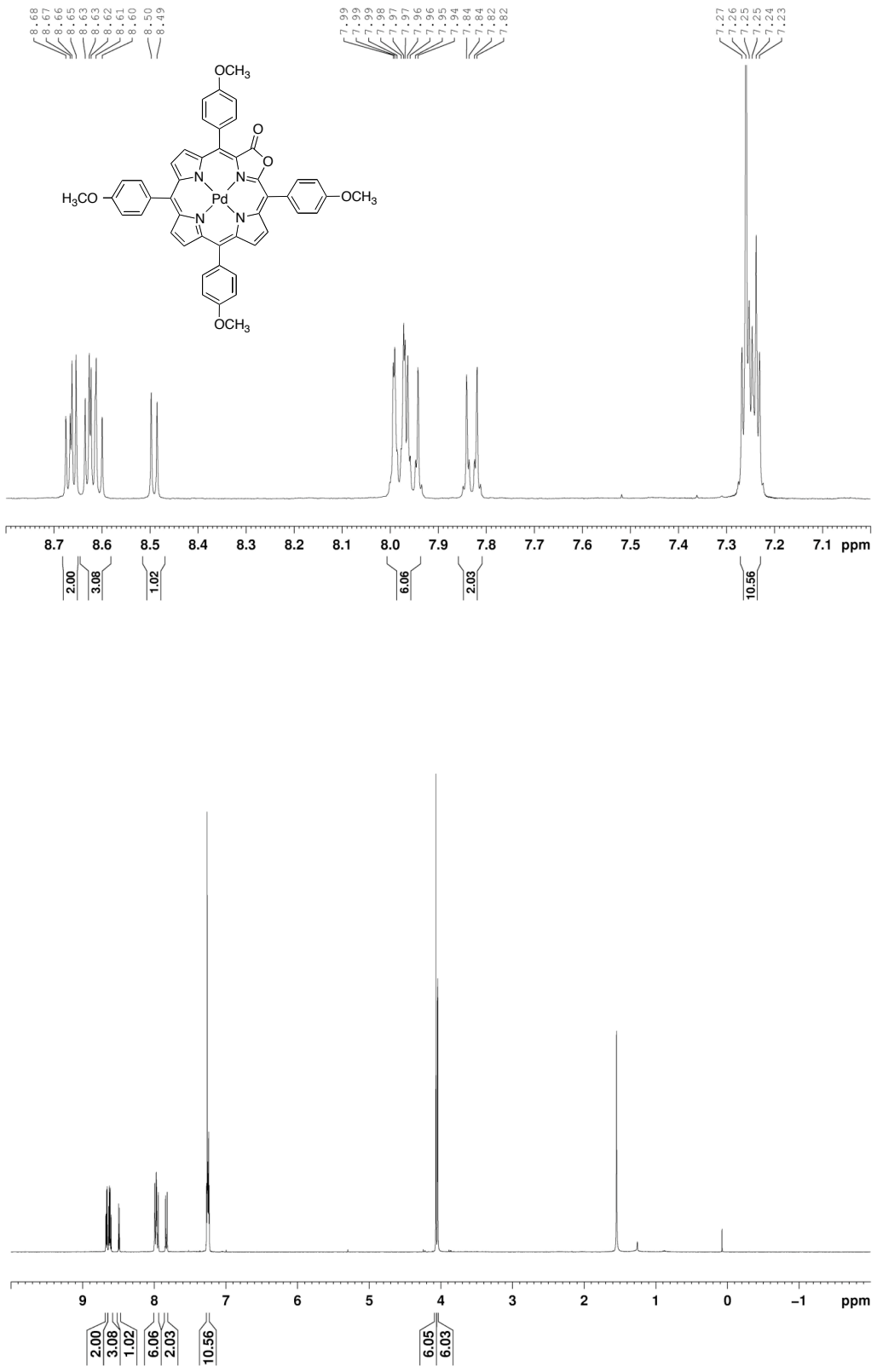

Figure S17. ^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of **5ePd**

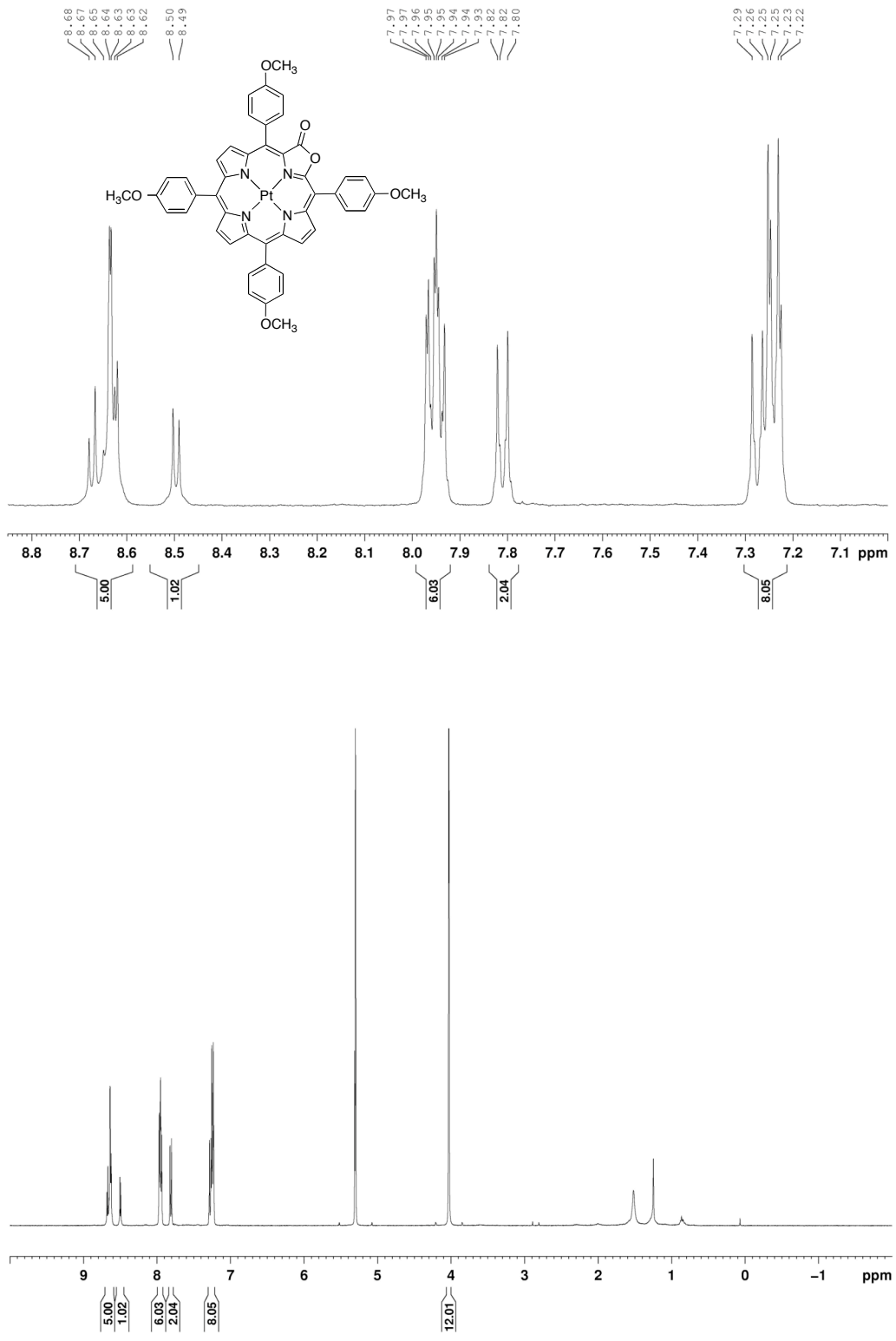

Figure S18. ^{1}H NMR Spectrum (400 MHz, CD_2Cl_2) of **5ePt**

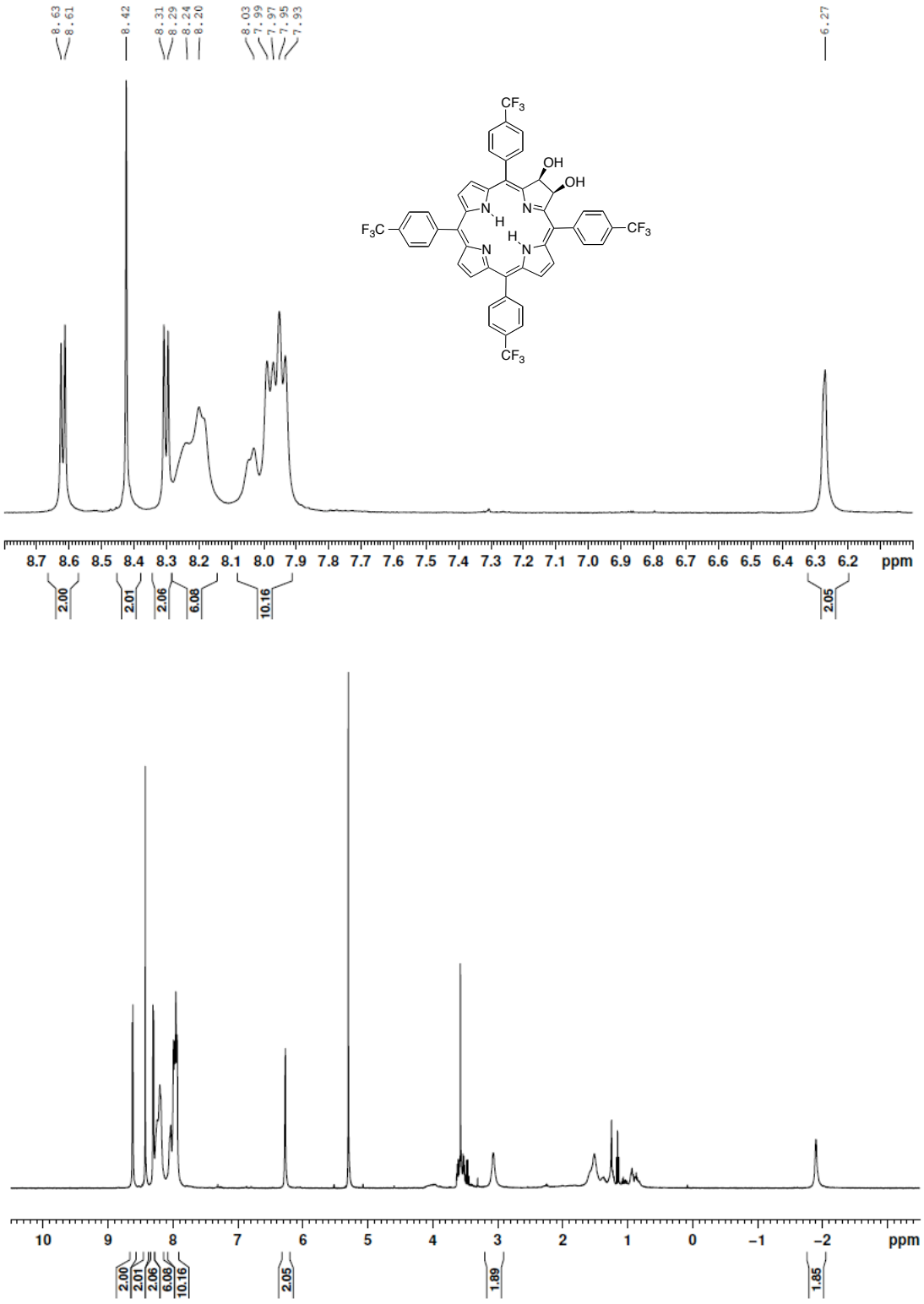

Figure S19. ^{1}H NMR (400 MHz, CD_2Cl_2) of **7fH$_2$**

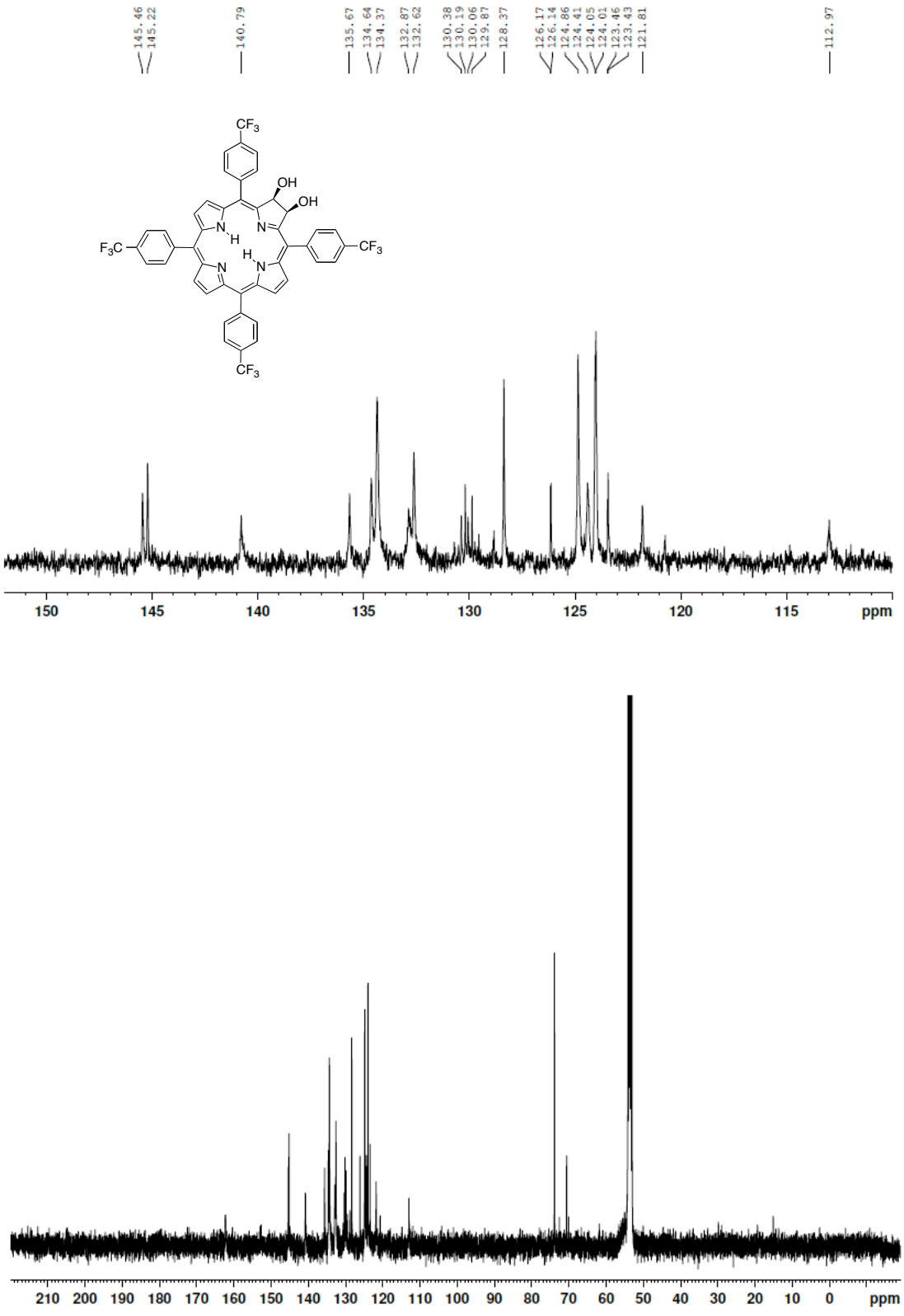

Figure S20. ^{13}C NMR Spectrum (100 MHz, CD_2Cl_2) of **7fH$_2$**

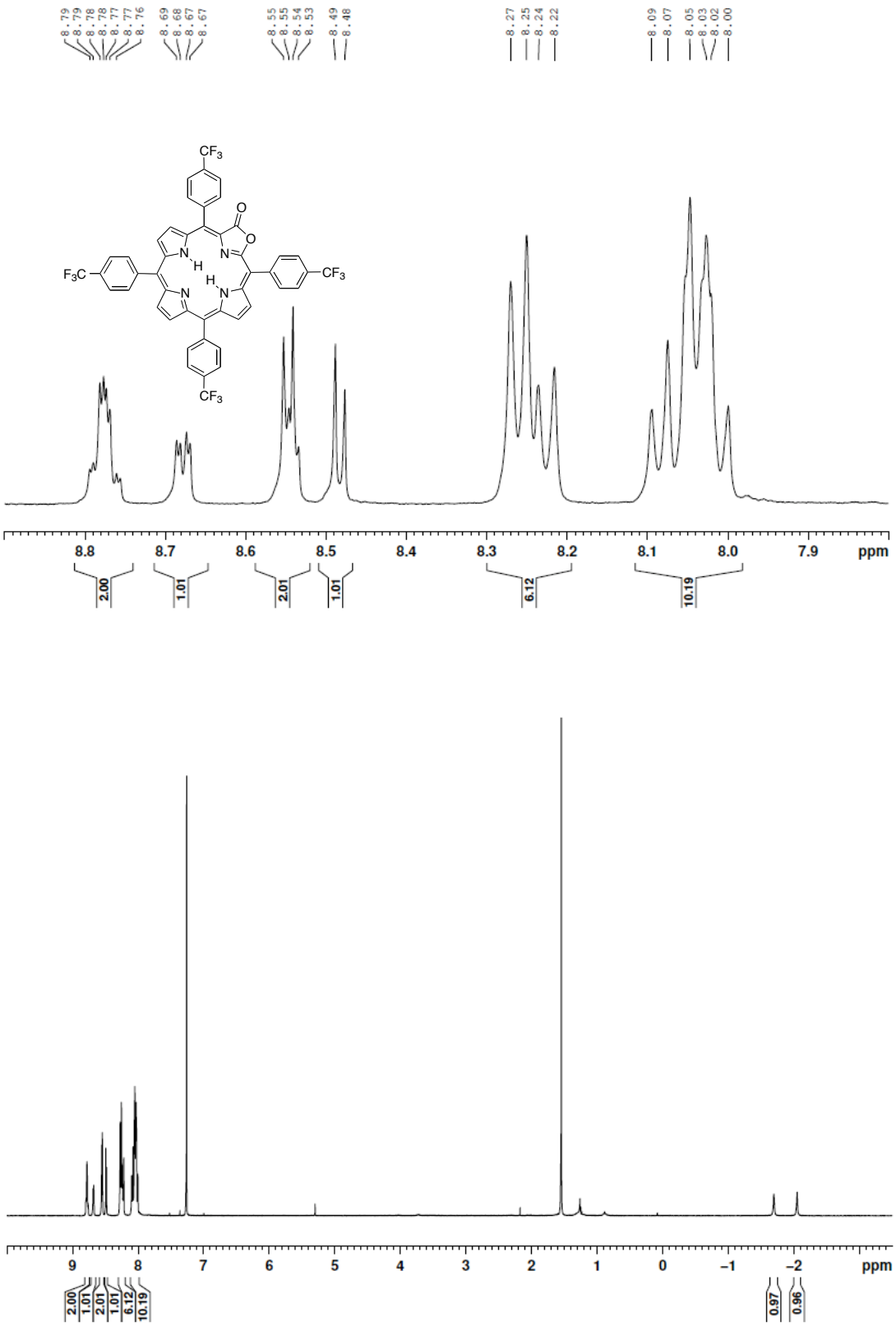

Figure S21. ^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of **5fH$_2$**

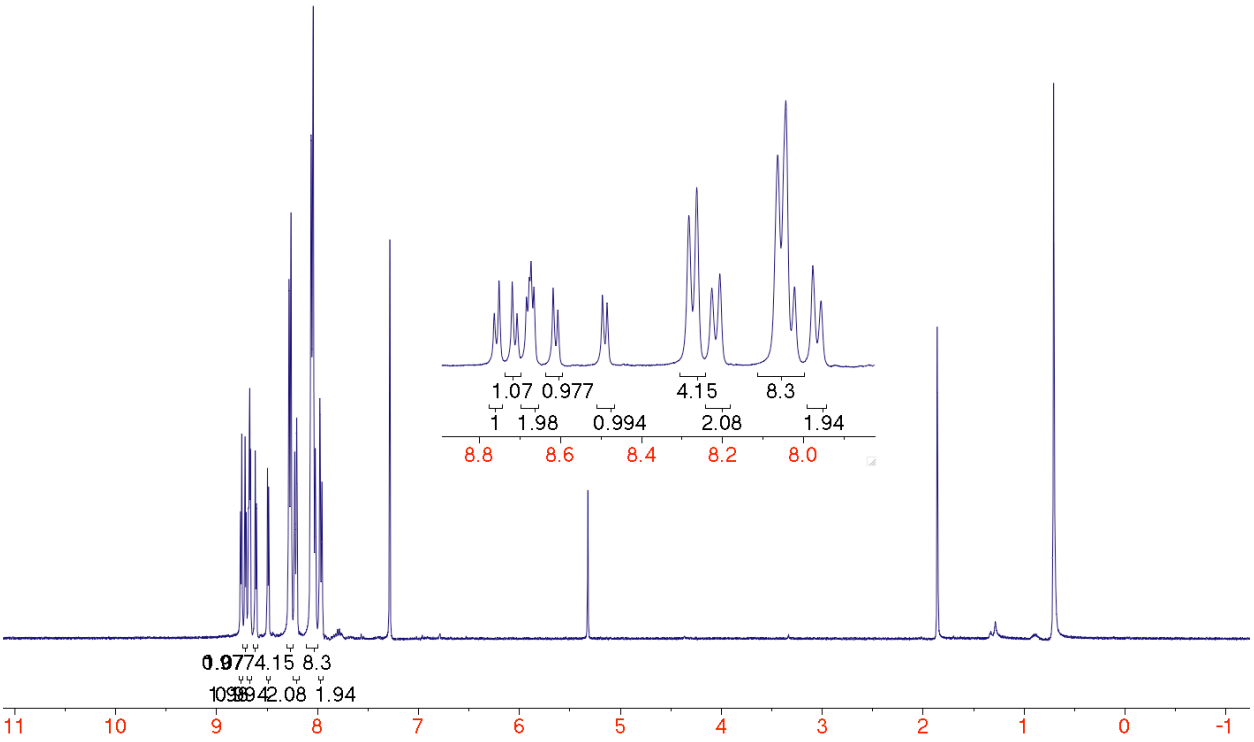

Figure S22. ^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of **5fZn**

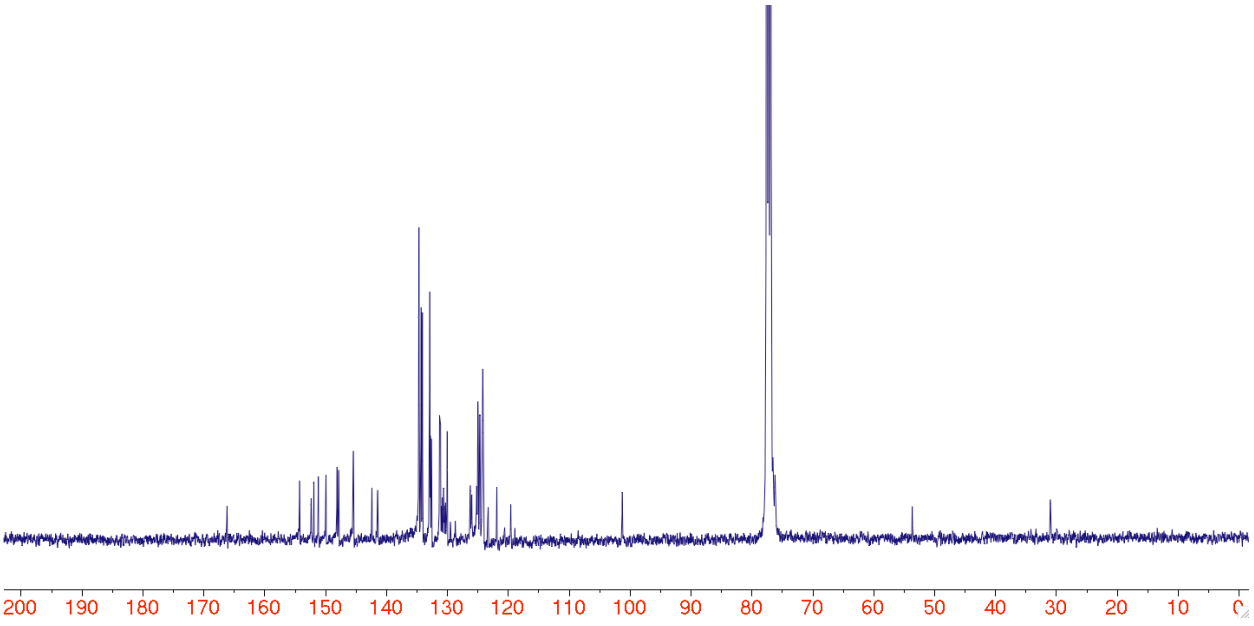

Figure S23. ^{13}C NMR Spectrum (400 MHz, $CDCl_3$) of **5fZn**

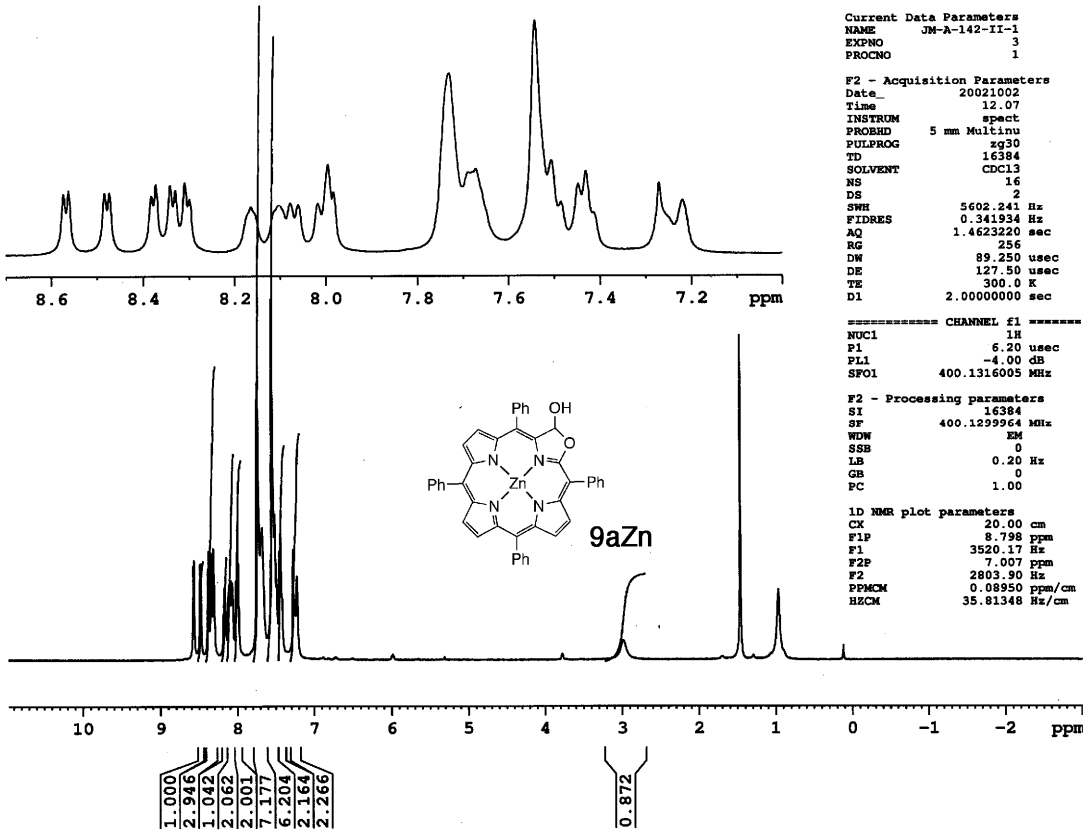

Figure S24. ^{1}H NMR Spectrum (100 MHz, $CDCl_3$) of **9aZn**

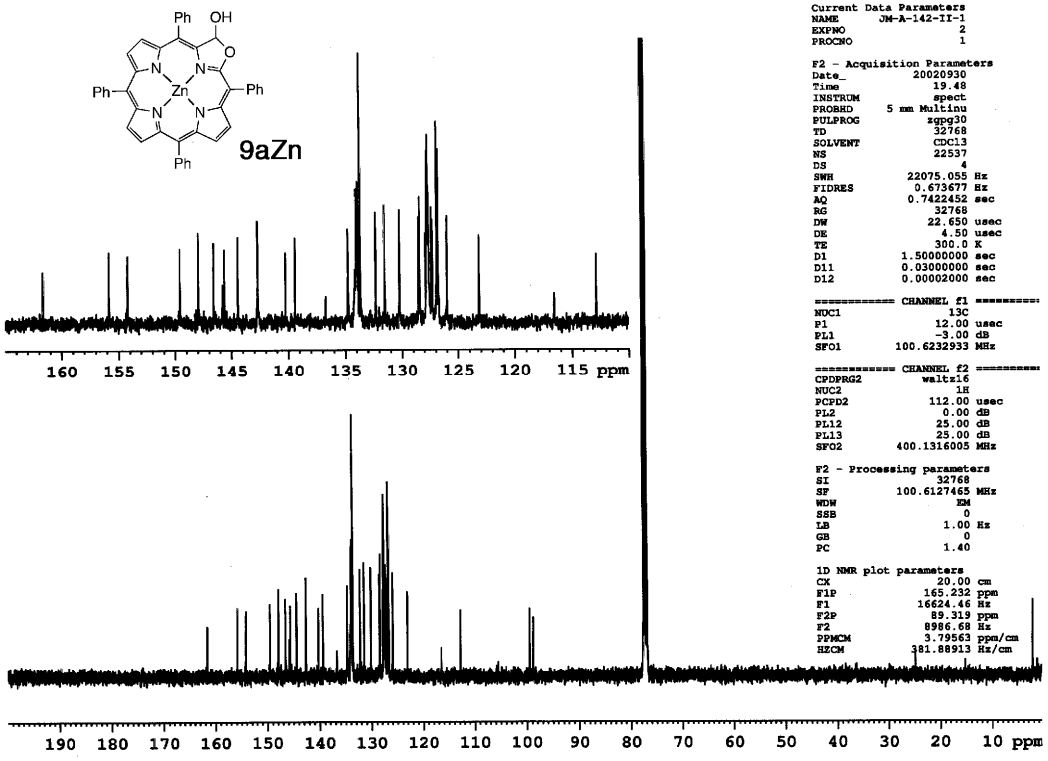

Figure S25. ^{13}C NMR Spectrum (100 MHz, $CDCl_3$) of **9aZn**

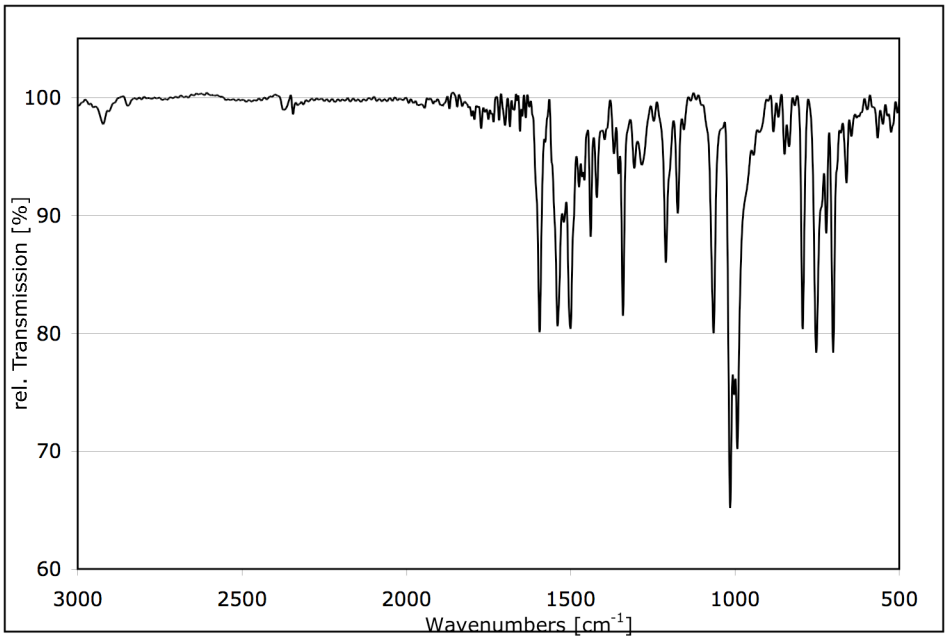

Figure S26. FT-IR Spectrum (KBr) of **9aZn**

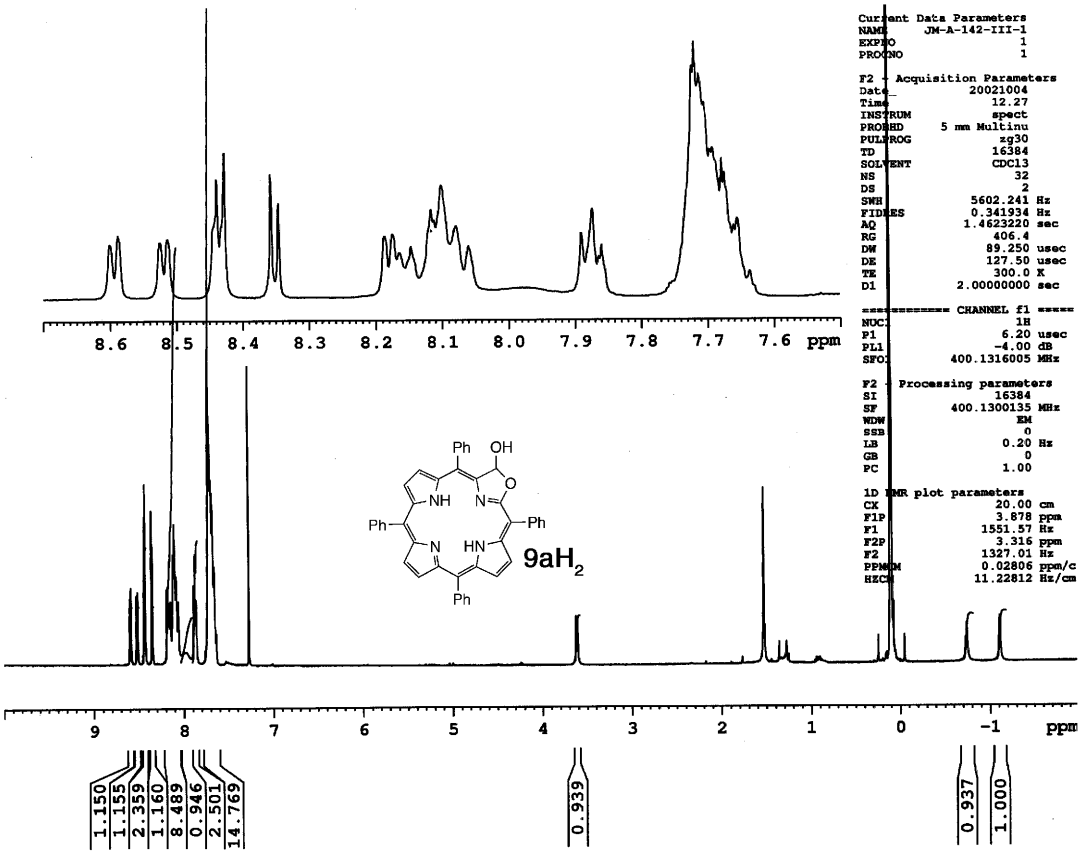

Figure S27. ^{1}H NMR Spectrum (100 MHz, $CDCl_3$) of **9aH$_2$**

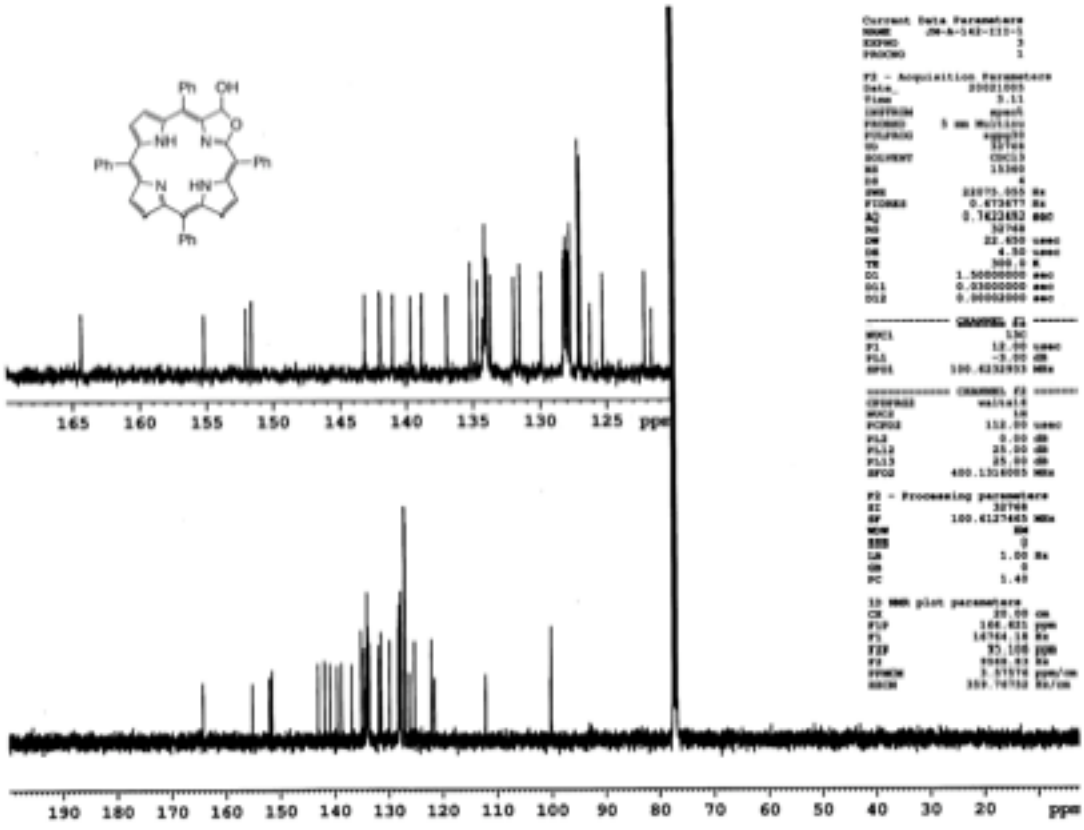

Figure S28. ^{13}C NMR Spectrum (100 MHz, $CDCl_3$) of **11aH$_2$**

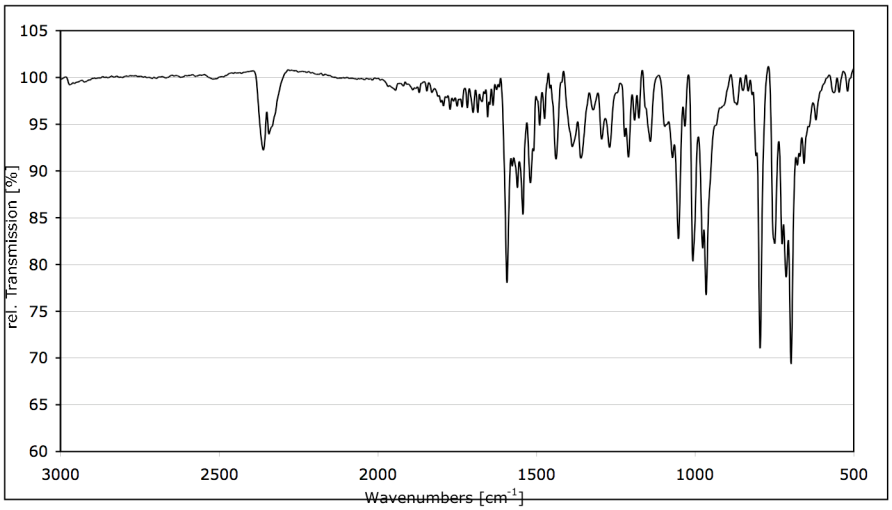

Figure S29. FT-IR Spectrum (KBr) of **11aH$_2$**

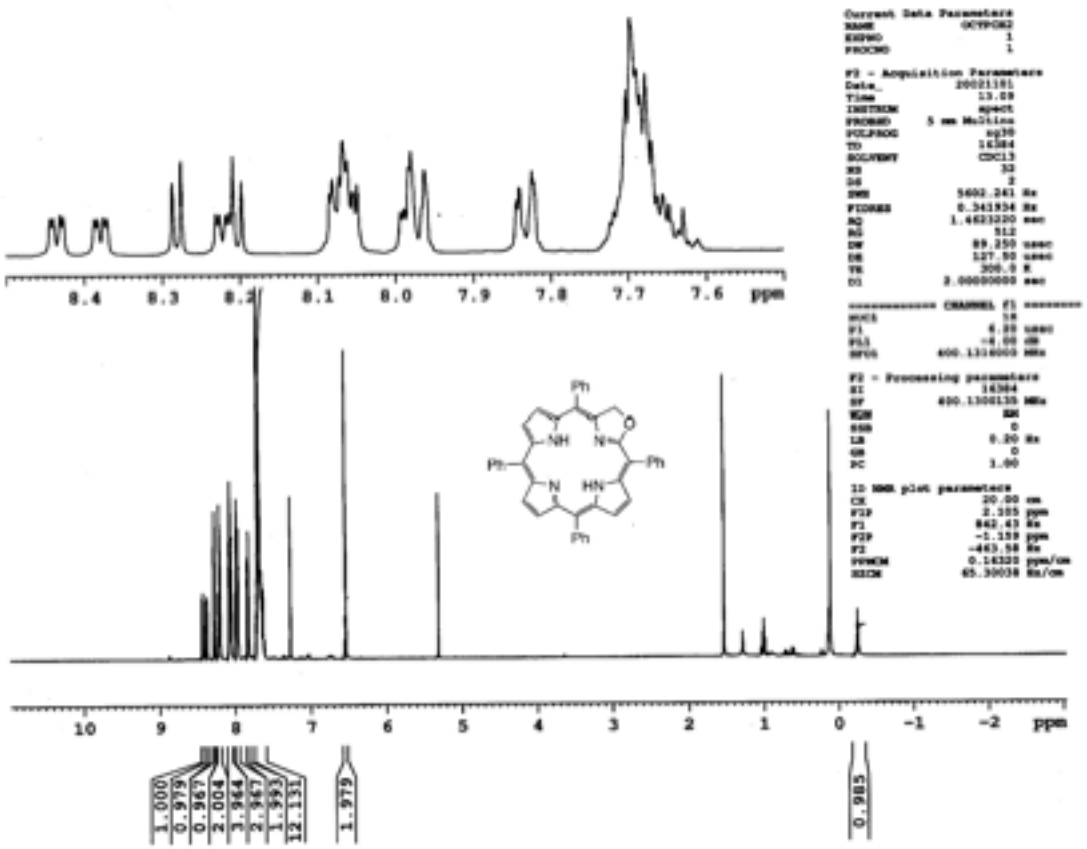

Figure S30. ^{1}H NMR Spectrum (100 MHz, $CDCl_3$) of **12aH$_2$**

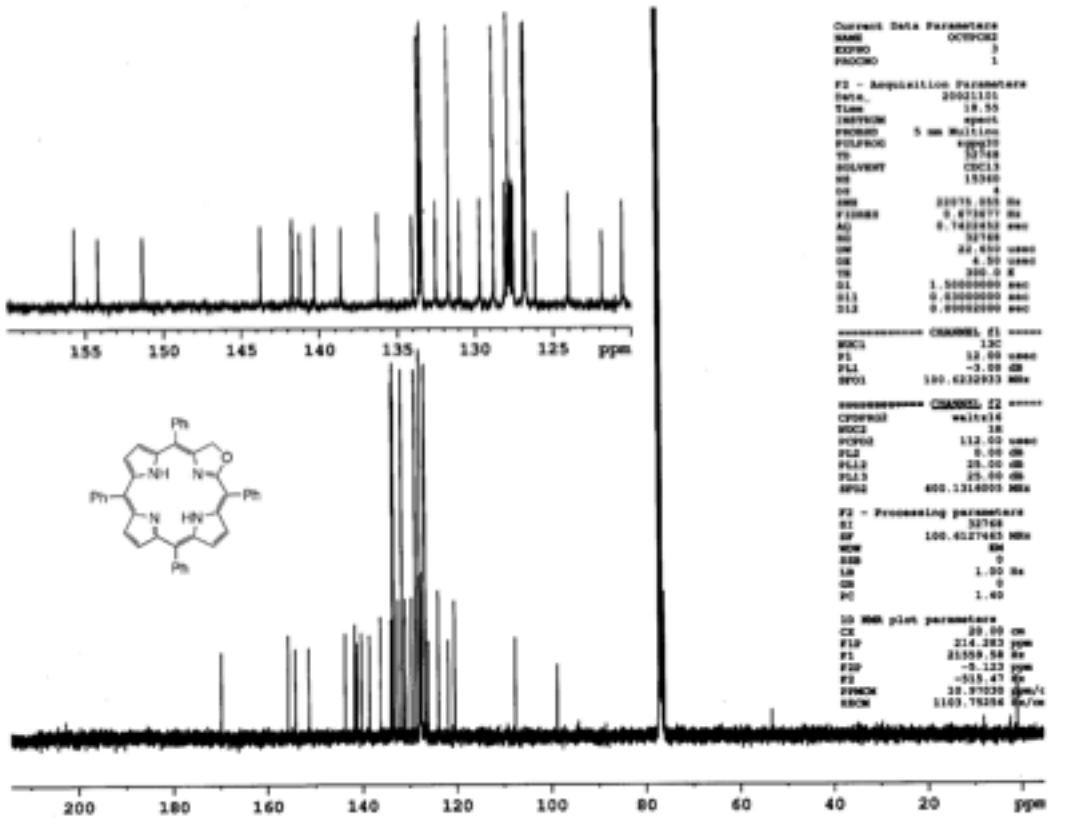

Figure S31. ^{13}C NMR Spectrum (100 MHz, $CDCl_3$) of **12aH$_2$**

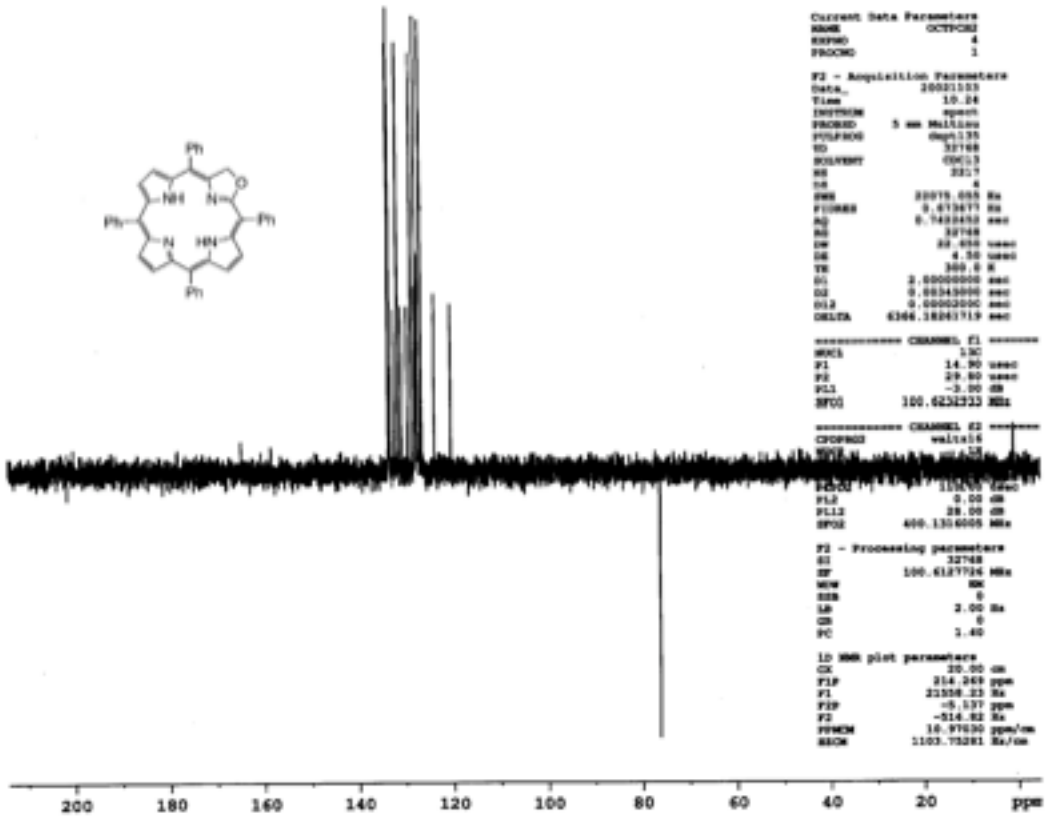

Figure S32. DEPT Spectrum (100 MHz, $CDCl_3$) of **12aH$_2$**

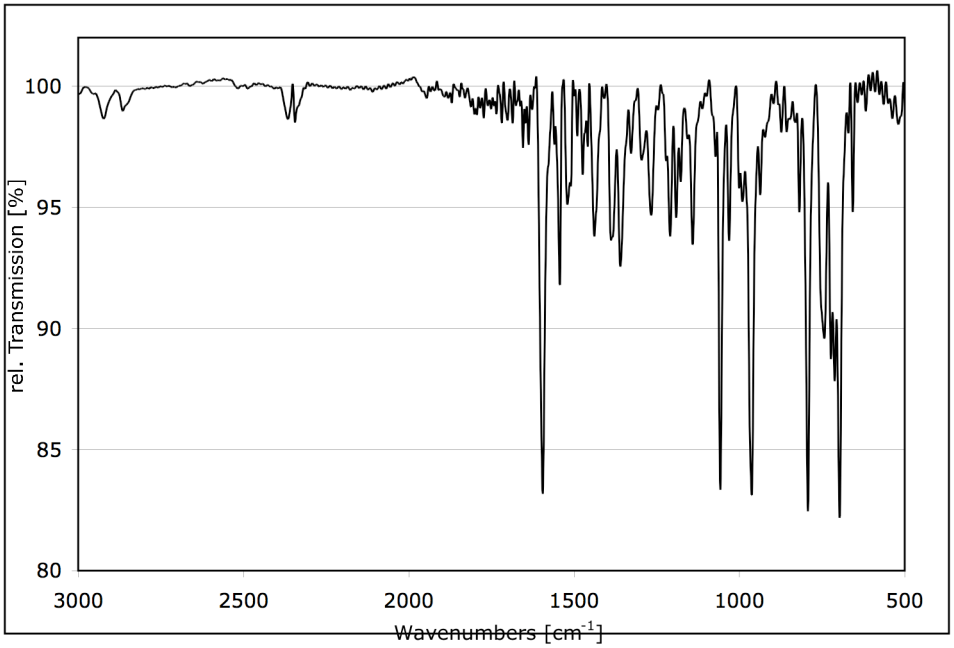

Figure S33. FT-IR Spectrum (KBr) of **12aH$_2$**

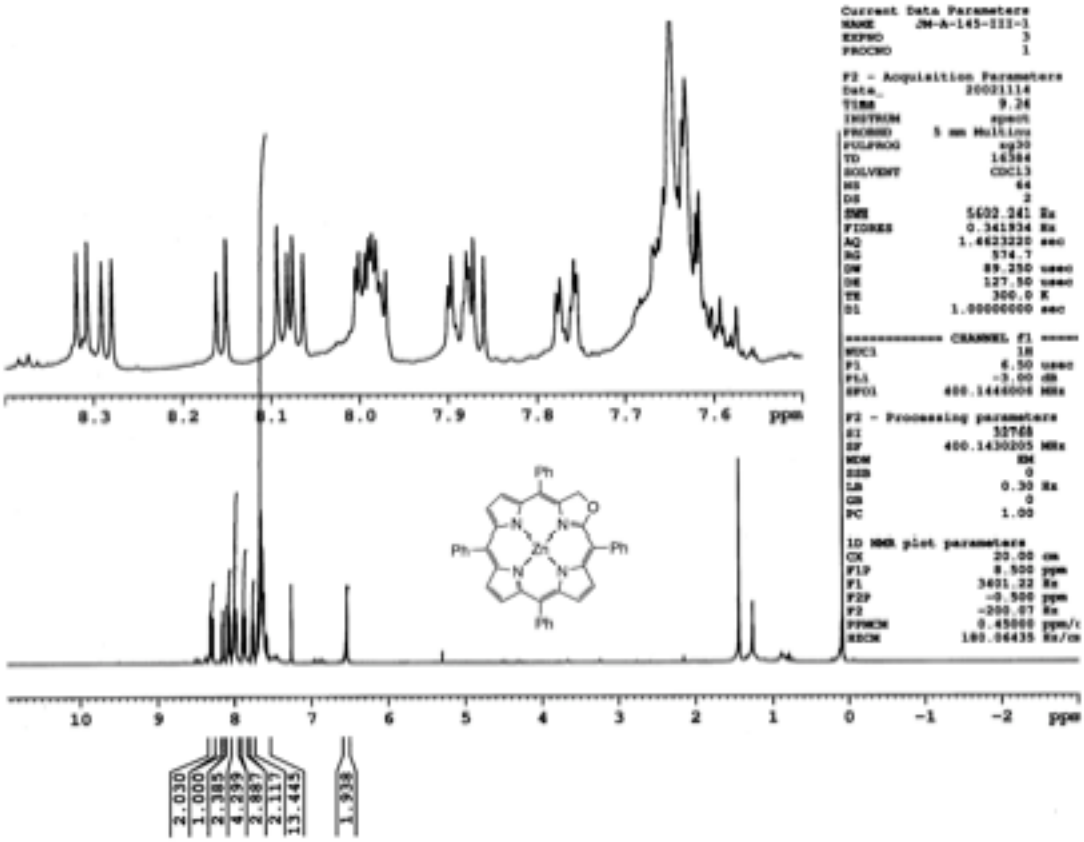

Figure S34. ^{1}H NMR Spectrum (100 MHz, $CDCl_3$) of **12aZn**

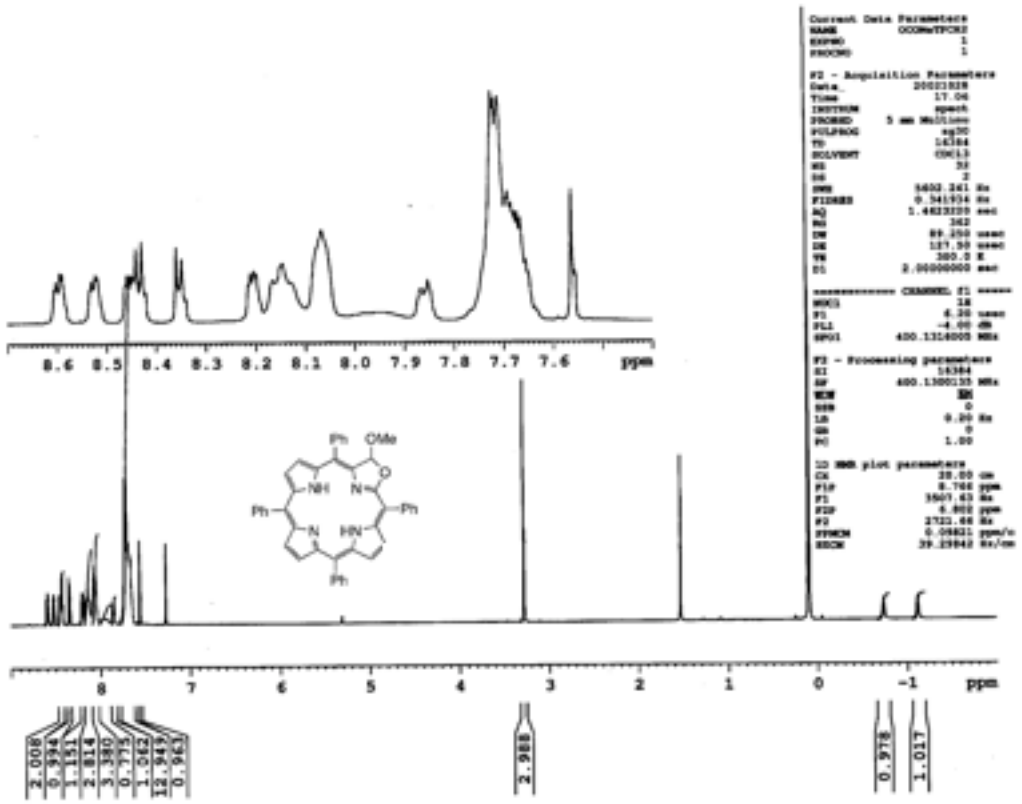

Figure S35. ^{1}H NMR Spectrum (100 MHz, $CDCl_3$) of **13a-OMe**

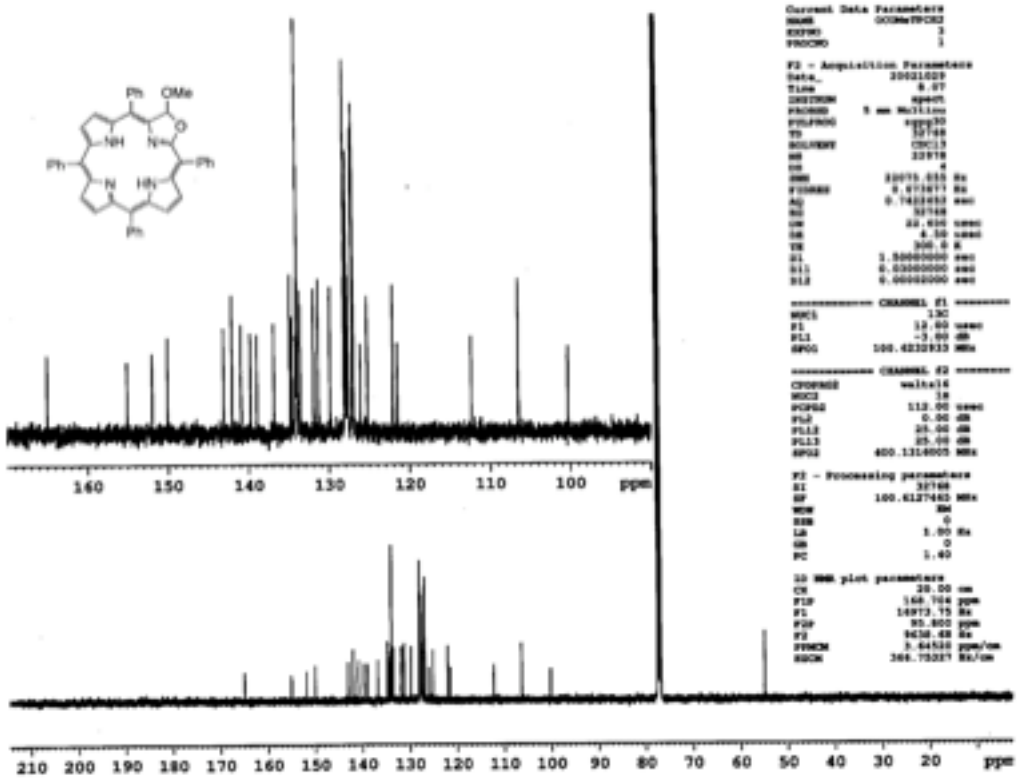

Figure S36. ^{13}C NMR Spectrum (100 MHz, $CDCl_3$) of **13a-OMe**

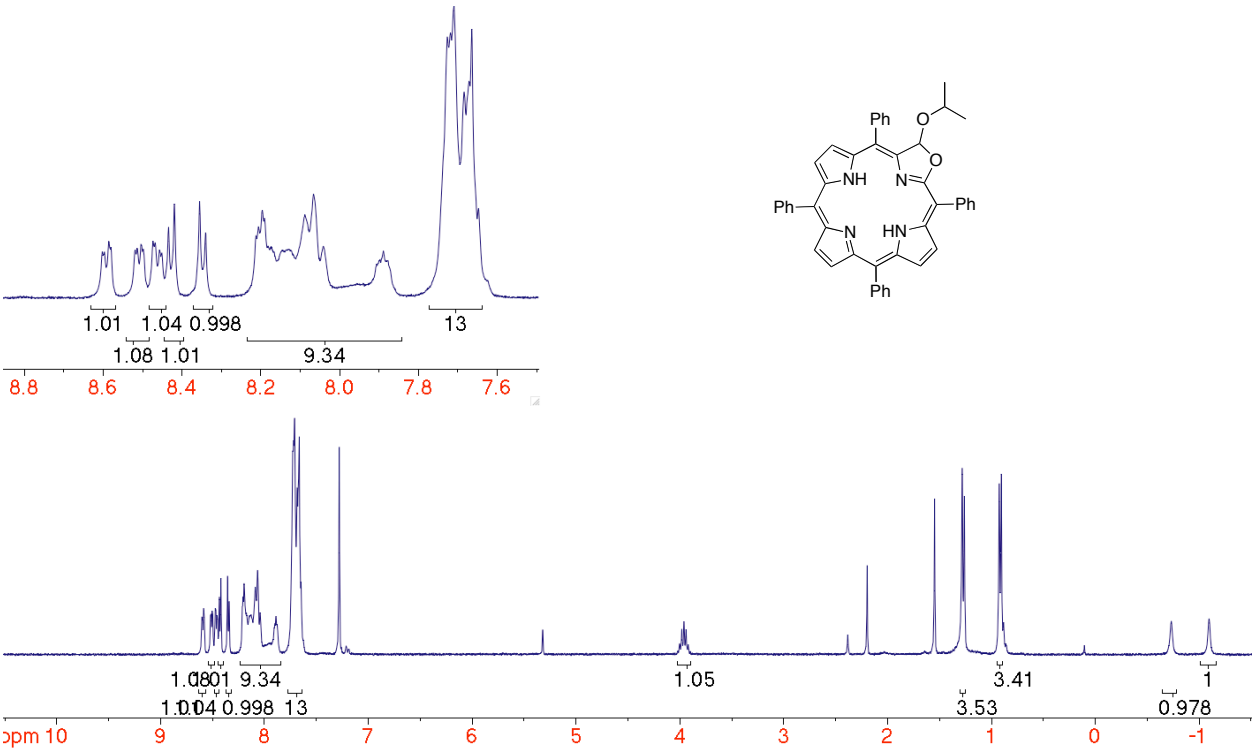

Figure S37. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of **13a-O^{i}Pr**

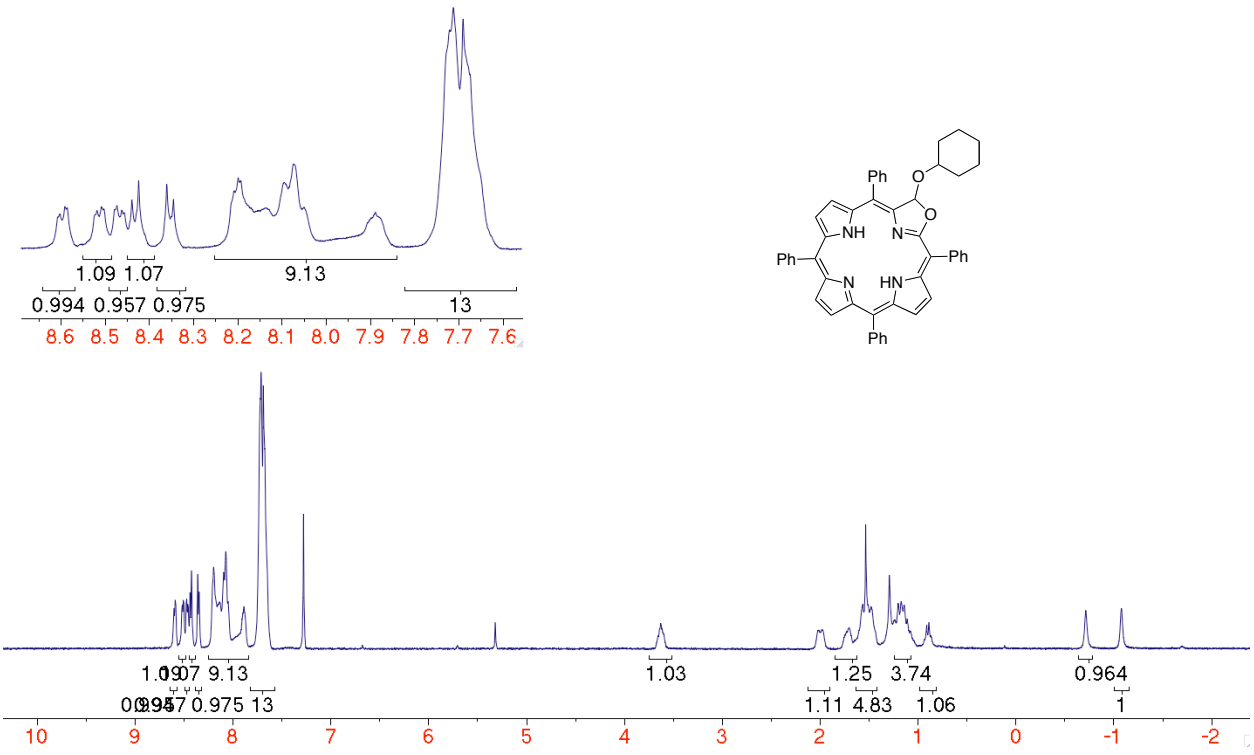

Figure S38. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of **13a-O^{c}Hex**

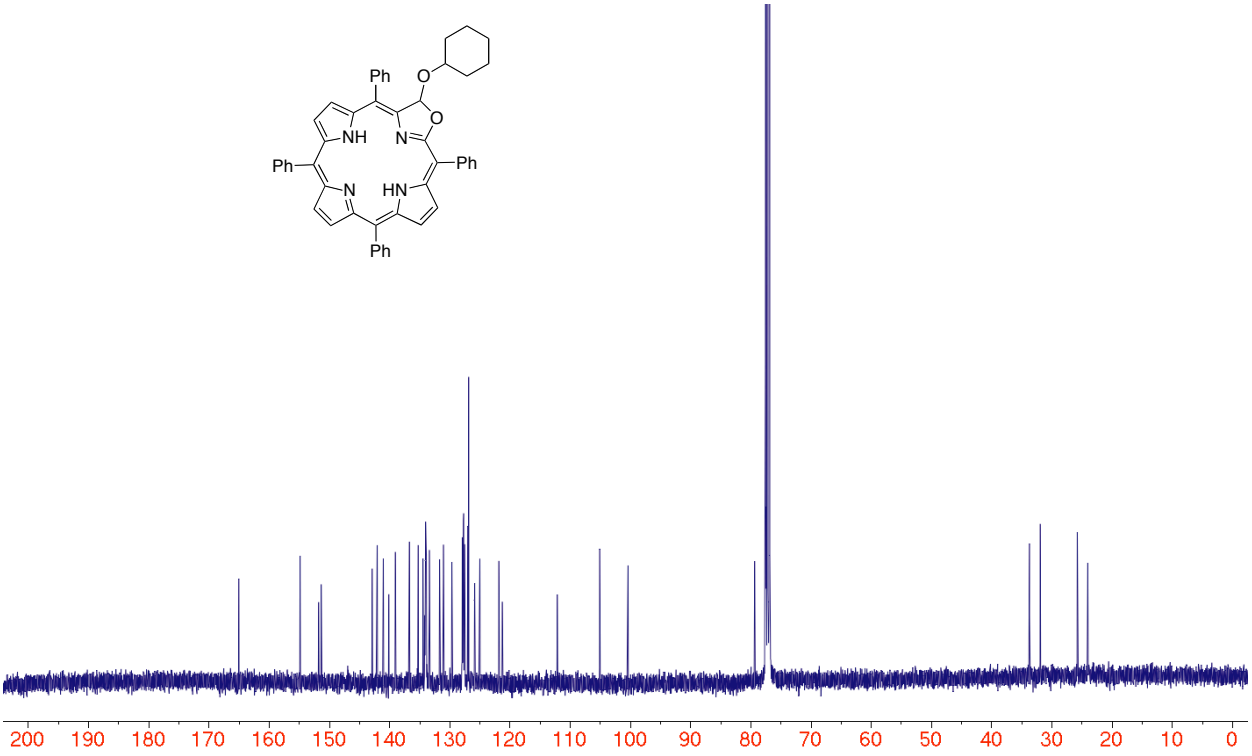

Figure S39. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **13a-O^{c}Hex**

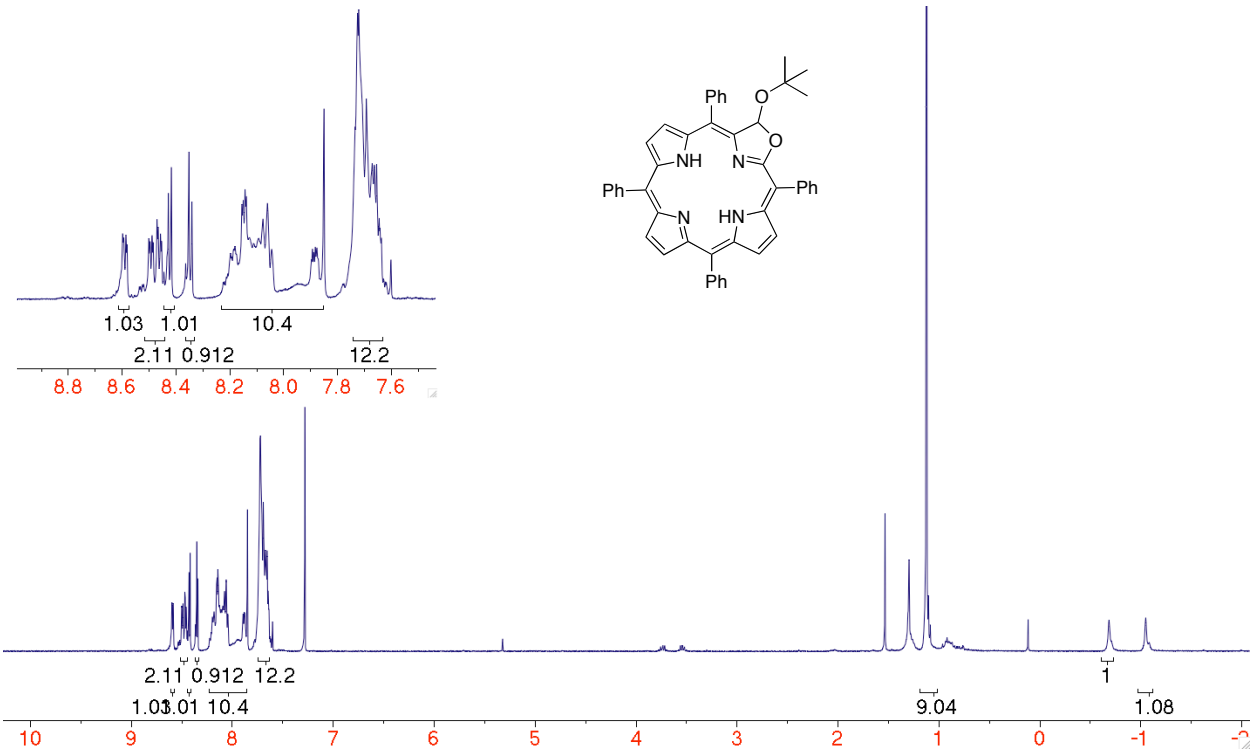

Figure S40. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of **13a-O^{t}Bu**

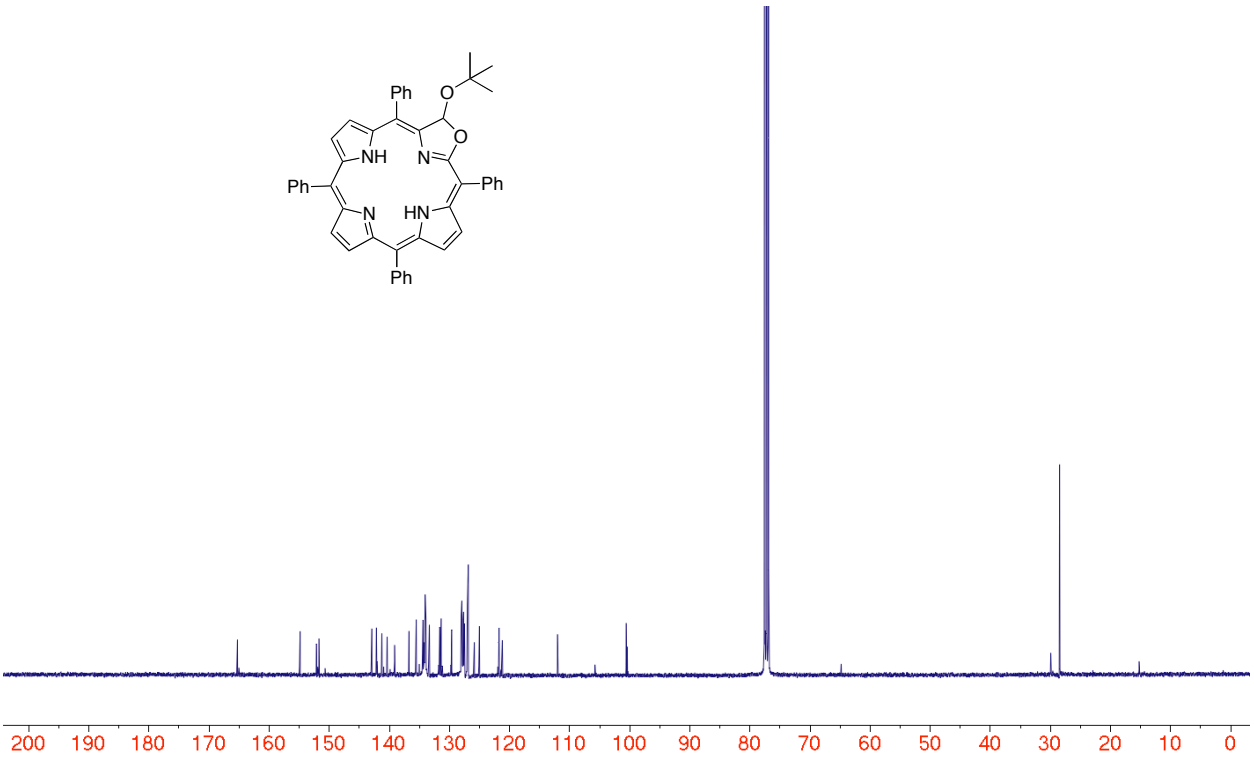

Figure S41. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **13a-O^{t}Bu**

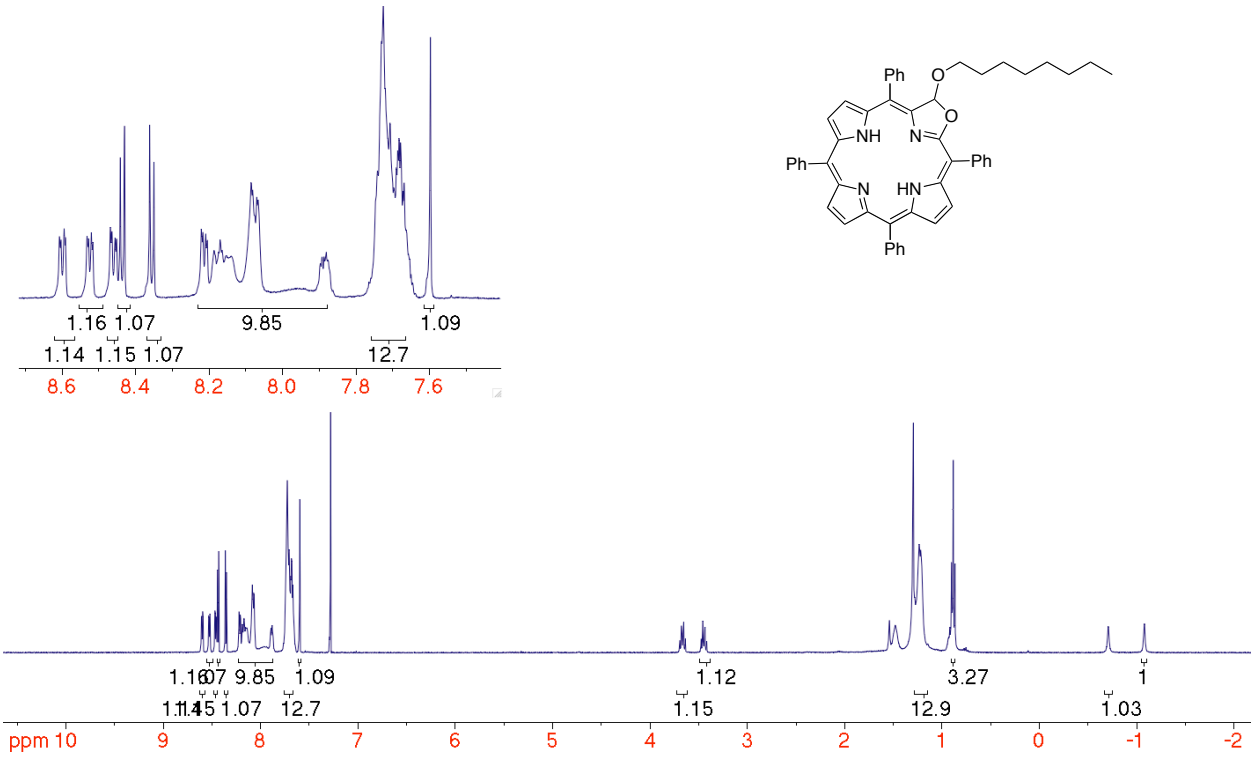

Figure S42. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of **13a-O^{n}Oct**

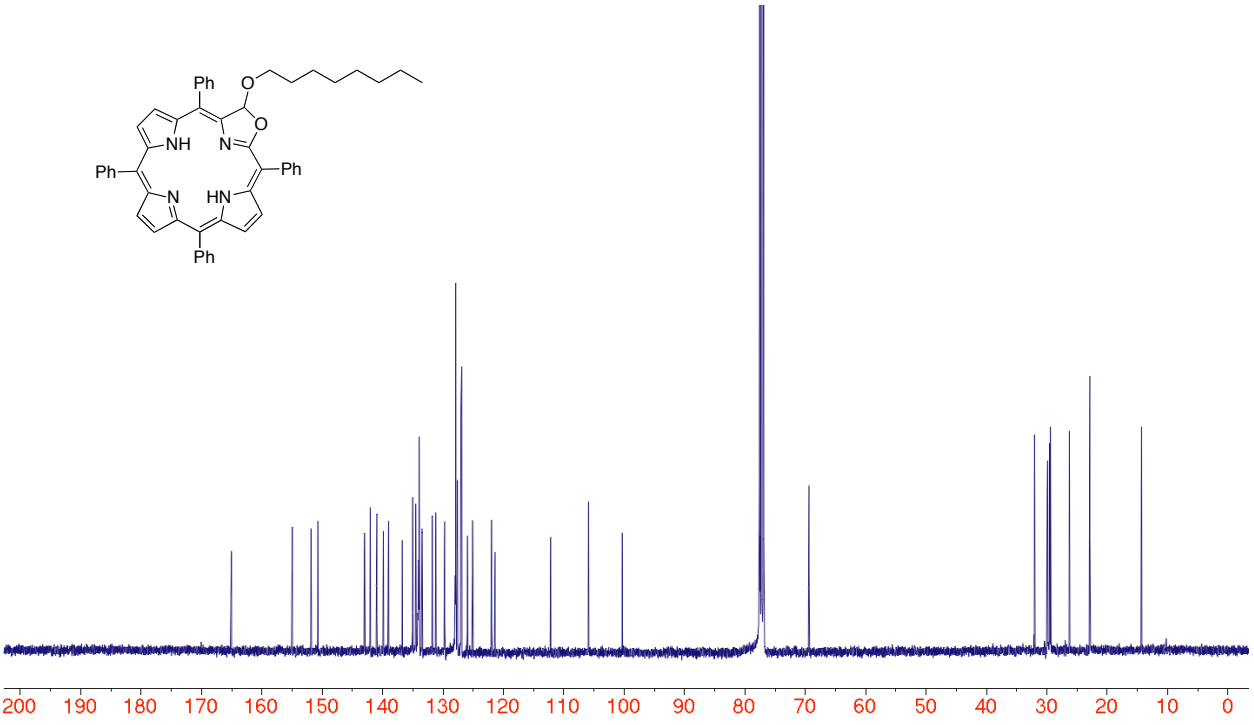

Figure S43. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **13a-O^{n}Oct**

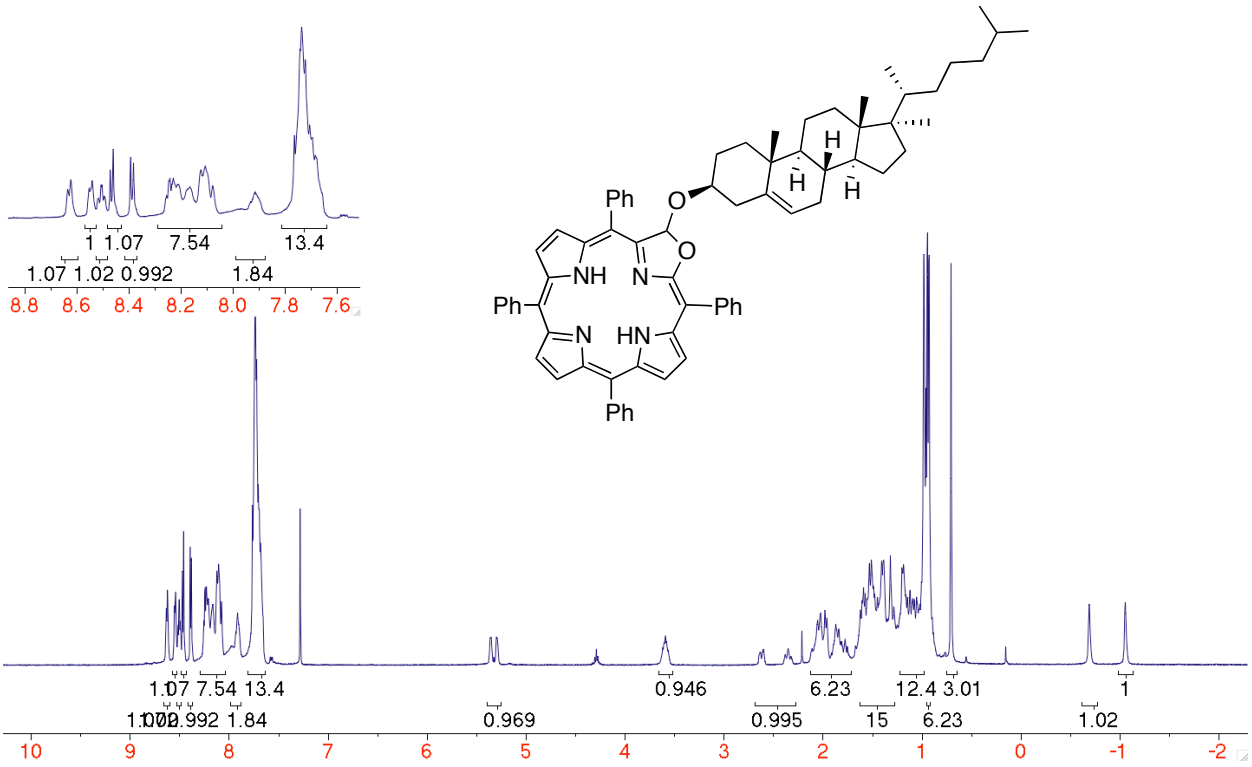

Figure S44. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **13a-OChol**

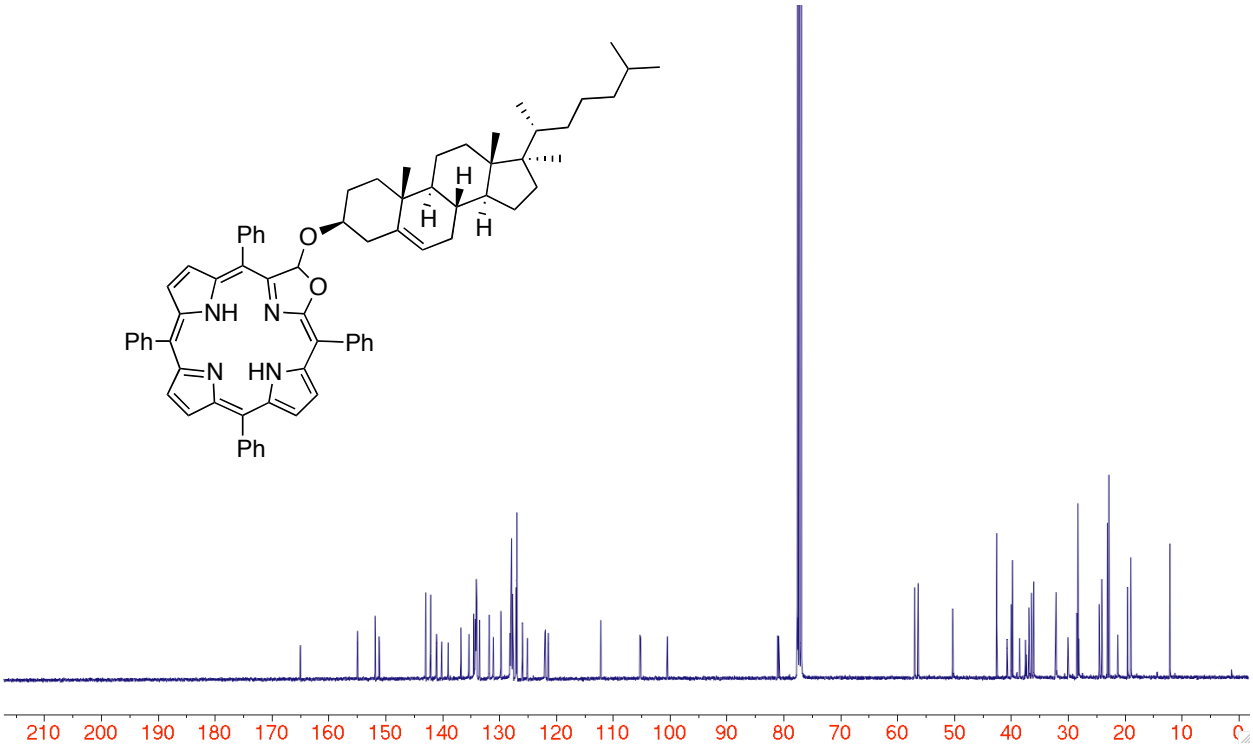

Figure S45. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **13a-OChol**

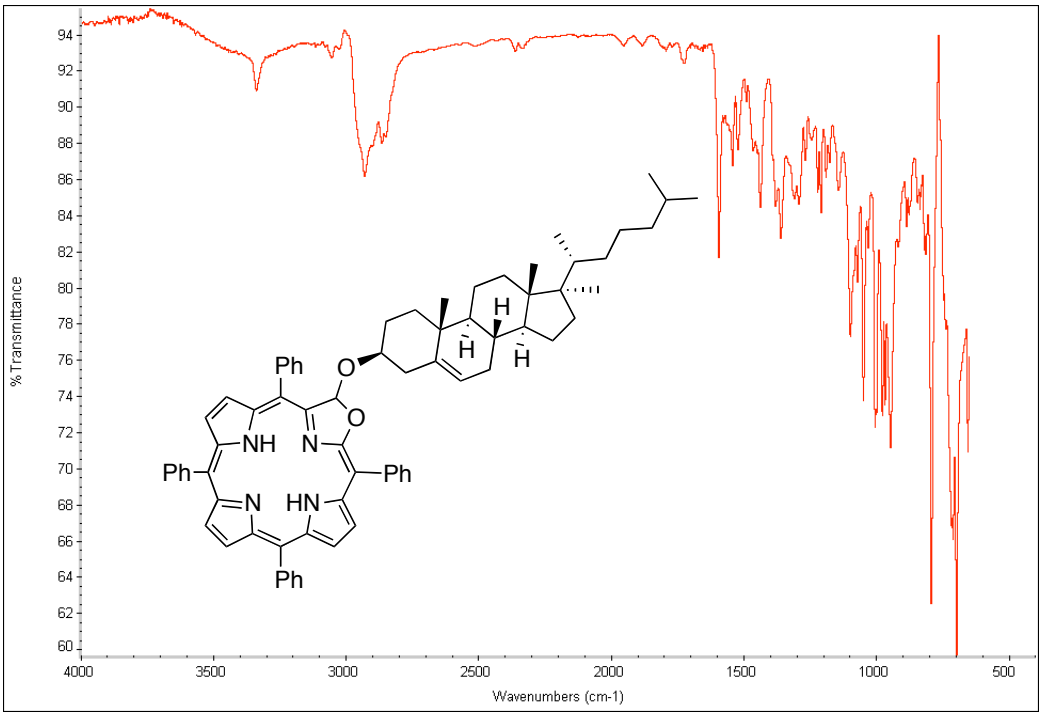

Figure S46. FT-IR spectrum (neat, diffuse reflectance) of **13a-OChol**

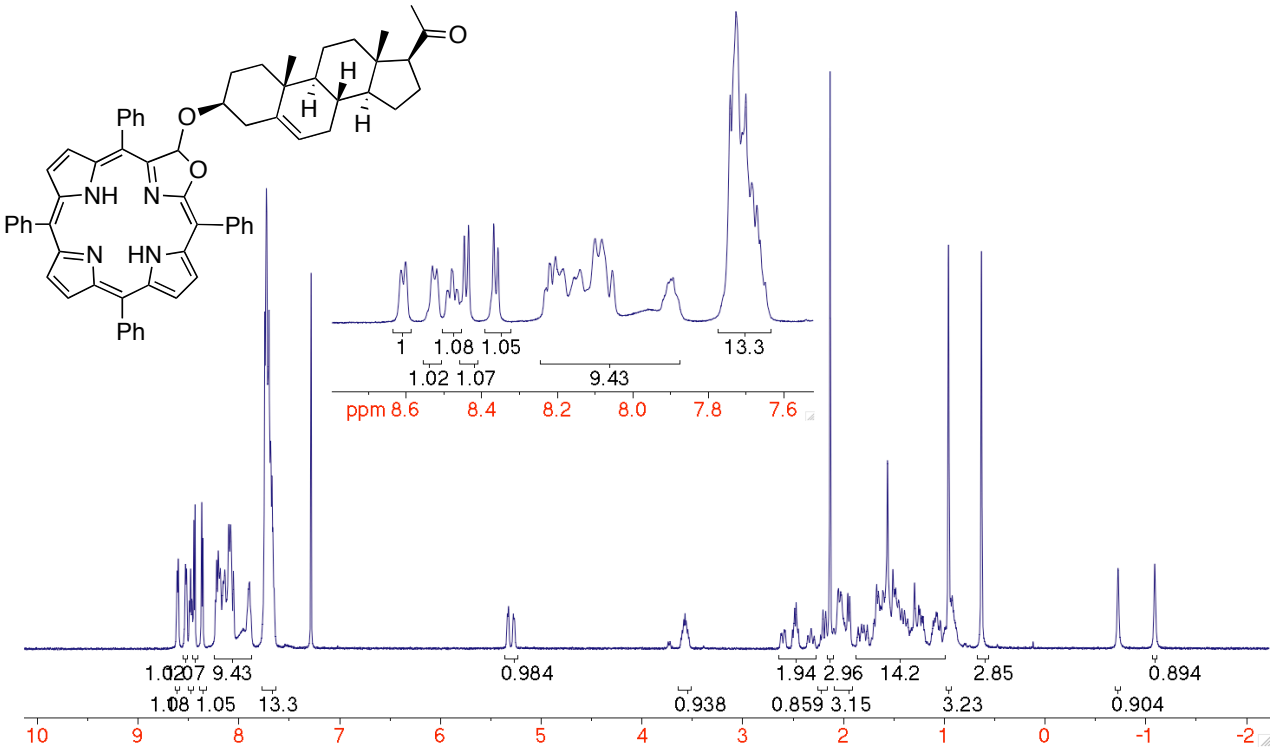

Figure S47. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **13a-OPreg**

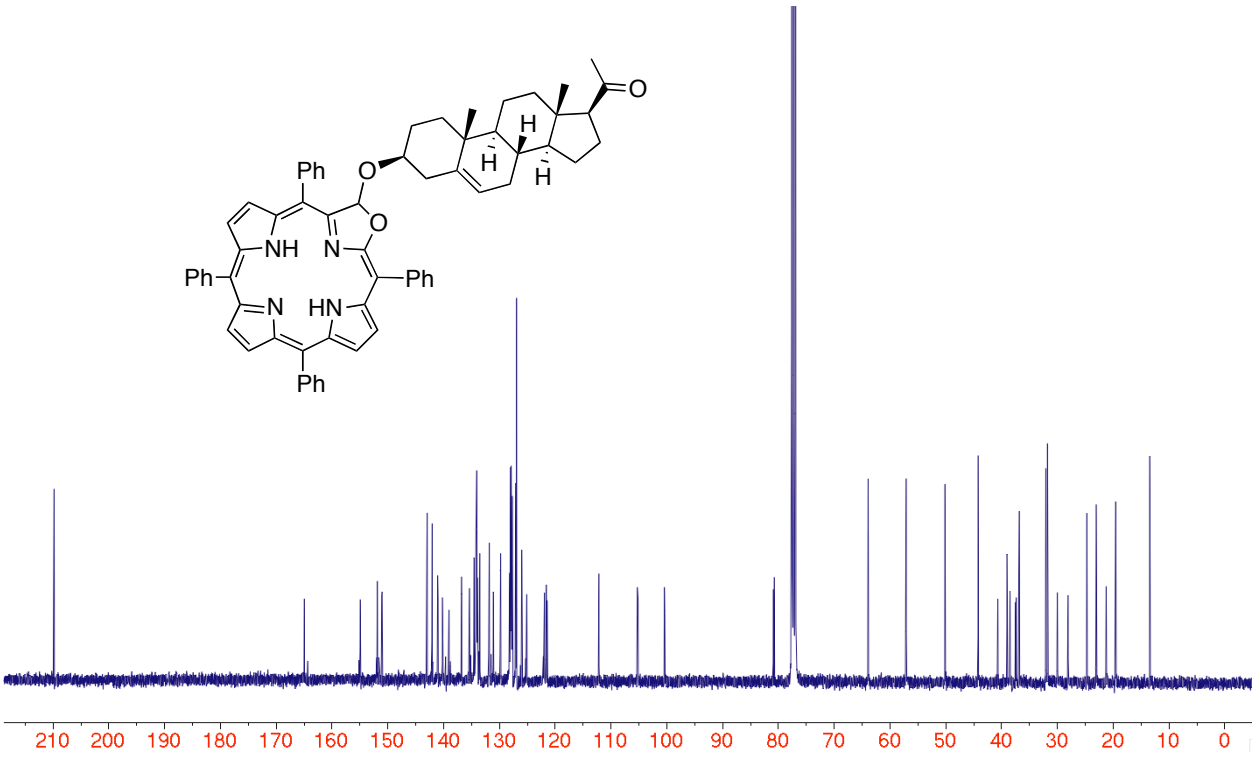

Figure S48. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **13a-OPreg**

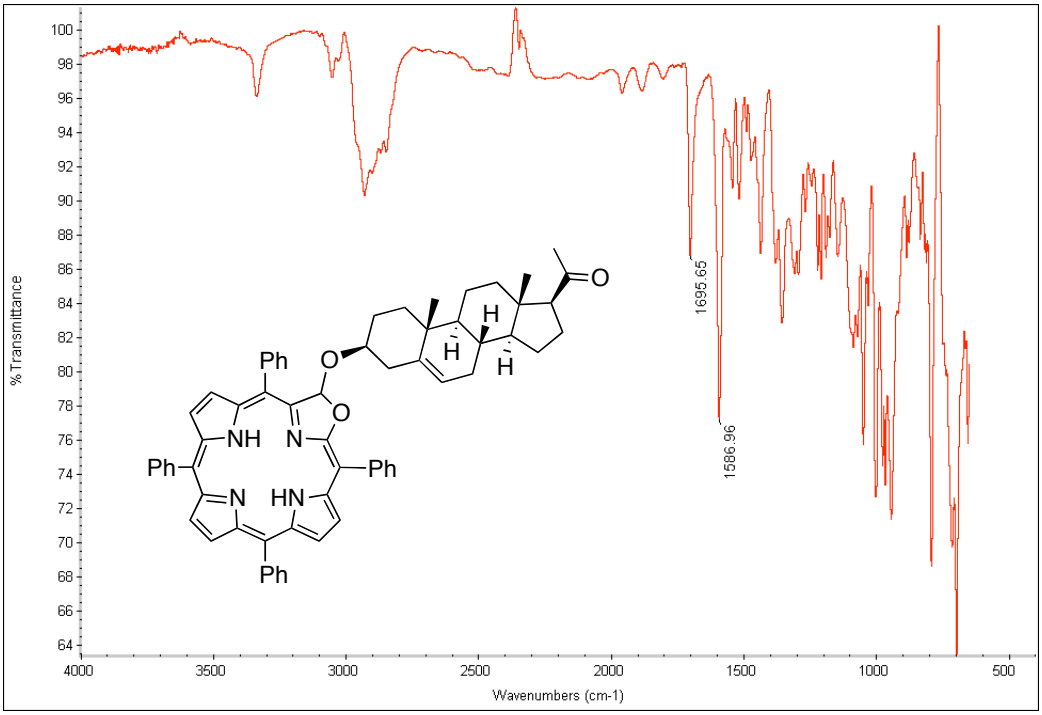

Figure S49. FT-IR spectrum (neat, diffuse reflectance) of **13a-OPreg**

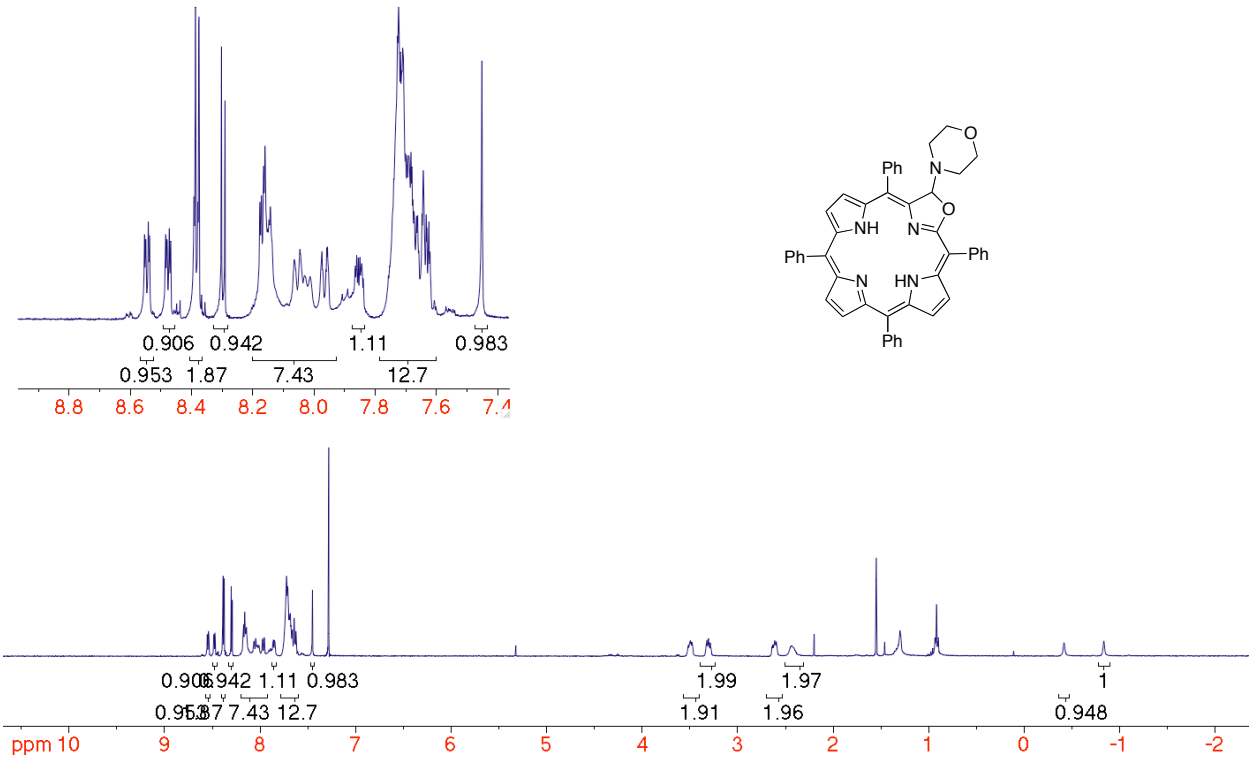

Figure S50. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of **13a-N^{morph}**

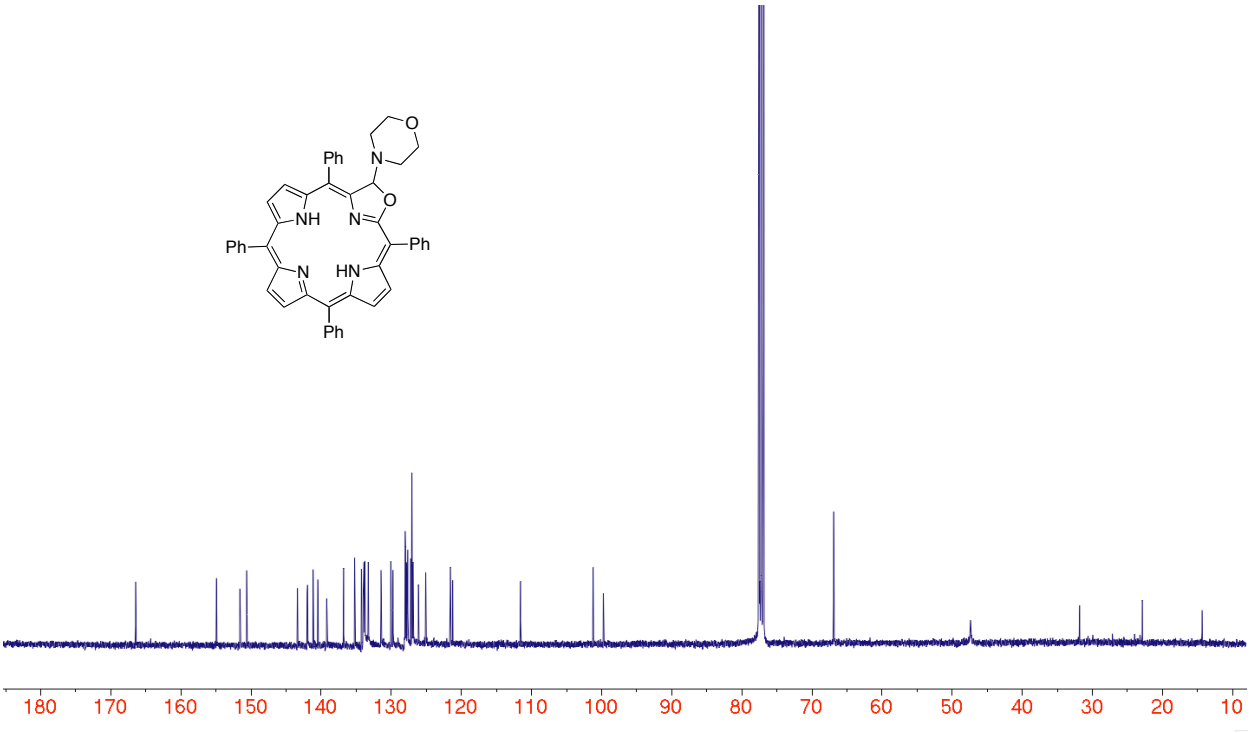

Figure S51. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **13a-N^{morph}**

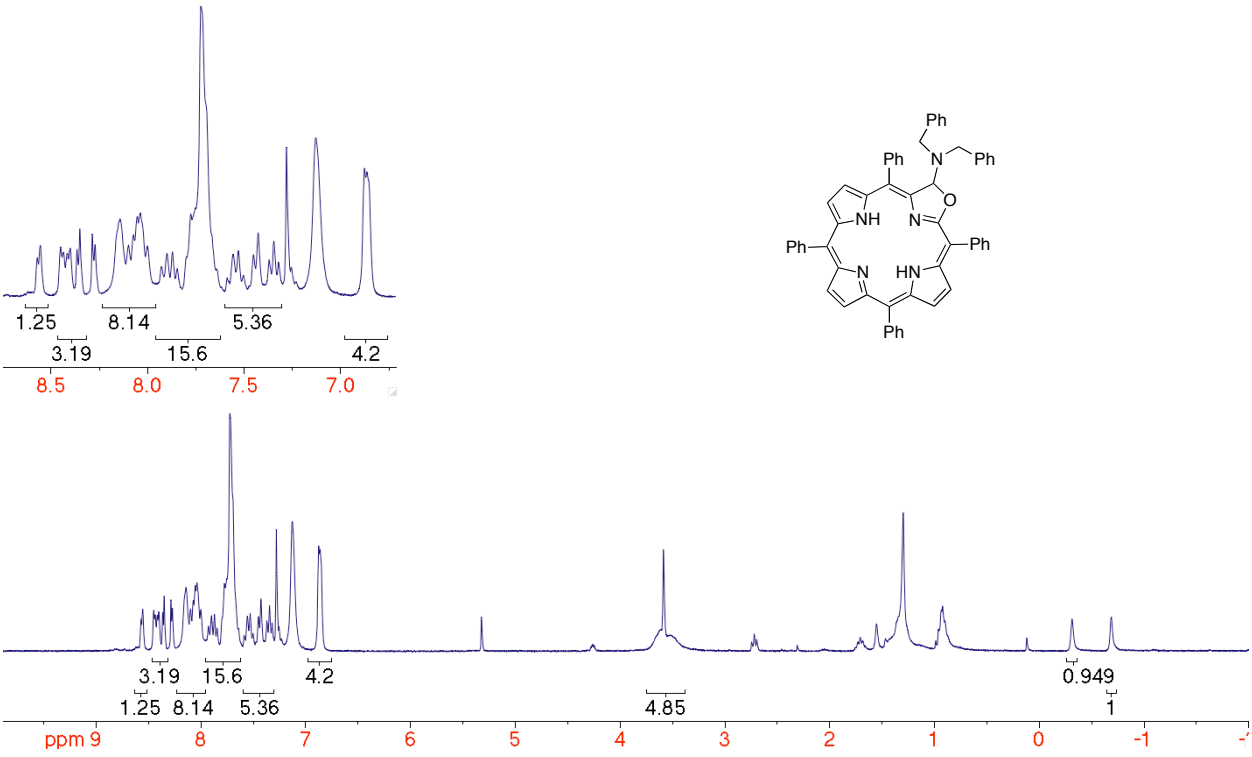

Figure S52. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of **13a-N(Bn)$_2$**

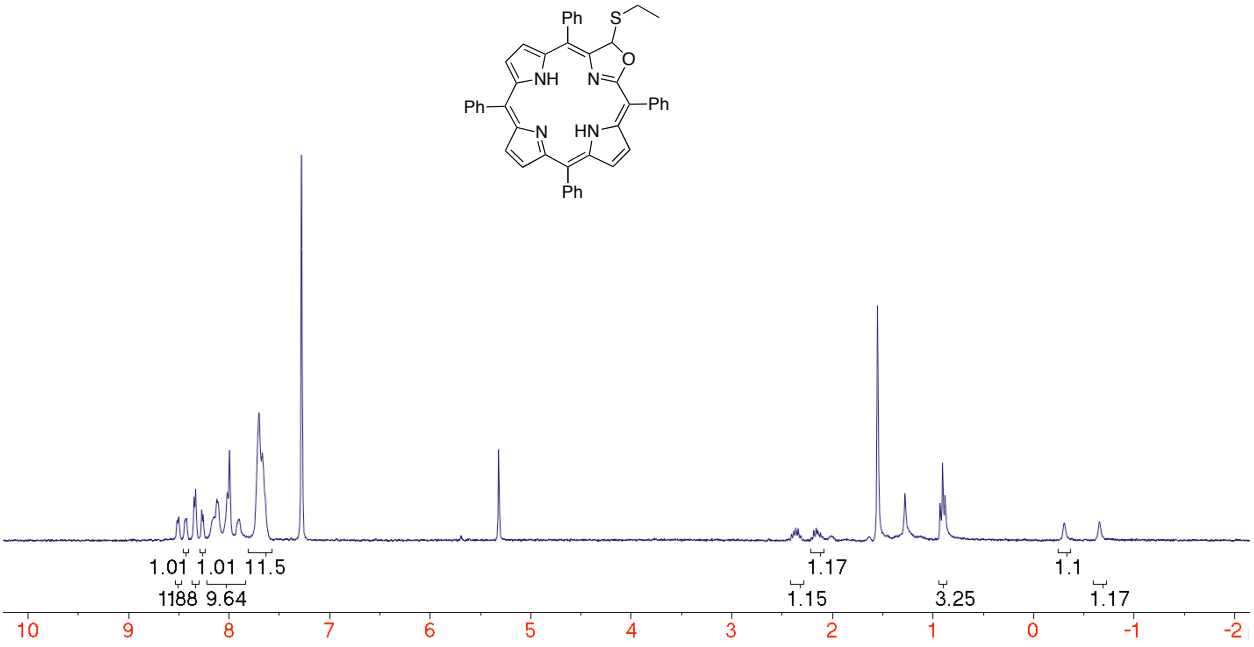

Figure S53. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of **13a-SEt**

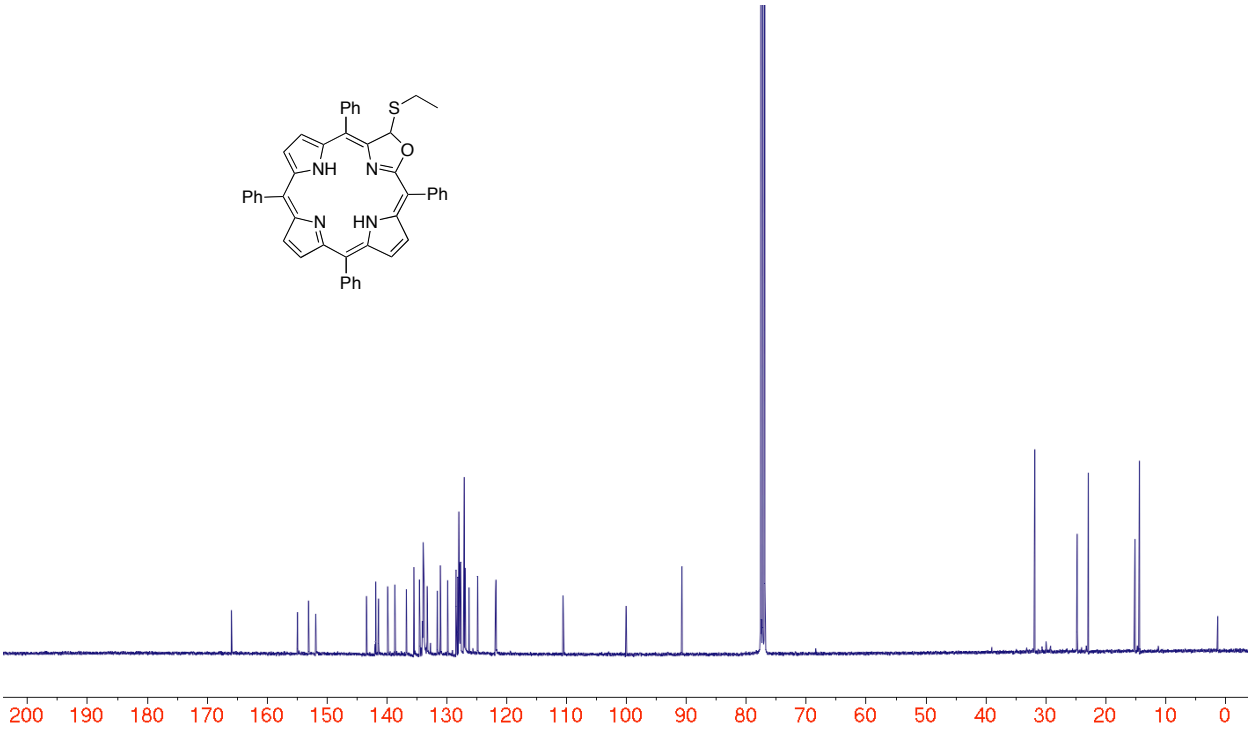

Figure S54. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **13a-SEt**

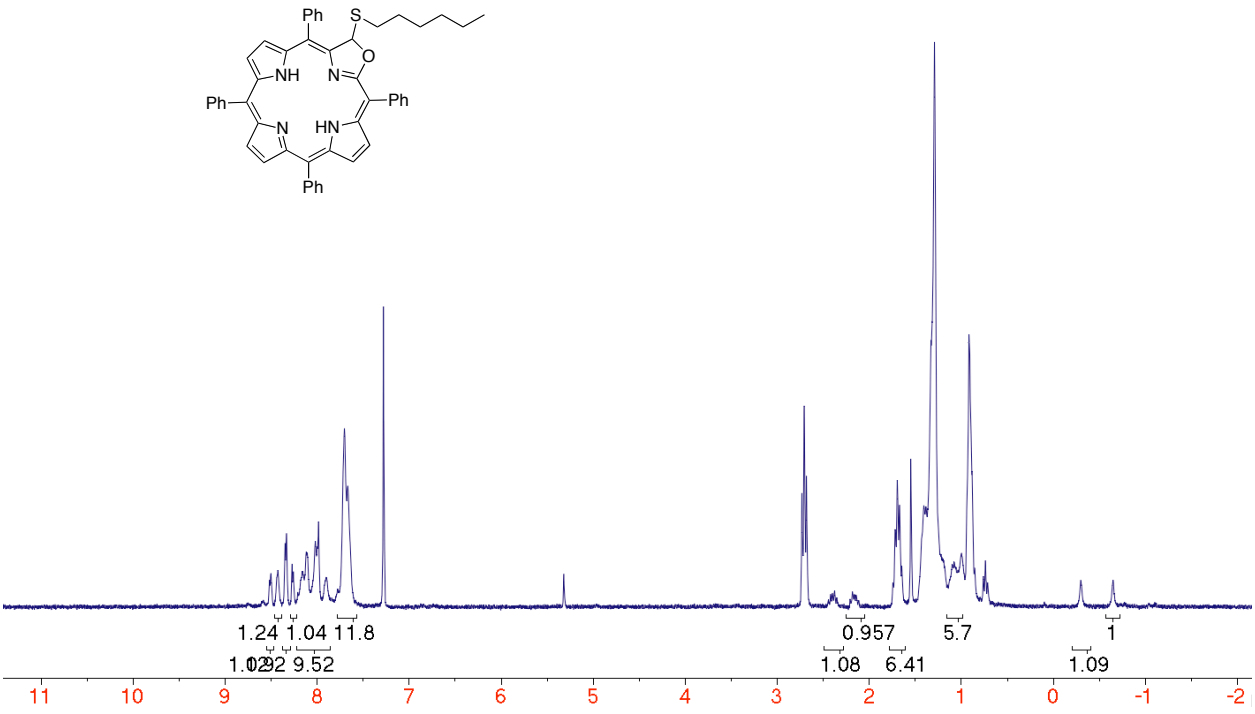

Figure S55. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of **13a-S^{n}Hex**

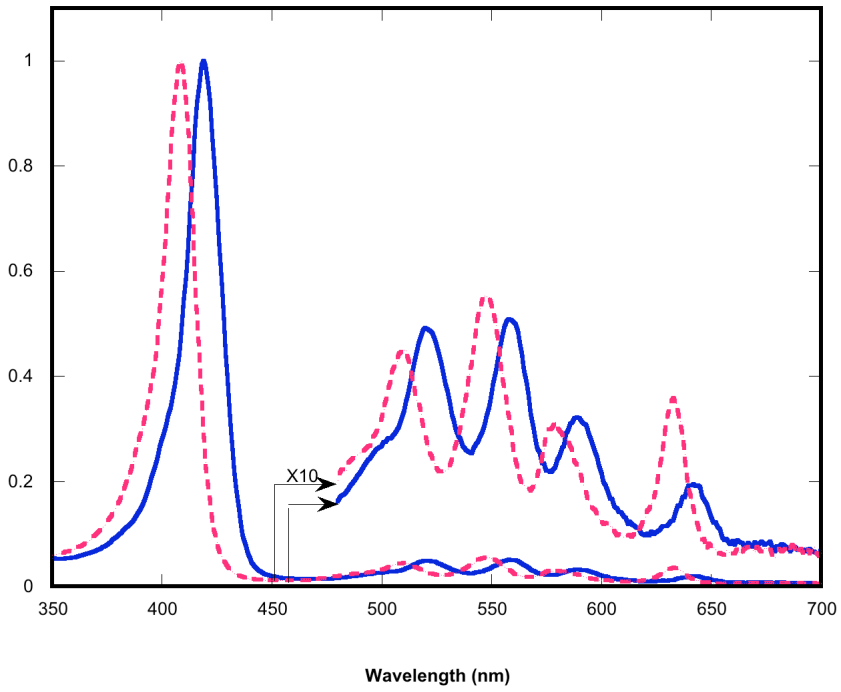

Figure S56. Normalized UV-visible spectra of porpholactones **5aH$_2$** (blue, solid trace) and **15-II-H$_2$** (red, dotted trace)

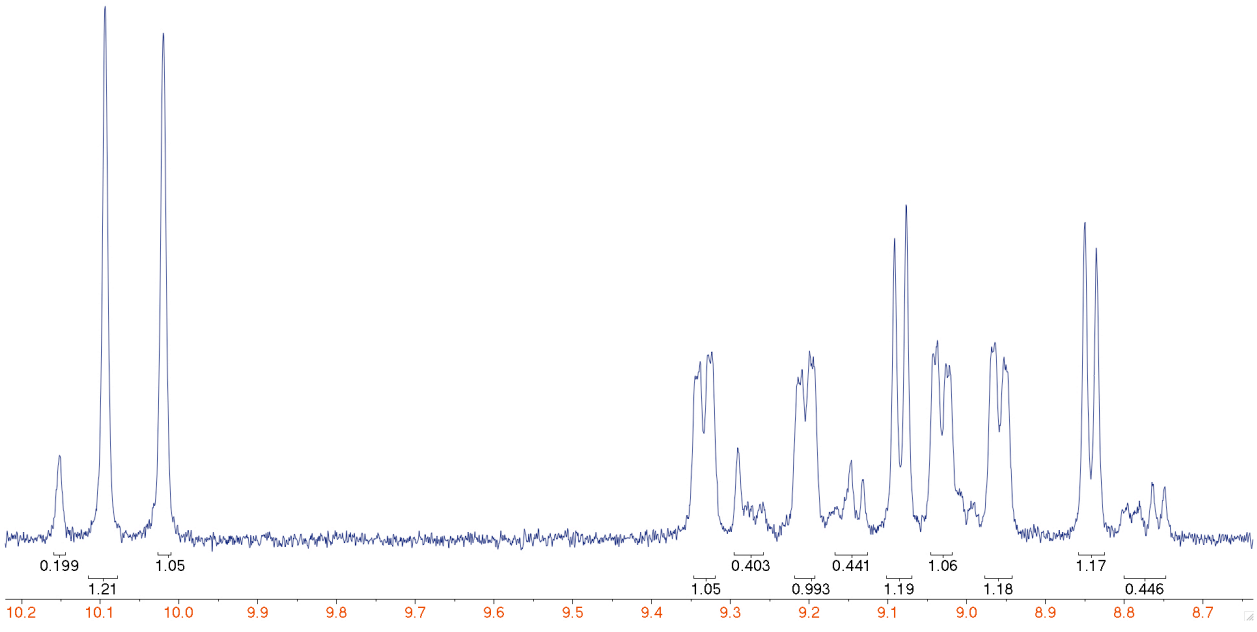

Figure S57. ^{1}H NMR (400 MHz, $CDCl_3$) of a mixture of the two regio-isomers of 5,15-diphenylporpholactones, **15-I-H$_2$** and **15-II-H$_2$**

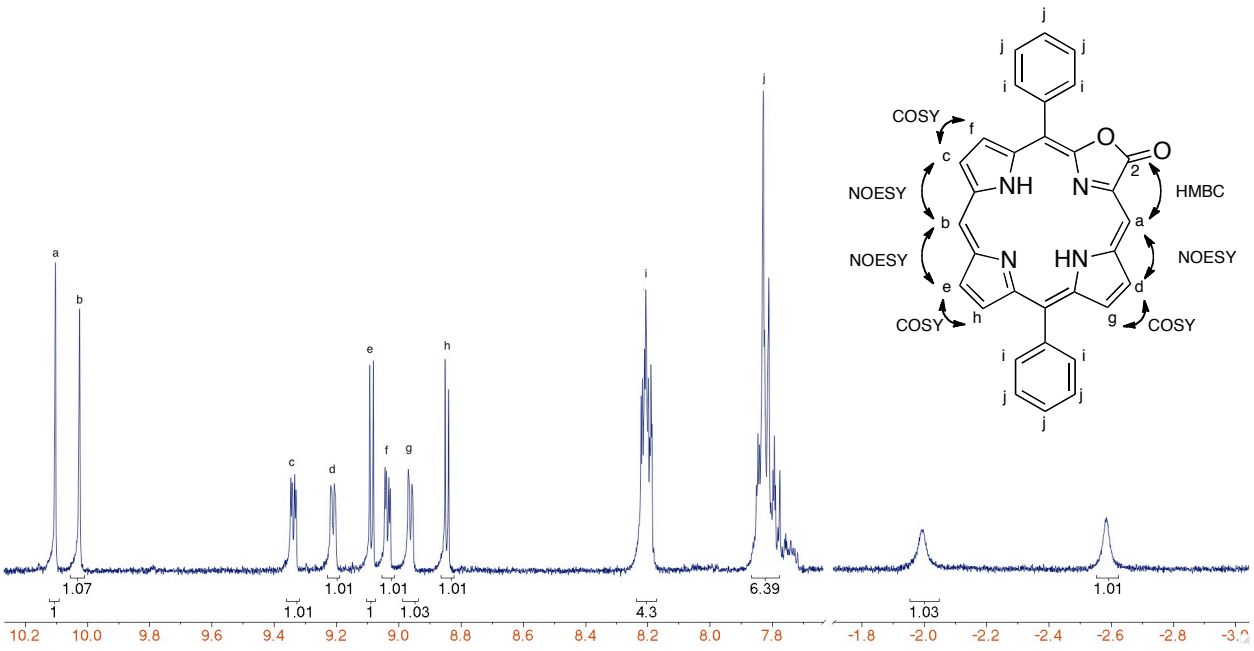

Figure S58. ^{1}H NMR (300 MHz, $CDCl_3$) of **15-II-H$_2$**. Assignment of proton signals as shown, and based on the 2D spectra shown below.

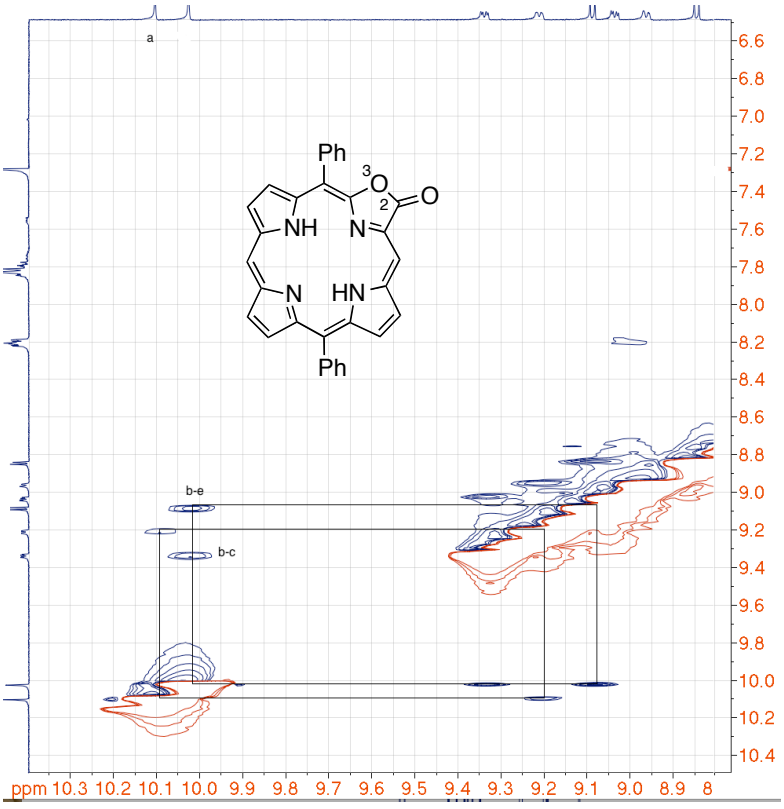

Figure S59. NOESY Spectrum (300 MHz, $CDCl_3$) of **15-II-H$_2$.**

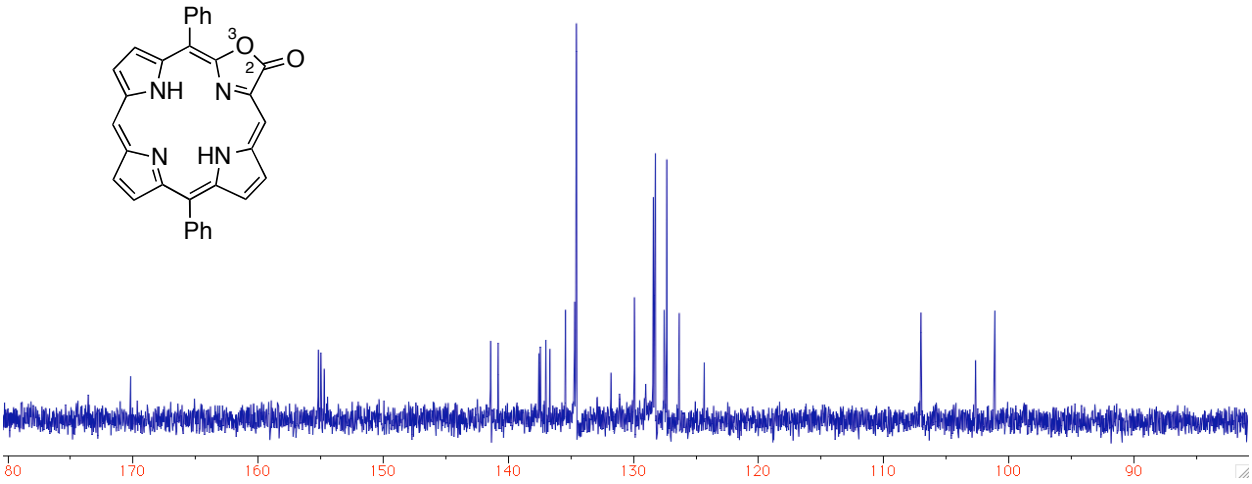

Figure S60. ^{13}C NMR (100 MHz, $CDCl_3$) of **15-II-H$_2$.**

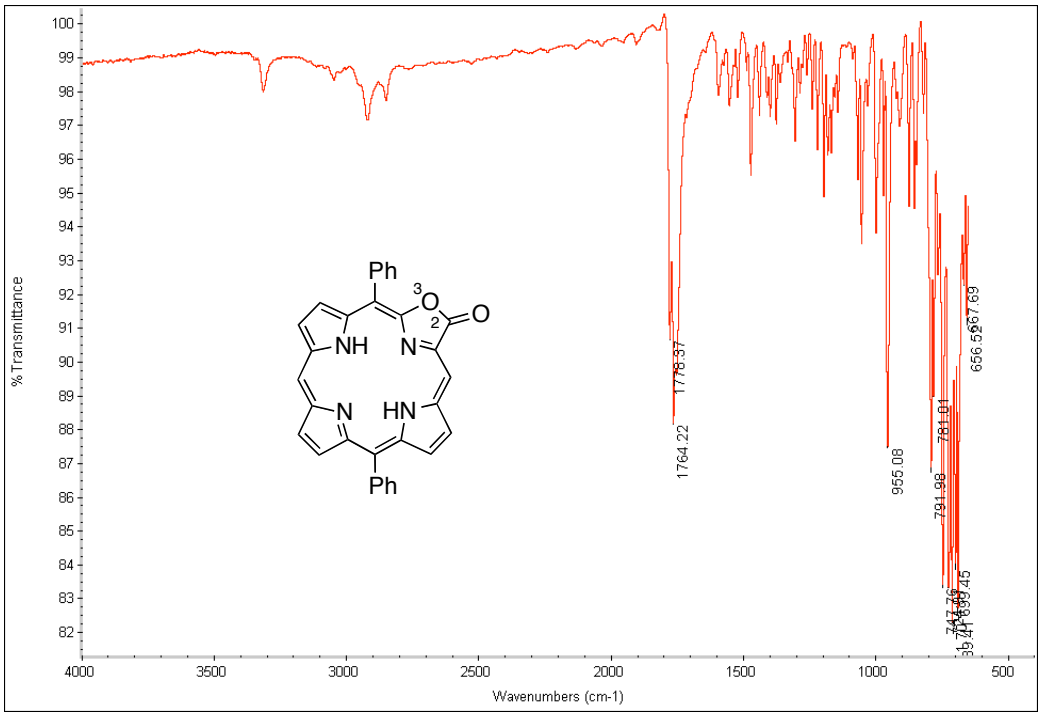

Figure S61. FT-IR spectrum (neat, diffuse reflectance) of **15-II-H$_2$**

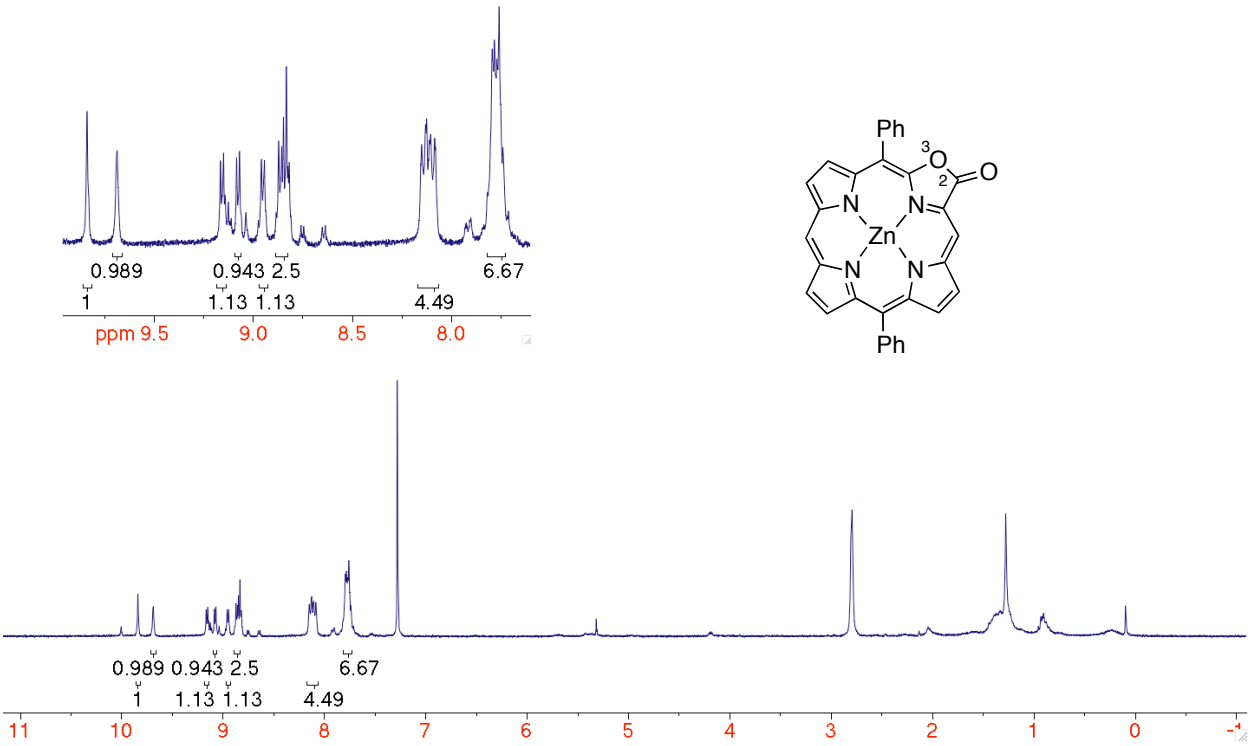

Figure S62. ^{1}H NMR (300 MHz, $CDCl_3$) of **15-II-Zn.**

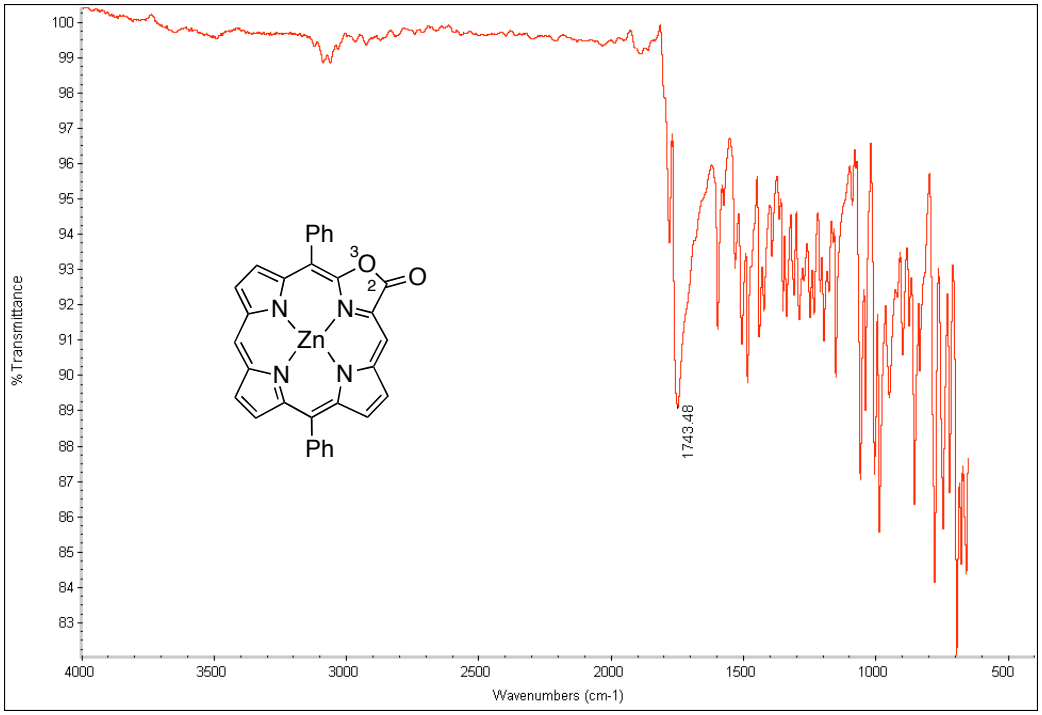

Figure S63. FT-IR spectrum (neat, diffuse reflectance) of **15-II-Zn.**

DETAILS OF THE SINGLE CRYSTAL X-RAY DIFFRACTOMETRY STUDIES

Table S1. Crystallographic data and structure refinement for **5aH$_2$.**

Identification code:	06mz049m
Empirical formula:	$C_{43}H_{28}N_4O_2$
Formula weight:	632.69
Temperature:	100(2) K
Wavelength:	0.71073 Å
Crystal system:	Triclinic
Space group:	P-1
Unit cell dimensions:	
	a = 6.3491(4) Å, α = 94.1750(10)°
	b = 10.3930(6) Å, β = 100.3440(10)°
	c = 12.2632(7) Å, γ = 90°
Volume, *Z*:	778.20(8) Å^3, 1
Density (calculated):	1.350 Mg/m^3
Absorption coefficient:	0.084 mm^{-1}
F(000):	330
Crystal size:	0.46 × 0.40 × 0.18 mm
Crystal shape, colour:	block, black
θ range for data collection:	1.70 to 28.28°
Limiting indices:	$-8 \le h \le 8$, $-13 \le k \le 13$ $-16 \le l \le 16$
Reflections collected:	7972
Independent reflections:	3842 (R(int) = 0.0187)
Completeness to θ = 28.28°:	99.4 %
Absorption correction:	multi-scan
Max. and min. transmission:	0.985 and 0.907
Refinement method:	Full-matrix least-squares on F^2
Data / restraints / parameters:	3842 / 45 / 238
Goodness-of-fit on F^2:	1.157
Final R indices [$I>2\sigma(I)$]:	R1 = 0.0565, wR2 = 0.1378
R indices (all data):	R1 = 0.0581, wR2 = 0.1389
Largest diff. peak and hole:	0.323 and -0.216 e × Å^{-3}

Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors

Comments:

The free base lactone **5aH$_2$** molecule (code 06mz049m) is located on an inversion center and the lactone moiety is disordered with the pyrrol units over three different positions. Two of the three are disordered with one of the two pyrrols (flip disordered with respect to themselves), and the third position is disordered with the second pyrrol. Occupancy restraints were applied as follows:

1. All pyrrol occupancies were restraint to sum up to 1.5 (half of 3 since molecule is located on an inversion center). The sum of the lactone occupancies was restrained to 0.5. For the pyrrol unit disordered with only one lactone moiety the occupancies of both were restrained to sum up to 1. The occupancies for the first site refined to 0.573(2) for the pyrrol, and 0.266(3) and 0.157(3) for the two lactone moieties. The occupancies for the second site refined to 0.927(2) for the pyrrol and 0.077(2) for the lactone.
2. For the disordered parts of the molecule additional restraints were applied. The two pyrrol and the three lactone units were restrained to have the same geometries within a standard deviation of 0.02 Å. The pyrrol units were restraint to be flat within a standard deviation of 0.1 Å^2. For the lactone equivalent 1,3 distances within the rings were restrained to be identical within a standard deviation of 0.02 Å, as were the keto C=O bond lengths. All anisotropic displacement parameters within the disordered parts of the rings were restrained to be identical and isotropic (within a standard deviation of 0.01). All anisotropic displacement parameters of the keto oxygen atoms were restrained to be identical.

One keto oxygen atom of one of the lactone units (that with the 15.9% occupancy) is forced into a close contact with an aromatic carbon atom of a neighboring molecule, which forces this lactone moiety out of the plane of the porpholactone molecule. The distance between the keto oxygen atom O3 and the carbon atom C14^{i} is 2.910(7) Å (symmetry operator (i) 2-x, 1-y, -z).

Treatment of hydrogen atoms:

All hydrogen atoms were located in the difference density Fourier map and were isotropically refined with a displacement parameter 1.2 times that of the adjacent carbon atom. The occupancy ratio for the two pyrrole hydrogen atoms was refined to 0.266(4) to 0.734(3).

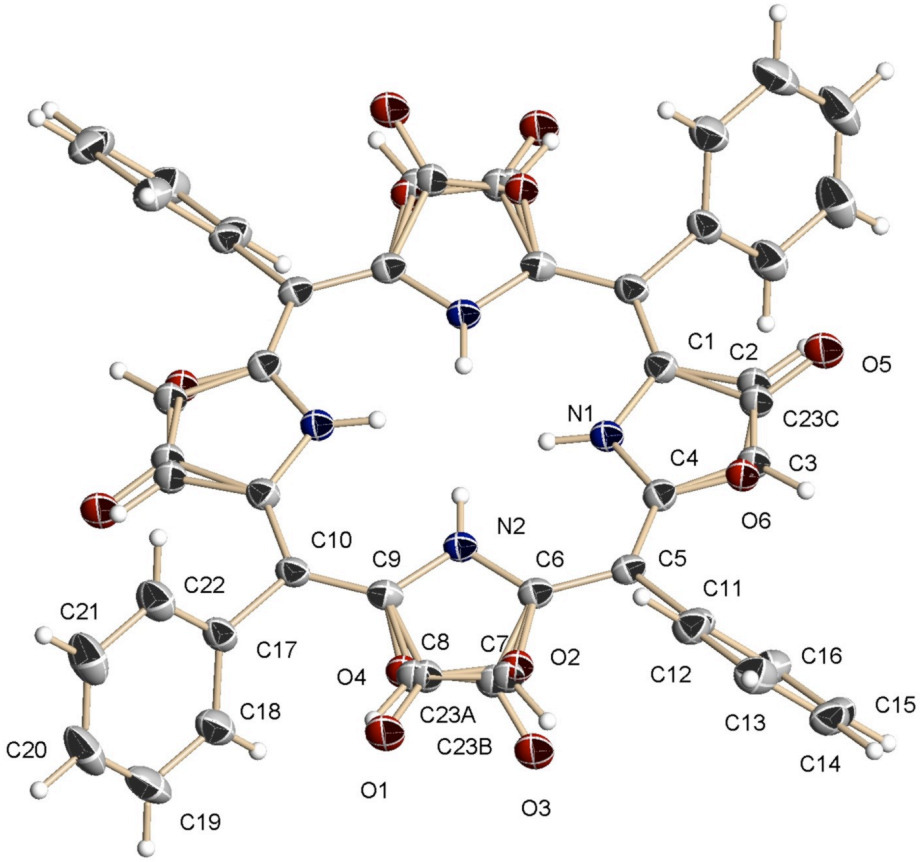

Figure S64. ORTEP representation and numbering scheme used in the crystal structure of **5aH$_2$**.

Table S2. Crystallographic data and structure refinement for **5aZn.**

Crystal shape: rod (black). Experiments were carried out at 100 K with Mo *K*α radiation using a Bruker AXS SMART APEX CCD diffractometer. Data collection used ω scans. Absorption was corrected for by multi-scan methods, Apex2 v2009.7-0 (Bruker, 2009). H-atom parameters were constrained.

Crystal data	
Chemical formula	$C_{48}H_{31}N_5O_2Zn$
M_r	775.19
Identification code	JA-B-152_09mz431
Crystal system, space group	Monoclinic, *C*2/*c*
a, *b*, *c* (Å)	14.863 (9), 17.010 (11), 14.667 (9)
α, β, γ (°)	90, 93.844 (10), 90
V (Å^3)	3700 (4)
Z	4
F(000)	1600
D_x (Mg m^{-3})	1.392
μ (mm^{-1})	0.71
Crystal size (mm)	0.55 × 0.20 × 0.10
Data collection	
Radiation source	fine-focus sealed tube
Monochromator	graphite
T_{min}, T_{max}	0.462, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	12911, 3385, 2252
R_{int}	0.066
θ values (°)	θ_{max} = 25.4, θ_{min} = 1.8
Range of *h*, *k*, *l*	*h* = -17→17, *k* = -20→20, *l* = -17→16
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.092, 0.213, 1.17
No. of reflections	3385
No. of parameters	486
No. of restraints	845
$\Delta\rangle_{max}$, $\Delta\rangle_{min}$ (e Å^{-3})	0.78, -0.65

Computer programs: Bruker Advanced X-ray Solutions SMART for WNT/2000 (Version5.628),

Bruker AXS Inc., Madison, WI, USA, 1997–2002. Apex2 v2009.7-0 (Bruker, 2009), Apex2 v2009.7-0, *SHELXTL* 6.14 (Bruker, 2000-2003; Sheldrick, 2008), *SHELXTL* 6.14.

Comments

The molecule **5aZn** as a whole is disordered over two positions related by a two fold axis running through the pyridine ligand and close to the Zn ion. In addition the pyridine ligand is disordered over two positions in a refined ratio of 0.60(2) to 0.40(2). The lactone unit is in addition flip disordered with an occupancy ratio of 0.62(2) to 0.38(2). Due to the proximity of the disordered atoms restraints and constraints needed to be applied to achieve a meaningful refinement. The two halves of the molecule related by pseudo two fold symmetry were restrained to have similar geometries (not including the phenyl rings). The phenyl and pyridyl rings were constrained to resemble ideal hexagons with C-C and C-N distances of 1.39 Å. All atoms were restrained to have ADPs similar to those of their neighbors using the SIMU and DELU restraints from Shelxtl (standard deviation 0.03). Atoms N3 and N3b were in addition constrained to have identical ADPs.

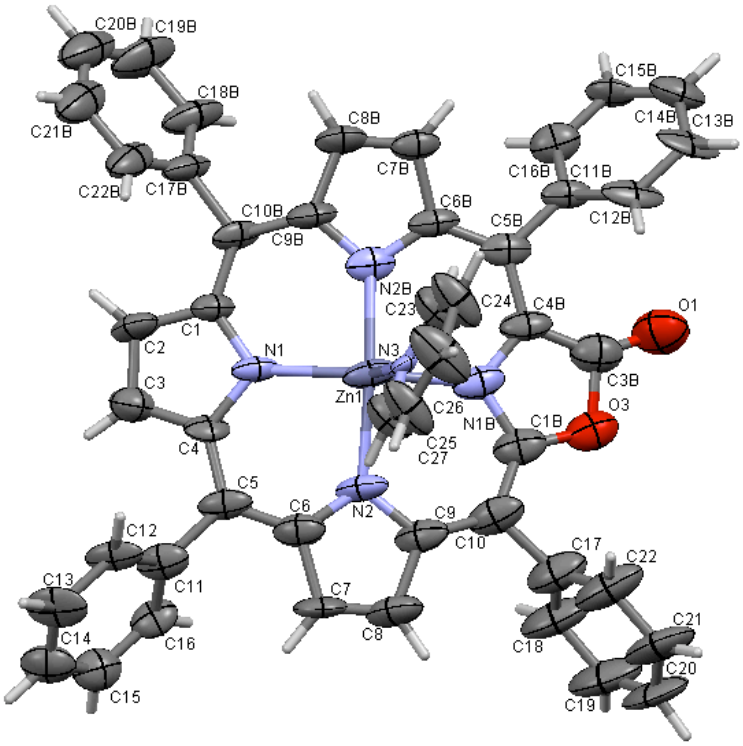

Figure S65. ORTEP representation and numbering scheme used in the crystal structure of **5aZn·py**. The second symmetry equivalent moiety created by the two fold axis and disorder of the pyridine and lactone units are omitted for clarity.

Table S3. Crystallographic data and structure refinement for **12aH$_2$.**

Crystal shape: rod (black). Experiments were carried out at 100 K with Mo *K*α radiation using a Bruker AXS SMART APEX CCD diffractometer. Data collection used ω scans. Absorption was corrected for by multi-scan methods, Apex2 v2009.7-0 (Bruker, 2009). H-atom parameters were constrained.

Crystal data	
Chemical formula	$C_{43}H_{30}N_4O$
Identification Code	JA-D-89-F1_oxazole_10mz584
M_r	618.71
Crystal system, space group	Triclinic, $P\bar{1}$
a, *b*, *c* (Å)	6.3603 (17), 10.378 (3), 12.263 (3)
α, β, γ (°)	94.826 (4), 99.465 (4), 101.113 (4)
V (Å^3)	777.8 (4)
Z	1
F(000)	324
D_x (Mg m^{-3})	1.321
μ (mm^{-1})	0.08
Crystal size (mm)	0.55 × 0.20 × 0.12
Data collection	
Radiation source	fine-focus sealed tube
Monochromator	graphite
T_{min}, T_{max}	0.692, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	11715, 3817, 2995
R_{int}	0.028
θ values (°)	θ_{max} = 28.3, θ_{min} = 2.0
Range of *h*, *k*, *l*	*h* = -8→8, *k* = -13→13, *l* = -16→16
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.045, 0.120, 1.06
No. of reflections	3817
No. of parameters	223
No. of restraints	0
$\Delta\rangle_{max}$, $\Delta\rangle_{min}$ (e Å^{-3})	0.35, -0.20

Computer programs: Apex2 v2009.7-0 (Bruker, 2009), Apex2 v2009.7-0, *SHELXTL* 6.14 (Bruker, 2000-2003; Sheldrick, 2008), *SHELXTL* 6.14.

Comments:

The oxazole unit was refined as disordered with the pyrrole units in a three to one ratio, with the oxazole ring in all four possible positions and orientations. The oxazole occupancies refined to 0.115(5), 0.084(5), 0.190(3) and 0.110(4) for the four crystallographically independent positions. To accomplish refinement the positions of minor C and O atoms were constrained to be the same as those of the major atom at the same site. No attempts were made to refine the geometry of the oxazole units.

Refinement of the structure as the parent compound tetraphenyl porphyrin gave a slightly higher R values:

R1 = 0.0496 for 2995 Fo > 4sig(Fo) and 0.0643 for all 3817 data

wR2 = 0.1380, GooF = S = 1.093, Restrained GooF = 1.093 for all data

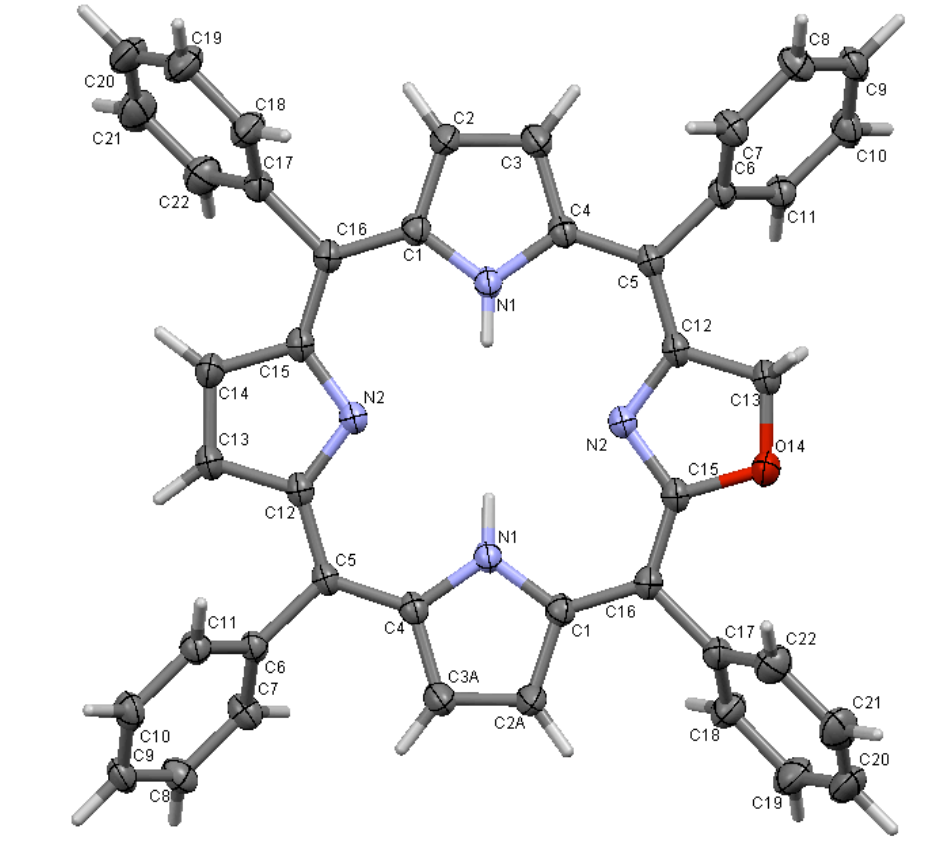

Figure S66. ORTEP representation and numbering scheme used in the crystal structure of **12aH$_2$**. Only the major of the of four realized positions and orientations of the oxazole unit is shown for clarity.

Table S4. Crystallographic data for **15-II-Zn·py.**

Chemical formula	$C_{36}H_{23}N_5O_2Zn$
M_r	622.96
Cell setting, space group	Triclinic, $P\bar{1}$
Temperature (K)	100 (2)
a, b, c (Å)	10.4629(19), 13.445(2), 20.798(4)
α, β, γ (°)	91.532(3), 91.461(3), 108.916(3)
V (Å^3)	2764.9(9)
Z	4
D_x (Mg m^{-3})	1.494
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.933
Crystal form, colour	block, dark green
Crystal size (mm)	0.20 × 0.20 × 0.10
Diffractometer	CCD area detector
Data collection method	phi and ω scans
Absorption correction	Multi-scan
T_{min}	0.3844
T_{max}	0.9124
No. of measured, independent and observed reflections	23458, 12485, 10192
Criterion for observed reflections	$I > 2\sigma(I)$
R_{int}	0.0250
θ_{max} (°)	28.40
Refinement	
Refinement on	F^2
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.0404, 0.1137, 0.1096
No. of relections	12485 reflections
No. of parameters	826
No. of restraints	0
H-atom treatment	Constrained to parent site
Weighting scheme	Calculated $w = 1/[\sigma^2(F_o^2) + (0.0617P)^2 + 0.7753P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$	<0.01
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.199, –0.525

Comments:

Purple crystals of **15-II-Zn·py** were grown by diffusion of MeOH into a CH_2Cl_2 solution of the complex. A 0.10 x 0.20 x 0.20 crystal was mounted and X-ray intensity data were measured at 100 K (Bruker KYRO-FLEX) on a Bruker SMART APEX CCD-based X-ray diffractometer system equipped with a Mo-target X-ray tube (λ = 0.71073 Å) operated at 2000 W power. The crystals were mounted on a cryoloop using Paratone N-Exxon oil and placed under a stream of nitrogen at 100 K. The detector was placed at a distance of 5.009 cm from the crystals. The data were corrected for absorption with the SADABS program. The structures were refined using the Bruker SHELXTL Software Package (Version 6.1), and were solved using direct methods until the final anisotropic full-matrix, least squares refinement of F^2 converged.

In the solid state structure of compound **15-II-Zn·py**, there are two molecules of Zn(DPPL)py per asymmetric unit. The orientation of the oxazolone ring is disordered in this compound, however the disorder manifests itself in different ways in each of the equivalents of Zn(DPPL)py in the asymmetric unit. In one of the two porpholactones, the disorder is primarily between cis positions on the ring, whereas in the second equivalent the disorder is along trans oxazolone positions. For all disordered moieties the overlapping C and O atoms were constrained to have identical ADPs. In the cis disorder, the occupancy was refined to 0.548(5) and 0.452(5) for the two positions, while in the trans disorder, the occupancy was refined to 0.715(5) and 0.285(5) for the two orientations. In both cases, the acyl group of the oxazolone ring is oriented away from the meso phenyl groups, and as such the oxygen atoms do not encounter any steric interactions and do not deviate from the plane of the porphyrinoid macrocycle. Residual electron density indicates additional disorder (the three largest Q peaks agree with possible alternative positions of oxazole keto oxygen atoms).

The Zn(II) ions are five coordinate with the equatorial positions occupied by the dianionic porpholactone ring, and the axial position occupied by pyridines. The equatorial Zn-N bonds range from 2.0499(19) to 2.0832(19) Å, while the axial Zn-N bonds are longer, with values of 2.1430(18) and 2.1587(18)Å. The zinc ion in each complex is pulled out of the plane of the porpholactone by 0.329 and 0.325 Å as measured by the distance of the metal to the plane defined by the four nitrogen atoms of the macrocycle.

Hydrogen atoms were assigned in ideal positions as riding atoms and refined isotropically.

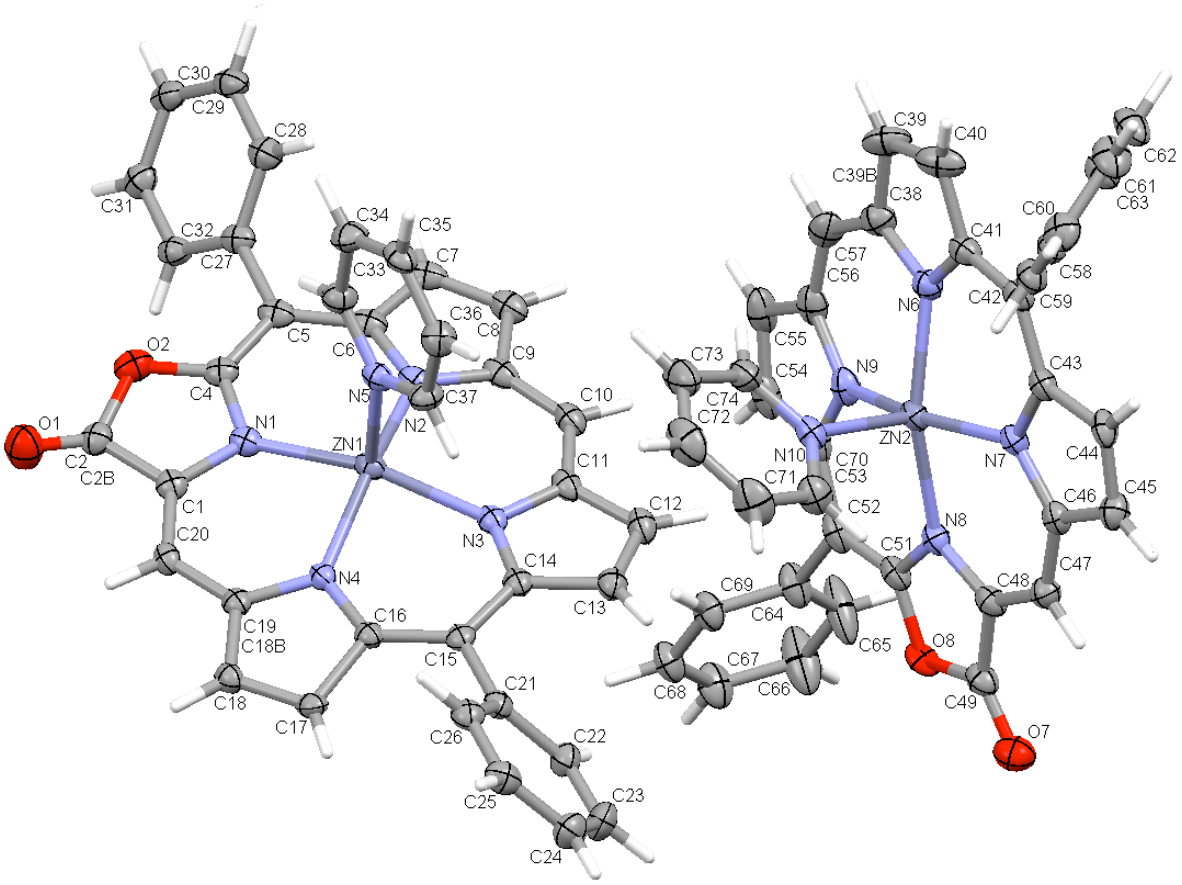

Figure S67. ORTEP representation and numbering scheme used in the crystal structure of **15-II-Zn·py**. Minor disordered moieties are omitted for clarity.

Table S5. Crystallographic data for **13a-OMe.**

Chemical formula	$C_{44}H_{33}N_4O_{2.5}$
M_r	657.74
Cell setting, space group	Tetragonal, *I*4/m
Temperature (K)	100 (2)
a, *b*, *c* (Å)	13.460(3), 13.460(3), 9.7678(18)
α, β, γ (°)	90, 90, 90
V (Å^3)	1769.6(6)
Z	2
D_x (Mg m^{-3})	1.234
Radiation type	Mo *K*α
μ (mm^{-1})	0.078
Crystal form, colour	block, yellow
Crystal size (mm)	0.38 × 0.22 × 0.18
Diffractometer	Bruker ApexII CCD area detector
Data collection method	phi and ω scans
Absorption correction	Multi-scan
T_{min}	0.6620
T_{max}	0.7455
No. of measured, independent and observed reflections	7481, 1046, 832
Criterion for observed reflections	$I > 2\sigma(I)$
R_{int}	0.0268
θ_{max} (°)	27.12
Refinement	
Refinement on	F^2
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.0531, 0.1651, 0.1530
No. of relections	1046 reflections
No. of parameters	95
No. of restraints	1
H-atom treatment	Constrained to parent site
Weighting scheme	Calculated $w = 1/[\sigma^2(F_o^2) + (0.0901P)^2 + 0.8333P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$	<0.01
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.309, –0. 182

Comments:

The oxazole unit is disordered with the pyrrole units in a 3:1 ratio. In addition the methoxy group is disordered over two alternative positons above or below the plane of the macrocycle. The methoxy groups of neighboring molecules are disordered around a four fold rotinversion axis with a combined site occupancy of 0.5. The remainder of the site is taken up by a half occupied water molecule (located directly on the four fold rotinversion axis.

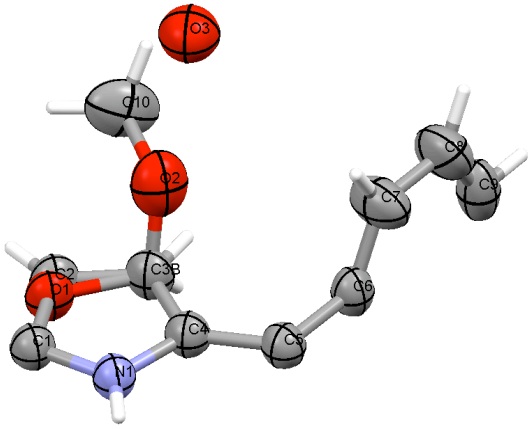

Figure S68. ORTEP representation and numbering scheme of the asymmetric unit of the crystal structure of **13a-OMe**.

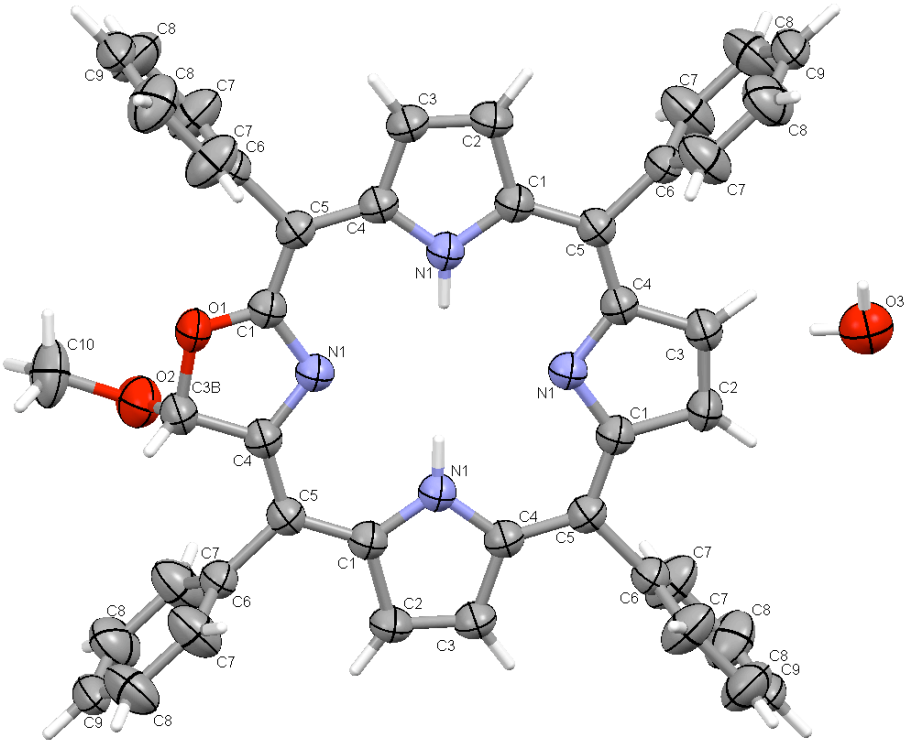

Figure S69. ORTEP representation and numbering scheme of the crystal structure of **13a-OMe**; Only one of the possible eight positions and orientations of the oxazole unit is shown for clarity.

DETAILS TO THE COMPUTATIONS

Table S2. Ratios of the oscillator strength of the Q_x band divided by the oscillator strength of the Soret band as a function of solvent and comparison to computed ratios.

	$\left(\int(Q_x) \Big/ \int(Q_{Soret})\right) \times 10^4$				
Solvent	**1aH_2**	**5aH_2**	**7aH_2**	**10aH_2**	**12aH_2**
$CHCl_3$	112	61	256	342	513
CH_2Cl_2	108	54	218	333	522
DMSO	104	85	231	348	515
Hexane	86	81	253	356	547
Acetone	78	71	219	334	490
EtOAc	76	68	223	354	492
MeCN	75	64	214	330	493
MeOH	75	65	208	334	465
THF	71	70	230	362	530
Pyridine	64	64	232	374	451
Toluene	58	72	250	361	474
Exp. Average[a]	82	69	230	348	499
SAC-CI[b]	0	120	115	303	377
MNDOCI[c]	51	21	6	28	117
Dipole Moment (D)[d]	0.0000	5.0056	3.5992	1.3018	1.1781
Dipole Moment* (D)[e]	0.0000	4.7023	0.8262	1.2315	1.3615

[a] Average of the results obtained in 11 solvents ($CHCl_3$, CH_2Cl_2, DMSO, *n*-hexane, acetone, EtOAc, MeCN, MeOH, THF, pyridine, toluene).

[b] From Figure 3 (left panel).

[c] From Figure 3 (right panel).

[d] B3LYP/6-31G(d) dipole moments computed without the phenyl rings.

[e] B3LYP/6-31G(d) dipole moments computed with the phenyl rings.

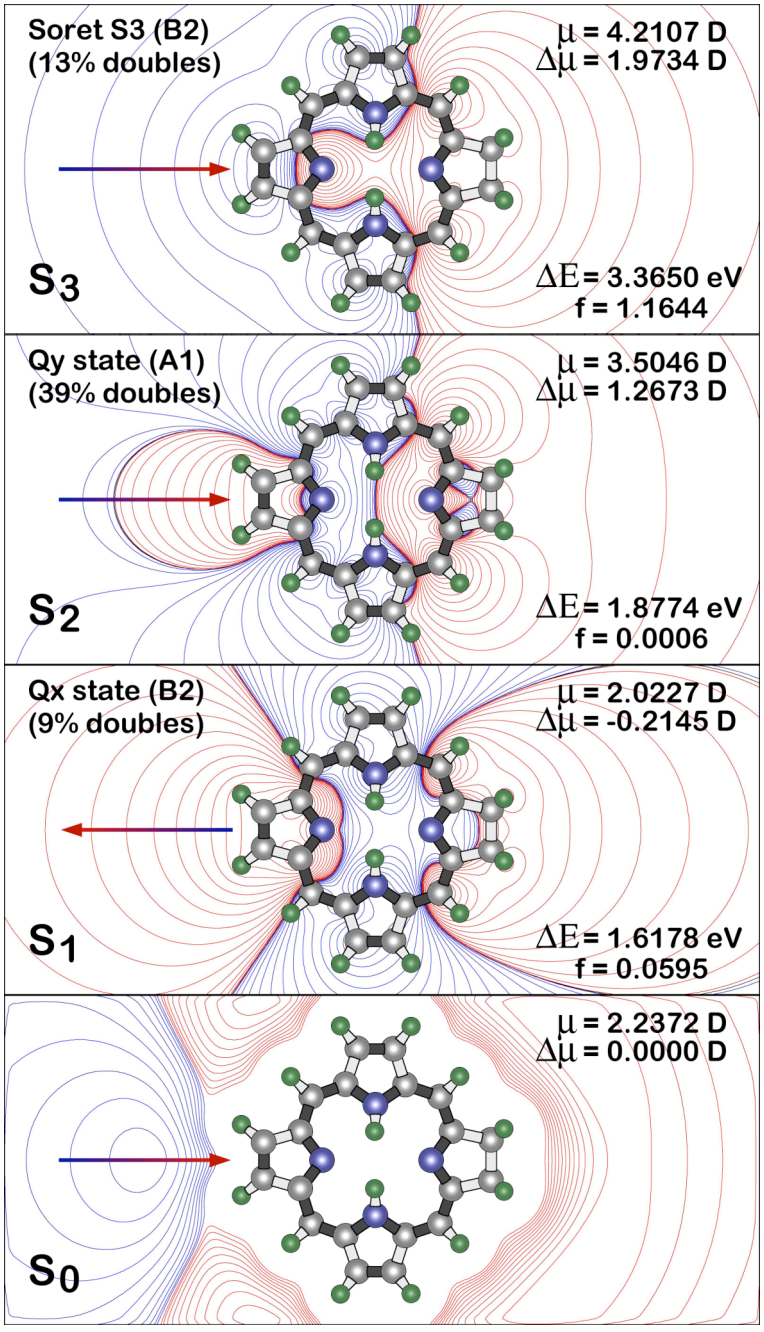

Figure S70. Ground and excited state charge behavior in chlorin (C_{2v}) based on SAC-CI molecular orbital theory using a full double-zeta D95 basis set and level two integral selection (see theoretical section). The ground state charge distribution is shown in the bottom panel, and the arrow indicates the direction of the ground state dipole moment (2.24 D). The upper three panels show the shift in electronic charge upon excitation into the lowest energy singlet states, with the arrows showing the charge shift directions (red is positive and blue is negative).

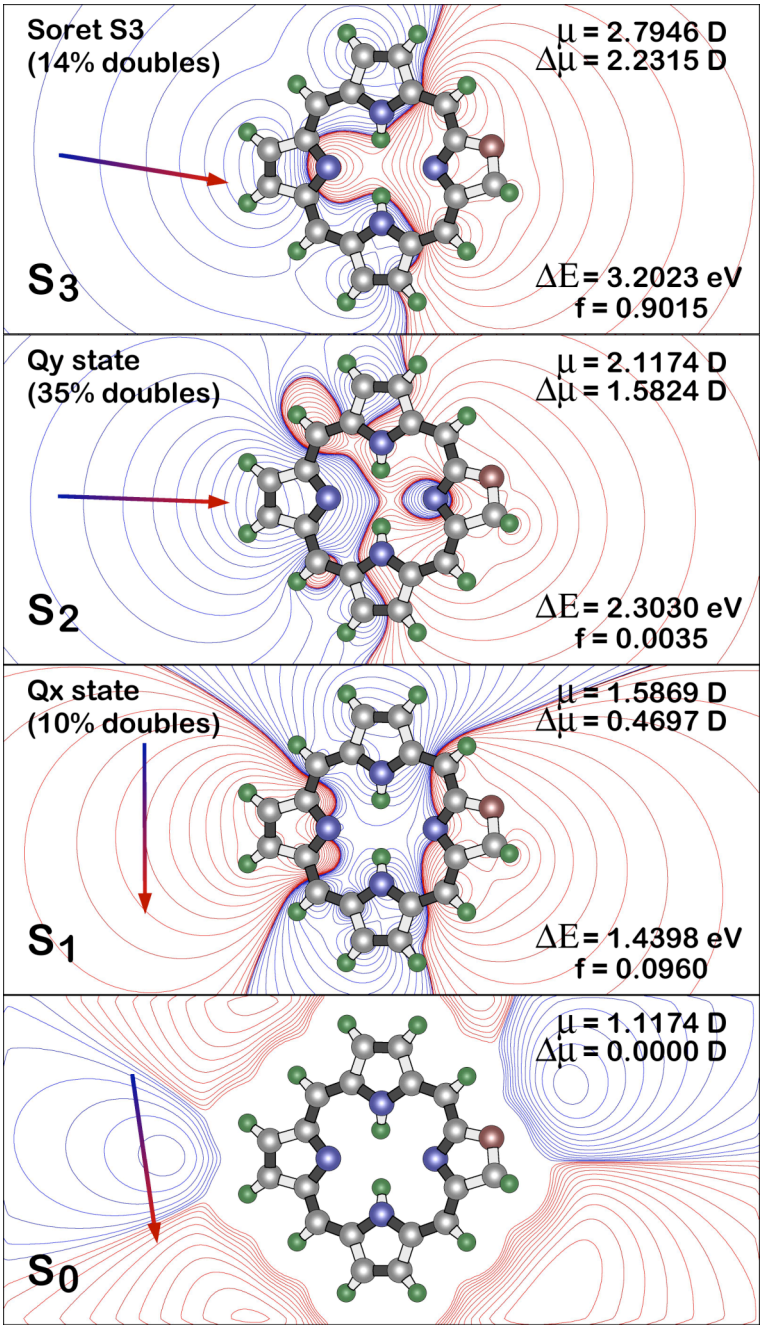

Figure S71. Ground and excited state charge behavior in **12aH$_2$** based on SAC-CI molecular orbital theory using a full double-zeta D95 basis set and level two integral selection (see theoretical section). The ground state charge distribution is shown in the bottom panel, and the arrow indicates the direction of the ground state dipole moment (2.24 D). The upper three panels show the shift in electronic charge upon excitation into the lowest energy singlet states, with the arrows showing the charge shift directions (red is positive and blue is negative).

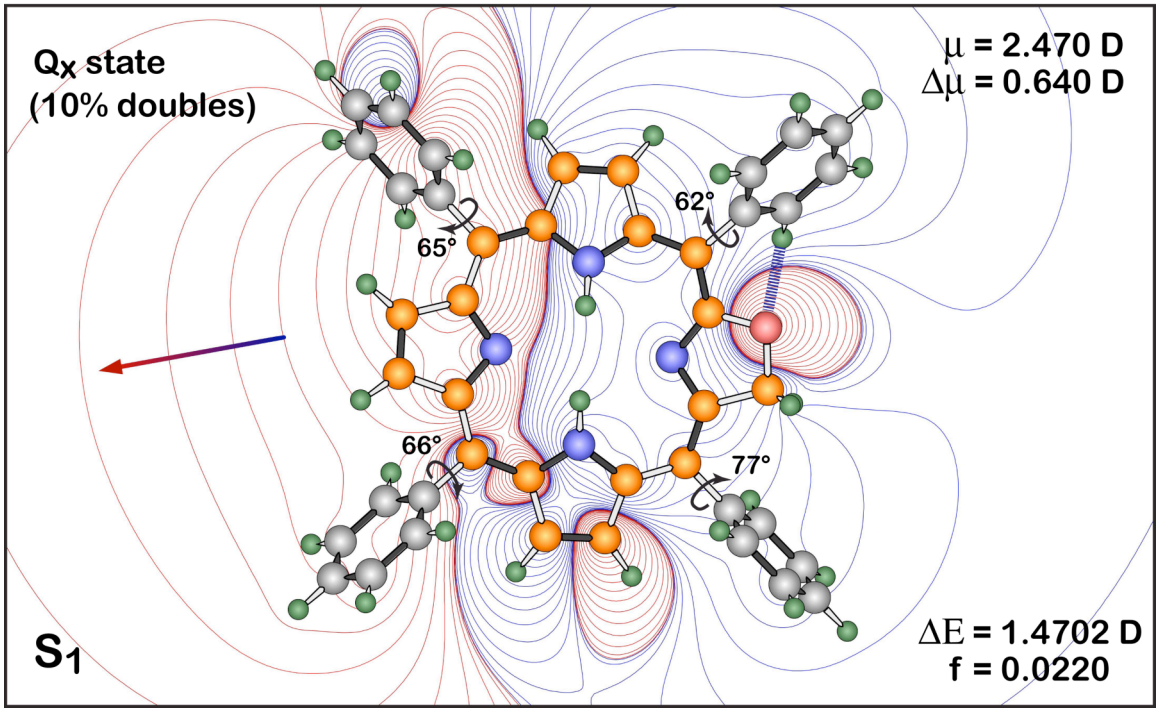

Figure S72. Charge shifts upon excitation into the lowest-lying Q_x state of **12aH$_2$** based on MNDO-PSDCI molecular orbital theory. The charge shift vector is shown at middle left. A key interaction involving the hydrogen atom off the phenyl group and the oxygen atom in the macrocycle is shown with the dashed blue line. The two atoms are separated by 2.8 Å and form a weak hydrogen bond that stabilizes the phenyl group and enhances the negative charge on the oxygen atom upon excitation.

Table S7. Ground State Coordinates of porphyrin $1aH_2$[(a)] w/o Ph

Atom	X(Å)	Y(Å)	Z(Å)	Charge
C 1	0.000000	4.239505	0.669450	-0.231406
C 2	0.000000	4.239505	-0.669450	-0.231406
C 3	0.000000	2.838607	-1.072824	0.328928
C 4	0.000000	2.424271	-2.400498	-0.303197
C 5	0.000000	1.119161	-2.859251	0.383216
C 6	0.000000	0.678048	-4.219123	-0.238680
C 7	0.000000	-0.678048	-4.219123	-0.238680
C 8	0.000000	-1.119161	-2.859251	0.383216
C 9	0.000000	-2.424271	-2.400498	-0.303197
C10	0.000000	-2.838607	-1.072824	0.328928
C11	0.000000	-4.239505	-0.669450	-0.231406
C12	0.000000	-4.239505	0.669450	-0.231406
C13	0.000000	-2.838607	1.072824	0.328928
C14	0.000000	-2.424271	2.400498	-0.303197
C15	0.000000	-1.119161	2.859251	0.383216
C16	0.000000	-0.678048	4.219123	-0.238680
C17	0.000000	0.678048	4.219123	-0.238680
C18	0.000000	1.119161	2.859251	0.383216
C19	0.000000	2.424271	2.400498	-0.303197
C20	0.000000	2.838607	1.072824	0.328928
N21	0.000000	2.034506	0.000000	-0.776446
N22	0.000000	0.000000	-2.092880	-0.917044
N23	0.000000	-2.034506	0.000000	-0.776446
N24	0.000000	0.000000	2.092880	-0.917044
H25	0.000000	0.000000	1.096318	0.514781
H26	0.000000	0.000000	-1.096318	0.514781
H27	0.000000	1.331702	-5.067969	0.224413
H28	0.000000	-1.331702	-5.067969	0.224413
H29	0.000000	-1.331702	5.067969	0.224413
H30	0.000000	1.331702	5.067969	0.224413
H31	0.000000	5.078424	1.337330	0.210947
H32	0.000000	5.078424	-1.337330	0.210947
H33	0.000000	-5.078424	-1.337330	0.210947
H34	0.000000	-5.078424	1.337330	0.210947
H35	0.000000	3.189761	-3.154855	0.215133
H36	0.000000	-3.189761	-3.154855	0.215133
H37	0.000000	-3.189761	3.154855	0.215133
H38	0.000000	3.189761	3.154855	0.215133

(a) Optimized using Gaussian03 and RHF/6-31G(d) procedures. Total energy = -983.250771778 Hartree. Point Group = d2h Dipole moment = 0.00000 D (0.00000, 0.00000, 0.00000) Mulliken charges are listed in last column.

Table S8. Ground State Coordinates of chlorin[(a)]

Atom	X(Å)	Y(Å)	Z(Å)	Charge
C 1	0.000000	0.678886	4.311213	-0.248609
C 2	0.000000	-0.678886	4.311213	-0.248609
C 3	0.000000	-1.069019	2.934707	0.271399
C 4	0.000000	-2.409668	2.486911	-0.236832
C 5	0.000000	-2.861571	1.203888	0.319814
C 6	0.000000	-4.216417	0.746490	-0.189217
C 7	0.000000	-4.211435	-0.605843	-0.286474
C 8	0.000000	-2.840381	-1.040911	0.455928
C 9	0.000000	-2.398603	-2.371880	-0.389551
C10	0.000000	-1.094201	-2.809783	0.387609
C11	0.000000	-0.764644	-4.292816	-0.377140
C12	0.000000	0.764644	-4.292816	-0.377140
C13	0.000000	1.094201	-2.809783	0.387609
C14	0.000000	2.398603	-2.371880	-0.389551
C15	0.000000	2.840381	-1.040911	0.455928
C16	0.000000	4.211435	-0.605843	-0.286474
C17	0.000000	4.216417	0.746490	-0.189217
C18	0.000000	2.861571	1.203888	0.319814
C19	0.000000	2.409668	2.486911	-0.236832
C20	0.000000	1.069019	2.934707	0.271399
N21	0.000000	0.000000	2.126454	-0.751772
N22	0.000000	-2.084225	0.058630	-0.919153
N23	0.000000	0.000000	-2.042558	-0.741730
N24	0.000000	2.084225	0.058630	-0.919153
H25	0.000000	1.088712	0.066267	0.506082
H26	0.000000	-1.088712	0.066267	0.506082
H27	0.000000	-5.053656	-1.267152	0.219211
H28	0.000000	5.053656	-1.267152	0.219211
H29	0.000000	-5.071213	1.393267	0.227912
H30	0.000000	5.071213	1.393267	0.227912
H31	0.000000	1.342185	5.154350	0.194267
H32	0.000000	-1.342185	5.154350	0.194267
H33	0.000000	-3.171328	-3.118296	0.194998
H34	0.000000	3.171328	-3.118296	0.194998
H35	0.000000	-3.168639	3.249408	0.220547
H36	0.000000	3.168639	3.249408	0.220547
H37	0.873426	-1.186736	-4.776872	0.197980
H38	-0.873426	-1.186736	-4.776872	0.197980
H39	0.873426	1.186736	-4.776872	0.197980
H40	-0.873426	1.186736	-4.776872	0.197980

(a) Optimized using Gaussian03 and RHF/6-31G(d) procedures. Total energy = -984.429436153 Hartree. Point Group = c2v Dipole moment = 2.62910 D (0.00000, 0.00000, -2.62910) Mulliken charges are listed in last column.

Table S9. Ground State Coordinates of chlorin $5aH_2$[(a)] w/o Ph

Atom	X(Å)	Y(Å)	Z(Å)	Charge
C 1	-4.224864	1.609003	0.000000	-0.177982
C 2	-4.525301	0.285035	0.000000	-0.180778
C 3	-3.249915	-0.420982	0.000000	0.345131
C 4	-3.146060	-1.823740	0.000000	-0.273011
C 5	-1.981777	-2.579038	0.000000	0.396272
C 6	-1.841601	-4.008150	0.000000	-0.185329
C 7	-0.503121	-4.304699	0.000000	-0.194426
C 8	0.227561	-3.066432	0.000000	0.414394
C 9	1.612236	-2.892554	0.000000	-0.308505
C10	2.255794	-1.658420	0.000000	0.598424
C11	2.743154	0.439135	0.000000	0.255353
C12	2.685306	1.822357	0.000000	-0.263021
C13	1.513415	2.590729	0.000000	0.400934
C14	1.385205	4.016454	0.000000	-0.194198
C15	0.044421	4.321902	0.000000	-0.190318
C16	-0.689741	3.092879	0.000000	0.393418
C17	-2.072161	2.908277	0.000000	-0.269545
C18	-2.770137	1.695303	0.000000	0.343347
N19	-2.203974	0.450273	0.000000	-0.674961
N20	-0.704630	-2.063930	0.000000	-0.768558
N21	1.707081	-0.441234	0.000000	-0.639090
N22	0.240937	2.081598	0.000000	-0.761016
C23	4.023726	-0.308571	0.000000	0.573521
O24	5.173837	0.046894	0.000000	-0.460438
H25	-0.500865	-1.069865	0.000000	0.415406
H26	0.000000	1.095820	0.000000	0.415546
H27	-2.669470	3.815774	0.000000	0.144615
H28	-4.903385	2.453344	0.000000	0.135196
H29	-5.501954	-0.183425	0.000000	0.134603
H30	-4.077178	-2.383191	0.000000	0.143389
H31	-2.671035	-4.702972	0.000000	0.151788
H32	-0.042235	-5.283412	0.000000	0.152891
H33	2.237216	-3.777642	0.000000	0.164280
H34	3.634338	2.348754	0.000000	0.170266
H35	2.220271	4.704155	0.000000	0.153133
H36	-0.407896	5.304777	0.000000	0.150034
O37	3.637346	-1.649393	0.000000	-0.510764

(a) Optimized using Gaussian03 and B3LYP/6-31G(d) procedures. Total energy = -1100.712248930 Hartree. Point Group = cs Dipole moment = 5.00560 D (-5.00060, 0.22220, 0.00000) Mulliken charges are listed in last column.

Table S10. Ground State Coordinates of chlorin $7aH_2$[(a)] w/o Ph

Atom	X(Å)	Y(Å)	Z(Å)	Charge
C 1	0.140477	-4.780436	0.679786	-0.183243
C 2	0.140477	-4.780436	-0.679786	-0.183243
C 3	0.071244	-3.384771	-1.085086	0.341281
C 4	0.059987	-2.965850	-2.424225	-0.273304
C 5	0.002695	-1.660522	-2.897929	0.388365
C 6	0.002389	-1.208180	-4.256418	-0.189008
C 7	-0.060923	0.163900	-4.247909	-0.200451
C 8	-0.103594	0.599854	-2.882650	0.409473
C 9	-0.182124	1.920260	-2.418583	-0.266150
C10	-0.241651	2.360155	-1.104723	0.338171
C11	-0.352685	3.846605	-0.781769	0.024924
C12	-0.352685	3.846605	0.781769	0.024924
C13	-0.241651	2.360155	1.104723	0.338171
C14	-0.182124	1.920260	2.418583	-0.266150
C15	-0.103594	0.599854	2.882650	0.409473
C16	-0.060923	0.163900	4.247909	-0.200451
C17	0.002389	-1.208180	4.256418	-0.189008
C18	0.002695	-1.660522	2.897929	0.388365
C19	0.059987	-2.965850	2.424225	-0.273304
C20	0.071244	-3.384771	1.085086	0.341281
N21	0.028077	-2.558686	0.000000	-0.677834
N22	-0.063644	-0.529168	-2.111387	-0.763755
N23	-0.208952	1.584234	0.000000	-0.601013
N24	-0.063644	-0.529168	2.111387	-0.763755
O25	0.726506	4.538613	1.390620	-0.600252
O26	0.726506	4.538613	-1.390620	-0.600252
H27	0.560143	5.490482	-1.311015	0.385967
H28	0.560143	5.490482	1.311015	0.385967
H29	-0.070748	-0.552457	-1.097961	0.407423
H30	-0.070748	-0.552457	1.097961	0.407423
H31	-0.077370	0.830799	-5.099745	0.142051
H32	-0.077370	0.830799	5.099745	0.142051
H33	0.047174	-1.862238	-5.117385	0.143079
H34	0.047174	-1.862238	5.117385	0.143079
H35	0.184087	-5.628495	1.352571	0.127222
H36	0.184087	-5.628495	-1.352571	0.127222
H37	-0.185168	2.689141	-3.184838	0.140258
H38	-0.185168	2.689141	3.184838	0.140258
H39	0.105409	-3.743595	-3.181615	0.136998
H40	0.105409	-3.743595	3.181615	0.136998
H41	-1.311897	4.236136	-1.157582	0.130375
H42	-1.311897	4.236136	1.157582	0.130375

(a) Optimized using Gaussian03 and B3LYP/6-31G(d) procedures. Total energy = -1141.171086680 Hartree. Point Group = cs Dipole moment = 3.59920 D (-2.09780, 2.92470, 0.00000) Mulliken charges are listed in last column.

Table S11. Ground State Coordinates of chlorin 10aH_2[(a)] w/o Ph

Atom	X(Å)	Y(Å)	Z(Å)	Charge
C 1	4.342203	-1.424616	0.067103	-0.181759
C 2	4.582811	-0.086509	0.110192	-0.184742
C 3	3.280812	0.560512	0.078738	0.340885
C 4	3.108956	1.958698	0.110276	-0.273193
C 5	1.913370	2.657619	0.087574	0.391252
C 6	1.703889	4.076901	0.123590	-0.184927
C 7	0.353331	4.310076	0.085631	-0.200437
C 8	-0.318471	3.039537	0.024095	0.418783
C 9	-1.695930	2.811903	-0.028126	-0.316560
C10	-2.304462	1.561861	-0.098377	0.593734
C11	-2.696908	-0.563085	-0.192598	0.250180
C12	-2.555543	-1.936252	-0.218709	-0.285509
C13	-1.341297	-2.648658	-0.185689	0.406756
C14	-1.151998	-4.066336	-0.214441	-0.204545
C15	0.201039	-4.315987	-0.166061	-0.189023
C16	0.881241	-3.060493	-0.106270	0.385908
C17	2.250536	-2.816590	-0.046665	-0.268512
C18	2.897489	-1.574909	0.009831	0.338445
N19	2.275927	-0.355903	0.018421	-0.675912
N20	0.658758	2.083623	0.027599	-0.770427
N21	-1.709268	0.361868	-0.114430	-0.613111
N22	-0.096717	-2.087520	-0.119645	-0.762723
C23	-4.056427	0.127727	-0.200943	0.284097
O24	-4.902585	-0.220344	0.850776	-0.578209
O25	-3.674211	1.517031	-0.160571	-0.525020
H26	-4.646009	-0.031623	-1.108051	0.167034
H27	-4.380348	-0.215641	1.671301	0.395991
H28	0.505764	1.081649	-0.008546	0.410964
H29	0.102322	-1.093461	-0.087531	0.412142
H30	-0.154018	5.265521	0.097518	0.146693
H31	-1.955636	-4.788850	-0.266018	0.143717
H32	0.693942	-5.279307	-0.171345	0.145024
H33	2.498525	4.809874	0.172257	0.147291
H34	5.537182	0.423834	0.158651	0.128652
H35	5.058671	-2.237182	0.072798	0.129168
H36	-2.350017	3.675796	-0.020653	0.152767
H37	-3.463361	-2.529821	-0.264883	0.145475
H38	4.012097	2.560631	0.159459	0.139194
H39	2.886504	-3.697783	-0.045119	0.140457

(a) Optimized using Gaussian03 and B3LYP/6-31G(d) procedures. Total energy = -1101.891047750 Hartree. Point Group = c1 Dipole moment = 1.30180 D (1.18340, -0.39620, 0.37030) Mulliken charges are listed in last column.

Table S12. Ground State Coordinates of chlorin 12aH_2[(a)] w/o Ph

Atom	X(Å)	Y(Å)	Z(Å)	Charge
C 1	4.302661	-0.657246	0.000335	-0.185986
C 2	4.295283	0.704001	0.000003	-0.183320
C 3	2.898323	1.101208	0.000062	0.337000
C 4	2.472303	2.437520	-0.000056	-0.267955
C 5	1.165983	2.914095	-0.000080	0.384324
C 6	0.711310	4.268900	-0.000278	-0.187941
C 7	-0.664978	4.257487	-0.000227	-0.207294
C 8	-1.096808	2.892634	-0.000080	0.409249
C 9	-2.419355	2.408449	-0.000063	-0.293525
C10	-2.806859	1.082747	0.000047	0.298233
C11	-4.252855	0.613362	0.000618	-0.086539
C12	-2.776197	-1.085684	0.000060	0.601770
C13	-2.385855	-2.422230	-0.000120	-0.318254
C14	-1.066886	-2.883176	-0.000134	0.421008
C15	-0.625030	-4.252589	-0.000248	-0.202452
C16	0.745985	-4.258629	-0.000151	-0.184434
C17	1.199020	-2.897358	-0.000029	0.389050
C18	2.497470	-2.417509	0.000005	-0.272524
C19	2.909510	-1.069360	0.000082	0.339210
N20	2.076223	0.007747	0.000240	-0.676010
N21	0.061261	-2.112233	0.000027	-0.771060
N22	-1.992524	-0.000213	0.000055	-0.607975
N23	0.032282	2.124463	0.000038	-0.764589
O24	-4.121304	-0.814806	-0.000301	-0.515533
H25	-4.814313	0.923879	-0.889691	0.171644
H26	0.057196	1.110792	0.000059	0.411228
H27	0.086967	-1.098496	0.000005	0.409820
H28	-1.290992	-5.105202	-0.000357	0.144338
H29	-1.332565	5.108927	-0.000315	0.139797
H30	1.363235	5.132663	-0.000391	0.143444
H31	1.401651	-5.119597	-0.000160	0.145657
H32	5.155910	-1.324841	0.000488	0.126430
H33	5.141239	1.380826	-0.000111	0.126848
H34	-3.177072	-3.162536	-0.000262	0.148765
H35	-3.200814	3.162841	-0.000162	0.129303
H36	3.283063	-3.168150	0.000009	0.137800
H37	3.250457	3.196225	-0.000174	0.138842
H38	-4.812380	0.923028	0.892483	0.171629

(a) Optimized using Gaussian03 and B3LYP/6-31G(d) procedures. Total energy = -1026.670810840 Hartree. Point Group = c1 Dipole moment = 1.17810 D (-0.90840, 0.75020, 0.00060) Mulliken charges are listed in last column.

Table S13. Ground State Coordinates of TPP[a]

Atom	X(Å)	Y(Å)	Z(Å)	Charge
C 1	-4.260254	0.676919	-0.184702	-0.181317
C 2	-4.260254	-0.676919	-0.184702	-0.181317
C 3	-2.865333	-1.087627	-0.053945	0.301535
C 4	-2.463557	-2.440654	-0.012586	-0.047044
C 5	-1.132653	-2.890891	0.022330	0.348277
C 6	-0.684685	-4.248655	0.135075	-0.190792
C 7	0.684685	-4.248655	0.135075	-0.190792
C 8	1.132653	-2.890891	0.022330	0.348277
C 9	2.463557	-2.440654	-0.012586	-0.047044
C10	2.865333	-1.087627	-0.053945	0.301535
C11	4.260254	-0.676919	-0.184702	-0.181317
C12	4.260254	0.676919	-0.184702	-0.181317
C13	2.865333	1.087627	-0.053945	0.301535
C14	2.463557	2.440654	-0.012586	-0.047044
C15	1.132653	2.890891	0.022330	0.348277
C16	0.684685	4.248655	0.135075	-0.190792
C17	-0.684685	4.248655	0.135075	-0.190792
C18	-1.132653	2.890891	0.022330	0.348277
C19	-2.463557	2.440654	-0.012586	-0.047044
C20	-2.865333	1.087627	-0.053945	0.301535
N21	-2.039718	0.000000	0.006234	-0.687437
N22	0.000000	-2.111182	-0.035000	-0.772895
N23	2.039718	0.000000	0.006234	-0.687437
N24	0.000000	2.111182	-0.035000	-0.772895
C25	-3.527030	3.496005	0.001404	0.015917
C26	-3.681694	4.377651	-1.080205	-0.157580
C27	-4.672359	5.360354	-1.064857	-0.134538
C28	-5.524702	5.480542	0.034207	-0.125729
C29	-5.380823	4.610673	1.116780	-0.134401
C30	-4.391497	3.627019	1.099974	-0.154155
C31	-4.391497	-3.627019	1.099974	-0.154155
C32	-5.380823	-4.610673	1.116780	-0.134401
C33	-5.524702	-5.480542	0.034207	-0.125729
C34	-4.672359	-5.360354	-1.064857	-0.134538
C35	-3.681694	-4.377651	-1.080205	-0.157580
C36	-3.527030	-3.496005	0.001404	0.015917
C37	3.527030	-3.496005	0.001404	0.015917
C38	3.681694	-4.377651	-1.080205	-0.157580
C39	4.672359	-5.360354	-1.064857	-0.134538
C40	5.524702	-5.480542	0.034207	-0.125729
C41	5.380823	-4.610673	1.116780	-0.134401
C42	4.391497	-3.627019	1.099974	-0.154155
C43	4.391497	3.627019	1.099974	-0.154155
C44	5.380823	4.610673	1.116780	-0.134401
C45	5.524702	5.480542	0.034207	-0.125729
C46	4.672359	5.360354	-1.064857	-0.134538

C47	3.681694	4.377651	-1.080205	-0.157580
C48	3.527030	3.496005	0.001404	0.015917
H49	4.278159	2.954399	1.945449	0.142299
H50	0.000000	-1.096559	-0.062448	0.412529
H51	0.000000	1.096559	-0.062448	0.412529
H52	-1.338733	-5.103551	0.218198	0.158485
H53	1.338733	-5.103551	0.218198	0.158485
H54	1.338733	5.103551	0.218198	0.158485
H55	-1.338733	5.103551	0.218198	0.158485
H56	-5.107979	1.339573	-0.282479	0.146577
H57	-5.107979	-1.339573	-0.282479	0.146577
H58	5.107979	-1.339573	-0.282479	0.146577
H59	5.107979	1.339573	-0.282479	0.146577
H60	-4.278159	2.954399	1.945449	0.142299
H61	-4.278159	-2.954399	1.945449	0.142299
H62	4.278159	-2.954399	1.945449	0.142299
H63	-3.025251	4.281078	-1.940557	0.139898
H64	-3.025251	-4.281078	-1.940557	0.139898
H65	3.025251	-4.281078	-1.940557	0.139898
H66	3.025251	4.281078	-1.940557	0.139898
H67	-6.295883	6.246124	0.046758	0.131149
H68	-6.295883	-6.246124	0.046758	0.131149
H69	6.295883	-6.246124	0.046758	0.131149
H70	6.295883	6.246124	0.046758	0.131149
H71	-6.037147	4.699162	1.978604	0.132857
H72	-6.037147	-4.699162	1.978604	0.132857
H73	6.037147	-4.699162	1.978604	0.132857
H74	6.037147	4.699162	1.978604	0.132857
H75	-4.780512	6.028970	-1.914927	0.132463
H76	-4.780512	-6.028970	-1.914927	0.132463
H77	4.780512	-6.028970	-1.914927	0.132463
H78	4.780512	6.028970	-1.914927	0.132463

(a) Optimized using Gaussian03 and B3LYP/6-31G(d) procedures.
Total energy = -1913.751108910 Hartree. Point Group = c2v
Dipole moment = 0.03760 D (0.00000, 0.00000, -0.03760)
Mulliken charges are listed in last column.

Table S14. Ground State Coordinates of TPP $1aH_2$[(a)]

Atom	X(Å)	Y(Å)	Z(Å)	Charge
C 1	4.260257	-0.677012	-0.184616	-0.181314
C 2	4.260305	0.676825	-0.184646	-0.181313
C 3	2.865390	1.087586	-0.053899	0.301520
C 4	2.463628	2.440597	-0.012600	-0.047000
C 5	1.132678	2.890826	0.022245	0.348249
C 6	0.684749	4.248575	0.135248	-0.190801
C 7	-0.684641	4.248592	0.135250	-0.190801
C 8	-1.132603	2.890854	0.022244	0.348249
C 9	-2.463565	2.440659	-0.012602	-0.047000
C10	-2.865362	1.087658	-0.053902	0.301520
C11	-4.260288	0.676934	-0.184642	-0.181313
C12	-4.260274	-0.676904	-0.184626	-0.181314
C13	-2.865325	-1.087564	-0.053838	0.301568
C14	-2.463584	-2.440603	-0.012493	-0.047066
C15	-1.132686	-2.890856	0.022465	0.348297
C16	-0.684745	-4.248645	0.135175	-0.190789
C17	0.684636	-4.248662	0.135176	-0.190789
C18	1.132611	-2.890885	0.022464	0.348297
C19	2.463521	-2.440665	-0.012495	-0.047066
C20	2.865297	-1.087637	-0.053836	0.301568
N21	2.039701	-0.000018	0.006238	-0.687443
N22	0.000027	2.111150	-0.035173	-0.772886
N23	-2.039700	0.000033	0.006231	-0.687443
N24	-0.000027	-2.111153	-0.034510	-0.772917
C25	3.526966	-3.496062	0.001406	0.015883
C26	3.681768	-4.377438	-1.080399	-0.157566
C27	4.672412	-5.360170	-1.065173	-0.134533
C28	5.524610	-5.480656	0.033963	-0.125732
C29	5.380614	-4.611038	1.116733	-0.134400
C30	4.391317	-3.627366	1.100045	-0.154150
C31	4.391771	3.626820	1.099821	-0.154179
C32	5.381091	4.610477	1.116606	-0.134400
C33	5.524749	5.480554	0.034173	-0.125731
C34	4.672175	5.360548	-1.064739	-0.134536
C35	3.681528	4.377840	-1.080064	-0.157589
C36	3.527063	3.495972	0.001414	0.015935
C37	-3.526973	3.496061	0.001412	0.015935
C38	-3.681415	4.377934	-1.080064	-0.157589
C39	-4.672037	5.360667	-1.064739	-0.134536
C40	-5.524609	5.480693	0.034171	-0.125731
C41	-5.380975	4.610611	1.116603	-0.134399
C42	-4.391680	3.626929	1.099818	-0.154179
C43	-4.391409	-3.627255	1.100047	-0.154149
C44	-5.380731	-4.610902	1.116736	-0.134400
C45	-5.524749	-5.480518	0.033967	-0.125732
C46	-4.672547	-5.360054	-1.065169	-0.134533

C47	-3.681879	-4.377346	-1.080396	-0.157567
C48	-3.527056	-3.495973	0.001408	0.015883
H49	-4.277947	-2.954851	1.945672	0.142293
H50	-0.000015	-1.096521	-0.062172	0.412533
H51	0.000015	1.096516	-0.062883	0.412527
H52	-1.338699	5.103448	0.218627	0.158485
H53	1.338829	5.103415	0.218624	0.158485
H54	-1.338836	-5.103499	0.218336	0.158484
H55	1.338706	-5.103532	0.218338	0.158484
H56	-5.107925	-1.339649	-0.282383	0.146583
H57	5.107993	1.339514	-0.282462	0.146582
H58	5.107891	-1.339780	-0.282367	0.146583
H59	-5.107960	1.339645	-0.282452	0.146582
H60	4.278596	2.954086	1.945221	0.142301
H61	4.277871	-2.954960	1.945670	0.142293
H62	-4.278523	2.954190	1.945217	0.142301
H63	-3.025569	-4.280562	-1.940820	0.139893
H64	3.024946	4.281398	-1.940319	0.139897
H65	3.025460	-4.280636	-1.940823	0.139893
H66	-3.024834	4.281477	-1.940319	0.139897
H67	-6.295768	6.246289	0.046703	0.131151
H68	6.295927	6.246131	0.046704	0.131151
H69	6.295779	-6.246244	0.046427	0.131149
H70	-6.295937	-6.246087	0.046432	0.131149
H71	-6.037453	4.698953	1.978317	0.132858
H72	-6.036943	-4.699602	1.978616	0.132857
H73	6.037570	4.698804	1.978321	0.132858
H74	6.036824	-4.699755	1.978613	0.132857
H75	4.780143	6.029302	-1.914716	0.132464
H76	-4.780803	-6.028439	-1.915400	0.132463
H77	-4.779987	6.029426	-1.914715	0.132464
H78	4.780651	-6.028557	-1.915405	0.132463

(a) Optimized using Gaussian03 and B3LYP/6-31G(d) procedures.
Total energy = -1913.751108900 Hartree. Point Group = c1
Dipole moment = 0.03790 D (0.00000, 0.00000, -0.03790)
Mulliken charges are listed in last column.

Table S15. Ground State Coordinates of TPC[(a)]

Atom	X(Å)	Y(Å)	Z(Å)	Charge
C 1	-4.292072	0.681837	-0.155263	-0.185769
C 2	-4.292967	-0.676145	-0.155739	-0.185767
C 3	-2.903775	-1.086147	-0.034756	0.296326
C 4	-2.495889	-2.442948	-0.013757	-0.042958
C 5	-1.171000	-2.892992	0.008227	0.335280
C 6	-0.712007	-4.247919	0.069795	-0.185289
C 7	0.658686	-4.237155	0.068027	-0.201488
C 8	1.096717	-2.873199	0.016001	0.374988
C 9	2.438565	-2.432582	0.004300	-0.081115
C10	2.879976	-1.106411	-0.016179	0.316659
C11	4.368283	-0.768416	-0.029997	-0.354251
C12	4.369286	0.762699	-0.032768	-0.354248
C13	2.881443	1.102681	-0.017201	0.316653
C14	2.441796	2.429438	0.003219	-0.081130
C15	1.100526	2.871792	0.015884	0.374985
C16	0.664272	4.236296	0.068401	-0.201491
C17	-0.706408	4.248812	0.071017	-0.185298
C18	-1.167171	2.894491	0.009375	0.335299
C19	-2.492657	2.446183	-0.012367	-0.042950
C20	-2.902333	1.089930	-0.034039	0.296315
N21	-2.076115	0.001322	0.025929	-0.692352
N22	-0.035283	-2.101542	-0.017319	-0.778391
N23	2.096233	-0.001346	-0.016985	-0.604913
N24	-0.032485	2.101591	-0.016878	-0.778389
C25	-3.555719	3.502197	-0.014699	0.016758
C26	-3.718596	4.358023	-1.115318	-0.157061
C27	-4.708657	5.341642	-1.114790	-0.134823
C28	-5.551532	5.488311	-0.011822	-0.125752
C29	-5.399369	4.643507	1.089450	-0.134662
C30	-4.411471	3.658406	1.087221	-0.152865
C31	-3.560301	-3.497601	-0.016942	0.016760
C32	-3.723917	-4.352632	-1.118066	-0.157053
C33	-4.715200	-5.335022	-1.118350	-0.134822
C34	-5.558575	-5.481234	-0.015706	-0.125752
C35	-5.405680	-4.637215	1.086069	-0.134664
C36	-4.416561	-3.653339	1.084651	-0.152870
C37	3.484891	-3.513675	0.019665	0.010088
C38	3.973419	-4.056211	-1.178238	-0.153149
C39	4.948341	-5.055492	-1.165895	-0.132536
C40	5.449663	-5.530231	0.047433	-0.126640
C41	4.969202	-5.001969	1.247052	-0.132561
C42	3.994729	-4.002344	1.231912	-0.153772
C43	3.489531	3.509178	0.017363	0.010096
C44	3.978602	4.049842	-1.181157	-0.153135
C45	4.954795	5.047901	-1.169974	-0.132532
C46	5.456863	5.523265	0.042796	-0.126640

C47	4.975885	4.996854	1.243026	-0.132566
C48	4.000148	3.998448	1.229046	-0.153787
H49	3.623489	3.592429	2.164463	0.135962
H50	-0.057287	1.088680	-0.030167	0.404952
H51	-0.058832	-1.088595	-0.030279	0.404954
H52	-1.352185	5.112952	0.116976	0.156407
H53	-1.358903	-5.111252	0.115195	0.156405
H54	1.328277	5.086944	0.106272	0.153823
H55	1.321599	-5.088643	0.106167	0.153824
H56	-5.141189	1.343549	-0.247751	0.142139
H57	-5.142947	-1.336685	-0.248680	0.142139
H58	-4.297355	-2.999622	1.943989	0.141966
H59	-4.292832	3.004084	1.946178	0.141964
H60	-3.069071	4.240551	-1.978225	0.139873
H61	-3.073997	-4.235506	-1.980723	0.139870
H62	-6.330156	-6.246565	-0.015202	0.130014
H63	-6.322160	6.254601	-0.010680	0.130014
H64	6.208063	-6.308594	0.058145	0.130413
H65	6.216253	6.300675	0.052612	0.130413
H66	-6.055465	-4.745763	1.950588	0.131789
H67	-6.048771	4.752394	1.954215	0.131788
H68	-4.830416	-5.983142	-1.983272	0.131462
H69	-4.823316	5.990369	-1.979332	0.131462
H70	5.351065	-5.369131	2.196231	0.131626
H71	5.358348	5.364506	2.191774	0.131627
H72	5.320905	5.455342	-2.108871	0.131441
H73	5.314057	-5.464369	-2.104322	0.131441
H74	3.580745	-3.690719	-2.123713	0.135341
H75	3.585324	3.683895	-2.126205	0.135335
H76	3.618447	-3.594912	2.166867	0.135956
H77	4.881235	1.189975	0.835838	0.167446
H78	4.877321	-1.192869	0.841761	0.167450
H79	4.860775	-1.197192	-0.909322	0.166969
H80	4.859949	1.187290	-0.915202	0.166971

(a) Optimized using Gaussian03 and B3LYP/6-31G(d) procedures. Total energy = -1914.964092050 Hartree. Point Group = c1 Dipole moment = 1.74590 D (1.74560, -0.00120, -0.03130) Mulliken charges are listed in last column.

Table S16. Ground State Coordinates of $5aH_2$[(a)]

Atom	X(Å)	Y(Å)	Z(Å)	Charge
C 1	-4.172395	1.458356	-0.212468	-0.179668
C 2	-4.430467	0.128026	-0.183718	-0.183141
C 3	-3.142355	-0.536680	-0.033238	0.301604
C 4	-3.007990	-1.948649	0.032838	-0.042384
C 5	-1.794229	-2.643006	0.061748	0.344146
C 6	-1.599016	-4.059527	0.188276	-0.184255
C 7	-0.254323	-4.311010	0.166325	-0.194251
C 8	0.435124	-3.057699	0.030370	0.361109
C 9	1.828309	-2.867078	-0.013787	-0.105264
C10	2.422465	-1.593764	-0.024831	0.570771
C11	2.869781	0.521225	0.000764	0.215994
C12	2.763986	1.911347	0.030271	-0.062460
C13	1.534518	2.609825	0.035574	0.366120
C14	1.360536	4.027474	0.100940	-0.192645
C15	0.014146	4.293798	0.077734	-0.188520
C16	-0.685456	3.048565	-0.006664	0.342763
C17	-2.077628	2.851386	-0.055269	-0.039673
C18	-2.728858	1.599647	-0.076345	0.297781
N19	-2.125297	0.370981	0.013235	-0.689955
N20	-0.533287	-2.085949	-0.021084	-0.783452
N21	1.850561	-0.388916	0.017833	-0.651861
N22	0.276118	2.061557	-0.022788	-0.775729
C23	-2.921881	4.088656	-0.080302	0.014824
C24	-3.759158	4.405523	1.001120	-0.153585
C25	-4.541423	5.560522	0.982124	-0.134366
C26	-4.501989	6.417083	-0.119705	-0.124713
C27	-3.674747	6.111973	-1.202008	-0.134466
C28	-2.889521	4.958690	-1.181622	-0.157266
C29	4.004794	2.755874	0.068433	0.038178
C30	4.462567	3.401110	-1.087904	-0.145167
C31	5.597201	4.212429	-1.045151	-0.131503
C32	6.283894	4.393161	0.156054	-0.122531
C33	5.830959	3.758481	1.314216	-0.130550
C34	4.699009	2.945851	1.270540	-0.130890
C35	4.165666	-0.206518	-0.074856	0.578837
O36	5.317082	0.138658	-0.128240	-0.455749
O37	3.798529	-1.548760	-0.087194	-0.504098
C38	2.709586	-4.073733	-0.052756	0.064225
C39	3.656240	-4.313882	0.955710	-0.133014
C40	4.465038	-5.447998	0.917265	-0.135826
C41	4.345034	-6.363154	-0.130783	-0.123417
C42	3.411701	-6.133923	-1.142279	-0.135405
C43	2.602301	-4.998055	-1.104279	-0.160683
C44	-4.255799	-2.775775	0.072854	0.016512
C45	-4.578328	-3.643841	-0.982382	-0.158883
C46	-5.740267	-4.415616	-0.942171	-0.134531

C47	-6.598781	-4.334196	0.155443	-0.124988
C48	-6.288941	-3.475142	1.211751	-0.134249
C49	-5.128656	-2.701898	1.170404	-0.154366
H50	-4.886980	-2.038715	1.996151	0.143497
H51	0.064892	1.069781	-0.033214	0.412450
H52	-0.365808	-1.086913	-0.068941	0.411397
H53	0.235495	-5.268751	0.255396	0.164473
H54	-0.461254	5.261948	0.123489	0.161001
H55	2.170561	4.738398	0.163478	0.164218
H56	-2.396709	-4.778979	0.296926	0.162867
H57	-5.388374	-0.362785	-0.276237	0.148466
H58	-4.878146	2.267472	-0.332168	0.149039
H59	3.755643	-3.606664	1.773238	0.137622
H60	-3.787136	3.743087	1.861576	0.143537
H61	-2.252544	4.719833	-2.028675	0.142092
H62	-3.917283	-3.701740	-1.842632	0.140986
H63	1.887905	-4.815201	-1.902181	0.137109
H64	4.349294	2.450820	2.172384	0.132391
H65	-7.503471	-4.935319	0.187484	0.133643
H66	-5.112239	7.316084	-0.135027	0.133782
H67	5.190130	-5.617348	1.708743	0.134276
H68	4.977736	-7.246157	-0.160479	0.131632
H69	3.930149	3.258610	-2.024456	0.133361
H70	7.167868	5.024432	0.189832	0.129322
H71	6.360303	3.894740	2.253524	0.130900
H72	-5.179251	5.792400	1.830956	0.135213
H73	-3.642298	6.769815	-2.066486	0.135244
H74	-6.949249	-3.408760	2.072415	0.135105
H75	-5.976300	-5.076665	-1.771906	0.134855
H76	5.944531	4.701040	-1.951700	0.130376
H77	3.317074	-6.834491	-1.967792	0.131786

(a) Optimized using Gaussian03 and B3LYP/6-31G(d) procedures.
Total energy = -2024.908032160 Hartree. Point Group = c1
Dipole moment = 4.70230 D (-4.69120, 0.20620, 0.24910)
Mulliken charges are listed in last column.

Table S17. Ground State Coordinates of $7aH_2$[(a)]

Atom	X(Å)	Y(Å)	Z(Å)	Charge
C 1	-4.563760	-0.328226	0.094318	-0.172821
C 2	-4.450984	1.022767	0.037737	-0.193987
C 3	-3.027743	1.311627	-0.051020	0.311075
C 4	-2.509128	2.628488	-0.081315	-0.039632
C 5	-1.152733	2.973222	-0.055651	0.328408
C 6	-0.596929	4.292663	-0.044768	-0.171729
C 7	0.766370	4.183071	0.031952	-0.179036
C 8	1.105844	2.789787	0.042217	0.356741
C 9	2.412788	2.252064	0.103077	-0.054837
C10	2.742792	0.893532	0.067505	0.286633
C11	4.202459	0.406647	0.111885	0.036185
C12	4.041790	-1.097846	-0.206453	0.030157
C13	2.545700	-1.312970	-0.048086	0.263986
C14	2.009146	-2.602452	-0.008993	-0.024331
C15	0.637923	-2.939016	0.057165	0.338931
C16	0.097862	-4.266431	0.064204	-0.206636
C17	-1.269625	-4.173358	0.083348	-0.199487
C18	-1.622889	-2.786634	0.096700	0.317242
C19	-2.911266	-2.236730	0.087079	-0.020528
C20	-3.208851	-0.854370	0.034700	0.262668
N21	-2.293152	0.158626	-0.046194	-0.682980
N22	-0.432528	-2.082681	0.084948	-0.760738
N23	1.866566	-0.140874	0.023407	-0.601963
N24	-0.079287	2.101292	-0.013726	-0.776087
C25	3.517638	3.262687	0.249332	-0.012691
C26	4.122921	3.471589	1.495458	-0.153465
C27	5.132273	4.424038	1.649900	-0.137072
C28	5.545090	5.189328	0.559202	-0.125516
C29	4.942830	4.996207	-0.686209	-0.140559
C30	3.939547	4.040265	-0.838740	-0.107970
O31	5.102935	1.039464	-0.769412	-0.613157
O32	4.391820	-1.344377	-1.582277	-0.618703
C33	3.491674	-4.277254	-1.205750	-0.111634
C34	4.358934	-5.371045	-1.190536	-0.145842
C35	4.710960	-5.974419	0.018685	-0.124997
C36	4.187634	-5.479427	1.214254	-0.138160
C37	3.317648	-4.387356	1.197675	-0.155079
C38	2.960283	-3.769170	-0.010553	-0.011590
C39	-4.052268	-3.206358	0.128380	0.019867
C40	-4.288346	-3.990075	1.268818	-0.158249
C41	-5.349500	-4.895688	1.305593	-0.136924
C42	-6.191731	-5.035144	0.201169	-0.123982
C43	-5.966766	-4.262087	-0.939610	-0.136828
C44	-4.907256	-3.355168	-0.975159	-0.157442
C45	-3.487703	3.764162	-0.120134	0.015610
C46	-3.664300	4.602818	0.991134	-0.161842

C47	-4.579148	5.656101	0.951903	-0.136151
C48	-5.331766	5.889182	-0.200430	-0.125177
C49	-5.164976	5.061488	-1.312440	-0.135585
C50	-4.251481	4.007566	-1.272141	-0.156077
H51	-4.121330	3.366012	-2.139114	0.144265
H52	5.325887	-1.605660	-1.597439	0.399863
H53	4.899036	0.655708	-1.642012	0.398616
H54	-0.171407	1.092417	-0.018242	0.401037
H55	-0.385862	-1.070577	0.056453	0.400833
H56	1.486507	4.985910	0.069871	0.166080
H57	0.693469	-5.166498	0.039649	0.159305
H58	-1.179328	5.200926	-0.084341	0.166119
H59	-1.980740	-4.985804	0.075938	0.158630
H60	-5.466232	-0.914947	0.187303	0.147999
H61	-5.243573	1.756194	0.074237	0.147010
H62	3.222989	-3.805272	-2.144836	0.151766
H63	-4.731457	-2.757850	-1.865270	0.146282
H64	-3.639220	-3.877547	2.132666	0.146069
H65	-3.085337	4.418300	1.891753	0.142411
H66	3.479467	3.884706	-1.810839	0.132990
H67	-7.017840	-5.740590	0.229300	0.130905
H68	-6.044000	6.709351	-0.231490	0.130621
H69	5.386006	-6.826108	0.028629	0.126444
H70	6.328980	5.932672	0.678018	0.128279
H71	-6.614731	-4.366687	-1.805876	0.132760
H72	-5.744545	5.237193	-2.214923	0.132568
H73	-4.706150	6.291528	1.824459	0.131976
H74	-5.520003	-5.488898	2.200190	0.132640
H75	4.453222	-5.943490	2.160568	0.127437
H76	5.259263	5.587304	-1.541813	0.129751
H77	5.589451	4.572175	2.624910	0.128885
H78	2.906242	-4.006630	2.129041	0.136392
H79	4.757296	-5.754791	-2.126393	0.127200
H80	3.791323	2.889875	2.352095	0.135923
H81	4.632449	-1.742581	0.449230	0.141166
H82	4.605170	0.549967	1.120338	0.159754

(a) Optimized using Gaussian03 and B3LYP/6-31G(d) procedures. Total energy = -2065.374775390 Hartree. Point Group = c1 Dipole moment = 0.82620 D (-0.48040, -0.58770, 0.32640) Mulliken charges are listed in last column.

Table S18. Ground State Coordinates of $10aH_2$[(a)]

Atom	X(Å)	Y(Å)	Z(Å)	Charge
C 1	4.296519	1.153434	0.168147	-0.183171
C 2	4.452200	-0.194803	0.133045	-0.186908
C 3	3.117668	-0.758029	0.002834	0.297649
C 4	2.871968	-2.158265	-0.045927	-0.041481
C 5	1.612000	-2.759785	-0.039390	0.339166
C 6	1.307008	-4.159041	-0.127097	-0.183949
C 7	-0.052459	-4.307388	-0.073890	-0.200195
C 8	-0.643794	-3.002395	0.038306	0.364883
C 9	-2.020873	-2.708547	0.089522	-0.110873
C10	-2.527989	-1.401084	0.051685	0.577238
C11	-2.798320	0.744389	-0.081315	0.265350
C12	-2.586590	2.114576	-0.060603	-0.054063
C13	-1.306804	2.728117	-0.030760	0.365854
C14	-1.031684	4.129841	-0.052605	-0.201349
C15	0.332068	4.298070	-0.028631	-0.187953
C16	0.940561	3.005776	0.016963	0.336531
C17	2.310838	2.702622	0.053348	-0.040430
C18	2.869253	1.404260	0.053766	0.294789
N19	2.172410	0.225061	-0.030916	-0.690183
N20	0.394584	-2.107172	0.050823	-0.783818
N21	-1.864899	-0.243699	-0.049812	-0.629952
N22	-0.095081	2.089871	0.007819	-0.776859
C23	3.246575	3.872282	0.093604	0.016033
C24	3.293803	4.716588	1.213951	-0.156383
C25	4.163658	5.807257	1.249125	-0.134865
C26	4.998309	6.074548	0.162604	-0.125255
C27	4.959451	5.242887	-0.958205	-0.134649
C28	4.092177	4.150538	-0.991877	-0.152958
C29	4.906975	-3.076209	-1.217068	-0.153561
C30	6.006378	-3.932804	-1.274710	-0.134550
C31	6.275155	-4.803414	-0.216551	-0.125484
C32	5.436680	-4.811779	0.899295	-0.134909
C33	4.335494	-3.956182	0.955662	-0.159057
C34	4.054078	-3.076264	-0.101468	0.017988
C35	-2.986680	-3.846864	0.173593	0.065329
C36	-2.943183	-4.743015	1.253334	-0.162525
C37	-3.830676	-5.817573	1.329088	-0.136221
C38	-4.781843	-6.012625	0.327226	-0.125480
C39	-4.839900	-5.124440	-0.749438	-0.139121
C40	-3.952203	-4.052748	-0.825182	-0.138666
C41	-4.180662	0.114849	-0.137170	0.263211
C42	-3.770997	3.037916	-0.011356	-0.006306
C43	-4.541407	3.309804	-1.151905	-0.134449
C44	-5.624993	4.187182	-1.084637	-0.140862
C45	-5.958343	4.804429	0.122404	-0.125609
C46	-5.200469	4.540849	1.264739	-0.135554

C47	-4.114779	3.666455	1.196446	-0.154484
O48	-4.711168	0.246347	-1.431682	-0.589216
O49	-3.892301	-1.253531	0.150551	-0.519136
H50	-4.885680	0.471223	0.621024	0.153394
H51	-5.620305	-0.095461	-1.414213	0.400508
H52	0.304357	-1.097540	0.073823	0.408388
H53	0.045481	1.085735	-0.009623	0.410933
H54	-0.614153	-5.227514	-0.129464	0.158993
H55	0.874914	5.231127	-0.049442	0.156852
H56	2.045219	-4.940096	-0.231188	0.159173
H57	-1.787040	4.900236	-0.094688	0.155488
H58	5.064820	1.905014	0.278223	0.143974
H59	5.371783	-0.756546	0.211417	0.143571
H60	-4.287637	2.825881	-2.088603	0.150472
H61	-4.001689	-3.364394	-1.663426	0.136407
H62	4.060092	3.507252	-1.866575	0.143125
H63	4.697703	-2.402890	-2.043393	0.143088
H64	2.650292	4.506627	2.063682	0.140398
H65	3.690845	-3.957134	1.830158	0.139797
H66	-2.212422	-4.587725	2.042290	0.136094
H67	5.674914	6.924555	0.189273	0.131063
H68	7.132672	-5.469523	-0.261121	0.130937
H69	-5.474077	-6.848492	0.384901	0.127947
H70	5.602762	5.445590	-1.810470	0.132959
H71	-6.802659	5.487042	0.172460	0.129768
H72	-3.522819	3.464978	2.085451	0.136787
H73	6.651455	-3.922190	-2.149414	0.132811
H74	4.191254	6.445572	2.128411	0.132414
H75	5.641515	-5.480928	1.730950	0.132198
H76	-5.452597	5.015348	2.209582	0.131077
H77	-3.781436	-6.497659	2.175609	0.129249
H78	-6.208033	4.390406	-1.979283	0.130752
H79	-5.575900	-5.269911	-1.536111	0.127846

(a) Optimized using Gaussian03 and B3LYP/6-31G(d) procedures.
Total energy = -2026.088614950 Hartree. Point Group = c1
Dipole moment = 1.23150 D (-1.05780, 0.30850, 0.55000)
Mulliken charges are listed in last column.

Table S19. Ground State Coordinates of $12aH_2$[(a)]

Atom	X(Å)	Y(Å)	Z(Å)	Charge
C 1	-4.316619	-0.472066	0.206606	-0.184483
C 2	-4.245435	0.884757	0.185419	-0.188509
C 3	-2.839470	1.218847	0.034883	0.295254
C 4	-2.364981	2.559621	-0.022337	-0.039657
C 5	-1.025175	2.947674	-0.049378	0.337009
C 6	-0.499632	4.278016	-0.162696	-0.182998
C 7	0.866828	4.204905	-0.145466	-0.201607
C 8	1.242647	2.822442	-0.025029	0.366682
C 9	2.556631	2.314672	0.008763	-0.120725
C10	2.850031	0.942382	0.007948	0.576613
C11	2.747994	-1.224809	-0.027505	0.259445
C12	2.304613	-2.539189	-0.045324	-0.076292
C13	0.944241	-2.939034	-0.042765	0.374080
C14	0.447150	-4.278160	-0.100545	-0.206240
C15	-0.926091	-4.225321	-0.080704	-0.186526
C16	-1.319682	-2.853510	-0.002590	0.332856
C17	-2.619455	-2.330378	0.042423	-0.039173
C18	-2.954626	-0.955442	0.066135	0.291878
N19	-2.071574	0.091569	-0.020008	-0.689912
N20	-0.147922	-2.115794	0.012937	-0.778170
N21	1.998902	-0.092692	-0.031207	-0.618547
N22	0.074462	2.107067	0.022831	-0.785025
C23	-3.380724	3.660200	-0.054842	0.017672
C24	-3.489063	4.573136	1.005944	-0.158631
C25	-4.434011	5.599648	0.971326	-0.134771
C26	-5.285683	5.732331	-0.126464	-0.125630
C27	-5.188322	4.830258	-1.187994	-0.134595
C28	-4.245818	3.802590	-1.151698	-0.153314
C29	-4.627852	-3.424002	-1.018600	-0.152907
C30	-5.665877	-4.355907	-1.005733	-0.134764
C31	-5.833991	-5.205031	0.089847	-0.125338
C32	-4.956356	-5.116950	1.171749	-0.134981
C33	-3.915502	-4.187458	1.157017	-0.157315
C34	-3.737041	-3.327419	0.062108	0.017982
C35	3.340892	-3.625581	-0.055410	0.006562
C36	4.039811	-3.940204	-1.231272	-0.159088
C37	5.012944	-4.940809	-1.239351	-0.132166
C38	5.300890	-5.647136	-0.070130	-0.125521
C39	4.609825	-5.348299	1.105542	-0.132650
C40	3.639095	-4.345258	1.112463	-0.154477
C41	4.218575	-0.845390	0.021185	-0.084337
O42	4.171696	0.583727	0.050168	-0.509783
C43	3.692656	3.287058	0.049419	0.067078
C44	3.830501	4.177429	1.125908	-0.161162
C45	4.878691	5.098162	1.164686	-0.135802
C46	5.811881	5.141441	0.128286	-0.125831

C47	5.689141	4.257708	-0.946270	-0.137330
C48	4.640278	3.340545	-0.984925	-0.134821
H49	4.548943	2.656917	-1.823720	0.130433
H50	0.003905	1.096761	0.059454	0.407087
H51	-0.130284	-1.102030	0.017556	0.409219
H52	1.567986	5.021755	-0.226321	0.158305
H53	-1.104020	5.167497	-0.260749	0.158873
H54	-1.611396	-5.058789	-0.122916	0.156386
H55	1.069588	-5.158860	-0.158654	0.151882
H56	-5.058103	1.590088	0.282809	0.142472
H57	-5.198383	-1.085557	0.323300	0.142666
H58	-4.497242	-2.765431	-1.872526	0.143154
H59	-4.169820	3.103831	-1.979958	0.142800
H60	-3.238432	-4.115419	2.003624	0.140317
H61	-2.832938	4.466614	1.865317	0.139775
H62	3.111853	4.139357	1.940082	0.135164
H63	6.057400	-6.427355	-0.075696	0.133032
H64	-6.643991	-5.929558	0.100701	0.130841
H65	-6.021086	6.532060	-0.154443	0.130653
H66	3.102794	-4.113151	2.028883	0.139428
H67	6.629759	5.856668	0.157662	0.127627
H68	-6.342278	-4.419664	-1.854188	0.132654
H69	5.541036	-5.172468	-2.160717	0.134031
H70	4.827193	-5.894700	2.019702	0.134228
H71	-5.844963	4.928078	-2.048660	0.132393
H72	-5.083156	-5.769382	2.031840	0.132125
H73	-4.506629	6.292757	1.805501	0.131989
H74	6.410189	4.285190	-1.759311	0.128248
H75	4.968184	5.776854	2.009134	0.128691
H76	3.806863	-3.401403	-2.146467	0.137146
H77	4.790300	-1.168253	-0.856511	0.172371
H78	4.732619	-1.212091	0.918279	0.175975

(a) Optimized using Gaussian03 and B3LYP/6-31G(d) procedures. Total energy = -1950.871519550 Hartree. Point Group = c1 Dipole moment = 1.36150 D (0.67030, -1.18500, -0.01630) Mulliken charges are listed in last column.