Supporting Information to:

meso-Tetraphenyl-2-oxabacteriochlorins and *meso*-Tetraphenyl-2,12/13-dioxabacteriochlorins

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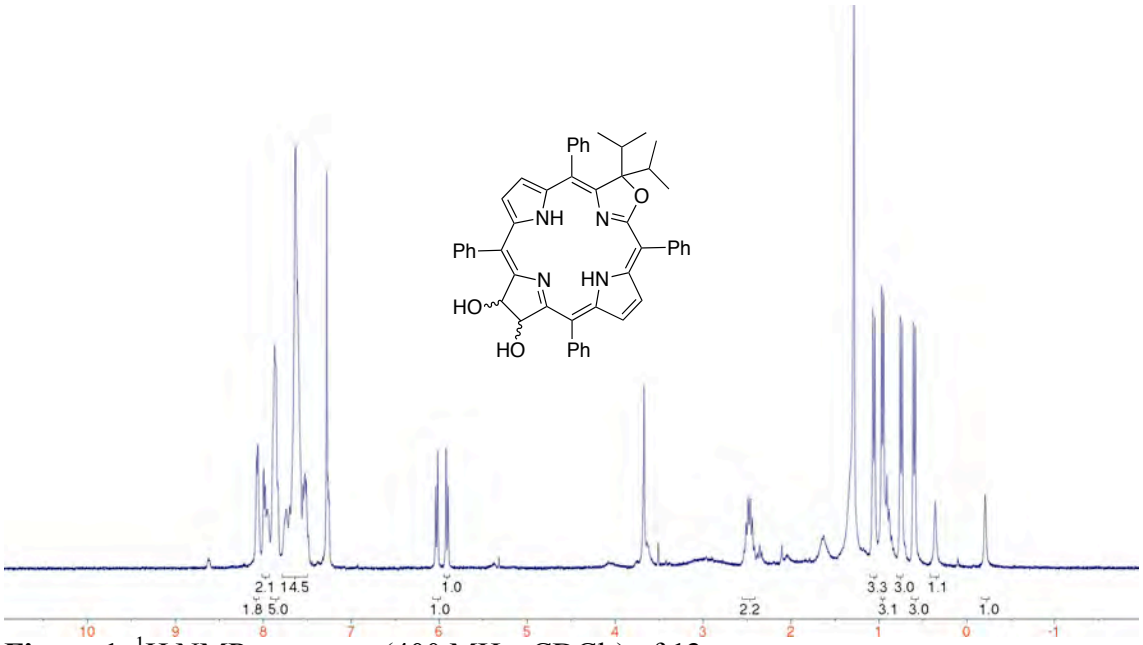


Figure 1. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **13**

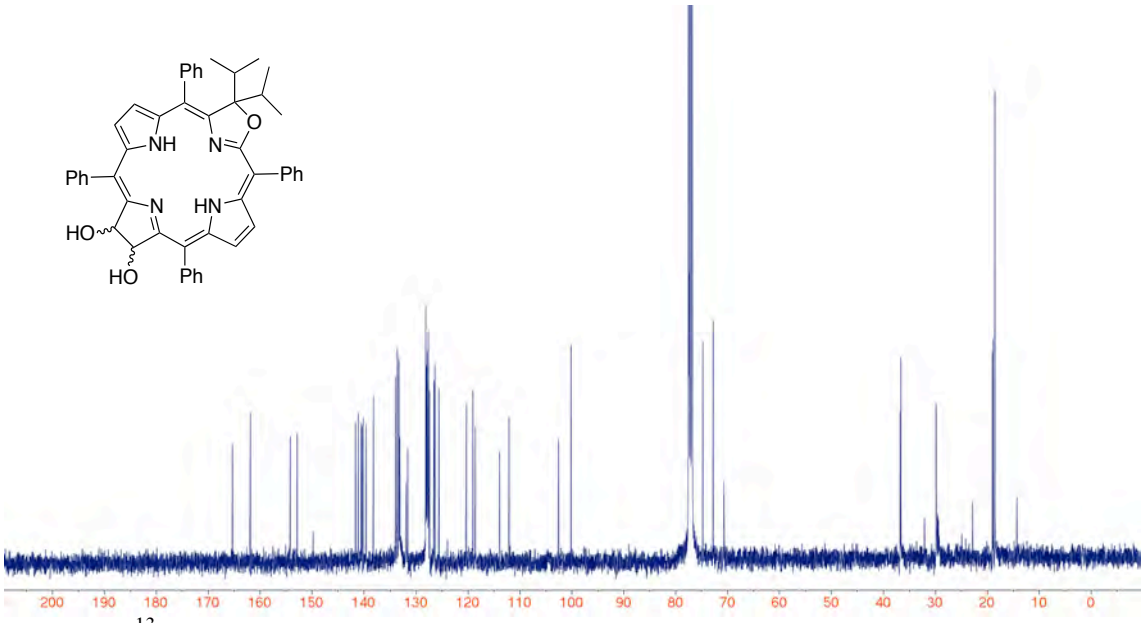


Figure 2. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **13**

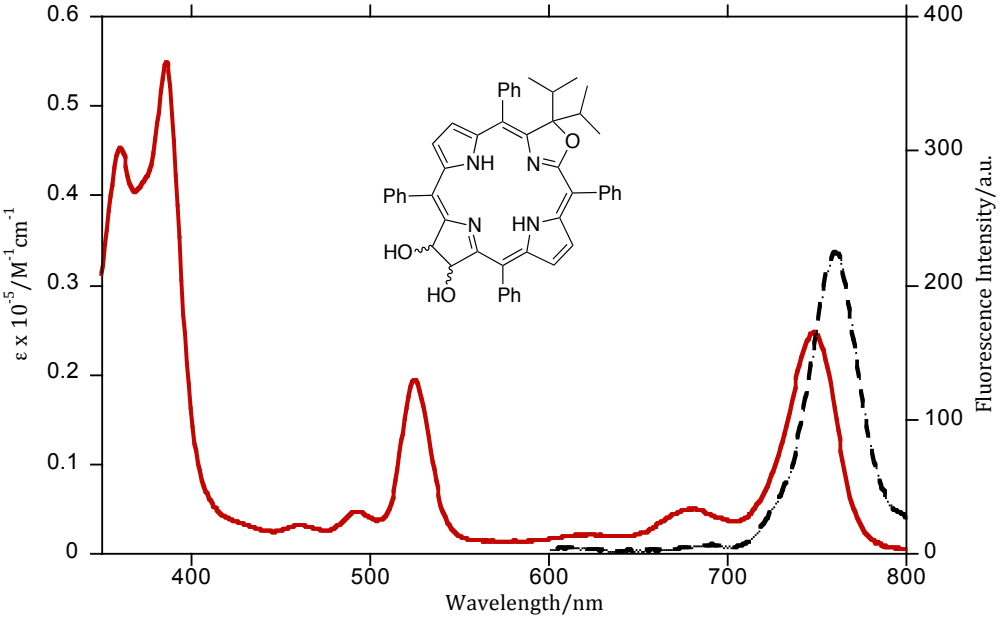


Figure 3. UV-vis (solid red trace) and fluorescence (broken black trace) spectra of **13** (CH_2Cl_2)

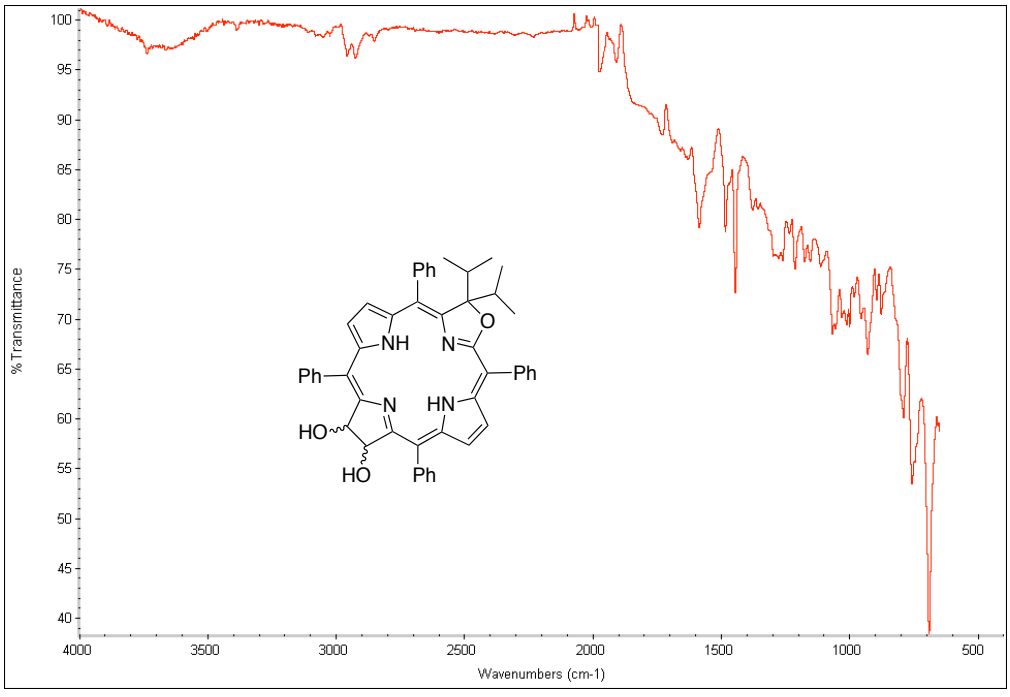


Figure 4. FT-IR spectrum (neat, diffuse reflectance) of **13**

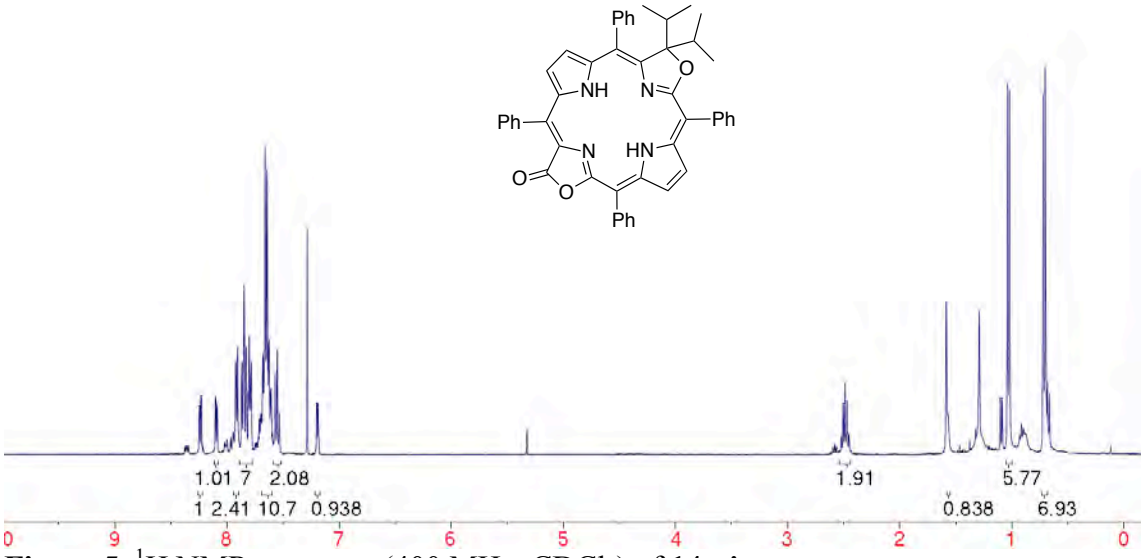


Figure 5. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **14-*cis***

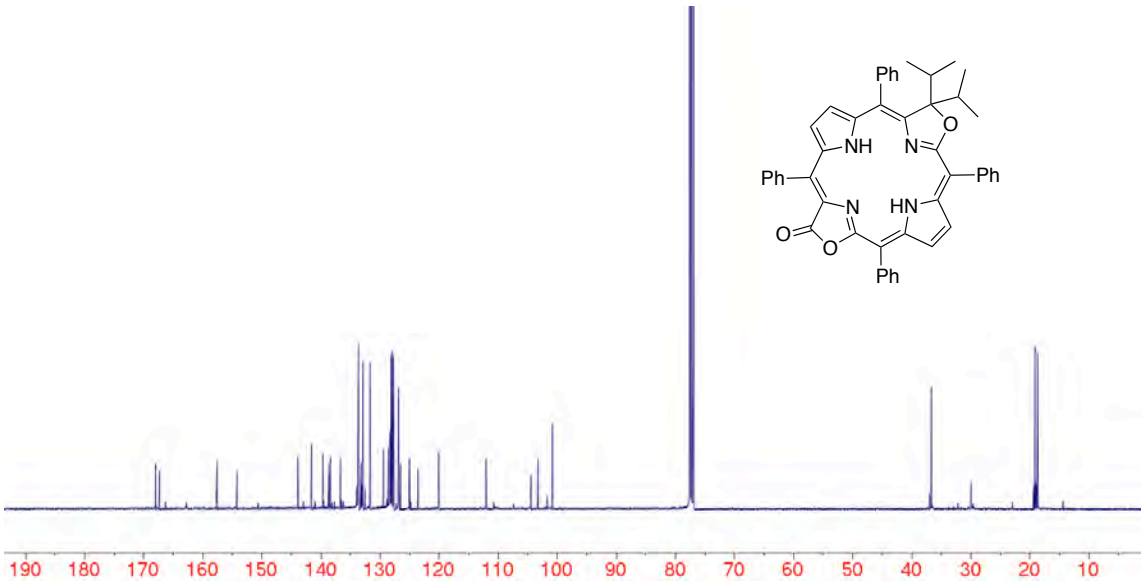


Figure 6. ^{13}H NMR spectrum (100 MHz, $CDCl_3$) of **14-*cis***

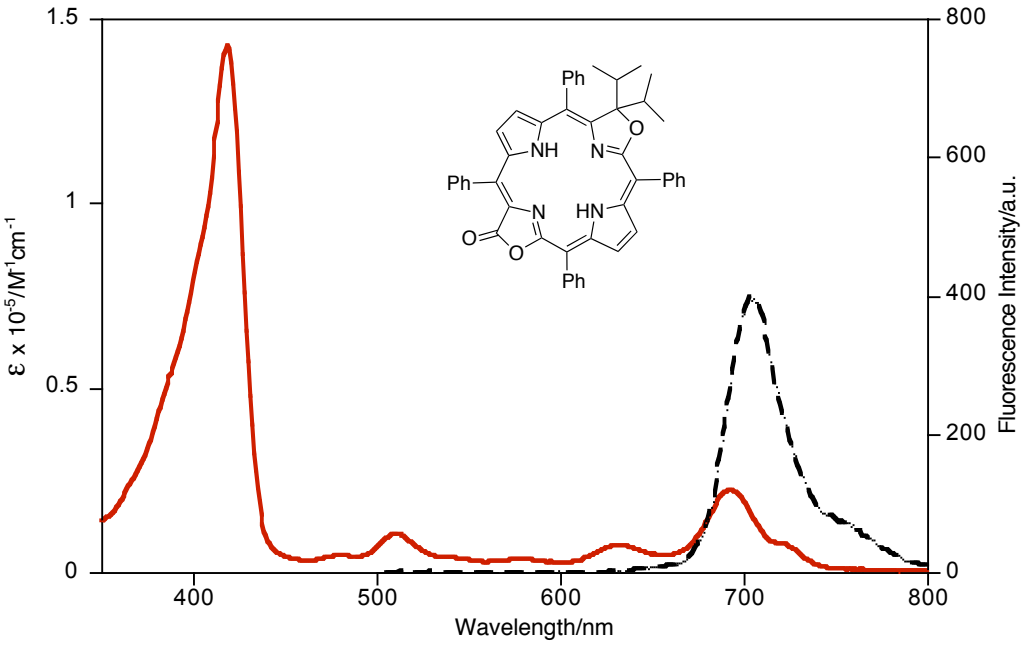


Figure 7. UV-vis (solid red trace) and fluorescence (broken black trace) spectra of **14-*cis*** (CH_2Cl_2)

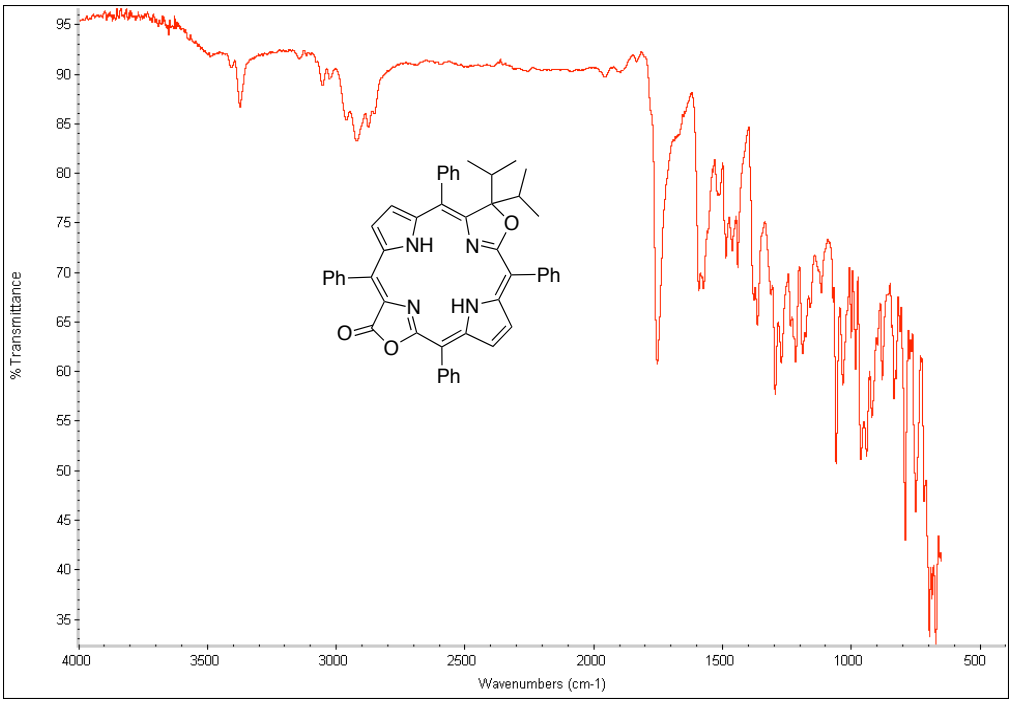


Figure 8. FT-IR spectrum (neat, diffuse reflectance) of **14-*cis***

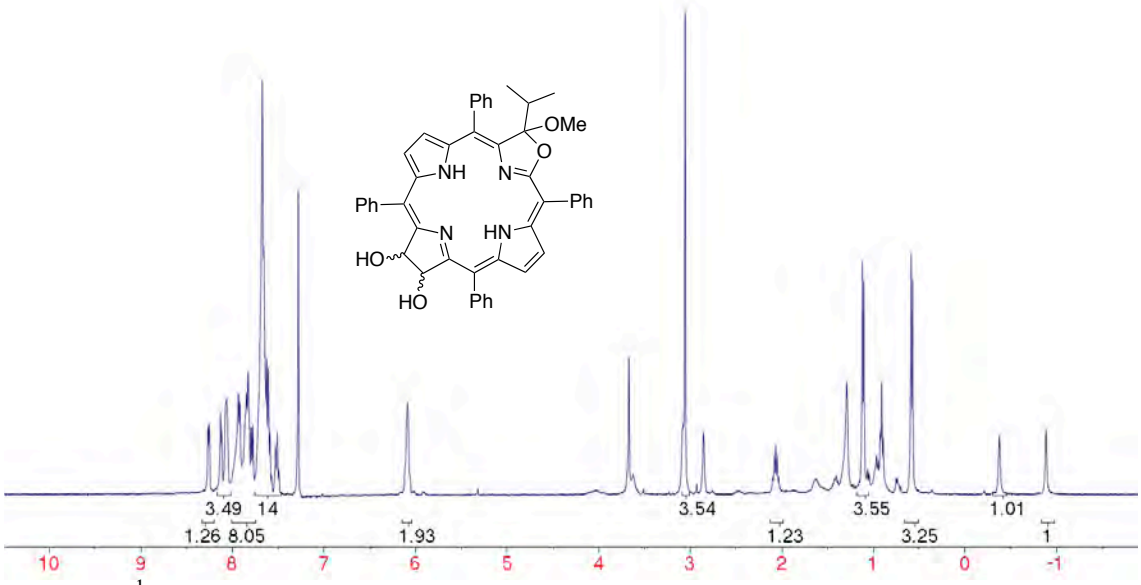
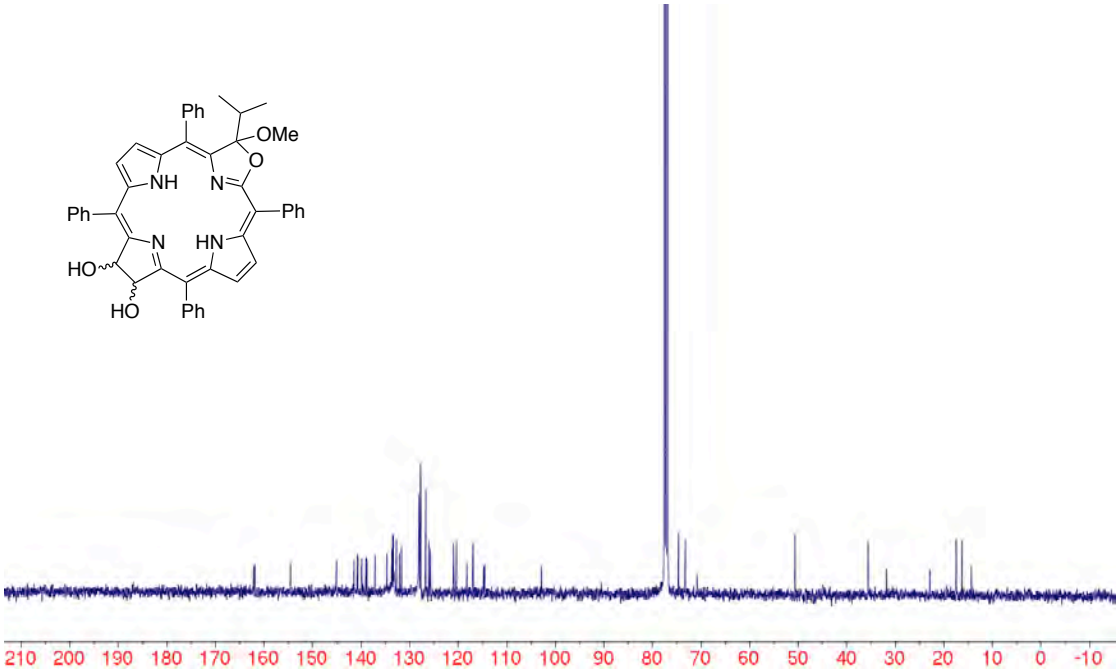


Figure 9. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **15**



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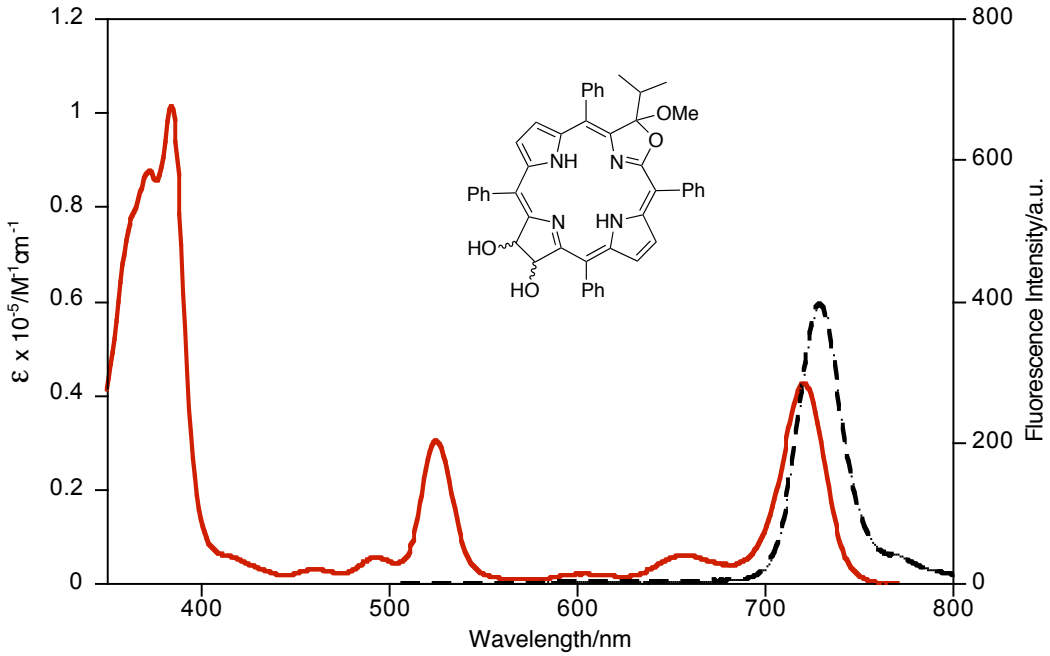


Figure 11. UV-vis (solid red trace) and fluorescence (broken black trace) spectra of **15** (CH_2Cl_2)

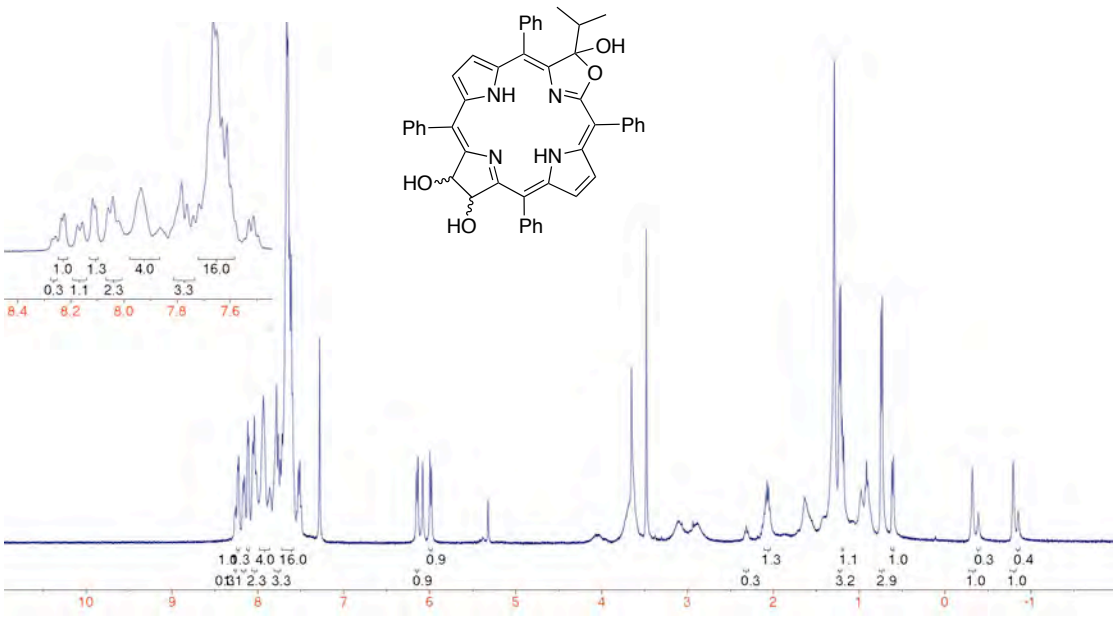


Figure 12. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **17**

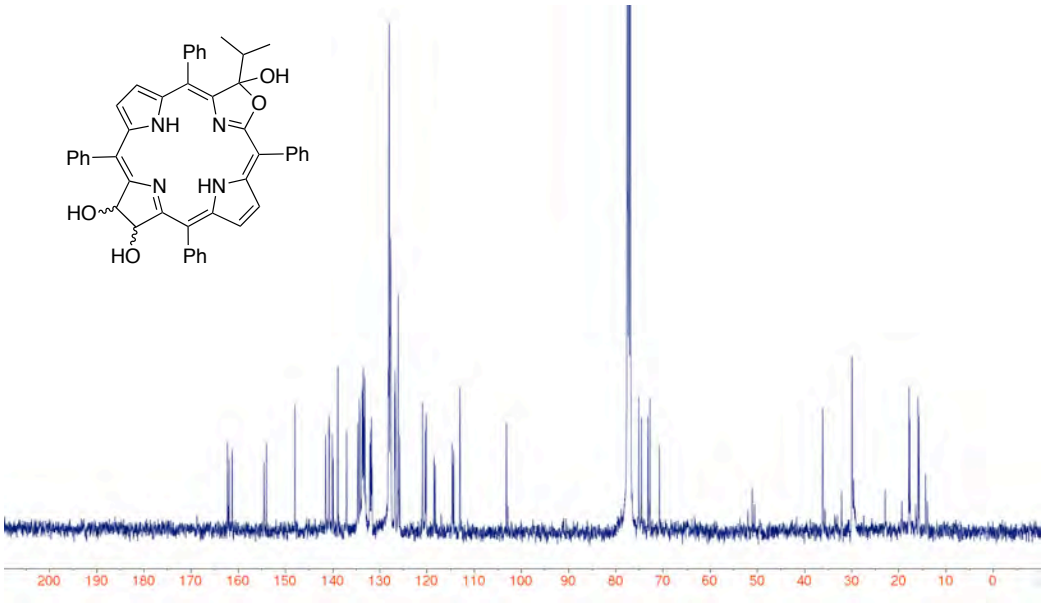


Figure 13. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **17**

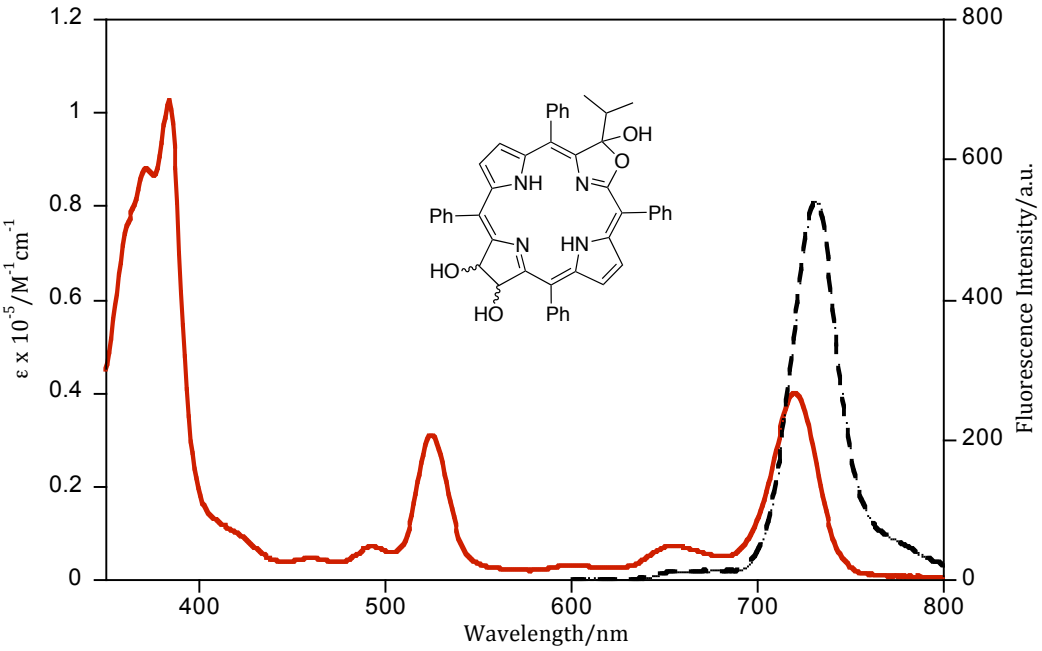


Figure 14. UV-vis (solid red trace) and fluorescence (broken black trace) spectra of **17** ($CHCl_3$)

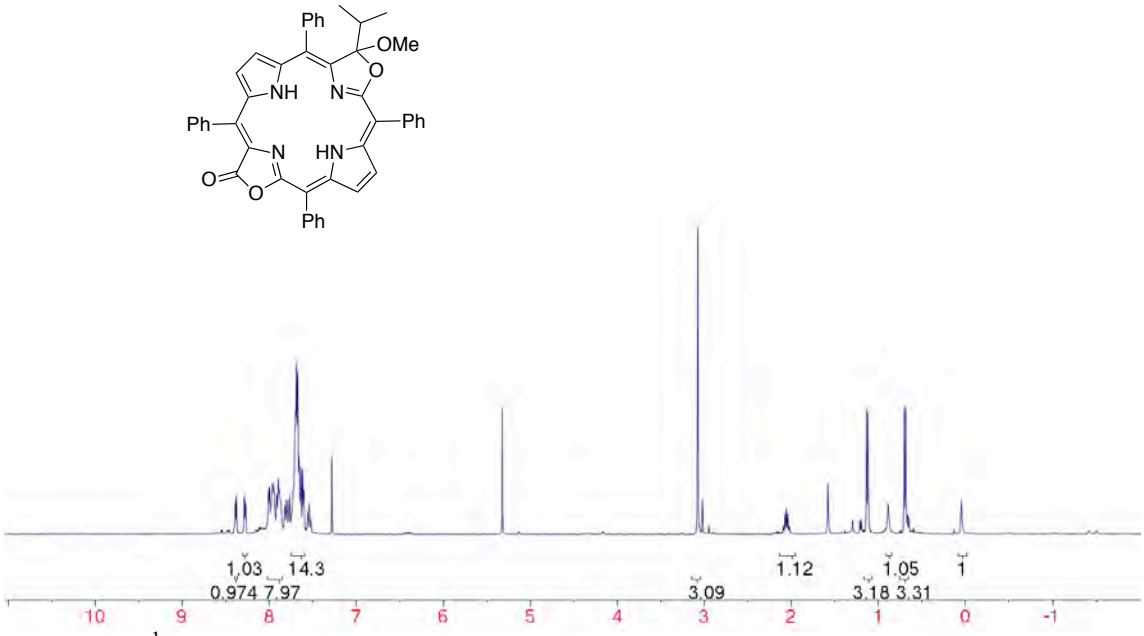


Figure 15. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **16-*cis***

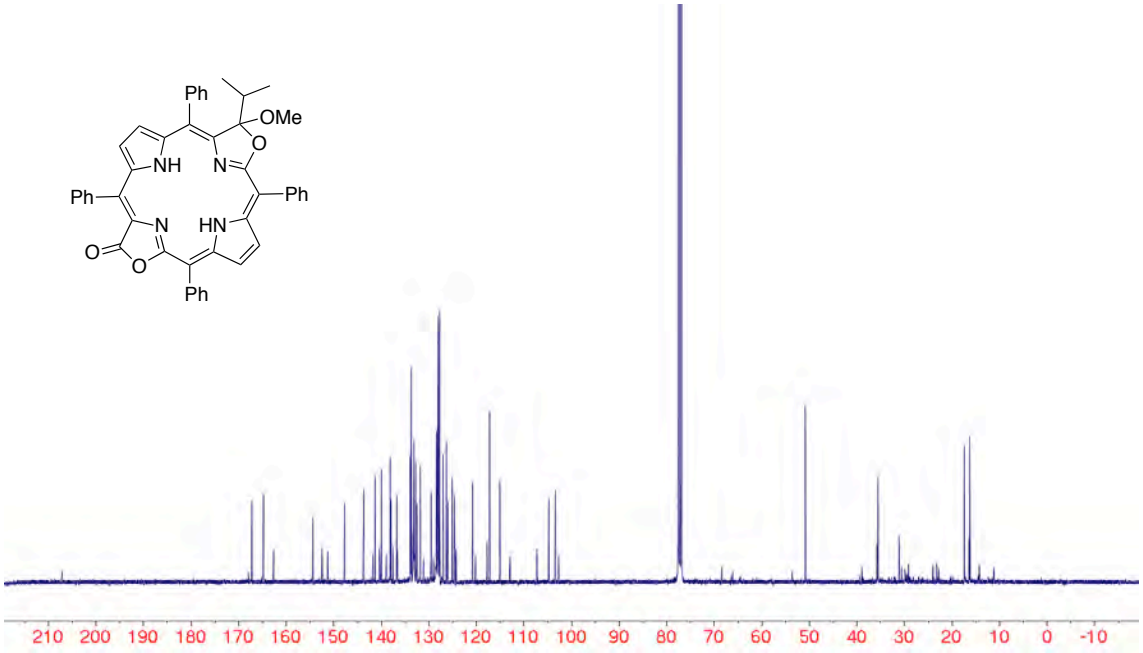
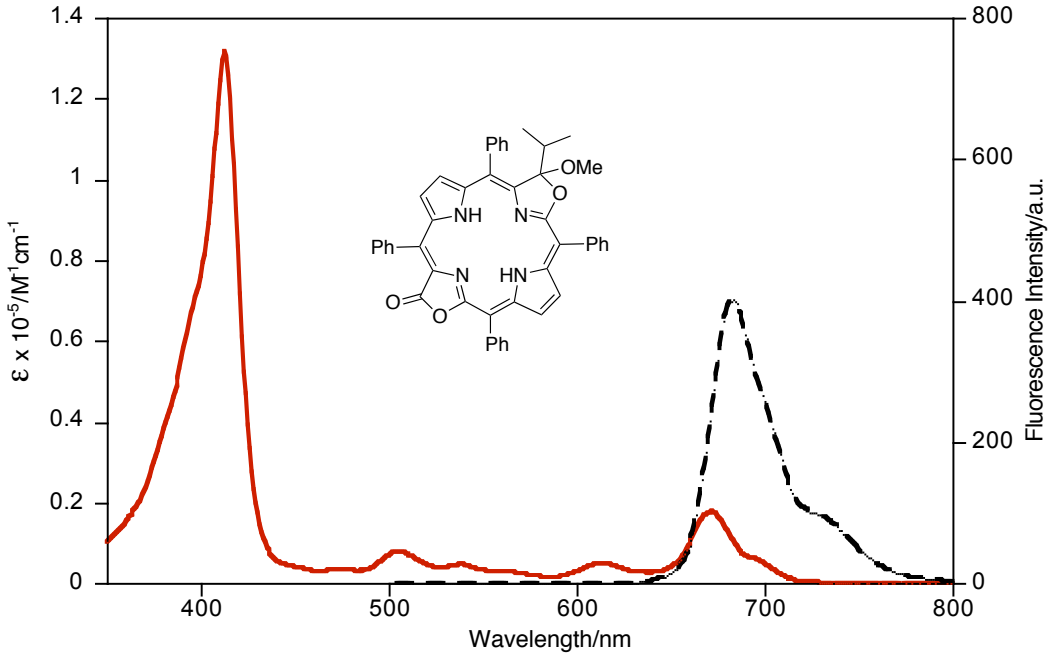


Figure 16. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **16-*cis***



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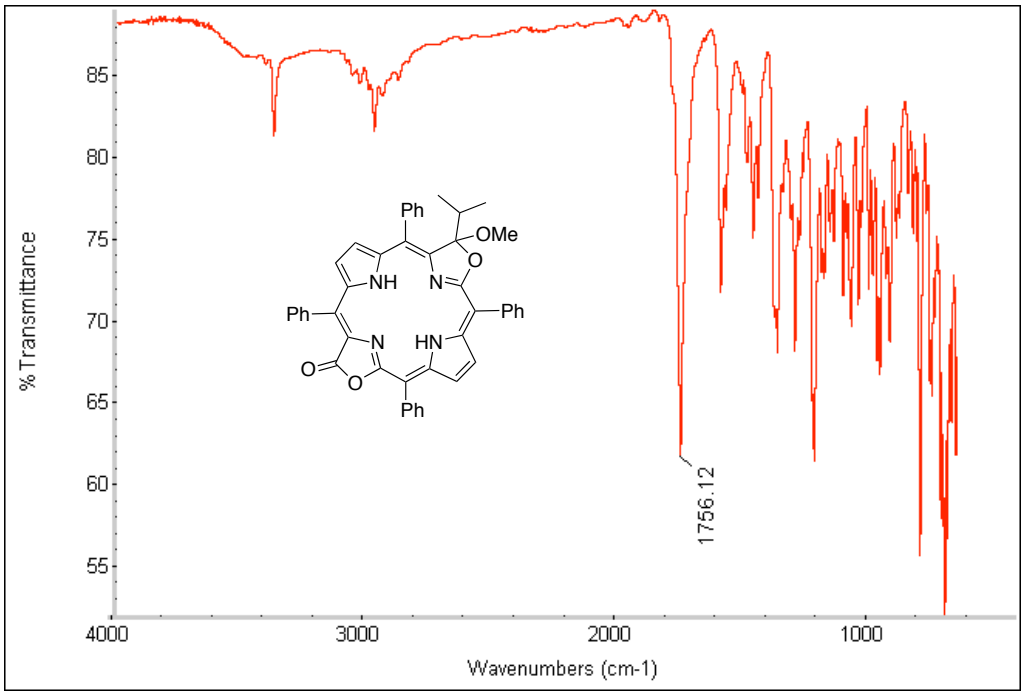


Figure 18. FT-IR spectrum (neat, diffuse reflectance) of **16-*cis***

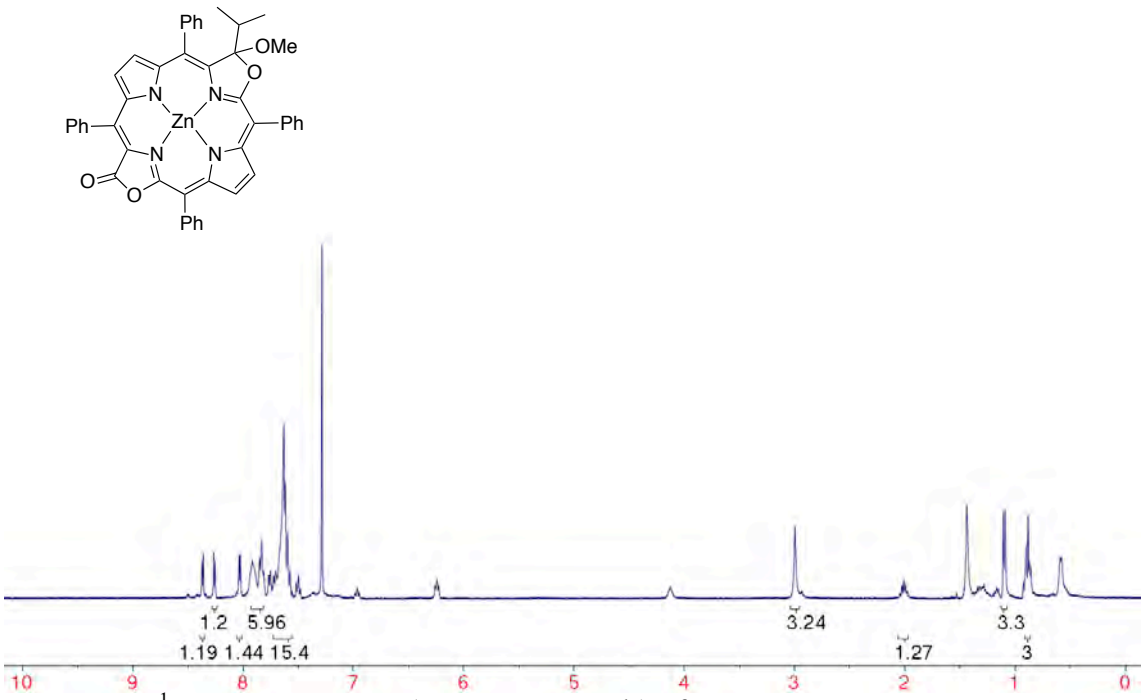


Figure 19. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **16Zn-*cis***

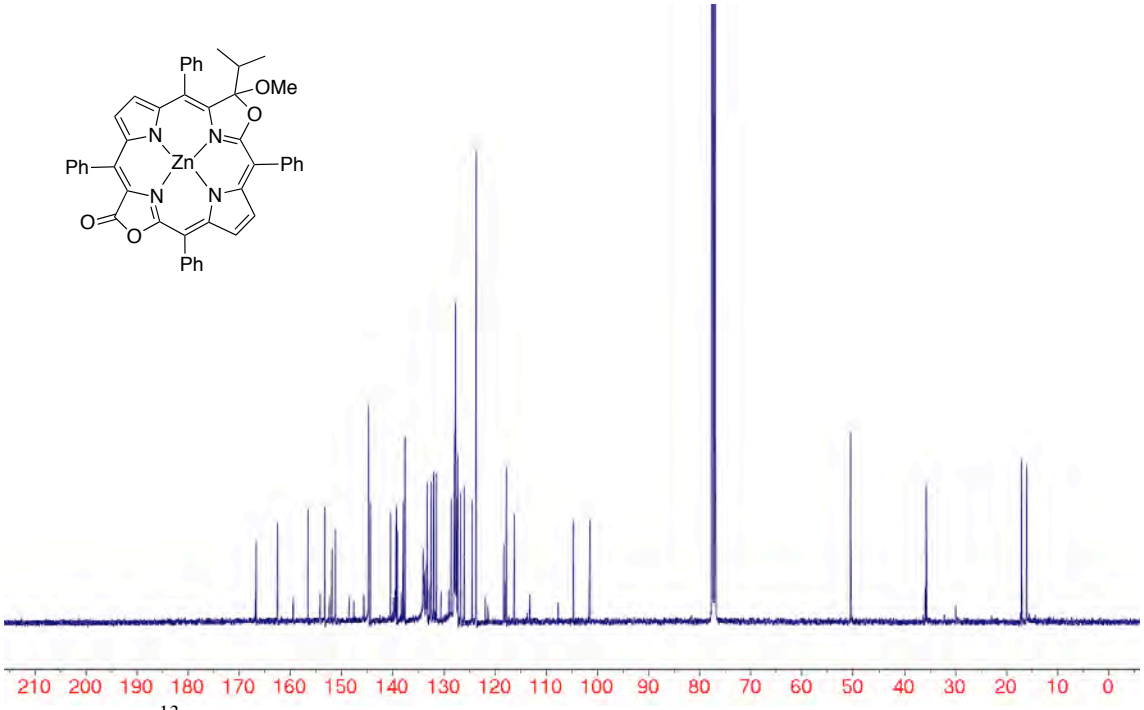
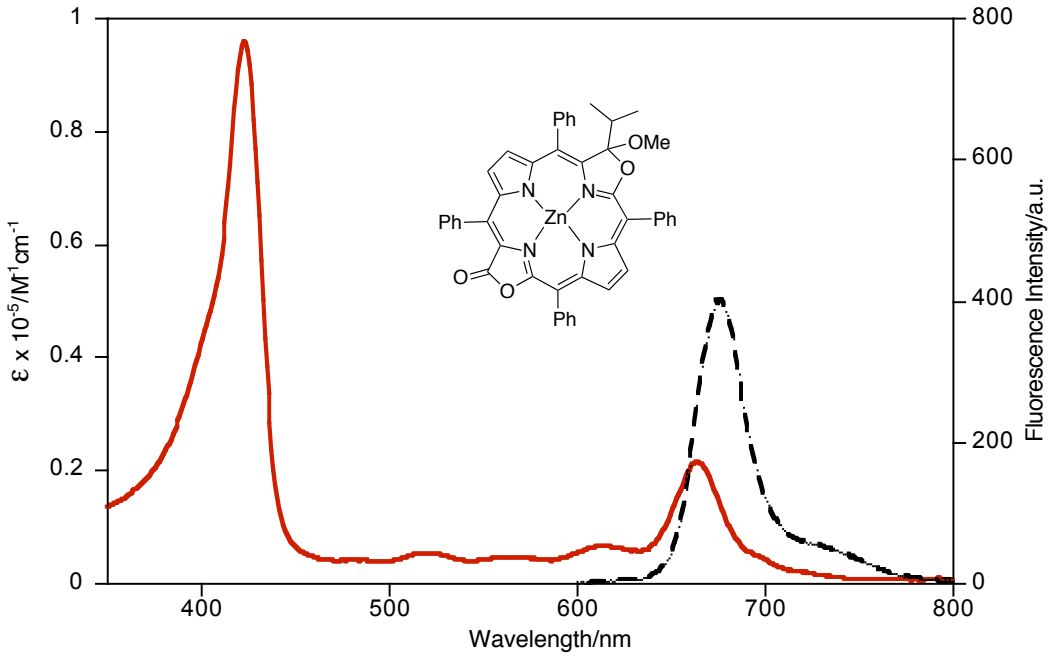


Figure 20. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **16Zn-*cis***



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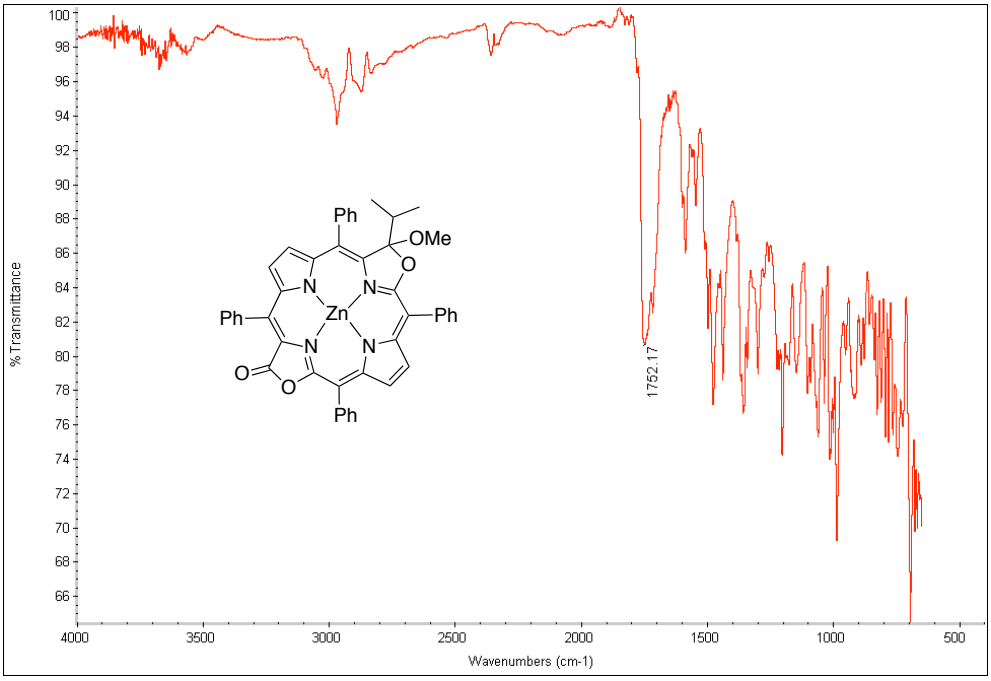

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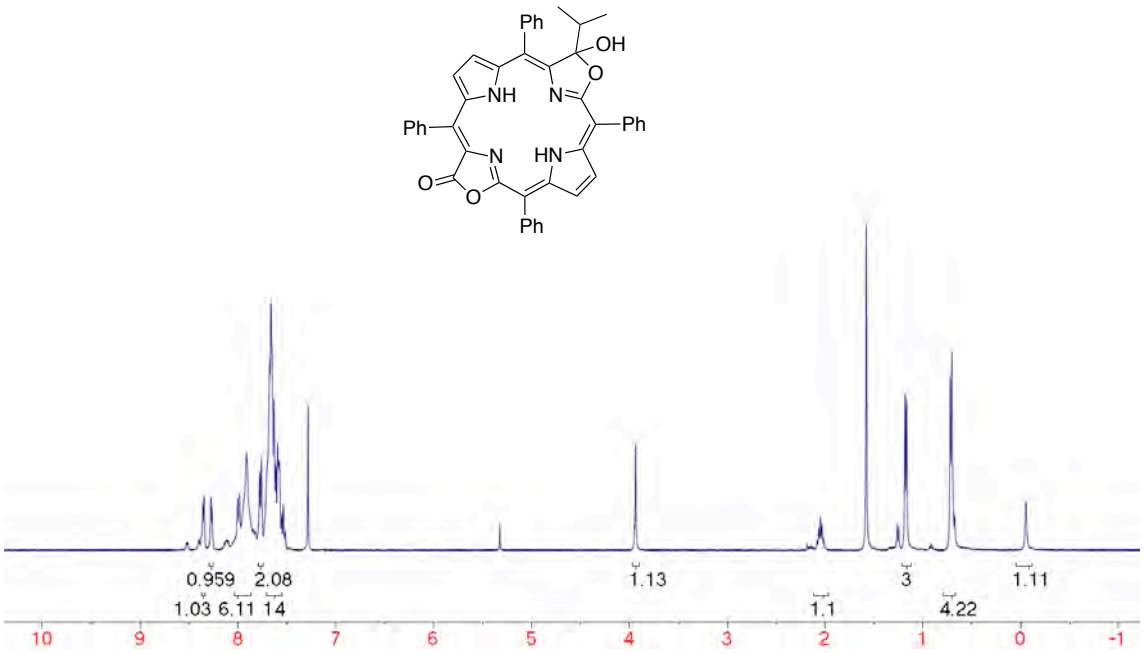
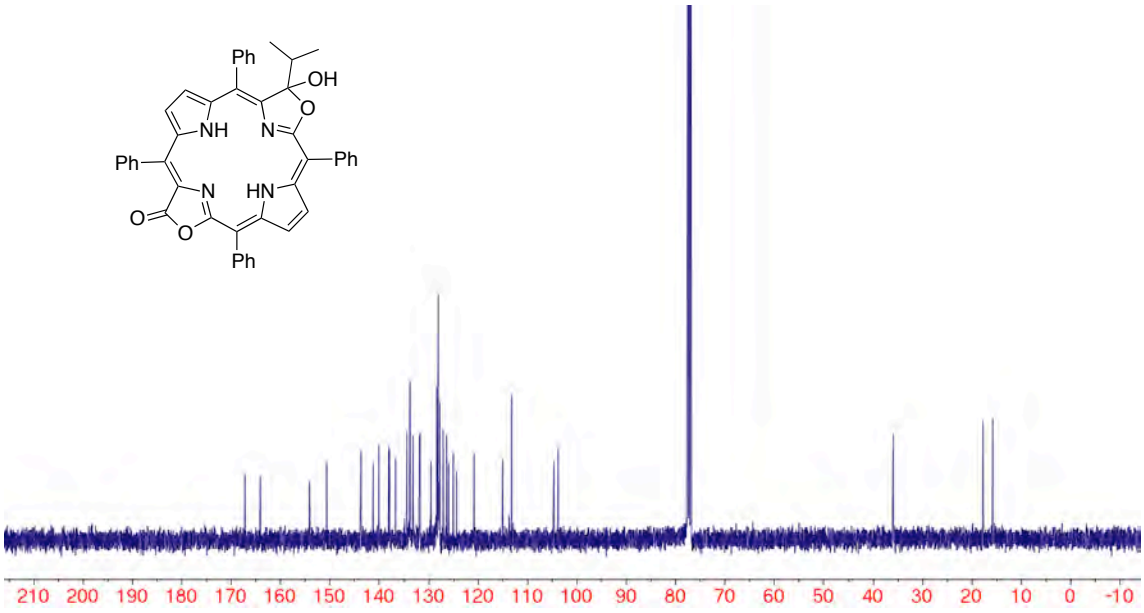


Figure 23. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **18-*cis***



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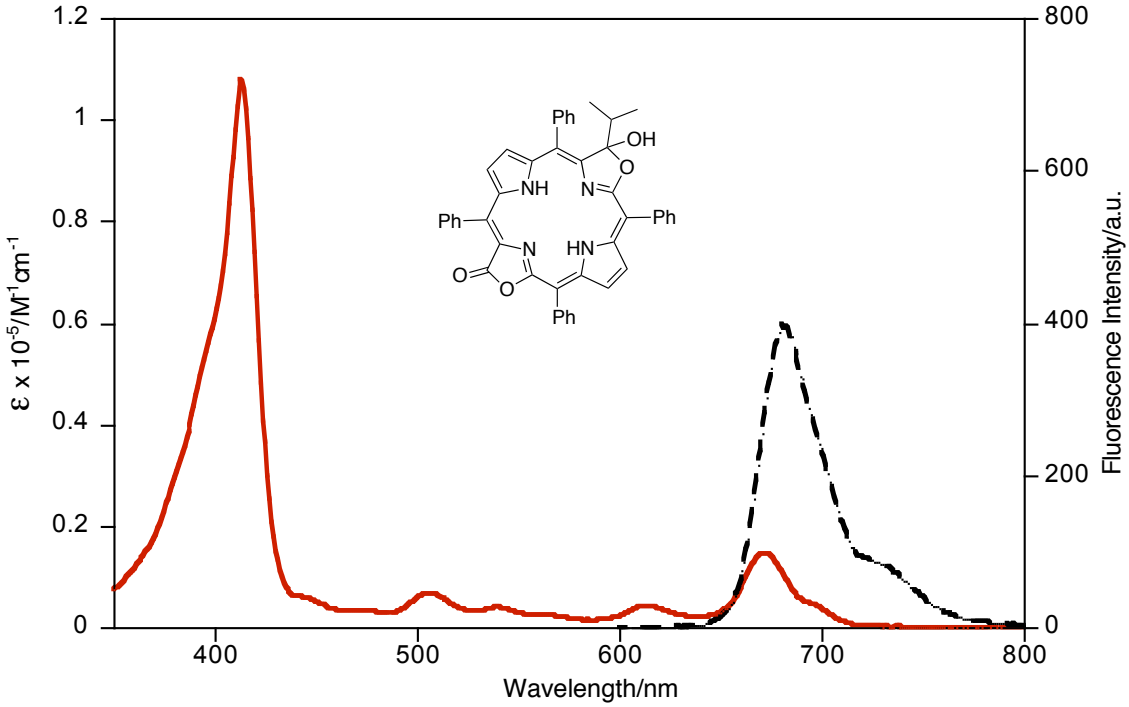

Figure 25. UV-vis (solid red trace) and fluorescence (broken black trace) spectra of **18-*cis*** (CH_2Cl_2)

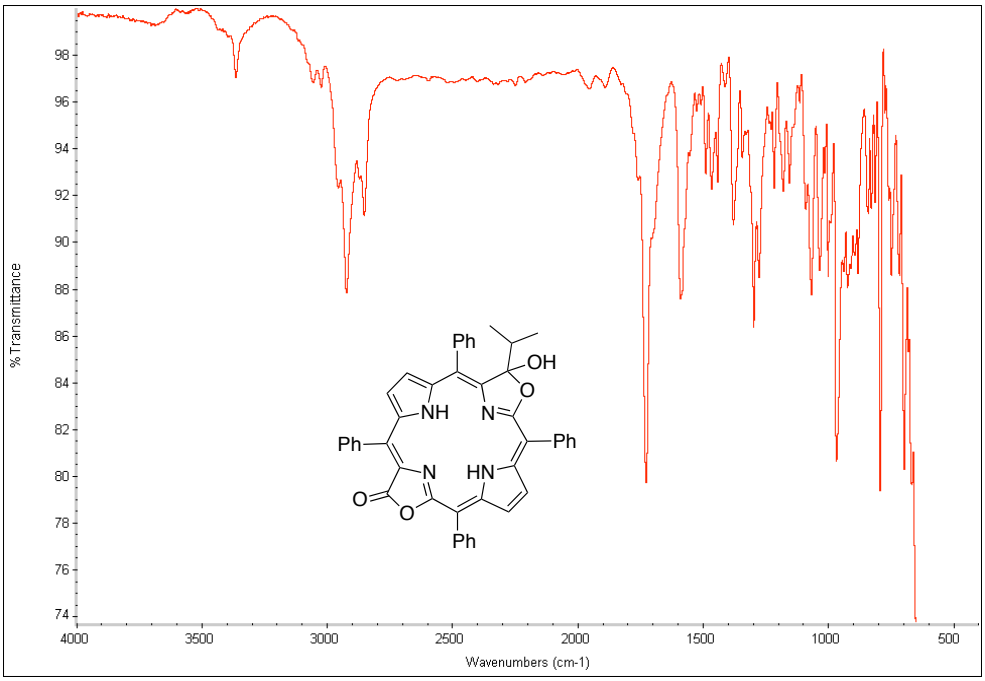

Figure 26. FT-IR spectrum (neat, diffuse reflectance) of **18-*cis***

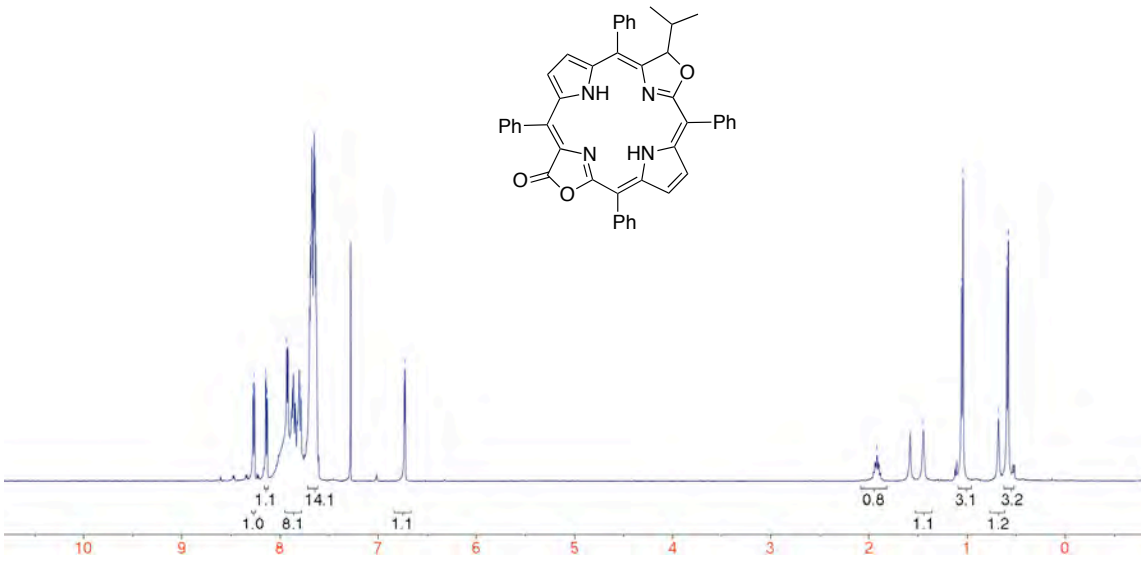

Figure 27. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **19-*cis***

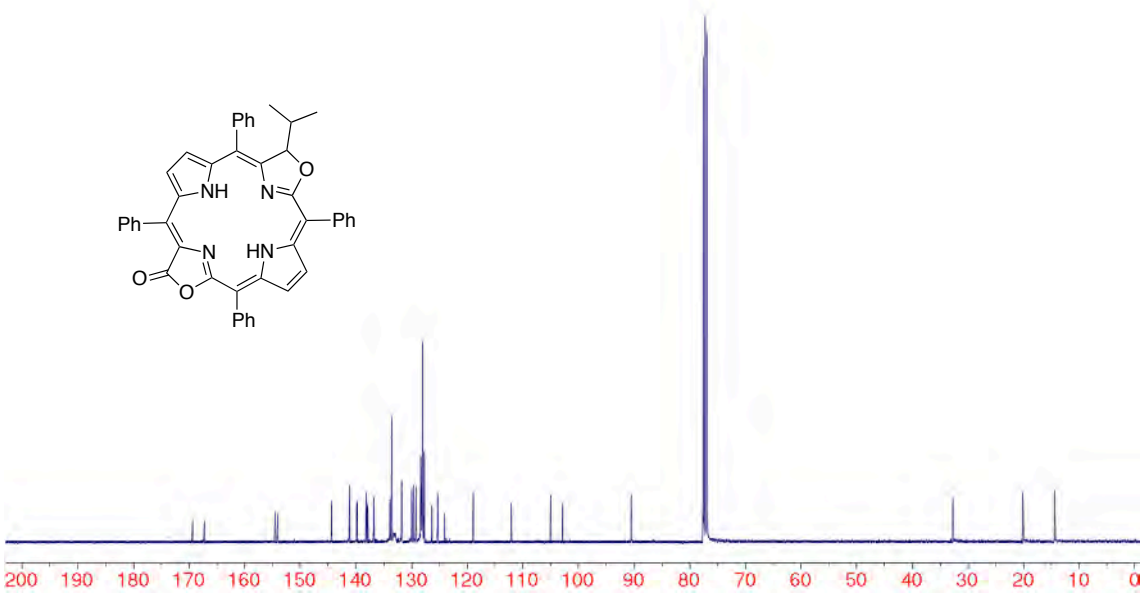

Figure 28. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **19-*cis***

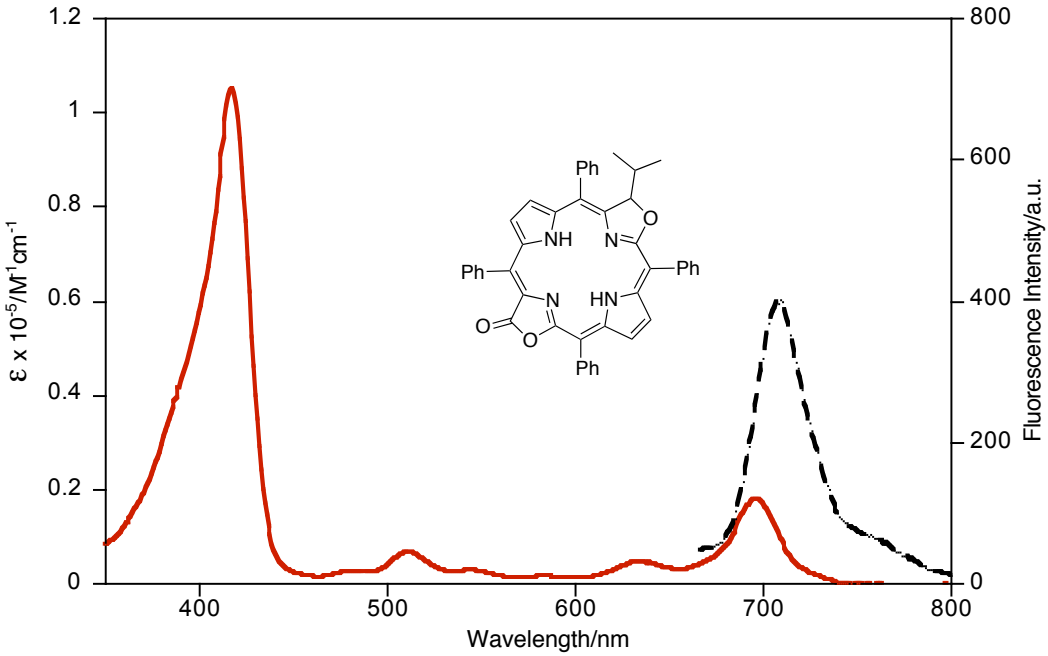

Figure 29. UV-vis (solid red trace) and fluorescence (broken black trace) spectra of **19-*cis*** (CH_2Cl_2)

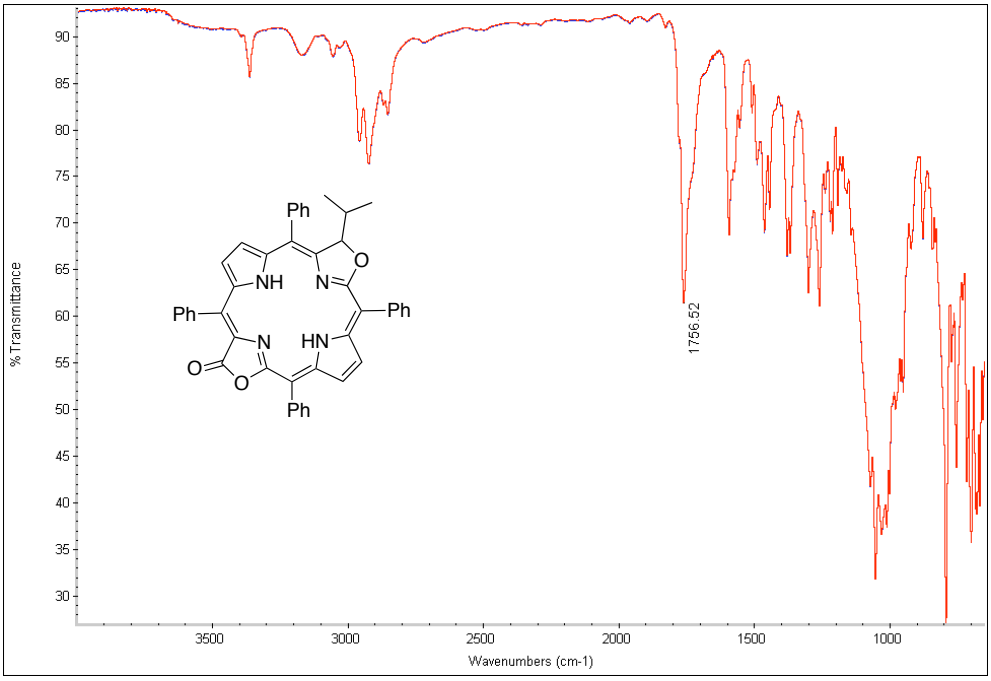

Figure 30. FT-IR spectrum (neat, diffuse reflectance) of **19-*cis***

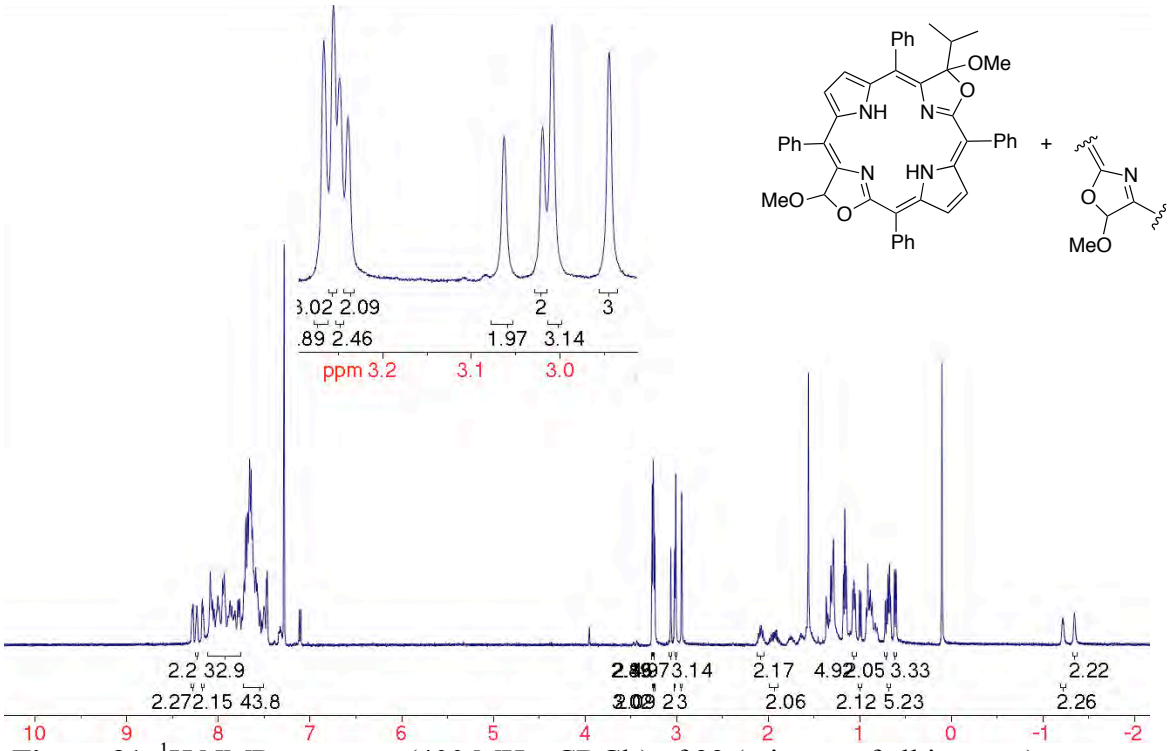

Figure 31. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **22** (mixture of all isomers)

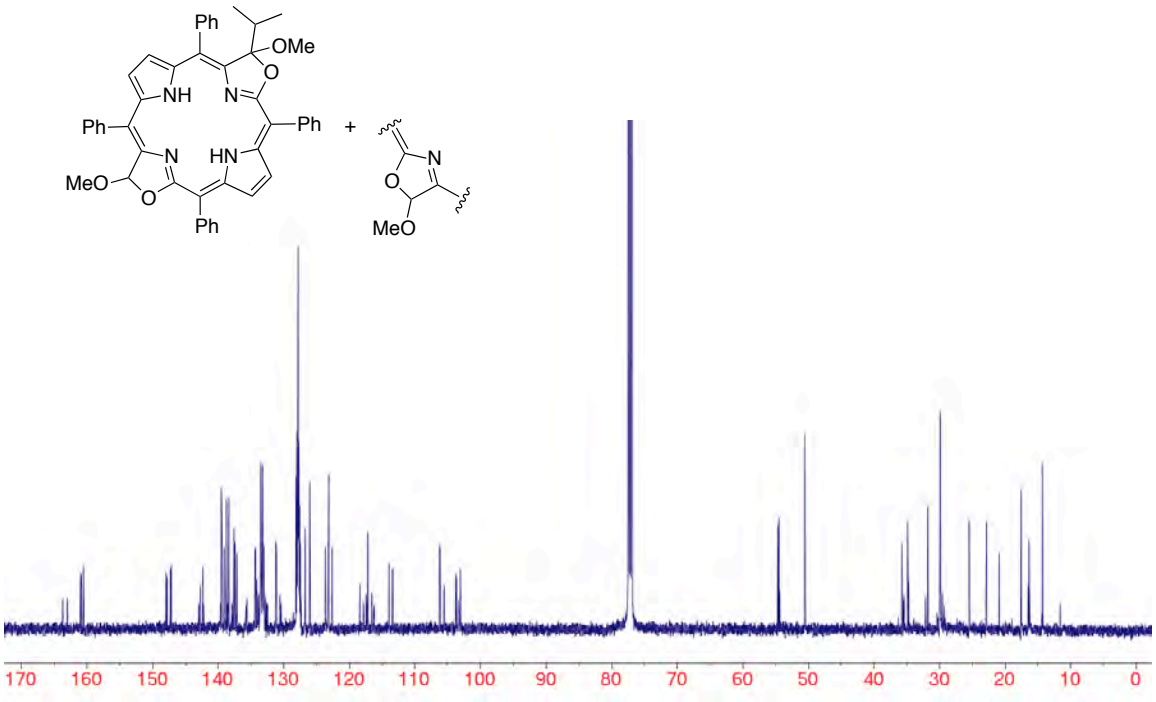

Figure 32. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **23** (mixture of all isomers)

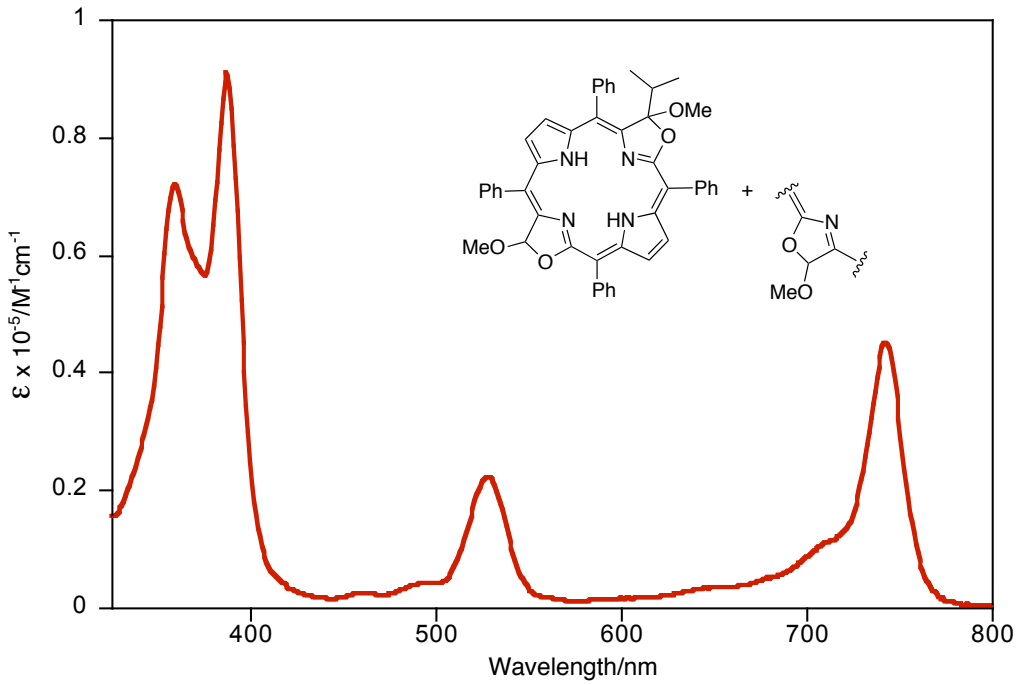

Figure 33. UV-vis spectrum of **23** (CH_2Cl_2, mixture of all isomers)

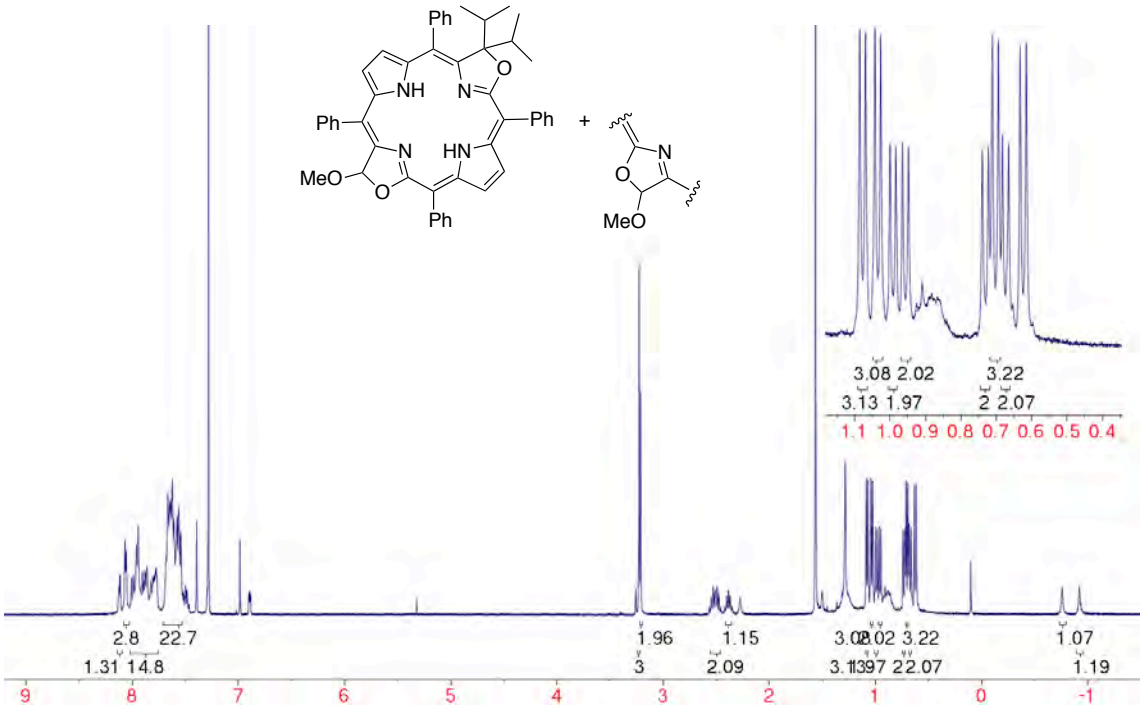

Figure 34. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **22-*cis* /*trans*** (mixture, 3:2 favoring **22-*cis)***

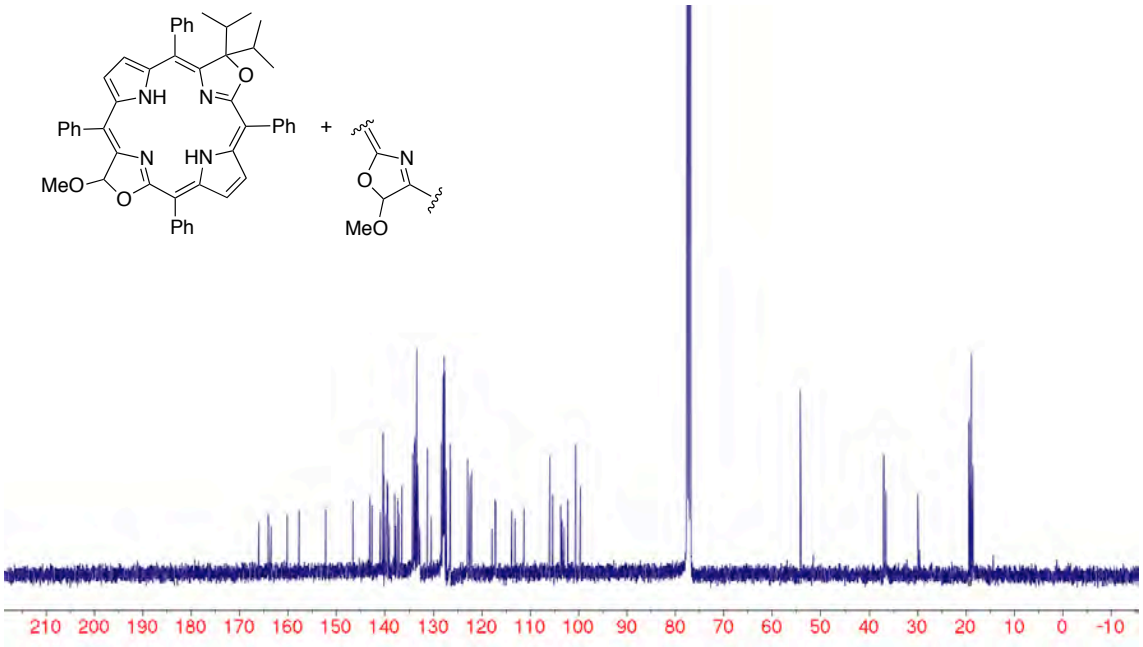

Figure 35. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **22-*cis* /*trans*** (mixture, 3:2 favoring **22-*cis***)

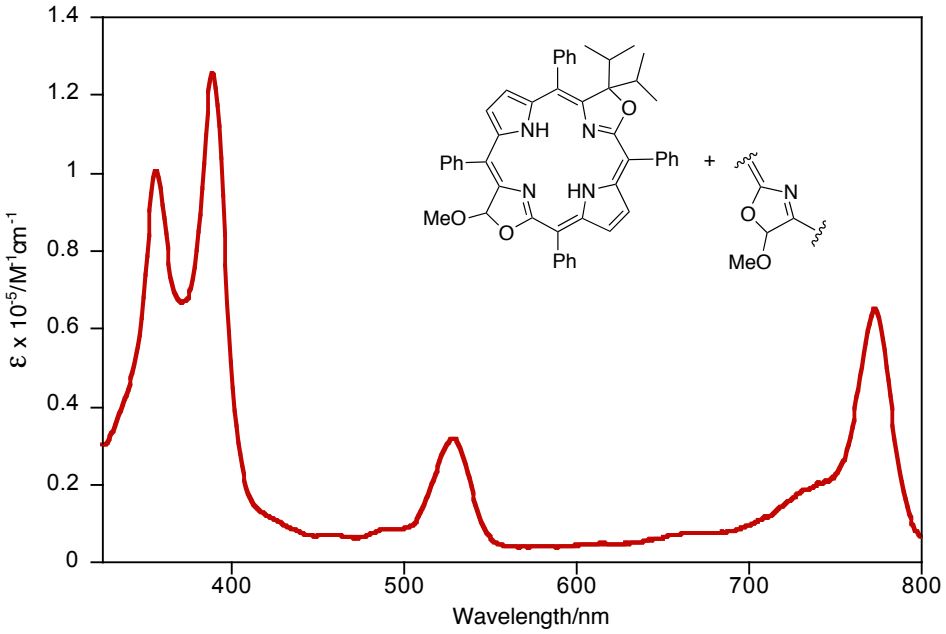

Figure 36. UV-vis spectrum of **22-*cis* /*trans*** (CH_2Cl_2, mixture, 3:2 favoring **22-*cis***)

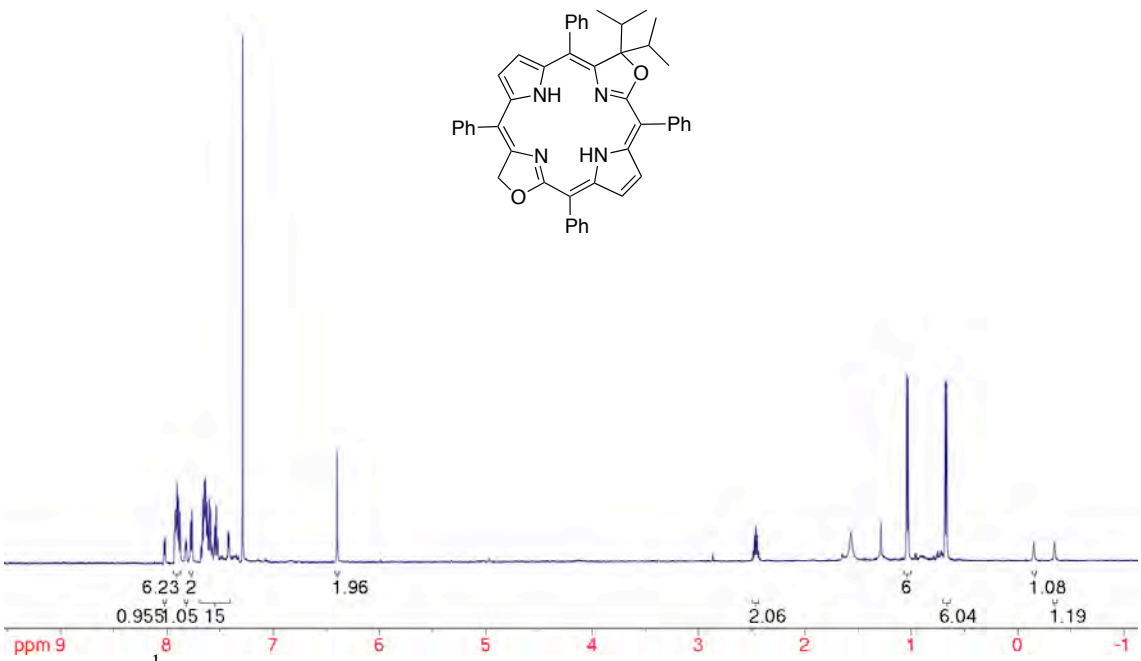

Figure 37. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of **24**

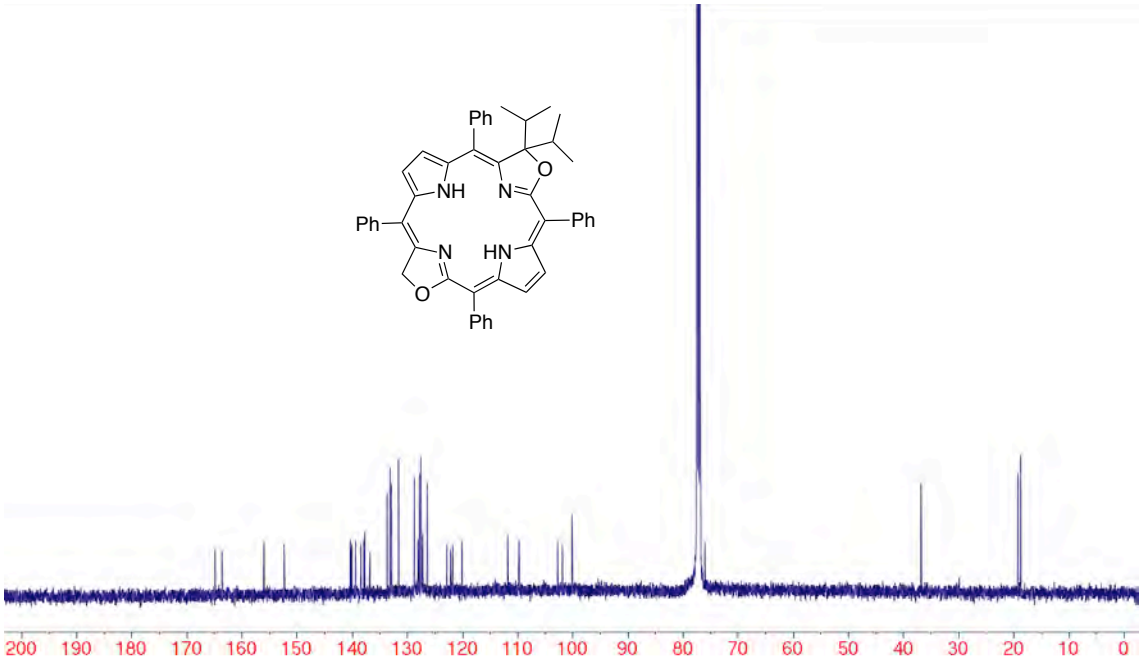

Figure 38. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **24**

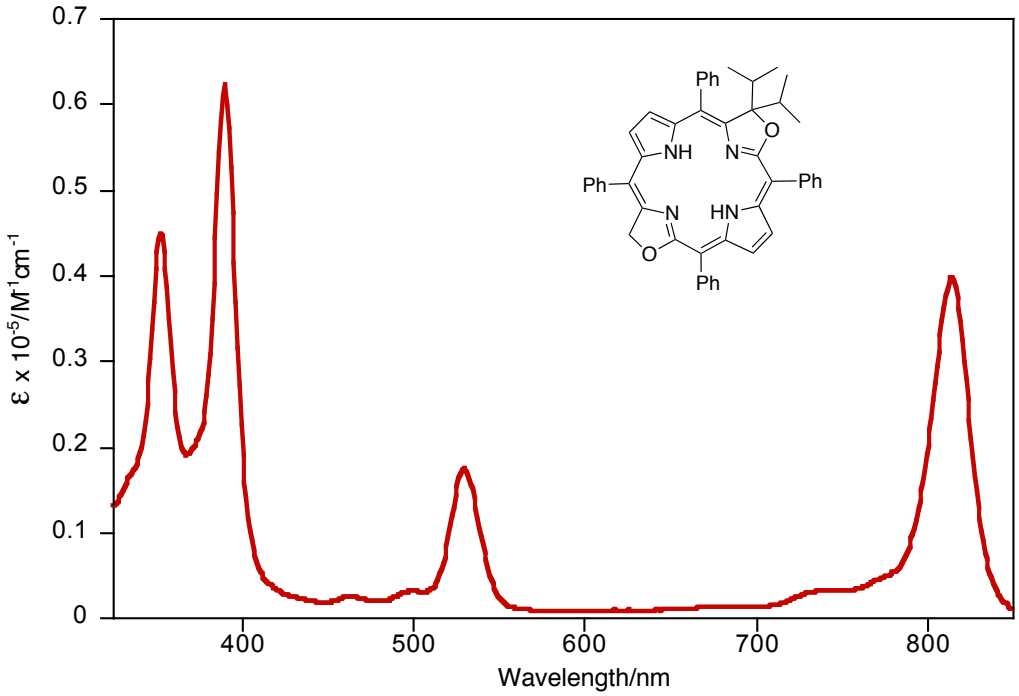

Figure 39. UV-vis spectrum of **24** (CH_2Cl_2)

Crystal Structure Report for 14-cis

A red block-like specimen of **14-cis**, approximate dimensions 0.13 mm × 0.14 mm × 0.19 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured. The integration of the data using a monoclinic unit cell yielded a total of 20276 reflections to a maximum θ angle of 62.99° (0.87 Å resolution), of which 5807 were independent (average redundancy 3.492, completeness = 96.5%, R_{int} = 4.80%, R_{sig} = 5.07%) and 4865 (83.78%) were greater than $2\sigma(F^2)$. The final cell constants of a = 11.4410(5) Å, b = 21.8550(10) Å, c = 18.5306(8) Å, β = 126.626(3)°, volume = 3718.6(3) $Å^3$, are based upon the refinement of the XYZ-centroids of reflections above 20 σ(I). The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.8892 and 0.9220.

The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group P2(1)/c, with Z = 4 for the formula unit, $C_{48}H_{40}N_4O_3$. The final anisotropic full-matrix least-squares refinement on F^2 with 573 variables converged at R1 = 8.74%, for the observed data and wR2 = 23.24% for all data. The goodness-of-fit was 1.082. The largest peak in the final difference electron density synthesis was 0.328 $e^-/Å^3$ and the largest hole was -0.226 $e^-/Å^3$ with an RMS deviation of 0.053 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.288 g/cm^3 and F(000), 1520 e^-.

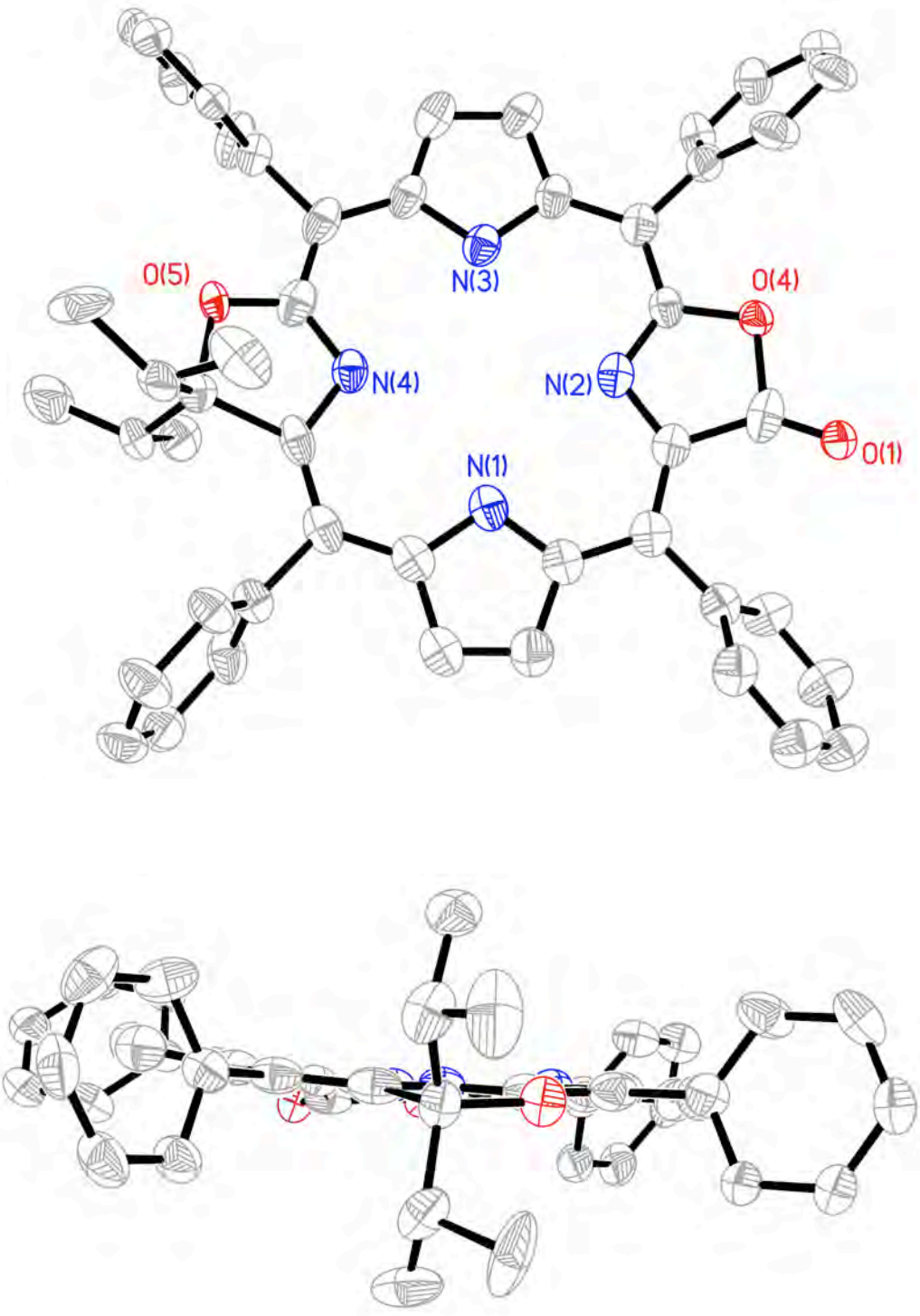

Figure 40. ORTEP Representation of the crystal structure of **14-*cis***, side and top views. Hydrogen atoms and disorder removed for clarity.

Table S1. Crystal data and structure refinement for **14-cis**.

Identification code	**14-cis**	
Empirical formula	$C_{48}H_{40}N_4O_3$	
Formula weight	720.84	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 11.4410(5) Å	α= 90°
	b = 21.8550(10) Å	β = 126.626(3)°
	c = 18.5306(8) Å	γ = 90°
Volume	3718.6(3) $Å^3$	
Z	4	
Density (calculated)	1.288 Mg/m^3	
Absorption coefficient	0.640 mm^{-1}	
F(000)	1520	
Crystal size	0.19 × 0.14 × 0.13 mm^3	
Theta range for data collection	3.59 to 62.99°.	
Index ranges	-13<=h<=11, -25<=k<=22, -21<=l<=20	
Reflections collected	20276	
Independent reflections	5807 [R(int) = 0.0480]	
Completeness to theta = 62.99°	96.5 %	
Absorption correction	SADABS	
Max. and min. transmission	0.9220 and 0.8892	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5807 / 0 / 573	
Goodness-of-fit on F^2	1.082	
Final R indices [I>2sigma(I)]	R1 = 0.0874, wR2 = 0.2245	
R indices (all data)	R1 = 0.0987, wR2 = 0.2324	
Largest diff. peak and hole	0.328 and -0.226 e.$Å^{-3}$	

Crystal Structure Report for 16-cis

A red plate-like specimen of **16-cis**, approximate dimensions 0.08 mm × 0.22 mm × 0.28 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured.

The integration of the data using a monoclinic unit cell yielded a total of 21363 reflections to a maximum θ angle of 64.61° (0.85 Å resolution), of which 6046 were independent (average redundancy 3.533, completeness = 96.4%, R_{int} = 3.03%, R_{sig} = 2.87%) and 5127 (84.80%) were greater than $2\sigma(F^2)$. The final cell constants of a = 23.6921(5) Å, b = 13.7480(3) Å, c = 25.7494(8) Å, β = 117.2340(10)°, volume = 7457.3(3) $Å^3$, are based upon the refinement of the XYZ-centroids of reflections above 20 σ(I). Data were corrected for absorption effects using the multi-scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.871. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.8320 and 0.9473.

The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group C 1 2/c 1, with Z = 4 for the formula unit, $C_{97}H_{77}N_9O_8$. The final anisotropic full-matrix least-squares refinement on F^2 with 518 variables converged at R1 = 5.16%, for the observed data and wR2 = 15.51% for all data. The goodness-of-fit was 0.967. The largest peak in the final difference electron density synthesis was 0.797 $e^-/Å^3$ and the largest hole was -0.386 $e^-/Å^3$ with an RMS deviation of 0.056 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.333 g/cm^3 and F(000), 3144 e^-.

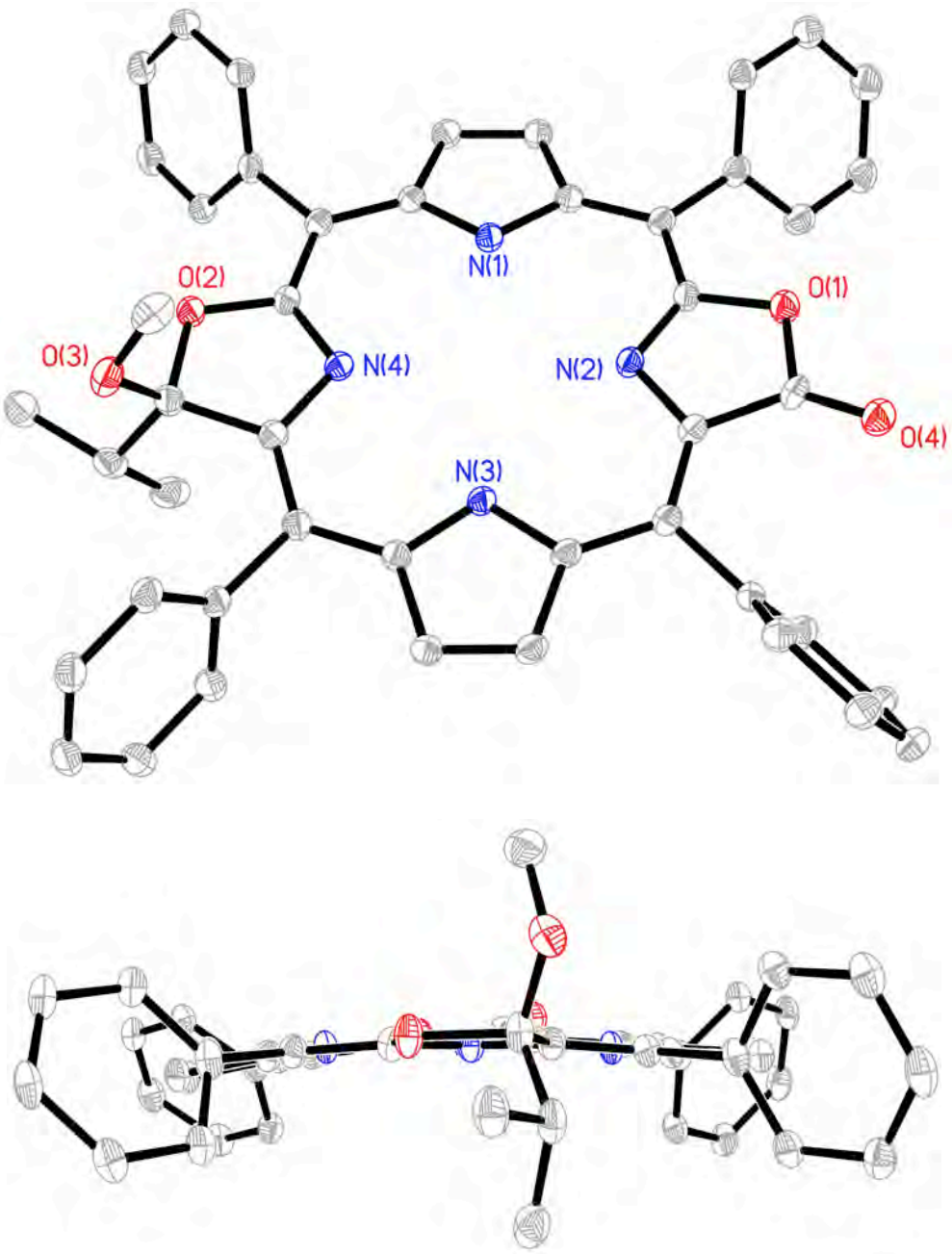

Figure 41. ORTEP Representation of the crystal structure of **16-*cis***, side and top views. Hydrogen atoms and disorder removed for clarity.

Table S2. Crystal data and structure refinement for **16-cis**.

Identification code	**16-cis**	
Empirical formula	$C_{97}H_{77}N_9O_8$	
Formula weight	1496.68	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 23.6921(5) Å	α = 90°
	b = 13.7480(3) Å	β = 117.2340(10)°
	c = 25.7494(8) Å	γ = 90°
Volume	7457.3(3) $Å^3$	
Z	4	
Density (calculated)	1.333 Mg/m^3	
Absorption coefficient	0.684 mm^{-1}	
F(000)	3144	
Crystal size	0.28 × 0.22 × 0.08 mm^3	
Theta range for data collection	3.84 to 64.61°.	
Index ranges	-27<=h<=26, -16<=k<=16, -30<=l<=29	
Reflections collected	21363	
Independent reflections	6046 [R(int) = 0.0303]	
Completeness to theta = 64.61°	96.4 %	
Absorption correction	SADABS	
Max. and min. transmission	0.9473 and 0.8320	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6046 / 0 / 518	
Goodness-of-fit on F^2	0.967	
Final R indices [I>2sigma(I)]	R1 = 0.0516, wR2 = 0.1466	
R indices (all data)	R1 = 0.0607, wR2 = 0.1551	
Largest diff. peak and hole	0.797 and -0.386 $e.Å^{-3}$	

Crystal Structure Report for 16Zn-cis

A green specimen of **16Zn-cis**, approximate dimensions 0.27 mm × 0.47 mm × 0.55 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured.

The integration of the data using a triclinic unit cell yielded a total of 23334 reflections to a maximum θ angle of 61.00° (0.88 Å resolution), of which 6348 were independent (average redundancy 3.676, completeness = 94.7%, R_{int} = 2.72%, R_{sig} = 2.19%) and 6109 (96.24%) were greater than $2\sigma(F^2)$. The final cell constants of a = 12.5921(4) Å, b = 12.9701(4) Å, c = 14.8500(5) Å, α = 111.9920(10)°, β = 96.5610(10)°, γ = 97.7270(10)°, volume = 2192.37(12) $Å^3$, are based upon the refinement of the XYZ-centroids of reflections above 20 σ(I). The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.5661 and 0.7434.

The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group P -1, with Z = 2 for the formula unit, $C_{47}H_{38}N_4O_5Zn$. The final anisotropic full-matrix least-squares refinement on F2 with 522 variables converged at R1 = 6.29%, for the observed data and wR2 = 17.48% for all data. The goodness-of-fit was 0.968. The largest peak in the final difference electron density synthesis was 1.736 $e^-/Å^3$ and the largest hole was -0.441 $e^-/Å^3$ with an RMS deviation of 0.080 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.218 g/cm^3 and F(000), 836 e^-.

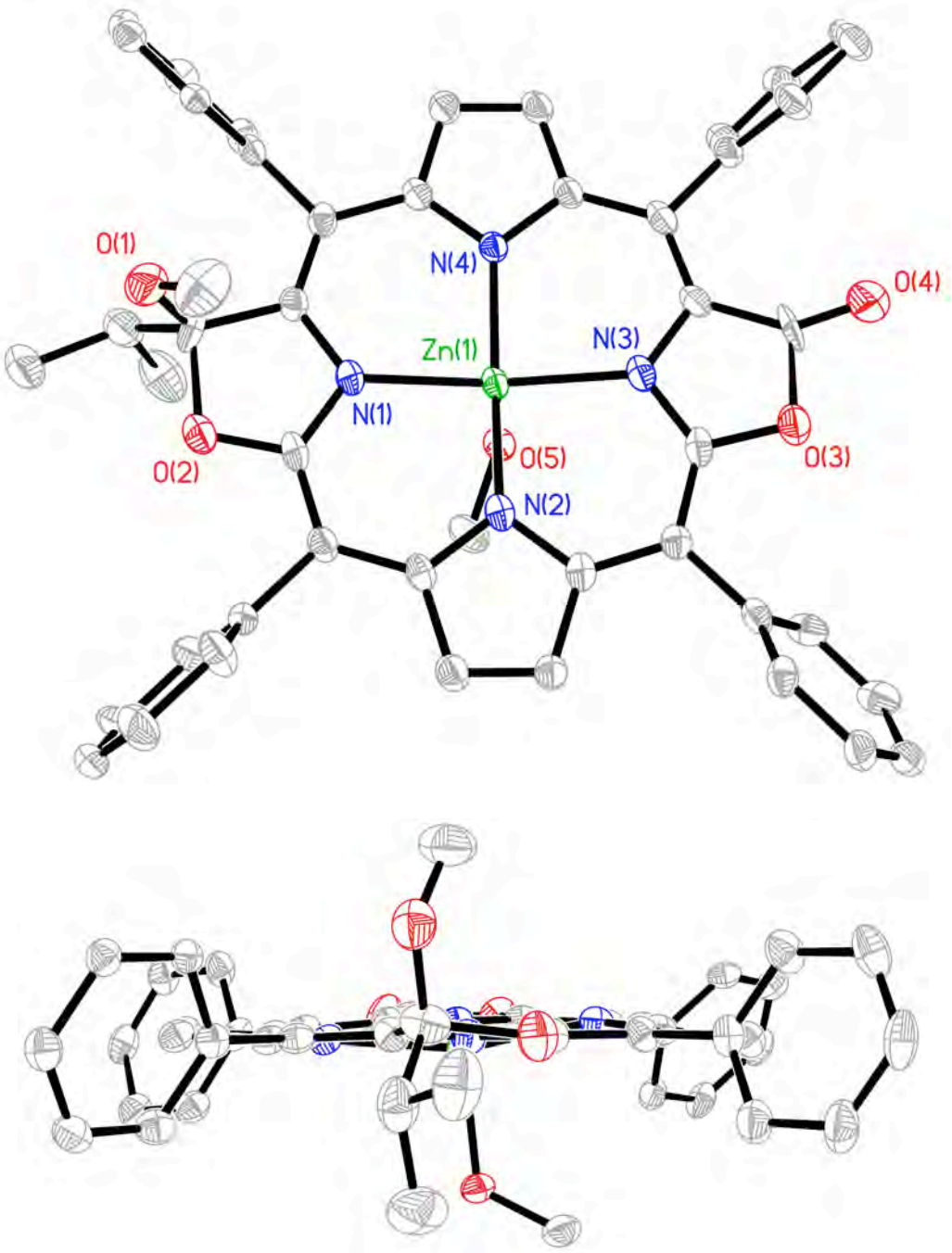

Figure 42. ORTEP Representation of the crystal structure of **16Zn-*cis***, side and top views. Hydrogen atoms and disorder removed for clarity.

Table S3. Crystal data and structure refinement for **16Zn-*cis***.

Identification code	**16Zn-*cis***	
Empirical formula	$C_{47}H_{38}N_4O_5Zn$	
Formula weight	804.18	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	P1	
Unit cell dimensions	a = 12.5921(4) Å	α = 111.9920(10)°
	b = 12.9701(4) Å	β = 96.5610(10)°
	c = 14.8500(5) Å	γ = 97.7270(10)°
Volume	2192.36(12) $Å^3$	
Z	2	
Density (calculated)	1.218 Mg/m^3	
Absorption coefficient	1.163 mm^{-1}	
F(000)	836	
Crystal size	0.55 × 0.47 × 0.27 mm	
Theta range for data collection	3.26 to 61.00°.	
Index ranges	-14<=h<=14, -14<=k<=11, -16<=l<=16	
Reflections collected	23334	
Independent reflections	6348 [R(int) = 0.0272]	
Completeness to theta = 61.00°	94.7 %	
Absorption correction	SADABS	
Max. and min. transmission	0.7434 and 0.5661	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6348 / 0 / 522	
Goodness-of-fit on F^2	0.968	
Final R indices [I>2sigma(I)]	R1 = 0.0629, wR2 = 0.1734	
R indices (all data)	R1 = 0.0645, wR2 = 0.1748	
Largest diff. peak and hole	1.736 and -0.441 $e.Å^{-3}$	

Crystal Structure Report for 23-*trans-E*

An orange plate-like specimen of **23-*trans-E***, approximate dimensions 0.09 mm × 0.10 mm × 0.21 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured.

The total exposure time was 33.52 hours. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using an orthorhombic unit cell yielded a total of 42976 reflections to a maximum θ angle of 63.00° (0.87 Å resolution), of which 6168 were independent (average redundancy 6.968, completeness = 100.0%, R_{int} = 7.20%, R_{sig} = 4.31%) and 5590 (90.63%) were greater than $2\sigma(F^2)$. The final cell constants of a = 9.4468(2) Å, b = 13.2846(3) Å, c = 30.4999(7) Å, volume = 3827.64(15) $Å^3$, are based upon the refinement of the XYZ-centroids of 9852 reflections above 20 σ(I) with 5.795° < 2θ < 123.8°. Data were corrected for absorption effects using the multi-scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.854. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.8772 and 0.9438.

The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group P2(1)2(1)2(1), with Z = 4 for the formula unit, $C_{47}H_{40}N_4O_4$. The final anisotropic full-matrix least-squares refinement on F2 with 519 variables converged at R1 = 8.08%, for the observed data and wR2 = 22.13% for all data. The goodness-of-fit was 0.945. The largest peak in the final difference electron density synthesis was 1.354 $e^-/Å^3$ and the largest hole was -0.389 $e^-/Å^3$ with an RMS deviation of 0.073 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.258 g/cm^3 and F(000), 1528 e^-.

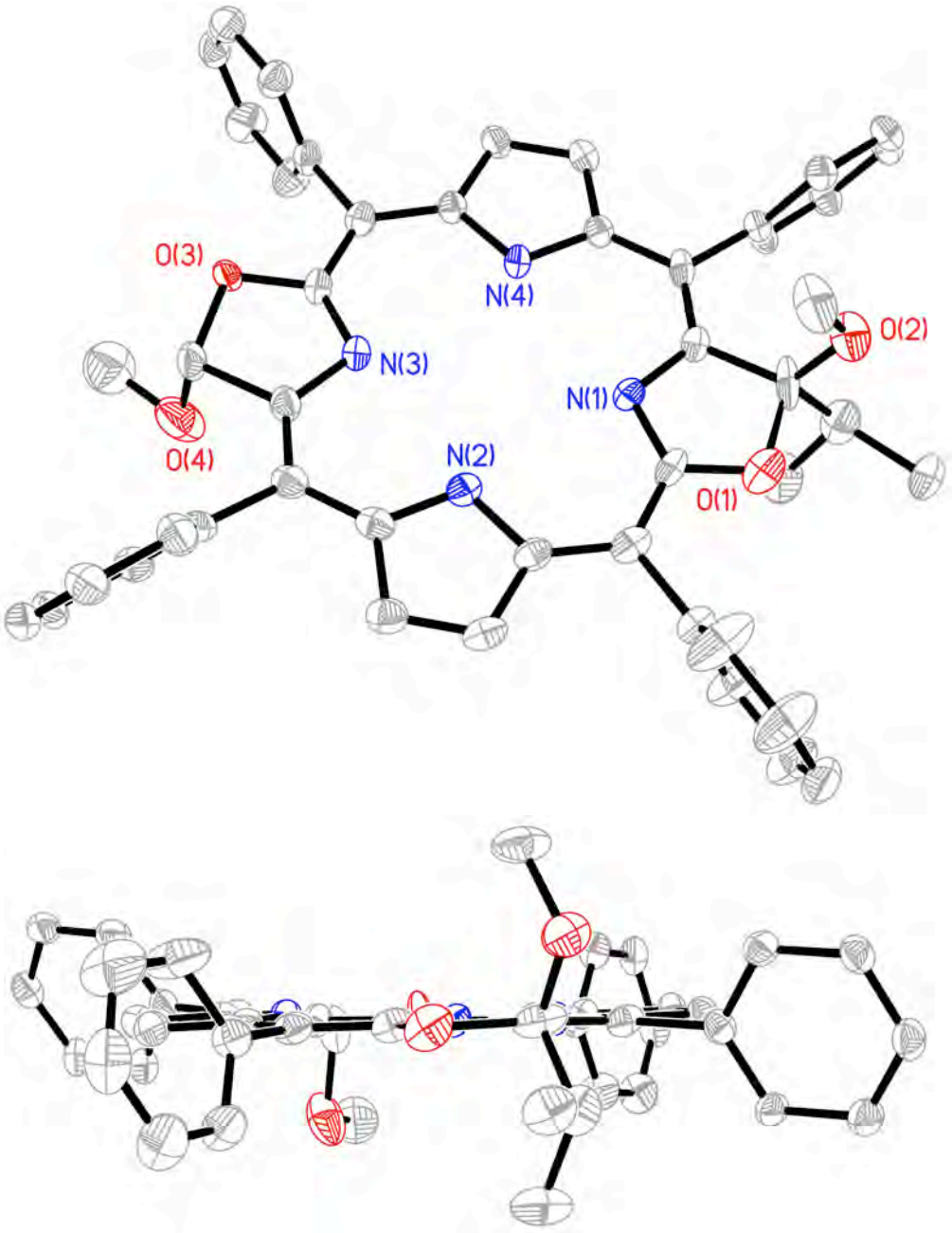

Figure 43. ORTEP Representation of the crystal structure of **23-*trans-E***, side and top views. Hydrogen atoms and disorder removed for clarity.

Table S4. Crystal data and structure refinement for **23-*trans-E***

Identification code	**23-*trans-E***	
Empirical formula	$C_{47}H_{40}N_4O_4$	
Formula weight	724.83	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 9.4468(2) Å	α = 90°
	b = 13.2846(3) Å	β = 90°
	c = 30.4999(7) Å	γ = 90°
Volume	3827.64(15) $Å^3$	
Z	4	
Density (calculated)	1.258 Mg/m^3	
Absorption coefficient	0.644 mm^{-1}	
F(000)	1528	
Crystal size	0.21 × 0.10 × 0.09 mm^3	
Theta range for data collection	2.90 to 63.00°.	
Index ranges	-9<=h<=10, -15<=k<=15, -35<=l<=35	
Reflections collected	42976	
Independent reflections	6168 [R(int) = 0.0720]	
Completeness to theta = 63.00°	100.0 %	
Absorption correction	SADABS	
Max. and min. transmission	0.9437 and 0.8772	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6168 / 24 / 519	
Goodness-of-fit on F^2	0.945	
Final R indices [I>2sigma(I)]	R1 = 0.0808, wR2 = 0.2144	
R indices (all data)	R1 = 0.0876, wR2 = 0.2213	
Absolute structure parameter	0.9(6)	
Largest diff. peak and hole	1.354 and -0.389 e.$Å^{-3}$	

Crystal Structure Report for 23-*trans-Z*

A orange specimen of **23-*trans-Z***, approximate dimensions 0.18 mm × 0.24 mm × 0.28 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured.

The total exposure time was 38.48 hours. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using a monoclinic unit cell yielded a total of 37579 reflections to a maximum θ angle of 61.98° (0.87 Å resolution), of which 5901 were independent (average redundancy 6.368, completeness = 99.8%, Rint = 4.98%, Rsig = 3.56%) and 4716 (79.92%) were greater than $2\sigma(F^2)$. The final cell constants of a = 20.5804(4) Å, b = 9.5370(2) Å, c = 19.1964(4) Å, β = 91.8000(10)°, volume = 3765.92(13) $Å^3$, are based upon the refinement of the XYZ-centroids of 164 reflections above 20 σ(I) with 17.70° < 2θ < 97.69°. Data were corrected for absorption effects using the multi-scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.824. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.8401 and 0.8891.

The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group P 2(1)/c, with Z = 4 for the formula unit, $C_{47}H_{40}N_4O_4$. The final anisotropic full-matrix least-squares refinement on F^2 with 519 variables converged at R1 = 8.14%, for the observed data and wR2 = 25.49% for all data. The goodness-of-fit was 0.894. The largest peak in the final difference electron density synthesis was 1.444 $e^-/Å^3$ and the largest hole was -0.439 $e^-/Å^3$ with an RMS deviation of 0.064 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.278 g/cm^3 and F(000), 1528 e^-.

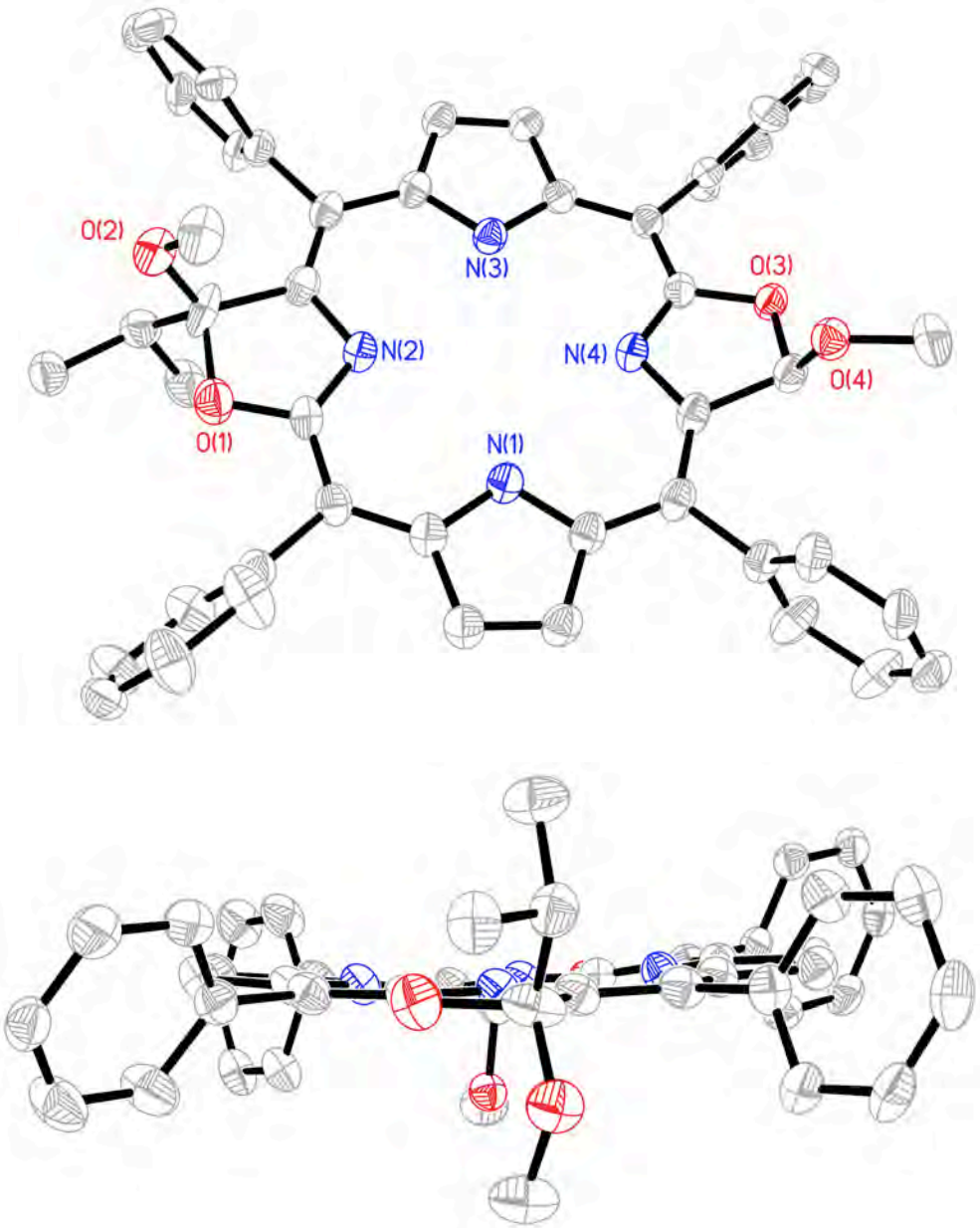

Figure 44. ORTEP Representation of the crystal structure of **23-*trans-Z***, side and top views. Hydrogen atoms and disorder removed for clarity.

Table S5. Crystal data and structure refinement for **23-*trans-Z***

Identification code	**23-*trans-Z***	
Empirical formula	$C_{47}H_{40}N_4O_4$	
Formula weight	724.83	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 20.5804(4) Å	α= 90°
	b = 9.5370(2) Å	β=91.80(10)°
	c = 19.1964(4) Å	γ = 90°
Volume	3765.92(13) $Å^3$	
Z	4	
Density (calculated)	1.278 Mg/m^3	
Absorption coefficient	0.654 mm^{-1}	
F(000)	1528	
Crystal size	0.28 × 0.24 × 0.18 mm^3	
Theta range for data collection	4.30 to 61.98°.	
Index ranges	-23<=h<=23, -10<=k<=10, -21<=l<=20	
Reflections collected	37579	
Independent reflections	5901 [R(int) = 0.0498]	
Completeness to theta = 61.98°	99.8 %	
Absorption correction	None	
Max. and min. transmission	0.8891 and 0.8401	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5901 / 0 / 519	
Goodness-of-fit on F^2	0.894	
Final R indices [I>2sigma(I)]	R1 = 0.0814, wR2 = 0.2308	
R indices (all data)	R1 = 0.0970, wR2 = 0.2549	
Largest diff. peak and hole	1.444 and -0.439 $e.Å^{-3}$	

Crystal Structure Report for 22-*cis*

A red specimen of **22-*cis*** , approximate dimensions 0.38 mm × 0.42 mm × 0.55 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured.

The integration of the data using a monoclinic unit cell yielded a total of 23323 reflections to a maximum θ angle of 64.45° (0.85 Å resolution), of which 6350 were independent (average redundancy 3.673, completeness = 96.1%, R_{int} = 3.15%, R_{sig} = 2.24%) and 5451 (85.84%) were greater than $2\sigma(F^2)$. The final cell constants of a = 20.3320(5) Å, b = 11.1841(3) Å, c = 18.4019(5) Å, β = 109.5870(10)°, volume = 3942.36(18) $Å^3$, are based upon the refinement of the XYZ-centroids of reflections above 20 σ(I). The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.7297 and 0.8006.

The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group P2(1)/c, with Z = 4 for the formula unit, $C_{49}H_{44}N_4O_3$. The final anisotropic full-matrix least-squares refinement on F2 with 585 variables converged at R1 = 8.25%, for the observed data and wR2 = 26.74% for all data. The goodness-of-fit was 1.037. The largest peak in the final difference electron density synthesis was 1.341 $e^-/Å^3$ and the largest hole was -0.423 $e^-/Å^3$ with an RMS deviation of 0.056 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.242 g/cm^3 and F(000), 1560 e^-.

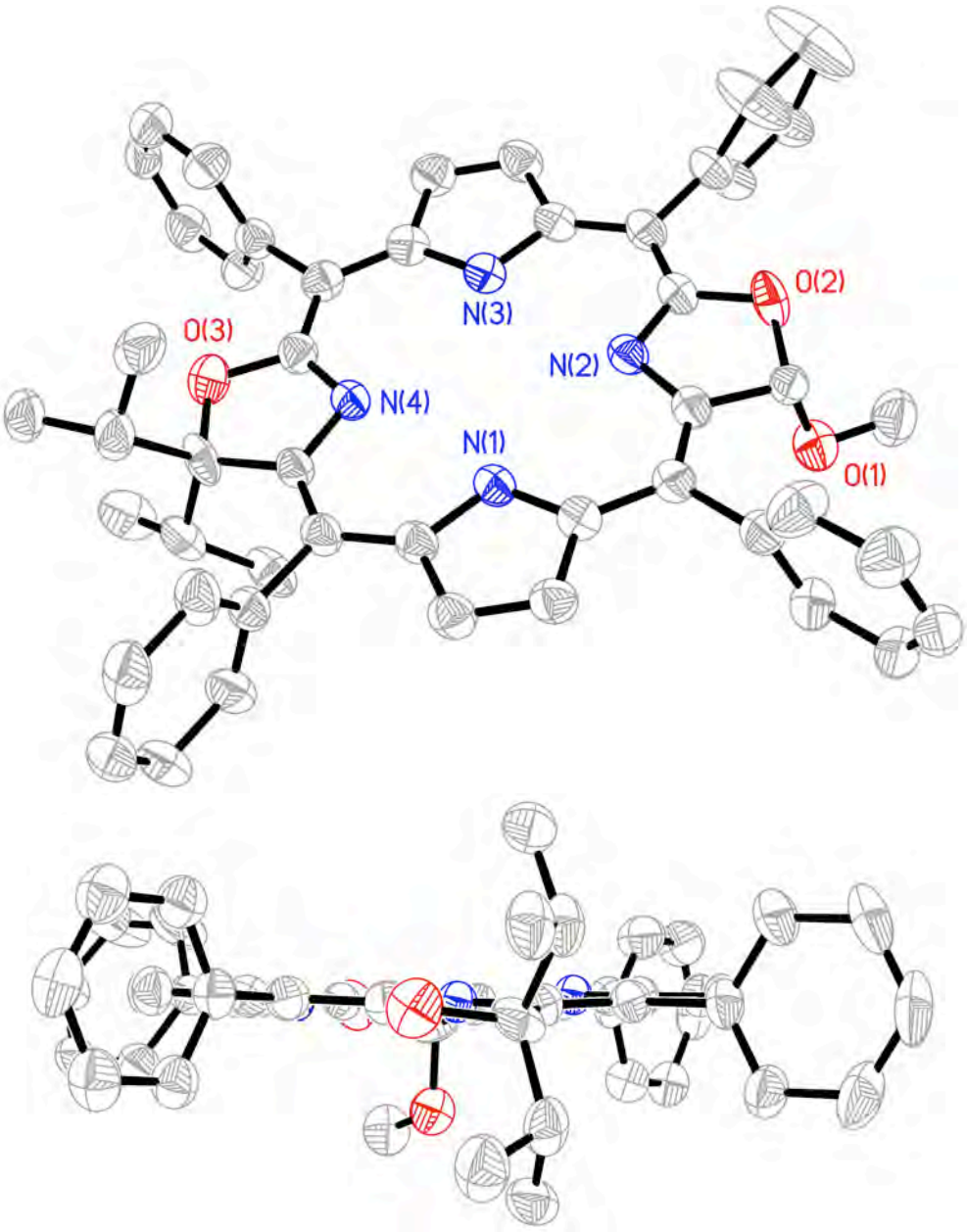

Figure 45. ORTEP Representation of the crystal structure of **22-*cis*** , side and top views. Hydrogen atoms and disorder removed for clarity.

Table S6. Crystal data and structure refinement for **22-cis**.

Identification code	**22-cis**	
Empirical formula	$C_{49}H_{44}N_4O_3$	
Formula weight	736.88	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 20.3320(5) Å	α = 90°
	b = 11.1841(3) Å	β= 109.5870(10)°
	c = 18.4019(5) Å	γ = 90°
Volume	3942.36(18) $Å^3$	
Z	4	
Density (calculated)	1.242 Mg/m^3	
Absorption coefficient	0.613 mm^{-1}	
F(000)	1560	
Crystal size	0.55 × 0.42 × 0.38 mm^3	
Theta range for data collection	2.31 to 64.45°.	
Index ranges	-23<=h<=22, -12<=k<=11, -20<=l<=19	
Reflections collected	23323	
Independent reflections	6350 [R(int) = 0.0315]	
Completeness to theta = 64.45°	96.1 %	
Absorption correction	SADABS	
Max. and min. transmission	0.8006 and 0.7297	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6350 / 6 / 585	
Goodness-of-fit on F^2	1.037	
Final R indices [I>2sigma(I)]	R1 = 0.0825, wR2 = 0.2563	
R indices (all data)	R1 = 0.0904, wR2 = 0.2674	
Largest diff. peak and hole	1.341 and -0.423 e.$Å^{-3}$	