Oligoamylose-Entwined Porphyrin: Excited-State Induced-Fit for Chirality Induction

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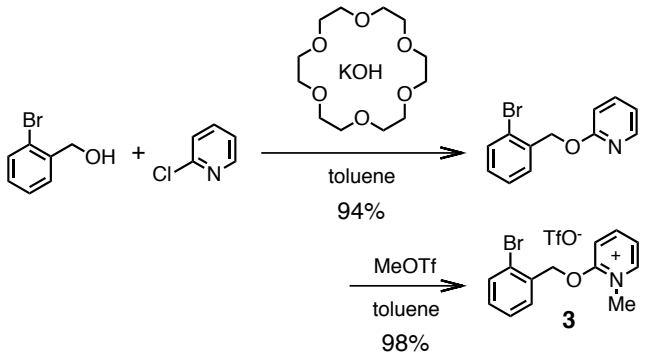
Experimental Section

1. General Procedures

NMR spectra were recorded on AV-300 (Brüker). MALDI-TOF MS spectra were observed by using α-cyanocynnamic acid as the matrix by Autoflex Speed (Brüker). Recycling gel-permeation chromatography (GPC) was carried out by LC-9101 (Japan Analytical Industry Co., Ltd.) connecting column of JAIGEL-3H and -2H with chloroform as the eluent. UV-visible spectra were recorded on the spectrophotometer (Multispec-1500, Shimadzu). CD and CPL spectra were recorded on a spectropolarimeter (JASCO J-720) and spectrofluoropolarimeter (JASCO CPL-200S), respectively. Time-resolved fluorescence measurements were carried out by employing a circularly polarized beam of 200-fs laser pulse at 450 nm, second harmonic generation (Spectra Physics, Model 3980) of a continuous wave (CW) from 200-fs Ti:sapphire laser (Spectra Physics, Mai Tai), and a streak camera (Hamamatsu Photonics, Streak Scope C4334) to detect the fluorescence, wherein the time-resolution was approximately 30 ps.

2. Synthesis

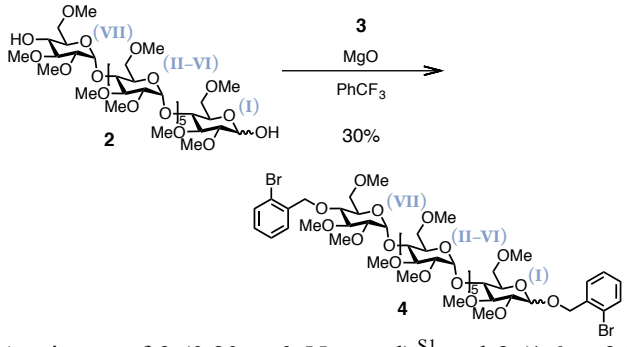
2.1. Synthesis of methyl 2-(2-bromophenylmethyloxy)pyridinium trifluoromethanesulfonate (3): A mixture of 2-bromophenylmethanol (2.0 g, 11 mmol), 2-chloropyridine (2.0 mL, 18 mL), potassium hydroxide (2.3 g, 35 mmol) and 18-crown-6 (62 mg, 0.24 mmol) dissolved in toluene (17 mL) was refluxed with azeotropic removal of generated water under nitrogen atmosphere for 28 h in a round-bottom flask equipped with Dean-Stark trap. The reaction mixture was washed with water (80 mL) and the organic layer was separated, and then the crude product was further extracted with ethyl acetate (60 mL). The combined organic layer was dried over anhydrous sodium sulfate, before removal of the solvent under reduced pressure. The crude product was subjected to chromatographic separation with *n*-hexane/ethyl acetate (5/0, v/v) as the eluent. 2-(2-Bromophenylmethoxy)pyridine was obtained as a pale yellow liquid (2.7 g, 10 mmol) in 94% yield. ^{1}H NMR (300 MHz, in $CDCl_3$): δ 8.18 (ddd, J = 5.1, 1.8, 0.6 Hz, 1H; Py), 7.61–7.52 (m, 3H; Ar), 7.30 (ddd, J = 7.5, 7.5, 1.2 Hz, 1H; Py), 7.15 (ddd, J = 7.8, 7.8, 1.5 Hz, 1H; Ar), 6.91–6.82 (m, 2H; Py), 5.46 (s, 2H; methylene). ^{13}C NMR (75 MHz, in $CDCl_3$): δ 163.4, 147.0, 138.7, 136.8, 132.7, 129.4, 129.2, 127.4, 123.0, 117.1, 111.2, 67.0.



To a solution of 2-(2-bromophenylmethoxy)pyridine (1.0 g, 3.9 mmol) in toluene (3.5 mL) was added dropwise methyltriflate (0.7 mL, 6.4 mmol) with stirring at 0 °C, followed by stirring at room temperature for 1.5 h. The solvent was removed from the resultant biphasic solution under reduced pressure. The colorless liquid obtained was added to excess *n*-hexane, and colorless precipitate was obtained. The titled compound **3** (1.6 g, 3.8 mmol) was obtained in 98% yield. ^{1}H NMR (300 MHz, in $CDCl_3$): δ 8.56 (dd, J = 6.3, 1.5 Hz, 1H; Py), 8.40 (ddd, J = 9.6, 8.1, 8.0, 1.5 Hz, 1H; Py), 7.70 (d, J = 8.7 Hz, 1H; Py), 7.64 (dd, J = 7.8, 1.2 Hz, Ar), 7.63 (dd, 7.5 1.8 Hz, 2H; Ar), 7.47 (ddd, J = 9.6, 6.3, 1.2 Hz, 1H; Py), 7.40 (ddd, J = 7.8, 7.5, 1.2 Hz, 1H; Ar), 7.31 (ddd, J = 7.8, 7.5, 1.8 Hz, 1H; Ar), 5.63 (s, 2H; methylene), 4.09 (s, 3H; Me). ^{13}C NMR (75 MHz, in $CDCl_3$): δ

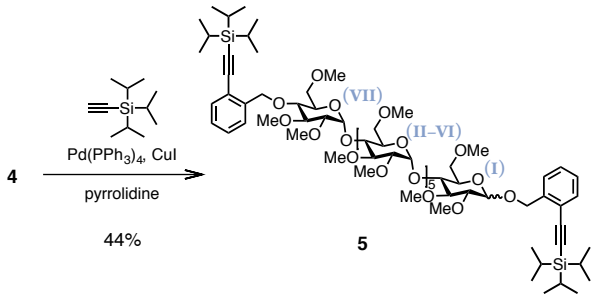
159.3, 148.3, 144.2, 133.3, 131.8, 131.7, 131.6, 128.3, 124.2, 119.4, 111.9, 74.0, 42.2.

2.2. Synthesis of $1^{(I)},4^{(VII)}$-*O*-bis(2-bromophenylmethyl)-2,3,6-*O*-trimethylmaltoheptaose (4):

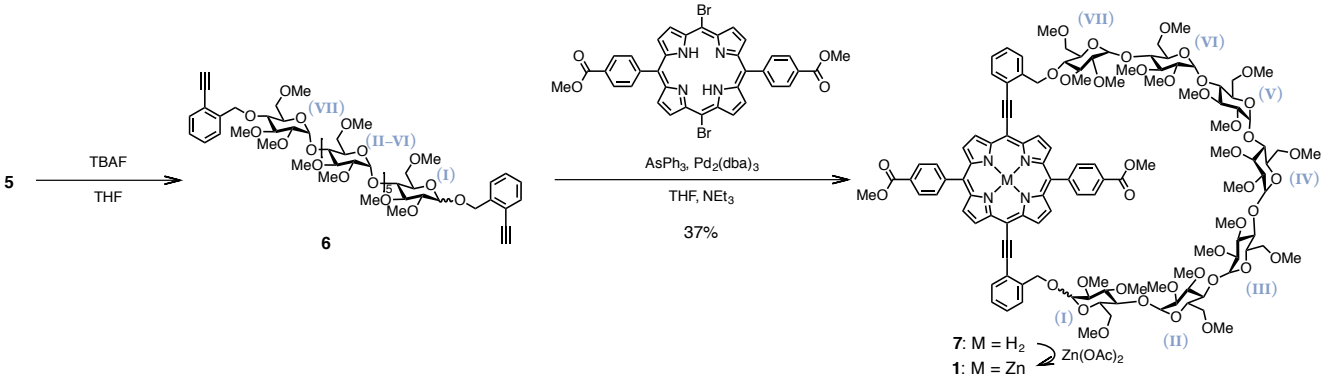


A mixture of **2** (0.80 g, 0.55 mmol)[S1] and **3** (1.6 g. 3.7 mmol) was refluxed with MgO (0.15 g, 3.8 mmol) in α,α,α-trifluoromethylbenzene (5.0 mL) under argon atmosphere for 2 days. The reaction mixture was diluted with 15 mL of toluene, and washed with saturated aqueous sodium hydrogencarbonate and brine. The organic layer separated was dried over anhydrous magnesium sulfate. The residue was subjected to column chromatography over silica gel with dichloromethane/methanol (15/1, v/v) as the eluent, followed by purification by preparative GPC. The titled compound **4** was obtained as a colorless viscous substance (0.31 g, 0.17 mmol) in 30% yield. The product included the diastereomers of α/β-anomeric connection of $1^{(I)}$-glucose to methylphenyl group, which were not separable by silica gel column and preparative GPC. ^{1}H NMR (300 MHz, in $CDCl_3$): δ 7.62–7.15 (m, 8H; Ar), 5.68 (d, J = 3.6 Hz, 1H; Glc$^{(VII)}$-1β), 5.63–5.53 (m, 5H; Glc$^{(II)–(VI)}$-1β), 5.11 (d, J = 3.6 Hz, 0.4H; Glc$^{(I)}$-1β), 5.00–4.64 (m, 4H; -OCH_2Ar), 4.41 (d, J = 7.8 Hz, 0.6H; Glc$^{(I)}$-1α), 3.90–3.22 (m, 105H; Glc and methyl protons). ^{13}C NMR (75 MHz, in $CDCl_3$): δ 137.72, 136.90, 136.73, 132.56, 132.37, 129.90, 129.41, 129.12, 129.02, 128.92, 128.25, 127.44, 127.33, 123.03, 122.54, 102.36, 86.93, 96.65, 96.24, 96.17, 86.18, 83.96, 83.30, 83.12, 82.95, 82.76, 82.06, 77.66, 77.23, 76.81, 73.89, 73.81, 73.51, 72.44, 71.46, 70.69, 70.62, 70.46, 70.14, 70.09, 70.03, 60.95, 60.34, 60.24, 60.18, 60.07, 59.79, 59.33, 59.15, 59.12, 59.09, 59.01, 58.98, 58.94, 58.87, 58.81, 58.77, 58.33. MALDI-TOF MS (α-cyanocynnamic acid as a matrix): *m/z* calculated for $C_{77}H_{124}Br_2O_{36}$: 1782.62; found: 1805.90 as $[M + Na]^+$ and 1821.97 as $[M + K]^+$. $[\alpha]^{20}_{D(589)}$ = +138 (c1.03 × 10^{-2} g·mL^{-1} at 20 °C in EtOH).

2.4. Synthesis of $1^{(I)},4^{(VII)}$-*O*-bis[2-{(triisopropyl)silylethynyl}phenylmethyl]-2,3,6-*O*-trimethylmaltoheptaose (5):



A solution of 4 (0.27 g, 0.15 mmol) and triisopropylsilylacetylene (0.33 mL, 1.5 mmol) in pyrrolidine (2.0 mL) was degassed by successive freeze–pump–thaw cycles in a Schlenk flask, before purging with argon gas. Then, $Pd(PPh_3)_4$ (0.15 g, 0.15 mmol) and CuI (0.14 g, 0.74 mmol) were added to the solution under argon stream. The mixture was stirred at 80 °C under inert atmosphere for 3 days. The mixture was washed with water and the crude material was extracted with dichloromethane (20 mL). The crude product was eluted from silica-gel column chromatography (dichloromethane/methanol = 15/1, v/v), and then purified by preparative GPC. The titled compound **5** was obtained as colorless solid (0.13 g, 0.066 mmol) in 44% yield. ^{1}H NMR (300 MHz, in $CDCl_3$): δ 7.52–7.19 (m, 8H, Ar), 5.70 (d, J = 3.6 Hz, 1H; Glc$^{(VII)}$-1β), 5.67–5.54 (m, 5H; Glc$^{(II)–(VI)}$-1β), 5.17 (d, J = 13.8 Hz, 0.4H; Glc$^{(I)}$-1β), 5.09–4.86 (m, 4H; -OCH_2Ar), 4.41 (d, J = 7.8 Hz, 0.6H; Glc$^{(I)}$-1α), 3.97–3.26 ppm (m, 105H; Glc and methyl protons), 1.15, 1.14 (s, s, 36H; *Me* of TIPS), 0.08 (s, 6H; C*H* of TIPS). ^{13}C NMR (75 MHz, in $CDCl_3$): δ 141.06, 140.11,139.82, 132.56, 132.31, 132.13, 128.58, 128.45, 128.32, 126.91, 126.78, 126.64, 126.30, 121.18, 121.04, 104.10, 104.05, 102.81, 96.96, 96.71, 96.17, 95.88, 95.80, 95.67, 86.30, 83.90, 83.33, 83.20, 82.98, 82.81, 82.17, 73.94, 73.42, 73.26, 72.50, 72.19, 71.99, 71.18,



70.74, 70.63, 70.18, 70.06, 69.49, 69.08, 67.27, 60.83, 60.39, 60.30, 60.19, 60.10, 60.02, 59.74, 59.64, 59.34, 59.18, 59.12, 59.04, 18.71, 18.67, 11. 26, 1.01. MALDI-TOF MS (α-cyanocynnamic acid as a matrix): *m/z* calculated for $C_{99}H_{166}O_{36}Si_2$: 1987.07; found: 2010.13 as $[M + Na]^+$ and 2026.14 as $[M + K]^+$. $[\alpha]^{20}_{D(589)} = +136$ ($c1.00 \times 10^{-2}$ g·mL^{-1} at 20 °C in EtOH).

2.5. Synthesis of oligoamylose-strapped metal-free porphyrin (7): A solution of **5** (77 mg, 0.046 mmol) in THF (8 mL) was treated with tetrabutylammonium fluoride (0.4 mM) at 0 °C for 2 h. Deprotection of TIPS-groups was confirmed by MALDI-TOF MS spectrometry. The mixture was diluted with ether (50 mL) and washed with brine (50 mL). The product was extracted with ether (50 mL × 3), and the combined organic layer was dried over anhydrous magnesium sulfate. Desilylated product **6** was used without further purification for

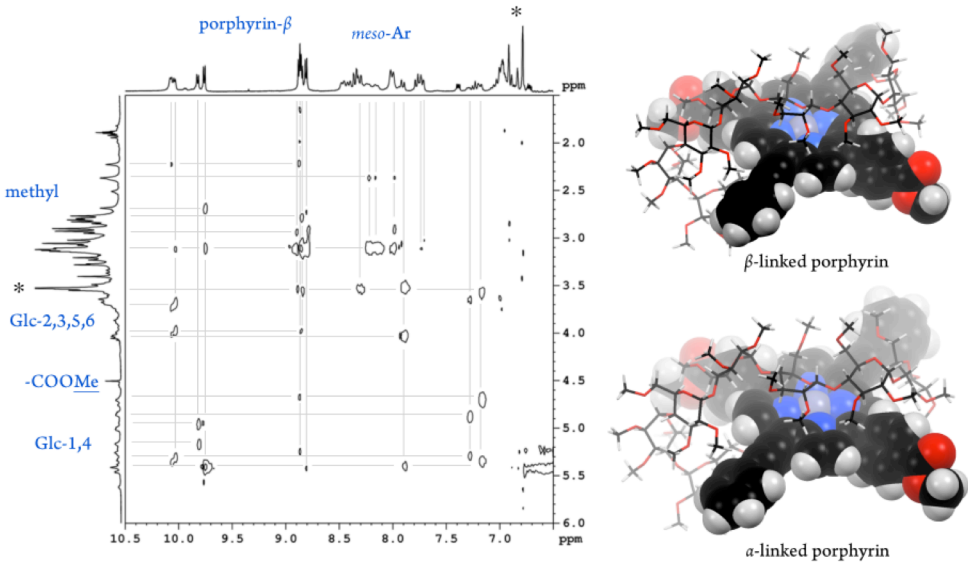


Figure S1. NOE spectrum of **1** in toluene-d_8 and the computer-optimized structures of **1** of β-linked (upper) and α-linked porphyrin (lower).

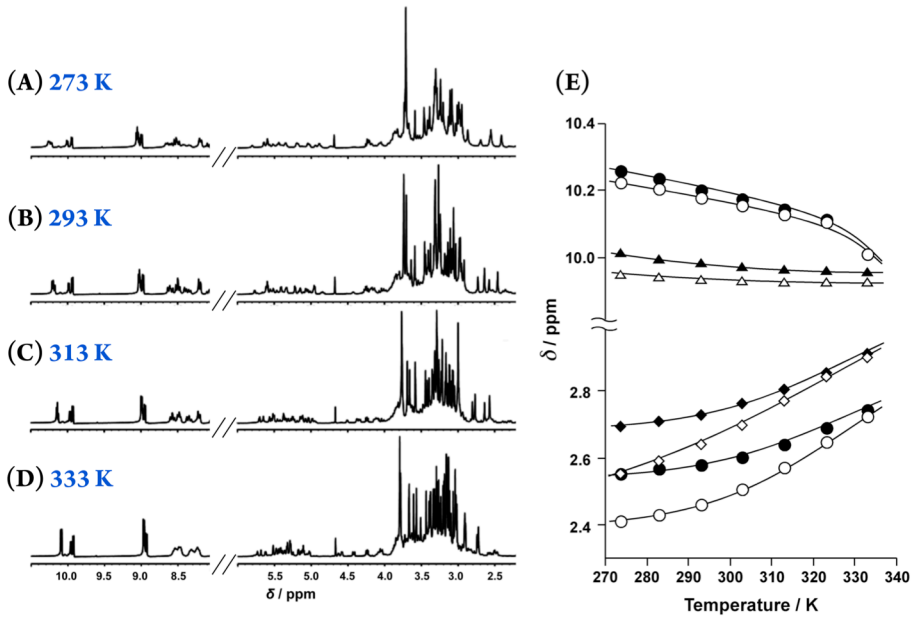


Figure S2. VT-NMR spectra of **1** at 273 K (A), 293 K (B), 313 K (C), and 333 K (D) in toluene-d_8. (E) Plot of the selected signal of **1**.

the next step.

The product **6**, dibromoporphyrin (34 mg, 46 μmol), $Pd_2(dba)_3$ (22 mg, 24 μmol) and Ph_3As (38 mg, 0.12 mmol) were dissolved in THF (40 mL) mixed with Et_3N (10 mL) in a Schlenk tube. The mixture was deoxygenated by freeze–pump–thaw cycles and then purged with argon, and then was stirred at 45 °C for 20 h. The solvent was removed under reduced pressure. The crude product was eluted from silica-gel column chromatography with chloroform/methanol (10/0 to 10/2, v/v) and then ethyl acetate/methanol (10/1, v/v) as the eluent. The oligoamylose-strapped porphyrin **7** was purified by preparative GPC. Free-base form of oligoamylose-strapped porphyrin **7** was green solid (38 mg, 17 μmol) in 37% yield. ^{1}H NMR (300 MHz, in $CDCl_3$): δ 9.77 (d, J = 3.6 Hz, 1H; porphyrin-β), 9.75 (d, J = 4.5 Hz, 1H; porphyrin-β), 9.71 (d, J = 4.8 Hz, 1H; porphyrin-β), 9.68 (d, J = 4.8 Hz, 1H; porphyrin-β), 8.81 (d, J = 3.6 Hz, 1H; porphyrin-β), 8.79 (d, J = 4.5 Hz, 1H; porphyrin-β), 8.75 (d, J = 4.8 Hz, 1H; porphyrin-β), 8.74 (d, J = 4.5 Hz, 1H; porphyrin-β), 8.48 (d, J = 8.4 Hz, 2H; Ar), 8.48 (d, J = 8.4 Hz, 2H; Ar-β to porphyrin), 8.27 (d, J = 8.4 Hz, 4H; Ar-α to porphyrin), 8.06–7.99 (m, 2H, Ar), 7.89 (d, J = 7.2 Hz, 0.4H; Ar), 7.78 (d, J = 7.2 Hz, 0.6H; Ar), 7.77–7.46 (m, 5H; Ar), 5.65–4.96 (m, 6H; $Glc^{(II)–(VII)}$-1β), 4.55 (d, J = 7.2 Hz, 0.4H; $Glc^{(I)}$-1β), 4.15 (s, 6H; ArCOO*Me*), 3.9–2.59 ppm (m, 105H; Glc and methyl protons), –2.02 (brs, 0.8H; inner pyrrole-N*H*), –2.03 (1.2 H; inner pyrrole-N*H*). ^{13}C NMR (75 MHz, in $CDCl_3$): δ 167.1, 145.9, 134.4, 129.9, 128.2, 120.7, 101.5, 96.4, 82.2, 70.6, 70.0, 69.7, 60.6, 60.1, 59.5, 59.0, 58.8, 58.6, 52.5, 29.7, 22.7. MALDI-TOF MS (α-cyanocynnamic acid as a matrix): m/z calculated for $C_{117}H_{148}N_4O_{40}$: 2248.97; found: 2272.34 as $[M + Na]^+$ and 2288.38 as $[M + K]^+$.

2.6. Synthesis of oligoamylose-strapped zinc porphyrin (1): A solution of **7** (38 mg, 17 mmol) dissolved in chloroform (30 mL) was stirred with saturated zinc acetate in methanol (2 mL) for 1 h, and the mixture was washed with saturated aqueous sodium hydrogencarbonate (5 mL). The organic layer separated was dried over anhydrous magnesium sulfate, and then subjected to silica-gel column chromatography with chloroform/MeOH (10/2, v/v). The target material **1** was quan-

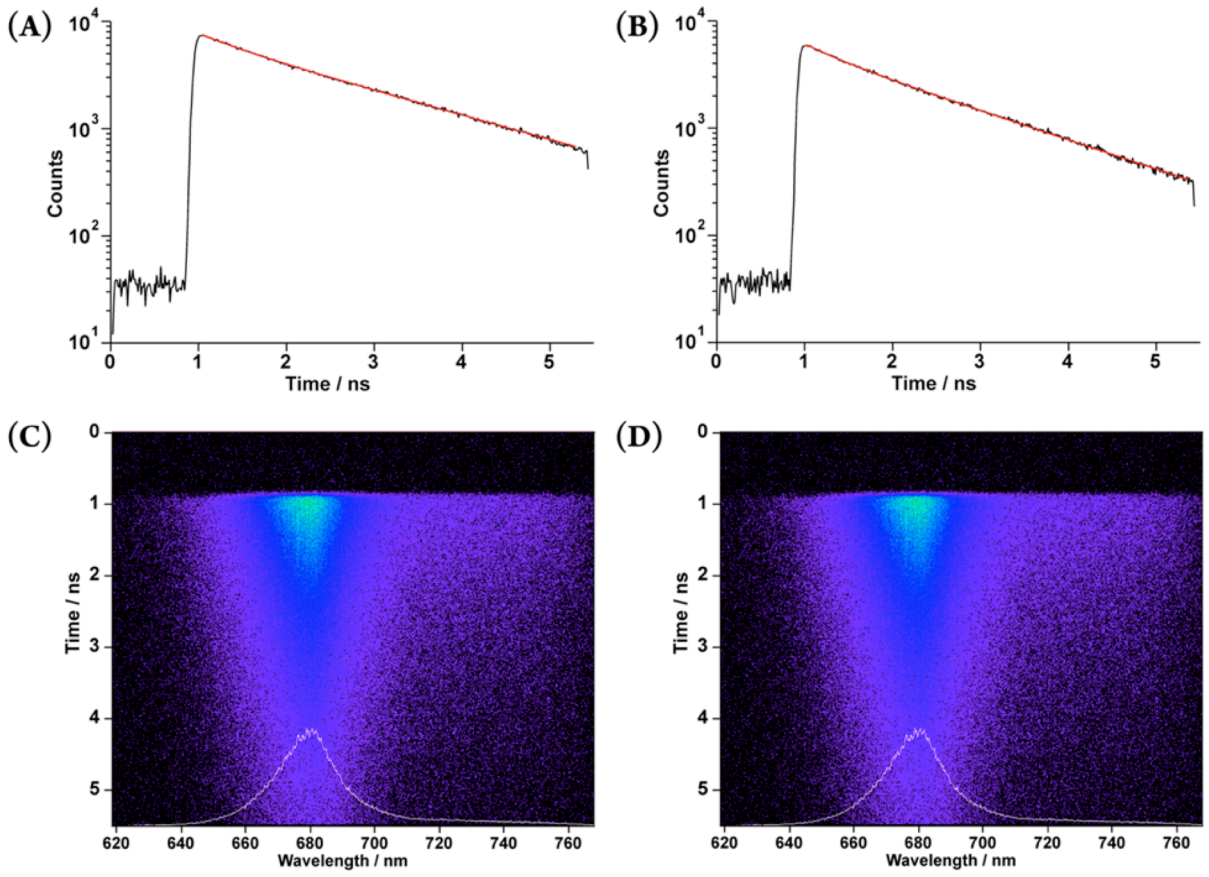


Figure S3. Fluorescence decay profiles and streak images of **1** (A, C) and **1**·Py (B, D) upon excitation at 455 nm in toluene. The decay profiles were fitted with red lines assuming τ_1 = 0.51 ns (19%) and τ_2 = 1.98 ns (81%) for **1**, and τ_1 = 0.44 ns (21%) and τ_2 = 1.68 ns (79%) for **1**·Py.

titatively obtained as a green substance. ^{1}H NMR (300 MHz, in toluene-d_8): δ 10.22 (d, J = 4.5 Hz, 1H; porphyrin-β), 10.21 (d, J = 4.5 Hz, 1H; porphyrin-β), 10.04 (d, J = 4.5 Hz, 1H; porphyrin-β), 9.98 (d, J = 4.5 Hz, 1H; porphyrin-β), 9.01 (d, J = 4.5 Hz, 3H; porphyrin-β), 8.97 (d, J = 4.5 Hz, 1H; porphyrin-β), 8.58 (d, J = 8.1 Hz, 1H; Ar-β to porphyrin), 8.56 (d, J = 9.9 Hz, 1H; Ar-β to porphyrin), 8.48 (td, J = 7.8, 1.6 Hz, 2H; Ar-β to porphyrin), 8.33 (d, J = 8.1 Hz, 1H; Ar-α to porphyrin), 8.30 (d, J = 9.9 Hz, 1H; Ar-α to porphyrin), 8.17 (d, J =

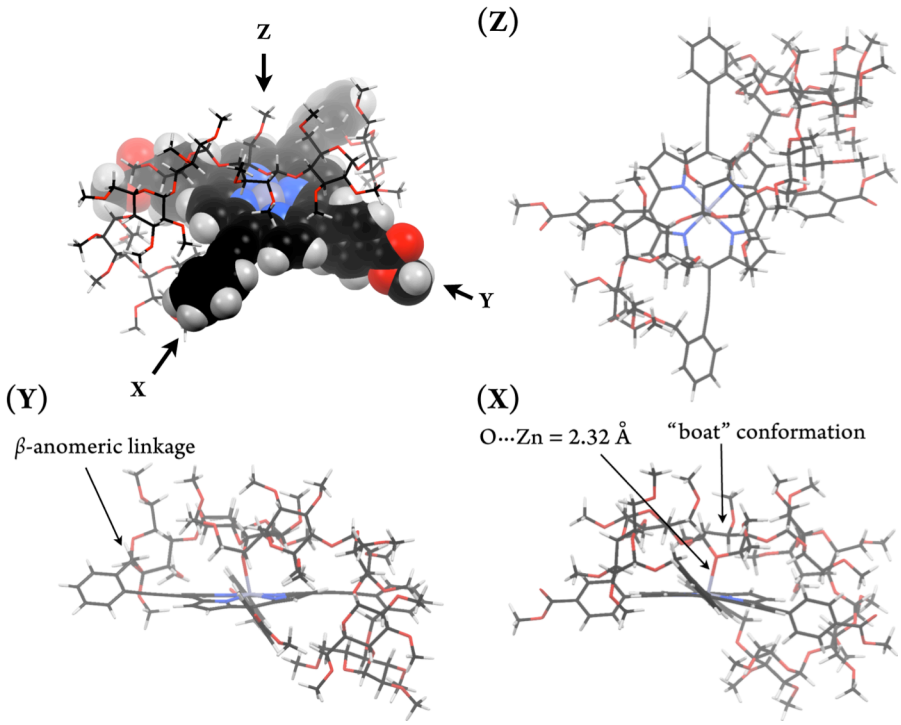


Figure S4. Orthographic projective views of B97D-optimized structures for β-linked **1**. Key geometrical parameters are given in Table S1.

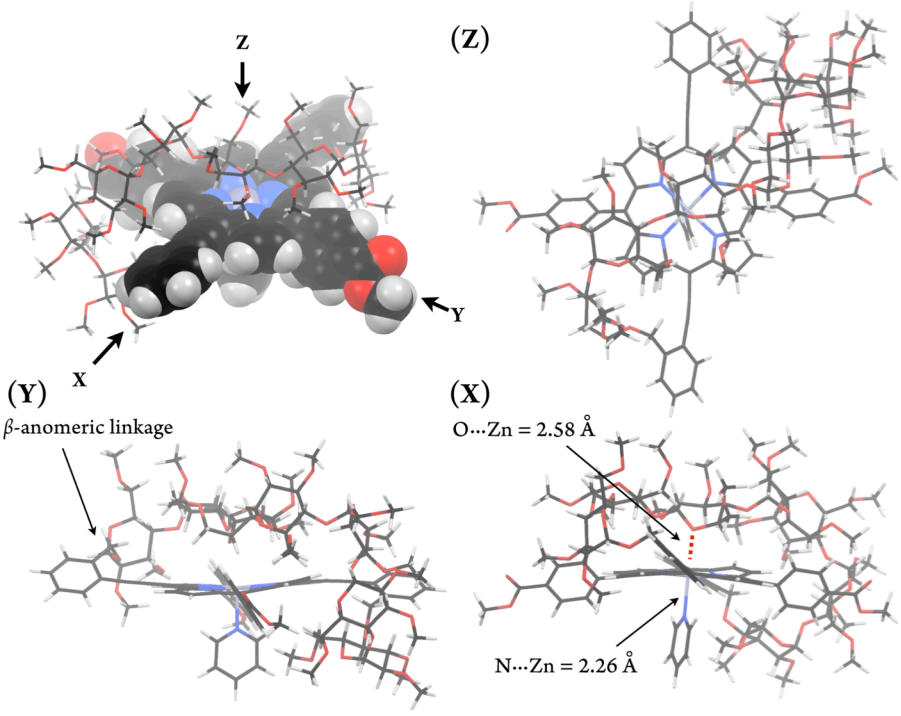


Figure S5. Orthographic projective views of B97D-optimized structures for β-linked **1**·Py. Key geometrical parameters are given in Table S1.

7.8 Hz, 2H; Ar-α to porphyrin), 8.1–7.9 (m, 2H; Ar), 7.6–7.1 (m, 6H, Ar), 5.7–2.2 (m, 121H; Glc and methyl protons, and ArCOO*Me*). ^{13}C NMR (75 MHz, in in toluene-d_8): δ 165.5, 151.7, 151.3, 148.9,146.7, 142.0, 133.7, 131.6, 81.8, 81.5, 70.6, 59.2, 59.0, 58.3, 57.7, 57.5, 57.3, 57.3, 57.0, 50.5, 31.1, 29.0, 28.6, 13.0. MALDI-TOF MS (α-cyanocynnamic acid): *m/z* calculated for $C_{117}H_{146}N_4O_{40}Zn$: 2310.88; found: 2334.37 as $[M + Na]^+$ and 2349.39 as $[M + K]^+$.

3.Computational Methods

We optimized oligoamylose-strapped porphyrins in the presence or absence of pyridine as axial ligand by using DFT calculations implemented in Gaussian 09

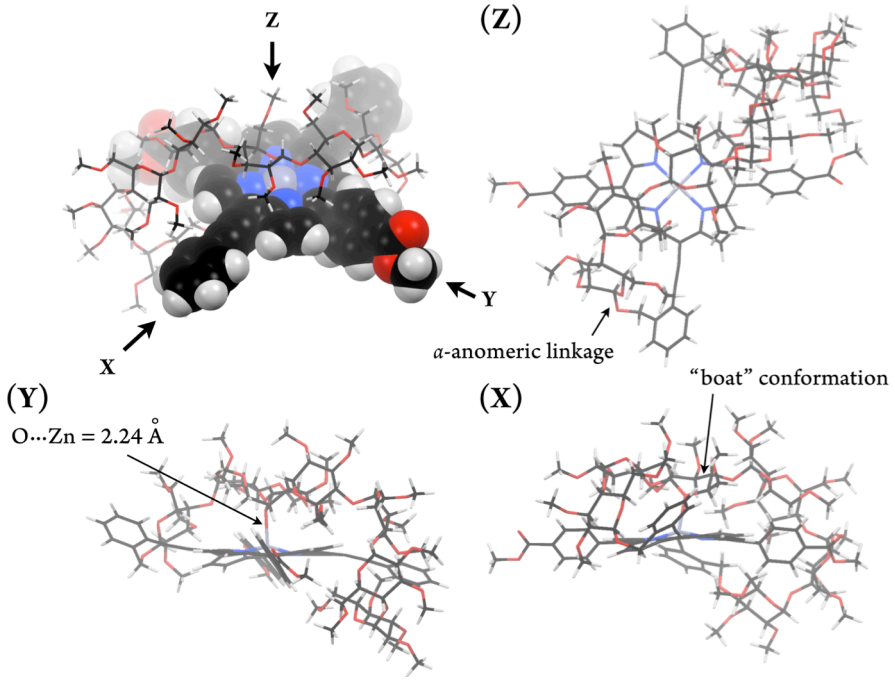


Figure S6. Orthographic projective views of B97D-optimized structures for α-linked **1**. Key geometrical parameters are given in Table S1.

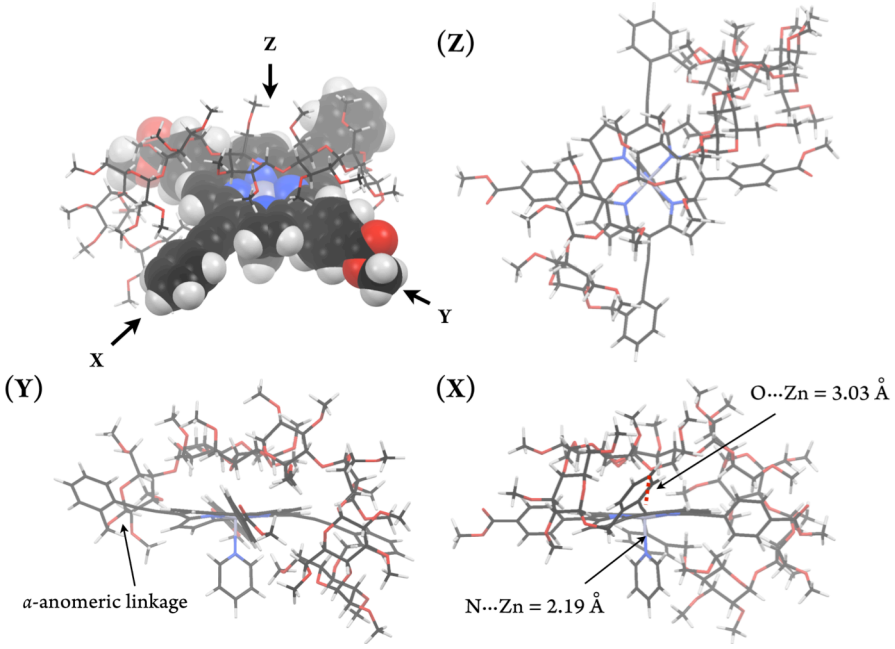


Figure S7. Orthographic projective views of B97D-optimized structures for α-linked **1**·Py. Key geometrical parameters are given in Table S1.

code.[S3] For determining self-folded conformations, host-guest interactions would be responsible. When DFT calculations are employed to investigate the structure of oligoamylose-strapped porphyrins, selection of DFT functionals is key to accurately describe host–guest interactions, such as CH–π interactions, that operate at long range. As is well known, standard functionals, such as the B3LYP functional, fail to describe long-range forces. To overcome this drawback of standard DFT calculations. B97-D functional, which adds an empirical atom-atom dispersion potential to GGA-based B97 functional, was devised.[S4] The B97-D functional is available as a functional that includes the empirical dispersion correction for the Gaussian 09 program. Therefore, the current study used the B97-D functional to analyze the geometrical properties of oligoamylose-strapped porphyrins. In discussing their electronic properties such as orbital energy levels, B97-D functional without including exact exchange terms is not suitable, because GGA-based calculations tend to underestimate the HOMO–LUMO gap of molecules. Instead, we performed single-point calculations based on standard B3LYP functional by using B97-D optimized geometries to estimate their electronic properties. We used the 6-311G* basis set for the zinc cation, and the 6-31G* basis set for the other atoms.

Table S1. Key parameters of optimized structures for α- or β-oligoamylose-strapped porphyrin [a].

Anomeric linkage of glucose-(I)	Pyridine	Zn···O(glucose)	Zn···N(pyridine)	Zn–N(porphyrin)
α-linked	presence	3.025	2.187	2.056, 2.067, 2.080, 2.090
α-linked	absence	2.239	–	2.067, 2.090, 2.092, 2.114
β-linked	presence	2.580	2.261	2.048, 2.066, 2.072, 2.085
β-linked	absence	2.318	–	2.040, 2.058, 2.071, 2.085

a) Optimized structures are given in Figure S4–S7. Bond lengths are given in Å.

Table S2. Electronic excitations of a small model of β-oligoamylose-strapped porphyrin.[a]

E_x/nm [b]	f [c]	Electronic transitions [d]
626.6	0.389	272→275 (0.31), 273→274 (0.63)
447.6	1.003	272→274 (0.55), 273→275 (0.39), 273→277 (0.21)
437.1	1.444	270→274 (0.18), 272→275 (0.59), 273→274 (–0.30)

a) This model is given in Figure S8A. b) E_x; excitation energy. c) f; oscillatory strength. d) Electronic transitions: Combination of occupied and unoccupied orbitals contributing to a certain electronic transition. Labels of the frontier orbitals; HOMO–n; 273–n, HOMO; 273, LUMO; 274, LUMO+m; 274+m, where n and m is an integer. Detailed orbital information is provided in Figure S8A. The values in parentheses indicate a CI coefficient in a certain excited configuration, as obtained from TD-DFT calculations.

Table S3. Electronic excitations of a small model of β-oligoamylose-strapped porphyrin in the presence of pyridine.[a]

E_x/nm [b]	f [c]	Electronic transitions [d]
639.1	0.397	293→296 (0.29), 294→295 (0.64)
455.5	0.926	293→295 (0.55), 294→296 (0.37), 294→298 (0.21)
442.3	1.224	290→295 (0.13), 293→296 (0.59), 294→295 (–0.28), 294→297 (–0.12)

a) This model is given in Figure S8B. b) E_x; excitation energy. c) f; oscillatory strength. d) Electronic transitions: Combination of occupied and unoccupied orbitals contributing to a certain electronic transition. Labels of the frontier orbitals; HOMO–n; 294–n, HOMO; 294, LUMO; 295, LUMO+m; 295+m, where n and m is an integer. Detailed orbital information is provided in Figure S8B. The values in parentheses indicate a CI coefficient in a certain excited configuration, as obtained from TD-DFT calculations.

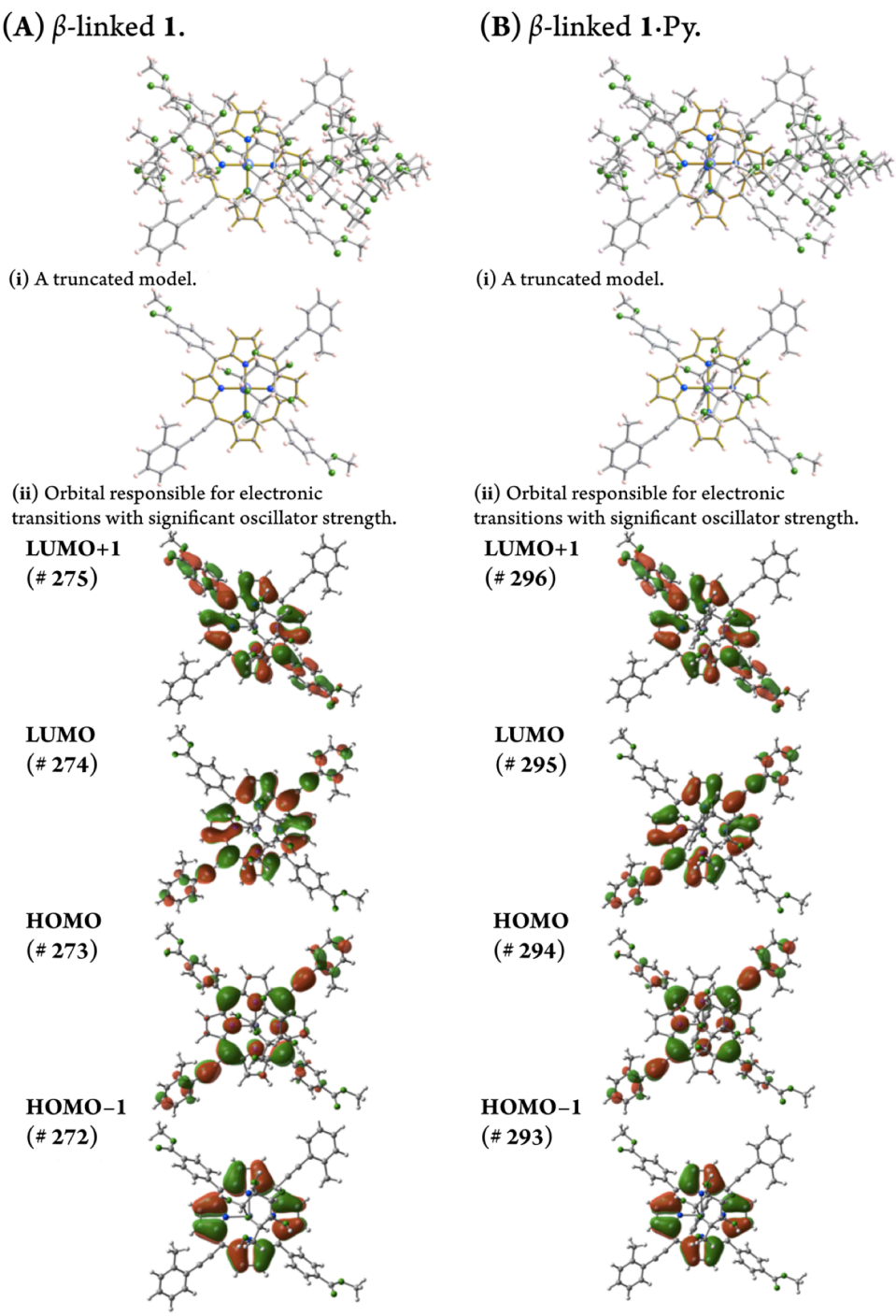


Figure S8. Orbitals responsible for electronic transitions with significant oscillator strengths, obtained from time-dependent DFT B3LYP calculations of truncated models of B97D-optimized β-oligoamylose-strapped porphyrin with or without pyridine as the axial ligand.

Figure S4–S7 show the optimized structures for both diastereomers **1** with α/β-anomeric connection of glucose-(I) in the presence or absence of pyridine as axial ligand. From a viewpoint of the energetics, β-oligoamylose-strapped porphyrin is more stable than α-linked diastereomer irrespective of the presence or absence of pyridine ligand: the energy differences are ~110 kcal/mol. At the same time, the molar contents of β-linked oligoamylose precursors **4** and **5** were approximately 60% judging from the α/β ratios in the ^{1}H NMR. Based on these facts, β-linked porphyrin **1** should be predominant. Thus, we confine our attention to the β-linked **1**. As shown in Figure S4, the distance between the zinc cation and the ring-membered oxygen atom of

glucose-(III) was calculated to be 2.32 Å in *β*-linked **1**, indicating formation of the Zn···O coordination bond. In *β*-linked **1** with pyridine ligand, the pyridine nitrogen atom binds into the zinc atom whose separation is 2.26 Å. The pyridine-to-zinc coordination bond slightly lengthens the Zn···O coordination bond (2.58 Å) (Figure S5). Although coordination environment of zinc atom in *β*-linked **1** changes significantly by the pyridine binding, self-folded conformations are kept, irrespective of the presence or absence of pyridine as the axial ligand.

In order to understand electronic transitions of *β*-linked **1** in the presence or absence of pyridine ligand, we tried time-dependent (TD) DFT calculations. For the TD-DFT calculations of *β*-linked **1** and **1**·Py, a considerable amount of memory was required, and therefore, we could not perform TD-DFT calculations. To overcome the limitations in the TD-DFT calculations, we removed some atoms from the *β*-oligoamylose-strapped porphyrins to create smaller models in the presence or absence of pyridine ($C_{65}H_{53}N_5O_{10}Zn$ and $C_{60}H_{48}N_4O_{10}Zn$, respectively), as shown in Figure S8. The models consist of zinc-porphyrins attached by *meso*-ethynylaryl and methoxycarbonylphenyl moieties, together with glucose-(III), corresponding to the first coordination ligand. Note that the atomic coordinates of the smaller models are the same as those of the remaining atoms in the *β*-oligoamylose-strapped porphyrins, and thus, the coordination environment of the zinc atom remains unchanged. Accordingly, the smaller models can relatively well reproduce orbital energies of the *β*-oligoamylose-strapped porphyrins.

Information regarding the electronic transitions obtained from the smaller models is given in Tables S2 and S3, together with orbitals responsible for the electronic transitions with significant oscillator strengths in Figure S8. The orbitals in Figure S8 come from frontier orbitals of metalloporphyrin coupled with orbitals of *meso*-ethynylaryl and methoxycarbonylphenyl moieties as small contributions, independent of the presence or absence of the pyridine ligand. Note that their orbitals do not have orbital contributions on the zinc atom and the glucose moiety. From Tables S2 and S3, we found maximum oscillator strength (*f*) in the strongest electronic excitation of the *β*-oligoamylose-strapped porphyrin in the absence and presence of pyridine at 437.1 and 442.3 nm, respectively, originating from the a_{1u}-like HOMO−1 to LUMO+1 that corresponds to an e_g-like porphyrin orbital plus π orbitals on both methoxycarbonylphenyl groups.[S5]

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S5 A. Ceulemans, W. Oldenhof, C. Görller-Walrand, L. G. Vanquickenborne, *J. Am. Chem. Soc.* 1986, **108**, 1155–1163.

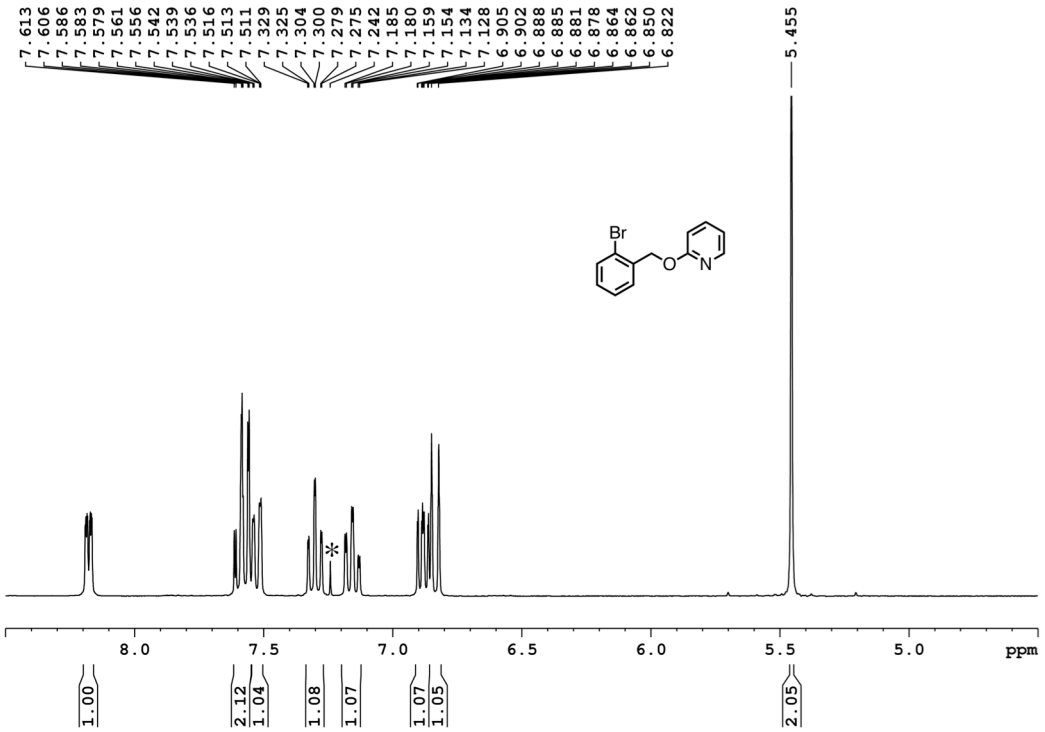

Figure S9. ^{1}H NNR spectrum (300 MHz) of 2-(2-bromophenylmethoxy)pyridine in $CDCl_3$.

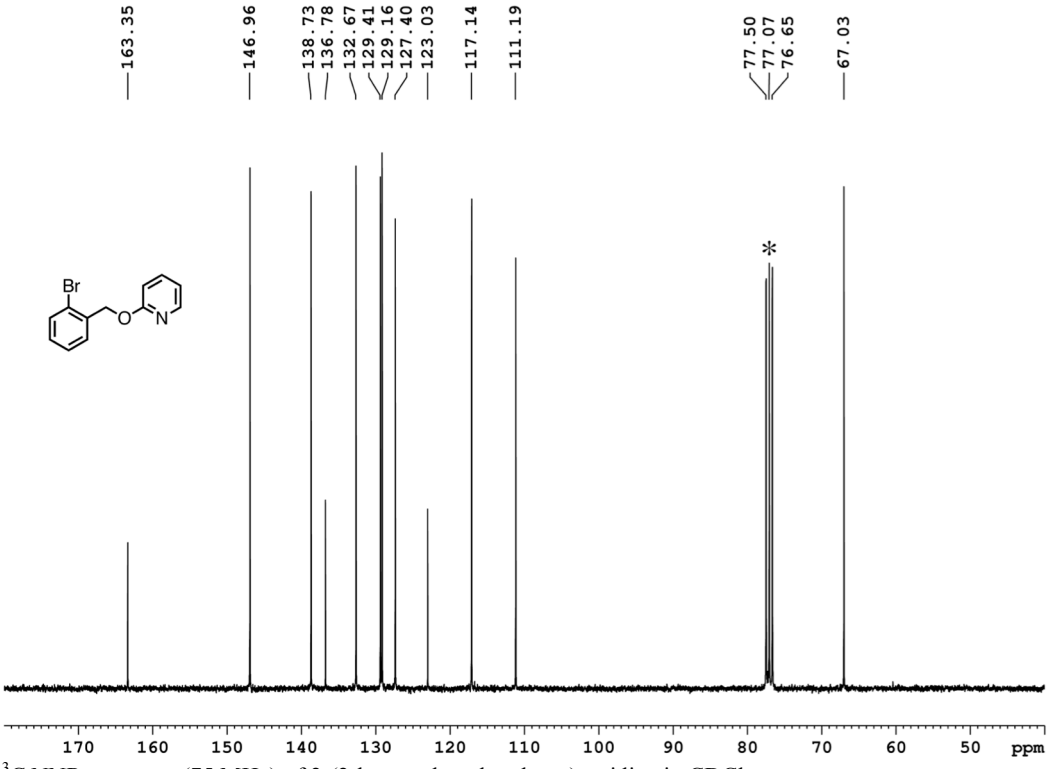

Figure S10. ^{13}C NNR spectrum (75 MHz) of 2-(2-bromophenylmethoxy)pyridine in $CDCl_3$.

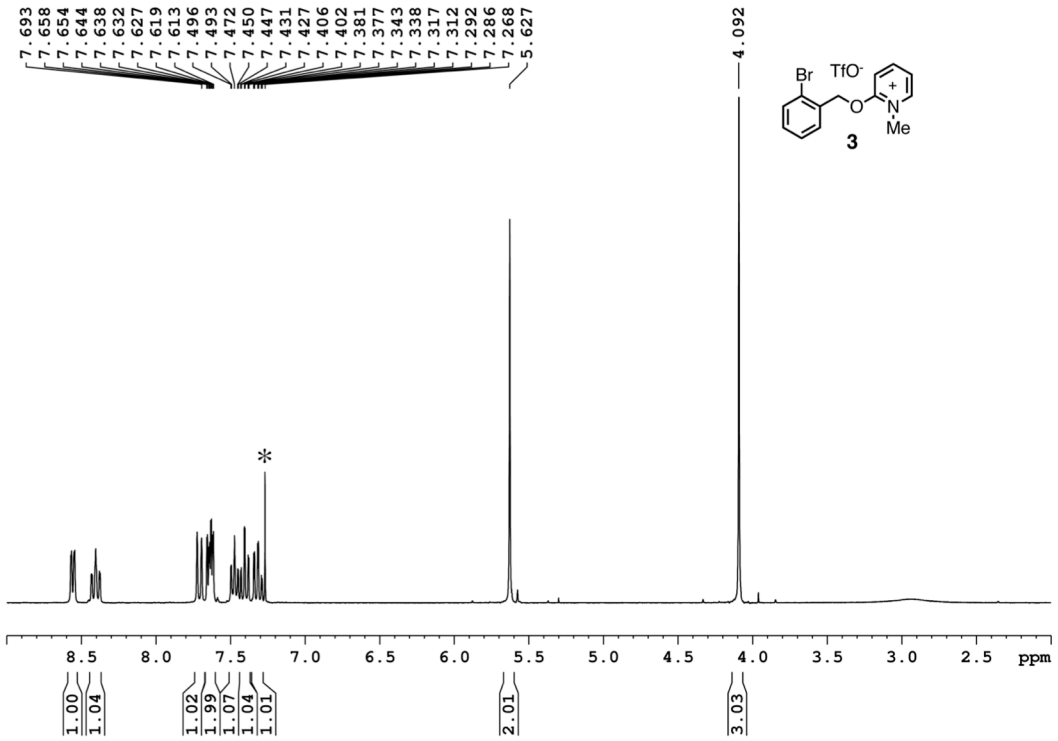

Figure S11. ^{1}H NNR spectrum (300 MHz) of **3** in $CDCl_3$.

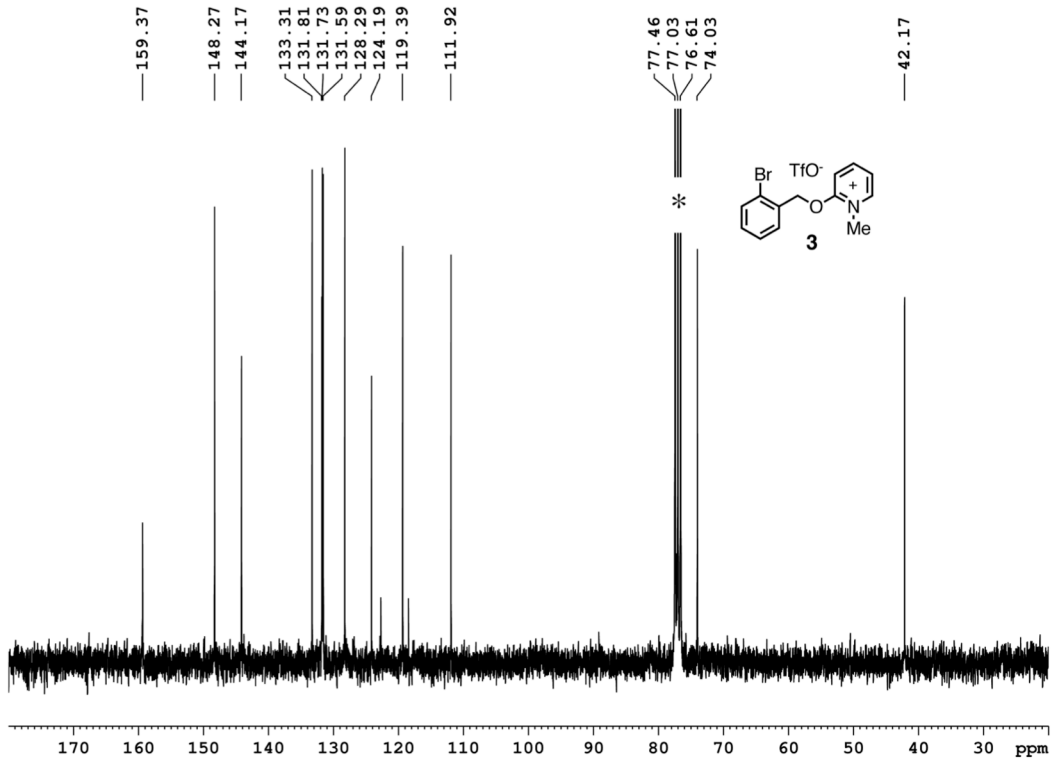

Figure S12. ^{13}C NNR spectrum (75 MHz) of **3** in $CDCl_3$.

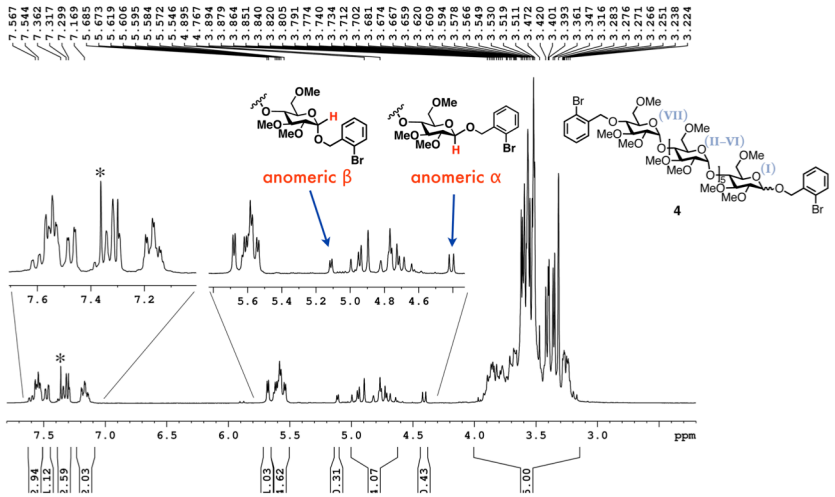

Figure S13. ^{1}H NNR spectrum (300 MHz) of **4** in $CDCl_3$.

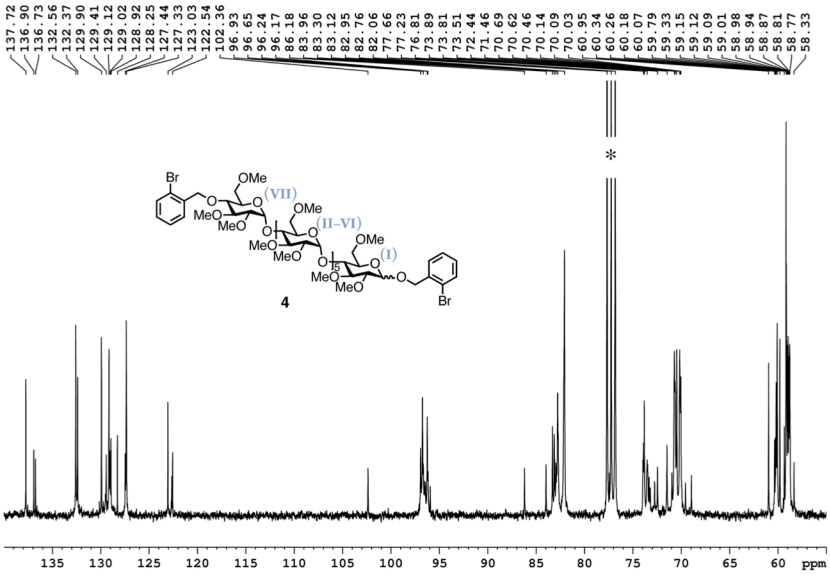

Figure S14. ^{13}C NNR spectrum (75 MHz) of **4** in $CDCl_3$.

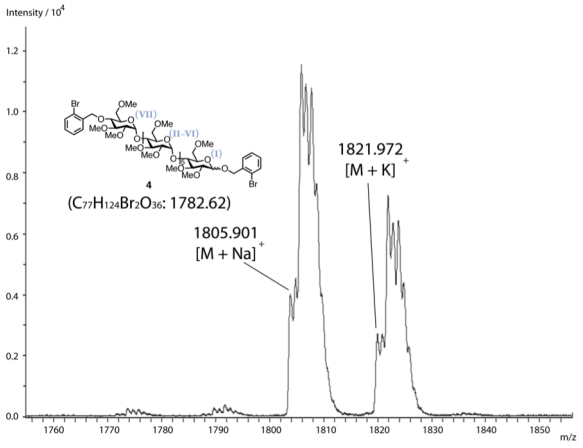

Figure S15. MALDI-TOF MS spectrum of **4** (α-cyanocynnamic acid as the matrix).

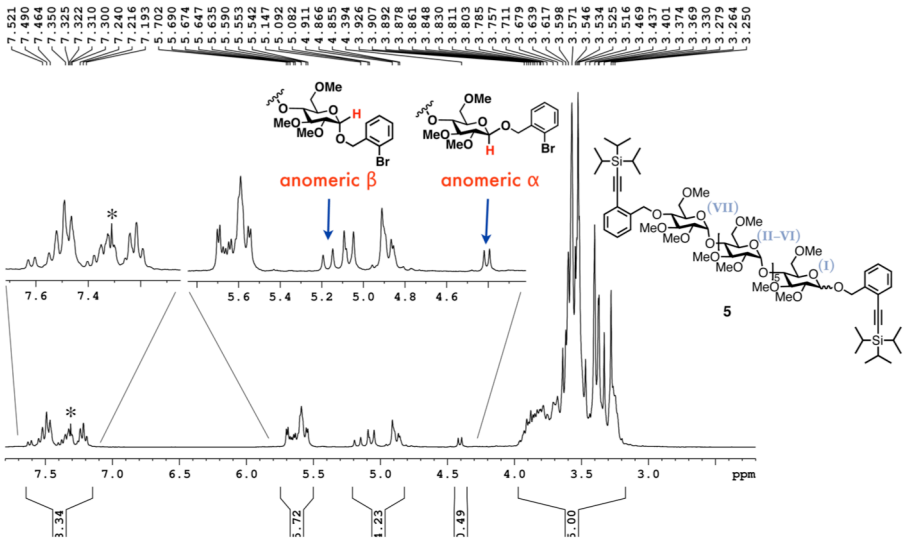

Figure S16. ^{1}H NNR spectrum (300 MHz) of **5** in $CDCl_3$.

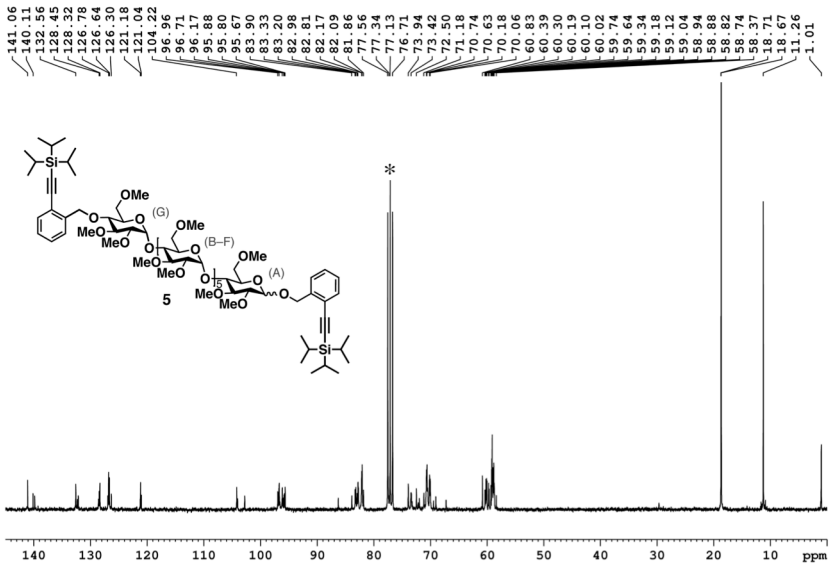

Figure S17. ^{13}C NNR spectrum (75 MHz) of **5** in $CDCl_3$.

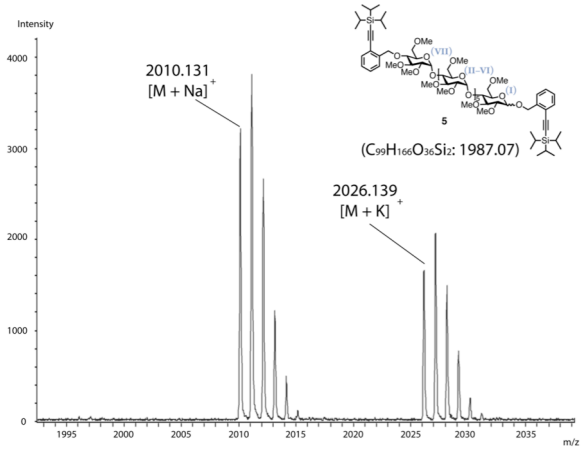

Figure S18. MALDI-TOF MS spectrum of **5** (α-cyanocynnamic acid as the matrix).

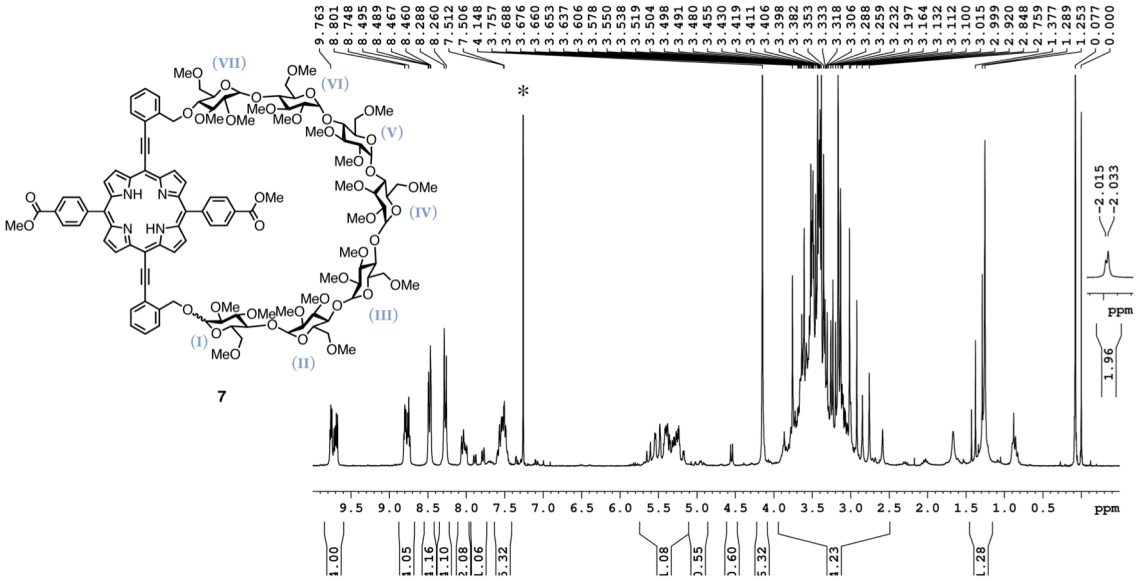

Figure S19. ^{1}H NNR spectrum (300 MHz) of **7** in $CDCl_3$.

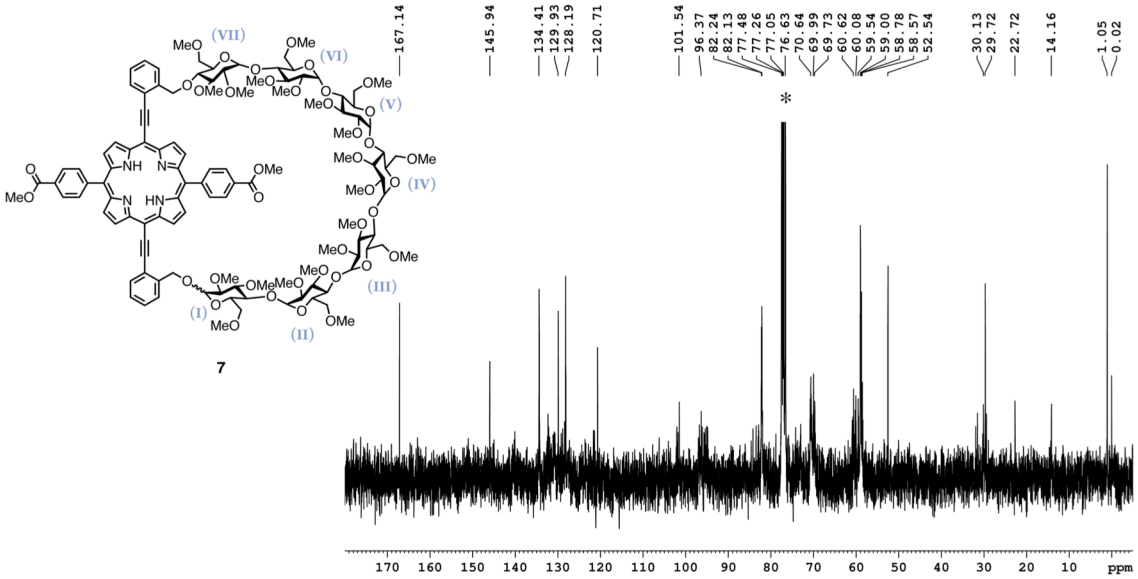

Figure S20. ^{13}C NNR spectrum (75 MHz) of **7** in $CDCl_3$.

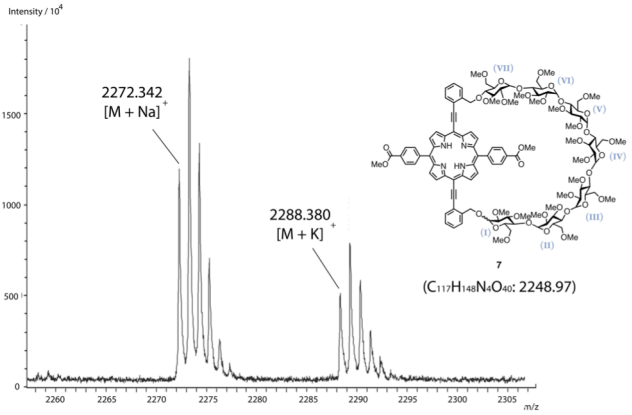

Figure S21. MALDI-TOF MS spectrum of **7** (α-cyanocynnamic acid as the matrix).

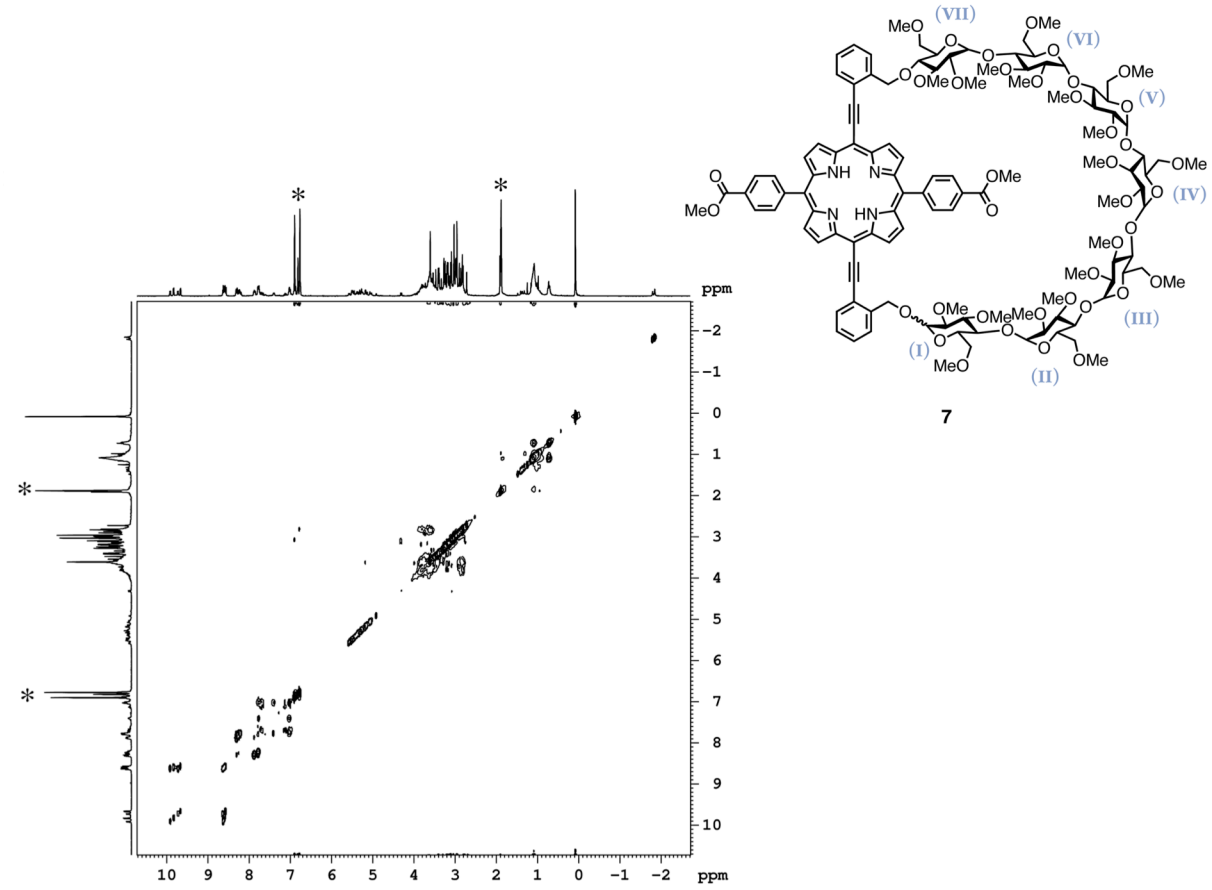

Figure S22. TOCSY spectrum of **7** in toluene-d_8.

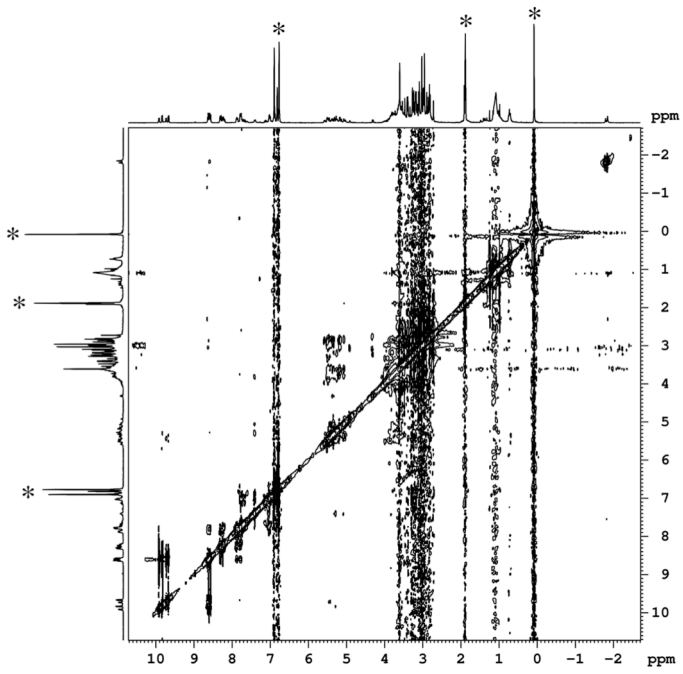

Figure S23. NOESY spectrum of **7** in toluene-d_8.

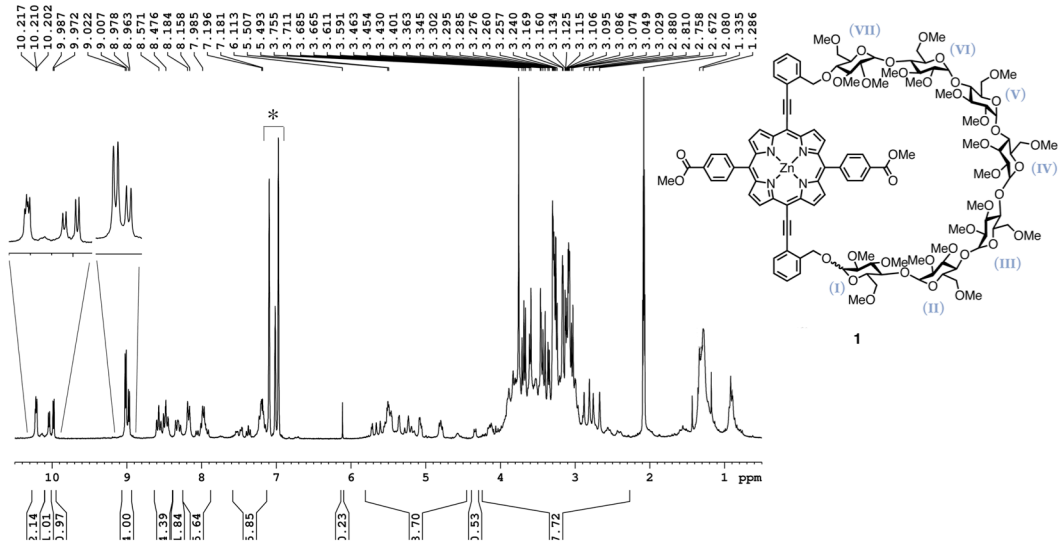

Figure S24. ^{1}H NNR spectrum (300 MHz) of **1** in toluene-d_8.

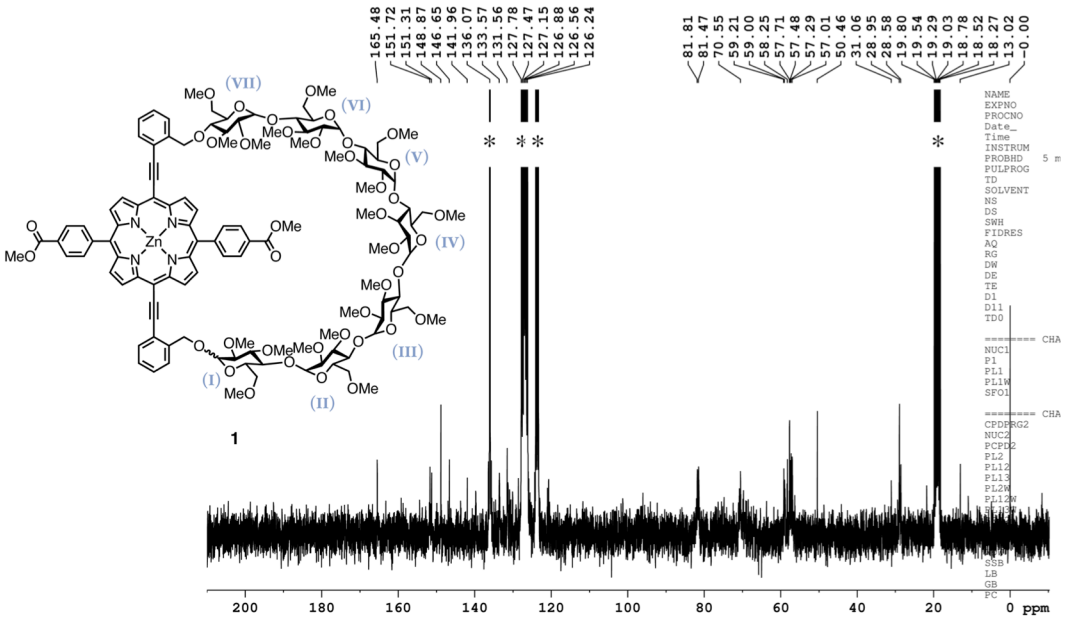

Figure S25. ^{13}C NNR spectrum (300 MHz) of **1** in toluene-d_8.

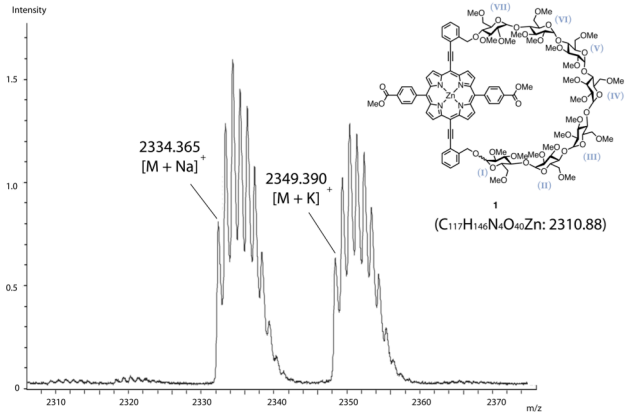

Figure S26. MALDI-TOF MS spectrum of **1** (α-cyanocynnamic acid as the matrix).

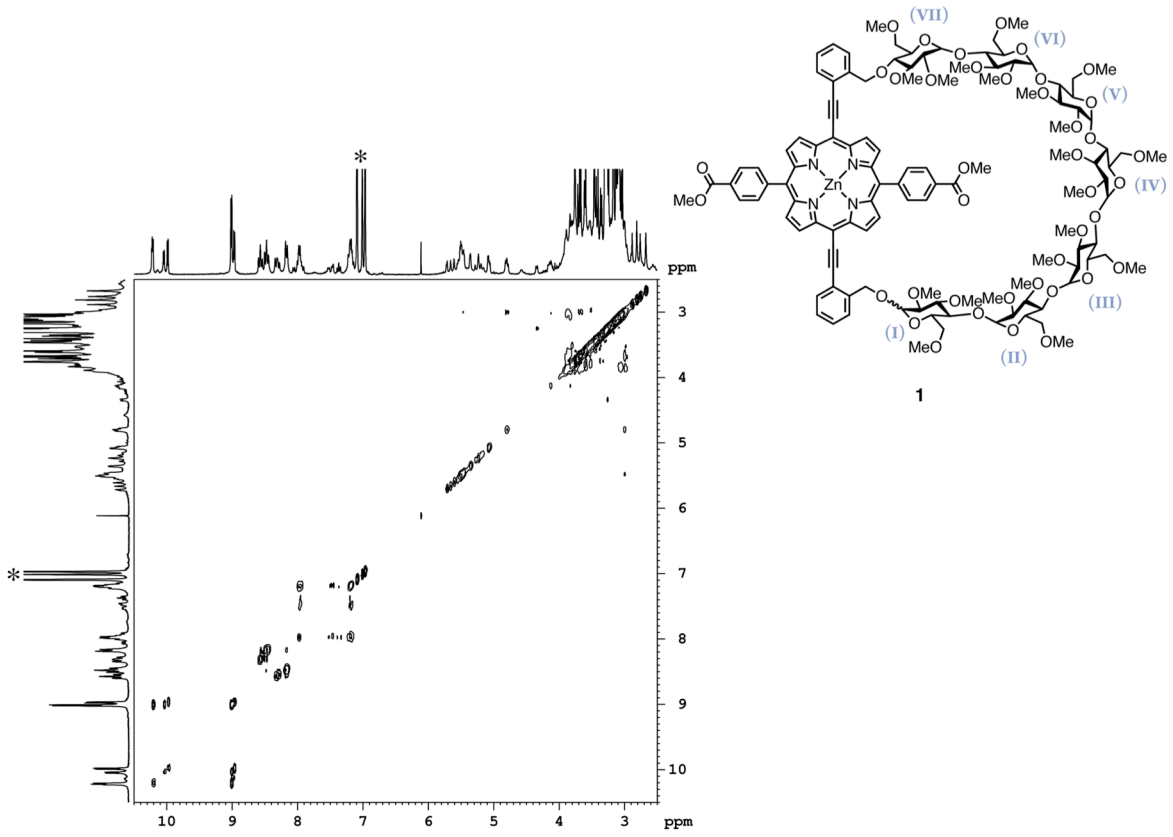

Figure S27. TOCSY spectrum of **1** in toluene-d_8.

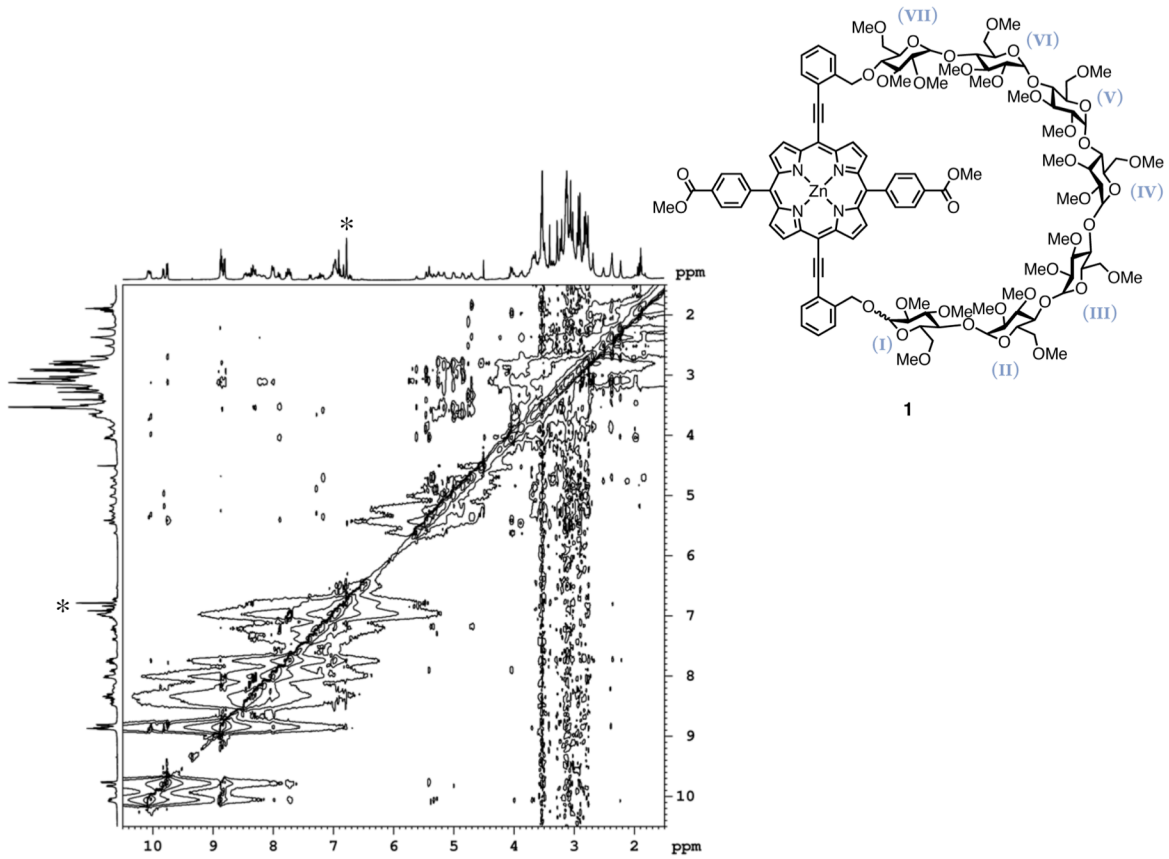

Figure S28. NOESY spectrum of **1** in toluene-d_8 (representative region is magnified in Figure S1).

Cartesian coordinates in optimized structures obtained from B97-D calculations

(a) β-oligoamylose-strapped porphyrin in the absence of pyridine.

C	-5.86924500	0.29455800	-3.44473200
C	-6.55647900	0.21795700	-2.06413500
C	-7.56326600	-0.95617600	-1.94483600
C	-7.16369600	-2.24151100	-2.73126300
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H	-2.15037100	-1.82506800	-3.77277600
H	-2.89594800	-2.04640100	-1.09291900
C	-1.25842100	-3.79663900	-2.13220100
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C	1.36926500	4.22031600	-0.66747100	H	1.39960300	3.17511500	-3.15751400
C	2.69996000	4.31890800	-0.35911000	C	0.23820500	-0.98542900	-5.07172500
C	4.37454900	2.77345000	0.77543300	H	0.80261500	-0.17552200	-5.57019800
C	-0.68550000	-1.74552200	2.20027800	H	0.89313700	-1.86202400	-4.94486600
H	-2.96650100	1.12669200	-0.66868700	H	-0.61778900	-1.28649100	-5.68932200
H	-3.18348400	-1.06692900	0.90778700	C	0.23352500	-4.97263200	-4.49465800
H	0.26633600	-3.99216100	3.78044300	H	0.86415700	-4.91592300	-5.39401500
H	2.98003700	-4.04548600	3.92918300	H	0.88834800	-4.95872900	-3.60205500
H	6.85521500	-0.68039300	2.67192600	H	-0.33413400	-5.92471100	-4.50647500
H	6.94456300	1.86739600	1.78930800	C	-3.95530300	-3.82263500	-5.68724600
H	3.37578800	5.13786600	-0.58277300	H	-3.48601000	-4.80043600	-5.47074600
H	0.73476200	4.94147900	-1.17499500	H	-4.96105700	-3.79061900	-5.23172000
C	10.72374500	2.66298200	0.84424700	H	-4.05473500	-3.71281400	-6.77680500
H	10.53231900	3.74330000	0.78496600	C	-5.05610800	2.51640000	-3.80991500
H	11.35748100	2.44168700	1.72024300	H	-5.55229800	2.54010600	-4.80204900
H	11.25135000	2.34487400	-0.07618300	H	-5.69682900	3.02654800	-3.07357300
C	9.20067900	0.53864100	3.84615000	H	-4.09628100	3.04646400	-3.87271500
H	9.44326600	0.99137800	4.81805100	C	-8.20159200	1.99066400	-2.41847700
H	8.49901300	1.19611600	3.30943000	H	-7.92713000	2.11807500	-3.48018800
H	8.73541100	-0.44690400	4.00298500	H	-9.09784000	1.35236800	-2.34292900

H	-8.43468800	2.97254400	-1.98428900	O	8.24790300	8.00589900	1.00003900
C	-11.82474200	-0.27094800	-1.28168500	C	-5.36272000	-4.86027000	3.66279200
H	-12.45514600	-0.80082100	-0.53953800	O	-5.51708200	-6.03845600	3.36929200
H	-11.91585400	0.81368800	-1.12362600	O	-6.35028200	-4.07504100	4.18434000
H	-12.15893900	-0.53787600	-2.29486100	C	-7.68745300	-4.62786500	4.22246500
C	-9.52074000	5.39178200	3.65019400	H	-8.35001700	-3.75441900	4.24320700
H	-10.61850700	5.37465900	3.72423000	H	-7.86986600	-5.24201800	3.32985300
H	-9.09592400	5.60734100	4.65246000	H	-7.80946800	-5.24906800	5.12288600
H	-9.20504000	6.18030500	2.94960700	C	9.31312900	8.98077900	0.99963500
C	5.42939200	3.82721700	0.66343400	H	8.87595400	9.88699200	1.43643900
C	5.23069900	5.10548900	1.24007600	H	10.16108400	8.62333700	1.60273400
C	6.66132300	3.57184400	0.02224900	H	9.66116900	9.16833400	-0.02709000
C	6.22614700	6.08587100	1.18565900	O	-8.33585200	-1.83953300	1.52006600
H	4.29028700	5.31247100	1.75252000	C	-9.39692400	0.67268100	0.58931300
C	7.65635800	4.54641000	-0.03483000	H	-8.61240400	0.97037500	-0.11276400
H	6.87418700	2.60051900	-0.41044300	O	-10.37277500	1.71392400	0.49352600
C	7.45826300	5.81075100	0.55078300	C	-11.29604600	1.80760200	1.57638800
H	6.06234400	7.05666300	1.65233300	H	-12.10068200	2.47357900	1.23142500
H	8.60061500	4.32375900	-0.52587300	H	-11.73591500	0.82582800	1.84066000
C	-1.82613300	-2.58734500	2.66311500	H	-10.81701400	2.25206900	2.46493900
C	-2.84615000	-1.99725500	3.44221300	O	-6.16975000	2.00823100	3.50529300
C	-1.94839300	-3.94737100	2.30662400	C	-6.93582500	4.39067900	2.04087900
C	-3.97547100	-2.72689900	3.81913800	H	-7.39346200	3.93870100	1.15250500
H	-2.74934100	-0.95152400	3.73703100	O	-7.09043000	5.79701200	1.82126400
C	-3.07558500	-4.68433600	2.68703000	C	-6.33630200	6.64586300	2.68508500
H	-1.18148300	-4.40396500	1.68128700	H	-6.70381100	7.66581200	2.50126900
C	-4.11274100	-4.07528000	3.42398500	H	-6.48977800	6.39944800	3.75329400
H	-4.75575300	-2.25010100	4.40853500	H	-5.25883900	6.59873400	2.45262800
H	-3.19643300	-5.72111200	2.37293800	O	8.39826100	0.71648500	-1.22142300
C	8.58949200	6.78146200	0.49866300	O	4.06435100	-0.03128500	-1.57851600
O	9.70822000	6.52734300	0.06510100	O	-0.77743900	-2.49235300	-1.83426300

O	-4.48970000	-1.49790000	-2.78358300	H	2.89706700	-5.97021000	-0.99354500
O	-7.57810400	-1.29822400	-0.53736900	C	-4.47922900	-3.28965200	-0.42667000
H	9.00045100	0.25140100	-3.14101000	H	-5.10363800	-2.38300600	-0.32112100
H	-0.50434000	-4.56019600	-1.87805200	H	-4.03086900	-3.52558300	0.55403500
H	-4.85689200	-1.11202800	-4.79492300	O	-5.27984400	-4.37582300	-0.88837700
H	-9.08459200	-2.69628100	-0.14563500	C	-6.28034900	-4.71706800	0.06944400
H	-8.08829400	1.86065500	4.14486700	H	-5.83383300	-5.20881300	0.95263100
O	-8.02377500	1.82539100	2.06865900	H	-6.84203400	-3.82323200	0.40216700
C	10.11818200	-2.08539700	-1.91609300	H	-6.96567800	-5.42226700	-0.42489100
H	9.71448500	-1.60553100	-2.81897000	C	-8.38578700	-3.08857100	-3.07212200
H	11.22316800	-1.98850000	-1.93723300	H	-8.84408100	-3.42435900	-2.12124000
O	9.73721700	-3.45890900	-1.89606800	H	-8.06631600	-3.99012000	-3.63183600
C	10.26387000	-4.15666500	-3.01304400	O	-9.31176500	-2.32669300	-3.83529000
H	9.93111800	-5.20110700	-2.92631600	C	-10.60986800	-2.89399500	-3.81260300
H	9.89228000	-3.73355000	-3.96954600	H	-11.25278200	-2.24639200	-4.42719200
H	11.37278000	-4.12555600	-3.02466400	H	-10.62069200	-3.91932900	-4.23748200
C	5.84207100	-2.48519600	-1.71984300	H	-11.00863000	-2.93083900	-2.77898400
H	4.98190200	-2.54756000	-1.03951200	C	-7.28858000	-0.97346400	3.47496800
H	6.69292200	-3.05138700	-1.29319500	H	-6.69190100	-1.89758500	3.43052100
O	5.40959500	-3.08574500	-2.93794600	H	-6.65006600	-0.15385700	3.84414300
C	6.46859700	-3.41548500	-3.84096900	O	-8.41698600	-1.15873300	4.33842400
H	6.05623900	-4.15204700	-4.54775700	C	-7.99903100	-1.26516600	5.69359500
H	6.82701000	-2.53054000	-4.39260500	H	-7.32753600	-2.13292600	5.84314800
H	7.32624600	-3.85338000	-3.29781200	H	-7.46608300	-0.34984700	6.02346400
C	1.92977400	-3.51581200	-0.44832100	H	-8.90659600	-1.39708900	6.30114800
H	1.10426500	-4.24105700	-0.28813200	C	-3.90976300	1.97875200	2.66332000
H	2.49672500	-3.43048400	0.49521500	H	-3.87691900	0.87815500	2.79180800
O	2.77778700	-3.94145200	-1.50997100	H	-3.31398100	2.22284500	1.76591300
C	3.54524800	-5.08656200	-1.16411200	O	-3.38055800	2.63301200	3.80645400
H	4.22659700	-5.26691100	-2.00467900	C	-1.98348400	2.39366700	3.91672000
H	4.13756900	-4.90461500	-0.24520800	H	-1.76225800	1.31221500	4.03124200

H	-1.43786100	2.75959000	3.02420400
H	-1.63396700	2.93130900	4.80997900

(b) β-oligoamylose-strapped porphyrin in the presence of pyridine.

C	-5.98830200	-0.03438000	-3.58753400
C	-6.68137300	-0.01041500	-2.20751200
C	-7.66258700	-1.19329100	-1.99528500
C	-7.23344900	-2.53040900	-2.67285400
C	-5.44914800	-1.45628200	-3.84121200
H	-5.87990500	-0.10893700	-1.46580100
H	-6.70713000	0.17288200	-4.40068800
H	-6.58200600	-3.06915900	-1.97136200
H	-8.66004500	-0.92519900	-2.35210600
C	-3.91342200	-3.00627700	-2.72686600
C	-2.75484500	-3.06718400	-3.74889700
C	-3.42523700	-3.07503000	-1.25656700
H	-4.63246000	-3.81718900	-2.90990300
C	-1.76608100	-4.18631400	-3.35413100
H	-2.21486000	-2.11610000	-3.69766700
H	-2.97951800	-2.09911000	-1.02671300
C	-1.31377300	-3.92166600	-1.89482400
H	-2.26570600	-5.17620300	-3.34482400
O	-6.54346600	-2.36085300	-3.92775100
O	-2.42550800	-4.10008000	-1.04798100
O	-4.89459400	0.87532900	-3.63508300
O	-7.26842300	1.26849600	-1.89287900
O	-3.19344400	-3.14634500	-5.11176200
O	-0.69739400	-4.20480800	-4.29539000
C	0.49943500	-2.25524100	-2.07857900
C	0.46631800	-0.84338300	-2.71570100
C	1.30408200	-2.20462300	-0.75130600
H	0.91089800	-2.99127800	-2.77940200
C	1.89331300	-0.27652900	-2.98193600
H	0.01384100	-0.18238400	-1.96474700
H	0.59167800	-1.89948600	0.01489500
C	2.90294700	-0.96313400	-2.02313400
H	2.21935900	-0.52538800	-4.01074300
O	2.32068200	-1.17801800	-0.73594600
O	-0.41729300	-0.76272500	-3.83319200
O	1.93281100	1.12712100	-2.80187700
H	3.17928100	-1.93999600	-2.45683100
C	5.13839000	-0.36893800	-2.67126100
C	5.65398300	1.03748600	-3.01486000
C	6.20069500	-1.22565800	-1.96425200
H	4.82537900	-0.87445700	-3.59836800
C	7.12484700	1.07047200	-3.48834500
H	5.56582600	1.63700900	-2.09845700
H	6.39920200	-0.78571100	-0.97201600
C	8.05249100	0.04658700	-2.77554500
H	7.12942100	0.76519300	-4.55412000
O	7.41555500	-1.22515700	-2.75318500
O	7.56418400	2.41787600	-3.36434300
O	4.81737200	1.56791100	-4.04225000
C	9.52732200	-0.07144300	-0.81692600
C	9.40350600	0.52418900	0.61668100
C	9.55236100	-1.63809100	-0.76130600
H	10.45120800	0.28450900	-1.31140300
C	10.40008600	-0.13363800	1.60438000
H	8.38667000	0.28084000	0.93871800
H	8.53296700	-1.98194700	-0.54035000
C	10.14631800	-1.65811300	1.57612500

H	11.42490900	-0.01643000	1.22077800	C	-3.31150000	4.63926700	-2.29916700
H	10.84621900	-2.19460500	2.23902700	C	-5.33457500	6.35346200	-3.27801000
O	10.46463500	-2.10296900	0.26333100	H	-6.58758500	5.46155600	-1.74661600
O	10.45512100	0.45814600	2.89096500	C	-3.04822600	5.53589900	-3.36842400
O	9.43881500	1.94574500	0.62115700	C	-4.05266600	6.37736100	-3.85621000
C	-8.82782900	-1.79426600	0.17611400	H	-6.11666200	7.01980600	-3.64740800
C	-10.03247600	-0.82743000	0.06452900	H	-2.04762000	5.55631800	-3.80318600
H	-10.77826000	-1.17549300	0.80605800	H	-3.83516800	7.05673300	-4.68301300
C	-7.83519400	-0.56729600	1.96719100	C	8.39898500	-4.01649500	3.14564700
C	-8.82889800	0.61423700	1.78753000	C	9.52647900	-4.73345200	3.57467500
H	-6.94282800	-0.34685300	1.36215800	C	7.25001500	-3.95427900	3.99483400
H	-9.55810400	0.58473100	2.61211600	C	9.54747200	-5.38506400	4.81814700
O	-10.57999600	-0.94215800	-1.24831700	H	10.39429500	-4.79083000	2.91292000
C	-7.70347800	2.48315000	2.95426900	C	7.27639200	-4.62818400	5.24184400
C	-7.88959800	4.00779800	2.76162600	C	8.41526700	-5.33273600	5.64854700
H	-7.49550100	4.50748200	3.66822800	H	10.43536700	-5.93725000	5.13194700
C	-5.47884700	2.51265900	2.08785400	H	6.39473900	-4.58321300	5.88292700
C	-5.58801500	4.01469200	1.72982600	H	8.41880100	-5.84289800	6.61395100
H	-5.79956600	1.90936300	1.22234200	C	6.10080700	-3.21731700	3.59051600
H	-5.17842200	4.56923900	2.58514600	C	5.16511500	-2.54377200	3.16375400
O	-9.28706300	4.24369400	2.63899500	C	-2.26864500	3.81579200	-1.79147100
O	8.80070900	-1.92608700	1.92552900	C	-1.37893200	3.12957500	-1.29398500
O	-4.74404400	4.38380100	0.63887900	C	4.17680500	-1.67122900	2.62959500
C	8.40434100	-3.32283200	1.80477500	C	-0.41321000	2.33803000	-0.61799100
H	7.39153000	-3.29291200	1.37974100	Zn	1.86785000	0.46433500	1.20216600
H	9.07148300	-3.83319500	1.09459200	N	1.96005800	2.20513600	0.09356500
C	-4.96360000	3.66657900	-0.59622400	N	-0.17654200	0.37314900	0.87823800
H	-4.32673800	2.76799500	-0.61802800	N	3.90512500	0.48108700	1.41161800
H	-6.00876000	3.33648300	-0.69282000	N	1.74987300	-1.33174300	2.25409200
C	-4.62068500	4.59663700	-1.73518900	C	2.80529800	-2.03333600	2.77302000
C	-5.60455900	5.47036700	-2.22233500	C	4.66525300	-0.47075400	2.02837700

C	4.74966500	1.51953400	1.08931200	H	8.75034400	-0.35691900	3.82107800
C	0.60427000	-1.98928000	2.64838100	C	8.85239500	2.66042000	-3.91255300
C	-1.04684200	-0.57578100	1.36750900	H	9.64742600	2.16344600	-3.32524200
C	-0.89826200	1.15223600	0.01026700	H	8.91541500	2.31818100	-4.96575000
C	0.92666900	2.82211700	-0.55591000	H	9.00929400	3.74734700	-3.87095100
C	3.07078300	2.99720500	-0.07871400	C	4.44383300	2.92973500	-3.82211500
C	6.04529700	-0.03994000	2.10691300	H	3.85481000	3.02280000	-2.89534900
C	6.09269800	1.21251200	1.55713000	H	5.32978500	3.58544200	-3.77299300
C	0.95664500	-3.13348200	3.47032400	H	3.81587500	3.21605500	-4.67843300
C	2.32727500	-3.17247100	3.52792600	C	1.26078200	1.84251000	-3.83421200
C	-2.34973900	-0.40783900	0.75182900	H	1.67917400	1.57763600	-4.82587700
C	-2.24904400	0.64814100	-0.11563900	H	0.17614400	1.64358700	-3.83544800
C	1.38008000	4.05413600	-1.16340600	H	1.44428100	2.90577100	-3.63320800
C	2.71539400	4.16220600	-0.87464800	C	0.05132900	-1.31769400	-5.06542900
C	4.37445800	2.70909700	0.41194100	H	0.60878400	-0.56031200	-5.64728600
C	-0.70929500	-1.62768200	2.25973700	H	0.68926000	-2.20147000	-4.90867300
H	-2.99938500	1.02584400	-0.80451300	H	-0.84053900	-1.63895500	-5.61970000
H	-3.21380600	-1.03789700	0.93250600	C	0.19142700	-5.30584200	-4.12876100
H	0.25012100	-3.81381200	3.93613300	H	0.81046900	-5.34710800	-5.03696300
H	2.96355500	-3.88724100	4.04358600	H	0.85546400	-5.17938100	-3.25246700
H	6.85577400	-0.61062500	2.54407000	H	-0.36557600	-6.25854900	-4.02313500
H	6.95686200	1.86265800	1.47757700	C	-3.97331200	-4.28908400	-5.45867800
H	3.40135300	4.94331600	-1.18600000	H	-3.47159500	-5.23515300	-5.18251100
H	0.75349000	4.72999600	-1.73899000	H	-4.97656500	-4.25676800	-4.99772800
C	10.72230000	2.54308500	0.43671100	H	-4.08375600	-4.25488600	-6.55219800
H	10.54006400	3.62033300	0.31999200	C	-5.22452600	2.16756600	-4.13548400
H	11.37290700	2.36435700	1.31016400	H	-5.72224100	2.09799300	-5.12498400
H	11.22558700	2.16815700	-0.47544700	H	-5.87487500	2.72521200	-3.44334000
C	9.21442300	0.61493700	3.59035000	H	-4.27577400	2.70996700	-4.24568400
H	9.47191700	1.13253000	4.52554000	C	-8.35941600	1.69197300	-2.71613700
H	8.50486900	1.23480100	3.02054800	H	-8.06934900	1.76122100	-3.77915600

H	-9.23623300	1.03047500	-2.61552600	O	9.72518500	6.34862800	-0.67646600
H	-8.63260700	2.69067100	-2.34863200	O	8.27419800	7.91865400	0.11287800
C	-11.94551000	-0.54355500	-1.36824700	C	-5.40030700	-4.60745700	3.94696400
H	-12.56150000	-1.01872500	-0.57835500	O	-5.55561700	-5.80447200	3.74358500
H	-12.05399300	0.54901100	-1.30101100	O	-6.38651100	-3.78632500	4.41405300
H	-12.28304800	-0.90035300	-2.35233200	C	-7.72250700	-4.33819300	4.49673100
C	-9.69067400	5.56668700	2.98129400	H	-8.38804500	-3.46817100	4.44861400
H	-10.79067800	5.55778900	3.00629500	H	-7.90361700	-5.02125100	3.65545300
H	-9.30987500	5.85358900	3.98369000	H	-7.84173500	-4.88717200	5.44331700
H	-9.33908100	6.30103300	2.24014700	C	9.34258600	8.88411400	0.00882200
C	5.43703000	3.73954100	0.20150200	H	8.90867300	9.83329600	0.34656100
C	5.24746400	5.06912200	0.65173200	H	10.18957100	8.59048200	0.64686700
C	6.66508700	3.41715300	-0.41661300	H	9.69147300	8.96035900	-1.03180300
C	6.24692200	6.03455800	0.49760700	O	-8.41741600	-1.82270900	1.52775400
H	4.30915900	5.32941900	1.14370800	C	-9.53156900	0.58710000	0.40817700
C	7.66490000	4.37573200	-0.57192900	H	-8.76382500	0.84567400	-0.32700200
H	6.86919800	2.40753600	-0.75616400	O	-10.53105800	1.59693100	0.24589800
C	7.47508600	5.69242800	-0.11239600	C	-11.44966700	1.74841700	1.32537800
H	6.08994300	7.04744100	0.86721900	H	-12.27757100	2.35905800	0.93567200
H	8.60451700	4.10052400	-1.04464800	H	-11.85667200	0.77825800	1.67229800
C	-1.85351300	-2.42779900	2.78267700	H	-10.98005200	2.27787700	2.17160400
C	-2.87124300	-1.77821500	3.51727900	O	-6.32787400	2.20701200	3.21626300
C	-1.98855200	-3.80754100	2.51681400	C	-7.06703200	4.43480300	1.51518600
C	-4.00688800	-2.47122400	3.94177500	H	-7.49848500	3.89659100	0.66244000
H	-2.76779600	-0.71463400	3.73670500	O	-7.22402100	5.81352900	1.16022600
C	-3.11956000	-4.50855500	2.94892600	C	-6.48584500	6.74283100	1.95179400
H	-1.22885200	-4.30964100	1.91835300	H	-6.85530000	7.73963300	1.67052500
C	-4.15131400	-3.84391800	3.64488600	H	-6.65269700	6.59379400	3.03601900
H	-4.78705300	-1.94852300	4.49178900	H	-5.40518800	6.67954600	1.73848400
H	-3.24801600	-5.56354900	2.70682700	O	8.38392400	0.50495400	-1.49120100
C	8.60926900	6.64827900	-0.26543800	O	4.03863900	-0.18892200	-1.77072900

O	-0.84111300	-2.59411100	-1.71497700	H	4.07497500	-4.95756900	-0.09764700
O	-4.57521100	-1.73234100	-2.76615500	H	2.79084500	-6.06317800	-0.69941300
O	-7.67478200	-1.42028900	-0.56517200	C	-4.54832600	-3.30396400	-0.25525700
H	8.96390600	-0.10167600	-3.37823300	H	-5.19167100	-2.40474900	-0.23302600
H	-0.55732000	-4.65506600	-1.56946400	H	-4.10085700	-3.44377000	0.74446600
H	-4.93173100	-1.52766500	-4.80580900	O	-5.32398800	-4.44330000	-0.62277300
H	-9.14759000	-2.82166900	-0.06699400	C	-6.31119100	-4.73271000	0.36492000
H	-8.25719600	2.11433100	3.83171700	H	-5.84826600	-5.14288900	1.28053900
O	-8.15548600	1.87627500	1.77070400	H	-6.89394200	-3.83026700	0.63067200
C	10.06346700	-2.35886100	-2.01192800	H	-6.98072100	-5.49145400	-0.06810300
H	9.65846400	-1.93436500	-2.94136600	C	-8.43837100	-3.42292400	-2.95267900
H	11.16892800	-2.26898000	-2.04304300	H	-8.90250900	-3.68383000	-1.98120400
O	9.67627000	-3.72648300	-1.90421000	H	-8.09925300	-4.36325100	-3.43131000
C	10.18387100	-4.49250800	-2.98450800	O	-9.36771200	-2.74322000	-3.78595400
H	9.84751300	-5.52806900	-2.83086200	C	-10.64797100	-3.34852100	-3.75231900
H	9.80048400	-4.12526200	-3.95923600	H	-11.29707400	-2.76231700	-4.41973300
H	11.29271400	-4.46835100	-3.01344900	H	-10.61782100	-4.39890300	-4.10981000
C	5.77333300	-2.67829500	-1.73995000	H	-11.06852700	-3.33381600	-2.72656100
H	4.91186600	-2.67134900	-1.05862100	C	-7.36914800	-0.78692200	3.39798500
H	6.61509900	-3.22005100	-1.26506800	H	-6.75856900	-1.70306200	3.42360700
O	5.33384200	-3.37125600	-2.90455900	H	-6.74122000	0.06959100	3.69280300
C	6.38745100	-3.78918100	-3.77578600	O	-8.48744900	-0.91577900	4.28558400
H	5.96569600	-4.57860000	-4.41715300	C	-8.05961100	-0.87366800	5.64130200
H	6.75527500	-2.95927400	-4.40193100	H	-7.36317000	-1.70297900	5.87226000
H	7.24127300	-4.18924700	-3.19824800	H	-7.55111800	0.08481600	5.87236900
C	1.88364600	-3.55012600	-0.32787900	H	-8.96015200	-0.96876300	6.26599500
H	1.05416300	-4.24204500	-0.07065000	C	-4.05446800	2.10157200	2.42340000
H	2.49432100	-3.40056800	0.57972700	H	-4.02096900	1.01657400	2.64681000
O	2.67691200	-4.08449800	-1.38478000	H	-3.43992000	2.27173800	1.52187500
C	3.44244700	-5.20799900	-0.97258600	O	-3.55338800	2.85317800	3.52009300
H	4.08692500	-5.47225600	-1.82026500	C	-2.14572900	2.70178500	3.62884200

H	-1.85177600	1.64441100	3.79030400
H	-1.63131000	3.05710600	2.71479300
H	-1.81812800	3.30124200	4.48991800
C	1.16607700	2.91958000	3.08075900
C	2.12873800	1.18707700	4.27412200
C	1.10491600	3.73616800	4.21815600
H	0.81185700	3.26552200	2.10925700
C	2.10748400	1.92743000	5.46360700
H	2.52800100	0.17295100	4.23926600
C	1.58438300	3.22884700	5.43472400
H	0.68899000	4.74194500	4.14672200
H	2.49463700	1.49249100	6.38597700
H	1.55340900	3.83631100	6.34156300
N	1.66575300	1.66933100	3.10471200

(c) α-oligoamylose-strapped porphyrin in the absence of pyridine.

C	5.99172300	0.75267300	3.13614900
C	6.65227700	0.52498700	1.75933800
C	7.68004400	-0.63671200	1.75187700
C	7.30546300	-1.83233000	2.67681800
C	5.52813400	-0.60460600	3.69966300
H	5.84133700	0.25183900	1.07299100
H	6.71941600	1.15526900	3.86287400
H	6.63428500	-2.49514300	2.11461900
H	8.66899600	-0.26888100	2.03711400
C	4.01738900	-2.40438700	3.02559300
C	2.92242800	-2.29224700	4.11439400
C	3.45772900	-2.79487100	1.63194800
H	4.78575600	-3.12996700	3.32715700
C	1.94448600	-3.48206000	4.00310000
H	2.35429700	-1.37727600	3.92027400
H	2.97787200	-1.89558400	1.22983700
C	1.40492100	-3.50997400	2.55219300
H	2.46840100	-4.44680400	4.15628000
O	6.66216000	-1.43478300	3.90733300
O	2.46508100	-3.84757700	1.69133100
O	4.85645600	1.60814300	3.02790900
O	7.18559200	1.73315800	1.18140400
O	3.44146500	-2.10181100	5.43744300
O	0.92580800	-3.33279600	4.98668900
C	-0.42200800	-1.84313200	2.49175300
C	-0.39001600	-0.35445700	2.91645700
C	-1.23129600	-1.98053100	1.17391600
H	-0.82939400	-2.47605700	3.28966400
C	-1.81882100	0.22154200	3.13812000
H	0.03747600	0.19341500	2.06686000
H	-0.54556200	-1.70434800	0.37775100
C	-2.86051500	-0.59991200	2.33826500
H	-2.10693100	0.11567800	4.20260500
O	-2.32227400	-1.01523500	1.05804100
O	0.51387800	-0.09426300	3.98599400
O	-1.89652000	1.58273200	2.76044300
H	-3.10229500	-1.51252200	2.90525800
C	-5.20485400	-0.18091500	2.73877800
C	-5.97627900	1.14527500	2.82107400
C	-5.99015800	-1.26897500	1.98699800
H	-4.97615400	-0.53170000	3.75717500
C	-7.47331000	0.97338800	3.14175500
H	-5.90137700	1.62210400	1.83316200
H	-6.07957500	-0.96970200	0.92969100

C	-8.10686700	-0.21438300	2.36436500	H	6.08366800	1.67873400	-1.58687600
H	-7.57349400	0.71762000	4.21615300	H	4.85729300	3.70789900	-3.50897100
O	-7.30838000	-1.37745600	2.57883700	O	8.93767000	4.13751500	-3.66302300
O	-8.07512800	2.22739700	2.87049800	H	-8.41581100	-0.73603100	-2.73739900
O	-5.38410600	1.96140700	3.82771500	O	4.42473700	3.97140500	-1.57309200
C	-9.22605600	-0.50297200	0.20380400	C	-8.96086100	-2.34744800	-4.56979100
C	-9.61511000	0.59036300	-0.82519300	C	4.74457400	3.70113900	-0.18839700
C	-8.67681000	-1.79380100	-0.48324900	H	4.13589000	2.85242700	0.15846900
H	-10.10140900	-0.75526400	0.83187400	H	5.80070100	3.42316400	-0.06929500
C	-10.35497200	0.03682000	-2.07166300	C	4.45124600	4.94292600	0.62279500
H	-8.65916600	1.01192500	-1.17063700	C	5.45353800	5.91374700	0.77307900
H	-7.63147300	-1.59177700	-0.78265100	C	3.17104100	5.17107700	1.21220000
C	-9.45351400	-1.09231600	-2.62093700	C	5.23063200	7.08303300	1.51517300
H	-11.30899300	-0.43143800	-1.79097200	H	6.41253200	5.75238500	0.27829100
O	-9.94047900	-1.58215700	-3.82683700	C	2.95768900	6.35603400	1.96580600
O	-9.46086100	-2.12813800	-1.63405300	C	3.97935500	7.29764900	2.11958300
O	-10.70961900	1.04973100	-3.00114600	H	6.02701200	7.82226000	1.62170900
O	-10.26983500	1.68844700	-0.19469000	H	1.97940200	6.52036500	2.42032200
C	8.84222300	-1.62908700	-0.26896000	H	3.79859000	8.20162000	2.70490500
C	10.07810800	-0.69550700	-0.29004300	C	-8.73909300	-3.75261600	-4.03926100
H	10.81788100	-1.17850200	-0.95838300	C	-9.79537900	-4.67369800	-4.12501500
C	7.95201000	-0.69800700	-2.29687300	C	-7.50543400	-4.16636100	-3.45903800
C	8.95411900	0.50112700	-2.24104700	C	-9.65868100	-5.98930100	-3.66436800
H	7.00933200	-0.37794400	-1.83111700	H	-10.74252100	-4.33921300	-4.55406500
H	9.70550500	0.34444400	-3.03196800	C	-7.37082100	-5.50880900	-3.01289400
O	10.60675100	-0.62080600	1.03145600	C	-8.43436300	-6.40787400	-3.11210900
C	7.66938700	2.10802100	-3.60326700	H	-10.49544400	-6.68645300	-3.74136000
C	7.60200400	3.65335600	-3.67425400	H	-6.42293700	-5.81717400	-2.57011000
H	7.10977700	3.90748800	-4.63369200	H	-8.31181800	-7.43354600	-2.75761900
C	5.54812400	1.95188900	-2.51261600	C	-6.40660300	-3.28217600	-3.26207600
C	5.34283500	3.47923000	-2.54928300	C	-5.42253800	-2.59554900	-2.98740500

C	2.10109800	4.25182700	1.02839800	H	-6.67017300	-0.25658900	-3.48251600
C	1.16925400	3.48486700	0.79331000	H	-6.83664500	2.23718700	-2.41024600
C	-4.39904400	-1.71484000	-2.54527900	H	-3.66847800	5.14539000	0.81925400
C	0.17110700	2.57829700	0.34853300	H	-0.98782300	5.04862300	1.23444200
Zn	-2.19204200	0.28960900	-0.75698200	C	-11.66696100	1.52281300	0.04139700
N	-2.21723600	2.32301500	-0.27464900	H	-11.97229900	2.39219100	0.63971000
N	-0.10402500	0.40605900	-0.81863900	H	-12.23315700	1.50916700	-0.90526400
N	-4.11202700	0.51873800	-1.48622500	H	-11.88730200	0.59819600	0.61088200
N	-2.01005100	-1.44641800	-1.95005600	C	-9.63695900	1.87863500	-3.44824400
C	-3.05994700	-2.18095400	-2.44456000	H	-10.05626700	2.50690800	-4.24628000
C	-4.80358600	-0.37849800	-2.25712300	H	-9.25868600	2.52835500	-2.63868200
C	-4.90604200	1.64548400	-1.40540200	H	-8.80053400	1.28626100	-3.86316700
C	-0.86855500	-2.16932500	-2.23974100	C	-9.45985900	2.29263900	3.18685800
C	0.77150800	-0.60318200	-1.17000600	H	-10.05956000	1.66598900	2.50361500
C	0.63369200	1.30474100	-0.08577900	H	-9.64912700	1.98548500	4.23582400
C	-1.17457900	3.02926800	0.26520900	H	-9.75708500	3.34212900	3.05183600
C	-3.33364800	3.12648000	-0.14361600	C	-4.79671500	3.15905400	3.31030900
C	-6.01923600	0.21273400	-2.75438200	H	-3.98403700	2.92372800	2.60736400
C	-6.08841200	1.47428800	-2.22466600	H	-5.55749300	3.78861500	2.81439400
C	-1.22215600	-3.39666800	-2.92919400	H	-4.38684200	3.69763500	4.17837700
C	-2.59008700	-3.41877600	-3.02365100	C	-1.20275100	2.46004800	3.64615900
C	2.06584800	-0.35785400	-0.57552400	H	-1.54724200	2.31102800	4.68874600
C	1.97483400	0.81706900	0.12176900	H	-0.11161400	2.30880000	3.60289000
C	-1.62814900	4.30537100	0.76718900	H	-1.45365700	3.47607300	3.31691000
C	-2.97863800	4.35421900	0.54561600	C	0.08650300	-0.45101600	5.30413800
C	-4.61070400	2.82384400	-0.67480200	H	-0.43759400	0.39628100	5.78369300
C	0.44829600	-1.76834700	-1.91101600	H	-0.57075200	-1.33400400	5.30371200
H	2.73062400	1.28939200	0.74267800	H	0.99420800	-0.70378000	5.86690900
H	2.93068500	-1.00096500	-0.68061400	C	0.06761200	-4.46448000	5.09681300
H	-0.51610200	-4.12638100	-3.31283500	H	-0.51838900	-4.32294400	6.01679500
H	-3.22741600	-4.16235600	-3.49541900	H	-0.62803300	-4.54750300	4.24012400

H	0.65090600	-5.40371600	5.17686800	C	1.59717400	-2.62694400	-2.31726100
C	4.27949900	-3.13916200	5.94397000	C	2.66051700	-2.06197700	-3.06204800
H	3.79882700	-4.13290800	5.87708600	C	1.69129400	-3.98076100	-1.92544900
H	5.25502200	-3.16719000	5.42700200	C	3.80170200	-2.81237600	-3.35937300
H	4.44624400	-2.89846100	7.00379700	H	2.59894700	-1.02183600	-3.38687200
C	5.11856500	2.97681000	3.32046800	C	2.82007100	-4.74104800	-2.24588700
H	5.60330500	3.08795100	4.31186600	H	0.89120600	-4.41725000	-1.32739500
H	5.75318800	3.44937200	2.55362800	C	3.89924100	-4.15771400	-2.94263300
H	4.14440700	3.48377500	3.33405400	H	4.62055600	-2.35303700	-3.91167300
C	8.24668900	2.37489200	1.89537900	H	2.91068800	-5.77492800	-1.91251800
H	7.91545600	2.73409500	2.88545100	C	-9.11188600	6.42396300	0.13721000
H	9.12540000	1.71962300	2.01836600	O	-10.16393800	6.04910800	0.63978900
H	8.53974000	3.23247800	1.27467100	O	-8.89265100	7.71568100	-0.25616400
C	11.98145600	-0.24575000	1.11359400	C	5.13828100	-4.97440500	-3.12212400
H	12.59499100	-0.85508200	0.41963700	O	5.23532400	-6.16765400	-2.86484900
H	12.12397800	0.81949200	0.87983100	O	6.18483400	-4.21050600	-3.54850100
H	12.29271200	-0.45342500	2.14752700	C	7.48227200	-4.85059200	-3.58610200
C	9.10541400	5.41514400	-4.27253000	H	8.19913300	-4.03096900	-3.71113500
H	10.19040500	5.57299900	-4.36574500	H	7.66280800	-5.39040100	-2.64585700
H	8.65031000	5.43833300	-5.28460100	H	7.52741800	-5.56215100	-4.42434900
H	8.66224100	6.21752800	-3.66228200	C	-10.00066700	8.61317300	-0.02966900
C	-5.73727200	3.78362300	-0.49215500	H	-9.66238900	9.58937200	-0.39828900
C	-5.62769500	5.15611900	-0.81906200	H	-10.88989800	8.27189900	-0.58036100
C	-6.97870300	3.31215500	-0.00214900	H	-10.24357700	8.66084700	1.04241100
C	-6.70436700	6.02879500	-0.62990100	O	8.45744000	-1.86888700	-1.60128400
H	-4.69220200	5.52867500	-1.23761200	C	9.62315500	0.65997000	-0.85437800
C	-8.05628700	4.17776700	0.18732700	H	8.84420700	1.04035500	-0.18808400
H	-7.10343200	2.26098200	0.24486200	O	10.64510300	1.66201900	-0.81411200
C	-7.92914500	5.54792300	-0.11487600	C	11.56265300	1.66811900	-1.90360300
H	-6.60372400	7.08223900	-0.88905500	H	12.39741800	2.31412900	-1.59459600
H	-9.00004600	3.79079800	0.56311200	H	11.95722000	0.65817100	-2.12975500

H	11.09567200	2.09103700	-2.81070000	O	-4.93476700	-3.10172100	3.31064200
O	6.34765900	1.57555300	-3.65625700	C	-5.99903200	-3.55696900	4.14328300
C	6.73246900	4.17438700	-2.49326600	H	-5.52788900	-4.06547500	4.99828000
H	7.25415200	3.88632100	-1.57052000	H	-6.63034300	-2.72814000	4.50302700
O	6.66545100	5.60074500	-2.42198800	H	-6.64593000	-4.27535600	3.60045600
C	5.77386600	6.22240100	-3.34750100	C	-1.70797800	-3.39801900	0.89083100
H	5.95151000	7.30344500	-3.25625500	H	-0.82237500	-4.01712100	0.63854400
H	5.97588500	5.91491800	-4.39137500	H	-2.37769200	-3.38510800	0.01193800
H	4.72301200	6.00195200	-3.09701500	O	-2.37403800	-3.91810900	2.03595700
O	-8.21914800	0.13700500	1.01135800	C	-3.03543900	-5.14543700	1.76297400
O	-3.99297400	0.14106800	2.03107400	H	-3.55264300	-5.43419500	2.68640900
O	0.90643000	-2.23578700	2.15228700	H	-3.77996900	-5.02297000	0.95193900
O	4.61703300	-1.12675400	2.75507300	H	-2.31457300	-5.93332700	1.46409300
O	7.68573600	-1.11197300	0.38328300	C	4.53454300	-3.21072300	0.64044700
H	-9.09557000	-0.47961700	2.77521000	H	5.13004800	-2.31728500	0.37252400
H	0.63362300	-4.28617800	2.42006200	H	4.04123400	-3.59017300	-0.27025300
H	5.05972900	-0.49442100	4.68557100	O	5.38839100	-4.20519700	1.20464400
H	9.12618200	-2.61141400	0.14322700	C	6.36496400	-4.63573300	0.25901100
H	8.19166700	1.68988100	-4.47987500	H	5.90427900	-5.25236900	-0.53393300
O	8.33282800	1.78526400	-2.41100200	H	6.88036800	-3.77480700	-0.20889200
C	-8.73166600	-3.03461400	0.40760900	H	7.09430400	-5.24712500	0.81182100
H	-8.51288400	-2.77877900	1.45518900	C	8.52518500	-2.65200400	3.08510300
H	-9.75530800	-3.45494800	0.34162900	H	8.97413300	-3.09477600	2.17460500
O	-7.77109500	-3.97542500	-0.07337500	H	8.19887600	-3.48530500	3.73985300
C	-7.96603600	-5.25769900	0.49719200	O	9.46411500	-1.82591600	3.75706000
H	-7.18592000	-5.91293500	0.08407700	C	10.72244800	-2.46199800	3.88651900
H	-7.87630800	-5.23383400	1.60412800	H	11.38368600	-1.76049600	4.41657100
H	-8.96136500	-5.66713900	0.23202000	H	10.65053800	-3.40236500	4.47208300
C	-5.34386700	-2.65452900	2.01798700	H	11.15619400	-2.69497700	2.89318900
H	-4.42510100	-2.61325900	1.42030900	C	7.64882700	-1.18890600	-3.70942200
H	-6.04108600	-3.37073100	1.54779400	H	6.93927500	-2.02913900	-3.63831300

H	7.16924800	-0.38163800	-4.28268000
O	8.85662900	-1.61741100	-4.34782500
C	8.62454300	-1.91270300	-5.71723700
H	7.87937800	-2.72483200	-5.83808700
H	8.25600100	-1.02233100	-6.26750900
H	9.58512700	-2.23439300	-6.14575800
C	4.26786700	1.12746900	-2.53627100
H	4.55376400	0.06178200	-2.55625100
H	3.73464600	1.31497000	-1.59620300
O	3.43210500	1.37332100	-3.66465700
C	2.25230700	2.12623200	-3.34194600
H	1.55720000	1.53351000	-2.72158600
H	2.50349200	3.05684100	-2.80598300
H	1.76889400	2.36412600	-4.30091700
H	-8.00553800	-1.79445600	-4.60340800
H	-9.37643800	-2.39335000	-5.58704000

(d) α-oligoamylose-strapped porphyrin in the presence of pyridine.

C	6.11089500	0.50869100	3.25861100
C	6.74060200	0.36408400	1.85739100
C	7.77532700	-0.78691600	1.76347600
C	7.42540000	-2.03652800	2.62574700
C	5.66486400	-0.88008400	3.75531600
H	5.91565800	0.12353500	1.17544000
H	6.85283500	0.87151500	3.99152400
H	6.74645500	-2.67174700	2.04176400
H	8.76691900	-0.42912500	2.05247500
C	4.14660500	-2.64972200	3.02591300
C	3.06182100	-2.59852600	4.12791800
C	3.56434100	-2.98259600	1.62753000
H	4.92577700	-3.38049900	3.28422400
C	2.12577900	-3.81764600	3.98560700
H	2.46410200	-1.69576600	3.96528200
H	3.04828300	-2.07741700	1.29171500
C	1.54752800	-3.79482400	2.54595400
H	2.69464300	-4.76590900	4.07120400
O	6.80873800	-1.71351800	3.88990800
O	2.60492900	-4.06454400	1.65249100
O	4.97294800	1.36679800	3.22206400
O	7.25021900	1.60909800	1.33781300
O	3.59629900	-2.42862100	5.44810500
O	1.13974200	-3.76553000	5.01000200
C	-0.33915400	-2.21300700	2.59739700
C	-0.39513800	-0.73872800	3.05032000
C	-1.21259000	-2.38350500	1.32268400
H	-0.66781400	-2.87461400	3.40780700
C	-1.84888800	-0.31704300	3.39705800
H	-0.08794000	-0.12807000	2.19444100
H	-0.57664900	-2.09932800	0.48281600
C	-2.87440600	-1.10229200	2.51072200
H	-2.07853800	-0.59275400	4.44513100
O	-2.31318400	-1.45764000	1.24483100
O	0.56425800	-0.42594700	4.06262100
O	-2.03017700	1.07999000	3.22940700
H	-3.16417600	-2.03020200	3.03491600
C	-5.26657300	-0.76042100	2.64224800
C	-6.01692800	0.50007900	3.09645500
C	-6.02634100	-1.42600200	1.48560900
H	-5.18571200	-1.47170700	3.47988500
C	-7.52755600	0.27053400	3.30896600

H	-5.89502500	1.24271900	2.29455200	C	5.51682100	2.03869400	-2.29253400
H	-6.13191300	-0.70200200	0.66004100	C	5.30785700	3.56520300	-2.23842200
C	-8.17115100	-0.65831800	2.23294700	H	6.08188200	1.71556400	-1.40106700
H	-7.65298200	-0.26206100	4.27369600	H	4.78593400	3.84353100	-3.16552900
O	-7.33790100	-1.78260400	1.99370200	O	8.86019700	4.29427500	-3.44395800
O	-8.11494300	1.56186200	3.37959400	H	-8.36461100	-0.57396700	-2.66718700
O	-5.44107800	0.97388300	4.31051100	O	4.42562900	3.99802100	-1.20274800
C	-9.42059900	-0.41090600	0.15906300	C	-8.80179500	-1.92394300	-4.69062100
C	-9.59569700	0.77193700	-0.83383400	C	4.80055000	3.64660300	0.15211800
C	-8.99985200	-1.74247400	-0.55238900	H	4.20536900	2.77845000	0.47219700
H	-10.36436400	-0.57548400	0.71464000	H	5.85979800	3.36246400	0.20967800
C	-10.28423200	0.36587200	-2.16378200	C	4.54599800	4.83757500	1.04821700
H	-8.57148300	1.08721600	-1.08094300	C	5.54238900	5.81696100	1.18296400
H	-7.90938400	-1.70423000	-0.72142700	C	3.30708700	5.00993200	1.73695800
C	-9.44216800	-0.81468600	-2.70037100	C	5.35426500	6.94070200	2.00122200
H	-11.29578100	-0.02488800	-1.98529500	H	6.46717400	5.70037100	0.61574900
O	-9.81977700	-1.16956200	-3.99135200	C	3.12859900	6.14941200	2.56604500
O	-9.68211700	-1.89953300	-1.80459400	C	4.14428000	7.10046500	2.69974400
O	-10.47356800	1.45458700	-3.05366900	H	6.14566800	7.68715200	2.09403900
O	-10.16016600	1.91410400	-0.20004600	H	2.18240700	6.27018500	3.09593700
C	8.90663700	-1.63817500	-0.33856300	H	3.99141400	7.96858500	3.34438300
C	10.12470000	-0.68154100	-0.33507300	C	-8.63183100	-3.35263600	-4.20449300
H	10.85823300	-1.11426200	-1.04338100	C	-9.69945100	-4.24901600	-4.37261000
C	7.95020400	-0.60860000	-2.28729000	C	-7.42840700	-3.81536500	-3.59901600
C	8.93940500	0.59806600	-2.19558100	C	-9.59905600	-5.58818700	-3.97660000
H	7.01948100	-0.32779200	-1.77429100	H	-10.62552500	-3.87574400	-4.81513700
H	9.67464200	0.49126200	-3.00958300	C	-7.33001500	-5.18114200	-3.21728000
O	10.68042000	-0.66542600	0.97715900	C	-8.40143800	-6.05575900	-3.40516400
C	7.60090000	2.25859600	-3.44082600	H	-10.44294100	-6.26625800	-4.11914100
C	7.52625000	3.80529800	-3.43291900	H	-6.40536400	-5.52766000	-2.75377800
H	7.00051000	4.10498900	-4.36108600	H	-8.30692900	-7.10100800	-3.10304100

C	-6.32125300	-2.96143600	-3.32234100	H	-0.47633400	-3.99848000	-3.26697100
C	-5.33357500	-2.30989400	-2.98154700	H	-3.18247700	-3.93445600	-3.50159300
C	2.24542400	4.07729500	1.58032400	H	-6.60696200	0.06913000	-3.15886400
C	1.32372400	3.29294100	1.36229900	H	-6.74894800	2.41065800	-1.78307700
C	-4.30157900	-1.48895900	-2.45088800	H	-3.56555300	4.74845600	1.92949700
C	0.31909800	2.40607900	0.89547800	H	-0.87710500	4.62333000	2.29684200
Zn	-1.94746900	0.57730300	-0.96377900	C	-11.57633100	1.89616700	-0.03299800
N	-2.07826800	2.24060000	0.27839800	H	-11.81428600	2.78786800	0.56335300
N	0.03669400	0.35556200	-0.47072000	H	-12.09472800	1.95180400	-1.00559600
N	-4.00733000	0.59699100	-1.13443700	H	-11.92111400	0.99521400	0.51180600
N	-1.90591600	-1.31847300	-1.84367700	C	-9.30181800	2.19974000	-3.37755300
C	-2.97302000	-1.99460400	-2.37967800	H	-9.60227700	2.90538900	-4.16481800
C	-4.70422900	-0.19228300	-2.00685800	H	-8.92768200	2.76878100	-2.50775900
C	-4.79424900	1.70350800	-0.89977500	H	-8.49298200	1.55466200	-3.76820200
C	-0.78261000	-2.06245200	-2.13879200	C	-9.50905800	1.55449800	3.65650100
C	0.89020400	-0.62480100	-0.92336000	H	-10.08684900	1.14454200	2.80833100
C	0.78307200	1.18578100	0.32244800	H	-9.73751500	0.97201700	4.57277000
C	-1.03868100	2.84019100	0.93498600	H	-9.80055100	2.60344300	3.80803600
C	-3.20719400	2.97635500	0.57241600	C	-4.98065900	2.32366600	4.21660600
C	-5.93263100	0.45168900	-2.40212700	H	-4.20398000	2.41601900	3.43998300
C	-5.99138400	1.63723300	-1.71680300	H	-5.81705400	3.01272300	4.00102100
C	-1.16301300	-3.25041800	-2.88330400	H	-4.54565100	2.56876500	5.19741700
C	-2.52969800	-3.22160100	-3.00408800	C	-1.47546300	1.85918600	4.28415600
C	2.20014700	-0.43237700	-0.33914800	H	-1.85089800	1.51128200	5.26755100
C	2.12966900	0.67922500	0.45837300	H	-0.37329300	1.82281900	4.28615600
C	-1.50669200	3.98590800	1.68188700	H	-1.81568100	2.88816900	4.11125200
C	-2.86262800	4.04838300	1.48994000	C	0.26819100	-0.85806000	5.39443300
C	-4.48603400	2.76334000	-0.00486600	H	-0.29896800	-0.08022600	5.93768300
C	0.53914900	-1.71253100	-1.76399600	H	-0.29730000	-1.80124300	5.41143800
H	2.89645700	1.08745700	1.11129400	H	1.23355200	-1.03626800	5.88654000
H	3.05933300	-1.06676200	-0.51916900	C	0.33569800	-4.94049100	5.08367700

H	-0.22438700	-4.87490600	6.02822600	H	-6.41991100	7.02604900	0.47283200
H	-0.38004500	-5.00585700	4.24408400	H	-8.88928000	3.57437800	1.29818000
H	0.96420600	-5.85395400	5.09602400	C	1.67108400	-2.55147000	-2.25346800
C	4.41220500	-3.49006000	5.93782300	C	2.70414500	-1.94545300	-3.00677200
H	3.88128100	-4.45979500	5.92369000	C	1.77560300	-3.92434800	-1.94100800
H	5.35767000	-3.57913700	5.37313200	C	3.82957100	-2.67873100	-3.39373800
H	4.64686200	-3.23024000	6.98010100	H	2.63080000	-0.88860400	-3.26978800
C	5.23224300	2.70918100	3.61935900	C	2.88843300	-4.66601900	-2.35016700
H	5.72111700	2.74423300	4.61418400	H	1.00097400	-4.39222000	-1.33321900
H	5.86216700	3.24278600	2.88884700	C	3.94004100	-4.04540700	-3.05708700
H	4.25650900	3.20894700	3.67676400	H	4.62702000	-2.18958900	-3.95162600
C	8.32861400	2.21366500	2.05858200	H	2.98998900	-5.71656200	-2.07759300
H	8.03422900	2.48140900	3.08826500	C	-8.96870400	6.24390600	1.29569600
H	9.22420500	1.57045200	2.08823100	O	-10.05304000	5.80579100	1.65964400
H	8.57670300	3.12731300	1.50141700	O	-8.71236800	7.58202800	1.16630800
C	12.05474500	-0.28743000	1.04723700	C	5.17054200	-4.84955900	-3.32777100
H	12.65710400	-0.86590200	0.31786700	O	5.28233700	-6.05159800	-3.12354600
H	12.18821100	0.78708600	0.85347000	O	6.19544100	-4.06536200	-3.77203600
H	12.38725700	-0.53447400	2.06580000	C	7.49481400	-4.69397400	-3.87592400
C	9.00341200	5.60349200	-3.98867200	H	8.20370400	-3.86412900	-3.97818100
H	10.08398800	5.77027300	-4.11244100	H	7.70363200	-5.27903400	-2.96930000
H	8.51178200	5.67988700	-4.98098400	H	7.52213700	-5.36172800	-4.75028400
H	8.58122200	6.36986600	-3.32009900	C	-9.82163300	8.44463200	1.49635600
C	-5.60381900	3.69303800	0.32471200	H	-9.45144900	9.46534500	1.33955900
C	-5.46952200	5.10007700	0.24073200	H	-10.68082100	8.23384200	0.84214800
C	-6.86181600	3.16851900	0.70702000	H	-10.12710500	8.29437400	2.54270600
C	-6.53970900	5.94580600	0.54997000	O	8.49405800	-1.80778600	-1.67471400
H	-4.51979400	5.52344900	-0.08822300	C	9.63409500	0.69370600	-0.81613900
C	-7.93287000	4.00637500	1.01580800	H	8.86105800	1.02140200	-0.11586000
H	-7.01029700	2.09406300	0.76468500	O	10.63820700	1.71134500	-0.73917400
C	-7.78410700	5.40528000	0.94626700	C	11.53269400	1.79566700	-1.84446100

H	12.35963500	2.44307400	-1.51778100	H	-4.45464600	-2.34980800	0.38834300
H	11.94451300	0.80829300	-2.13161700	H	-6.06659300	-3.13164400	0.17759700
H	11.03818500	2.25511300	-2.71854500	O	-4.94512100	-3.63742600	1.86611000
O	6.27834900	1.72516600	-3.48010200	C	-6.00856900	-4.39777800	2.43808400
C	6.69726000	4.26199200	-2.19728400	H	-5.54485700	-5.28097900	2.90420400
H	7.25161500	3.93057900	-1.30895400	H	-6.56018800	-3.82260400	3.20120700
O	6.63003900	5.68323600	-2.05188600	H	-6.72683200	-4.71665600	1.66060700
C	5.70405200	6.34729700	-2.91029000	C	-1.64343900	-3.83595700	1.08990000
H	5.88172700	7.42310800	-2.76981300	H	-0.78696900	-4.39142700	0.65128200
H	5.86883800	6.09515300	-3.97545100	H	-2.47310700	-3.85213500	0.36098100
H	4.66339200	6.10937600	-2.63356200	O	-2.03663000	-4.45510300	2.31406200
O	-8.41982900	0.08606800	1.06744500	C	-2.59820300	-5.73963300	2.08729400
O	-3.98036800	-0.30705500	2.22614200	H	-2.86244800	-6.15205800	3.07234200
O	1.00165300	-2.52475300	2.21040600	H	-3.50588800	-5.66149100	1.46308000
O	4.73262700	-1.35462200	2.80717200	H	-1.87004300	-6.41594500	1.59238300
O	7.75847800	-1.18205500	0.36893200	C	4.62644800	-3.30907700	0.58873400
H	-9.11479400	-1.09011500	2.61043800	H	5.20149900	-2.38900600	0.37002700
H	0.79999100	-4.59055400	2.39763200	H	4.12140200	-3.63585000	-0.33559000
H	5.22122100	-0.82625900	4.75705800	O	5.50888000	-4.32395200	1.06659500
H	9.21814700	-2.63721400	0.00843600	C	6.45924600	-4.68502500	0.06735800
H	8.09721500	1.88614600	-4.35235400	H	5.97860000	-5.25236600	-0.75050700
O	8.30055800	1.88218600	-2.28657200	H	6.95677500	-3.79204000	-0.35863600
C	-9.36572300	-3.01116600	0.22317400	H	7.20788000	-5.32611900	0.55737300
H	-9.19756100	-2.89820000	1.30466300	C	8.65915600	-2.87037100	2.95518800
H	-10.44370800	-3.20930400	0.05229500	H	9.08618900	-3.25393500	2.00790100
O	-8.57364500	-4.07626300	-0.28917400	H	8.35468500	-3.74340000	3.56696400
C	-9.06154100	-5.34323300	0.11325700	O	9.61205200	-2.07955500	3.65056700
H	-8.41304100	-6.09545400	-0.35687400	C	10.87610800	-2.71419300	3.70813000
H	-9.03133000	-5.46625700	1.21633600	H	11.54935100	-2.04022000	4.25847400
H	-10.10431400	-5.49905000	-0.23042600	H	10.82537000	-3.68699800	4.24061900
C	-5.36783800	-2.67380700	0.90178300	H	11.28255800	-2.88805000	2.69133200

C	7.60487400	-1.02430900	-3.71377100
H	6.91729400	-1.88386400	-3.66527400
H	7.08701900	-0.19602800	-4.21996900
O	8.79579300	-1.38713200	-4.42182600
C	8.51853600	-1.59387200	-5.79885500
H	7.77993700	-2.40721300	-5.94816200
H	8.11930700	-0.67413500	-6.27476200
H	9.46717200	-1.87174300	-6.28141500
C	4.23535400	1.21883500	-2.31669900
H	4.51437100	0.15455400	-2.39711200
H	3.73139200	1.36226000	-1.35368600
O	3.36493100	1.52727900	-3.40512000
C	2.17557700	2.21658100	-2.99535400
H	1.52237200	1.56566400	-2.38814400
H	2.41708200	3.12185900	-2.41156100
H	1.64659500	2.49479600	-3.91769900
H	-7.83904300	-1.38474800	-4.63539000
H	-9.14436900	-1.92324500	-5.73578600
N	-1.56725800	1.70223600	-2.80012900
C	-1.25664900	3.01381300	-2.74674100
C	-1.60013800	1.09364100	-4.00278400
C	-0.97284400	3.76911500	-3.89101600
H	-1.23915800	3.45014500	-1.74757600
C	-1.32650500	1.76929300	-5.19882300
H	-1.85189300	0.03261600	-3.98296500
C	-1.00861900	3.13427900	-5.14163400
H	-0.72461600	4.82696500	-3.79818800
H	-1.36245500	1.23428000	-6.14838100
H	-0.78988700	3.69217900	-6.05424000