SUPPORTING INFORMATION

G-quadruplex binding optimization by gold(III) insertion into the center of a porphyrin

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Content

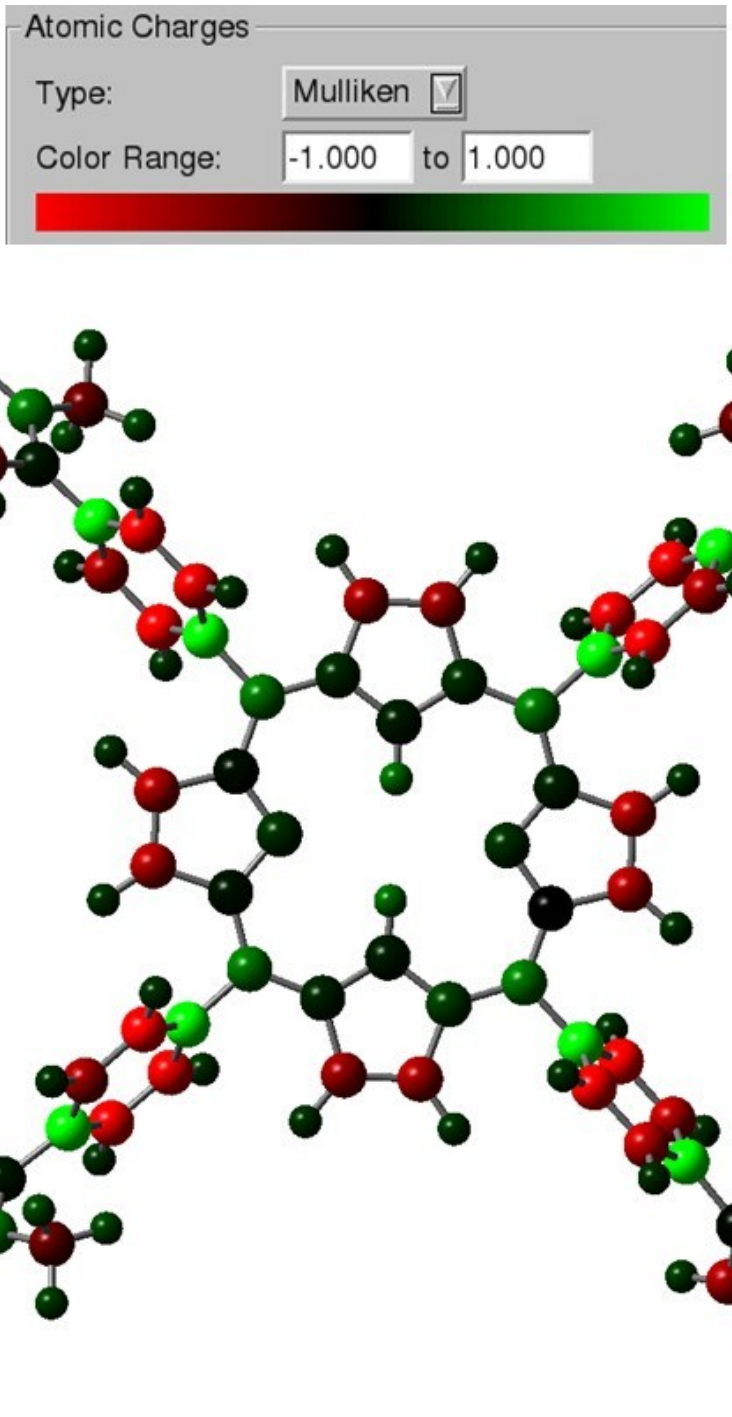

Figure S1. Calculated Mulliken atomic charges of the tetracationic non-metallated porphyrin H2MA. Color picture of the charges within a -1 to +1 color range.

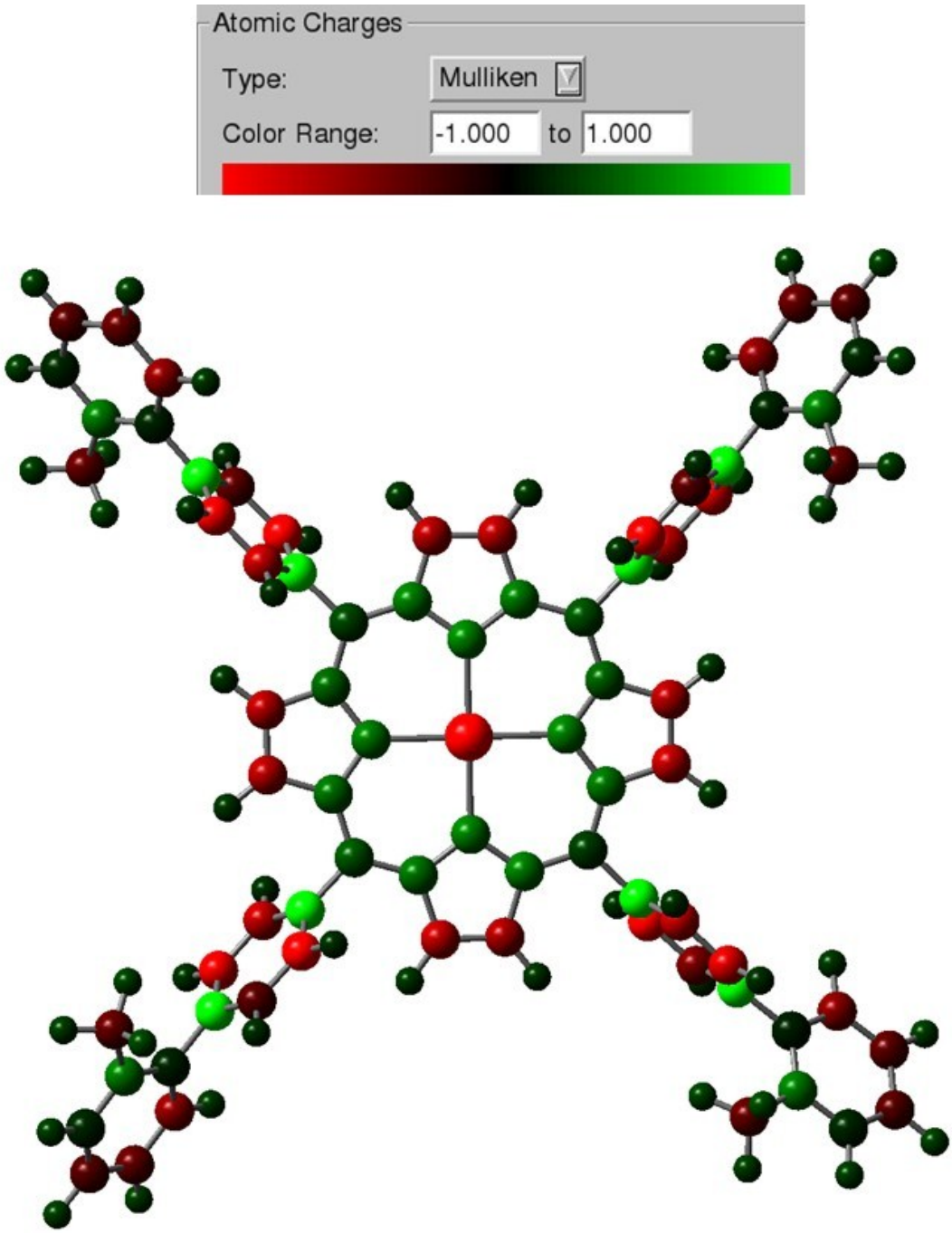

Figure S2. Calculated Mulliken atomic charges of the pentacationic gold(III)-porphyrin AuMA. Color picture of the charges within a -1 to +1 color range.

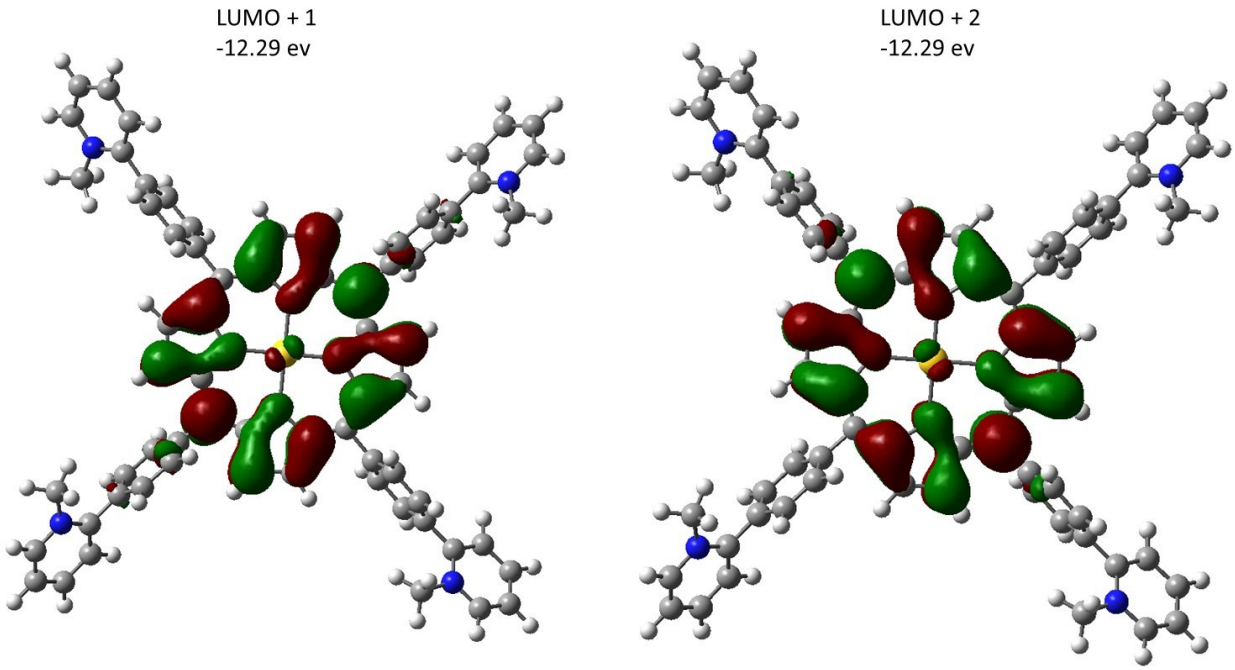

Figure S3. LUMO + 1 and LUMO + 2 of AuMA

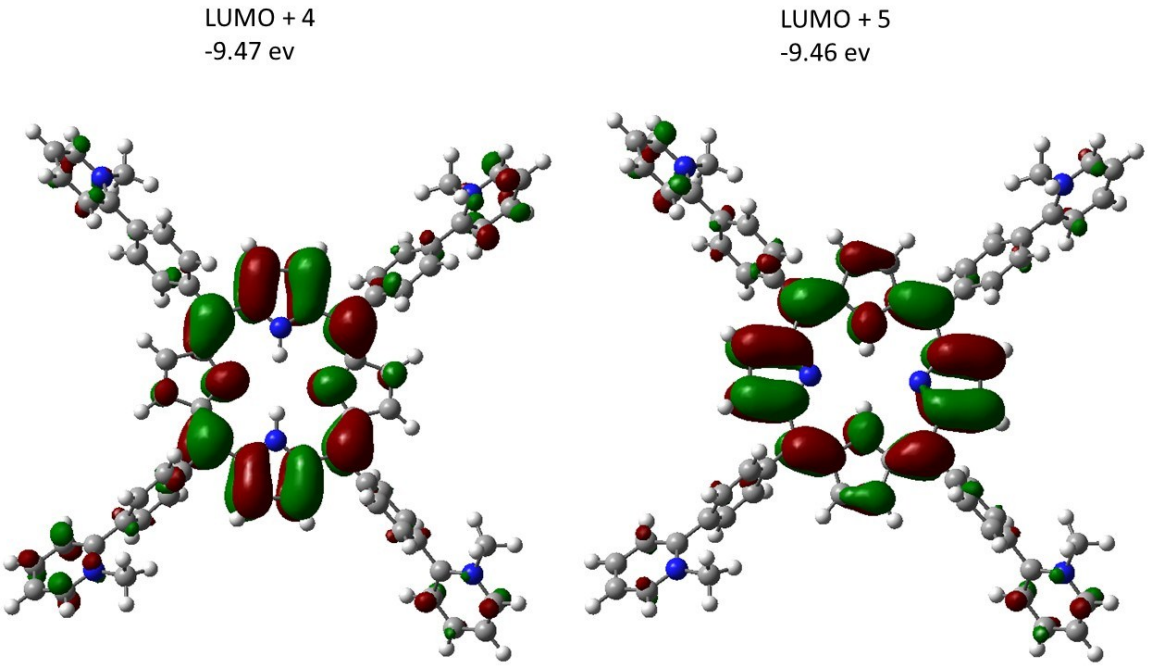

Figure S4. LUMO + 4 and LUMO + 5 of H2MA

Preparation of *meso*-5,10,15,20-tetrakis(4-(*N*-methyl-pyridinium-2-yl)phenyl)-porphyrinatogold(III) pentachloride (AuMA)

Tetrakis-(4-(*N*-methyl-pyridinium-2-yl)phenyl)porphyrin tetrakis(trifluoroacetate) (89 mg, 0.062 mmole) was dissolved in degassed water (10 mL). Aqueous 0.1M NaOH was added (248 µL, 0.248 mmole). Potassium tetrachloroaurate(III) (47 mg, 0.124 mmole) was dissolved in degassed water (2 mL) and added to the porphyrin solution. The mixture was refluxed for 3 hours under argon. The reaction was monitored by UV-visible spectroscopy and was stopped when the Soret band shift was complete (from 437 to 406 nm, H_2O, acidic pH). Desalting of the porphyrin was performed by reverse phase chromatography on a C18 Sep-Pak cartridge (5 g, Waters) by elution with Milli-Q water followed by acetonitrile containing 0.1% trifluoroacetic acid. The collected fractions were evaporated to dryness and the product was taken in methanol/water (50/50). Anion exchange was performed on DOWEX 1x8-200 resin (chloride form, 3 g) during 20 hours at room temperature. The solution was filtered off and evaporated to dryness under vacuum. The residue was taken in methanol and precipitated by the addition of diethyl ether, filtered, washed with diethyl ether and dried under vacuum. Yield: 64 mg (0.047 mmole, 76%) vermilion solid. TLC Rf $CH_3CN/H_2O/KNO_3$sat (6/1/1) 0.24. UV-visible (H_2O) λ = 406 nm ε = 400 10^3 M^{-1} cm^{-1} and λ = 521 nm ε = 20 10^3 M^{-1} cm^{-1}. HRMS (+ESI): calcd for $[C_{68}H_{52}AuN_8]^{5+}$: 235.4796, found: 235.4795. ^{1}H NMR (400 MHz, MeOD) δ_H (ppm) = 9.61 (s, 8H, pyrrole), 9.26 (d, 4H, J_{HH} = 6 Hz, pyr), 8.86 (dd, 4H, J_{HH} = 8 and 9 Hz, pyr), 8.67 (d, 8H, J_{HH} = 8 Hz, phe), 8.51 (d, 4H, J_{HH} = 8 Hz, pyr), 8.31-8.21 (m, 12H, phe+pyr), 4.66 (s, 12H,CH_3).

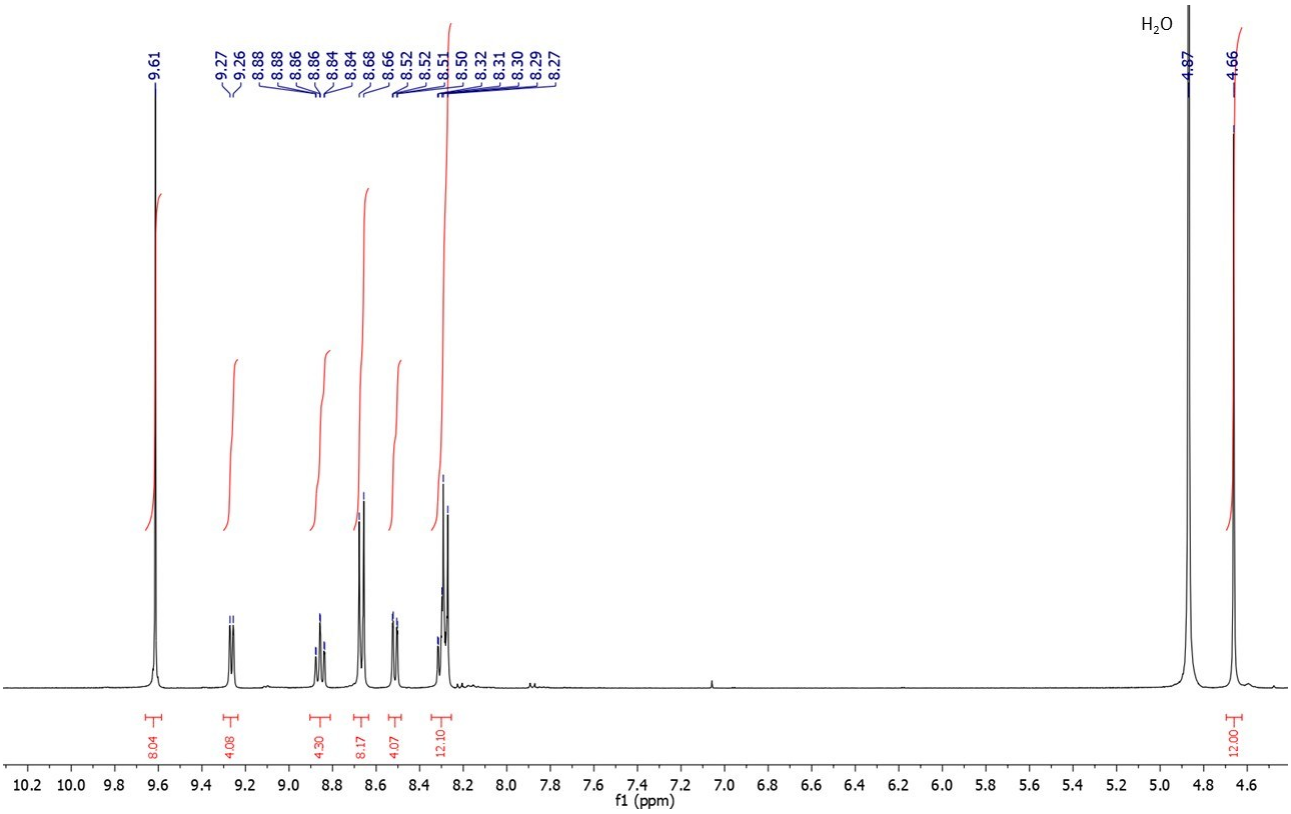

Figure S5. ^{1}H-NMR spectrum of AuMA (400 MHz, MeOD).

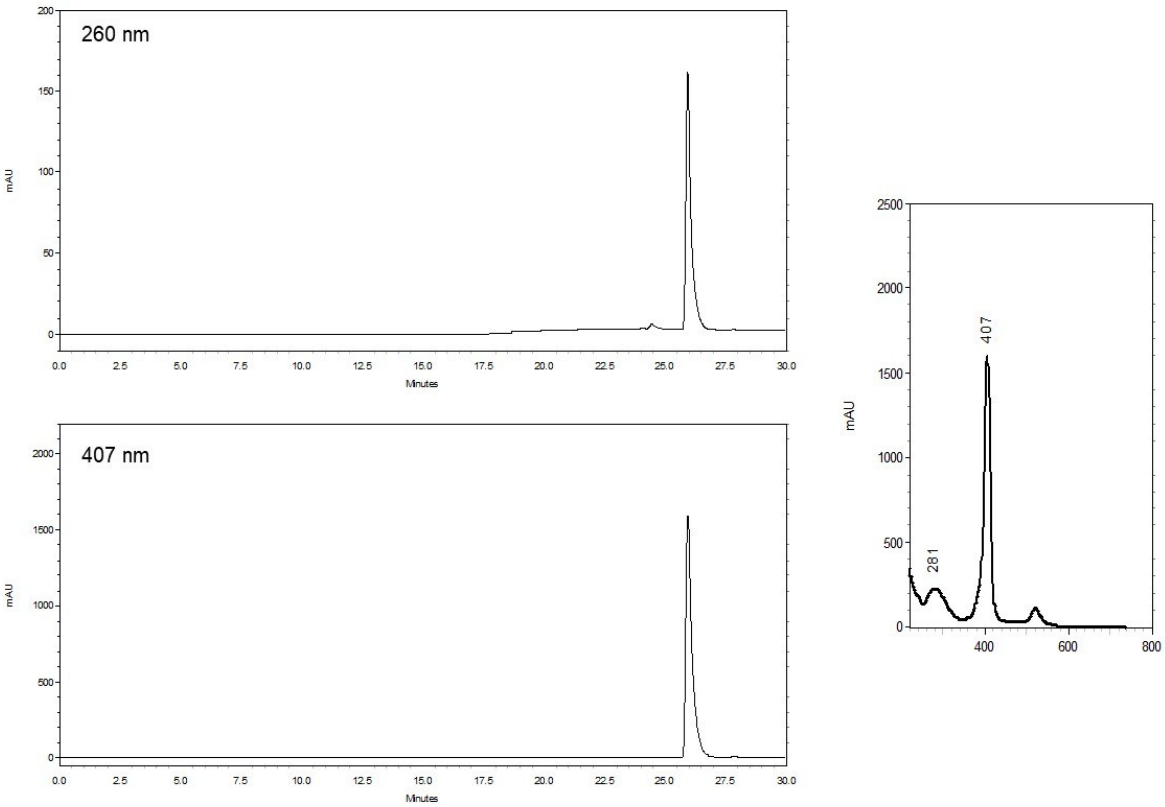

Figure S6. HPLC trace of AuMA with detection at 260 nm (upper trace) and at 407 nm (Soret band) (lower trace). The analysis was done on a nucleosil reverse phase C18 10µ column eluted with a gradient of water + 0.1% trifluoroacetic acid and acetonitrile + 0.1% trifluoroacetic acid, at a flow rate of 0.5 mL/min. After 5 min at 100% water, the percentage of acetonitrile increased to 90% in 25 min and it remained at 90% for 5 min before returning to the initial conditions. A diode array detector recorded the in-line UV-visible spectrum of AuMA at 26 min (spectrum: from 200 to 800 nm).