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Supporting Information

Mercury instructed assembly (MiA): Architecting of a clathrin triskelion inspired highly functional C_3-symmetric triskelion nanotorus functional structures into microtorus structures

Khushboo Kesharwani[a], Ramesh Singh[a,+], Nikunj Kumar[b,+], Narendra Singh[c], Puneet Gupta*[b] and Khashti Ballabh Joshi*[a]

[a.]Department of Chemistry, School of Chemical Science and Technology, Dr. Harisingh Gour Vishwavidyalaya (A Central University),
Sagar, M.P., 470003, India; E-mail: kbjoshi77@gmail.com; kbjoshi@dhsgsu.ac.in
[b.]Department of Chemistry, Indian Institute of Technology Roorkee-247667,
E-mail: puneet.gupta@cy.iitr.ac.in
[c.]Department of Chemistry, Indian Institute of Technology of Kanpur, U.P. 208016
[+] These authors contributed equally to this work.

Experimental section

1.0 General experimental procedures and technical details: The solvents and reagents used in this study were purchased from different commercial sources according to the requirement. Amino acids; L-tryptophan and D-Biotin were purchased from Spectrochem, Mumbai, India. Tris-(2-aminoethyl) amine (TREN) liker was purchased from Sigma Aldrich. Peptide Coupling Agents such as N, N´-dicyclohexylcarbodiimide(DCC), NHS (N-hydroxysuccinimide), N-hydroxybenzotriazole (HOBt), 1-ethyl-3-(3- dimethylaminopropyl) carbodiimide (EDC. HCl) were purchased from Spectrochem, Mumbai, India. Protecting reagent; Di-tert-butyl dicarbonate (Boc anhydride) and deprotecting reagent; Trifluoroacetic acid (TFA) were purchased from Spectrochem Pvt. Ltd. Organic bases such as triethylamine (Et_3N), diisopropylethylamine (DIPEA), 4-Dimethylamino pyridine (DMAP) were obtained from S D fine-chem Ltd. Strong anion exchange resin (Dowex 1-X8) was from HiMedia Laboratories Pvt. Ltd. India and strong cation exchange resin (Amberlite IR- 120 Na form) was purchased from Spectrochem Pvt. Ltd., Mumbai, India. Silica gel 60-120 and 100-200 mesh and precoated aluminum sheets for thin-layer chromatography (TLC Silica gel 60 F254) were purchased from Merck Chemicals, India. Solvents; such as **m**ethanol (MeOH), ethanol (EtOH), dichloromethane (DCM), ethyl acetate (EtOAc), acetone (Ac_2O), chloroform ($CHCl_3$),

dimethylsulfoxide (DMSO), diethyl ether (Et_2O), acetonitrile (ACN), pyridine, N, N-dimethylformamide (DMF), and tetrahydrofuran (THF), etc were purchased from S D Fine Chemicals Ltd., India. Other HPLC grade solvent such as; HPLC grade solvents, Deuterated solvents for recording nuclear magnetic resonance (NMR) spectra, were purchased from Merck Pvt. Ltd. Used ***Metal salts*** of mercury, zinc, and cadmium were purchased from Himedia Laboratories Pvt. Ltd., Mumbai, India. All other reagents needed were purchased from HiMedia.

2.0 Peptide synthesis. The C_3-Symmetric triskelion peptide-1 was synthesized by using the standard protocol mentioned in the research paper published by our group.[21, 24] Purity and identity were confirmed prior to use. All the experiments have been carried out at room temperature.

3.0 Spectroscopy Measurements. The steady-state absorption and emission spectra were recorded in a commercial spectrophotometer (LabIndia UV-Vis 3000^+ and Thermo Scientific, Multiskan Go UV-Vis Spectrophotometer, in 10 mm quartz cell at 25±0.1 °C) and spectrofluorometer (RF-5301PC, Shimadzu), respectively. The kinetics of metal ion addition were examined in a commercial spectrofluorimeter (RF-5301PC, Shimadzu). All samples were excited at 280 nm wavelength and the concentration-dependent dependent fluorescence intensity was recorded at 350 nm wavelength. Luminescence Cary eclipsed with the 10 mm quartz cell at 25±0.1°C. All samples were excited at λ_{ex} = 270 nm wavelength. The emission spectra were recorded from 280 nm to 500 nm range. A 15 mM stock solution of each metal ion salt was prepared in water. Ethanolic solution of each peptide (20 µM) was titrated with each metal ion up to 80 µM.

4.0 UV Titration Experiment Details. The 50µM solution of peptide1 in ethanol was titrated with an aqueous solution of metal ions till the 1:1 peptide-metals concentrations. Titration graphs with each metal ion were plotted in origin 8.0 and each plot between A/A^0 versus $[M^{n+}]$ was fitted with a linear fit.

5.0 Procedure for Preparation of Samples for Microscopic studies. The triskelion peptide was separately dissolved in pure ethanol. The final concentration of each solution was 1

mM. Therefore the 1 mM solution was used to perform metal ion instructed assembly. Now 2-10 µL aliquots were placed over the different substrates (mica for AFM and carbon-coated copper grid for TEM) and dried under a high vacuum. The samples were mounted under a microscope and imaged. The sample-coated substrates were dried in a dust-free space under a 60W lamp for 1h followed by high vacuum drying and subsequently examined under AFM/TEM.

6.0 Atomic Force Microscopy (AFM). Untreated and co-incubated solutions of **1** with different metal ion salts at different concentrations were imaged with an atomic force microscope. The samples were placed on freshly cleaved muscovite mica surfaces followed by imaging with an atomic force microscope (INNOVA, ICON analytical equipment, Bruker), operating under the acoustic AC mode (AAC or tapping mode), with the aid of a cantilever [NSC 12(c) from MikroMasch, Silicon Nitride Tip] by NanoDrive™ version 8 software. The force constant was ~2.0 N/m, while the resonant frequency was ~280 kHz. The images were taken in air at room temperature, with a scan speed of ~1.5 lines/sec. The data analysis was done using nanoscope analysis software.

7.0 Transmission Electron Microscopy (TEM). The sample(s) were placed on a 300 mesh carbon-coated copper grid. After 30 sec-1 minutes, excess fluid was removed and the samples were imaged using a FEI Tecnai 20 U Twin Transmission Electron Microscope, operating at 80 kV.

8.0 Purification of Hg(II) embedded microtorus samples. Purification of Hg(II) and other metal ions embedded nanobangles colloid samples is done by using the centrifugation method before using it for the imaging/analysis. The metal-containing solution was centrifuged at 12,000g for 15 minutes followed by removal of the supernatant and washing with ethanol. The residue/pallets were re-dissolved in an appropriate volume of solvent and used for further analysis. It is observed that the colloid solution was stable for 1-2 weeks.

9.0 Fourier Transform Infrared Spectroscopy. FT-IR spectra of peptide **1** alone and **1**-metal ions were performed in the range of 4000 cm^{-1} to 500 cm^{-1} using Bruker Alfa II ATR, FTIR spectrometer. Spectra were processed and smoothed using OPUS 7.0 software and

removed unwanted noise. Further, the IR spectra of the amide I region (1,600-1,700 cm^{-1}) were fitted by multiple Gaussian peaks, and the proportion of each secondary structure constituent was calculated through the origin 8.0 software.[1]

10.0 NMR Spectroscopy. Samples were prepared by dissolving the 15 mg of triskelion peptide-1 in DMSO-d_6. An increasing amount of $HgCl_2$ in DMSO-d_6(1mM) was added. After each incremental addition of Hg(II), ion solution ^1H NMR spectrum was recorded. All the experiments were carried out at 25 °C on 500 MHz JEOL ECX spectrometers. Each spectrum was recorded for 1000 scans.

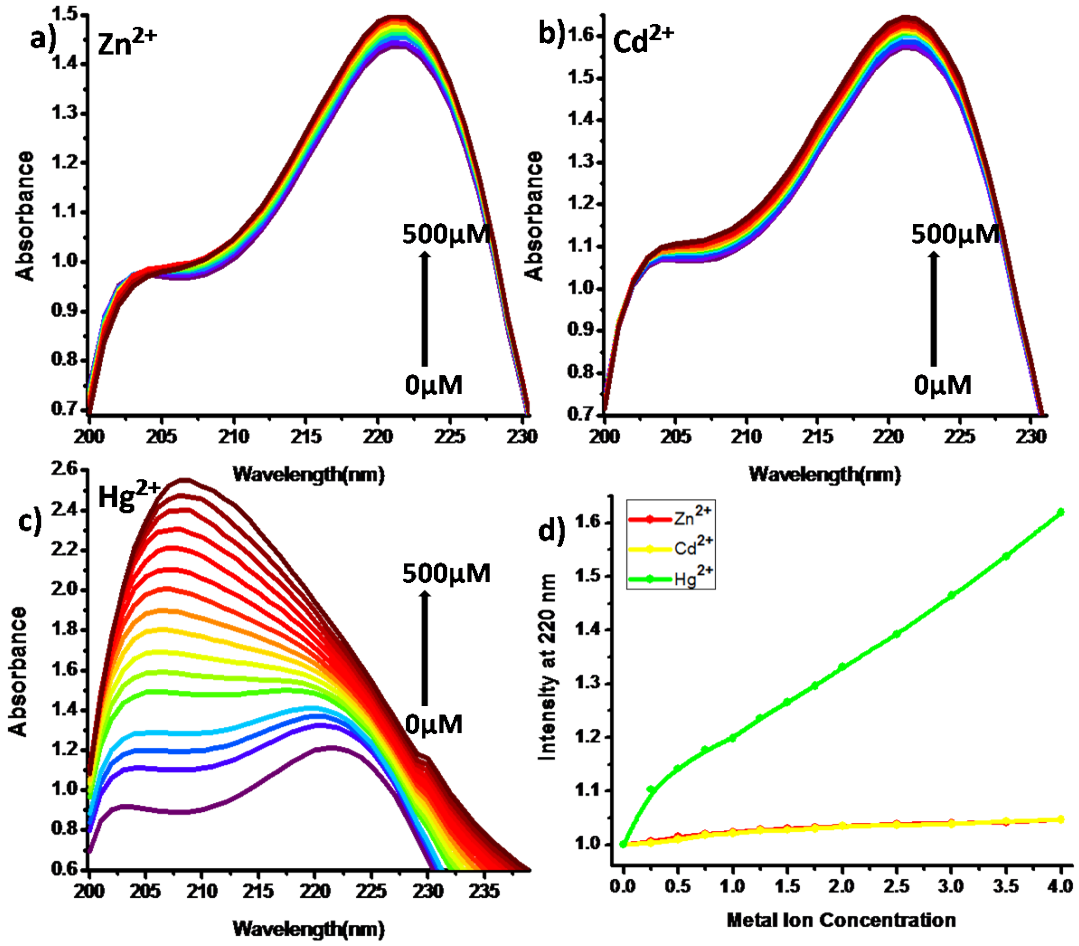


Figure S1: UV/Vis titration spectra of **1** (50 µM) with gradual addition of different metal ions: a) Zn(II), b) Cd(II) and c) Hg(II), and d) a comparative analysis of increase in absorbance intensity at 220 nm for amide and ureido region with the gradual addition of different metal ions.

	Structure	Wavenumber	Peak	Percent

	β-Sheet	1610-1640 cm^{-1}	1620, 1634 cm^{-1}	20.09%
	Random coil	1640-1650 cm^{-1}	1649 cm^{-1}	23.49%
	α-Helix	1650-1660 cm^{-1}	-	-
	Antiparallel β-Sheet	1660-1695 cm^{-1}	1669, 1682 & 1695 cm^{-1}	56.42%

Peptide 1	**Structure**	**Wavenumber**	**Peak**	**Percent**
1+ Hg(II)	β-Sheet	1610-1640 cm^{-1}	1612, 1630 cm^{-1}	28.47%
	Random coil	1640-1650 cm^{-1}	1645 cm^{-1}	12.55%
	α-Helix	1650-1660 cm^{-1}	-	-
	Antiparallel β-Sheet	1660-1695 cm^{-1}	1665 & 1698 cm^{-1}	58.98%

Table S1. The percentage contribution of β-sheet, α-helix, antiparallel β-sheet and random coil pattern of secondary structure of triskelion peptide-1

Table S2. The percentage contribution of β-sheet, α-helix, antiparallel β-sheet and random coil pattern of secondary structure of triskelion peptide-1 with Hg(II) ions.

	Structure	**Wavenumber**	**Peak**	**Percent**
1+ Cd(II)	β-Sheet	1610-1640 cm^{-1}	1613, 1632 cm^{-1}	17.87%
	Random coil	1640-1650 cm^{-1}	1646	04.49%
	α-Helix	1650-1660 cm^{-1}	-	-
	Antiparallel β-Sheet	1660-1695 cm^{-1}	1660, 1689 & 1693 cm^{-1}	77.64%

Table S3. The percentage contribution of β-sheet, α-helix, antiparallel β-sheet and random coil pattern of secondary structure of triskelion peptide-1 with Cd(II) ions.

	Structure	**Wavenumber**	**Peak**	**Percent**
1+ Zn(II)	β-Sheet	1610-1640 cm^{-1}	1613 cm^{-1}	2.56%
	Random coil	1640-1650 cm^{-1}	1648 cm^{-1}	54.91%
	α-Helix	1650-1660 cm^{-1}	-	-
	Antiparallel β-Sheet	1660-1695 cm^{-1}	1670 & 1687 cm^{-1}	42.52%

Table S4. The percentage contribution of β-sheet, α-helix, antiparallel β-sheet and random coil pattern of secondary structure of triskelion peptide-1 with Zn(II) ions.

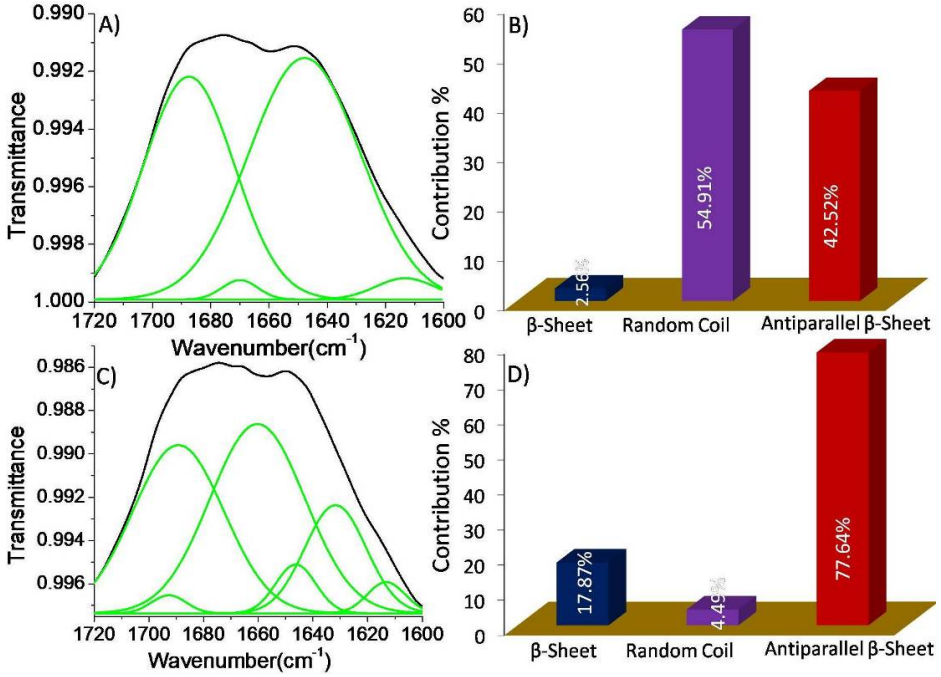


Figure-S2: Depicts FT-IR spectra of peptide 1 with (A) Zn(II) and (B) Cd(II) metal conjugate 500µM (1:1) in the amide I region, ranging from 1,600 to 1,700 cm^{-1} was fitted by multiple Gaussian peaks. A) FT-IR spectrum of Zn(II)- peptide **1** (solid line) and its deconvolution (green lines), B) corresponding secondary structure contribution in self-assembly, C) FT-IR spectrum of Cd(II)-Peptide **1** (solid line) and its deconvolution (green line), D) Corresponding quantitative contribution of different types of secondary structures; α-helix, β-sheet, anti-parallel β-sheet and random coil, contribution in self-assembly.[1-6]

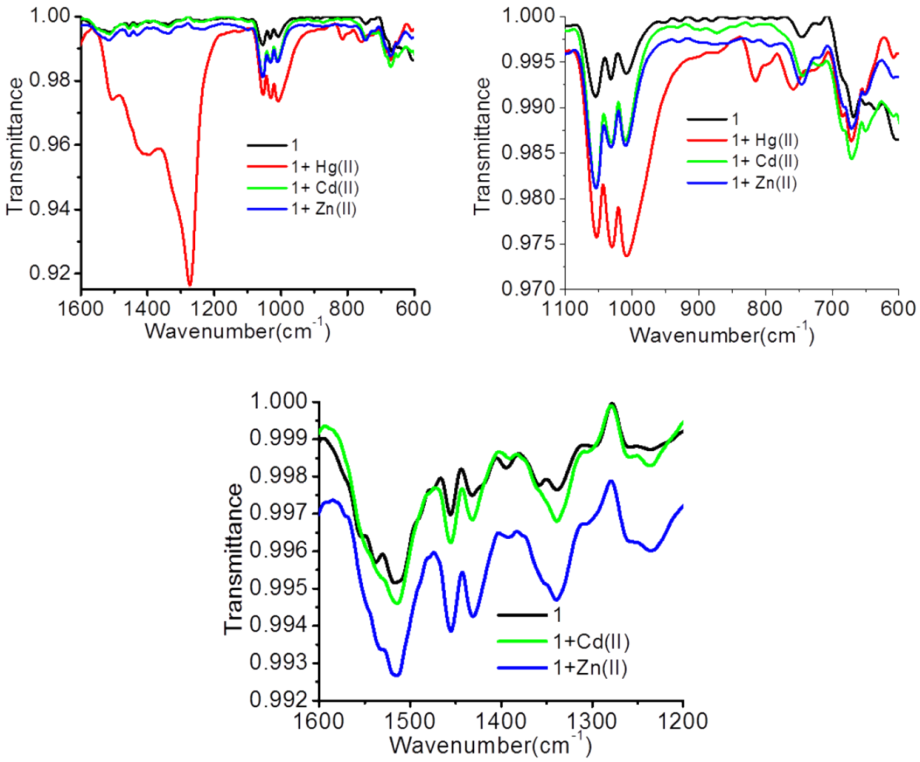


Figure S3. FT-IR spectra of peptide **1** and peptide **1** in the presence of Zn(II), Cd((II) and Hg(II) ions.

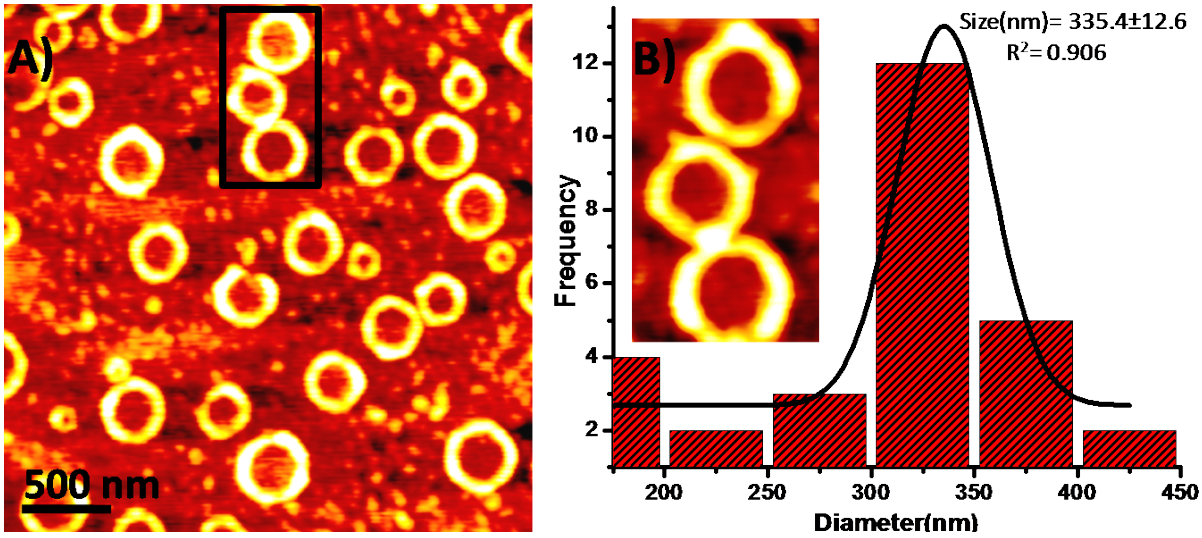


Figure-S4: Depicts, (A) AFM images of peptide-1 with 0.2 equivalent of Hg(II) ions (D) its corresponding particle(ring diameter) sized distribution histogram showing the enlargement of ring diameter.[1-6]

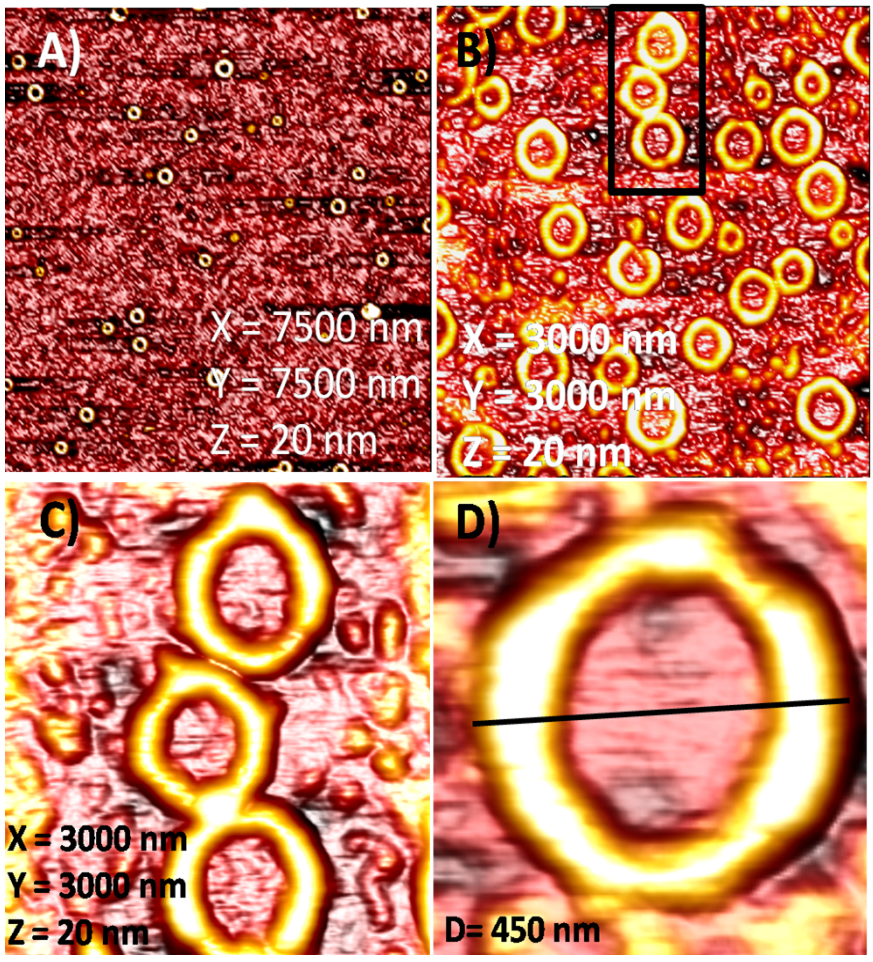


Figure-S5: Depicts, (A) 3D AFM images of **Peptide-1** and (B), (C) and (D) are the 3D AFM images of peptide-**1** with 0.2 equivalent of Hg(II) ions showing ring's diameter up to 450 nm.

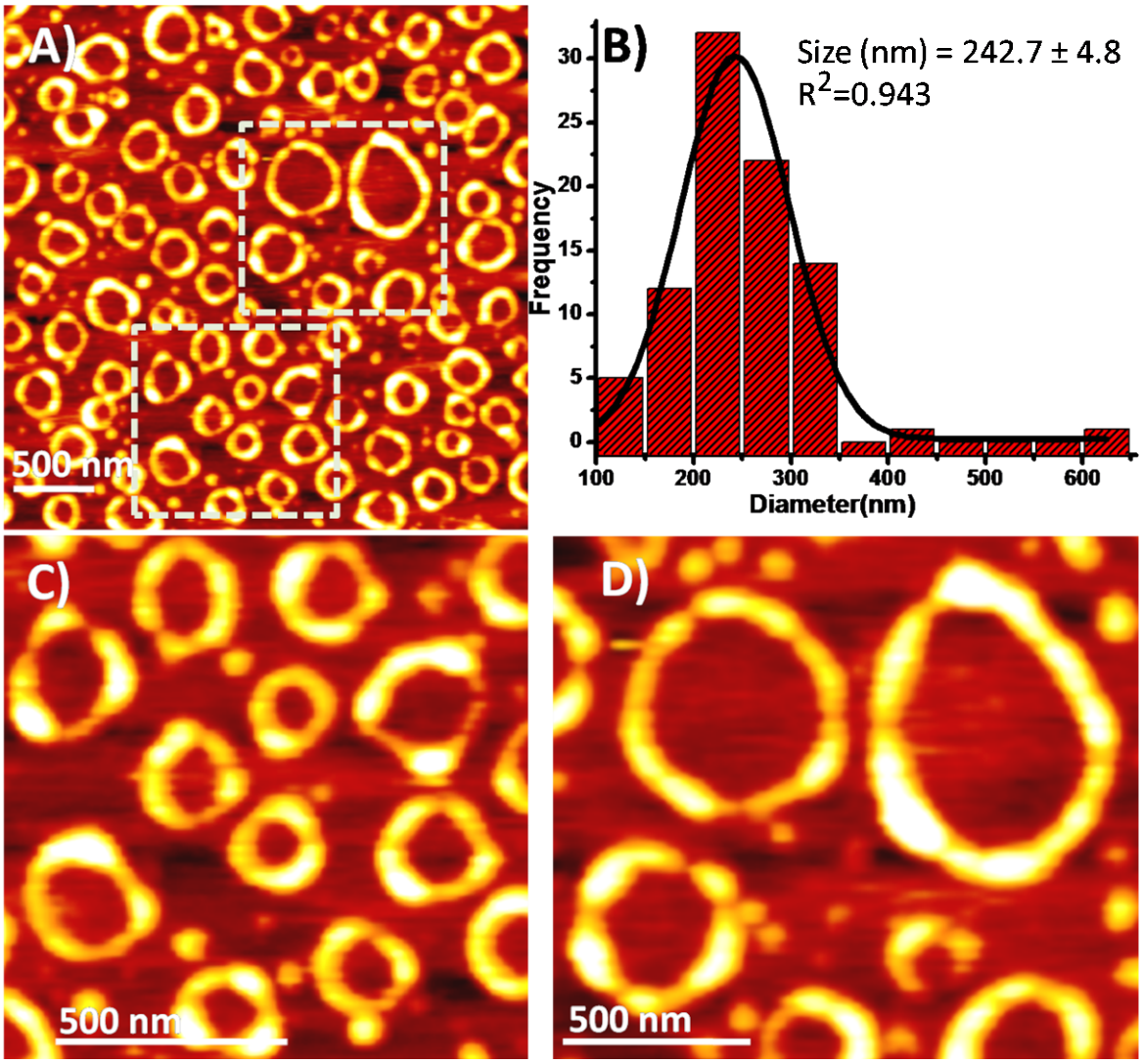


Figure-S6: Depicts, (A) AFM images of **Peptide-1 with** and 0.4 equivalent of Hg(II) ions (B) its corresponding particle(ring diameter) sized distribution histogram.[1-6] (C & D) AFM images of marked area showing the further enlargement of ring's diameter that is going up to ~700 nm.

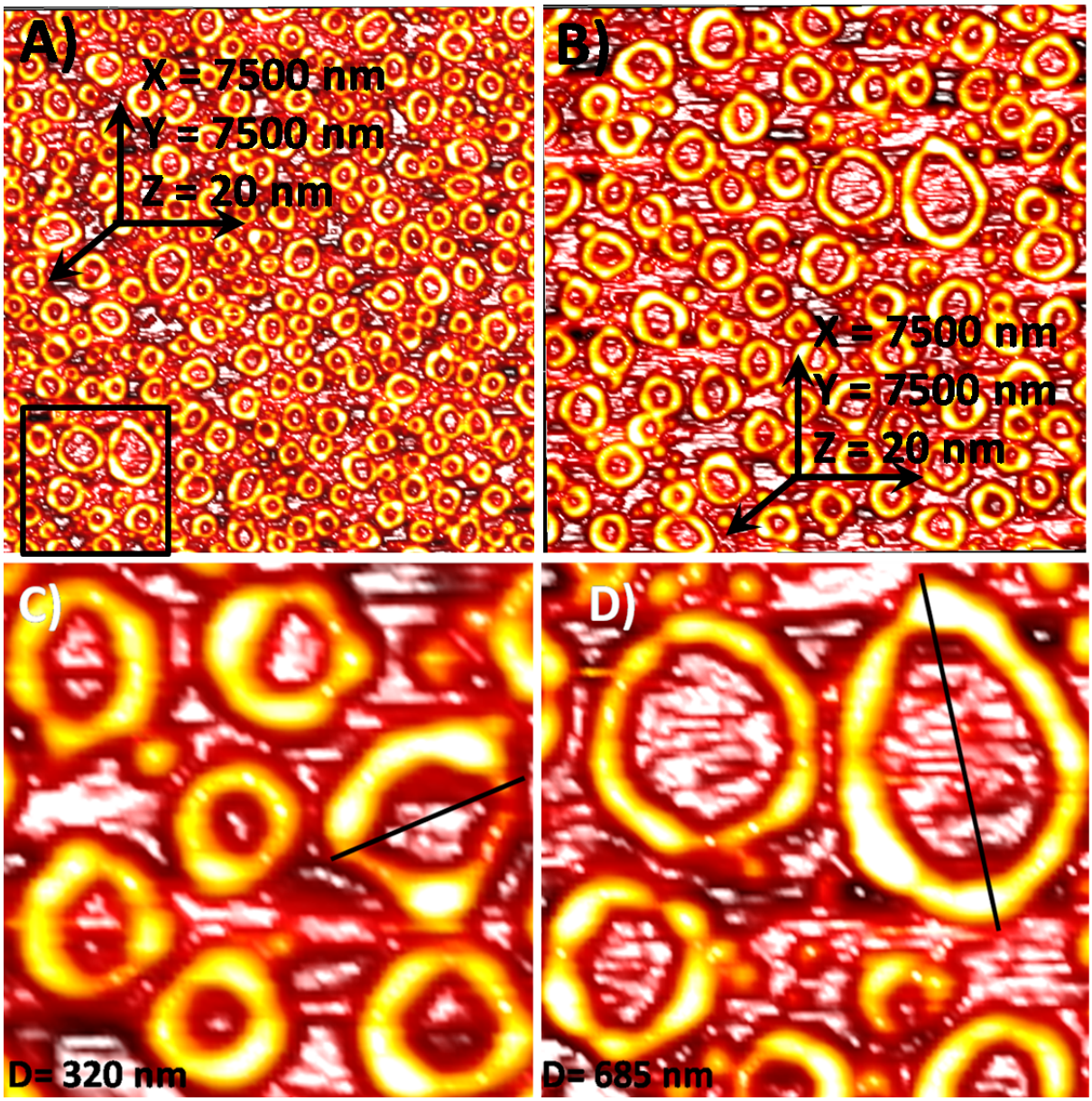


Figure-S7: Depicts, 3D AFM images of (A) **Peptide-1** with 0.4 eq. of Hg(II), (B), (C) and (D) are the 3D AFM images showing the further enlargement of ring's diameter that is ranging from 320 nm up to 685 nm.

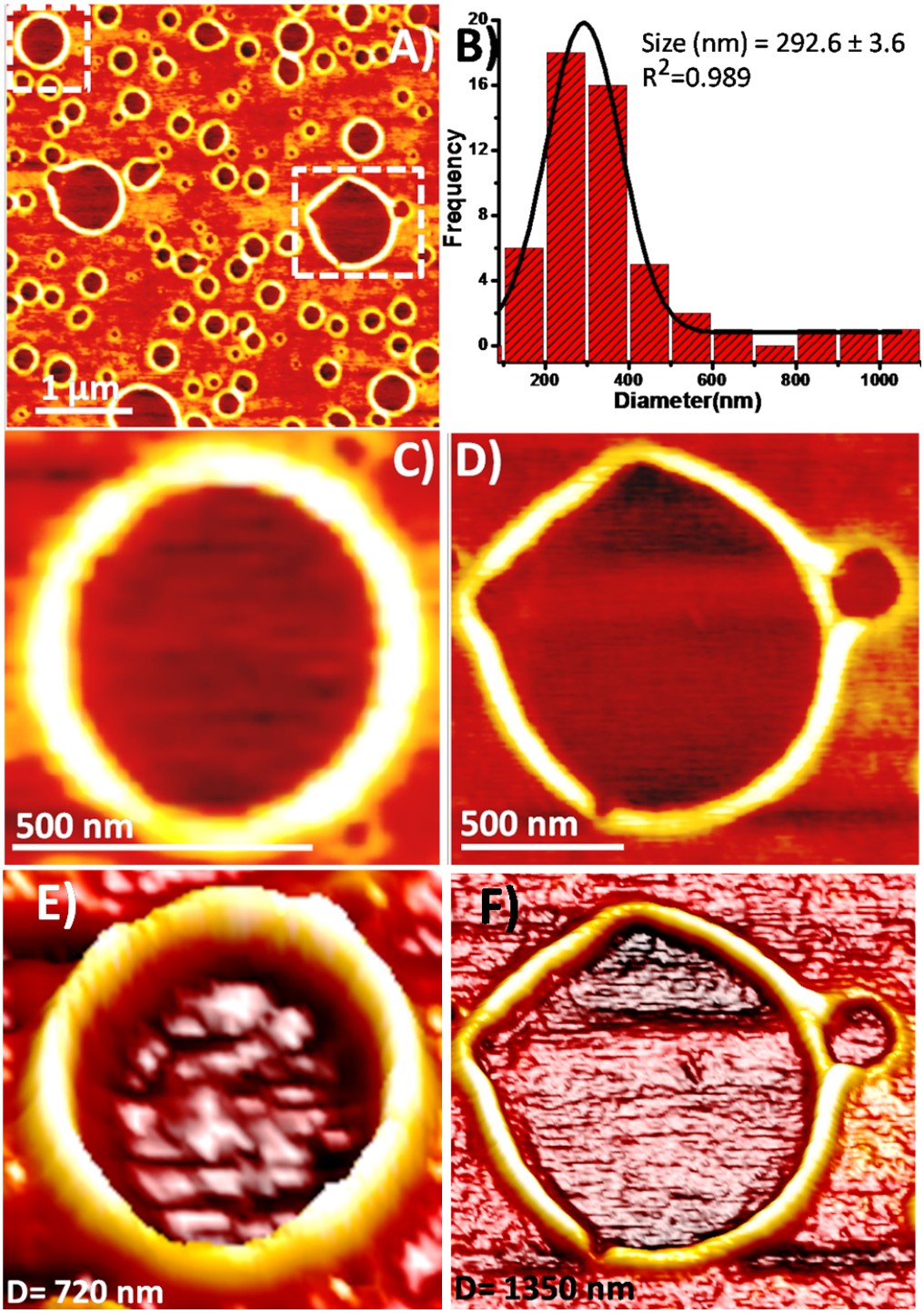


Figure-S8: Depicts, (A) AFM images of **Peptide-1** with 0.6 equivalent of Hg(II) ions (B) its corresponding particle (ring diameter) sized distribution histogram.[1-6] (C) AFM images fine and intact enlarged ring of 720 nm diameter and (D) showing 1350 nm diameter loop formation with small ring of ~200 nm diameter confirming the fusion of two rings. (E) and (F) are there corresponding 3D AFM images.

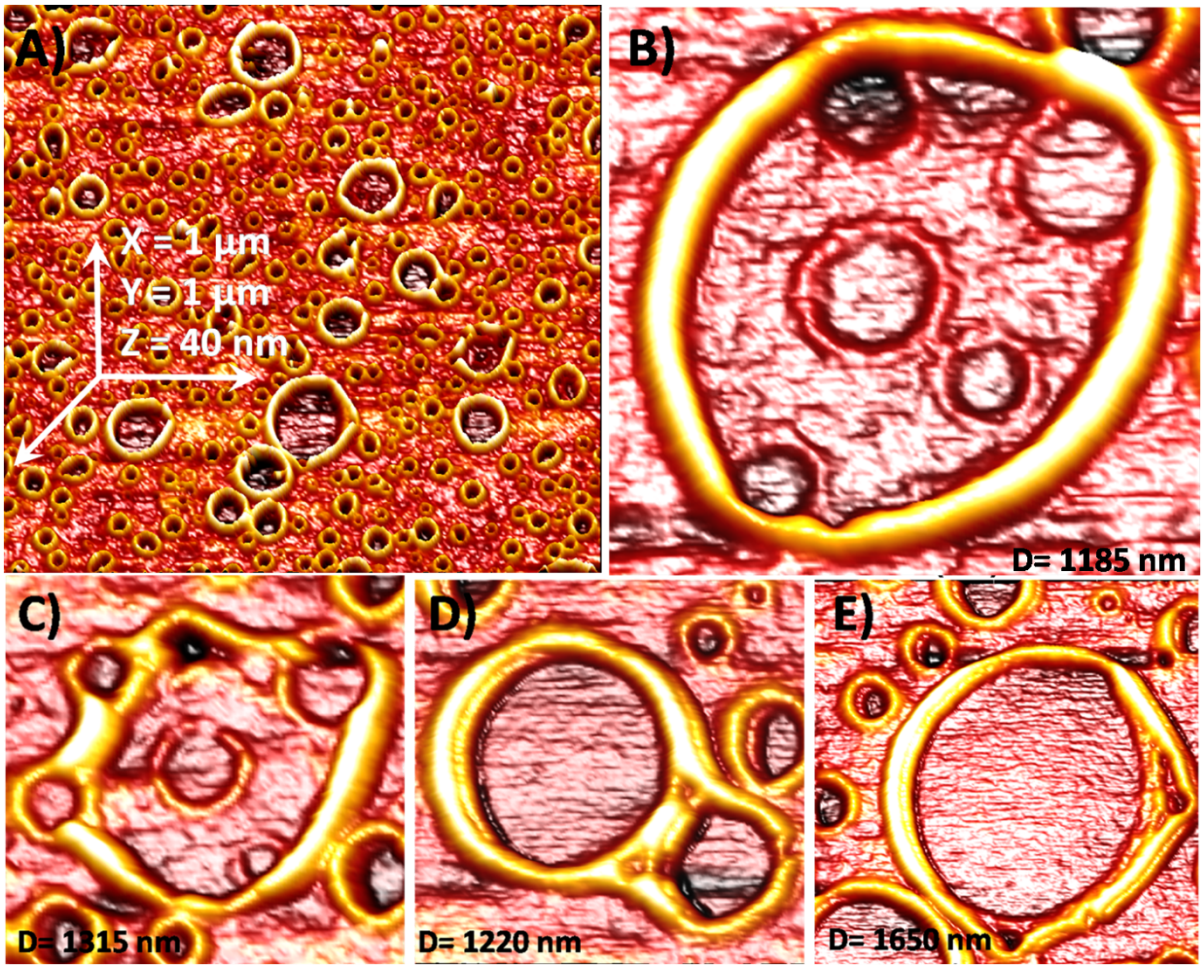


Figure-S9: Depicts, 3D AFM images of figure 4(main text) of **Peptide-1** with 1.0 equivalent of Hg(II) ions. These images are clearly representing the fusion of multiple small rings instructed by Hg(II) metal ions hence producing micro sized rings.

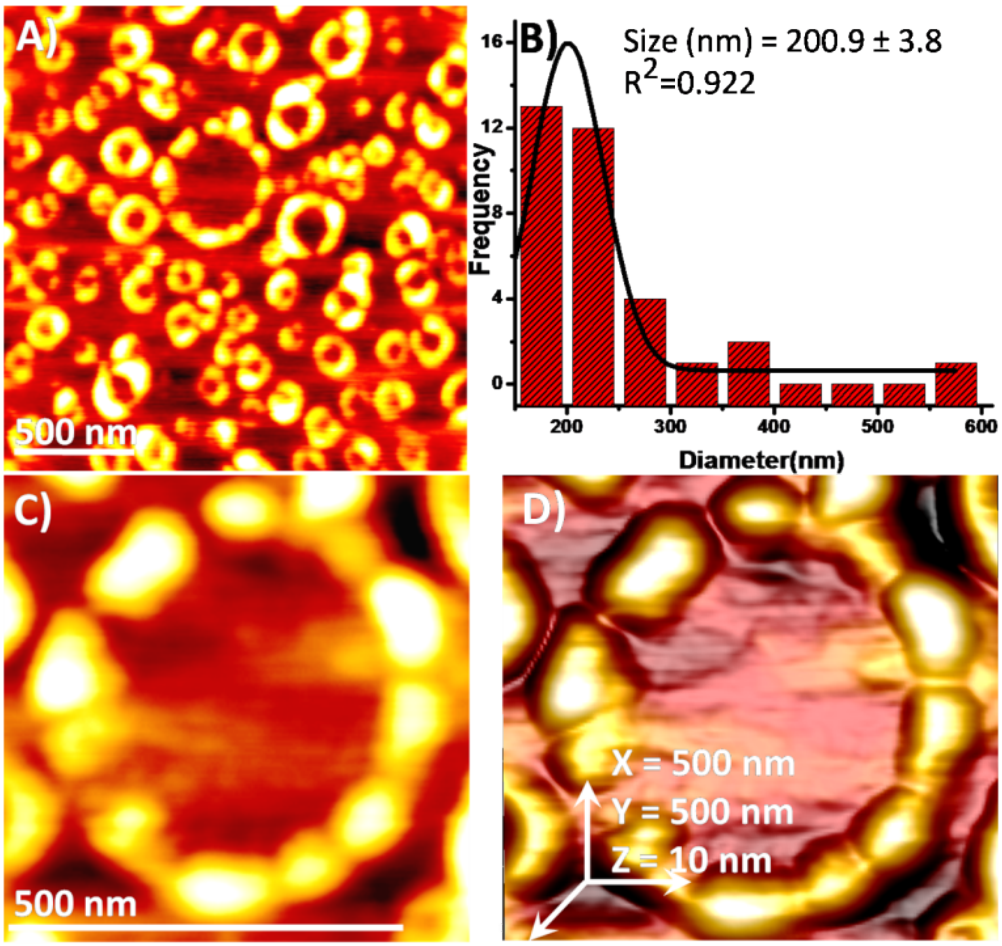


Figure S10: Depicts AFM images of self-assembled structures of **1** in the presence of excess Hg(II) metal ions in (1: 2) peptide: metal ions composition. (A&B) *Left:* AFM images of disintegrated nanotori of compound **1** in the presence of excess Hg(II) metal ions; *Right:* corresponding ring (particle) size distribution histogram. (C)&(D) Depicts single 2D and 3D AFM images of broken nanotori of 500 μm diameter

11.0 Computational studies.

11.1. DFT details

All Density functional theory (DFT) calculations were performed with the ORCA quantum chemical package[7] version 4.2.1. Geometries were optimized applying the BP86[8,9] generalized gradient approximation (GGA) functional in conjunction with the split valence basis set def2-SVP[10]. The RI[11-13](resolution-of-identity) approximation was used to accelerate the calculations. Dispersion corrections were included in all calculations via the Grimme D3 correction incorporating a Becke-Johnson (D3BJ) damping[14] function. Harmonic vibrational frequency analysis was carried out to verify the nature of the stationary points. Corrections for solvation were considered in all calculations by invoking the implicit

Conductor-like Polarizable Continuum Model (CPCM[15]) with the selection of ethanol as the solvent. The relative Gibbs free energies reported in the studies were obtained by performing solvation corrected single point energy calculations at BP86/def2-TZVP[10]/CPCM(Ethanol)//BP86-D3/def2-SVP.

11.2. Molecular Orbitals of the triskelion peptide

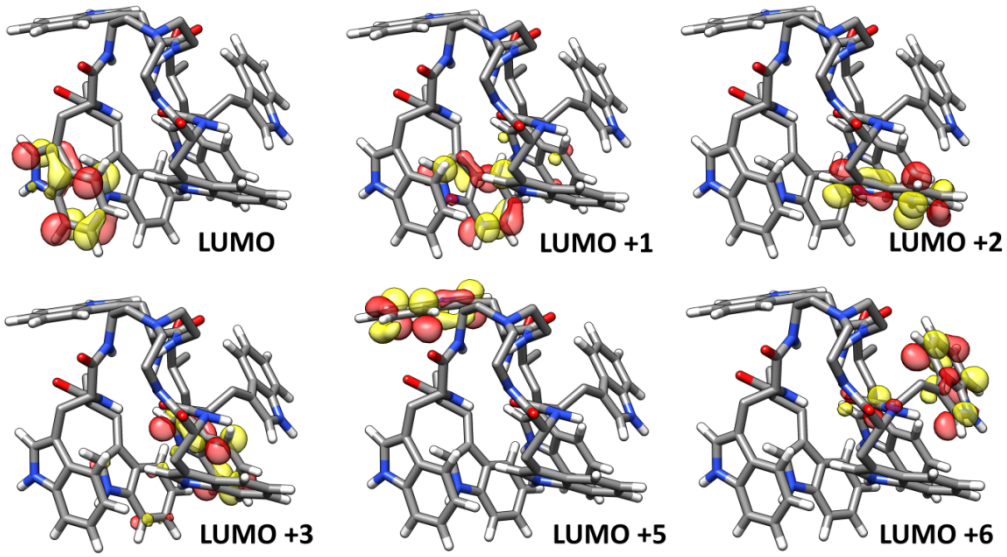


Figure-S11: Depicts the various HOMOs localized on the tryptophan rings of the triskelion peptide.

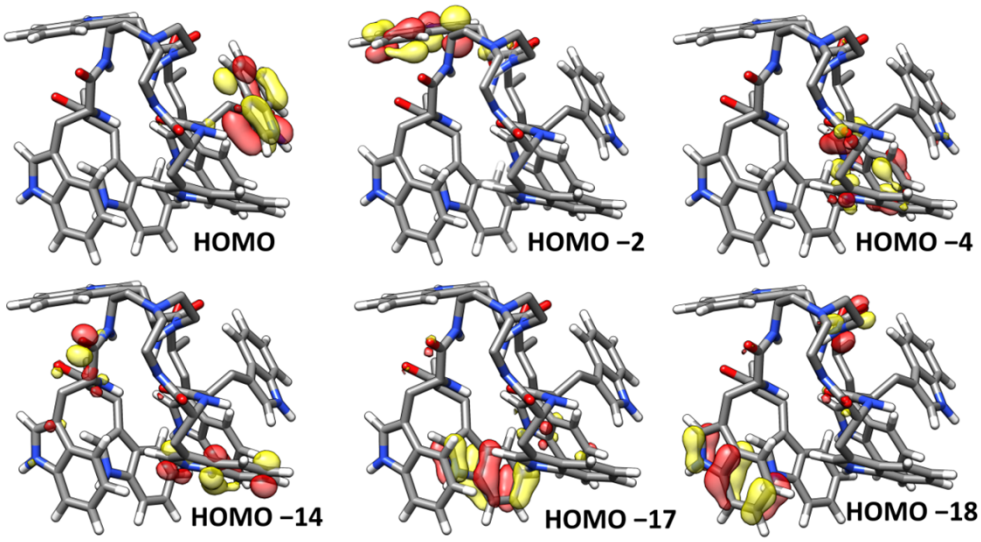


Figure-S12: Depicts the various LUMOs localized on the tryptophan rings of the triskelion peptide.

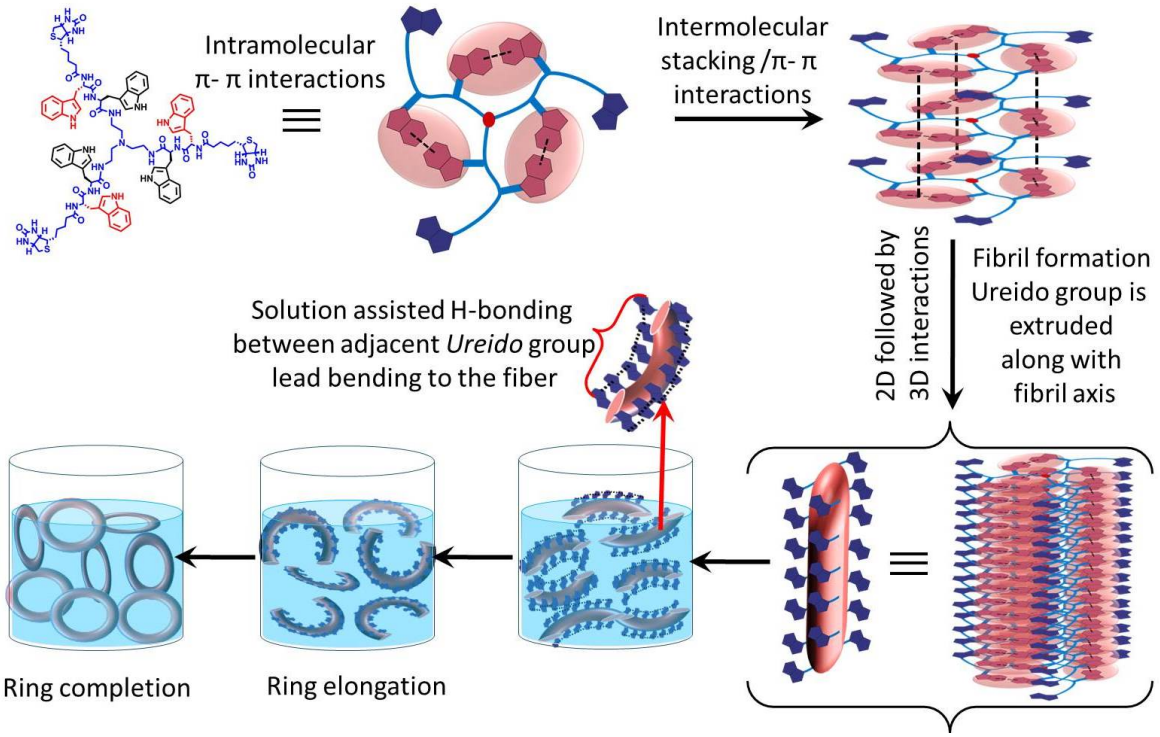


Figure S13. Depicts; proposed mechanism of formation of nanotorus by peptide-1. The formation of nanotorus is initiated via the formation of nanotube/fibril by pi-pi stacking interactions. The uriedo groups of biotin are extruded from the nanotube and are therefore responsible for bending of nanotubes which ultimately lead nanotorus assembly. The step wise shape transformation is supported by microscopy observations and this work is already published as reference number 21 and 24.

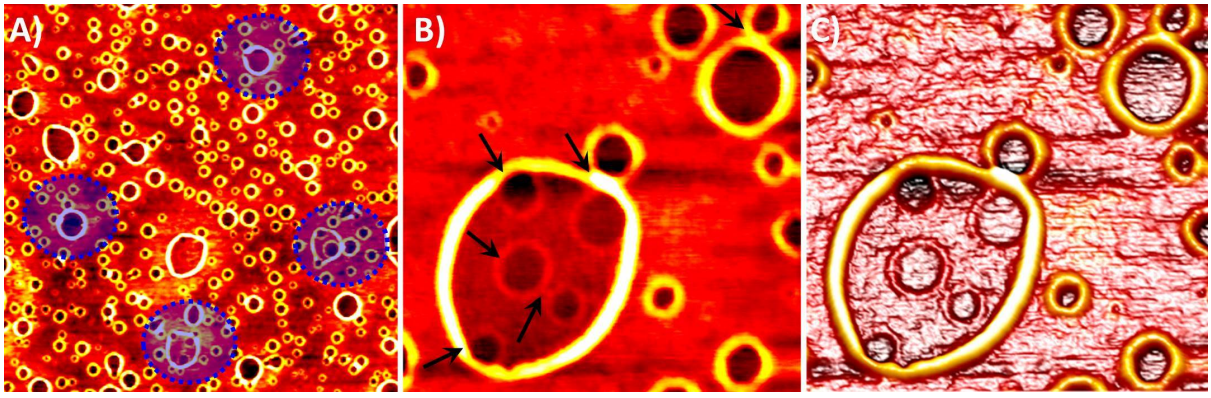
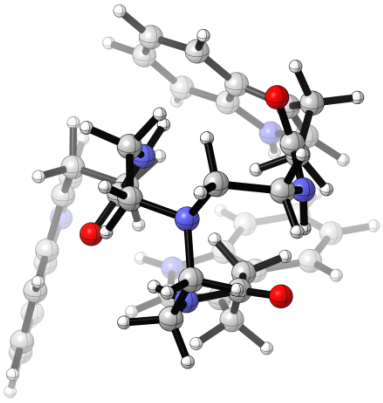


Figure S14: Represent the higher populations of nanotorus due to their smaller size. Howevere the marked area by blue and black arrow clearly depicts the presence of nanotorus inside the microtorus and their fusion points which may lead microloop formation.

11.3. Cartesian coordinates of the optimized structures

DFT optimization method: BP86-D3/def2-SVP

Truncated Model (M)



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C	-8.515271000	-13.631259000	2.643946000
O	-8.058475000	-13.700150000	3.798664000
N	-9.829926000	-13.400547000	2.375551000
C	-7.932634000	-15.202773000	0.684477000
H	-9.027221000	-15.380963000	0.653399000
H	-7.496973000	-16.029840000	1.284735000
C	-7.405091000	-15.196168000	-0.721231000
C	-8.179210000	-15.076581000	-1.867541000
N	-7.367316000	-14.933972000	-2.980131000
H	-7.715316000	-14.734401000	-3.920796000
C	-6.045869000	-14.956867000	-2.588208000
C	-6.027867000	-15.138522000	-1.158146000
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C	-3.601358000	-15.156399000	-1.251512000
C	-3.639905000	-14.948975000	-2.656133000
H	-2.696923000	-14.878808000	-3.219197000
C	-4.862057000	-14.848785000	-3.341332000
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H	-11.495766000	-11.795833000	4.930785000
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C	-6.717070000	-10.253605000	3.707338000
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N	-7.269785000	-11.004372000	4.703983000
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H	-5.169920000	-9.223510000	1.921884000
C	-4.835606000	-10.739682000	0.429743000
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N	-4.500047000	-11.999969000	-1.435525000
H	-4.228871000	-12.804233000	-2.010862000
C	-5.255280000	-10.924160000	-1.846999000
C	-5.488422000	-10.100987000	-0.687635000
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C	-6.504921000	-9.399050000	-3.220876000
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H	-6.877536000	-11.274669000	1.881905000
H	-7.381778000	-12.014488000	4.510546000
H	-7.351846000	-7.662151000	-2.212906000
C	-8.266957000	-10.403130000	5.573999000
H	-7.820103000	-9.543276000	6.114025000
H	-8.551668000	-11.157075000	6.334631000
C	-9.488018000	-9.890864000	4.782360000
H	-9.170139000	-8.964744000	4.267434000
H	-10.302191000	-9.607401000	5.502828000
C	-8.825317000	-11.591702000	-1.283916000
C	-9.659799000	-11.202006000	-0.075289000
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N	-9.156818000	-10.216687000	0.716935000
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N	-8.887019000	-13.450372000	-5.442006000
H	-8.540503000	-13.674137000	-6.374011000
C	-9.928855000	-14.118975000	-4.804633000
C	-10.302952000	-13.325217000	-3.672795000

C	-11.299569000	-13.797053000	-2.787637000
H	-11.559512000	-13.214674000	-1.889299000
C	-11.902229000	-15.030871000	-3.059801000
C	-11.528204000	-15.798412000	-4.192718000
H	-12.021662000	-16.764309000	-4.377053000
C	-10.536009000	-15.357592000	-5.079333000
H	-10.244457000	-15.963448000	-5.950988000
H	-7.860134000	-11.562937000	-5.127503000
H	-8.780738000	-12.698084000	-1.297646000
H	-8.263627000	-9.817453000	0.410054000
H	-12.677548000	-15.418596000	-2.381620000
C	-9.918333000	-9.427361000	1.692369000
H	-10.620893000	-8.761754000	1.140297000
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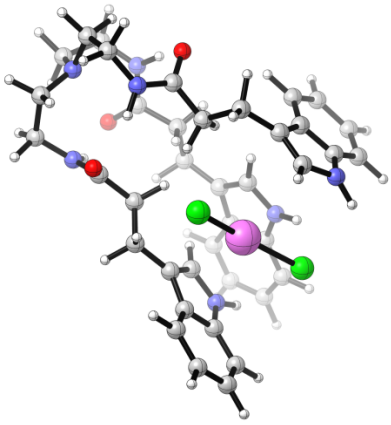
Truncated Model Metal Complex (HgM)



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H	-4.604459000	-18.603238000	-1.712544000
C	-11.311417000	-13.435457000	3.476650000
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C	-6.599361000	-7.658670000	-2.224524000
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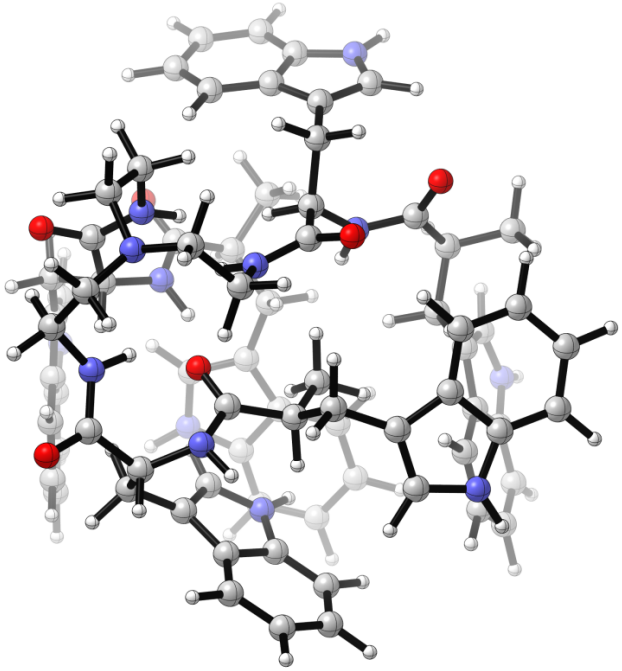
Extended Model (E)



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C	-2.872572000	-16.000473000	2.203249000
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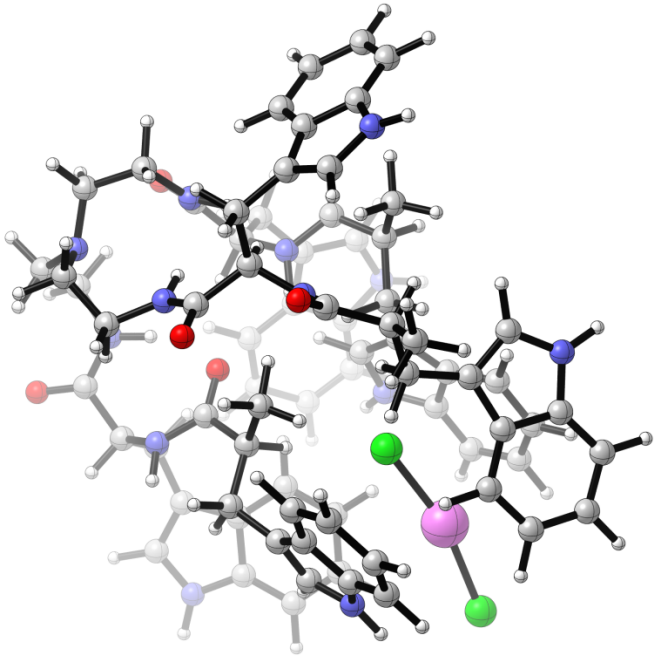
Extended Model Metal Complex (HgE)



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C	-3.167066000	-15.998106000	1.430149000
C	-2.611798000	-14.833149000	2.009594000

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C	-0.416485000	-15.444838000	1.093632000
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N	-8.434311000	-15.378155000	2.545355000
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O	-11.562455000	-14.891945000	4.210279000
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C	-9.704282000	-17.787028000	1.262912000
C	-9.817897000	-18.990735000	1.949860000
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C	-8.140833000	-17.189170000	-0.772844000
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C	-7.161907000	-17.731993000	-1.611983000
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C	-11.710948000	-12.419305000	2.951543000
H	-12.653663000	-12.903438000	3.278658000
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C	-5.691375000	-10.006698000	1.417064000
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C	-8.895779000	-10.785554000	4.634355000
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H	-0.344877000	-10.679810000	-1.141862000
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C	-8.346434000	-10.431163000	-2.215037000
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C	-6.789754000	-15.285269000	-4.223196000
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H	-4.192174000	-13.035674000	-4.624362000
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H	-3.286066000	-14.999189000	-5.879461000
C	-5.016584000	-16.271955000	-5.510290000
H	-4.581493000	-17.129764000	-6.044406000
C	-6.288990000	-16.395797000	-4.926155000
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C	-10.532010000	-12.228770000	-4.115279000
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C	-11.537752000	-14.722954000	-1.619002000
H	-11.787072000	-14.303241000	-0.632599000
C	-11.563549000	-16.107577000	-1.827066000
C	-11.242064000	-16.667173000	-3.090781000
H	-11.269837000	-17.759555000	-3.219869000
C	-10.893400000	-15.852067000	-4.177625000
H	-10.641270000	-16.285170000	-5.157484000
H	-10.250043000	-11.284851000	-4.594565000
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H	-10.112283000	-12.319169000	-0.130573000
H	-8.520518000	-9.716202000	0.498421000
H	-11.836698000	-16.781610000	-1.002525000
C	-9.554836000	-8.804533000	2.153357000
H	-9.995553000	-7.835232000	1.827877000
H	-8.534429000	-8.584218000	2.528347000
C	-10.430465000	-9.365371000	3.292214000
H	-11.465869000	-9.414755000	2.910608000
H	-10.415005000	-8.603144000	4.115082000
C	-6.083733000	-9.421552000	-2.616059000
H	-5.170433000	-9.469358000	-3.242459000
H	-6.620995000	-8.482693000	-2.843502000
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Hg	-3.707396000	-16.768389000	-2.664473000
Cl	-4.549551000	-14.898532000	-1.555856000
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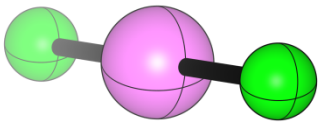
$HgCl_2$



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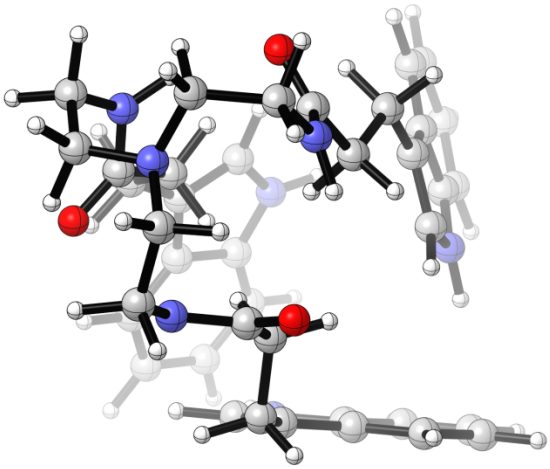
Truncated Model (M) without the dispersion correction



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N	-9.752463000	-13.678859000	3.324440000
C	-8.176565000	-15.548467000	1.194910000
H	-9.233545000	-15.855270000	1.338500000
H	-7.565116000	-16.216428000	1.837893000
C	-7.792674000	-15.694573000	-0.254193000
C	-8.655353000	-15.611919000	-1.341024000
N	-7.946960000	-15.653746000	-2.526362000
H	-8.366060000	-15.527368000	-3.454126000
C	-6.600684000	-15.751778000	-2.246768000
C	-6.461127000	-15.786138000	-0.813584000
C	-5.161688000	-15.889868000	-0.259822000
H	-5.020744000	-15.930936000	0.832098000
C	-4.054165000	-15.947609000	-1.115831000
C	-4.214694000	-15.904955000	-2.527518000
H	-3.326443000	-15.967940000	-3.175388000
C	-5.488871000	-15.809674000	-3.109000000
H	-5.616794000	-15.786010000	-4.202504000
H	-9.747050000	-15.508810000	-1.357295000
H	-6.934645000	-13.796801000	1.577054000
H	-10.360433000	-13.496576000	2.516103000
H	-3.041915000	-16.036424000	-0.691986000
C	-10.313170000	-13.451537000	4.649460000
H	-9.963272000	-14.255265000	5.332044000
H	-11.412144000	-13.561055000	4.561689000
C	-9.931640000	-12.104047000	5.301708000
H	-8.869466000	-12.183169000	5.600139000
H	-10.529513000	-12.006485000	6.250480000
N	-10.070573000	-10.948698000	4.426706000

C	-6.495064000	-10.782498000	1.552972000
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N	-7.190869000	-10.498981000	3.873771000
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H	-5.019498000	-9.323795000	0.896284000
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H	-4.420413000	-13.441061000	-2.262878000
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C	-5.349805000	-9.023435000	-2.722241000
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C	-5.114051000	-8.926008000	-4.099835000
C	-4.681547000	-10.051585000	-4.851111000
H	-4.486001000	-9.940345000	-5.929082000
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H	-4.129417000	-12.166876000	-4.816564000
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H	-5.256731000	-7.960961000	-4.610642000
C	-7.854859000	-9.891384000	5.019929000
H	-7.448287000	-8.868850000	5.176029000
H	-7.563543000	-10.483918000	5.909567000
C	-9.388140000	-9.757307000	4.908476000
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N	-10.670362000	-9.957091000	1.686904000
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C	-9.720719000	-11.526856000	-2.814046000
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N	-7.986845000	-11.411769000	-4.286752000
H	-7.092274000	-11.107324000	-4.682322000
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C	-8.401090000	-13.552494000	-5.576798000
H	-7.541607000	-13.461947000	-6.259042000
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C	-11.568357000	-9.721262000	2.809043000
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H	-12.096860000	-10.322801000	4.820233000
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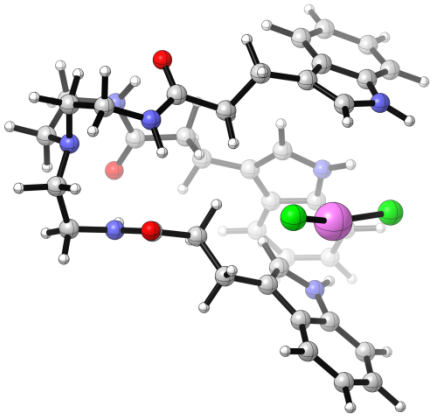
Truncated Model Metal Complex (HgM) without the dispersion correction



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C	-7.656900000	-15.187437000	-1.285219000
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H	-7.878706000	-14.523675000	-4.463112000
C	-6.985195000	-16.115983000	-3.313839000
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H	-5.216902000	-18.840002000	-4.330446000
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H	-11.161649000	-13.108125000	1.425260000
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C	-11.246244000	-13.646807000	3.489866000
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C	-9.761337000	-11.710909000	-4.045429000
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H	-11.877486000	-12.260120000	-4.169508000
C	-10.718861000	-13.048138000	-5.833248000
C	-9.446921000	-13.156120000	-6.454233000
H	-9.350724000	-13.715653000	-7.397291000
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H	-7.620529000	-10.056385000	-2.073592000
H	-9.264059000	-11.062722000	-0.151921000
H	-10.012374000	-9.009292000	1.826937000
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H	-12.491894000	-11.431045000	3.105086000
H	-12.567224000	-10.452172000	4.603741000
H	-9.497839000	-9.316855000	-0.390388000
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Hg	-5.130177000	-13.706600000	-1.356400000
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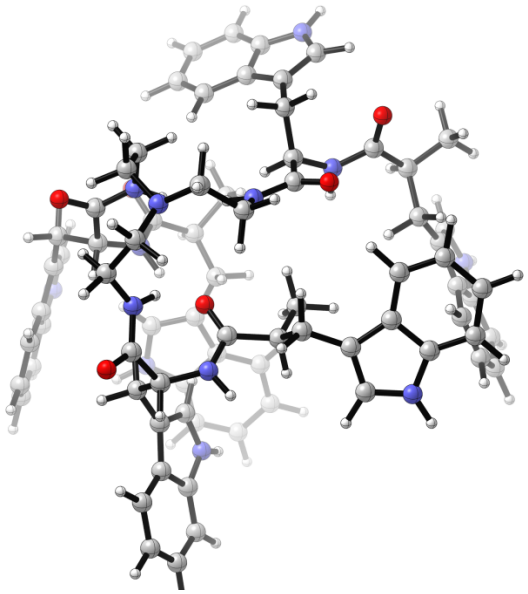
Cl	-4.731199000	-14.076397000	0.941890000

Extended Model (E) without the dispersion correction



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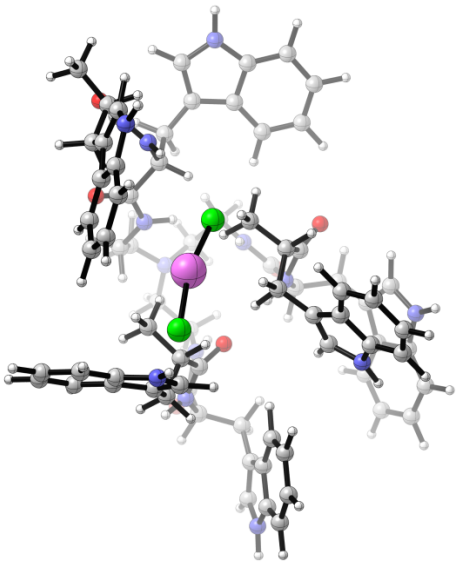
Extended Model Metal Complex (HgE) without the dispersion correction



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H	-1.214939000	-17.198116000	4.128120000
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H	0.541339000	-17.700020000	2.425216000
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H	-0.064404000	-17.978939000	-0.003089000
H	-4.821602000	-17.590538000	-1.578679000
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C	-10.211590000	-15.003081000	3.656484000
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H	-5.326461000	-9.464840000	0.014815000
H	-6.749501000	-10.143371000	1.788326000
H	-8.751681000	-7.917442000	-3.198727000
C	-6.269930000	-10.891686000	3.712729000
H	-5.382415000	-10.695269000	4.349059000
H	-6.410489000	-11.995006000	3.675235000
C	-7.531730000	-10.234847000	4.295712000
H	-7.447002000	-9.134417000	4.155064000
H	-7.540877000	-10.397448000	5.400968000
C	0.095288000	-7.435168000	0.455921000
H	1.080477000	-7.672830000	0.007327000
H	-0.183353000	-6.403765000	0.163026000
H	0.200101000	-7.442063000	1.558874000
C	-7.336816000	-12.096471000	-2.668873000
C	-8.725035000	-11.580607000	-2.226365000
O	-9.209685000	-10.570078000	-2.747603000
C	-7.074529000	-13.616689000	-2.525870000
H	-7.235876000	-13.919268000	-1.467778000
H	-5.989322000	-13.775218000	-2.708757000
C	-7.857187000	-14.515438000	-3.444053000
C	-9.080981000	-15.120454000	-3.188370000
N	-9.475061000	-15.880128000	-4.275682000
H	-10.362283000	-16.383053000	-4.327872000
C	-8.527424000	-15.777858000	-5.276293000
C	-7.483698000	-14.919771000	-4.783800000
C	-6.371054000	-14.652239000	-5.617593000
H	-5.552755000	-14.002786000	-5.267322000
C	-6.323471000	-15.223662000	-6.894942000
H	-5.464174000	-15.017605000	-7.552180000
C	-7.366078000	-16.065669000	-7.361842000
H	-7.300368000	-16.501346000	-8.370593000
C	-8.477836000	-16.356494000	-6.559553000
H	-9.282281000	-17.017001000	-6.920103000
H	-9.727016000	-15.051091000	-2.306623000
H	-7.293773000	-11.828387000	-3.745044000
N	-9.329193000	-12.244111000	-1.182052000
C	-10.664911000	-11.956922000	-0.653525000
C	-10.710823000	-10.850182000	0.434837000
O	-11.783058000	-10.519572000	0.951098000
N	-9.516410000	-10.289790000	0.779732000
C	-11.761502000	-11.630741000	-1.712202000
H	-11.537013000	-10.635992000	-2.137873000
H	-12.700853000	-11.535765000	-1.130041000

C	-11.917057000	-12.620556000	-2.829562000
C	-11.460879000	-12.445295000	-4.128995000
N	-11.814588000	-13.532125000	-4.911041000
H	-11.546544000	-13.660277000	-5.885325000
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C	-12.577592000	-13.910055000	-2.808296000
C	-13.245235000	-14.662170000	-1.812010000
H	-13.351304000	-14.264520000	-0.790525000
C	-13.775803000	-15.916612000	-2.138570000
C	-13.665190000	-16.440132000	-3.451741000
H	-14.094082000	-17.427668000	-3.680244000
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H	-10.891167000	-11.606037000	-4.544289000
H	-8.859593000	-13.062193000	-0.770817000
H	-10.973682000	-12.881782000	-0.119227000
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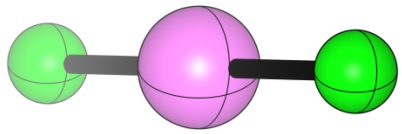
H	-14.289959000	-16.508051000	-1.365607000
C	-9.418102000	-9.215779000	1.760322000
H	-10.161294000	-8.429972000	1.505039000
H	-8.416040000	-8.747763000	1.658748000
C	-9.680561000	-9.663983000	3.208972000
H	-10.722906000	-10.036721000	3.228079000
H	-9.663181000	-8.757851000	3.867183000
C	-6.251177000	-11.282342000	-1.936632000
H	-5.245595000	-11.519052000	-2.340964000
H	-6.425989000	-10.193749000	-2.057109000
H	-6.235156000	-11.530090000	-0.852676000
Hg	-1.298842000	-15.040097000	-3.219953000
Cl	-2.340679000	-12.959190000	-3.364354000
Cl	-0.638238000	-17.298652000	-3.401329000

$HgCl_2$ without the dispersion correction



Hg	0.145991000	-3.289158000	-2.370959000
Cl	0.145991000	-3.289158000	-4.676396000
Cl	0.145991000	-3.289158000	-0.065517000

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