Supporting Information

Improved Electro- and Photocatalytic Water Reduction by Confined Cobalt Catalysts in Streptavidin

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1. EXPERIMENTAL SECTION

1.1. Materials and reagents

Reagents and solvents were purchased from commercial sources and used as received unless otherwise stated. Triethylamine (Et_3N) ≥ 99 % purity) and triethanolamine (TEOA ≥ 99 % purity) were purchased from Sigma-Aldrich® and used without further purification. Photosensitizer $[Ir(bpy)(ppy)_2]PF_6$ (**PS_{Ir}**) was synthesized according to literature procedures.[1] Ethyl [(3aS, 4S, 6aR)-2-oxo-hexahydro-thieno[3,4-d]imidazole-4-yl]pentanoate (**^{COOEt}Biotin**) was synthesized following the reported method from the literature.[2] Anhydrous acetonitrile was purchased from Scharlab. Water (18.2 MΩ·cm) was purified with a Milli-Q Millipore Gradient AIS system. All solvents were thoroughly degassed and stored under anaerobic conditions.

1.2. Instrumentation and experimental procedures

Physical methods

UV/Vis spectra were acquired on a Varian Cary 50 Bio Spectrophotometer. Gas chromatography was carried out on a SRI instruments, Model no. 310C GC using a 5Å molecular sieve column with a thermal conductivity detector and argon carrier gas.

NMR spectra were recorded in $CDCl_3$ on a Varian 400 or 500 MHz instrument, as noted. Low temperature NMR spectra of **Cat^{Bio}**, **Cat^{Bio}**$\subset$**SA** and **SA** were recorded in CD_3CN:H_2O tris buffer · HCl pH 7.5 mixtures (3:7, v/v) at 2 mM concentration. Circular Dichroism (CD) spectra measurements were carried out on an Applied Photophysics Chirascan Circular Dichroism spectrometer equipped with a photomultiplier detector, dual polarising prism design monochromator, photoelastic modulator (PEM) and 150 W Xenon light source. An average of 3 scans per sample were measured. All samples were were prepared in 100 mM Tris buffer (pH = 7.5) at 5 µM concentration, unless otherwise indicated.

Crystal Structure Determination and data collection: Crystals of **1^{Amide}** were grown by slow diffusion of Et_2O to a CH_2Cl_2 solution of the complex. The crystals for this samples were selected using a Zeiss stereomicroscope using polarized light and prepared under inert conditions immersed in perfluoropolyether as protecting oil for manipulation. Crystal structure determinations for **1^{Amide}** was carried out using a Apex DUO Kappa 4-axis goniometer equipped with an APPEX 2 4K CCD area detector, a Microfocus Source E025 IuS using MoK_α radiation, Quazar MX multilayer Optics as monochromator and an Oxford Cryosystems low temperature device Cryostream 700 plus (T = -173 °C). *Programs used:* Bruker Device: Data collection APEX-2,[3] data reduction Bruker Saint[4] V/.60A and absorption correction SADABS[5] or TWINABS[6]. Structure Solution and Refinement: Crystal structure solution was achieved using the computer program SHELXT. Visualization was performed with the program SHELXle[7]. Missing atoms were subsequently located from difference Fourier synthesis and added to the atom list. Least-squares refinement on F^2 using all measured intensities was carried out using the program SHELXL 2015[8]. All non-hydrogen atoms were refined including anisotropic displacement parameters.

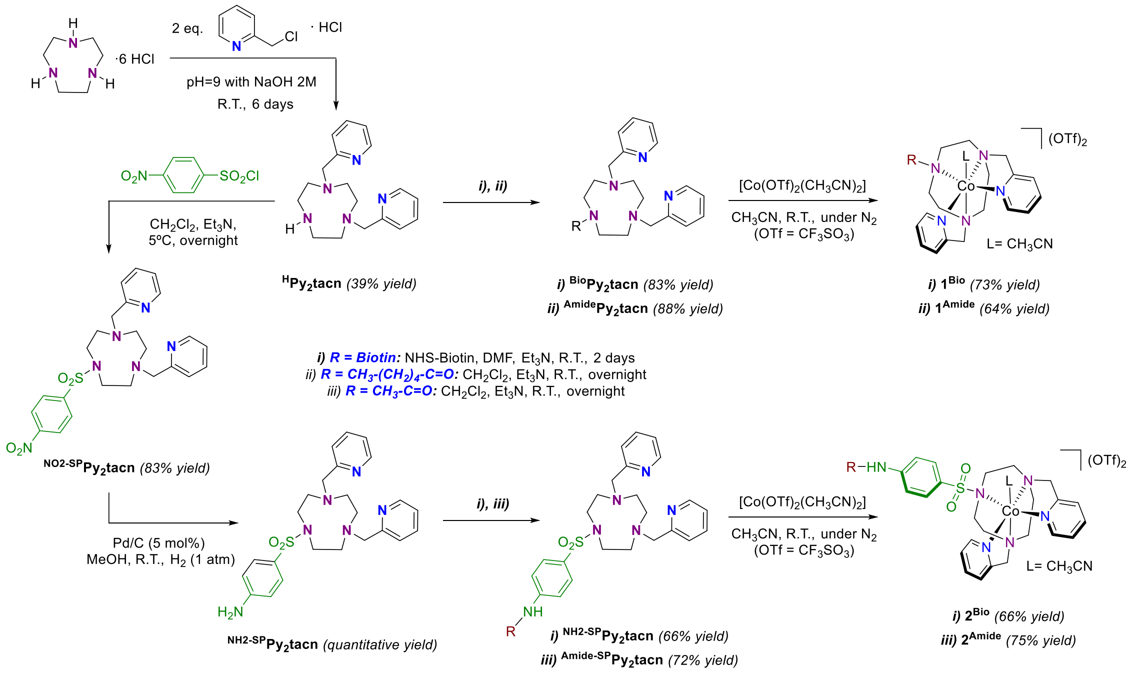
Electrochemical experiments were carried out on a CH-instruments 1242B potentiostat and a VSP potentiostat from Bio-Logic, equipped of the EC-Lab software. For all electrochemical measurements, a three-electrode system was used: a 3-mm diameter glassy carbon working electrode with a surface area of 0.28 cm^2, platinum mesh counter electrode, and saturated calomel reference electrode, unless otherwise specified. Working electrodes were polished with 1 μM alumina for 5 minutes, followed by 10 minutes of sonication, prior to use. Cyclic voltammetry was carried out on samples prepared in 100 mM citrate and 25 mM NaCl buffer of desired pH (3.5, 4.0, 4.5, 5.0, 5.5 and 6.0); scans were performed at 100 $mV \cdot s^{-1}$ scan rate. All potentials are quoted versus SCE. All electrolyte solutions were degassed by freeze and pump techniques. Samples were prepared by diluting the catalyst from a stock solution (10 mM) in water containing 5% DMSO to solubilize the catalyst. The final percentage of DMSO in the electrochemical cell was 0.5%. Electrochemical experiments **Cat^{Bio}** ⊂ **SA** were done by preparing a thin film of **Cat^{Bio}** ⊂ **SA** over the glassy carbon electrodes (0.28 cm^2 surface area) by drop-casting of 10 μL of a stock solution of metalloprotein of 10 μM and drying, otherwise indicated. After drying, electrochemical measurements were performed by directly submerging the glassy carbon electrode into the solution. For the Controlled Potential Electrolysis (CPE) experiments a VSP potentiostat from Bio-Logic, equipped of the EC-Lab software was used. A three-electrode configuration was used: a carbon mesh as working electrode, Pt wire as counter electrode and SCE as reference electrode. A solution of 4.1 ml of catalyst (**2^{Bio}** or **2^{Bio}** ⊂ **SA**) at 73 μM concentration in 100 mM citrate buffer 100 mM NaCl pH 3.5 under N_2 atmosphere at E_{appl} = –1.4 V vs SCE. A CV of the solution was taken before and after each CPE using a glassy carbon electrode (GC) of a surface area of 0.28 cm^2.

Electron Paramagnetic Resonance: An EMX Micro X-band EPR spectrometer from Bruker was used to collect data on 0.35 mM solution samples in a mixture of aqueous buffer and MeCN (7:3, buffer = Tris·HCl 100 mM, pH 7.5) using a finger Dewar at 77 K and He cryostat from Oxford Instruments at 50 K and 15 K. Data was acquired in perpendicular mode with a modulation frequency of 100 KHz, a modulation amplitude of 10 G, a 10.24 ms time constant and 19.02 ms conversion time with a microwave power was 0.1851 mW. Spectra were simulated using the EasySpin software package.[9]

X-ray Absorption Spectroscopy: Samples were recorded as 0.35 mM solutions in a mixture of aqueous buffer and MeCN (7:3, buffer = Tris·HCl 100 mM, pH 7.5) at the SOLEIL synchrotron (2.75 GeV, 400mA storage ring) SAMBA Beamline equipped with a Helium cryostat (20 K) and using a Si(220) double crystal monochromator together with a 36 channel Ge detector. Data calibration and normalization was carried out using the Athena software package.[10] Energies were calibrated to the first inflection point of Co foil spectra set at 7709.5 eV. A linear pre-edge function and a quadratic polynomial for the post-edge were used for background subtraction and normalization of the edge jump.

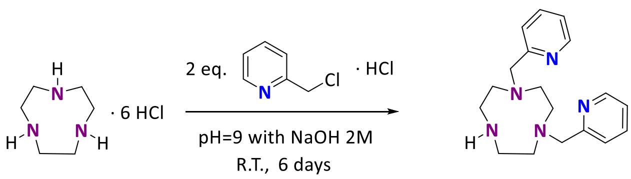
Photoinduced H_2 production Irradiation was performed using a 450W xenon lamp with a 400 nm cutoff filter, irradiating at a constant 1100 W/m^2 throughout the experiment. For each experiment, 400 µL of reaction mixture containing all of the reagents, were added to an airtight 1 mm cuvette and degassed extensively with argon prior to illumination. During irradiation time course 100 µL samples of the headspace were removed with a gas-tight syringe and injected directly for analysis by GC. A GC calibration curve was obtained by injecting various volumes of a 1% H_2, 99% N_2 gas mixture.

1.3. Synthesis of Ligands



Scheme S1. Synthesis of the biotinylated cobalt complexes used in this work.

Synthesis of 1,4-bis(2-pyridylmethyl)-1,4,7-triazacyclononane, ^{H}Py$_2$tacn.

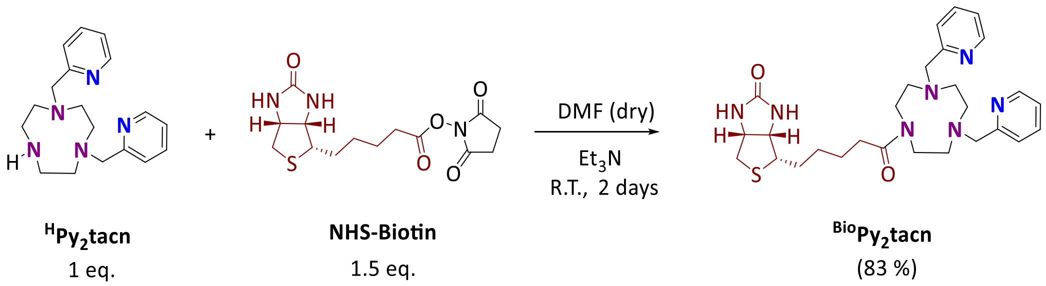


tacn · 6 HCl **^{H}Py$_2$tacn** (39 %)

Scheme S2. Synthesis of the basic structure **Py$_2$^{H}tacn**.

In a 100 mL flask tacn·6HCl (1 g, 2.87 mmol), 2-Pycolyl chloride hydrochloride (0.94 g, 5.74 mmol), and water (30 mL) were mixed and stirred to achieve a complete dissolution. The pH was adjusted to 9 by addition of NaOH 2 M. The resulting red solution was stirred for 3 days at room temperature: pH was readjusted to 9 with NaOH 2 M. The mixture was stirred for another 3 days, and then quenched by adding NaOH 2 M to pH 13. The solution was evaporated under reduced pressure and the resulting red oil was redissolved with NaOH 2 M and extracted with CH_2Cl_2 (3 x 60mL). The combined organic layers were then dried over anhydrous $MgSO_4$, filtered and the solvent was removed with rotary evaporator. The resulting crude red mixture was purified by basic alumina column chromatography (AcOEt : MeOH : drops of ammonia) to provide 0.344 g (1.105 mmol, 39 %) of the desired product. ^{1}H-NMR ($CDCl_3$, 300 MHz, 300K) δ, ppm: 8.53 (d, J= 4.5 Hz, 2H, $\mathbf{H_2}$ of py), 7.61 (dt, J= 7.8 Hz, 2H, $\mathbf{H_4}$ of py), 7.44 (d, J= 7.8 Hz, 2H, $\mathbf{H_5}$ of py), 7.15 (m, 2H, $\mathbf{H_3}$ of py), 3.88 (s, 4H, C$\mathbf{H_2}$), 2.81-2.73 (m, 8H, N-C$\mathbf{H_2}$-CH_2), 2.66 (s, 4H, N-C$\mathbf{H_2}$-CH_2).

Synthesis of ^{Bio}Py$_2$tacn. ^{Bio}Py$_2$tacn was synthesized by functionalizing the endocyclic secondary free amine on the tacn backbone with biotin *N*-hydroxysuccinimide (NHS-biotin) in the presence of Et_3N in DMF, using the general procedure described in the literature.[11]

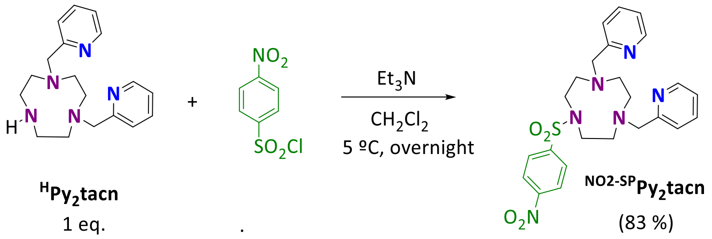


Scheme S3. Synthesis of **^{Bio}Py$_2$tacn**.

Biotin *N*-hydroxysuccinimide active ester of D-biotin (NHS-biotin) (180 mg, 0.500 mmol), **^{H}Py$_2$tacn** (104 mg, 0.333 mmol, 1 eq.), and triethylamine (0.17 mL, 1.2 mmol) were mixted in 4.5 mL of dry DMF. The reaction mixture was stirred at room temperature for 2 days under argon atmosphere. After that, it was slowly diluted with water (10 mL) and acidified with HCl (2 M) to pH 1. The solution was extracted with CH_2Cl_2 (3x10 mL) in order to remove the unreacted NHS-biotin. Then, the aqueous solution was basified to pH 10 by the addition of NaOH (2M), and extracted with CH_2Cl_2 (3x10 mL). The combined organic layers were then dried over anhydrous $MgSO_4$, filtered and the solvent was removed on a rotary evaporator. After drying under vacuum a pale yellow solid was obtained (0.148g, 0.275 mmol, 83 % yield) and used without further purification. ^{1}H-NMR ($CDCl_3$, 500 MHz, 300K) δ, ppm: 8.49 (m, 2H, **Ha** and **Ha'**), 7.62 (m, 2H, **Hc** and **Hc'**), 7.35 (m, 2H, **Hd** and **Hd'**), 7.13 (m, 2H, **Hb** and **Hb'**), 6.24 (s, 1H, **Hp**), 5.80 (s, 1H, **Hq**), 4.45 (m, 1H, **Ho**), 4.25 (m, 1H, **Hr**), 3.83 (s, 2H, **He**), 3.81 (m, 1H, **He**), 3.41 (m, 2H, **Hh**), 3.30 (m, 2H, **Hf**), 3.23 (m, 2H, **Hf´**), 3.11 (m, 1H, **Hm**), 2.96 (s, 2H, **Hg**), 2.84 (m, 2H, **Hn**), 2.71 (s, 2H, **Hg'**), 2.69 (s, 2H, **Hn'**), 2.57 (br, 2H, **Hh'**), 2.29 (t, *J* = 8.05 Hz, 2H, **Hi**), 1.70-1.59 (m, 4H, **Hl** and **Hj**), 1.38 (m, 2H, **Hk**). ^{13}C-NMR ($CDCl_3$, 126 MHz, 300K) δ, ppm: 173.2

(C_{10}), 163.8 (C_{17}), 159.9 (C_5), 159.7 ($C_{5'}$), 149.1 (C_1), 149.0 ($C_{1'}$), 136.5 (C_3), 136.3 ($C_{3'}$), 123.0 (C_4), 122.9 ($C_{4'}$), 122.1 (C_2), 121.9 ($C_{2'}$), 63.9 (C_6), 63.5 ($C_{6'}$), 61.9 (C_{16}), 60.2 (C_{18}), 57.2 ($C_{8'}$), 55.6 (C_{15}), 54.8 ($C_{9'}$), 54.3 ($C_{7'}$), 53.6 (C_8), 50.6 (C_7), 50.1 (C_9), 40.5 (C_{19}), 33.3 (C_{11}), 28.5 (C_{13}), 28.4 (C_{14}), 25.1 (C_{12}). MALDI-TOFMS (m/z): 538.7327 $[M+H]^+$.

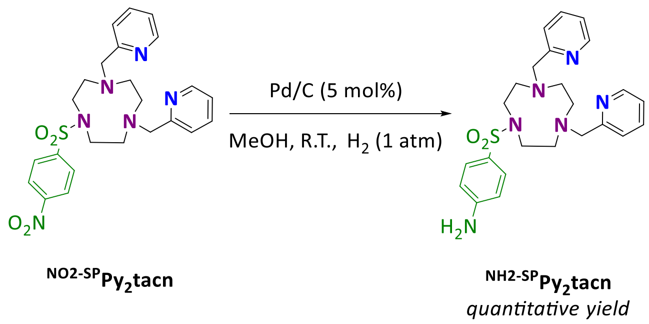
Synthesis of $^{NO2\text{-}SP}$Py$_2$tacn. The introduction of the 4-nitrobenzenesulfonyl moiety into the Py$_2$tacn backbone was performed following the general procedure described in the literature.[12]



Scheme S4. Synthesis of **$^{NO2\text{-}SP}$Py$_2$tacn**.

A CH_2Cl_2 solution (10 mL) containing 4-nitrophenylsulfonyl chloride (224 mg, 0.981 mmol, 1.1 eq.) was added dropwise at 5 °C to a solution of **^{H}Py$_2$tacn** (278 mg, 0.892 mmol, 1 eq.) and Et_3N (0.3 mL) in CH_2Cl_2 (25 mL). The yellowish solution was left stirring overnight at room temperature. The solvent was removed under reduced pressure and 10 mL of water at pH 1 was added. The aqueous solution was then washed with CH_2Cl_2 (3x10 mL) in order to remove the unreacted 4-nitrophenylsulfonyl chloride. The pH of the resulting aqueous solution was brought to 10 by the addition of NaOH (2M), and extracted with CH_2Cl_2 (3 x 10 mL). The combined organic layers were then dried over $MgSO_4$, filtered and the solvent was removed with rotary evaporator. After drying under vacuum a orange oil was obtained (367 mg, 0.740 mmol, 83 % yield). ^{1}H-NMR ($CDCl_3$, 400 MHz, 300K) δ, ppm: 8.53-8.52 (m, 2H), 8.36-8.33 (m, 2H), 7.97-7.95 (m, 2H), 7.68-7.64 (m, 2H), 7.46-7.44 (m, 2H), 7.19-7.15 (m, 2H), 3.89 (s, 4H), 3.31 (m, 4H), 3.19 (m, 4H), 2.79 (s, 4H). ^{13}C-NMR ($CDCl_3$, 101 MHz, 300K) δ, ppm: 159.65, 149.87, 149.08, 144.74, 136.42, 128.21, 124.30, 123.20, 122.04, 63.75, 55.94, 50.78. MALDI-TOFMS (m/z): 497.1945 $[M+H]^+$.

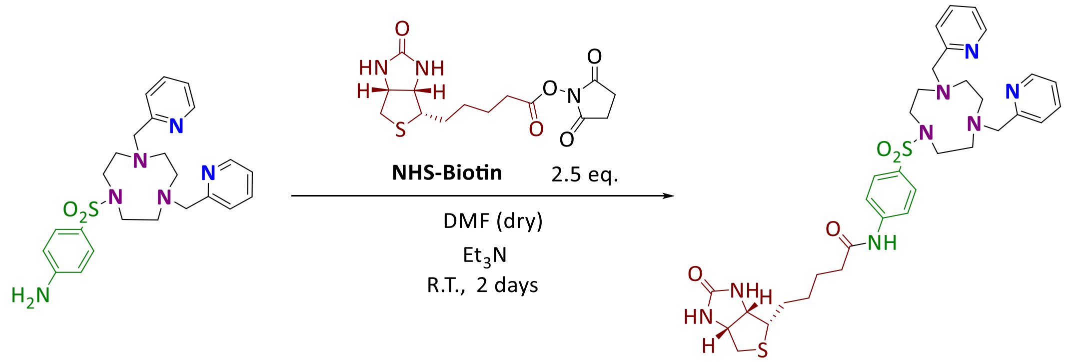
Synthesis of $^{NH2\text{-}SP}$Py$_2$tacn. Reduction of NO_2 group to NH_2 was performed following the general procedure described in the literature.[12]



Scheme S5. Synthesis of **$^{NH2\text{-}SP}$Py$_2$tacn**.

A flame dried round bottom flask containing a suspension of Pd/C (19.59 mg, 5 mol%) in MeOH (20 mL) was charged with **$^{NO2\text{-}SP}$Py$_2$tacn** (177 mg, 0.356 mmol). The Schlenk line was purged three times with argon and filled with hydrogen (1 atm). The reaction was vigorously stirred for 4 hours at RT, after which the hydrogen was carefully released. The suspension was removed by filtration through a Celite plug. The organic solvent was evaporated and the resulting product dried under vacuum, offering a pale yellow solid (165 mg, 0.356 mmol, quantitative yield). This compound is found to be very unstable and it was rapidly used in the next step without further purification. ^{1}H-NMR ($CDCl_3$, 400 MHz, 300K) δ, ppm: 8.52-8.51 (m, 2H), 7.67-7.61 (m, 4H), 7.50-7.48 (m, 2H), 7.18-7.16 (m, 2H), 7.02-7.00 (m, 2H), 7.19-7.15 (m, 2H), 3.89 (s, 4H), 3.21 (m, 4H), 3.14 (m, 4H), 2.83 (s, 4H). MALDI-TOFMS (m/z): 467.5017 $[M+H]^+$.

Synthesis of $^{Bio\text{-}SP}$Py$_2$tacn. The biotinylated ligand **$^{Bio\text{-}SP}$Py$_2$tacn** was synthesized according to the general procedure described in the literature.[11]



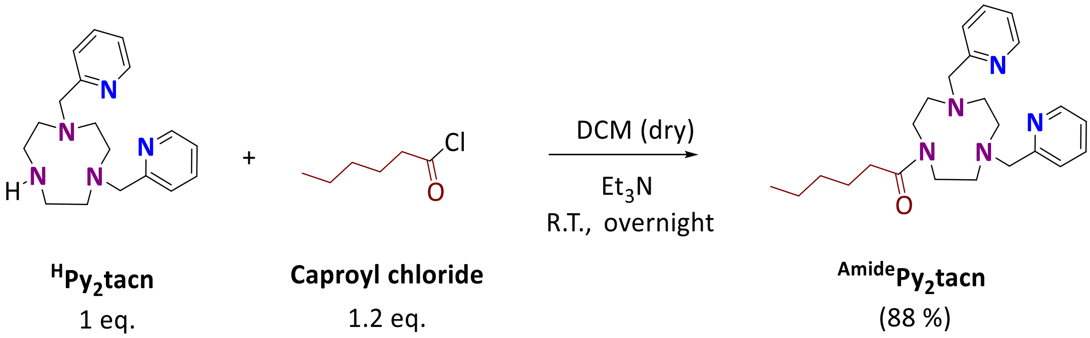
$^{NH2\text{-}SP}$Py$_2$tacn

$^{Bio\text{-}SP}$Py$_2$tacn
(66 %)

Scheme S6. Synthesis of **$^{Bio\text{-}SP}$Py$_2$tacn**.

Biotin *N*-hydroxysuccinimide active ester of D-biotin (NHS-biotin) (91.5 mg, 0.268 mmol, 2.5 eq.), **$^{NH2\text{-}SP}$Py$_2$tacn** (50 mg, 0.107 mmol, 1 eq.), and triethylamine (0.1 mL, 0.8 mmol) were mixted in 2.5 mL of dry DMF. The reaction mixture was stirred at room temperature for 2 days under argon atmosphere. After that, it was slowly diluted with water (10 mL) and acidified with HCl (2 M) up to pH 1. The solution was extracted with CH_2Cl_2 (3x10 mL) in order to remove the unreacted NHS-biotin. Then, the aqueous solution was further basified up to pH 10 by the addition of NaOH (2M), and extracted with CH_2Cl_2 (3x10 mL). The combined organic layers were then dried over anhydrous $MgSO_4$, filtered and the solvent was removed with rotary evaporator. After drying under vacuum a pale yellow solid was obtained (0.049 g, 0.071 mmol, 66 % yield) and used without further purification. ^{1}H-NMR ($CDCl_3$, 500 MHz, 300K) δ, ppm: 8.51-8.50 (m, 2H), 7.66-7.46 (m, 8H), 7.17-7.15 (m, 2H), 4.49 (m, 1H), 4.30 (m, 1H), 3.88 (s, 4H), 3.27-3.13 (m, 8H), 2.79 (s, 4H), 1.80-1.27 (m, 6H). MALDI-TOFMS (m/z): 693.53 $[M+H]^+$.

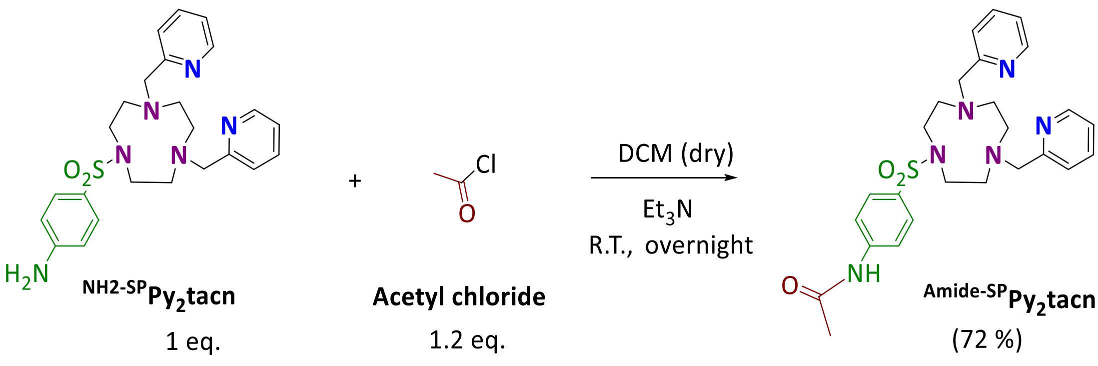
Synthesis of ^{Amide}Py$_2$tacn.



Scheme S7. Synthesis of ^{Amide}**Py$_2$tacn**.

To a flame-dried 25 mL round-bottomed flask was added ^{NH2}**Py$_2$tacn** (100 mg, 0.32 mmol), Et_3N (0.34 mL) and anhydrous CH_2Cl_2 (8.5 mL). Caproyl chloride (53.1 μL, 0.39 mmol) was then added dropwise through a syringe needle while the solution was stirred at room temperature under argon atmosphere. After stirring overnight, excess caproyl chloride was quenched by the addition of water (1 mL). The reaction mixture was extracted and washed with CH_2Cl_2 (2x10 mL) and the organic layers dried over $MgSO_4$, filtered and the solvent removed until dryness. Pure ^{Amide}**Py$_2$tacn** (116 mg, 0.28 mmol, 88 % yield) was obtained as a yellow oil following column chromatography on silica gel (5-10 % MeOH in $CHCl_3$ as eluent). ^{1}H-NMR ($CDCl_3$, 500 MHz, 300 K) δ, ppm: 8.54-8.52 (m, 2H), 7.68-7.61 (m, 2H), 7.43-7.41 (m, 2H), 7.19-7.13 (m, 2H), 3.88 (s, 1H), 3.49-3.48 (m, 2H), 3.38-3.35 (m, 2H), 3.25-3.24 (m, 2H), 3.03 (s-br, 2H), 2.78 (s-br, 2H), 2.63 (s-br, 2H), 2.29-2.27 (m, 2H), 1.63-1.58 (m, 2H), 1.32-1.24 (m, 4H), 0.90-0.86 (m, 3H). ^{13}C-NMR ($CDCl_3$, 126 MHz, 300K) δ, ppm: 207.23, 149.47, 54.12, 34.23, 32.09, 31.27, 30.05, 25.30, 22.92, 14.35, 1.37.

Synthesis of $^{Amide\text{-}SP}$Py$_2$tacn.

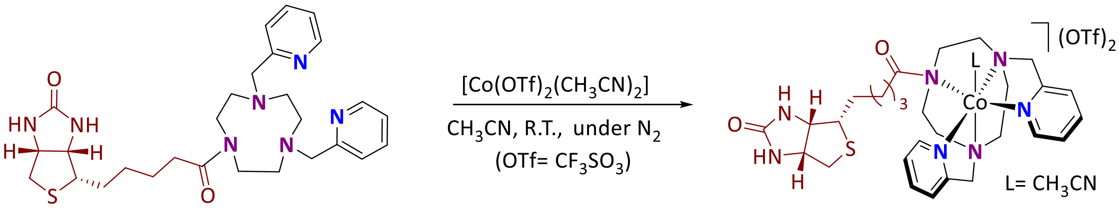


Scheme S8. Synthesis of $^{Amide\text{-}SP}$**Py$_2$tacn**.

To a flame-dried 25 ml round-bottomed flask was added $^{NH2\text{-}SP}$**Py$_2$tacn** (117.2 mg, 0.25 mmol), Et_3N (0.40 ml) and anhydrous CH_2Cl_2 (10 ml). Acetyl chloride (22 μl, 0.30 mmol) was then added dropwise through a syringe needle while the solution was stirred at 5ºC under argon atmosphere. After stirring overnight, excess acetyl chloride was quenched by the addition of water (1 ml). Then the reaction mixture was adjusted to pH 1 by the addition of HCl (1 M) and extracted with CH_2Cl_2 (1x10 mL). Then the pH was adjusted to 10 and extracted with CH_2Cl_2 (4x10 mL). The combined organic layers were then dried over anhydrous $MgSO_4$, filtered and the solvent was removed with rotary evaporator. After drying under vacuum **$^{Amide-SP}$Py$_2$tacn** was obtained as a pale yellow oil (92.1 mg, 0.18 mmol, 72 % yield) and used without further purification. ^{1}H-NMR ($CDCl_3$, 400 MHz, 300K) δ, ppm: 8.51-8.50 (m, 2H), 7.79-7.76 (m, 2H), 7.67-7.63 (m, 2H), 7.60-7.58 (m, 2H), 7.48-7.46 (m, 2H), 7.16-7.13 (m, 2H), 3.87 (s, 4H), 3.26-3.15 (m, 8 H), 2.78 (s, 4H), 2.28 (s, 3H). ^{13}C NMR ($CDCl_3$, 101 MHz, 300K) δ, ppm: 167.76, 159.94, 149.04, 142.44, 136.41, 128.09, 123.22, 121.97, 63.83, 55.97, 50.87, 45.82, 21.63, 18.32.

1.4. Synthesis of Cat^{Bio} and Cat^{Amide} and characterization.

Synthesis of [Co(^{Bio}Py$_2$tacn)(MeCN)](OTf)$_2$ (1^{Bio}).



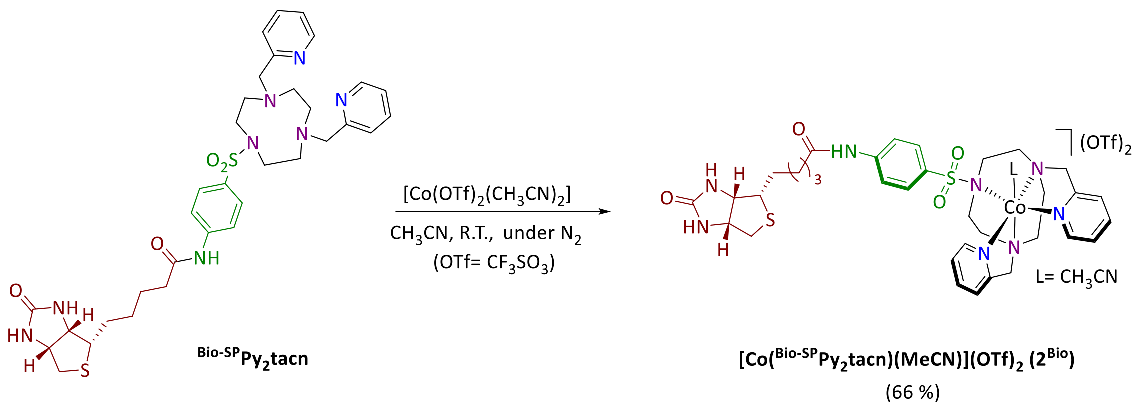
^{Bio}Py$_2$tacn

[Co(^{Bio}Py$_2$tacn)(MeCN)](OTf)$_2$ (1^{Bio})
(73 %)

Scheme S9. Synthesis of **[Co(^{Bio}Py$_2$tacn)(MeCN)](OTf)$_2$ (1^{Bio}).**

In a glovebox, a suspension of [Co(OTf)$_2$(MeCN)$_2$] (0.117 g, 0.266 mmol) in anhydrous CH_3CN (2 mL) was added dropwise to a vigorously stirred solution of **^{Bio}Py$_2$tacn** (0.143 g, 0.266 mmol) in anhydrous CH_3CN (2 mL). The cobalt triflate salt was quickly solubilized, and after few minutes the solution became red. After stirring for an additional 24 h the solution was passed through Celite, concentrated under vacuum (to 2 mL); slow diffusion of diethyl ether over the resultant solution yielded a pink powder (0.182 g, 0.194 mmol, 73% yield). ^{1}H-NMR (CD_3CN, 500 MHz, 240 K) δ, ppm: 368.1, 288.6, 264.2, 219.7, 156.3, 106.5, 90.1, 72.9, 56.3, 54.3, 40.3, 39.1, 31.2, 18.4, 17.3, 12.5, -7.2, -16.0, -18.1, -34.2, -38.5, -49.2. HR-MS-ESI (m/z) = 744.2467 [M-OTf]$^+$, 298.1124 [M-2·OTf]$^{2+}$. UV/Vis (H_2O) λ_{max} (ε)= 261 (5639 $M^{-1}\cdot cm^{-1}$).

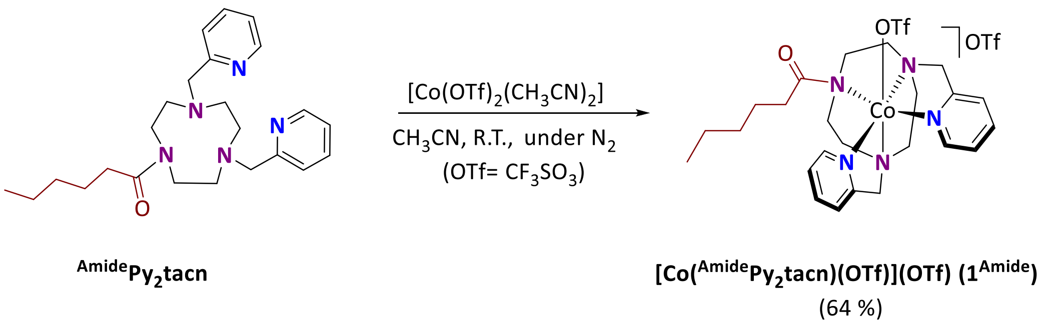
Synthesis of [Co($^{Bio-SP}$Py$_2$tacn)(MeCN)](OTf)$_2$ (2^{Bio}).



Scheme S10. Synthesis of **[Co($^{Bio\text{-}SP}$Py$_2$tacn)(MeCN)](OTf)$_2$ (2^{Bio}).**

In a glovebox, a suspension of [Co(OTf)$_2$(MeCN)$_2$] (0.046 g, 0.104 mmol) in anhydrous CH_3CN (2 mL) was added dropwise to a vigorously stirred solution of **$^{Bio\text{-}SP}$Py$_2$tacn** (0.072 g, 0.104 mmol) in anhydrous CH_3CN (2 mL). The cobalt triflate salt was quickly solubilized, and after few minutes the solution became red. After stirring for an additional 24 h the solution was passed through Celite, concentrated under vacuum (to 2 mL) and the slow diffusion of diethyl ether over the resultant solution afforded a pink powder compound (0.073 g, 0.068 mmol, 66% yield). ^{1}H-NMR (CD_3CN, 500 MHz, 240 K) δ, ppm: 286.8, 264.2, 170.5, 137.4, 125.8, 121.1, 109.8, 98.6, 88.2, 66.1, 61.8, 60.2, 57.0, 53.9, 42.3, 25.9, -10.6, -28.5, -66.6. HR-MS-ESI (m/z) = 674.0989 [M-biotin-OTf]$^+$, 262.5750 [M-biotin-2·OTf]$^{2+}$.UV/Vis (H_2O) λ_{max} (ε)= 264 (17716 $M^{-1}\cdot cm^{-1}$).

Synthesis of [Co(^{Amide}Py$_2$tacn)(MeCN)](OTf)$_2$ (1^{Amide}).

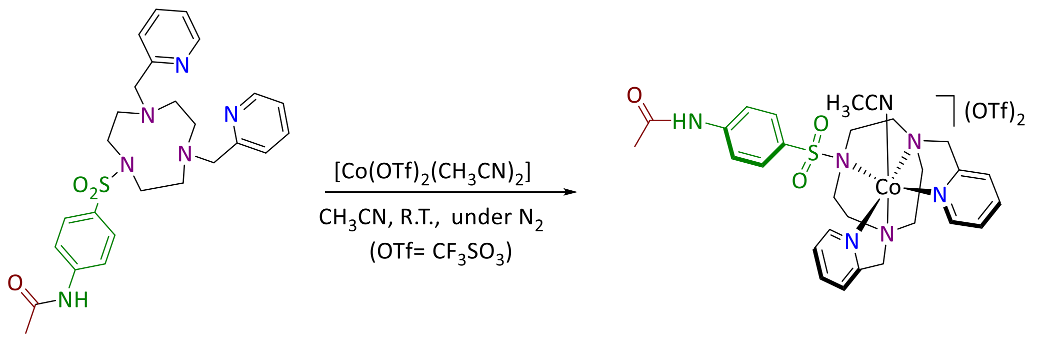


Scheme S11. Synthesis of **[Co(^{Amide}Py$_2$tacn)(MeCN)](OTf)$_2$ (1^{Amide}).**

In a glovebox, a suspension of [Co(OTf)$_2$(MeCN)$_2$] (0.124 g, 0.283 mmol) in anhydrous CH_3CN (1.5 mL) was added dropwise to a vigorously stirred solution of **^{Amide}Py$_2$tacn** (0.116 g, 0.283 mmol) in anhydrous CH_3CN (1.5 mL). The cobalt triflate salt was quickly solubilized, and after few minutes the solution became dark red. After stirring for an additional 12 h the solution was passed through Celite and concentrated under vacuum (to 1.5 mL). Slow diffusion of diethyl ether over the resultant solution yielded a dark pink powder (0.145 g, 0.180 mmol, 64 % yield). ^{1}H-NMR (CD_3CN, 400 MHz, 298 K) δ, ppm:

217.8, 211.2, 135.0, 128.9, 108.1, 89.9, 81.1, 68.8, 53.6, 47.7, 38.0, 24.6, 15.9, 3.5, 1.62, 1.31, 1.15, 0.9, -1.02, -2.4, -5.6, -14.8, -17.8, -84.3.

Synthesis of [Co($^{Amide-SP}$Py$_2$tacn)(MeCN)](OTf)$_2$ (2^{Amide}).



$^{Amide-SP}$Py$_2$tacn

[Co($^{Amide-SP}$Py$_2$tacn)(MeCN)](OTf)$_2$ (2^{Amide})
(75 %)

Scheme S12. Synthesis of **[Co($^{Amide-SP}$Py$_2$tacn)(MeCN)](OTf)$_2$ (2^{Amide}).**

In a glovebox, a suspension of [Co(OTf)$_2$(MeCN)$_2$] (0.071 g, 0.161 mmol) in anhydrous CH_3CN (1.5 mL) was added dropwise to a vigorously stirred solution of **$^{Amide-SP}$Py$_2$tacn** (0.082 g, 0.161 mmol) in anhydrous CH_3CN (1.5 mL). The cobalt triflate salt was quickly solubilized, and after few minutes the solution became dark pink. After stirring for an additional 12 h the solution was passed through Celite and concentrated under vacuum (to 1.5 mL). Slow diffusion of diethyl ether over the resultant solution yielded a dark pink powder (0.110 g, 0.121 mmol, 75 % yield). ^{1}H-NMR (CD_3CN, 400 MHz, 298 K) δ, ppm: 122.0, 55.13, 4.16, 3.41, 3.13, 1.23, 1.11, 0.65, -1.55, -1.63, -9.1.

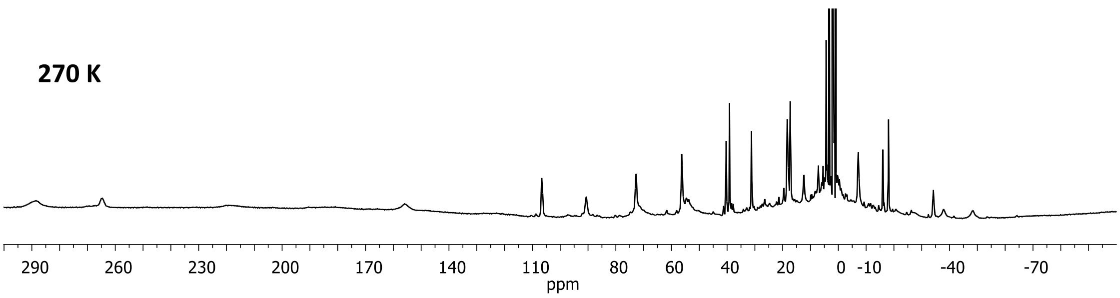


Figure S1. ^{1}H-NMR spectra (500 MHz) of **1^{Bio}** in CD_3CN at 270K.

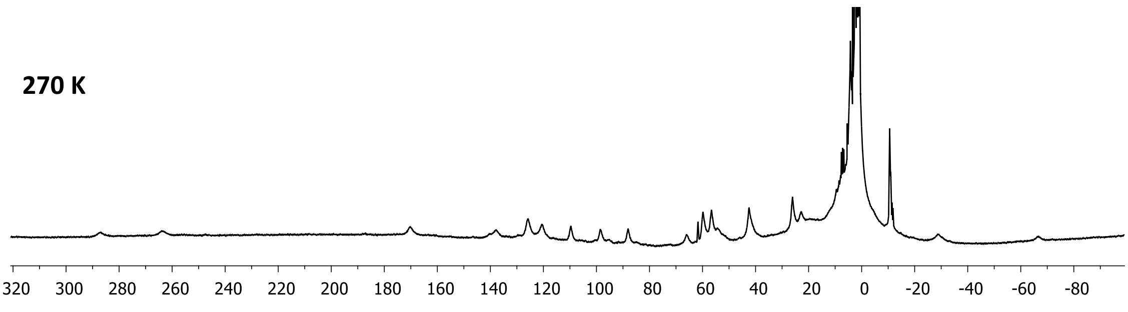


Figure S2. ^{1}H-NMR spectra (500 MHz) of **2^{Bio}** in CD_3CN at 270 K.

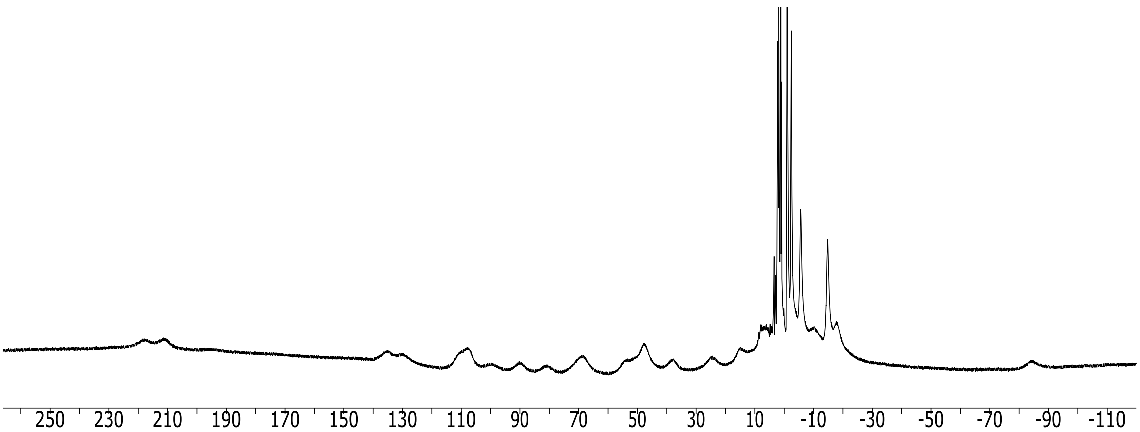


Figure S3. ^{1}H-NMR spectra (400 MHz) of **1^{Amide}** in CD_3CN at 298 K.

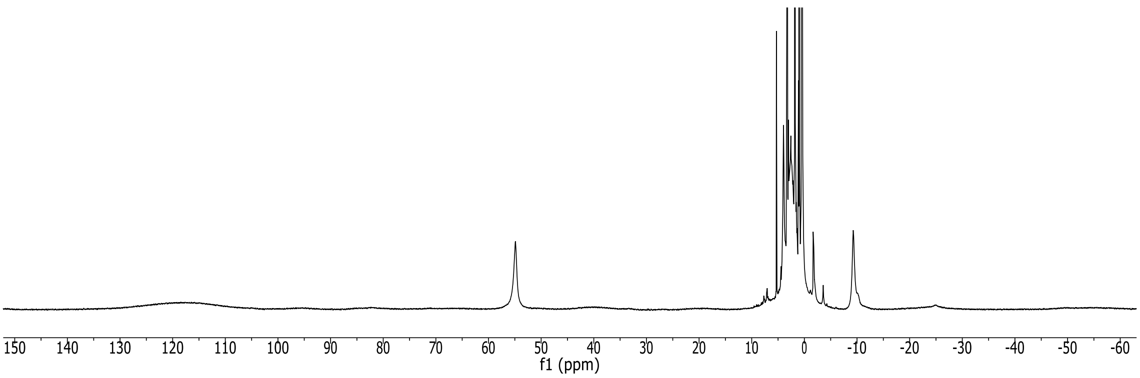


Figure S4. ^{1}H-NMR spectra (400 MHz) of **2^{Amide}** in CD_3CN at 298 K.

The magnetic susceptibility (μ_{eff}) values for complexes **1^{Bio}** and **2^{Bio}** were measured by ^{1}H-NMR following the Evans' method[13] under catalytic conditions (MeCN:aqueous Tris·HCl buffer (0.1 M) pH 7.5, 3:7 v/v) at 270, 280, 290 and 298 K. As shown in Figure SI.5, complexes **1^{Bio}** and **2^{Bio}** present reasonably constant μ_{eff} values (3.6 - 4.4 BM) between 270 and 298 K, in good agreement with d^{7} high-spin Co^{II} complexes reported in the literature[14] and our DFT calculations.

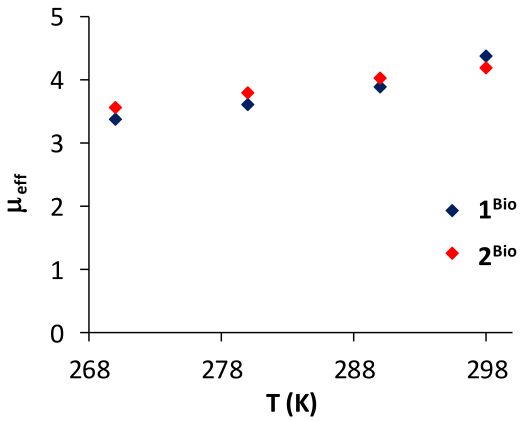


Figure S5. Representation of the effective magnetic moment (μ_{eff}) of **1**^{Bio} and **2**^{Bio} under catalytic conditions (MeCN:aqueous Tris·HCl buffer (0.1 M) pH 7.5, 3:7 v/v) as function of temperature.

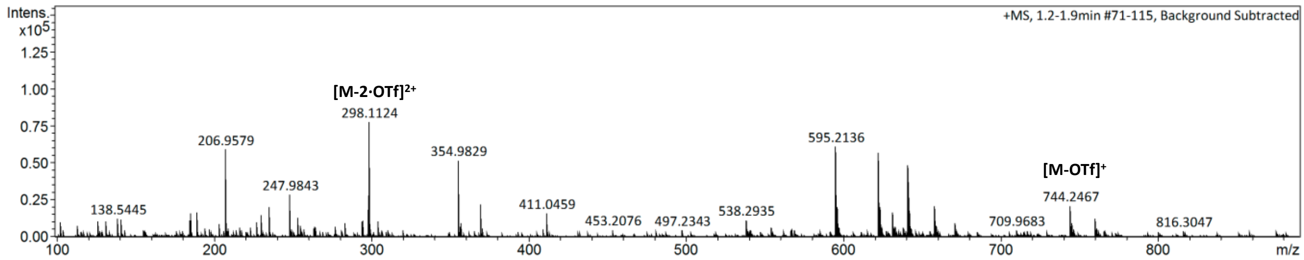


Figure S6. HR-MS-ESI spectrum of **1**^{Bio}. $[M\text{-}2\cdot OTf]^{2+}$ and $[M\text{-}OTf]^{+}$ stand for $[Co(^{Bio}Py_2tacn)]^{2+}$ and $[Co(^{Bio}Py_2tacn)(OTf)]^{+}$, respectively.

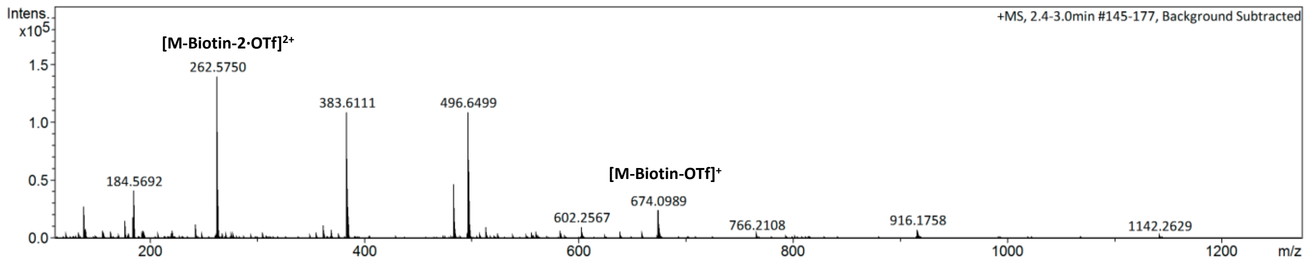


Figure S7. HR-MS-ESI spectrum of **2**^{Bio}. $[M\text{-biotin-}2\cdot OTf]^{2+}$ and $[M\text{-biotin-}OTf]^{+}$ stand for $[Co(^{SP}Py_2tacn)]^{2+}$ and $[Co(^{SP}Py_2tacn)(OTf)]^{+}$, respectively.

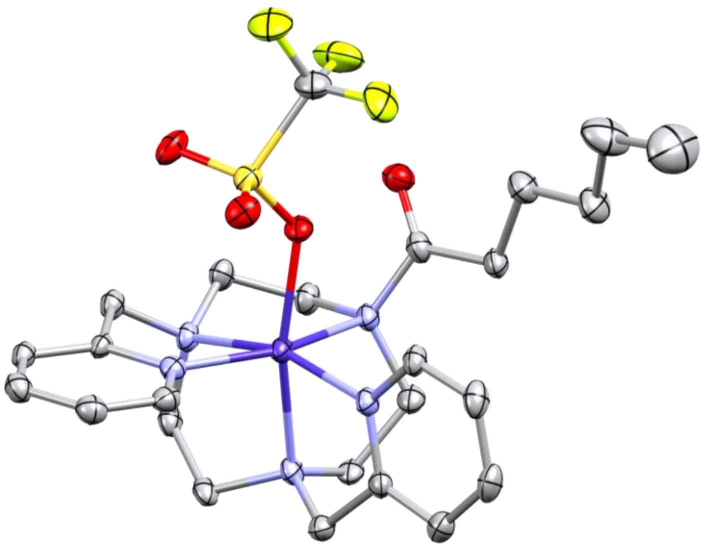


Figure S8. ORTEP drawing (thermal ellipsoids drawn at a 50 % probability level) showing the structure of ***1**^{Amide}*. OTf counteranion and hydrogen atoms have been omitted in the sake of clarity. Selected bond lengths (Å): Co-O1 2.063(2), Co-N1 2.087(2), Co-N3 2.132(3), Co-N4 2.128(2), Co-N2 2.136(3), Co-N5 2.374(2). Selected angles (º): O1-Cu-N1 95.10(9), O1-Co-N2 166.81(9), O1-Co-N3 93.50(9), O1-Co-N4 102.60(9), O1-Co-N5 87.69(9).

Table S1. Crystal data and structure refinement for complex **1^{Amide}.**

Identification code	mo_CCS01146_0m	
Empirical formula	C26 H35 Co F6 N5 O7 S2	
Formula weight	766.64	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 12.511(2)Å	α= 90°.
	b = 8.8444(16)Å	β = 93.865(5)°.
	c = 29.209(6)Å	γ = 90°.
Volume	3224.6(11) Å^3	
Z	4	
Density (calculated)	1.579 Mg/m^3	
Absorption coefficient	0.748 mm^{-1}	
F(000)	1580	
Crystal size	0.60 x 0.25 x 0.05 mm^3	
Theta range for data collection	1.818 to 30.762°.	
Index ranges	-17<=h<=9,-12<=k<=9,-42<=l<=40	
Reflections collected	25914	
Independent reflections	9207[R(int) = 0.0652]	
Completeness to theta =30.762°	91.6%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.964 and 0.625	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9207/ 0/ 426	
Goodness-of-fit on F^2	1.013	
Final R indices [I>2sigma(I)]	R1 = 0.0553, wR2 = 0.1162	
R indices (all data)	R1 = 0.1120, wR2 = 0.1340	
Largest diff. peak and hole	0.902 and -0.679 e.Å^{-3}	

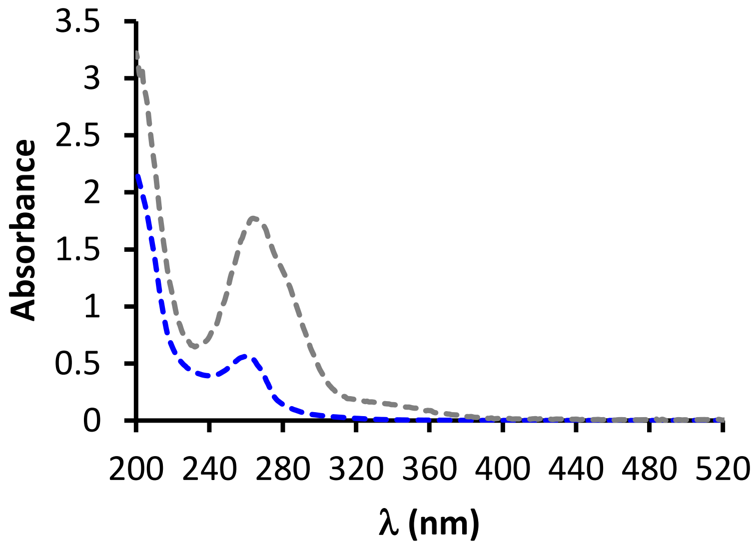


Figure S9. UV/Vis absorption spectra of **1**^{Bio} (0.1 mM, blue) and **2**^{Bio} (0.1 mM, grey) in H_2O at 298 K.

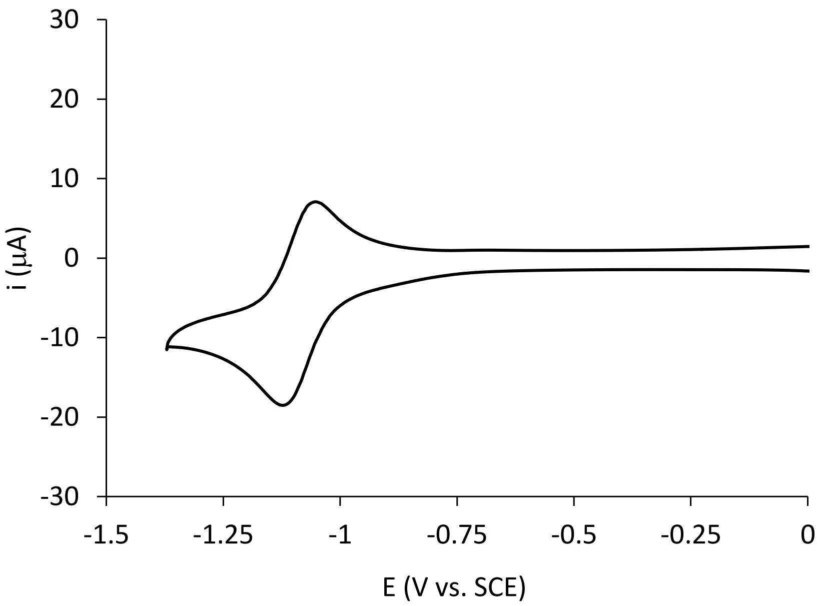


Figure S10. CVs of **1**^{Bio} (1 mM) in dry MeCN. Experimental conditions: Bu_4NPF_6 (0.1 M) as supporting electrolyte in acetonitrile, using a 0.28 cm^2 glassy carbon as working and SCE as reference electrodes. Scan rate of 100 $mV{\cdot}s^{-1}$.

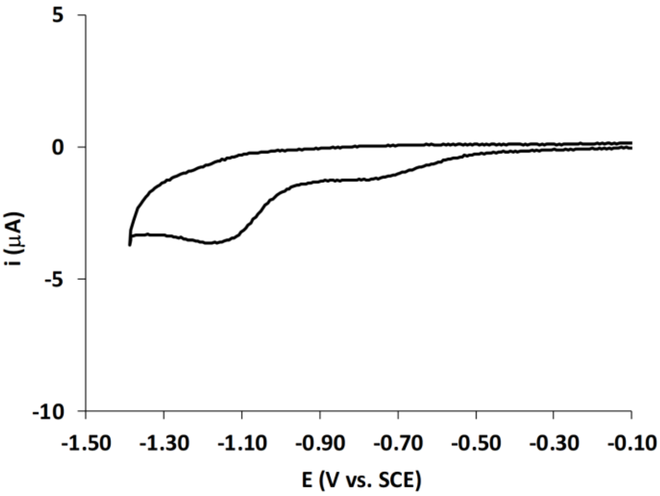


Figure S11. CVs of **2**^{Bio} (0.25 mM) in dry MeCN. Experimental conditions: Bu_4NPF_6 (0.1 M) as supporting electrolyte in acetonitrile, using a 0.28 cm^2 glassy carbon as working and SCE as reference electrodes. Scan rate of 100 mV·s^{-1}.

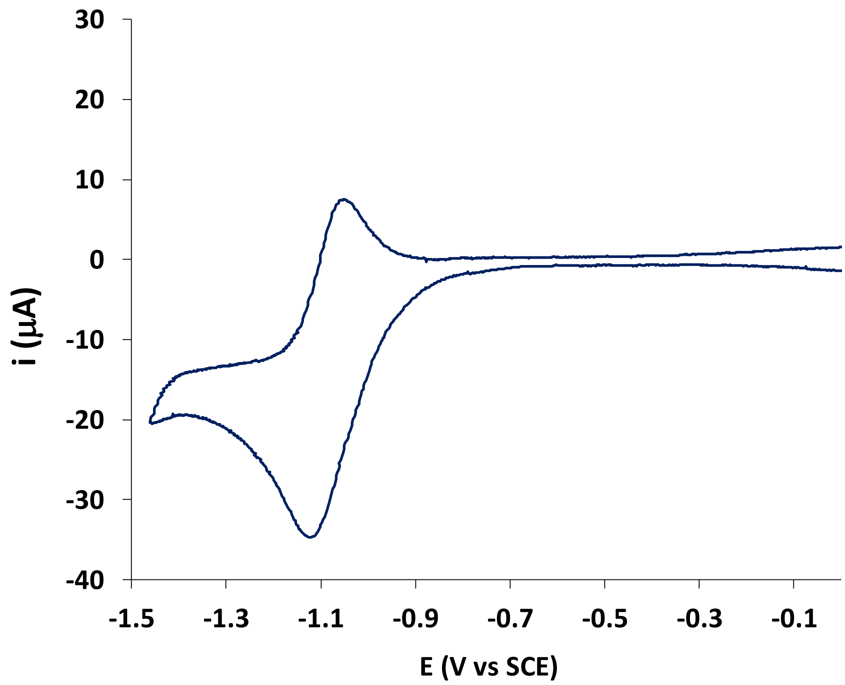


Figure S12. CV of **1**^{Amide} (1 mM) in dry MeCN. Experimental conditions: Bu_4NPF_6 (0.1 M) as supporting electrolyte in acetonitrile, using a 0.28 cm^2 glassy carbon as working and Ag pseudoreference and the Fc/Fc$^+$ couple as reference electrodes. Scan rate of 100 mV·s^{-1}.

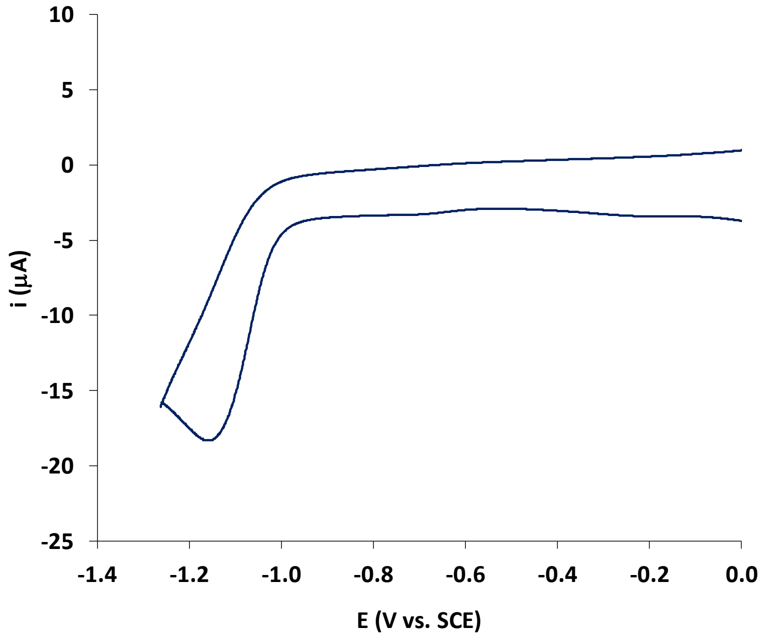


Figure S13. CV of **2**$^{\mathbf{Amide}}$ (1 mM) in dry MeCN. Experimental conditions: Bu_4NPF_6 (0.1 M) as supporting electrolyte in acetonitrile, using a 0.28 cm^2 glassy carbon as working and Ag pseudoreference and the Fc/Fc^+ couple as reference electrodes. Scan rate of 100 $mV \cdot s^{-1}$.

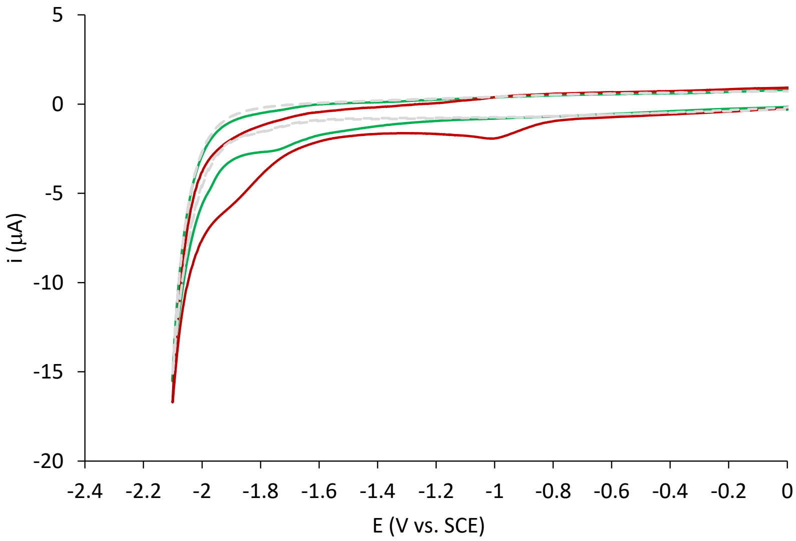


Figure S14. Cyclic voltammograms in CH_2Cl_2 containing 100 mM Bu_4NPF_6 in the absence (dashed grey trace), and presence of 0.5 mM of $^{\mathbf{Bio}}$**Py$_2$tacn** (green trace) and $^{\mathbf{Bio\text{-}SP}}$**Py$_2$tacn** (red trace) ligands. Scan rate of 100 $mV \cdot s^{-1}$ using a 0.28 cm^2 glassy carbon working electrode. Potentials are quoted versus SCE.

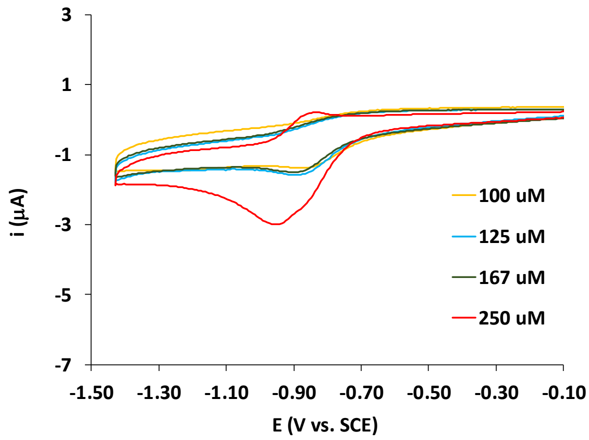


Figure S15. CVs of **biotin** (from 250 – 100 μM) in dry MeCN. Experimental conditions: Bu_4NPF_6 (0.1 M) as supporting electrolyte in acetonitrile, using a 0.28 cm^2 glassy carbon as working and SCE as reference electrodes. Scan rate of 100 $mV{\cdot}s^{-1}$.

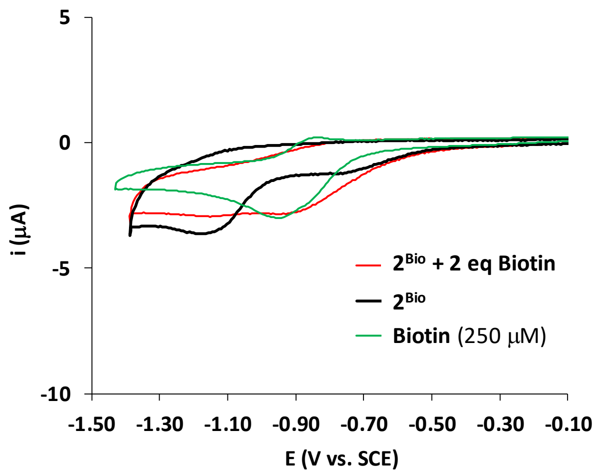


Figure S16. CVs of **biotin** (0.25 mM), $\mathbf{2^{Bio}}$ (0.25 mM) and $\mathbf{2^{Bio}}$ after the addition of 2 eq of biotin in dry MeCN. Experimental conditions: Bu_4NPF_6 (0.1 M) as supporting electrolyte in acetonitrile, using a 0.28 cm^2 glassy carbon as working and SCE as reference electrodes. Scan rate of 100 $mV{\cdot}s^{-1}$.

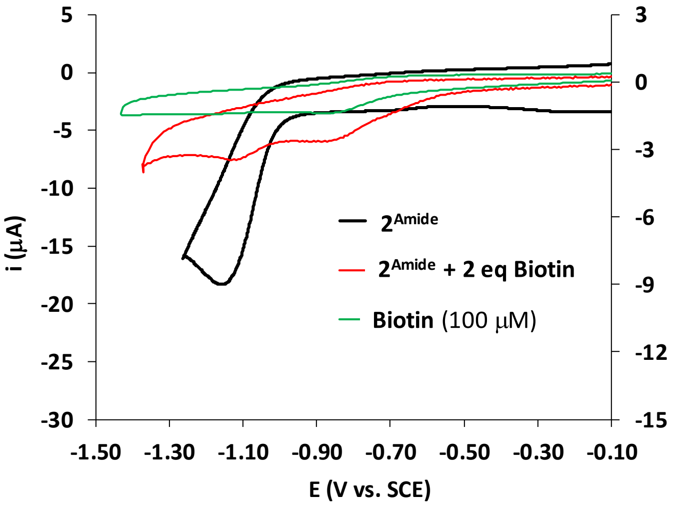


Figure S17. CVs of **biotin** (0.1 mM), $\mathbf{2}^{\mathbf{Amide}}$ (1 mM) and $\mathbf{2}^{\mathbf{Amide}}$ (0.25 mM) after the addition of 2 eq of biotin in dry MeCN. Experimental conditions: Bu_4NPF_6 (0.1 M) as supporting electrolyte in acetonitrile, using a 0.28 cm^2 glassy carbon as working and SCE as reference electrodes. Scan rate of 100 $mV{\cdot}s^{-1}$.

1.5. Determination of the stability constant

The stability constant of the complexes was estimated using a well-stablished 2-(4'-hydroxyazobenzene)benzoic acid (HABA) displacement assay.[15] HABA binds to SA with lower affinity than biotin, and thus it can be stoichiometrically replaced by biotin in a titration experiment. The HABA ⊂ SA complex absorbs in the visible range, with a characteristic band centered at 506 nm. The addition of biotinylated compounds causes the displacement of HABA resulting in loss of absorbance of the HABA ⊂ SA complex. The host protein SA (14 μM) was initially loaded with a large excess of HABA (1066.6 μM, ~ 80 eq) and incubated for 30 min in Phosphate buffer (0.3 M) pH 7 at room temperature in order to ensure the complete saturation of the binding sites of SA. This solution was then used for spectrophotometric titration with D-biotin and the biotinylated catalyst, respectively. From the saturated HABA ⊂ SA complex solution 200 μl were placed in a UV-vis quartz cuvete cell and diluted with 200 μl Phosphate buffer (0.3 M) pH 7 (final concentration HABA 533.35 μM and SA 7 μM) and the UV-vis spectrum recorded at rt from 200 to 700 nm. Then the UV-vis monitored titration was performed by subsequent addition of 4 μl of a stock solution (125 μM) of the corresponding D-biotin or the biotinilatd catalysts to see the decay of the band at 506 nm (HABA ⊂ SA complex). The stock solutions of D-biotin and the biotinilaed catalysts were prepared in the same phosphate buffer (0.3 M) pH 7 with a 0.5% addition of acetonitrile to ensure complete solubility of the cobalt catalysts. After each addition the mixture was shook for one minute prior to recording the UV-vis spectrum. As depicted in Figure SI.18, the addition of the biotinylated complexes $\mathbf{1}^{\mathbf{Bio}}$ and $\mathbf{2}^{\mathbf{Bio}}$ was followed by a concomitant decrease of the UV-vis signal at 506 nm, demonstrating the HABA displacement. The association constant of the cobalt complexes is estimated to be significantly higher than the HABA constant K_{HABA} = 10000 M^{-1}).

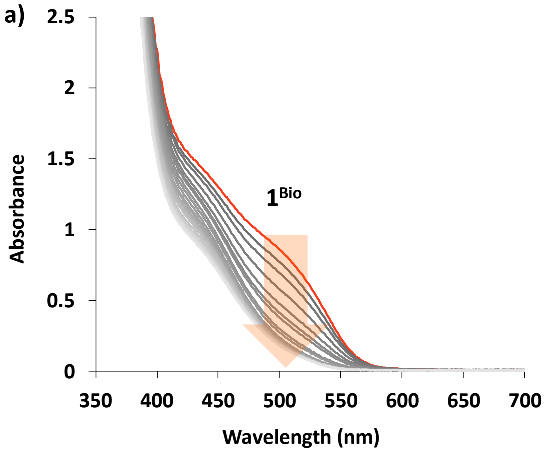


Figure S18. UV/Vis absorption decay in of the HABA ⊂ SA complex upon the addition of different amounts of $\mathbf{1}^{\mathbf{Bio}}$ (*Top*) and $\mathbf{2}^{\mathbf{Bio}}$ (*Bottom*) in 300 mM phosphate, pH 7 and saturated with 533.35 μM HABA.

The association constant for the equilibrium depicted in Eq 2 can be obtained as follow.

$$\mathrm{HABA} + \mathrm{SA} \rightleftharpoons \mathrm{HABA} \subset \mathrm{SA} \qquad (1)$$

$$\mathrm{HABA} \subset \mathrm{SA} + [\mathbf{Cat}^{\mathbf{Bio}}] \rightleftharpoons \mathbf{Cat}^{\mathbf{Bio}} \subset \mathrm{SA} + \mathrm{HABA} \qquad (2)$$

Considering the stability constant of HABA ⊂ SA complex reported in the literature (log K_{HABA} = 4.0)[16] we have estimated the stability constant of [$\mathbf{Cat}^{\mathbf{Bio}}$] ⊂ SA ($K_{[\mathbf{CatBio}] \subset \mathrm{SA}}$) according to eq. 5.

$$\mathrm{K_{HABA}} = \frac{[\mathrm{HABA} \subset \mathrm{SA}]}{[\mathrm{HABA}] \times [\mathrm{SA}]} \qquad (3)$$

$$\mathrm{K_{exch}} = \frac{[\mathbf{Cat}^{\mathbf{Bio}} \subset \mathrm{SA}] \times [\mathrm{HABA}]}{[\mathrm{HABA} \subset \mathrm{SA}] \times [\mathbf{Cat}^{\mathbf{Bio}}]} \quad (4)$$

$$K_{[\mathbf{Cat}^{\mathbf{Bio}}] \subset \mathrm{SA}} = \frac{[\mathbf{Cat}^{\mathbf{Bio}} \subset \mathrm{SA}]}{[\mathbf{Cat}^{\mathbf{Bio}}] \times [SA]} = K_{HABA} \times K_{exch} \qquad (5)$$

Arranging Eq. 5 leads to a single quadratic equation (Eq. 6) to calculate the exchange constant, K_{exch}. Variables $[\mathrm{HABA}]_{\mathrm{total}}$, $[\mathrm{SA}]_{\mathrm{total}}$ and $[\mathbf{Cat}^{\mathbf{Bio}}]_{\mathrm{total}}$ are known or can be calculated from the UV-Vis titration [HABA ⊂ SA].

$$(1 - K_{exch}) \times [HABA \subset SA]^2 + (K_{exch} \times \{[SA]_{total} - [\mathbf{CAt}^{\mathbf{Bio}}]\} - [HABA]_{total-} [SA]_{total}) \times [HABA \subset SA] + [HABA]_{total} \times [SA]_{total} = 0 \qquad (6)$$

Estimated association constant for $\mathbf{1}^{\mathbf{Bio}}$ and $\mathbf{2}^{\mathbf{Bio}}$ are approximatly $1{\cdot}10^7$ M^{-1}.

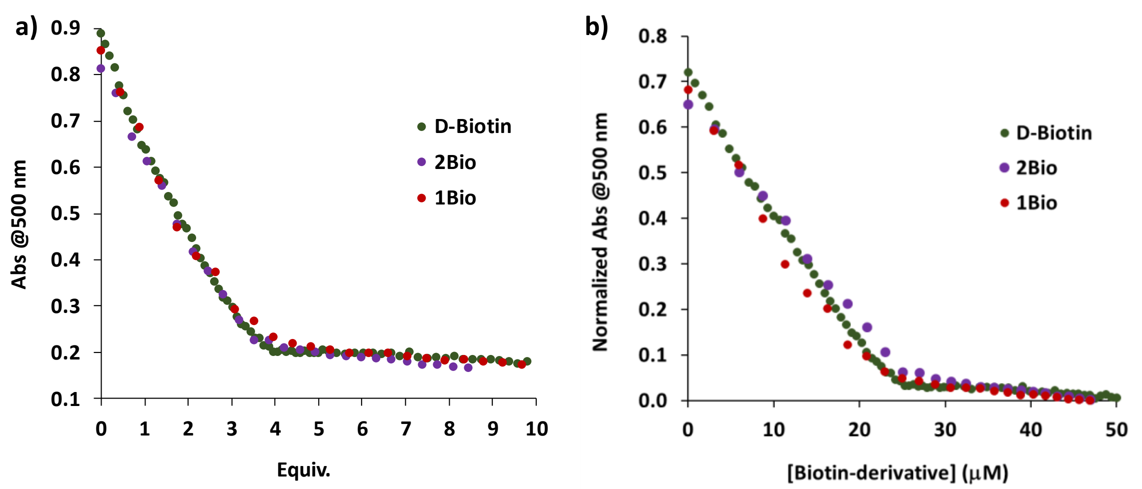


Figure S19. HABA displacement assay of SA by **1**^{Bio} (red dots) and **2**^{Bio} (purple dots). a) Absorbance at 500 nm monitored as a function of the biotinylated compound concentration. b) Normalized absorbance at 500 nm monitored as a function of the biotinylated compound added equivalents. A titration curve with free D-biotin (green dots) has been included for comparative purposes.

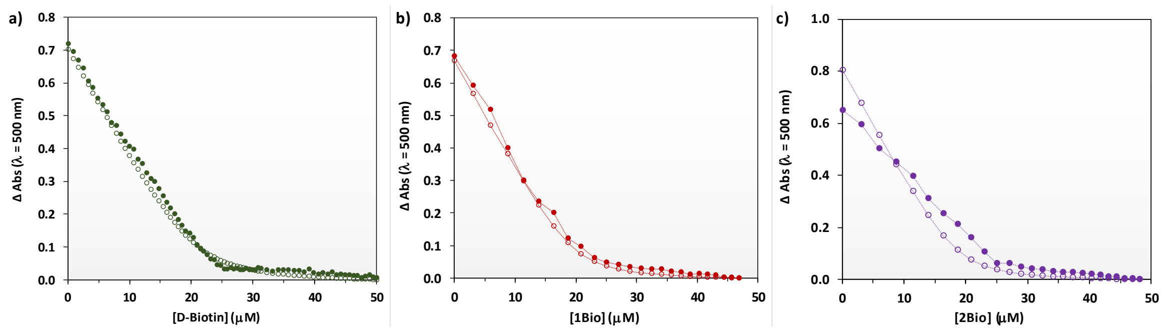


Figure S20. Fitting (empty dots) for the HABA displacement assay of SA by **D-biotin** (green dots, a) **1**^{Bio} (red dots, b) and **2**^{Bio} (purple dots, c).The fitting has been performed by taking into account a K_{exch} of 3, obtaining an association constant of about $1 \cdot 10^7$ M^{-1} for the biotinylated catalysts.

1.6. Synthesis of [Cat^{Bio}] $\subset$ SA and characterization

Synthesis of **Cat**^{Bio} $\subset$ **SA** adducts was carried out by combining the corresponding cobalt catalyst with streptavidin. 5 mg of SA were dissolved in 2.5 mL of 100 mM Tris·HCl buffer pH 7.5 and incubated with 4-fold excess of **Cat**^{Bio}. After mixing for 30 minutes at room temperature, the solution was purified by filtration through a PD-10 desalting column (Sephadex G-25; Exclusion limit M_r 5000, GE healthcare) previously equilibrated with the same buffer. Because of the extremely high affinity of SA for biotin, SA-incorporated biotinylated cobalt catalyst can be purified away from unbound biotinylated cobalt catalyst using a PD-10 desalting column, which eleiminates the potential free biotinylated cobalt complex in solution Fractions were collected every 1 mL and analyzed by UV-vis spectroscopy. The concentration of purified SA was determined spectrophotometrically using a molar extinction coefficient of 41820 $M^{-1} \cdot cm^{-1}$ at 280 nm for SA.[17] The combined protein fractions yielded a concentration of 19.3 μM of **1**^{Bio} $\subset$ **SA** and 25.2 μM of **2**^{Bio} $\subset$ **SA**.

1.6.1. Characterization by UV/Vis spectroscopy and circular diachroism

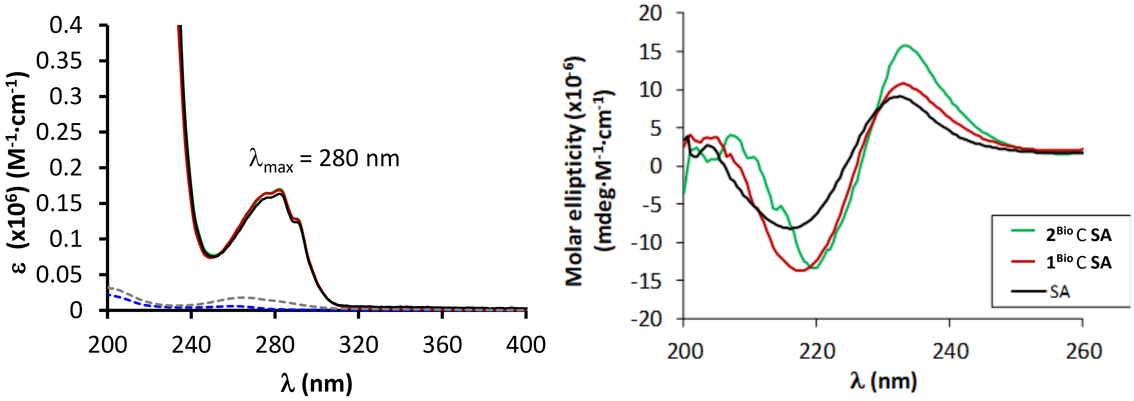


Figure S21. *Left*: UV/Vis spectra of 5 μM solution of SA (solid black trace), **1**^{Biot} ⊂ **SA** (solid red trace) and **2**^{Bio} ⊂ **SA** (solid green trace) measured in 100 mM Tris·HCl buffer, pH 7.5 at 20 ºC. The absorption of **1**^{Bio} (dashed blue trace) and **2**^{Bio} (dashed grey trace) are included for comparison. *Right*: CD spectra of SA (Black trace), **1**^{Bio} ⊂ **SA** (green trace) and **2**^{Bio} ⊂ **SA** (red trace). Conditions: 5 μM protein, 100 mM Tris·HCl buffer, pH 7.5 at 20 ºC.

1.6.2. Characterization by ^{1}H-NMR

The ^{1}H-NMR spectrum of the free SA shows diamagnetic signals of the residues present in the protein scaffold expanding from 10 to 1 ppm at 280 K (Figure S24). Upon encapsulation of the paramagnetic cobalt(II) **2**^{Bio} complex there are clear changes in the ^{1}H-NMR spectrum. For instance, some of the aromatic signals centered at about 7.5 ppm and the aliphatic signals at around 2.5 ppm disappear. The modification of the ^{1}H signals can be attributed to the effect of the paramagnetic Co(II) center in the protein residues, producing faster relaxation times (signal broadening) and chemical shifts. As a note, there is not broadening in the solvent peaks, which ensures that the paramagnetic effect is manifested on the ^{1}H-NMR protein signals due to close proximity interactions. In the paramagnetic spectrum some weak paramagnetic signals are found from 250 to -50 ppm, which could be attributed to the biotinylated Co(II) paramagnetic complex (Figure S22). We also noticed that the paramagnetic signals in the paramagnetic spectra recorded for **2**^{Bio} ⊂ **SA** are slightly shifted compared to complex **2**^{Bio} alone, under the same experimental conditions. (Figure S22).

Besides, the ^{1}H-NMR spectra of **2**^{Bio} is clearly modified from pure CD_3CN to Tris·HCl pH 7.5 buffer and 30 % CD_3CN mixtures; the conditions employed for measuring the free protein and the metalloprotein. The ^{1}H-NMR differences show the expected CD_3CN to Cl^- ligand exchange since the buffer contains a high concentration of chloride anion. Moreover, the ^{1}H-NMR spectra of **2**^{Bio} in CD_3CN also resembles the non-biotinylated complex [Co(OTf)($Py_2{}^{Ts}$tacn)](OTf) (**2**), and equally changes when the ^{1}H-NMR is recorded in Tris·HCl buffer:CD_3CN (7:3) mixtures (see Figure S25). The ligand exchange was also detected in the EPR measurements of [Co(X)($Py_2{}^{Ts}$tacn)](X) (X: -Cl, -OTf) in isobutyronitrile and H_2O:MeCN (7:3) mixtures in 0.1 M Tris·HCl buffer pH 7.5.

As a summary, the paramagnetic ^{1}H-NMR studies performed indicate that i) the main proton resonance features of the cobalt complex are present with slight modifications and ii) some ^{1}H-RMN features of the SA protein are also altered in the $\mathbf{2^{Bio}} \subset$ **SA** sample. The former observation suggests that the $\mathbf{2^{Bio}}$ structure is intact, which is in agreement with XAS and EPR studies, and both observations are consistent with the supramolecular assembly. Nevertheless, the broad nature of the signals complicates an analysis on the localization of the Cobalt-complex-protein contact interactions.

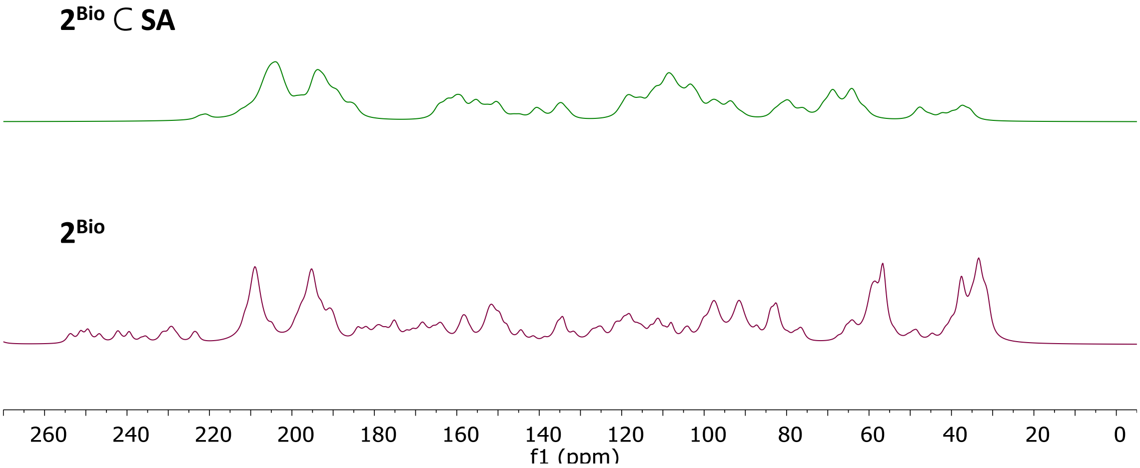


Figure S22. ^{1}H-NMR spectra (500 MHz, Tris·HCl buffer pH 7.5:CD_3CN (7:3) at 280 K) of $\mathbf{2^{Bio}} \subset$ **SA** and $\mathbf{2^{Bio}}$. The broad buffer signal from water of the ^{1}H-NMR spectra have been removed for clarity and the phases adjusted for a proper observation of the paramagnetic signals of the complexes.

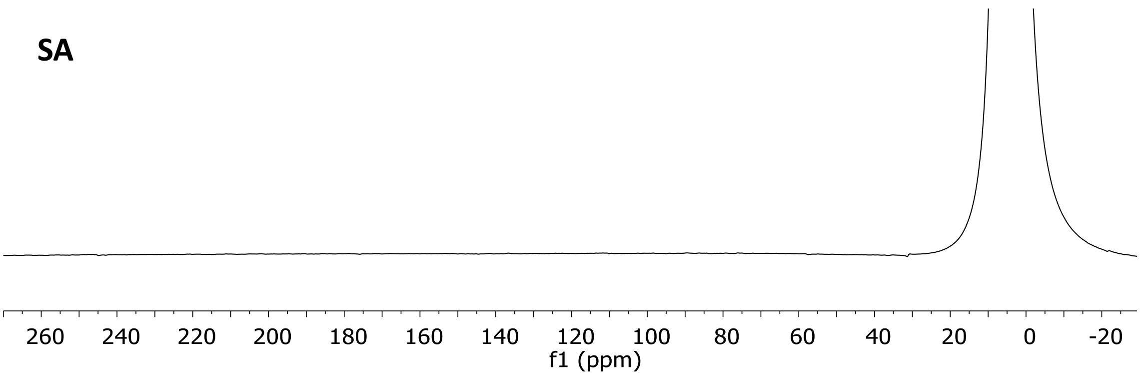


Figure S23. ^{1}H-NMR spectra (500 MHz, Tris·HCl buffer pH 7.5:CD_3CN (7:3) at 280 K) of SA.

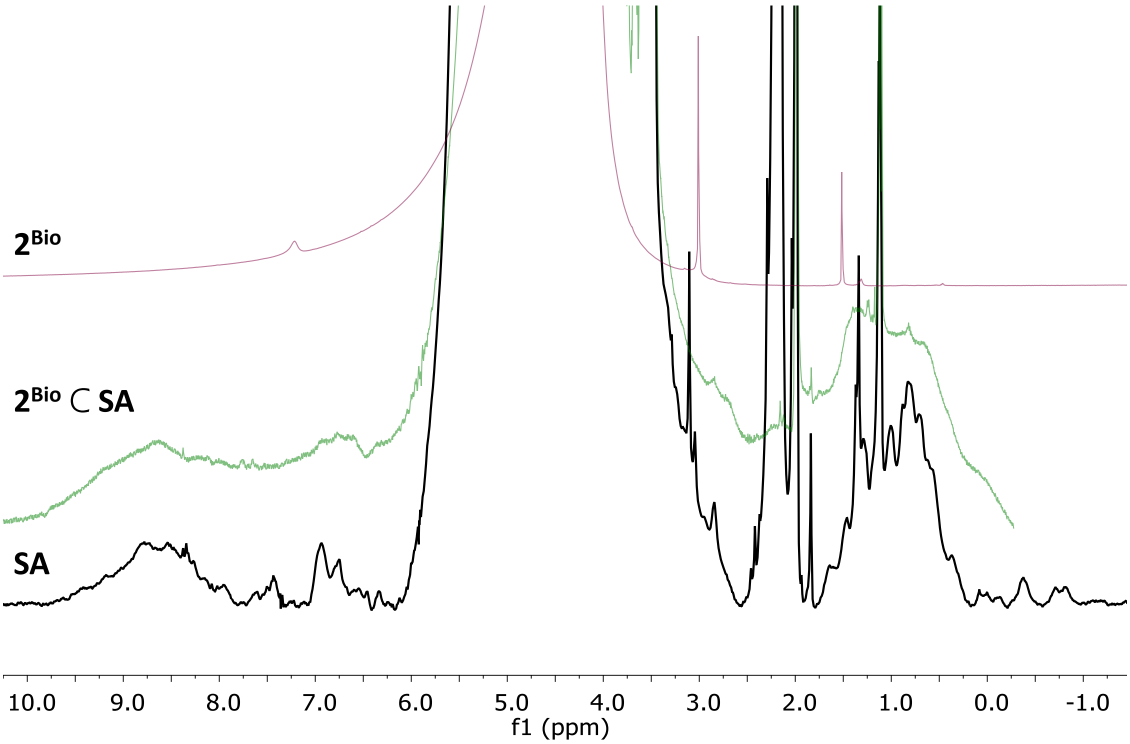


Figure S24. From *top* to *bottom*: Magnification of the diamagnetic region of the ^{1}H-NMR spectra (500 MHz, Tris·HCl buffer pH 7.5:CD_3CN (7:3) at 280 K) of **2^{Bio}**, **2^{Bio}** ⊂ **SA** and **SA**.

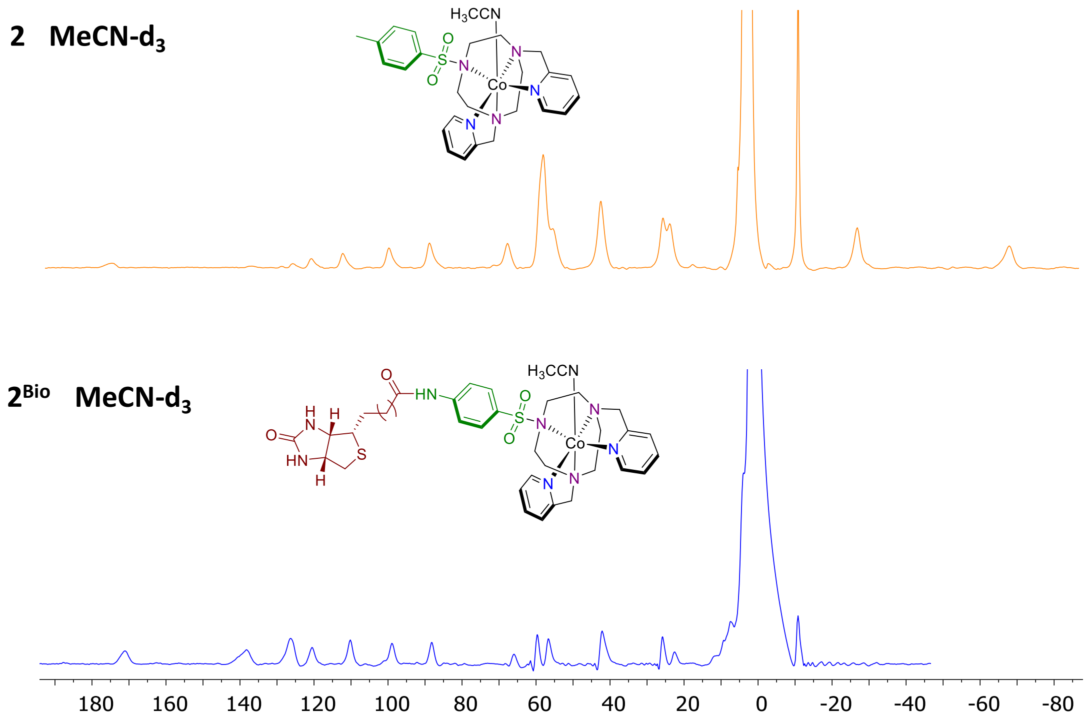


Figure S25. ^{1}H-NMR spectra (500 MHz at 273 K) of **2** in CD_3CN, **2^{Bio}** in Tris·HCl buffer pH 7.5:CD_3CN (7:3) and **2^{Bio}** in CD_3CN (from *top* to *bottom*, respectively).

1.6.3. Characterization by XAS and EPR

Furthermore we applied metal K-edge X-ray absorption spectroscopy (XAS) and EPR as direct probes of electronic and geometric structure of the metal coordination environment. The Co K-edge XAS spectra of $\mathbf{2}^{Bio}$ and $\mathbf{2}^{Bio}\subset\mathbf{SA}$ have a comparable profile suggesting a similar coordination environment and oxidation state. The rising edges centered around 7719.3 eV are consistent with a Co(II) center (Figure S26).[18] Furthermore, the intensity of the pre-edges at 7710.4 eV, of 0.06 normalized units, suggests a centrosymetric pseudo-octahedral environment.[19] This is further supported by EPR experiments of $\mathbf{2}^{Bio}$ and $\mathbf{2}^{Bio}\subset\mathbf{SA}$ which at liquid nitrogen temperatures show low spin Co(II) signals with gx and gy values centered around a g of 2.2 and gz values approaching 2.0 similar to previously reported values for elongated distorted pseudo octahedral Co(II) complexes (Figure S27B).[20] On the other hand the EPR spectra of $\mathbf{1}^{Bio}$ and $\mathbf{1}^{Bio}\subset\mathbf{SA}$ suggest an axially compressed pseudo-octahedral environment at the Co(II) center with g_z values centered around a g of 2.3 and g_x, g_y values close to 2.0 (Figure S27A).[20] For both series of complexes the XAS and EPR spectroscopic data indicate analogous coordination environments for $\mathbf{Cat}^{Bio}$ and $\mathbf{Cat}^{Bio}\subset\mathbf{SA}$ with minor modulations upon encapsulation. This data suports the hypothesis of a catalytic H_2 evolution enhancement based on second coordination sphere interactions between the catalytic center and the protein pocket.

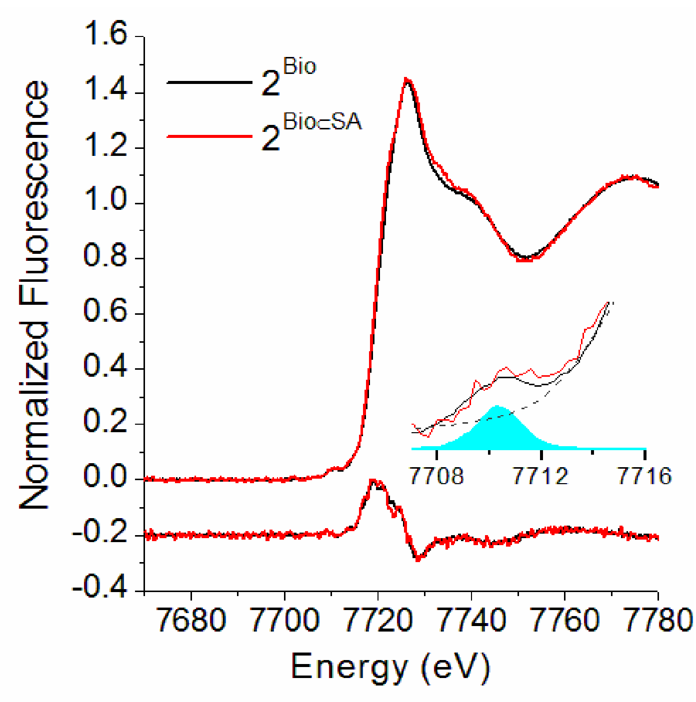


Figure S26. Co K-edge XANES spectra of $\mathbf{2}^{Bio}$ and $\mathbf{2}^{Bio}\subset\mathbf{SA}$ and the corresponding derivative. Inset: Pre-edge area and fit centered at 7710.4 eV with an intensity of 0.06 (cyan).

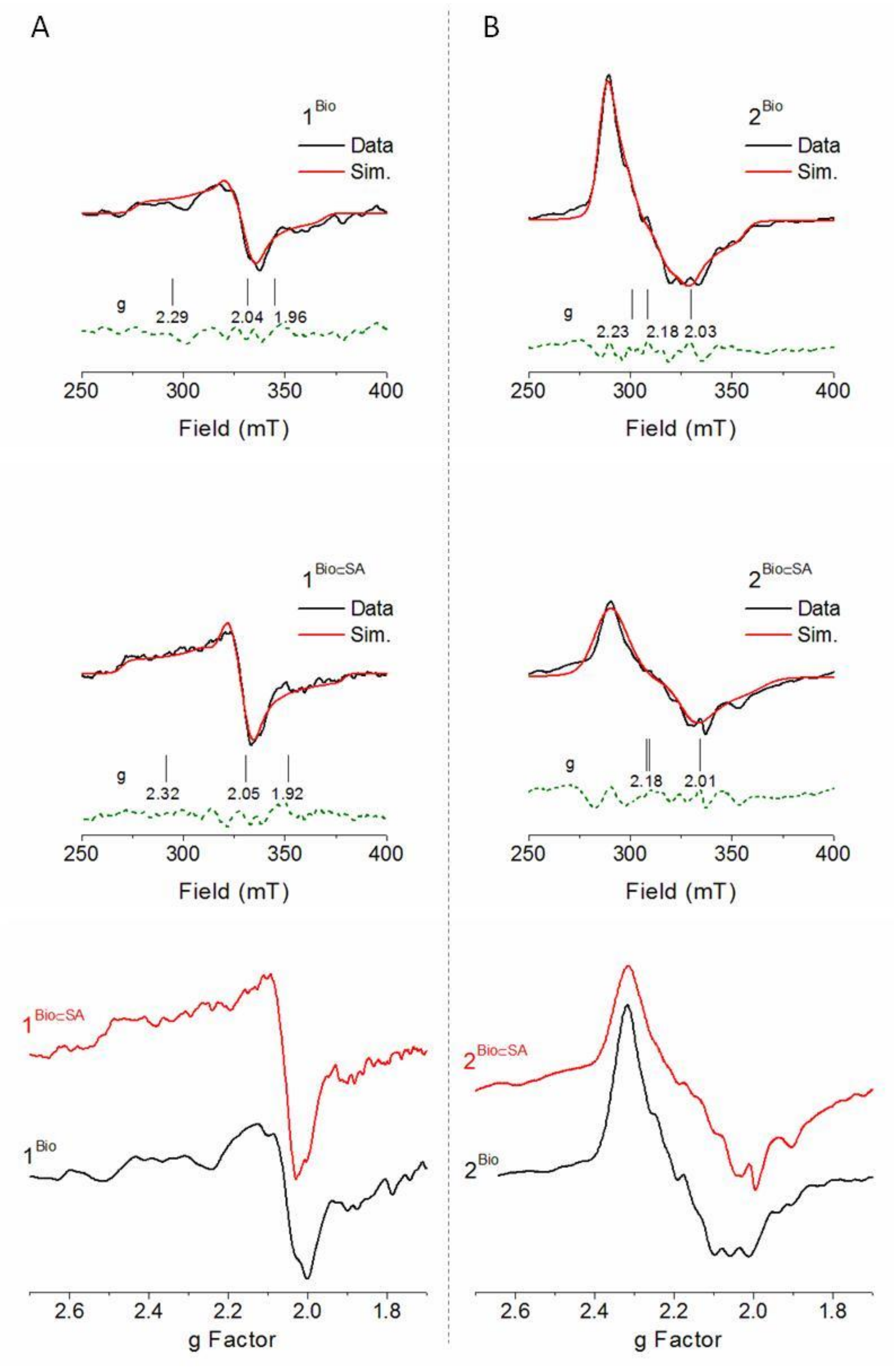


Figure S27. (A) EPR spectra and simulation of **1^{Bio}** (Az, Ax, Ay= 152.0, 5.6, 163.4, MHz), and **1^{Bio}** ⊂ **SA** (Az, Ax, Ay= 174.6, 2.8, 182.0, MHz). (B) EPR spectra and simulation of **2^{Bio}** (Az, Ax, Ay= 161.9, 105.1, 190.7 MHz), and **2^{Bio}** ⊂ **SA** (Az, Ax, Ay= 150.2, 169.1, 221.9, MHz) measured at 77K.

We have also preformed new EPR experiments (at 15 K or 50 K) of complexes [Co(OTf)(Py$_2$^{Ts}tacn)](OTf) (**2**) and [Co(Cl)(Py$_2$^{Ts}tacn)](Cl) (**2Cl**), **1**^{Bio}, **1**^{Bio} ⊂ **SA**, **2**^{Bio} and **2**^{Bio} ⊂ **SA** to provide less noisy spectra.

First we performed power saturation studies as suggested by the reviewer (Figures S28 – S31) and we clearly see the low spin Co(II) signals having a distinct saturation profile from the high spin component. We further analyzed the signals in this series at 25 db attenuation as it offered the best signal to noise ratio for both the high and low spin forms and allowed characterization of the low spin components at a non-saturating power.

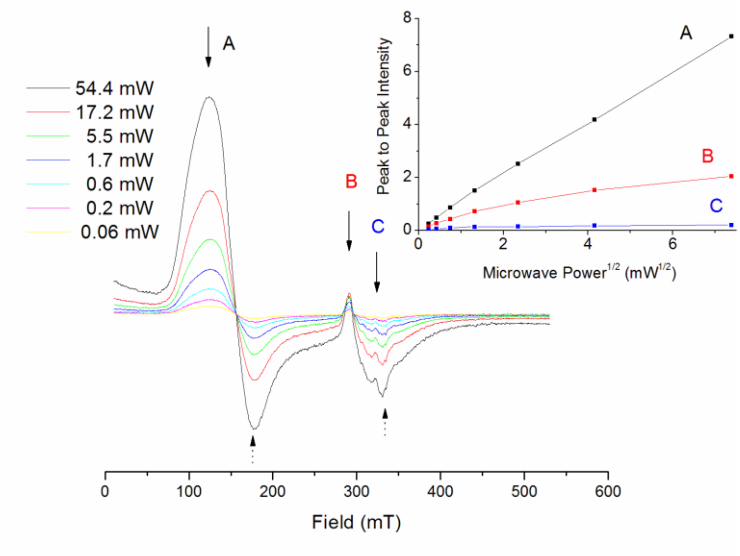


Figure S28. EPR power saturation of **1**^{Bio} at 15K.

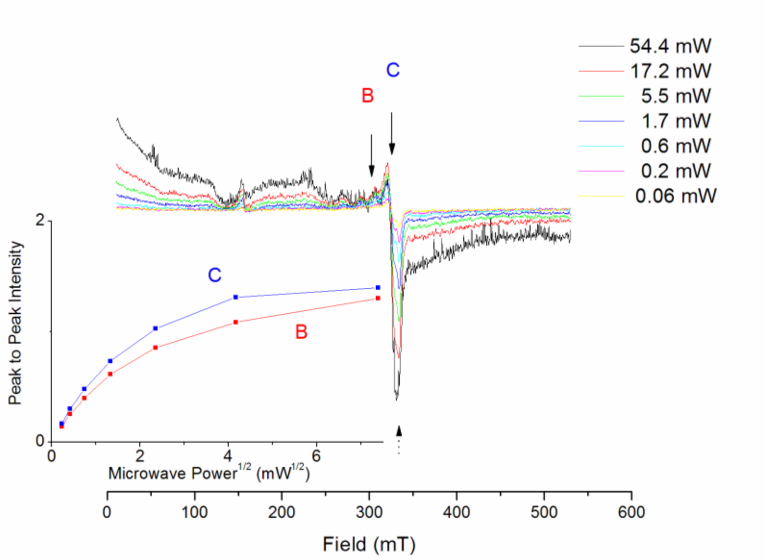


Figure S29. EPR power saturation of **1**^{Bio} ⊂ **SA** at 15K.

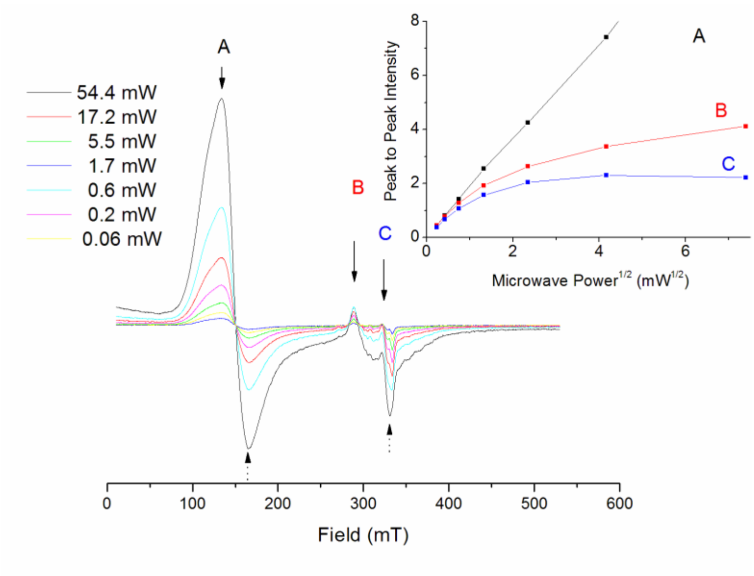


Figure S30. EPR power saturation of $\mathbf{2}^{\mathbf{Bio}}$ at 15K.

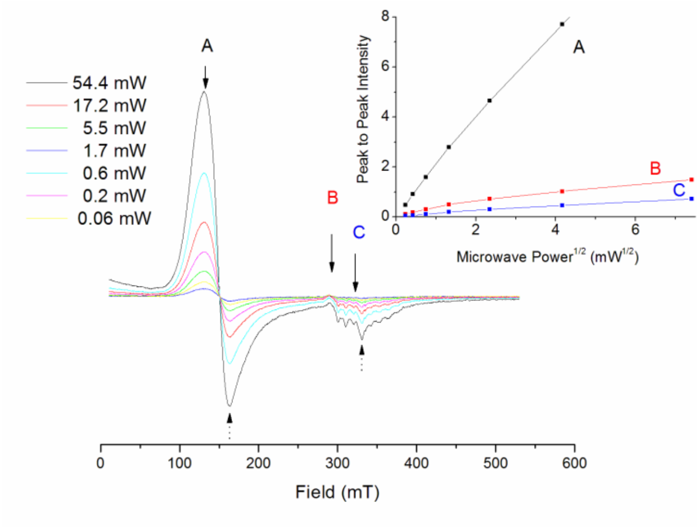


Figure S31. EPR power saturation of $\mathbf{2}^{\mathbf{Bio}} \subset$ **SA** at 15K.

Then we have analyzed standard complexes [Co(OTf)($Py_2{}^{Ts}$tacn)](OTf) (**2**) and [Co(Cl)($Py_2{}^{Ts}$tacn)](Cl) (**2Cl**) (Figure S32). The EPR of complex [Co(OTf)($Py_2{}^{Ts}$tacn)](OTf) in isobutyronitrile shows a dominant axially symmetric signal with g-values centered around 2.2 and 2.0 similar to previously reported values of elongated distorted pseudo octahedral Co(II) complexes (Nishida, Y.; Ida, K.; Kida, S. *Inorg. Chim. Acta* **1980**, *38*, 113.). However, replacing the OTf^- by a Cl^- anion as the sixth ligand ([Co(Cl)($Py_2{}^{Ts}$tacn)](Cl) (**2Cl**)) in the same solvent (isobutyronitrile) leads to a dominant broad high-spin Co(II) signal with transitions to the lower Kramer doublet (m_s ½) (Weckhuysen, B. M.; Verberckmoes, A. A.; Uytterhoeven, M. G.; Mabbs, F. E.; Collison, D.; de Boer, E.; Schoonheydt, R. A. *J. Phys. Chem. B* **2000**, *104*, 37) with simulated real g-values of 2.85, 2.22 and 1.89 and a E/D ratio of 0.041. In addition, a small low spin (1/2) Co(II) contribution to the EPR spectrum is also present with g-values and hyperfine coupling constants (A) close the ones of the biotinated-complexes (Table S2).

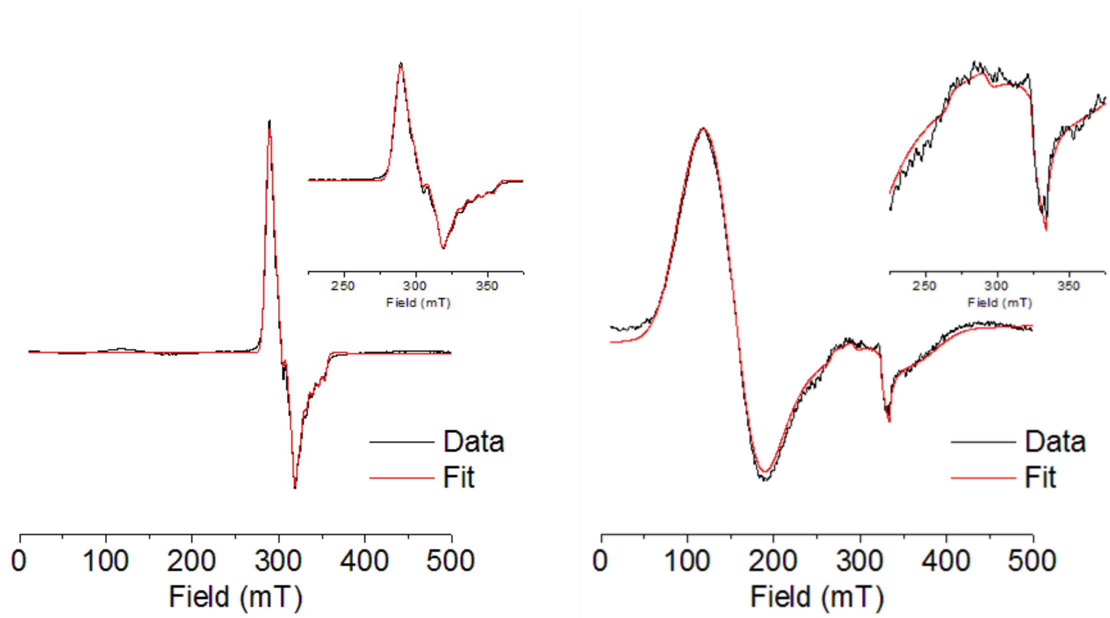


Figure S32. EPR spectra (black line) and simulation (red line) of $[Co(OTf)(Py_2{}^{Ts}tacn)](OTf)$ (left) and $[Co(Cl)(Py_2{}^{Ts}tacn)](Cl)$ (right) (0.35 mM) in isobutyronitrile at 5 db of power and 50 K.

Table S2. Results from simulation of sample EPR spectra.

Sample	Spin 3/2			Spin 1/2			Spin 1/2		
	g values g_1 g_2 g_3	E/D ratio	weight	g values g_1 g_2 g_3	A (MHz) A_1 A_2 A_3	weight	g values $g_{\parallel}$ $g_{\perp}$	A (MHz) $A_{\parallel}$ $A_{\perp}$	weight
1^Bio [a]	2.47 2.46 2.04	0.085	1	2.33 2.08 2.03	163 9 41	0.01	2.22 2.04	92 219	0.04
1^Bio ⊂ **SA** [a]	-	-	-	2.37 2.07 2.03	300 2 32	1	2.23 1.92	99 35	0.14
2^Bio [a]	2.58 2.29 2.01	0.052	1	2.33 2.06 2.04	246 7 35	0.06	2.23 2.02	102 218	0.03
2^Bio ⊂ **SA** [a]	2.45 2.37 2.03	0.002	1	2.38 2.07 2.03	287 7 37	0.008	2.20 1.99	115 296	0.03
$([Co(Cl)({}^{Ts}Py_2tacn)]Cl)$ (**2**) [b]	2.85 2.22 1.89	0.041	1	2.39 2.06 2.03	112 6 38	0.014	-	-	-
$([Co(OTf)({}^{Ts}Py_2tacn)](OTf))$ (**2Cl**) [b]	-	-	-	-	-	-	2.22 2.04	114 198	1

[a] EPR (25 db and 15 K) measurements in MeCN:0.1M Tris.HCl buffer pH 7.5 (3:7) at 0.35 mM concentration. [b] EPR measurements (5 db and 50 K) in isobutyronitrile at 0.5 mM concentration.

The EPR spectrum of complex **1**^Bio and **2**^Bio in H_2O:MeCN (7:3) with Tris·HCl buffer (0.1 M) at pH 7.5 measured at 25 db power and 15 K showed mainly a broad high-spin Co(II) signal, which is in agreement with a Cl^- anion as the sixth ligand coordinated to the metal center. In addition, two minor low-spin Co(II) signals appear. An axially symmetric signal with g-values centered around 2.2 and 2.0 similar to previously reported values of elongated distorted pseudo octahedral Co(II) complexes, that is also observed as the dominant signal in the $[Co(OTf)(Py_2{}^{Ts}tacn)](OTf)$ reference sample, and is in agreement with CH_3CN as the sixth ligand coordinated to the metal center. The second one corresponds to a rhombic signal with g-values centered at 2.33, 2.07, 2.03, consistent with an axially compressed pseudo-octahedral environment at the Co(II) center, which could be due to coordination of a water molecule or coordination vacancy.

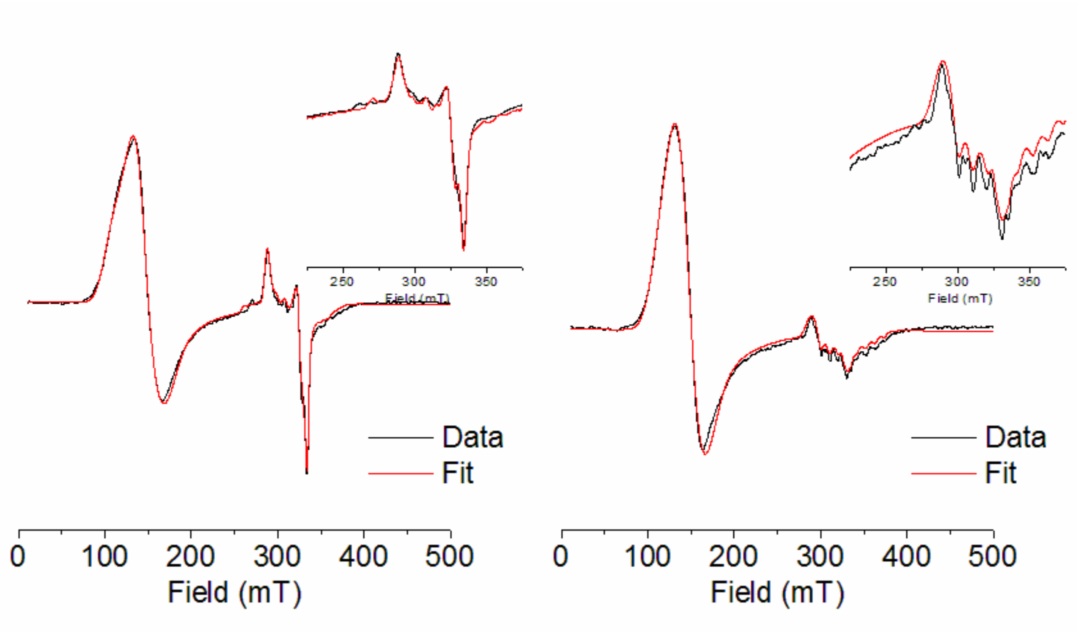


Figure S33. EPR spectra (black line) and simulation (red line) of **2**^{Bio} (left) and **2**^{Bio} ⊂ **SA** (right) (0.35 mM) in H_2O:MeCN (7:3, 0.1 M Tris.HCl buffer pH 7) at 25 db power and 15 K.

The basic EPR features observed in the **2**, **2Cl**, **1**^{Bio} and **2**^{Bio} series guide to understand the EPR of **1**^{Bio} ⊂ **SA** and **2**^{Bio} ⊂ **SA** (Figures S33 and S34). Interestingly, while the EPR spectrum of **2**^{Bio} ⊂ **SA** is similar to **2**^{Bio}, in the case of **1**^{Bio} ⊂ **SA** it is essentially different to **1**^{Bio}. The EPR spectrum of **2**^{Bio} ⊂ **SA** recorded at 15 K presents three different Co center environments as for **2**^{Bio} (Figure S33). The predominant is the Co(II) high spin (S = 3/2), and two minor signals that can be assigned to low spin Co(II) centers with a different coordinated sixth ligand (CH_3CN and H_2O). In contrast, the main feature in the EPR spectrum of **1**^{Bio} ⊂ **SA** corresponds to the rhombic signal with g-values centered at 2.37, 2.07 and 2.03, which is in agreement with the coordination of a water molecule. This correlates with the fact the cobalt complex in **1**^{Bio} ⊂ **SA** is more internalized into the protein cavity as judged by the Molecular Dynamics simulations. Therefore, the presence of mainly the low spin Co(II) rhombic signal may suggest that the protein pocket environment may regulate the binding ligand at the metal center. In the case of the **2**^{Bio} ⊂ **SA** the Molecular Dynamics simulations show both that the cobalt complex is exposed to the protein surface, but much more exposed to the reaction media than **1**^{Bio} ⊂ **SA**.

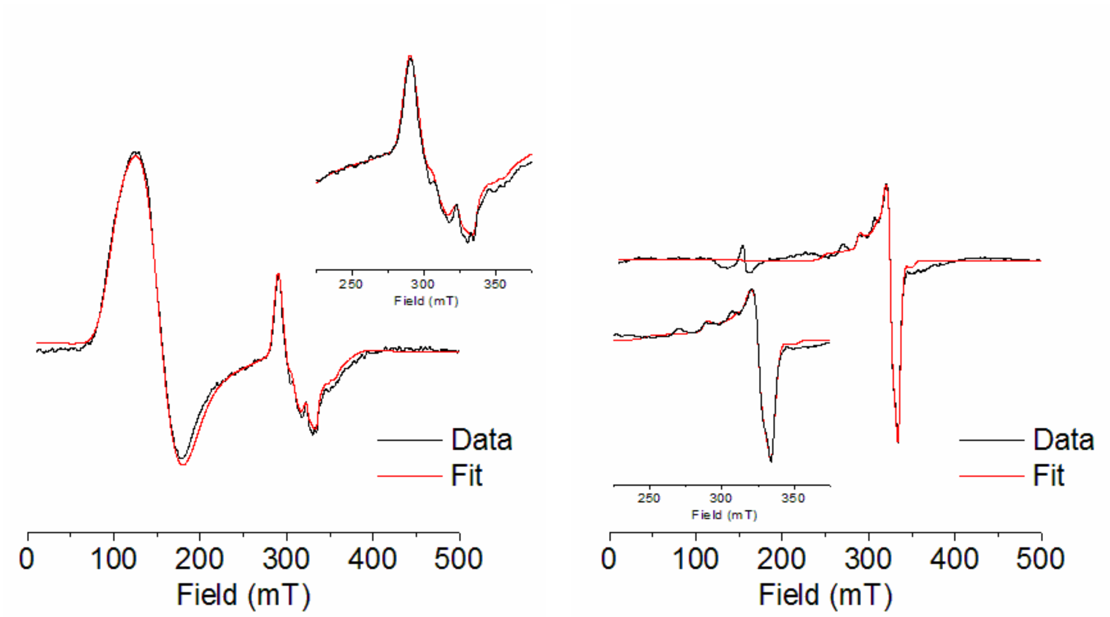


Figure S34. EPR spectra (black line) and simulation (red line) of **1**^{Bio} (left) and **1**^{Bio} ⊂ **SA** (right) (0.35 mM) in H_2O:MeCN (7:3, 0.1 M Tris.HCl buffer pH 7.5) at 25 db power and 15 K.

1.7. Electrocatalytic water reduction

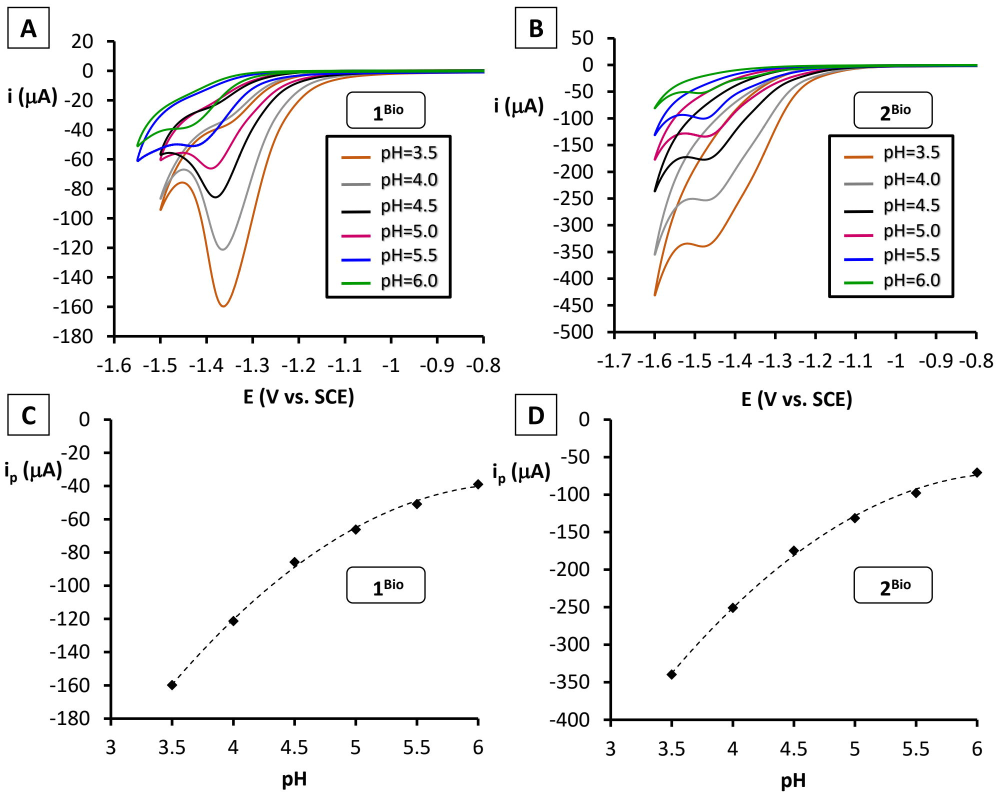


Figure S35. Cyclic voltammograms (CV) of **A**) **1**^{Bio} (1 mM) and **B**) **2**^{Bio} (1 mM) in buffer (citrate 100 mM, NaCl 100 mM) in the pH 3.5 - 6.0 range. Scan rate: 100 mV·s^{-1}. Working electrode glassy carbon (0.28 cm^2). Maximum peak intensity values versus pH for C) **1**^{Bio} and D) **2**^{Bio}.

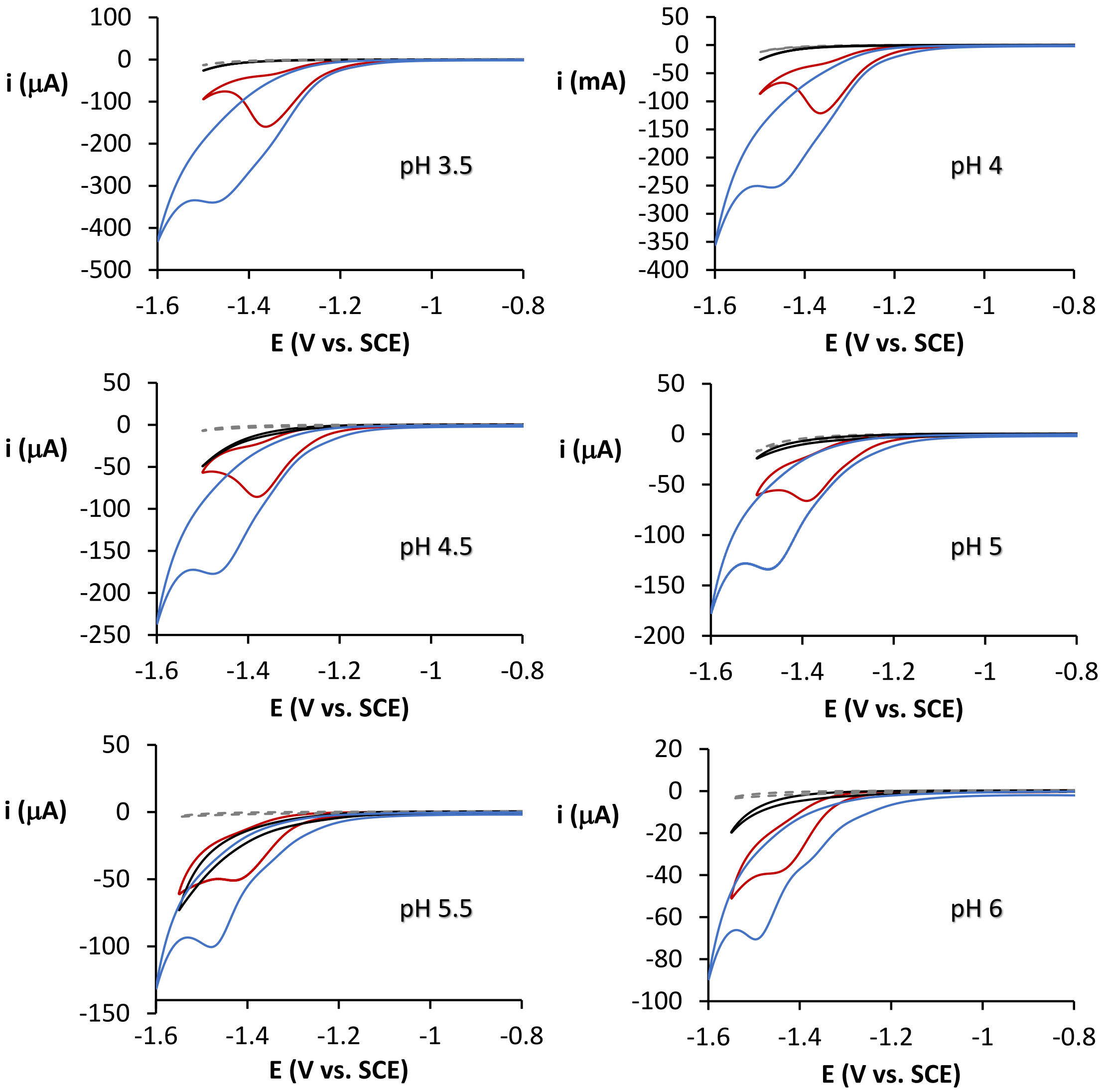


Figure S36. Cyclic voltammograms in 100 mM citrate buffer, 100 mM NaCl, at different pH values in the absence (dashed grey trace), and presence of 1 mM catalyst **1**^{Bio} (red trace) and **2**^{Bio} (blue trace). The black CV correspond to the electrocatalytic current obtained after rinsing the electrode after the measurement of the cobalt solution. Scan rate of 100 mV·s^{-1} using a 0.28 cm^2 glassy carbon working electrode. Potentials are quoted versus SCE

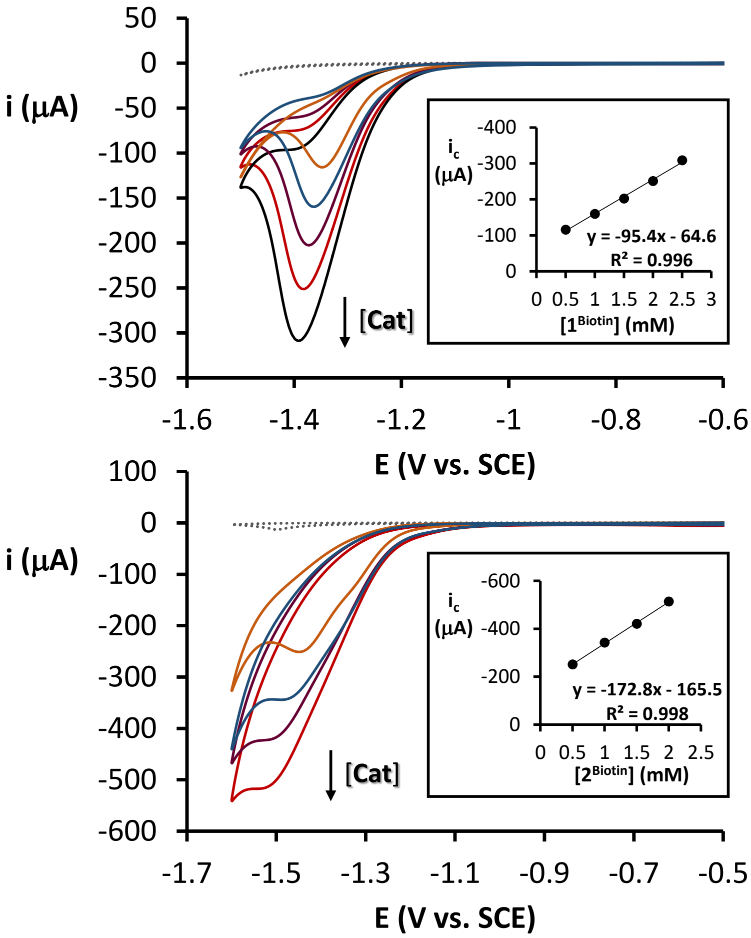


Figure S37. CVs at increasing concentrations of **1**^{Bio} (Top) and **2**^{Bio} (Bottom). Conditions: 100 mM citrate buffer, 100 mM NaCl, at pH 3.5 using different catalyst concentrations: 0 mM (dashed grey) 0.5 mM (orange), 1 mM (blue), 1.5 mM (purple), 2 mM (red) and 2.5 mM (black). Scan rate of 100 mV·s^{-1} using a 0.28 cm^2 glassy carbon working electrode. Potentials are quoted versus SCE. Inset: Electrocatalytic current (i_c) versus [Catalyst] showing a first order kinetics.

To study the electrocatalytic response of **Cat**^{Bio} ⊂ **SA** we prepared a thin film of **Cat**^{Bio} ⊂ **SA** over the glassy carbon electrode by drop-casting and drying. The modified electrode gave a significant catalytic wave attributed to proton reduction (Figure S38, red CV), which disappeared after the second scan due to protein detachment during electrocatalysis. The nature of the catalytic wave was attributed to the **Cat**^{Bio} ⊂ **SA** since no electrocatalytic activity was observed when SA alone was deposited on the same conditions (Figure S38, green CV).

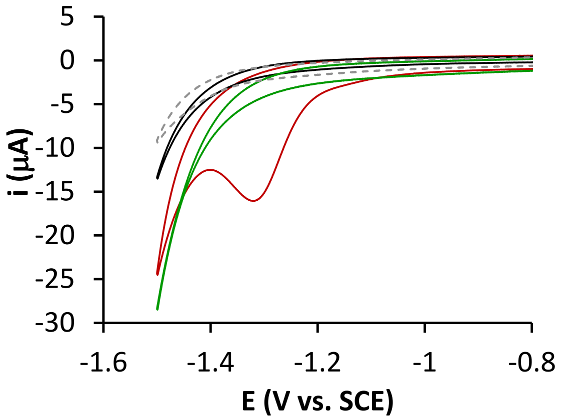


Figure S38. CV of a 10 μM **1**^{Bio} ⊂ **SA** in solution (green trace) and as a thin film (red trace), bare electrode (dashed grey trace) and the CV of a thin film of **SA** (black trace). Conditions: 100 mM citrate buffer, 100 mM NaCl, at pH 3.5. Scan rate: 100 mV·s^{-1}. Working electrode: glassy carbon (0.28 cm^2).

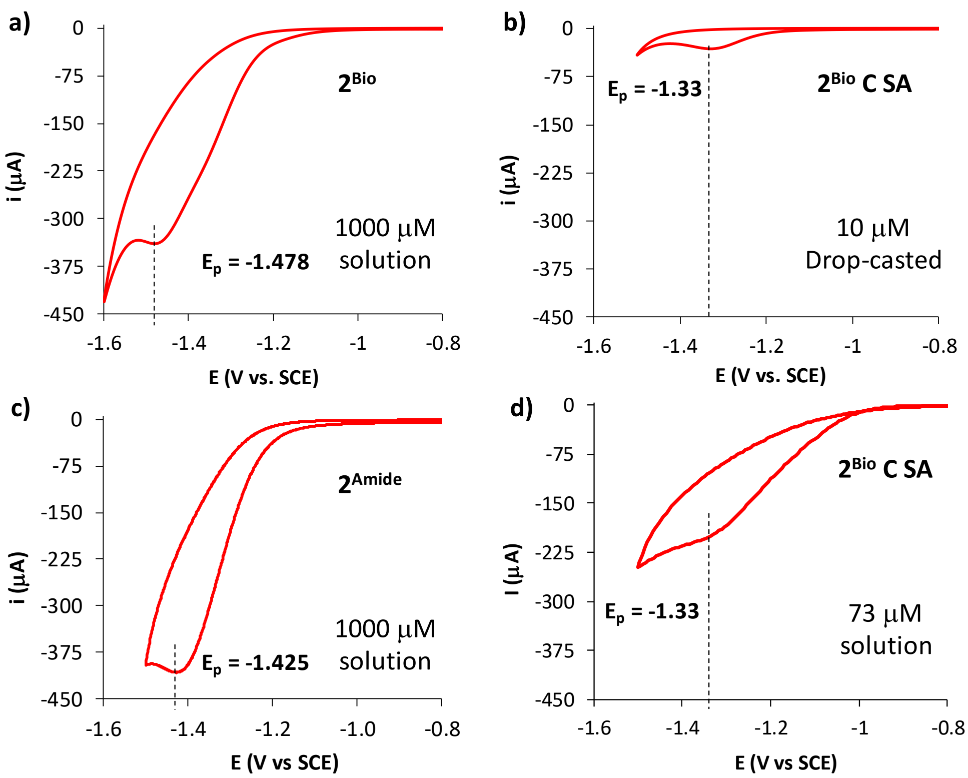


Figure S39. Cyclic voltammograms (CV) of a) **2**^{Bio} (1000 μM, solution), b) **2**^{Bio} ⊂ **SA** (10 μM, thin film), c) **2**^{Amide} (1000 μM, solution) and d) **2**^{Bio} ⊂ **SA** (73 μM, solution) in buffer (citrate 100 mM, NaCl 100 mM) at pH 3.5. Scan rate: 100 mV·s^{-1} in all cases except for c) in which the scan rate was 10 mV·s^{-1} in order to better see the Co$^{II/I}$ electrochemical process. Working electrode glassy carbon (0.28 cm^2).

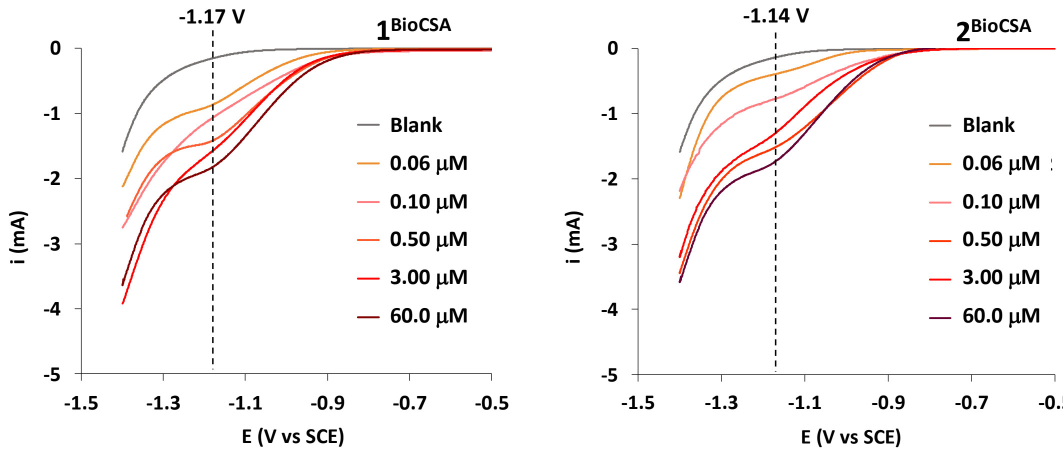


Figure S40. Cyclic voltammograms of the thin film electrochemistry of *Left*) $\mathbf{1}^{Bio \subset SA}$ and *Right*) $\mathbf{2}^{Bio \subset SA}$ in buffer (citrate 100 mM, NaCl 100 mM) at pH 3.5 at increasing concentrations (from 0.06 to 60 µM) of the metalloprotein onto the surface of the carbon fabric working electrode (1 cm^2 surface). Scan rate of 10 mV·s^{-1}. Potentials are quoted versus SCE.

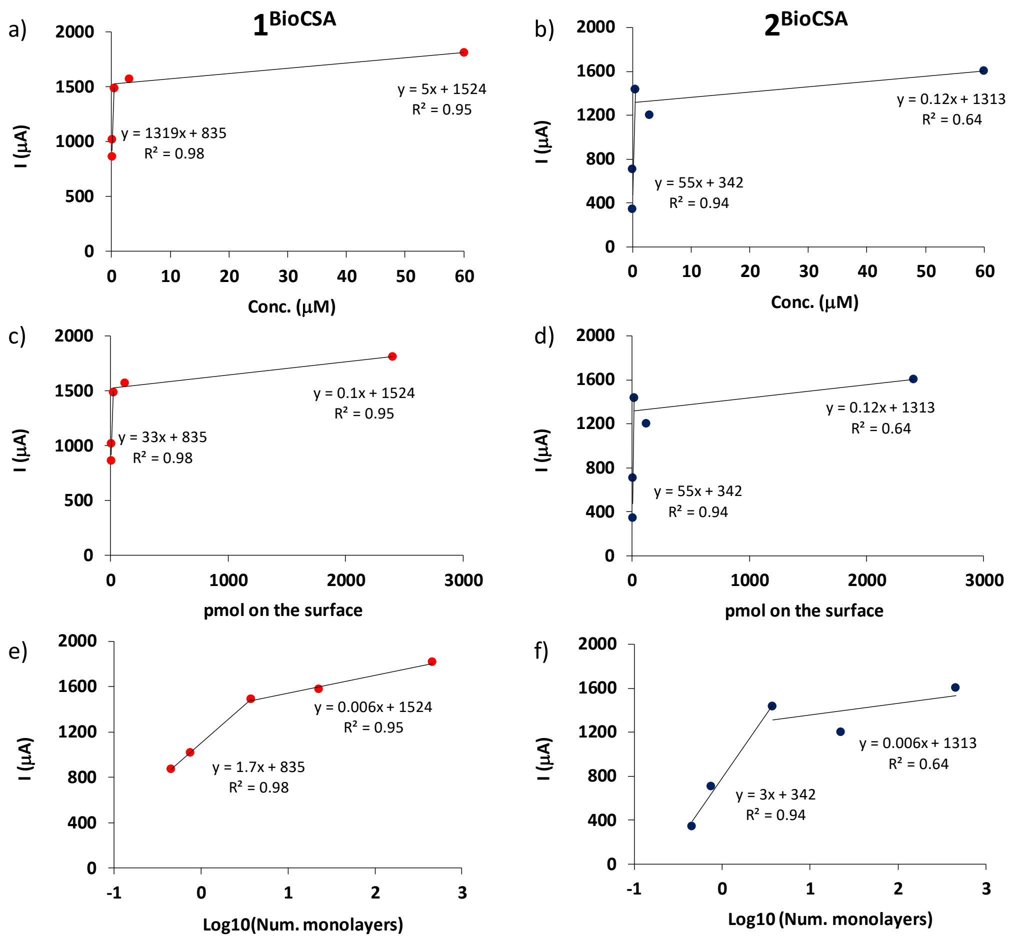


Figure S41. Plot of the current intensity at the peak potential (E_p) of $Co^{II/I}$ of the thin film CV of *Left*) $\mathbf{1}^{Bio \subset SA}$ and *Right*) $\mathbf{2}^{Bio \subset SA}$ in buffer (citrate 100 mM, NaCl 100 mM) at pH 3.5 as a function of the *a,b)* [metalloprotein], *c,d)* n(metalloprotein) deposited and *e,f)* logarithm of the estimated number of monolayers on the working electrode surface (carbon fabric, 1 cm^2) at 10 mV·s^{-1} scan rate. Potentials are quoted versus SCE.

Calculation for the estimation of the occupation of the surface of the carbon fabric working electrode.

The different electrode surface coverages (2.4, 4, 20, 120 and 2400 pmol·cm^{-2}) were obtained by drop casting of 40 μL of citrate buffer containing known metalloprotein concentrations (0.06 to 60 μM) onto a surface of carbon fabric working electrode (1 cm^2). CVs were recorded at scan rates of 10 mV·s^{-1} and potentials quoted versus SCE (Figures S40 and S41). Protein thin film electrochemical studies showed that independently of the amount of metalloprotein deposited the $Co^{II/I}$ reduction process appears at the same redox potential (Figure S40), excluding any interaction between neighboring metalloproteins. Interestingly, the current intensity at the peak potential (E_p) of $Co^{II/I}$ increases with the concentration of protein at the electrode until reaching a saturation at 3 μM concentration (Figure S41).

Taking into account the packing sphere model that considers that the highest-density lattice arrangement of spheres is a hexagonal packing arrangement and each sphere is surrounded by 6 other spheres the density of the occupied surface is 90% of the total surface.[7d-g] Considering SA as a sphere of about 30 Å in radius, each SA occupies an area of 2827.4 Å^2, and a 1 cm^2 of surface is fully covered by 3.18·10^{12} SA metalloproteins (or 5.29·10^{-12} moles of metalloprotein). Having these values as threshold, we can estimate the percentage of occupation of the electrode surface (% occup) as follows:

$$Area\ SA = \pi\ X\ 30^2 = 2827.4\ \text{Å}^2$$

$$max\ number\ molec\ surface = \frac{useful\ electrode\ area}{Area\ SA} = \frac{9 \cdot 10^{15}}{2827.4}$$

$$max\ number\ molec\ surface = 3.18 \cdot 10^{12}\ molecules\ metalloprotein$$

$$\%\ occup = \frac{mol\ deposited}{theoretical\ maximum\ mol\ number} X\ 100$$

A stock solution of metalloprotein (40 μL) at different concentrations was deposited onto a 1 cm^2 of carbon fabric. For each concentration, the pmol of metalloprotein deposited per cm^2 and the occupation percentage has been estimated following the procedure described above (table S3).

Table S3. Estimation of quantity and occupation of metalloprotein at the electrode surface.

Entry	V_{add} (μL)	$Conc_{add}$ (μM)	V_{add} (L)	$Conc_{add}$ (M)	mol deposited	molecules deposited	pmol/cm^2	Num. monolayers
1	40	60.0	4.0E-05	6.0E-05	2.4E-09	1.4E+15	2400	454
2	40	3.0	4.0E-05	3.0E-06	1.2E-10	7.2E+13	120	23
3	40	0.5	4.0E-05	5.0E-07	2E-11	1.2E+13	20	4
4	40	0.1	4.0E-05	1.0E-07	4E-12	2.4E+12	4	0.76
5	40	0.06	4.0E-05	6.0E-08	2.4E-12	1.4E+12	2.4	0.45
6*	10	10.0	1.0E-05	1.0E-05	1E-10	6.0E+13	353	67

*drop casted 10 μL of metalloprotein stock (10 μM) onto a 6 mm glassy carbon electrode (0.28 cm^2 surface area).

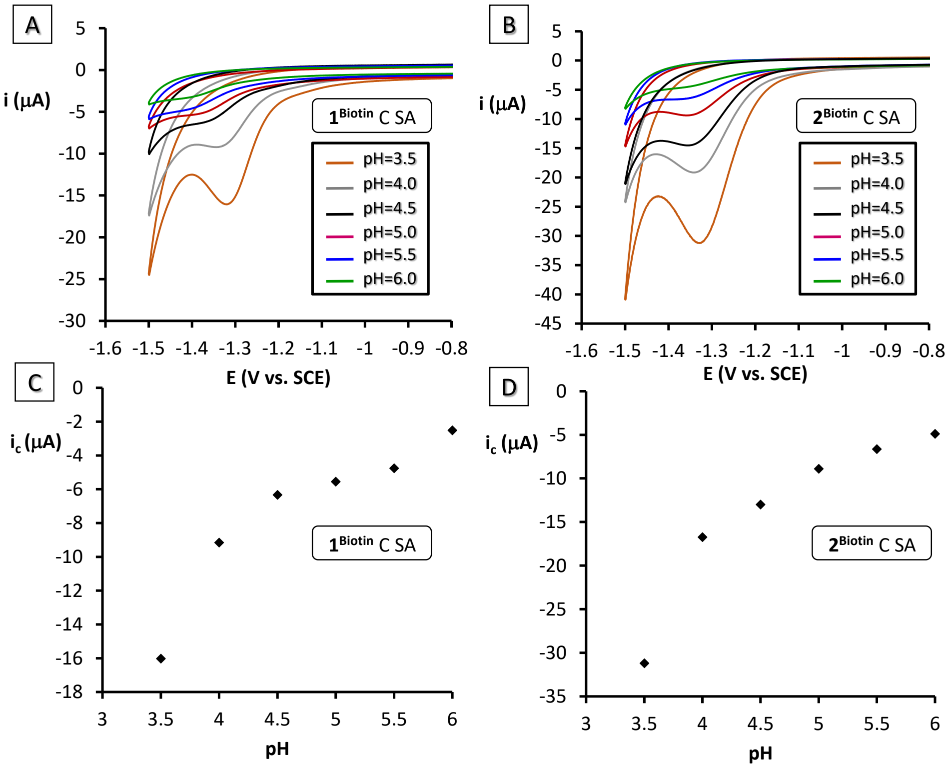


Figure S42. CV of thin films of A) $\mathbf{1^{Bio}} \subset$ **SA** (A and B) $\mathbf{2^{Bio}} \subset$ **SA** adducts in buffer (citrate 100 mM, NaCl 100 mM) in the pH 3.5 - 6.0 range. Scan rate of 100 mV·s^{-1} using a 0.28 cm^2 glassy carbon working electrode. Potentials are quoted versus SCE. Maximum peak intensity values versus pH for C) $\mathbf{1^{Bio}} \subset$ **SA** and D) $\mathbf{2^{Bio}} \subset$ **SA**.

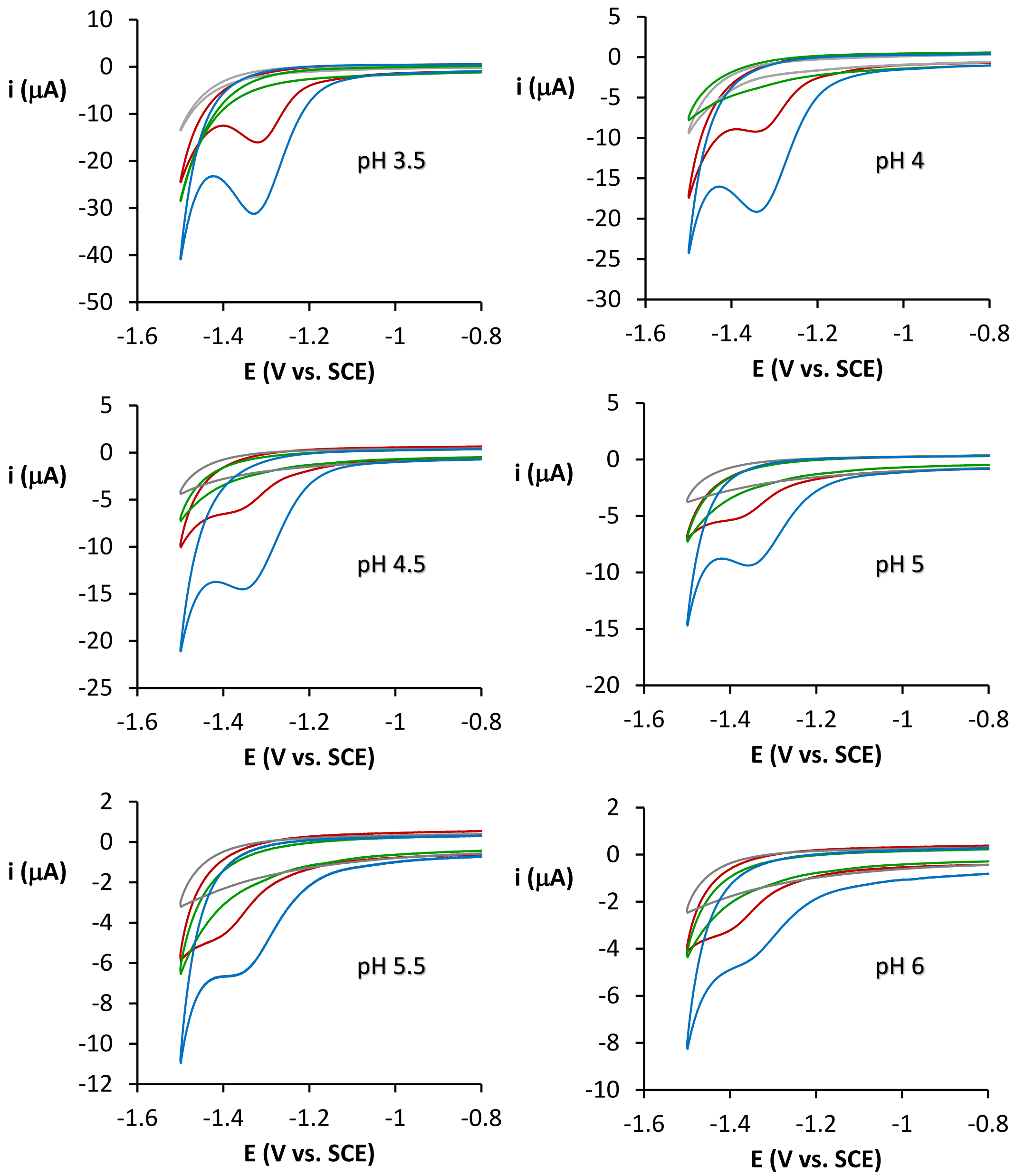


Figure S43. Cyclic voltammograms of **1**^{Bio} ⊂ **SA** (red trace) and **2**^{Bio} ⊂ **SA** (blue trace) in 100 mM citrate buffer, 100 mM NaCl, at pH in the 3.5 to 6.0 range. The CV scan for bare electrode under the same conditions (green trace) and the CV obtained from a thin film of SA alone (grey trace) are included. Scan rate of 100 mV·s^{-1} using a 0.28 cm^2 glassy carbon working electrode. Potentials are quoted versus SCE.

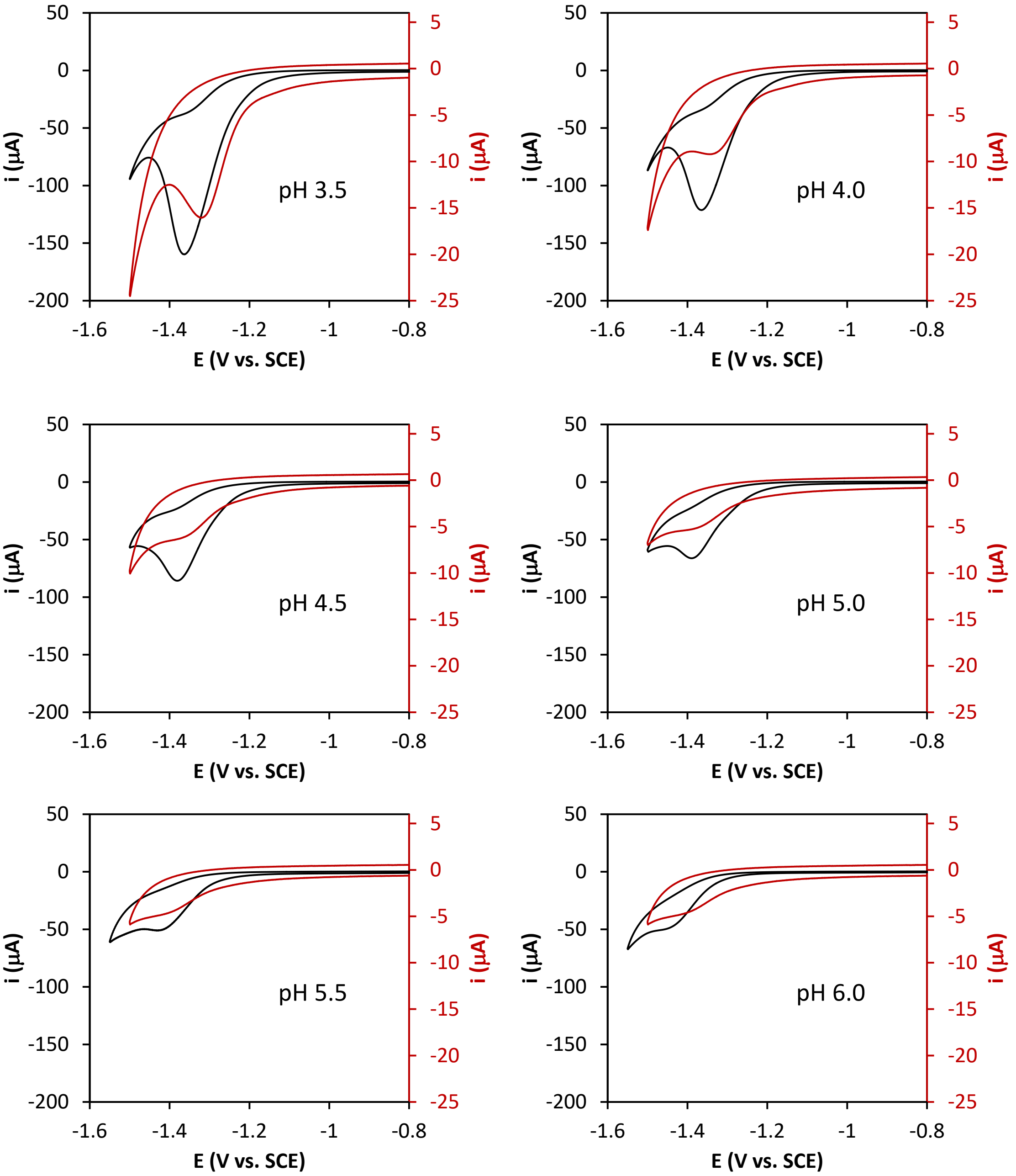


Figure S44. Cyclic voltammograms of **1**^{Bio} (black trace) **1**^{Bio}⊂ **SA** (red trace). CVs measured in 100 mM citrate buffer, 100 mM NaCl, at diferent pH values, at scan rate of 100 mV·s^{-1} using a 0.28 cm^2 glassy carbon working electrode. Potentials are quoted versus SCE.

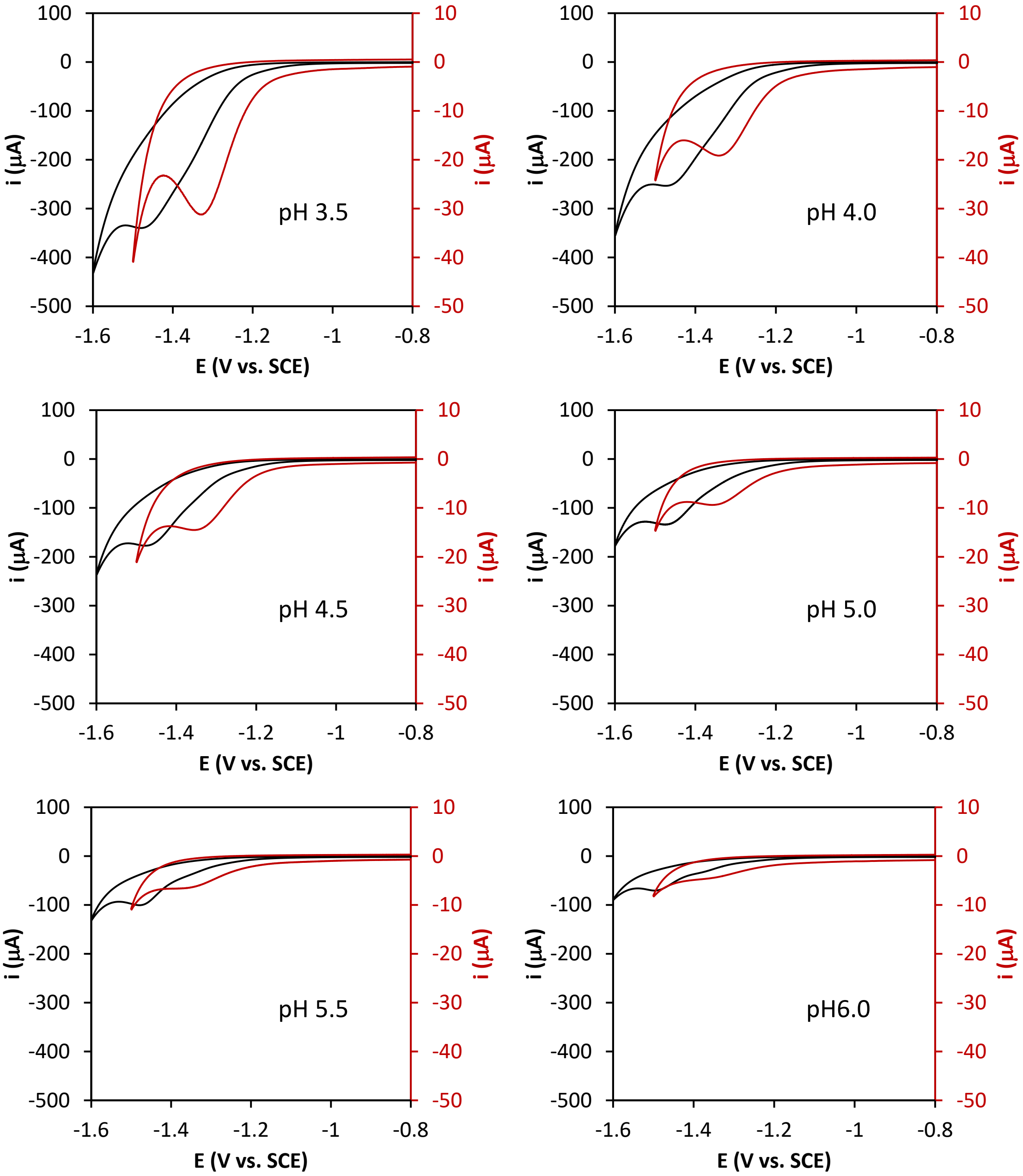


Figure S45. Cyclic voltammograms of **2**^{Bio} (black trace) **2**^{Bio} ⊂ **SA** (red trace). CVs measured in 100 mM citrate buffer, 100 mM NaCl, at diferent pH values. Scan rate of 100 mV·s^{-1} using a 0.28 cm^2 glassy carbon working electrode. Potentials are quoted versus SCE.

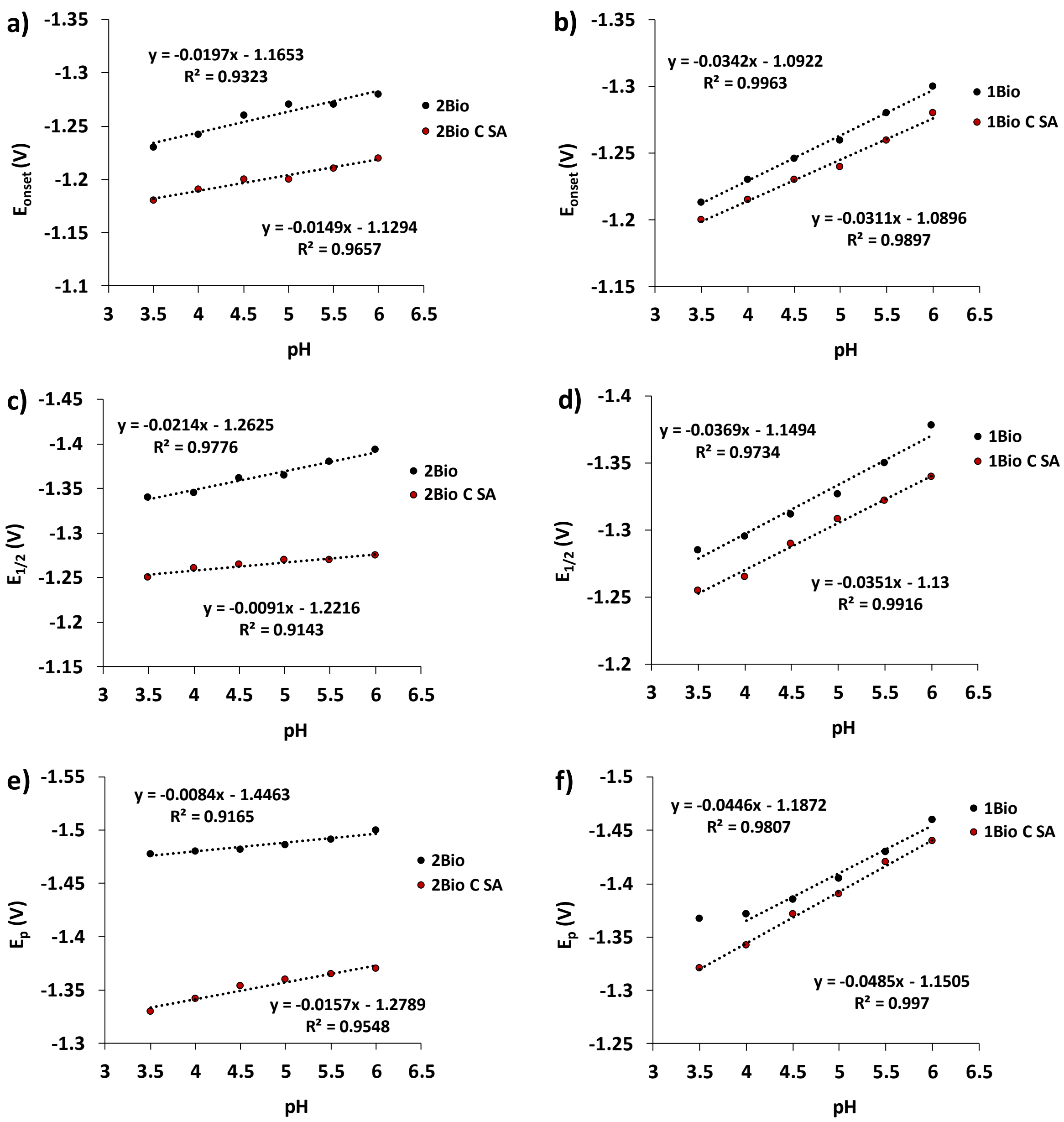


Figure S46. Plots of **a-b**) the onset potential (E_{onset}), **c-d**) half peak potential ($E_{1/2}$), and **e-f**) peak potential (E_p) as a function of pH of $\mathbf{1}^{\mathbf{Bio}}$ (1 mM) and $\mathbf{1}^{\mathbf{Bio}} \subset$ **SA** (thin film) and $\mathbf{2}^{\mathbf{Bio}}$ (1 mM) and $\mathbf{2}^{\mathbf{Bio}} \subset$ **SA** (thin film) in buffer (citrate 100 mM, NaCl 100 mM) in the pH 3.0 - 6.0 range. Scan rate: 100 $mV \cdot s^{-1}$. Working electrode glassy carbon (0.28 cm^2).

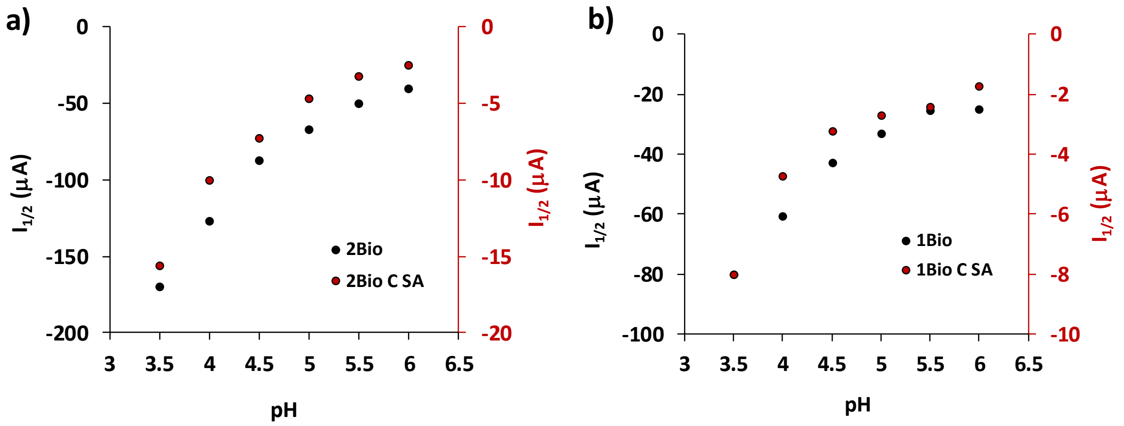


Figure S47. Plot of the half peak intensity values ($I_{1/2}$) vs the pH of **2**^{Bio} (1 mM) and **2**^{Bio} ⊂ **SA** (thin film) (a) and **1**^{Bio} (1 mM) and **1**^{Bio} ⊂ **SA** (thin film) (b) in buffer (citrate 100 mM, NaCl 100 mM) in the pH 3.0 - 6.0 range. Scan rate: 100 mV·s^{-1}. Working electrode glassy carbon (0.28 cm^2).

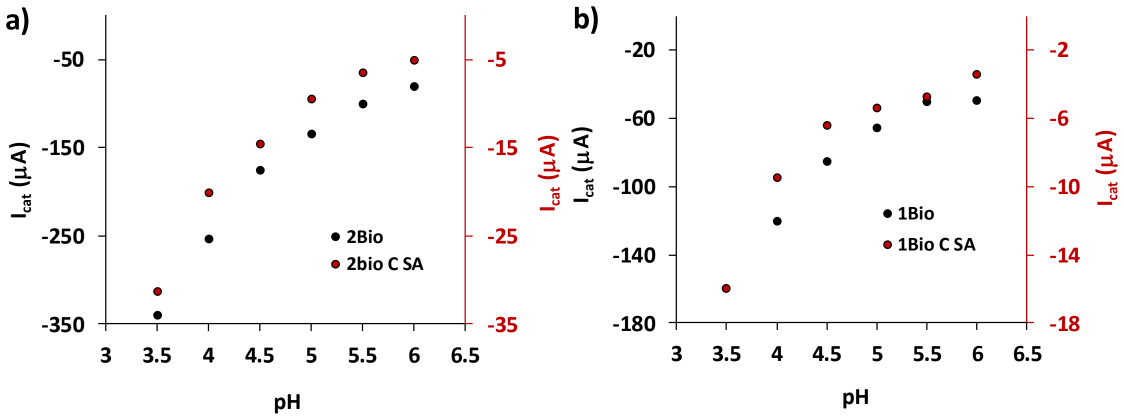


Figure S48. Plot of the maximum peak intensity values vs the pH of **2**^{Bio} (1 mM) and **2**^{Bio} ⊂ **SA** (thin film) (a) and **1**^{Bio} (1 mM) and **1**^{Bio} ⊂ **SA** (thin film) (b) in buffer (citrate 100 mM, NaCl 100 mM) in the pH 3.0 - 6.0 range. Scan rate: 100 mV·s^{-1}. Working electrode glassy carbon (0.28 cm^2).

Controlled Potential Electrolysis (CPE) studies were performed for **2^Bio^** and **2^Bio^ ⊂ SA** (Figures S49-S51). For **2^Bio^ ⊂ SA** good Faraday Yield is observed for H_2 production (70 TON H_2 as quantified by GC-TCD). In contrast, for **2^Bio^** despite the good Faraday yield for H_2 production (560 TON H_2 as quantified by GC-TCD), the catalyst suffers an activation process along the CPE (see Figure S51).

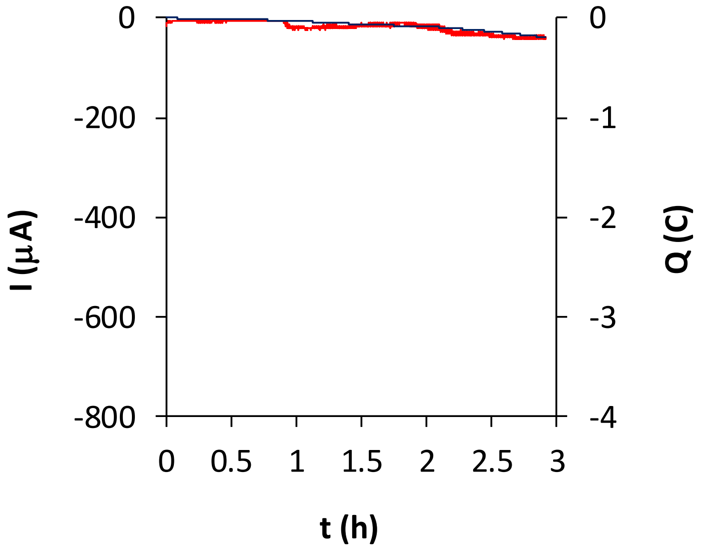


Figure S49. Bulk electrolysis of 100 mM citrate buffer 100 mM NaCl pH 3.5 under N_2 atmosphere at E_{appl} = –1.4 V vs SCE using a carbon mesh as working electrode, Pt wire as counter electrode and SCE as reference electrode. Represented are the current (red) and charge (blue) passed over 3 h.

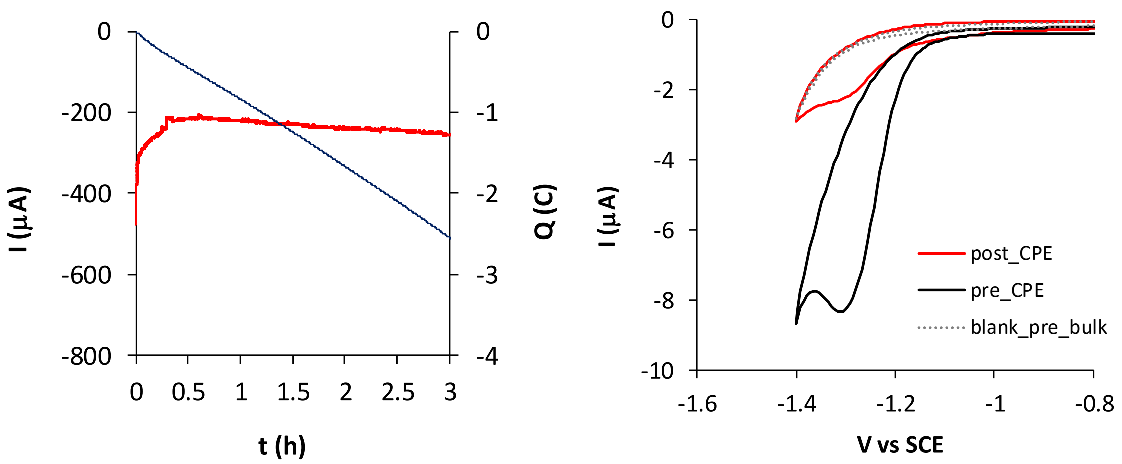


Figure S50. *Left*) Bulk electrolysis of **2^Bio^ ⊂ SA** (73 µM) in 100 mM citrate buffer 100 mM NaCl pH 3.5 under N_2 atmosphere at E_{appl} = –1.4 V vs SCE using a carbon mesh as working electrode, Pt wire as counter electrode and SCE as reference electrode. Represented are the current (red) and charge (blue) passed over 3 h. *Right*) CV before (blank) and after (red) the CPE.

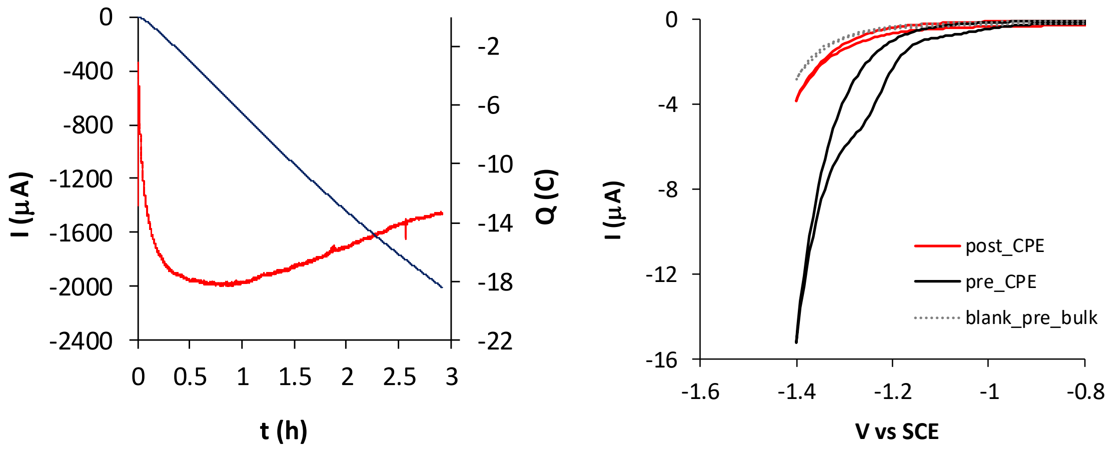


Figure S51. *Left*) Bulk electrolysis of **2**^{Bio} (73 μM) in 100 mM citrate buffer 100 mM NaCl pH 3.5 under N_2 atmosphere at E_{appl} = –1.4 V vs SCE using a carbon mesh as working electrode, Pt wire as counter electrode and SCE as reference electrode. Represented are the current (red) and charge (blue) passed over 3 h. *Right*) CV before (blank) and after (red) the CPE.

1.8. Evaluation of the coordination avility of the biotin moiety to the cobalt complexes.

The differences observed in the catalytic performance between synthesized metalloenzymes (**Cat**^{Bio} ⊂ **SA**) and coordination cobalt complexes (**Cat**^{bio}) could originate form changes in geometry, electronics, or second sphere interactions. In order to discard that the catalytic enhacement observed upon encapsulation of the catalyst in Streptavidin (SA), is due to possible changes in the first coordination sphere, the potential coordination of biotin to the cobalt center was investigated. Although in the streptavidin – biotin adduct biotin is no longer accessible for coordination to the cobalt center, in the biotinylated precursors there is the possibility that biotin interacts inter- or intramolecularly with the cobalt centers.

To clarify this aspect, we have first synthesized the homologous non-biotinylated **1**^{Amide} and **2**^{Amide} complexes (Figure S52) to study how the absence of biotin affects their behavior and performed the following experiments.

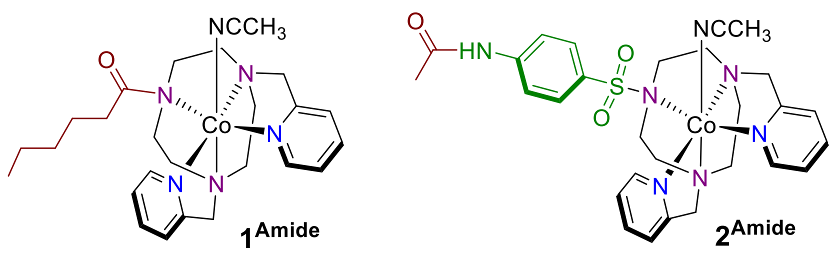


Figure S52. Model non-biotinylated versions (**1**^{Amide} and **2**^{Amide}) of the biotinylated complexes **1**^{Bio} and **2**^{Bio}.

Electrochemical studies:

Indeed, under electrochemical conditions, $\mathbf{1}^{Amide}$ and $\mathbf{2}^{Amide}$ behave equivalently to the biotinylated complexes $\mathbf{1}^{Bio}$ and $\mathbf{2}^{Bio}$, which is an indication that biotin does not interact with the metal center (Figures S53 – S56).

- Titration experiments of $\mathbf{1}^{Amide}$ and $\mathbf{2}^{Amide}$ (1 mM) with esterified biotin (^{COOEt}**Biotin**, the biotin was esterified for solubility reasons) showed negligible influence on the cyclic voltammograms for biotin concentrations of up to 20 mM (See Figures S53 and S54).
- Bimolecular biotin interactions appear negligible as there is a linear correlation between the current intensity and concentration of added biotinylated complexes $\mathbf{1}^{Bio}$ and $\mathbf{2}^{Bio}$ (Figure S37).
- We have also studied the pH effect (from 3.5 to 6) in the water reduction activity for the non-biotinylated complexes $\mathbf{1}^{Amide}$ and $\mathbf{2}^{Amide}$ (Figures S55 and S56). The electrochemistry and the observed behavior for both non-biotinylated complexes is analogous to complexes $\mathbf{1}^{Bio}$ and $\mathbf{2}^{Bio}$, negating any effect from a possible coordination of the biotin motif.
- We have also studied the effect of the concentration of the protein deposited onto the surface of the working electrode in protein thin film electrochemical studies (from 0.06 to 60 μM) for the synthesized metalloproteins $\mathbf{1}^{Bio} \subset$ **SA** and $\mathbf{2}^{Bio} \subset$ **SA** (Figures S40 and S41). Protein thin film electrochemical studies show that independently of the concentration of metalloprotein deposited, the electrochemical peak of the $Co^{II/I}$ redox process appears at the same potential (Figure S40), negating the possibility of interaction between neighbouring metalloproteins impacting reactivity. Interestingly, the current intensity at the peak potential (E_p) of $Co^{II/I}$ increases with the concentration of the thin film until reaching a maximum at 3 μM concentration (Figure S41) indicating a saturation of the electrode surface. We have estimated the quantity of metalloprotein supported onto the electrode according to the sphere packing model (see below and table S3) and an overoccupancy of the electrode surface (> 20 pmol/cm^2) is observed at concentrations ≥ 3 μM.

Density Functional Theory Studies:

We have studied computationally (B3LYP-3D/6-31+G** level of theory) possible coordination modes for the N, O and S atoms of biotin to the cobalt center in oxidation states I and II. All optimized structures showed that intramolecular coordination of biotin to the cobalt center is largely endergonic. In addition, an exchange between a coordinated pyridine (or tacn backbone) and a N, O or S atom of biotin is also highly endergonic. Therefore, the coordination of biotin to the cobalt center can be discarded (See Figures S78 - S87). In addition, the pKa values for complexes $\mathbf{1}^{Bio}$ and $\mathbf{2}^{Bio}$ have been calculated by DFT at the B3LYP/6-31+G** 6d level of theory (*see S.2.2.1. Computational details for further information*). The theoretical obtained pKa value for $\mathbf{1}^{Bio}$ is 4.4 and for $\mathbf{2}^{Bio}$ 2.9, which could explain the observed electrochemical behaviour for both catalysts.

As a summary, we can conclude that a coordination or interaction of the biotin to the cobalt center is discarded, and that the observed enhancement of the catalytic activity of the synthesized metalloenzimes is most likely due to second coordination sphere effects. The conclusions are supported by electrochemical, EPR, XAS and DFT analysis.

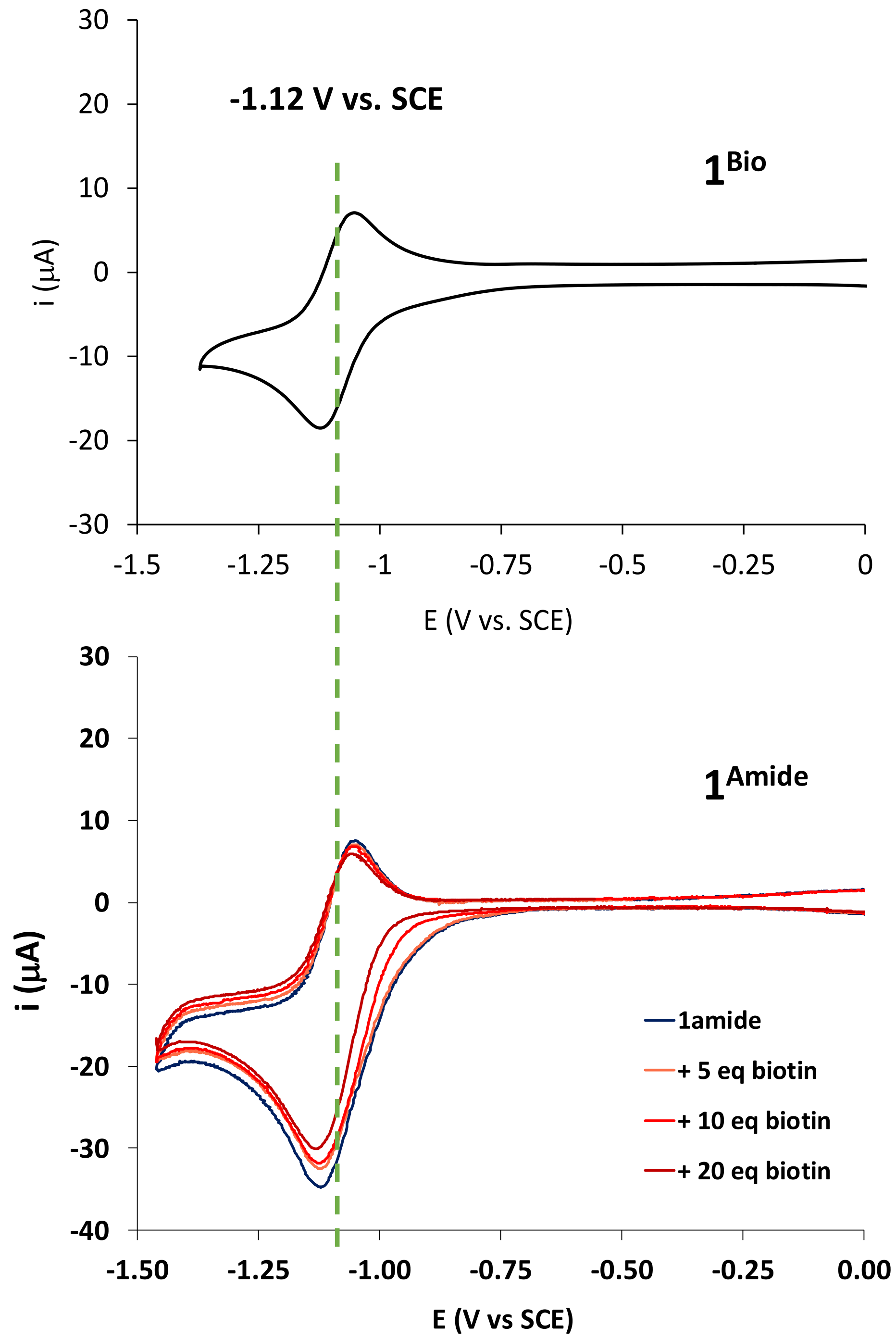


Figure S53. CVs of *Top*) **1**^{Bio} (1 mM) in dry MeCN and *Bottom*) CV of **1**^{Amide} (1 mM) in dry MeCN and CVs of the subsequent addition of biotin ethyl ester (from 5 to 20 eq). Experimental conditions: Bu_4NPF_6 (0.1 M) as supporting electrolyte in acetonitrile, using a 0.28 cm^2 glassy carbonas working and Ag pseudoreference and the Fc/Fc$^+$ couple as reference electrodes. Scan rate of 100 mV·s^{-1}.

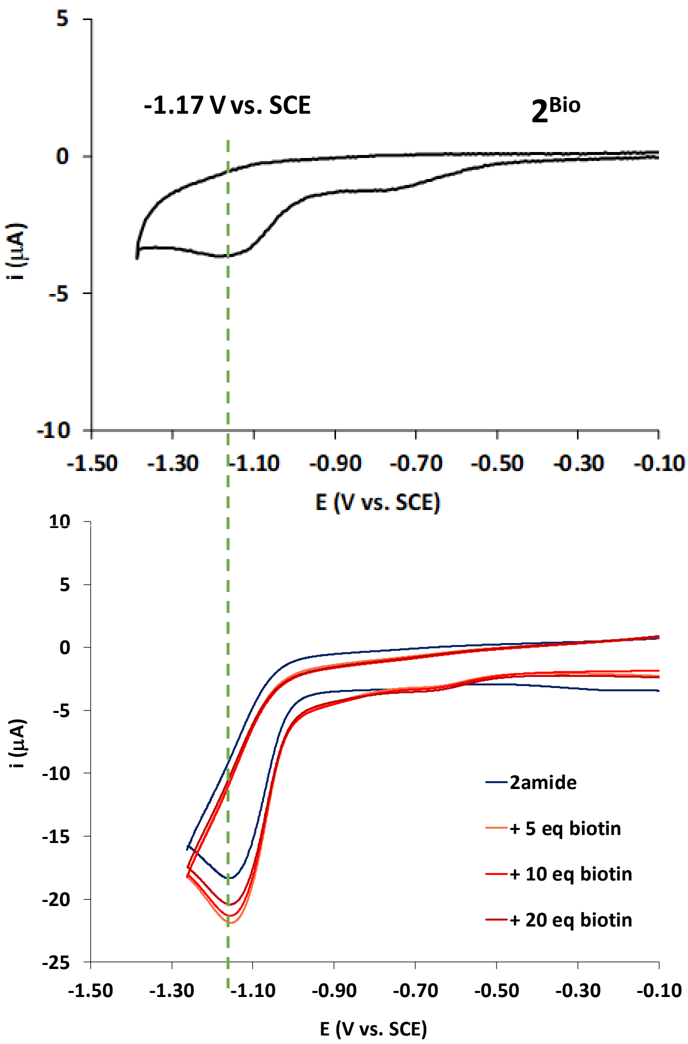


Figure S54. CVs of *Top*) **2**^{Bio} (0.25 mM) in dry MeCN and *Bottom*) **2**^{Amide} (1 mM) in dry MeCN and CVs of the subsequent addition of biotin ethyl ester (from 5 to 20 eq). Experimental conditions: Bu_4NPF_6 (0.1 M) as supporting electrolyte in acetonitrile, using a 0.28 cm^2 glassy carbon as working and Ag pseudoreference and the Fc/Fc^+ couple as reference electrodes. Scan rate of 100 $mV{\cdot}s^{-1}$.

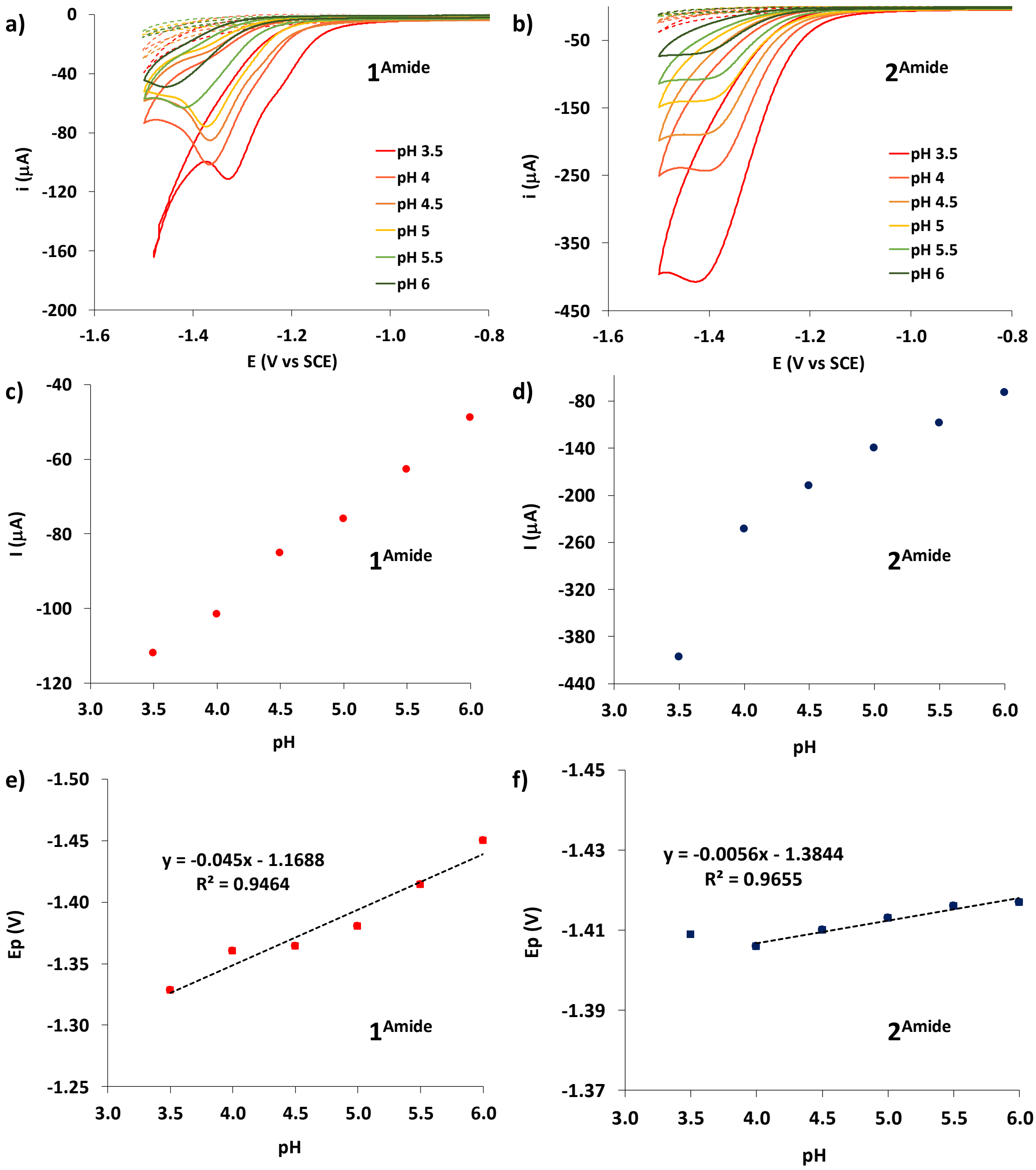


Figure S55. Cyclic voltammograms (CV) of a) $\mathbf{1}^{\mathbf{Amide}}$ (1 mM) and b) $\mathbf{2}^{\mathbf{Amide}}$ (1 mM) in buffer (citrate 100 mM, NaCl 100 mM) in the pH 3.5 - 6.0 range. Scan rate: 100 mV·s^{-1}. Working electrode glassy carbon (0.28 cm^2). Maximum peak intensity values versus pH for c) $\mathbf{1}^{\mathbf{Amide}}$ and d) $\mathbf{2}^{\mathbf{Amide}}$. Plot of the peak potential (Ep) as a function of pH of e) $\mathbf{1}^{\mathbf{Amide}}$ and f) $\mathbf{2}^{\mathbf{Amide}}$.

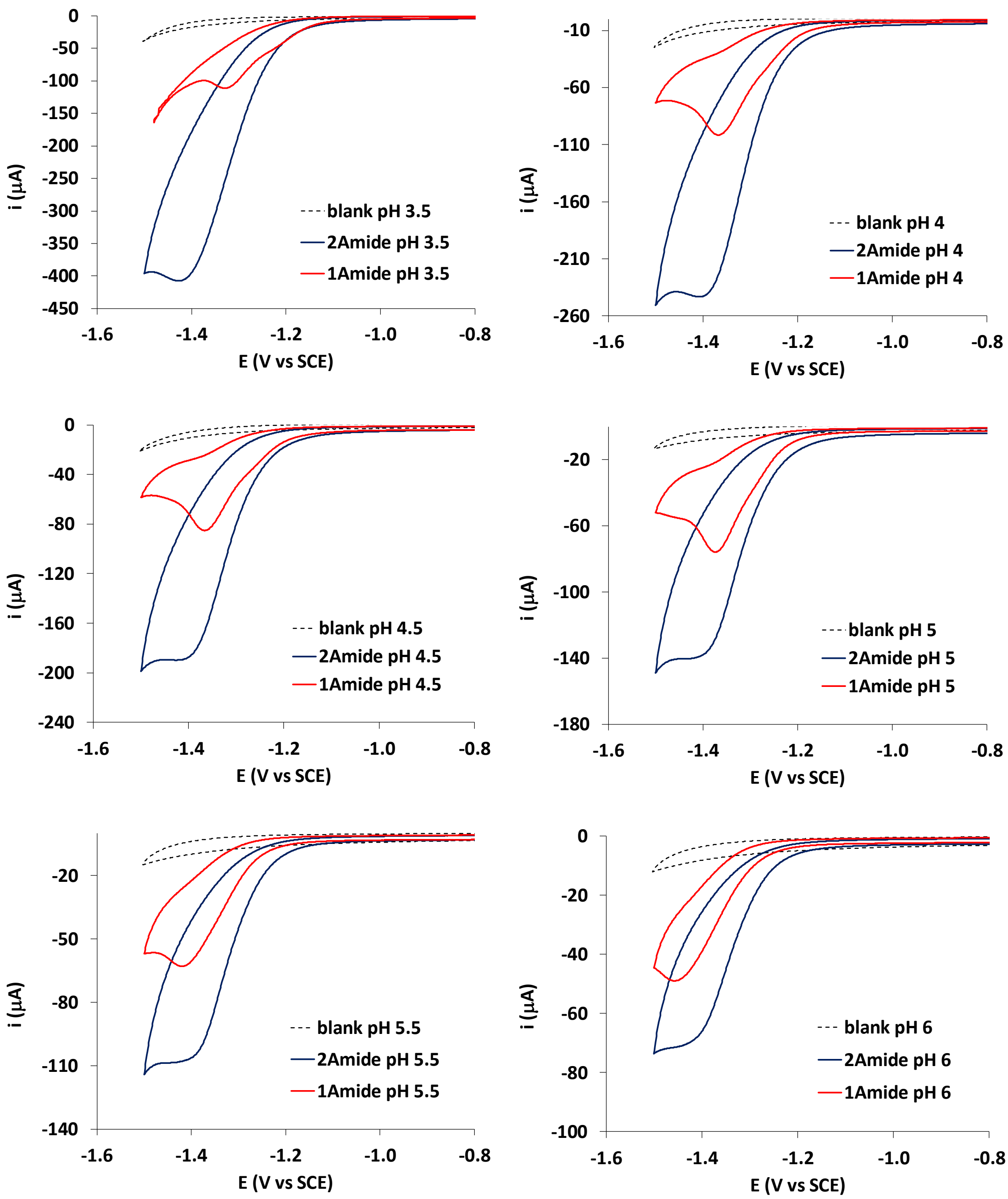


Figure S56. Cyclic voltammograms of **1**^{Amide} and **2**^{Amide} in buffer (citrate 100 mM, NaCl 100 mM) in the pH 3.5 - 6.0 range. Scan rate of 100 mV·s^{-1} using a 0.28 cm^2 glassy carbon working electrode. Potentials are quoted versus SCE.

1.9. Photocatalytic proton reduction

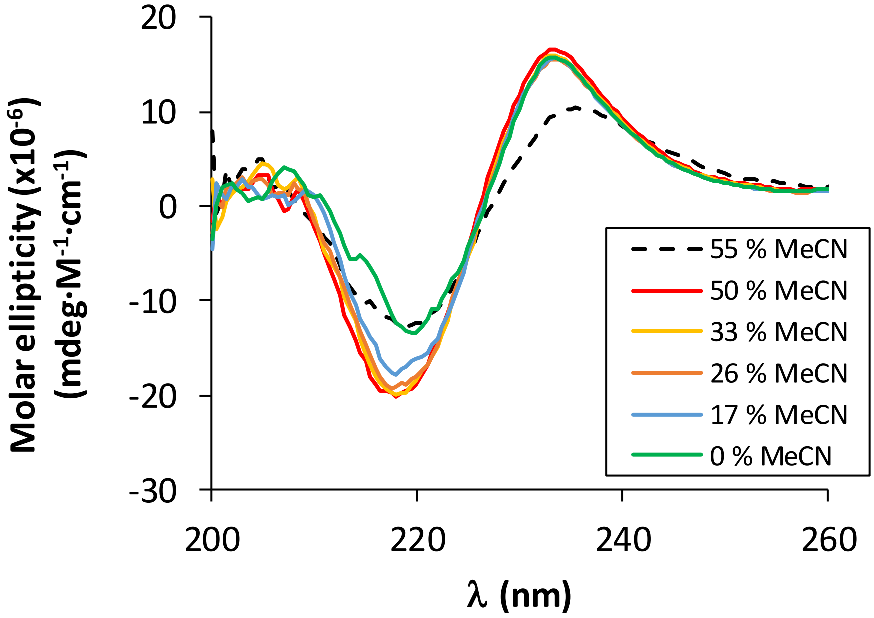


Figure S57. CD spectra of **2**^{Bio} ⊂ **SA** at different percentages of MeCN in the solvent mixture. Conditions: 5 μM protein, 100 mM Tris·HCl buffer, pH 7.5 at 20 ºC. The CD signals were corrected according to the dilution of the addition.

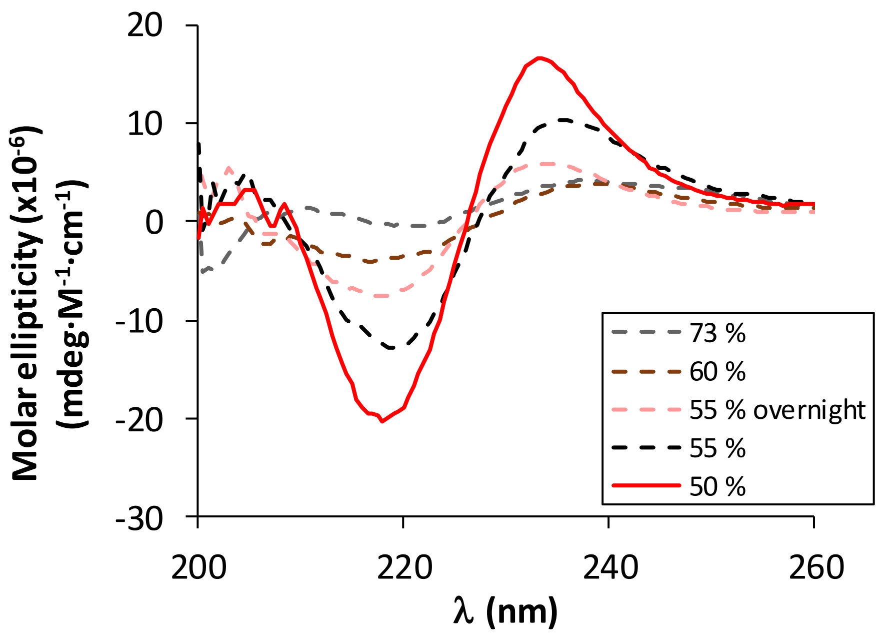


Figure S58. CD spectra of **2**^{Bio} ⊂ **SA** at different percentages of MeCN in the solvent mixture. Conditions: 5 μM protein, 100 mM Tris·HCl buffer, pH 7.5 at 20 ºC. The CD signals were corrected according to the dilution of the addition.

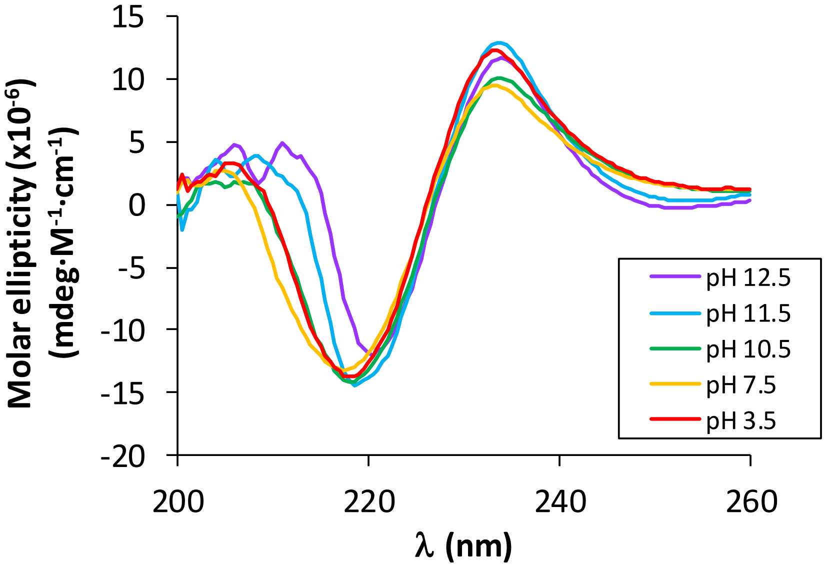


Figure S59. CD spectra of $\mathbf{2^{Bio}}$⊂**SA** at different pHs analogous to photocatalytic (pH 7.5 to 12.5) and electroctalytic (pH 3.5) conditions: 5 µM $\mathbf{2^{Bio}}$⊂**SA**, 100 mM phosphte buffer:MeCN mixtures (3:7, v/v) at 20 ºC. The CD at pH 7.5 has been measured in 100 mM Tris · HCl buffer pH 7.5.

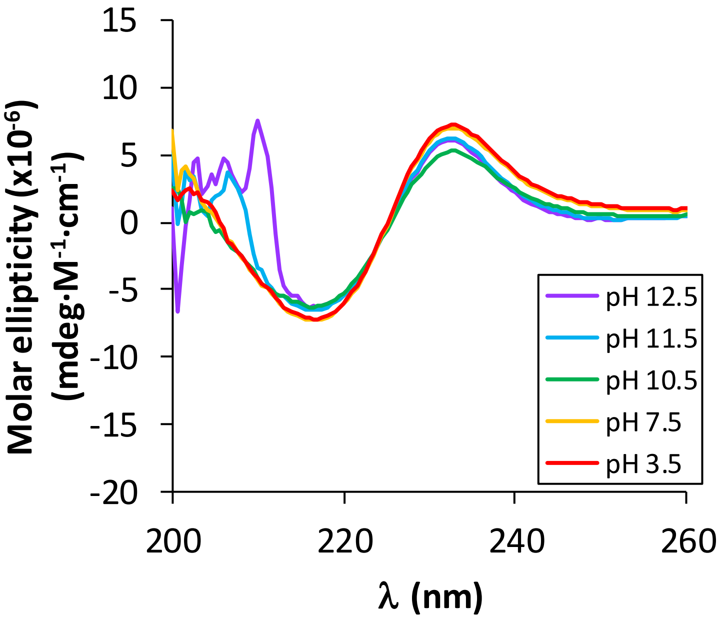


Figure S60. CD spectra of **SA** at different pHs analogous to photocatalytic (pH 7.5 to 12.5) and electroctalytic (pH 3.5) conditions: 5 µM **SA**, 100 mM phosphte buffer:MeCN mixtures (3:7, v/v) at 20 ºC. The CD at pH 7.5 has been measured in 100 mM Tris · HCl buffer pH 7.5.

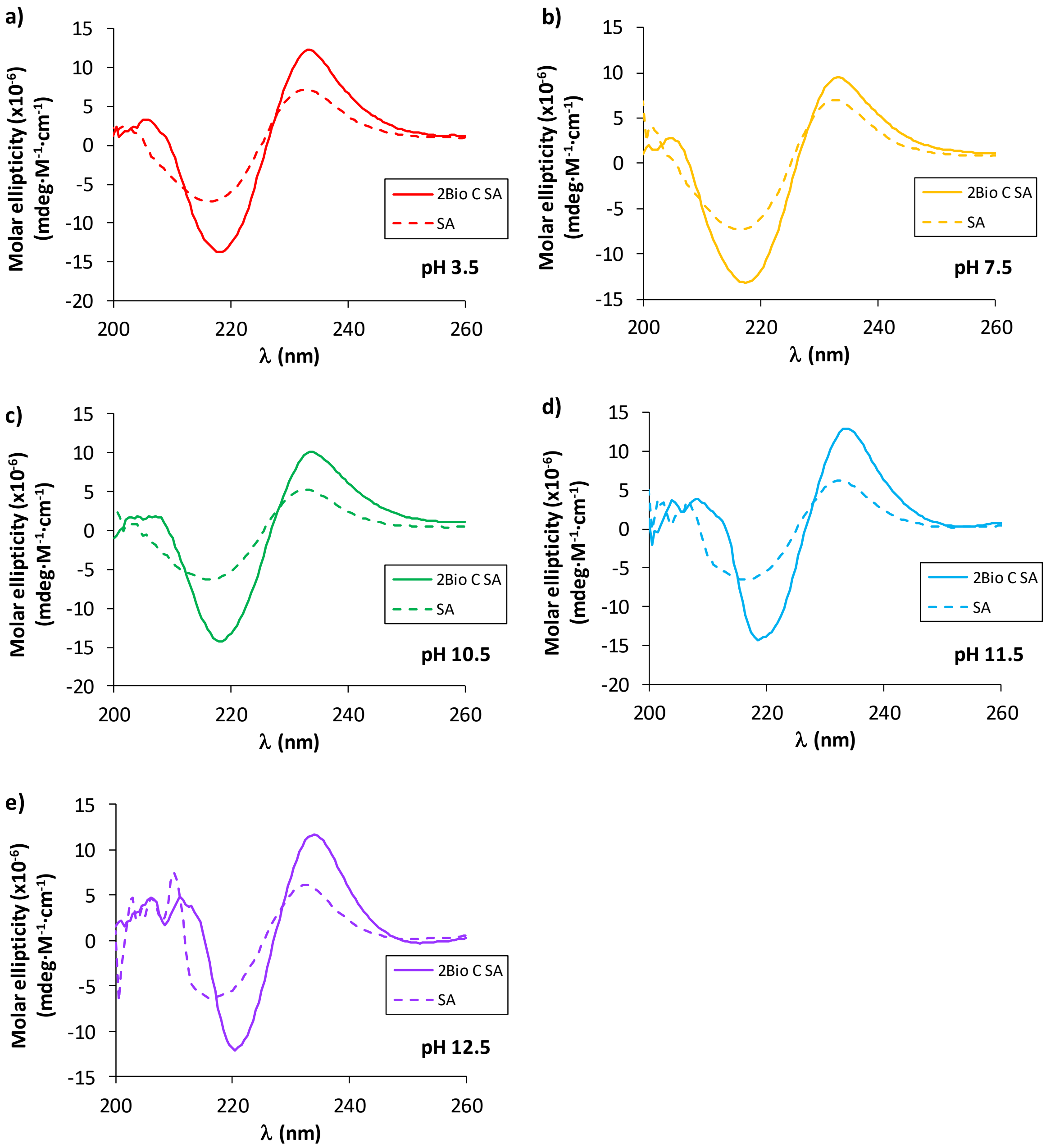


Figure S61. Comparison of the CD spectra of **2**^{Bio} ⊂ **SA** and **SA** at different pHs analogous to photocatalytic (pH 7.5 to 12.5) and electroctalytic (pH 3.5) conditions: 5 μM **2**^{Bio} ⊂ **SA** or **SA**, 100 mM phosphte buffer:MeCN mixtures (3:7, v/v) at 20 ºC. The CD at pH 7.5 has been measured in 100 mM Tris · HCl buffer pH 7.5.

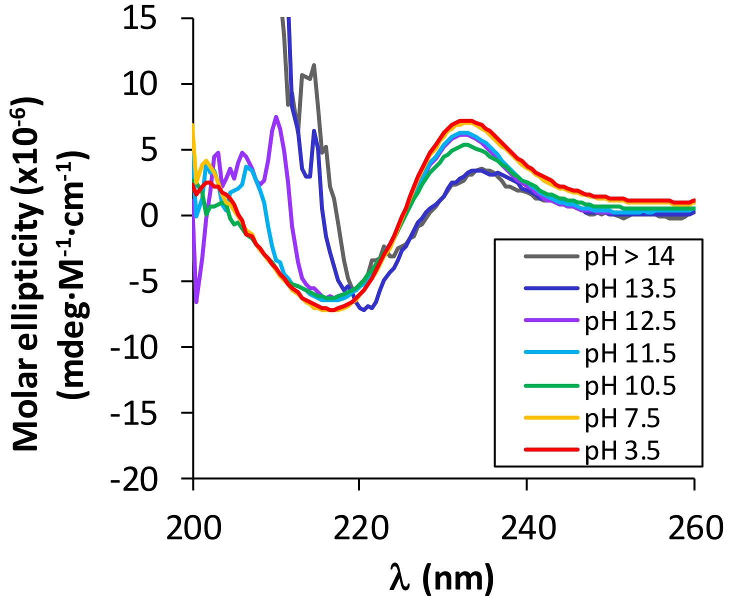


Figure S62. CD spectra of **SA** at different pHs analogous to photocatalytic (pH 7.5 to 12.5) and beyond (pH 13.5 and >14) and electroctalytic (pH 3.5) conditions: 5 μM **SA**, 100 mM phosphte buffer:MeCN mixtures (3:7, v/v) at 20 ºC. The CD at pH 7.5 has been measured in 100 mM Tris · HCl buffer pH 7.5.

Table S4. Catalytic activity of $\mathbf{2^{Bio}}$ and $\mathbf{2^{Bio}} \subset$ **SA** in light-driven proton reduction at different pH values.

pH	$\mathbf{2^{Bio}}$		$\mathbf{2^{Bio}} \subset$ **SA**		Enhancement factor	
pH	TON	TOF (h^{-1})	TON	TOF (h^{-1})	TON$2^{Bio} \subset$SA / TON2^{Bio}	TOF$2^{Bio} \subset$SA / TOF2^{Bio}
7.5	8	2	13	6	1.6	2.6
8.5	14	7	33	9	2.4	1.4
9.0	17	13	45	18	2.7	1.4
9.5	36	20	67	33	1.9	1.7
10.5	89	49	106	63	1.2	1.3
11.5	46	16	166	88	3.6	5.5
12.5	9	4	93	53	10.5	13.4

[a] Cobalt catalyst (5 μM), $\mathbf{PS_{Ir}}$ (250 μM), TEOA (0.4 M) in MeCN:H_2O (3:7, 0.4 mL), phosphate buffer (100 mM), NaCl (100 mM). pH: 7.5-12.5. Irradiation with 1100 W·m^{-2} of visible light (λ > 400 nm).

Additional catalytic tests show that the catalytic activity cannot be recovered after reaching the plateau under photocatalytic conditons by the addition of any of the catalytic components separately or together neither for **2**$^{\mathbf{Bio}}$ nor **2**$^{\mathbf{Bio}}$ $\subset$ **SA** (Figures S63 and S64). These experiments suggest that the catalytic activity stops due to the formation of a poisoning species in the due course of the catalysis. This behaviour was already observed.[21]

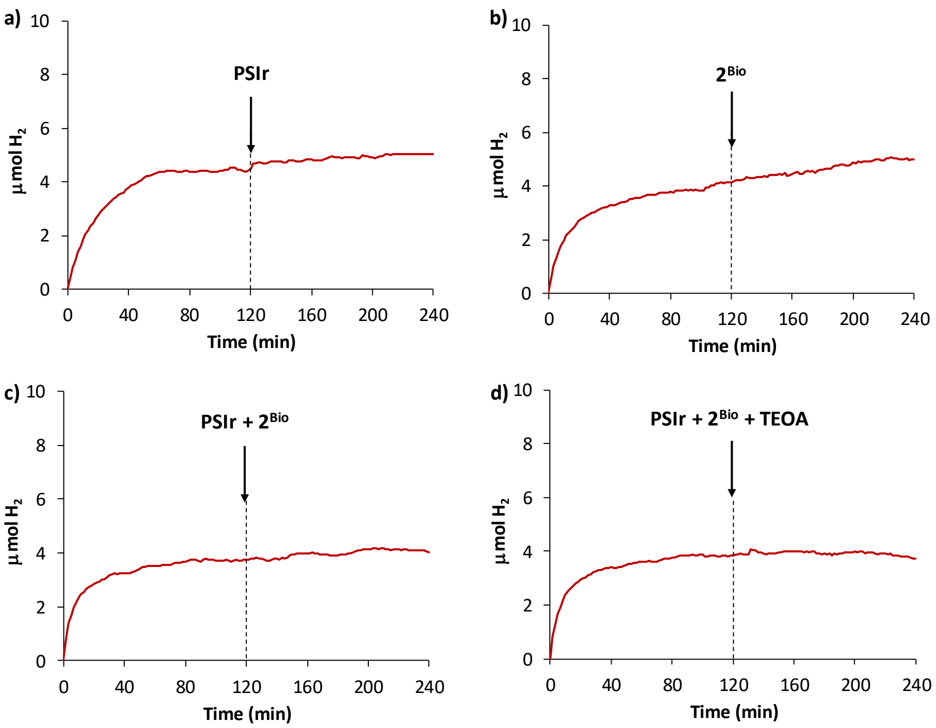


Figure S63. Time traces of the photoinduced H_2 production and recovery using **2**$^{\mathbf{Bio}}$ (5 µM), **PS**$_{\mathbf{Ir}}$ (250 µM), TEOA (0.4 M) in 4.2 mL of CH_3CN:phosphate buffer (3:7 *v/v*) (100 mM) at pH 10.5 after 4 h irradiation (1100 W·m^{-2}, λ > 400 nm). a) Addition of **PSIr**, b) addition of **2**$^{\mathbf{Bio}}$, c) addition of **PSIr** + **2**$^{\mathbf{Bio}}$ and d) addition of **PSIr** + **2**$^{\mathbf{Bio}}$ +TEOA after reaching the plateau after 2 h of irradiation.

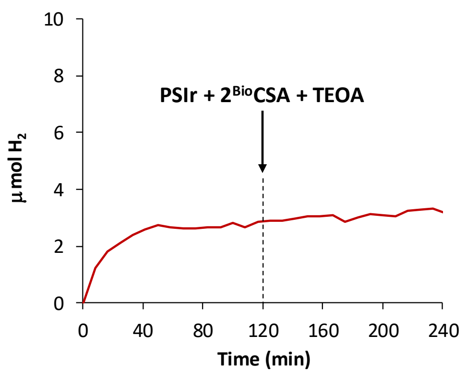


Figure S64. Time traces of the photoinduced H_2 production and recovery using **2**$^{\mathbf{Bio}}$ $\subset$ **SA** (5 µM), **PS**$_{\mathbf{Ir}}$ (250 µM), TEOA (0.4 M) in 4.2 mL of CH_3CN:phosphate buffer (3:7 *v/v*) (100 mM) at pH 10.5 after 4 h irradiation (1100 W·m^{-2}, λ > 400 nm) and after further addition of **PS**$_{\mathbf{Ir}}$ + **2**$^{\mathbf{Bio}}$ +TEOA after reaching the plateau after 2 h of irradiation.

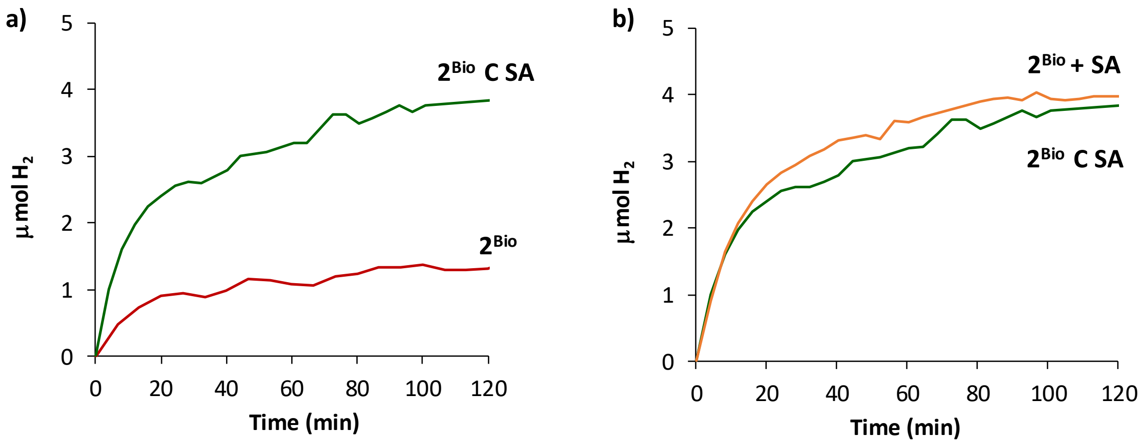


Figure S65. Time traces of the photoinduced H_2 production by a) **2**$^{\text{Bio}}$ and **2**$^{\text{Bio}}$ ⊂ **SA** (5 μM); and b) **2**$^{\text{Bio}}$ ⊂ **SA** (5 μM) and the "*in situ*" generated **2**$^{\text{Bio}}$ ⊂ **SA** by mixing **2**$^{\text{Bio}}$ + **SA** (5 μM), together with **PS**$_{\text{Ir}}$ (250 μM), TEOA (0.4 M) in 4.2 mL of CH_3CN:phosphate buffer (3:7 *v/v*) (100 mM) at pH 11.5 after 2 h irradiation (1100 W·m^{-2}, λ > 400 nm).

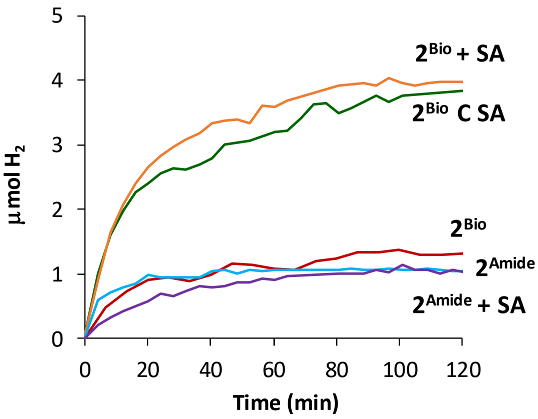


Figure S66. Time traces of the photoinduced H_2 production by (from *top* to *bottom*) the "*in situ*" generated **2**$^{\text{Bio}}$ ⊂ **SA** by mixing **2**$^{\text{Bio}}$ + **SA** (5 μM, yellow trace), **2**$^{\text{Bio}}$ ⊂ **SA** (5 μM, green trace); **2**$^{\text{Bio}}$ (5 μM, red trace), **2**$^{\text{Amide}}$ (5 μM, cian trace) and **2**$^{\text{Amide}}$ + **SA** (5 μM, purple trace), together with **PS**$_{\text{Ir}}$ (250 μM), TEOA (0.4 M) in 4.2 mL of CH_3CN:phosphate buffer (3:7 *v/v*) (100 mM) at pH 11.5 after 2 h irradiation (1100 W·m^{-2}, λ > 400 nm).

2. COMPUTATIONAL SECTION

2.1. Methodology for the molecular dynamic simulations

Molecular Dynamics Simulations. MD simulations in explicit water were performed using AMBER 16 package[22] on our in-house GPU cluster *Galatea*. $\mathbf{1}^{\mathbf{Bio}}$ and $\mathbf{2}^{\mathbf{Bio}}$ parameters for the MD simulations were generated within the *antechamber* module of AMBER 16 using the general AMBER force field (GAFF).[23] We have used the bonded model for Co (quadruplet state as the lowest in energy) and ligand moiety, in particular we used the Seminario method approach to obtain the metal parameters needed for the simulation as implemented in Prof. Ryde's program.[24] The optimization, frequencies and partial charge set to fit the electrostatic potential generated at the UB3LYP/6-31G(d) level by the restrained electrostatic potential (RESP) model using Gaussian 09. The charges were calculated according to the Merz-Singh-Kollman scheme. We have docked $\mathbf{1}^{\mathbf{Bio}}$ and $\mathbf{2}^{\mathbf{Bio}}$ complexes in the biotin pocket by using the pair-fitting tool in Pymol (http://www.pymol. org) using the biotin moiety of the crystal structure (PDB: 1MK5) as a reference and the optimized structure of the complex creating the tetramer enzyme. Amino acid protonation states and the data needed for the electrostatic map were set up using the Propka3.0 server (http://nbcr-222.ucsd.edu/pdb2pqr_2.0.0/).[25]Then, the enzyme was solvated in a pre-equilibrated truncated cuboid box with a 10-Å buffer of TIP3P[26] water molecules using the AMBER16 *leap* module, resulting in the addition of *ca.* 9,000 solvent molecules. The systems were neutralized by addition of explicit counterions (Na^+ and Cl^-). All subsequent calculations were carried out using the widely tested Stony Brook modification of the Amber 99 force field (ff14SB).[27] The structure used was 1MK5 from the protein data bank (PDB).

A two-stage geometry optimization was performed. The first stage minimizes the positions of solvent molecules and ions imposing positional restraints on solute by a harmonic potential with a force constant of 500 kcal mol^{-1} $Å^{-2}$, and the second stage is an unrestrained minimization of all the atoms in the simulation cell. The systems are gently heated using six 50-ps steps, incrementing the temperature 50 K each step (0–300 K) under constant volume and periodic boundary conditions. Water molecules were treated with the SHAKE algorithm such that the angle between the hydrogen atoms is kept fixed. Long-range electrostatic effects were modeled using the particle-mesh-Ewald method.[28]

A 8-Å cutoff was applied to Lennard-Jones and electrostatic interactions. Harmonic restraints of 10 kcal/mol were applied to the solute, and the Langevin equilibration scheme was used to control and equalize the temperature. The time step was kept at 1 fs during the heating stages, allowing potential inhomogeneities to self-adjust. Each system was then equilibrated without restrains for 2 ns with a 2-fs timestep at a constant pressure of 1 atm and temperature of 300 K. After the systems were equilibrated in the NPT ensemble, 3 independent 250 ns MD simulations for $\mathbf{1}^{\mathbf{Bio}}$ and $\mathbf{2}^{\mathbf{Bio}}$ (i.e. 750 microsecond accumulated) were performed under the NVT ensemble and periodic-boundary conditions.

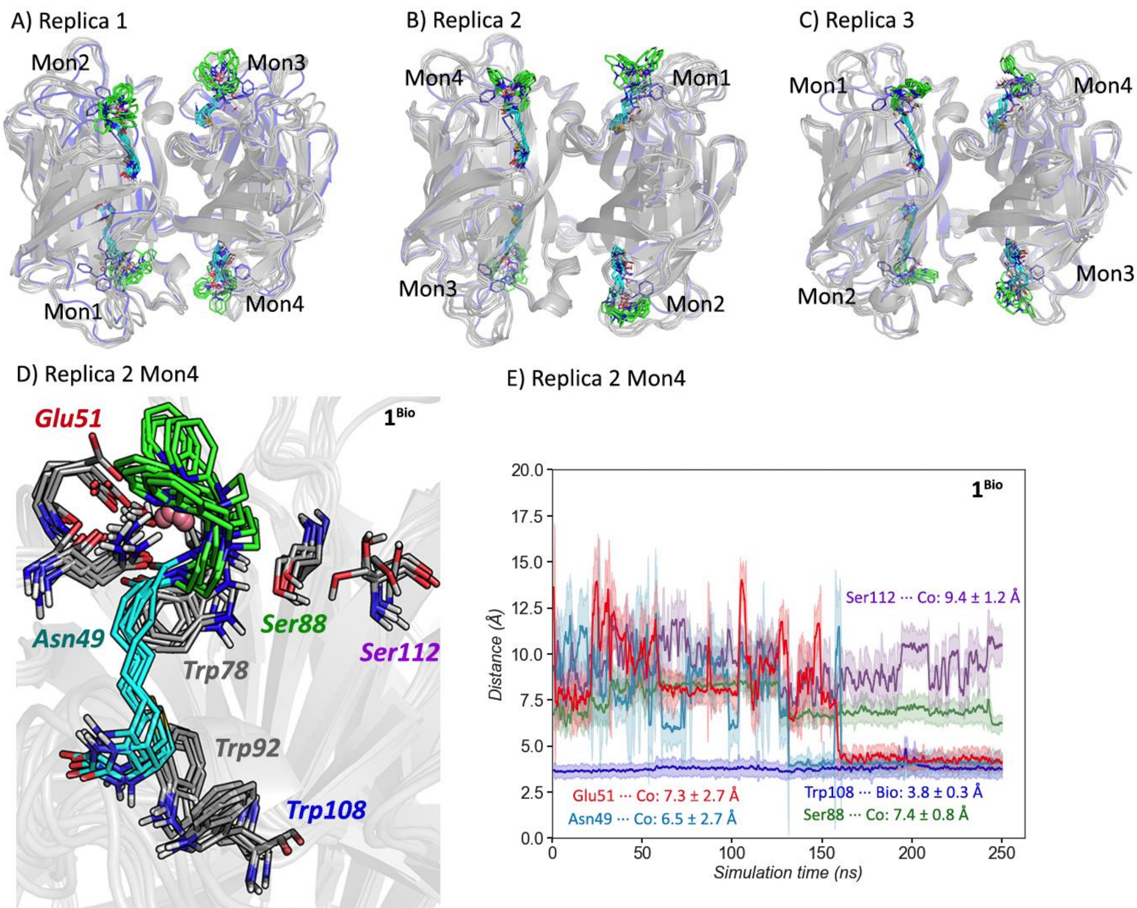
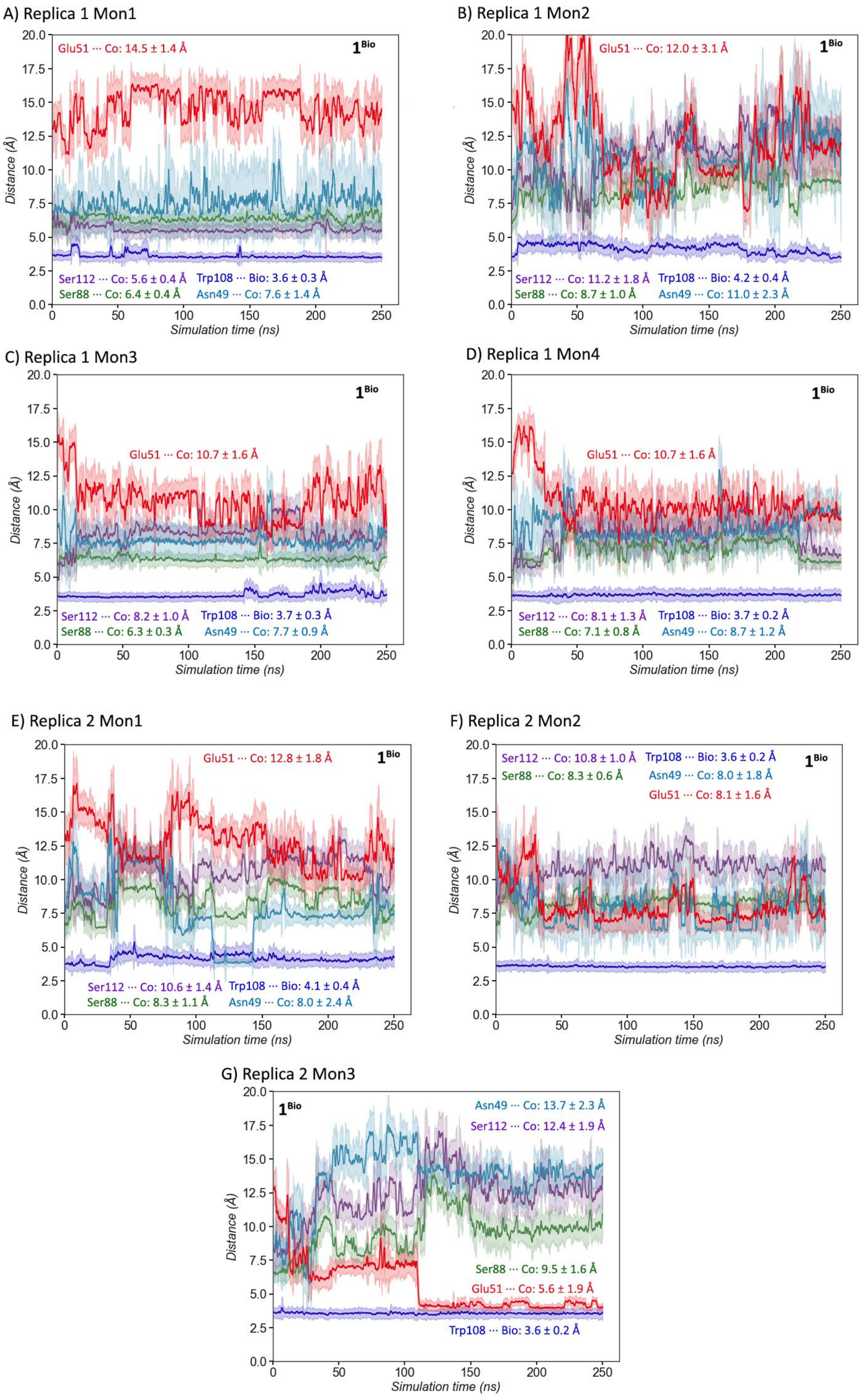


Figure S67. Overlay of representative snapshots visited along the Molecular Dynamics (MD) simulations of 3 independent replicas for **1**$^{\mathbf{Bio}}$: A) Replica 1, A) Replica 2, and C) Replica 3. The starting structure for the MD simulations is displayed in blue. The conformational dynamics of the binding pocket for replica 2 Mon4 are shown in D), where the most important residues surrounding the biotin complexes are represented. Some selected distances (in Å) are displayed in E). The distances have been computed from the metal center and either the sidechain of Ser112 (oxygen atom, in purple) and Ser88 (oxygen atom, in green), or Asn49 (carbonyl group, teal). In the case of Trp108, the distance has been computed from the center of mass of the indole ring and the tetrahydrothiophene ring of biotin, in blue. The average distances and the standard deviations are also shown.


A) Replica 1 Mon1
1^Bio
Glu51 ··· Co: 14.5 ± 1.4 Å
Ser112 ··· Co: 5.6 ± 0.4 Å
Trp108 ··· Bio: 3.6 ± 0.3 Å
Ser88 ··· Co: 6.4 ± 0.4 Å
Asn49 ··· Co: 7.6 ± 1.4 Å
B) Replica 1 Mon2
1^Bio
Glu51 ··· Co: 12.0 ± 3.1 Å
Ser112 ··· Co: 11.2 ± 1.8 Å
Trp108 ··· Bio: 4.2 ± 0.4 Å
Ser88 ··· Co: 8.7 ± 1.0 Å
Asn49 ··· Co: 11.0 ± 2.3 Å
C) Replica 1 Mon3
1^Bio
Glu51 ··· Co: 10.7 ± 1.6 Å
Ser112 ··· Co: 8.2 ± 1.0 Å
Trp108 ··· Bio: 3.7 ± 0.3 Å
Ser88 ··· Co: 6.3 ± 0.3 Å
Asn49 ··· Co: 7.7 ± 0.9 Å
D) Replica 1 Mon4
1^Bio
Glu51 ··· Co: 10.7 ± 1.6 Å
Ser112 ··· Co: 8.1 ± 1.3 Å
Trp108 ··· Bio: 3.7 ± 0.2 Å
Ser88 ··· Co: 7.1 ± 0.8 Å
Asn49 ··· Co: 8.7 ± 1.2 Å
E) Replica 2 Mon1
1^Bio
Glu51 ··· Co: 12.8 ± 1.8 Å
Ser112 ··· Co: 10.6 ± 1.4 Å
Trp108 ··· Bio: 4.1 ± 0.4 Å
Ser88 ··· Co: 8.3 ± 1.1 Å
Asn49 ··· Co: 8.0 ± 2.4 Å
F) Replica 2 Mon2
1^Bio
Ser112 ··· Co: 10.8 ± 1.0 Å
Trp108 ··· Bio: 3.6 ± 0.2 Å
Ser88 ··· Co: 8.3 ± 0.6 Å
Asn49 ··· Co: 8.0 ± 1.8 Å
Glu51 ··· Co: 8.1 ± 1.6 Å
G) Replica 2 Mon3
1^Bio
Asn49 ··· Co: 13.7 ± 2.3 Å
Ser112 ··· Co: 12.4 ± 1.9 Å
Ser88 ··· Co: 9.5 ± 1.6 Å
Glu51 ··· Co: 5.6 ± 1.9 Å
Trp108 ··· Bio: 3.6 ± 0.2 Å
Distance (Å)
Simulation time (ns)

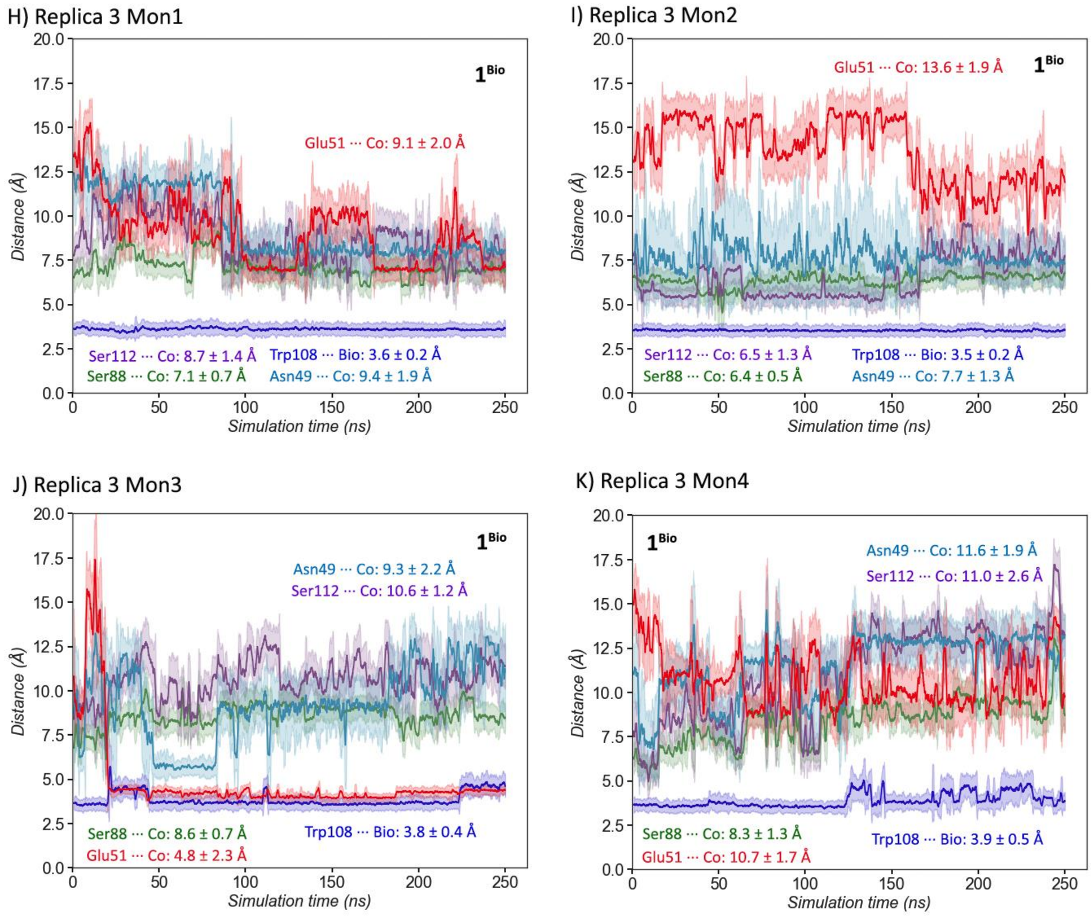


Figure S68. Representation of some selected distances (in Å) for each monomer of all replicas in **1**^{Bio}. The distances have been computed from the metal center and either the sidechain of Ser112 (oxygen atom, in purple) Ser88 (oxygen atom, in green), or Asn49 (carbonyl group, teal). In the case of Trp108, the distance has been computed from the center of mass of the indole ring and the tetrahydrothiophene ring of biotin, in blue. The average distances and the standard deviations are also shown.

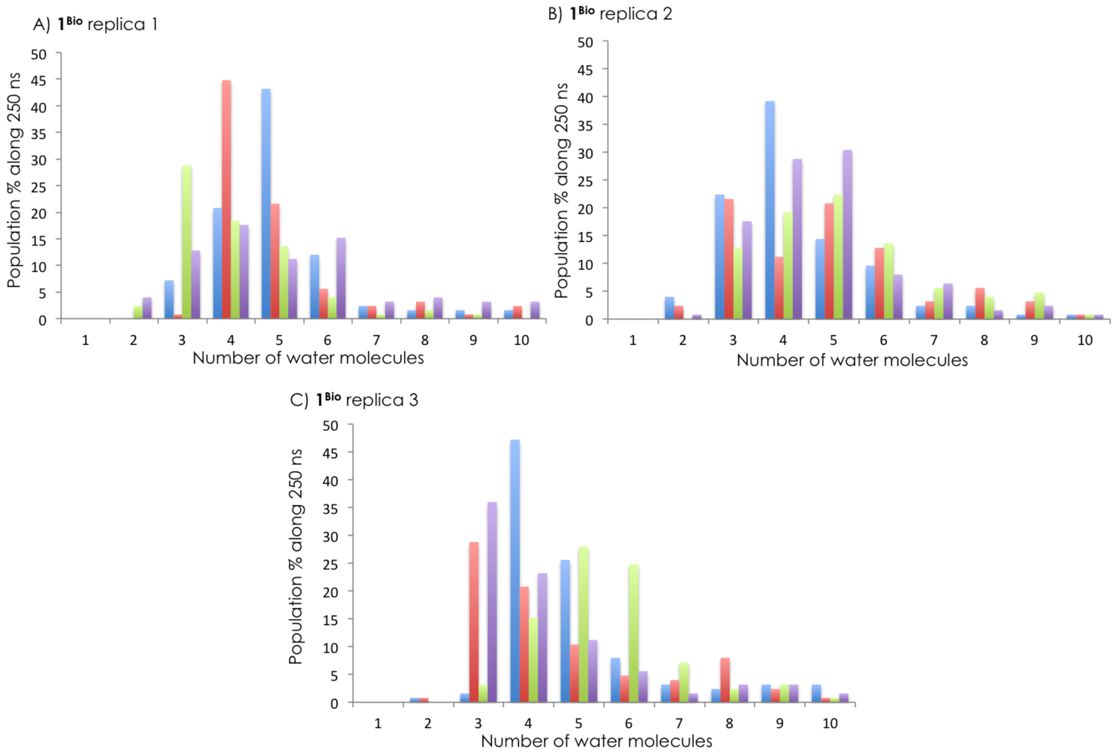


Figure S69. Watershell estimation along the MD trajectories for $\mathbf{1}^{\mathbf{Bio}}$ for all monomers (the different colors are referred to the different monomers)**.** The analysis suggests that around 3-5 water molecules are present near the metal center.

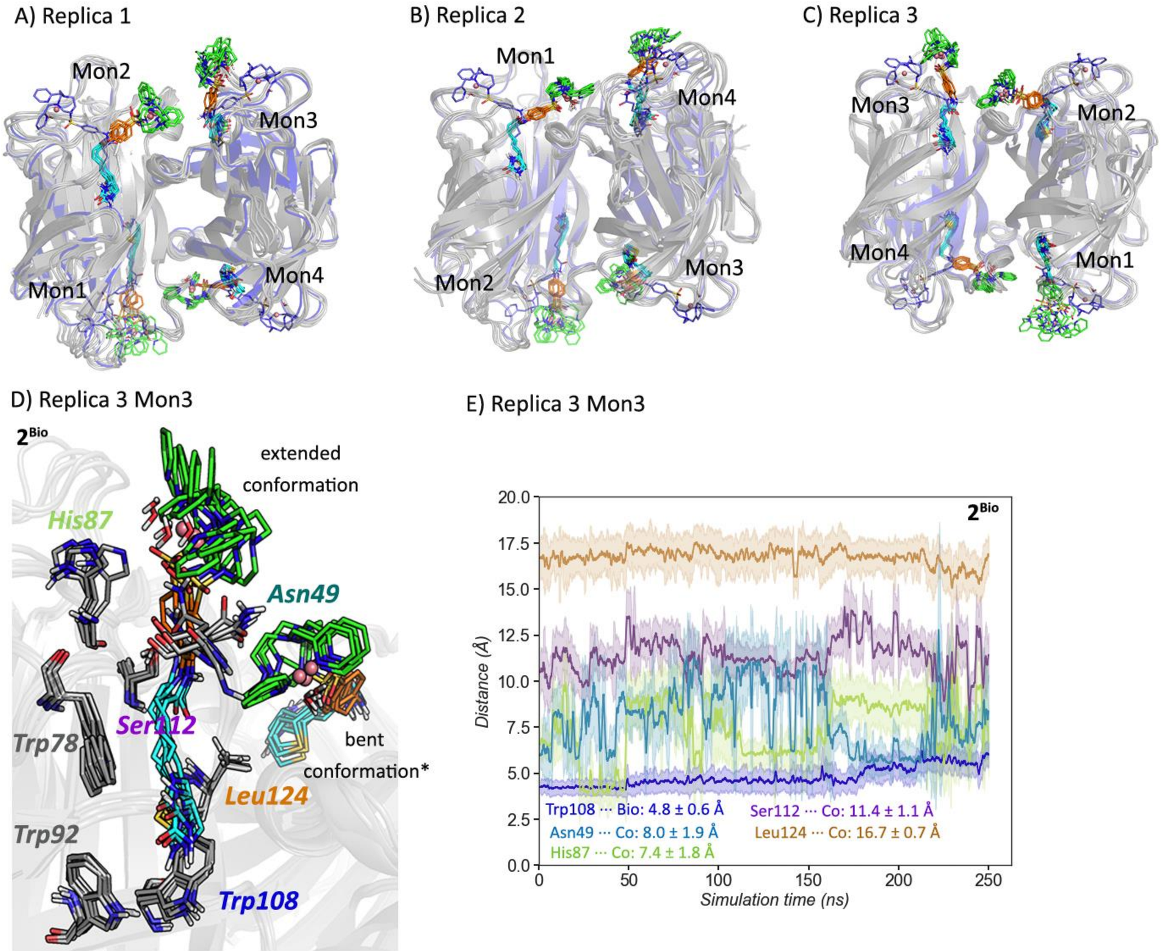
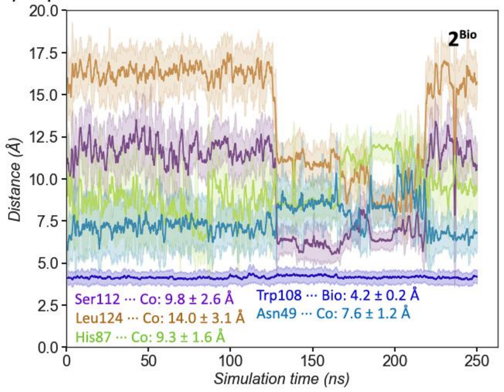
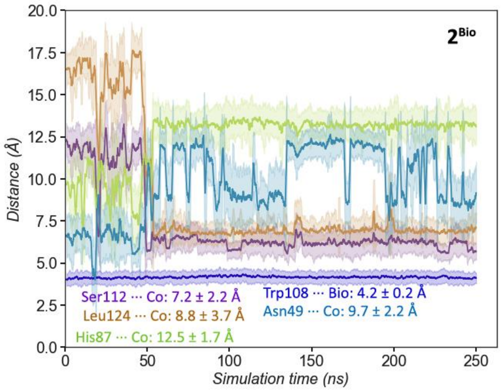


Figure S70. Overlay of representative snapshots visited along the Molecular Dynamics (MD) simulations of 3 independent replicas for **2**$^{\mathbf{Bio}}$: A) Replica 1, A) Replica 2, and C) Replica 3. The starting structure for the MD simulations is displayed in blue. The conformational dynamics of the binding pocket for replica 3 Mon3 are shown in D), where the most important residues surrounding the biotin complexes are represented. Some selected distances (in Å) are displayed in E). The distances have been computed from the metal center and either the sidechain of Ser112 (oxygen atom, in purple), His87 (deprotonated nitrogen, in light green), Leu124 (the terminal carbon of isobutyl side chain, in orange), and Asn49 (carbonyl group, teal). In the case of Trp108, the distance has been computed from the center of mass of the indole ring and the tetrahydrothiophene ring of biotin, in blue. The average distances and the standard deviations are also shown.***2**$^{\mathbf{Bio}}$ from the other monomer.

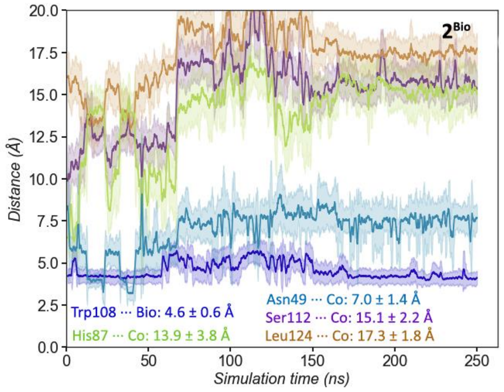
A) Replica 1 Mon1



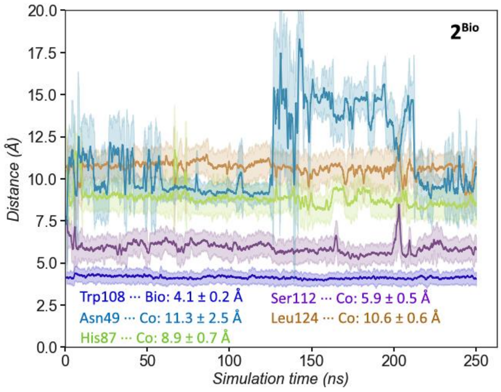
B) Replica 1 Mon2



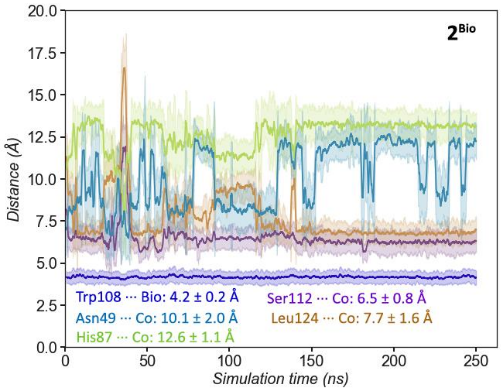
C) Replica 1 Mon3



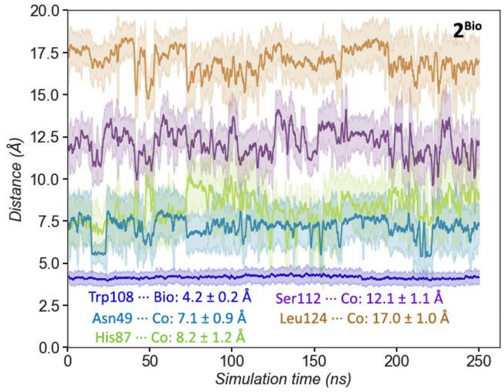
D) Replica 1 Mon4



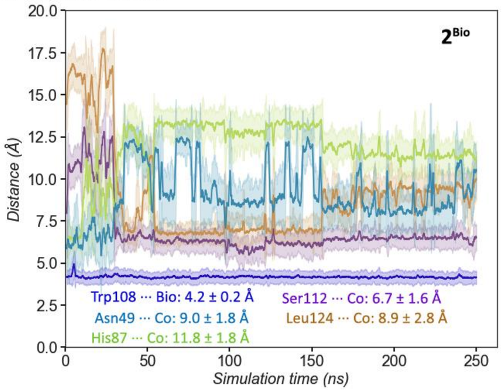
E) Replica 2 Mon1



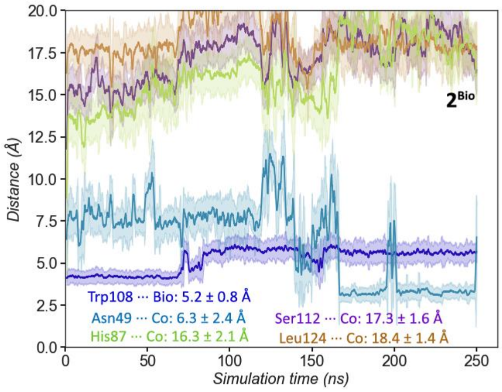
F) Replica 2 Mon2



G) Replica 2 Mon3



H) Replica 2 Mon4



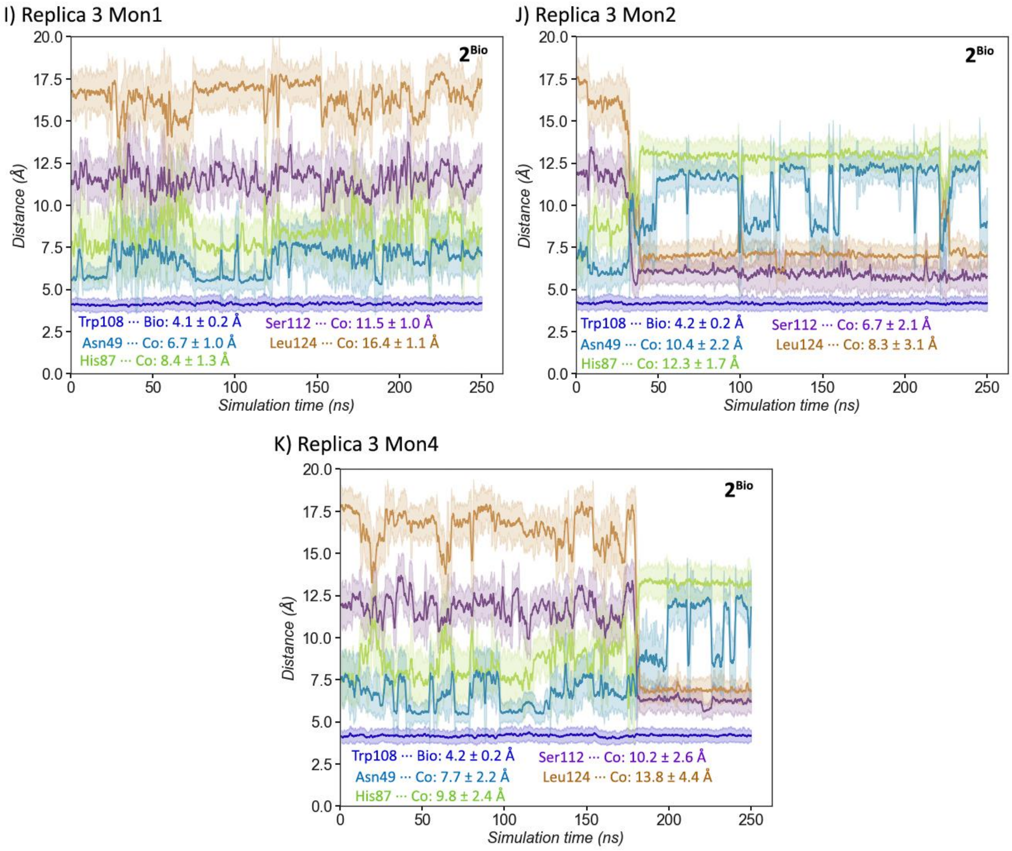


Figure S71. Representation of some selected distances (in Å) for each monomer of all replicas in **2**$^{\mathbf{Bio}}$. The distances have been computed from the metal center and either the sidechain of Ser112 (oxygen atom, in purple), His87 (deprotonated nitrogen, in light green), Leu124 (the terminal carbon of isobutyl side chain, in orange), and Asn49 (carbonyl group, teal). In the case of Trp108, the distance has been computed from the center of mass of the indole ring and the tetrahydrothiophene ring of biotin, in blue. The average distances and the standard deviations are also shown.

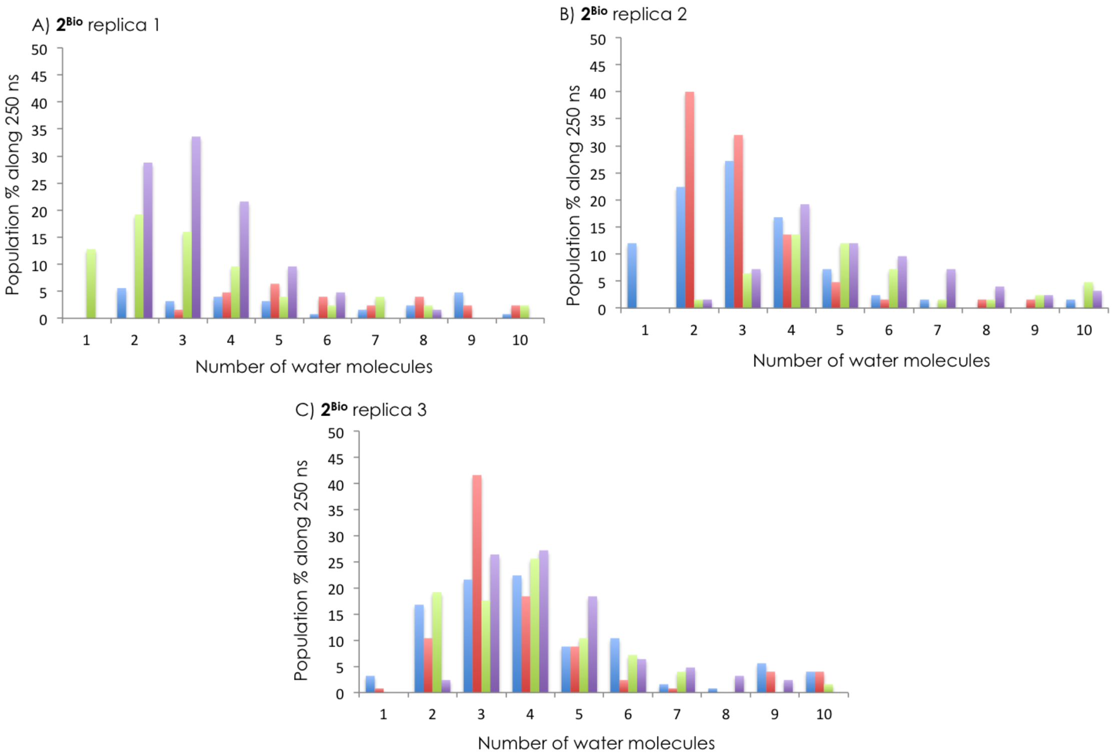


Figure S72. Watershell estimation along the MD trajectories for **2**$^{\mathbf{Bio}}$ for all monomers (the different colors are referred to the different monomers)**.** The analysis suggests that around 2-4 water molecules are present near the metal center.

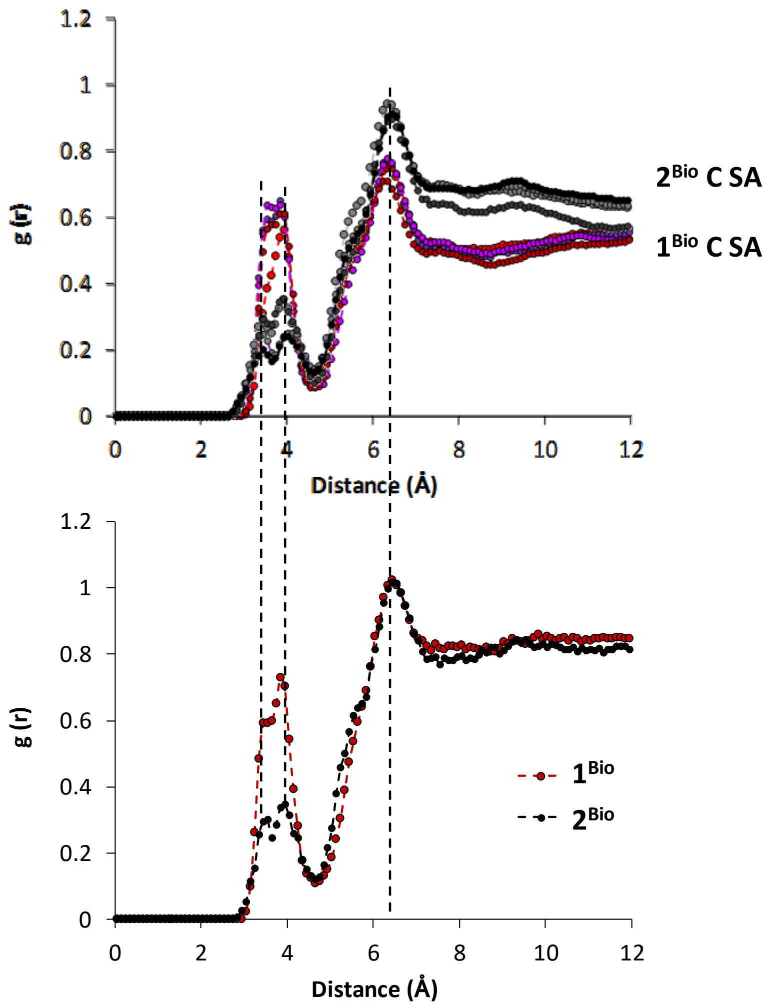


Figure S73. Radial distribution (**g(r)**) of water molecules in the second coordination sphere around the metal center for **2**^{Bio}, **1**^{Bio}, **2**^{Bio} ⊂ **SA** and **1**^{Bio} ⊂ **SA**. The **g(r)** of complexes **1**^{Bio} and **2**^{Bio} presents two clear peaks at about 3.9 and 6.2 Å, where the differences are at distances shorter than ca. 5 Å. The inclusion of the complexes in the protein pocket only slightly modifies the values at shorter distances than 5 Å. At longer distances, the **g(r)** value is reduced in both cases, being the reduction higher when the complex is deeper into the protein pocket (**1**^{Bio}).

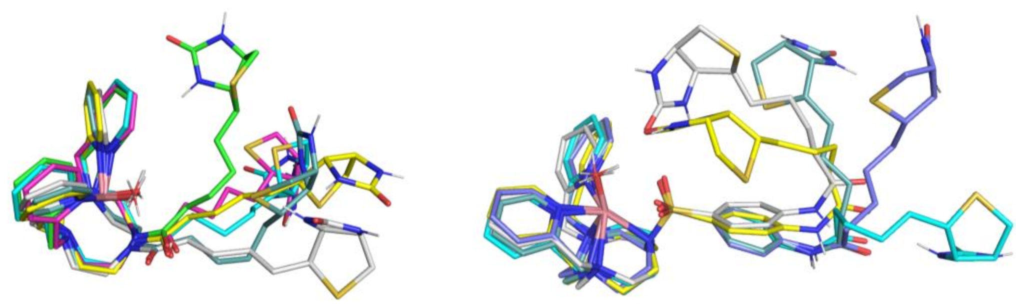


Figure S74. *Left*) Overlay of the representative conformations of complex **1**^{Bio}, *Right*) Overlay of the representative conformations of complex **2**^{Bio}.

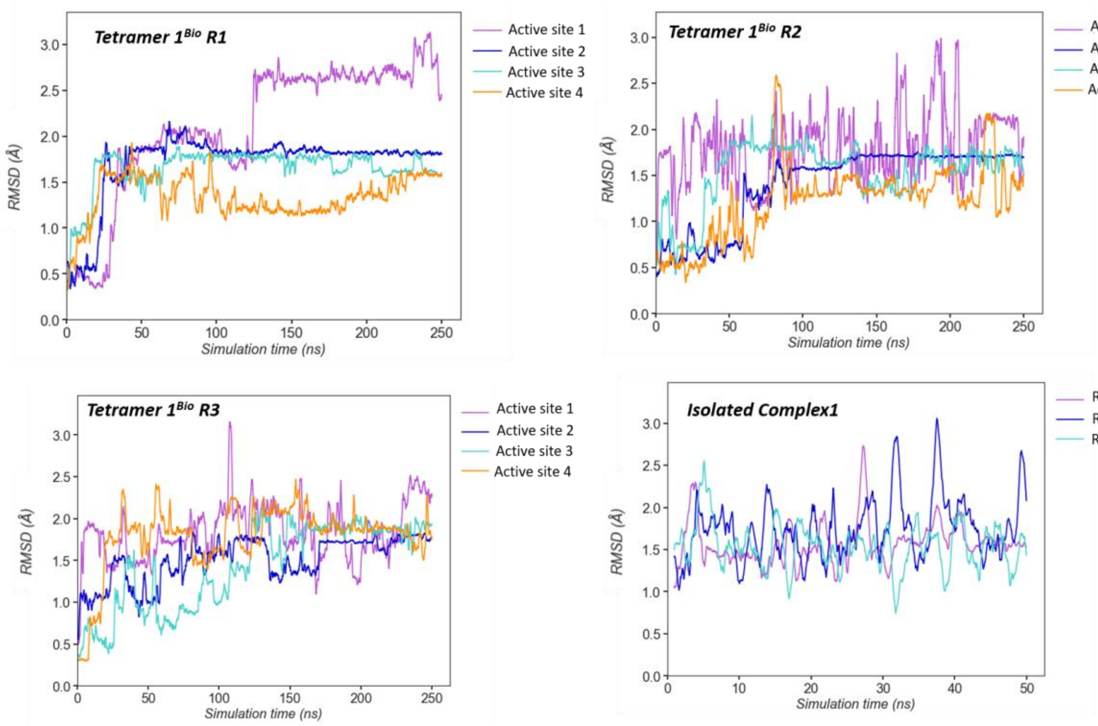


Figure S75. Calculation for the 3 replicas and 4 active sites of **1**^{Bio} in the tetramer, and for the complex **1**^{Bio} isolated.

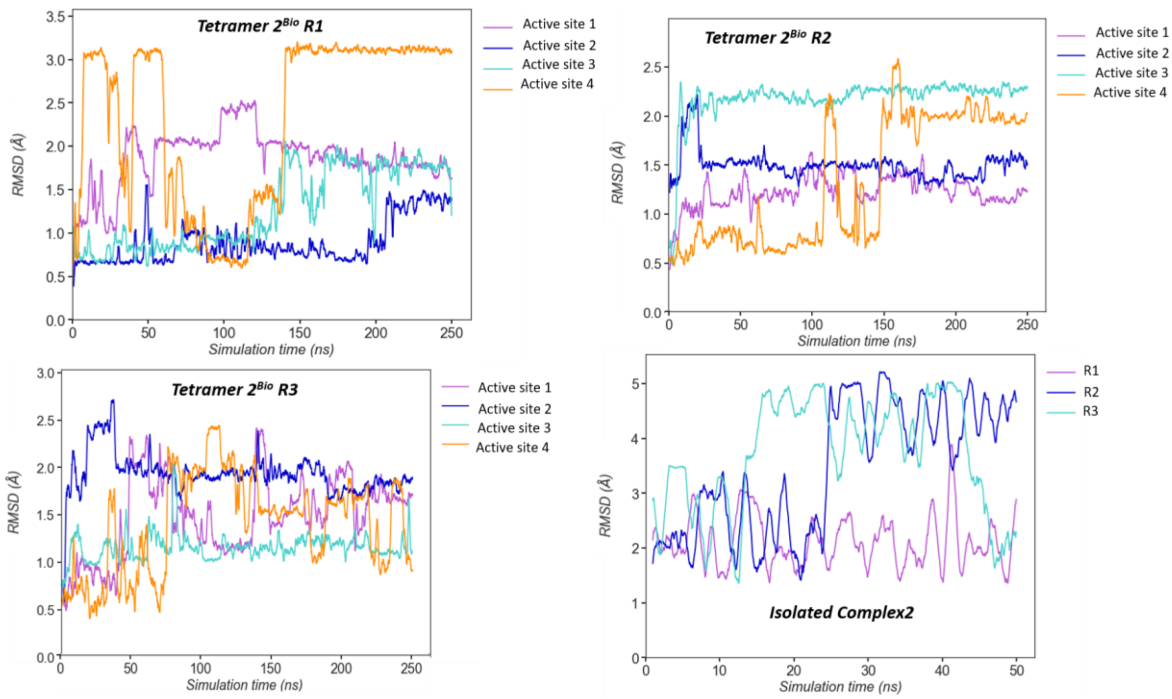


Figure S76. RMSD calculation for the 3 replicas and 4 active sites of **2**^{Bio} in the tetramer, and for the complex **2**^{Bio} isolated.

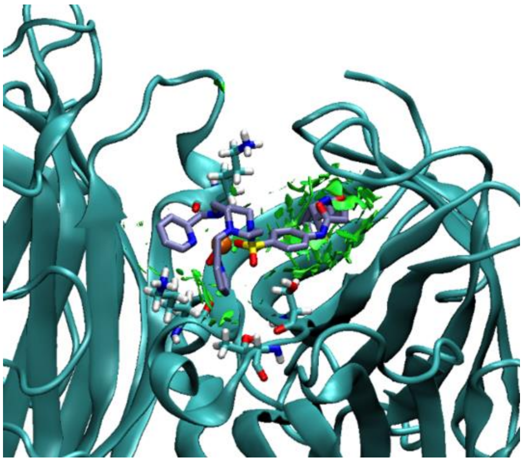


Figure S77. Representation of the non-covalent interactions for two representative conformations of **2^{Bio}** of the tetramer computed with the computational tool NCIplot.[29]

2.2. DFT study of potential external biotin coordination

2.2.1. Computational details

We have studied the coordination ability of the biotinated ligands **^{Bio}Py$_2$tacn** and **$^{Bio-SP}$Py$_2$tacn** to the metal center and the possibility of binding the biotin fragment to the metal center in complexes **1^{Bio}** and **2^{Bio}** computationally by density functional theory (DFT) using the Gaussian09 program. Geometry optimizations were performed in the unrestricted spin formalism, with the B3LYP hybrid exchange-correlation functional[31] and the standard 6-31+G** 6d basis set for all atoms. An extra quadratic convergent SCF step was added when the first-order SCF did not converge ("scf = xqc" keyword). The solvation effect of acetonitrile was introduced in geometry optimizations and energy through the IEFPCM-SMD polarizable continuum model.[32] Dispersion effects were also included using the Grimme D_3 correction.[33] The geometries have been edited with the Chemcraft program.[34] The located stationary points were characterized by analytical frequency calculations at the same level of theory than geometry optimizations. Gibbs energy values (G) were obtained by including thermal, solvation and Grimme corrections to the potential energy computed with the 6-31+G** 6d basis set on equilibrium geometries.

2.2.2. Protonation reactions

The standard dissociation free energy change between an acid (AH) and its conjugate base (A^-) in acetonitrile (ΔG*) may be expressed as:[35]

$$\Delta G^* = G(A^-_{MeCN}) + G(H^+_{MeCN}) - G(AH_{MeCN}) + \Delta G^{o/*} \quad (1)$$

$$G(H^+_{MeCN}) = G(H^+_{gas}) + \Delta G^{H+}_{solv} \quad (2)$$

where $G(AH_{MeCN})$ and $G(A^-_{MeCN})$ are standard free energies of the acid and its conjugate base in acetonitrile, respectively. The $G(H^+_{MeCN})$ is the free energy of the proton in acetonitrile, obtained from the experimental solvation free energy ($\Delta G^{H+}_{solv} = -260.2\ kcal \cdot mol^{-1}$)[35] and its gas-phase free energy ($G(H^+_{gas}) = -6.3\ kcal \cdot mol^{-1}$). $\Delta G^{o/*}$ is the free energy change associated with the conversion from a standard state of 1 M in the aqueous phase and 1 atm in gas phase, to the desired concentration in both phases. ΔG^* values are derived with the following expression:

$$\Delta G^{o/*} = RT\ \ln(24.45 * c) \quad (3)$$

where *R* is the universal gas constant (1.987 $cal \cdot mol^{-1} \cdot K^{-1}$), *T* is the temperature in Kelvin and *c* the concentration in $mol \cdot L^{-1}$.

In other to obtain more realistic thermodynamic values, the final free energies were adjusted to account for the following concentrations: 1 mM for biotin, 10^{-12} M for protons (due to the pH ≈ 12), 19.1 M for acetonitrile (the concentration of acetonitrile is derived from the electrocatalytic conditions). The previous concentrations translate into free energy correction values to the final free energy ($\Delta G^{o/*}$ at 298.15 K) of -2.2 $kcal \cdot mol^{-1}$ for biotin, -14.5 $kcal \cdot mol^{-1}$ for protons and 3.6 $kcal \cdot mol^{-1}$ for acetonitrile.

Taking into account the previous equations, the pKa of n acid H in solution is computed as:

$$pKa = \frac{\Delta G^*}{RT\ \ln(10)} \quad (4)$$

For the calculation of the pKa, the most stable isomers have been taken into account to calculate the ΔG* associated to each process. The change on the solvent concentration has been corrected through the addition of $\Delta G^{o/*}$.

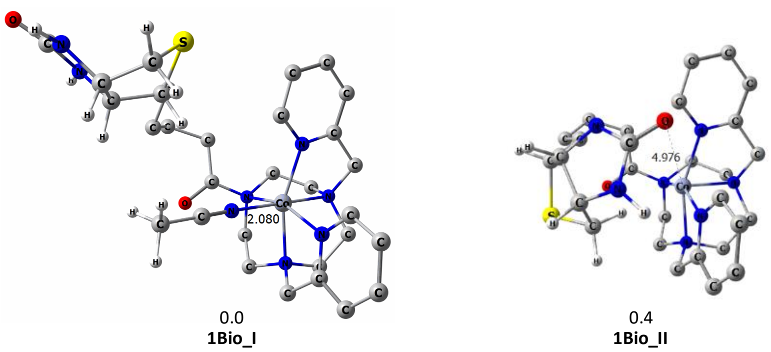
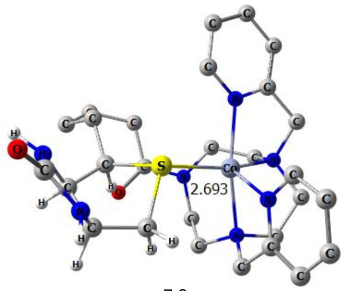
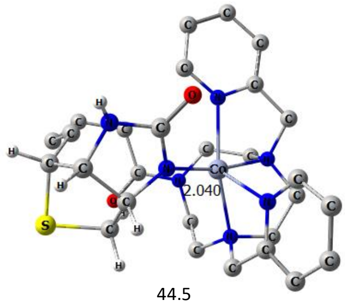


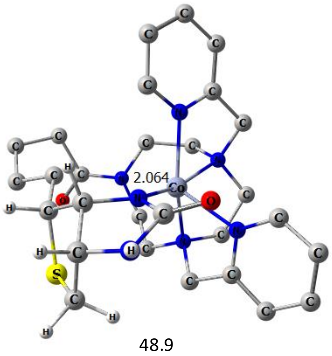
Figure S78. Optimized geometries of the lowest in energy **1Bio** complexes with and without acetonitrile bonded to the metal center. Selected hydrogen atoms are omitted for clarity. Relevant bond distances are in Å. Free energy values in $kcal \cdot mol^{-1}$ and referenced to **1Bio_I**.



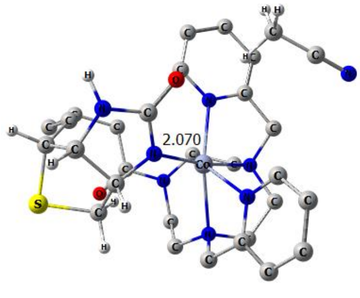
7.9
1Bio_III



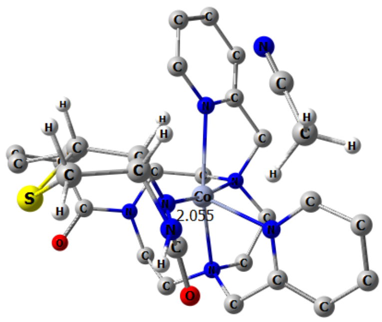
44.5
1Bio_IV



48.9
1Bio_V



51.0
1Bio_VI



51.2
1Bio_VII

Figure S79. Optimized geometries of the lowest in energy **1Bio** complexes with the biotin bonded to the metal center. We have noticed that the biotin oxygen cannot bond to the metal center due to geometrical constrains. Selected hydrogen atoms are omitted for clarity. Relevant bond distances are in Å. Free energy values in kcal·mol^{-1} and referenced to **1Bio_I**.

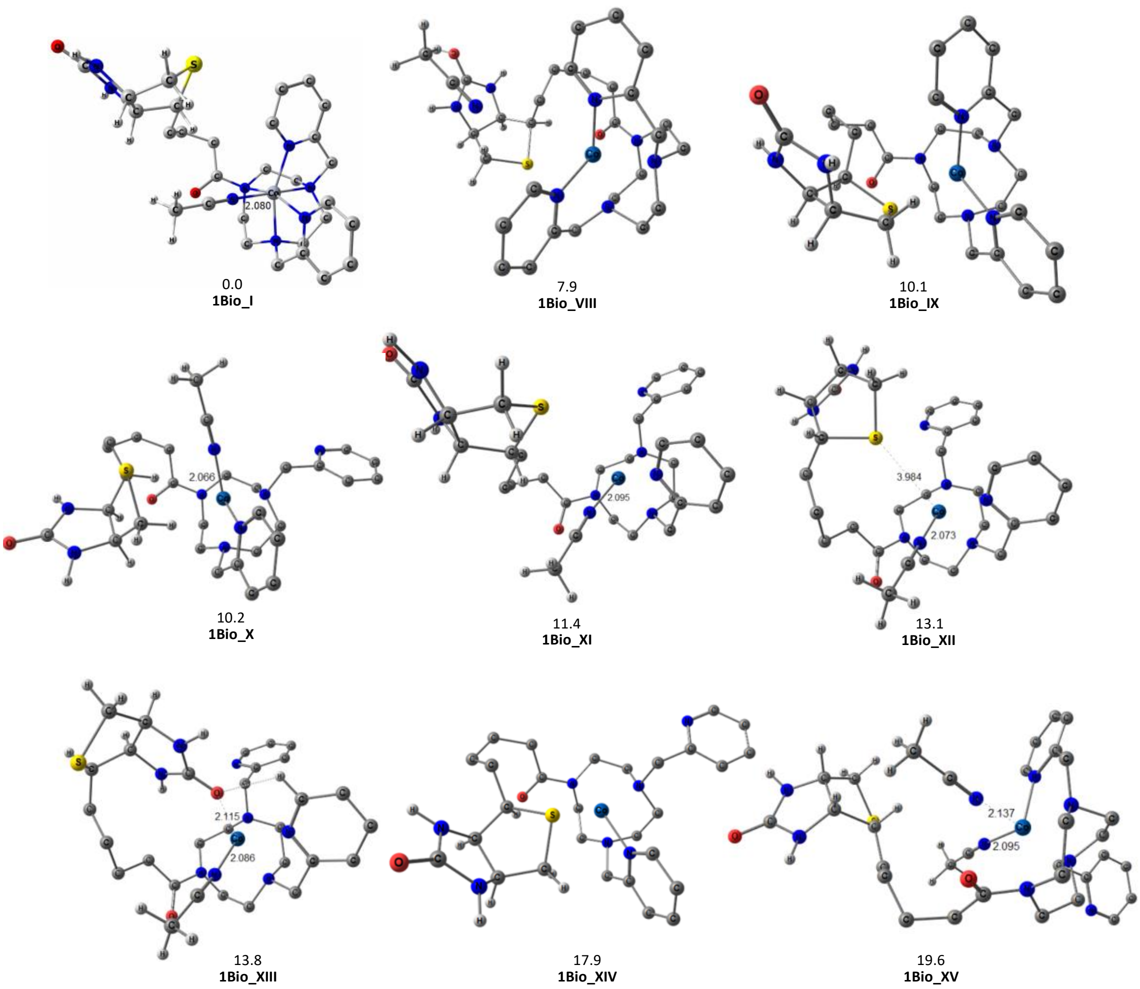


Figure S80. Optimized geometries of the lowest in energy possible isomers of **1Bio** complexes with a decoordinated pyridine and with and without the biotin bonded to the metal center. Selected hydrogen atoms are omitted for clarity. Relevant bond distances are in Å. Free energy values in kcal·mol^{-1} and referenced to **1Bio_I**.

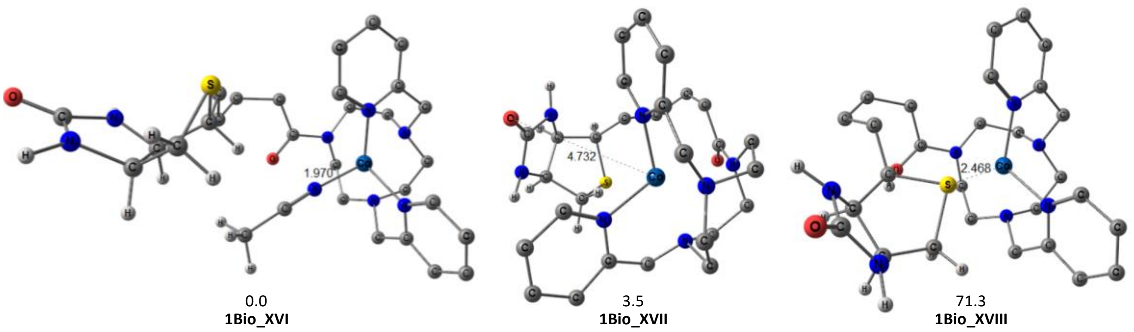


Figure S81. Optimized geometries of the lowest in energy **1Bio** complexes for Co (I) with biotin bonded and unbonded to the metal center. We have noticed that the biotin oxygen cannot bond to the metal center due to geometrical constrains. Selected hydrogen atoms are omitted for clarity. Relevant bond distances are in Å. Free energy values in kcal·mol^{-1} and referenced to **1Bio_XVI**.

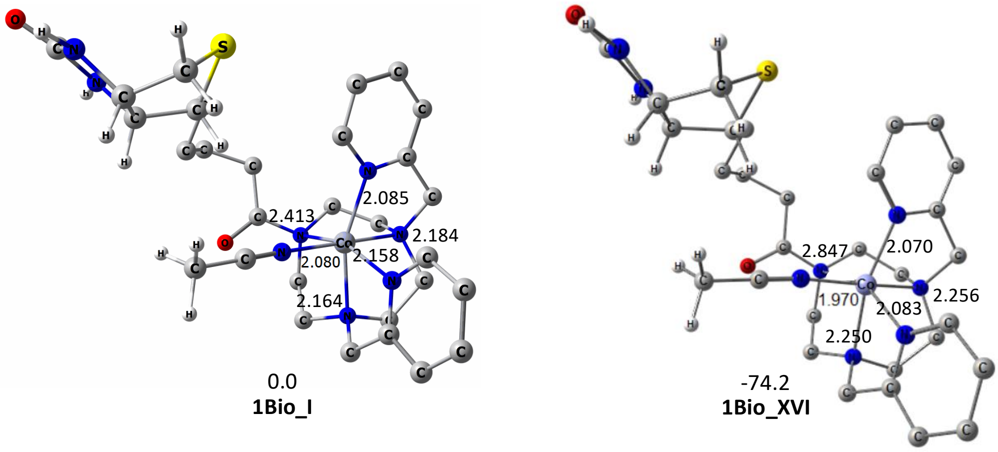


Figure S82. Optimized geometries of the lowest in energy **1**$^{\mathbf{Bio}}$ complexes for the Co (II) (**1Bio_I**) and the Co (I) (**1Bio_XVI**) oxidation state with acetonitrile bounded to the metal center. Relevant bond distances with the nitrogen atoms of the first coordination sphere are in Å. Free energy values in kcal·mol^{-1} and referenced to **1Bio_I**.

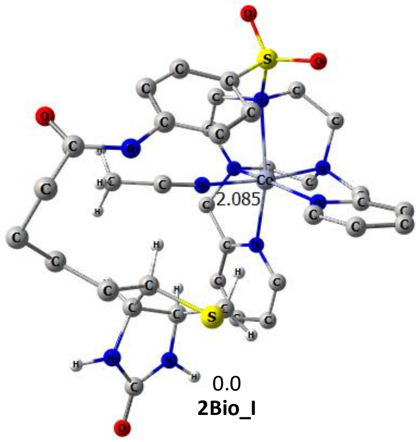


Figure S83. Optimized geometries of the lowest in energy **2Bio** complex. Selected hydrogen atoms are omitted for clarity. Relevant bond distances are in Å. Free energy values in kcal·mol^{-1} and referenced to **2Bio_I**.

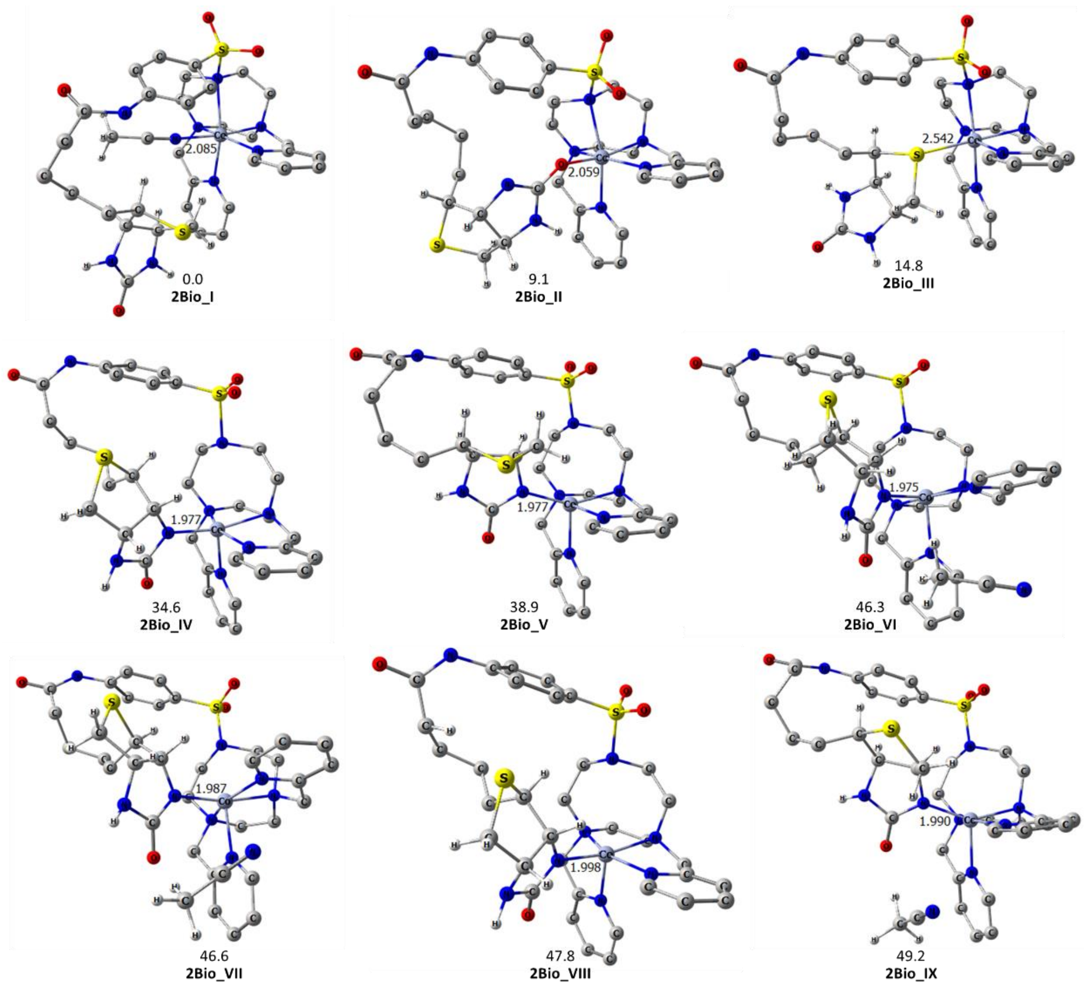


Figure S84. Optimized geometries of the lowest in energy **2Bio** complexes with and without the biotin bonded to the metal center. Selected hydrogen atoms are omitted for clarity. Relevant bond distances are in Å. Free energy values in kcal·mol^{-1} and referenced to **2Bio_I**.

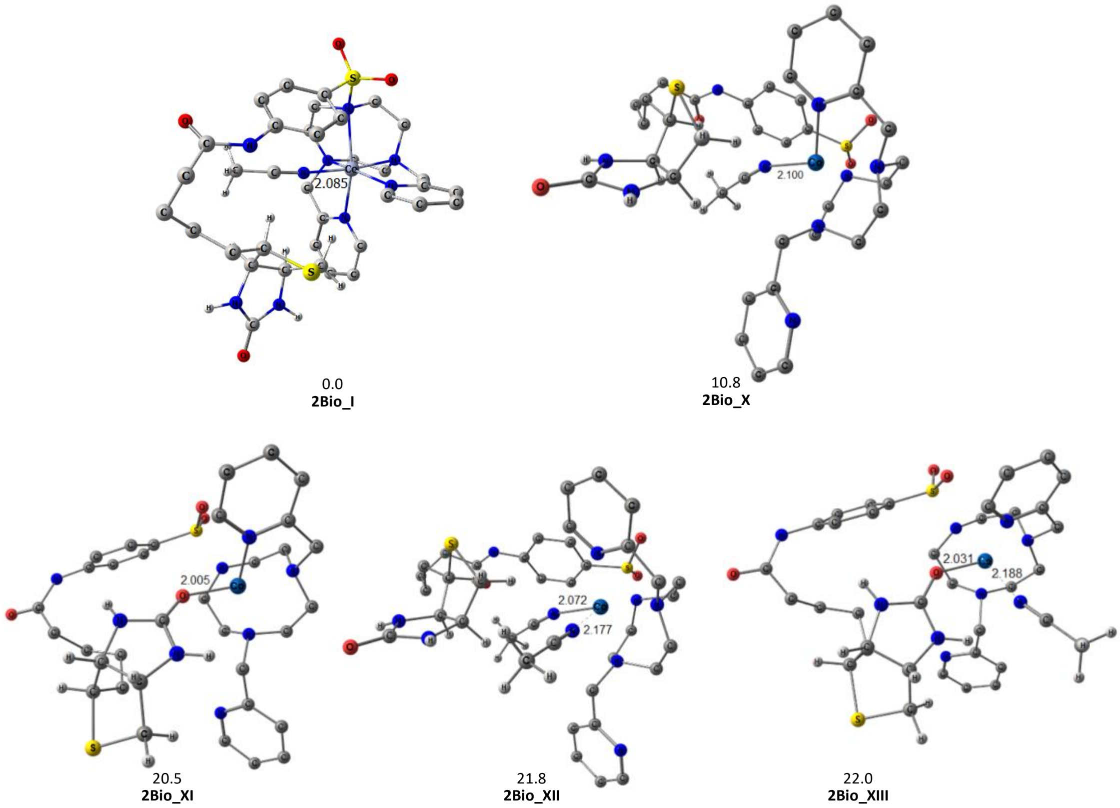


Figure S85. Optimized geometries of the lowest in energy possible isomers of **2Bio** complexes with a decoordinated pyridine and with and without the biotin bonded to the metal center. Selected hydrogen atoms are omitted for clarity. Relevant bond distances are in Å. Free energy values in kcal·mol^{-1} and referenced to **2Bio_I**.

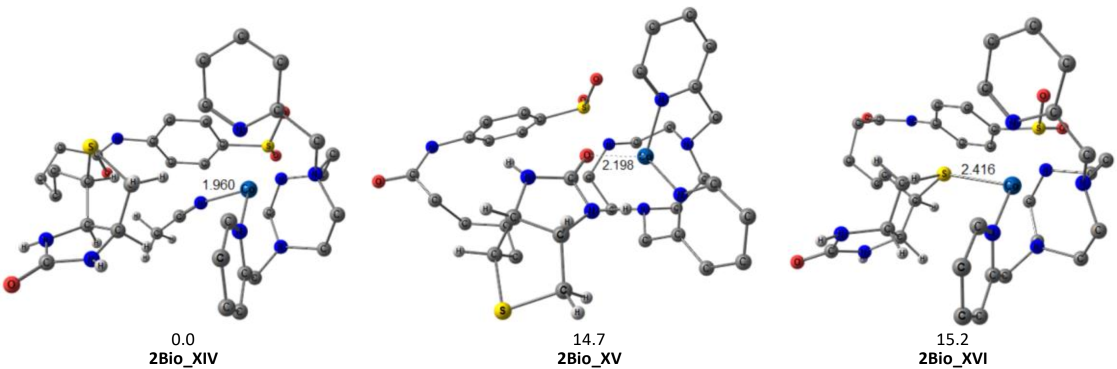


Figure S86. Optimized geometries of the lowest in energy **2Bio** complexes complexes for Co (I) with biotin bonded and unbonded to the metal center. Selected hydrogen atoms are omitted for clarity. Relevant bond distances are in Å. Free energy values in kcal·mol^{-1} and referenced to **2Bio_XIV**.

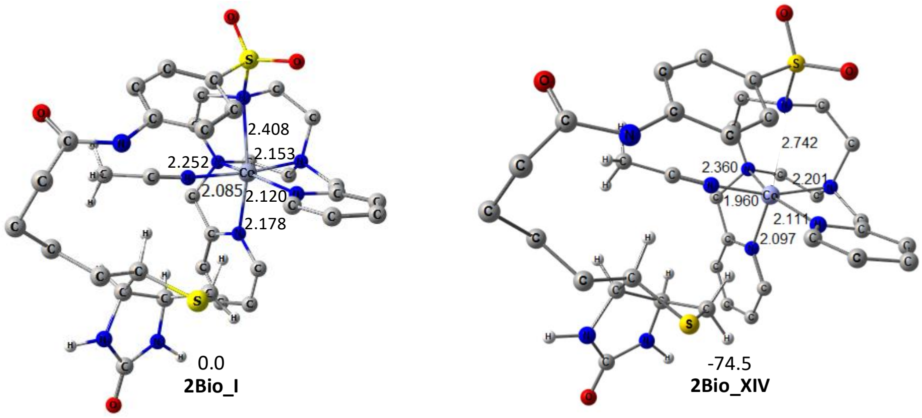


Figure S87. Optimized geometries of the lowest in energy **2^{Bio}** complexes for the Co (II) (**2Bio_I**) and the Co (I) (**2Bio_XIV**) oxidation state with acetonitrile bounded to the metal center. Relevant bond distances with the nitrogen atoms of the first coordination sphere are in Å. Free energy values in kcal·mol^{-1} and referenced to **2Bio_I**.

2.2.3. Cartesian coordinates

In parenthesis are the Gibbs energies (G) in hartrees and the spin state of each cobalt intermediate.

1Bio_I
(G = -3537.31306) (Quadruplet)

6	-0.496778000	-2.778705000	-0.731561000
8	-0.146601000	-2.837652000	-1.905103000
6	0.470787000	-3.018623000	0.414562000
6	1.903843000	-3.290938000	-0.060202000
6	2.654296000	-2.036416000	-0.535804000
6	3.210743000	-1.198930000	0.628124000
6	3.646470000	0.197844000	0.190146000
1	0.100659000	-3.878054000	0.986513000
1	0.433123000	-2.162042000	1.097542000
1	1.869715000	-4.030951000	-0.866124000
1	2.456418000	-3.751501000	0.768285000
1	1.979821000	-1.425901000	-1.144077000
1	3.476814000	-2.335714000	-1.196350000
1	4.057309000	-1.724036000	1.086526000
1	2.445502000	-1.095566000	1.404649000
16	4.293439000	1.228222000	1.585678000
6	4.916554000	2.442347000	0.355081000
6	5.493661000	1.622810000	-0.814216000
6	4.748669000	0.241229000	-0.891986000
7	5.827421000	-0.716475000	-0.673528000
6	7.069019000	-0.132047000	-0.654689000
7	6.880513000	1.225379000	-0.602677000
8	8.156436000	-0.722483000	-0.652435000
1	5.742720000	-1.684880000	-0.948910000
1	7.652729000	1.848612000	-0.793282000
1	2.777756000	0.731395000	-0.212324000
1	5.672324000	3.086834000	0.809814000
1	4.084261000	3.062513000	0.006628000
1	4.288485000	0.085389000	-1.872332000
1	5.391778000	2.191041000	-1.744397000
7	-3.438959000	-0.320790000	-1.653441000
6	-4.787735000	-0.513486000	-1.027498000
6	-4.800813000	-0.144282000	0.458868000
7	-3.607899000	-0.686891000	1.166391000
6	-3.666325000	-2.174540000	1.301064000
6	-2.355027000	-2.863919000	0.928370000
7	-1.847640000	-2.481740000	-0.422132000
6	-3.006871000	-1.507772000	-2.440311000
6	-2.780575000	-2.737438000	-1.560324000
6	-3.398250000	-0.006929000	2.468882000
6	-1.933688000	0.125245000	2.810929000
7	-1.102333000	0.291101000	1.762041000
6	-1.465526000	0.174051000	4.123379000
6	-0.109500000	0.415916000	4.348350000
6	0.741741000	0.604655000	3.256716000
6	0.203635000	0.530629000	1.976743000
6	-3.376562000	0.923428000	-2.455759000
6	-3.254247000	2.136105000	-1.560080000
6	-3.763838000	3.385488000	-1.913917000
6	-3.559153000	4.465893000	-1.054607000
6	-2.857469000	4.265249000	0.136659000
6	-2.387531000	2.986422000	0.422665000
7	-2.580378000	1.948754000	-0.407502000
27	-1.939128000	-0.091133000	-0.109678000
1	-5.089619000	-1.551287000	-1.165993000
1	-5.531247000	0.098845000	-1.546657000
1	-5.730520000	-0.506872000	0.916256000
1	-4.771577000	0.939482000	0.568642000
1	-4.489442000	-2.549185000	0.693030000
1	-3.898823000	-2.449423000	2.335140000
1	-2.500587000	-3.949563000	0.982055000
1	-1.599961000	-2.583040000	1.659407000
1	-2.066209000	-1.246900000	-2.928630000
1	-3.746105000	-1.752323000	-3.215011000
1	-2.368436000	-3.527560000	-2.191536000

1	-3.716582000	-3.112345000	-1.151661000
1	-3.945782000	-0.499849000	3.278937000
1	-3.791374000	1.011318000	2.380482000
1	-2.156516000	0.027096000	4.946940000
1	0.277581000	0.456328000	5.361912000
1	1.800160000	0.800382000	3.385248000
1	0.814576000	0.658207000	1.090421000
1	-4.243223000	1.016898000	-3.120193000
1	-2.481661000	0.873518000	-3.083873000
1	-4.312589000	3.500889000	-2.843015000
1	-3.947717000	5.447734000	-1.307609000
1	-2.680909000	5.076680000	0.834414000
1	-1.844351000	2.771273000	1.336597000
7	-0.346173000	0.353170000	-1.371648000
6	0.515659000	0.659440000	-2.079096000
6	1.601641000	1.025179000	-2.967163000
1	2.228179000	0.147828000	-3.150629000
1	1.190345000	1.387304000	-3.914239000
1	2.202899000	1.812562000	-2.504334000

1Bio_II

(G = -3404.56137) (Quadruplet)

6	-1.218407000	2.973743000	0.615033000
8	-0.785639000	3.530265000	1.618618000
6	-0.725647000	3.320703000	-0.775525000
6	0.513994000	4.229558000	-0.792528000
6	1.747942000	3.719313000	-0.028099000
6	2.197965000	2.311926000	-0.425908000
6	3.451207000	1.853981000	0.331977000
1	-1.541527000	3.824164000	-1.309401000
1	-0.541651000	2.389729000	-1.319946000
1	0.239096000	5.212857000	-0.393755000
1	0.777679000	4.382289000	-1.847022000
1	1.540701000	3.742208000	1.044520000
1	2.575290000	4.418704000	-0.210606000
1	2.415856000	2.299557000	-1.501319000
1	1.389806000	1.587407000	-0.260582000
16	3.085340000	1.514153000	2.129834000
6	2.717541000	-0.233173000	1.727360000
6	3.863997000	-0.639465000	0.794883000
6	4.108607000	0.539954000	-0.202580000
7	3.524508000	0.013856000	-1.433221000
6	3.292646000	-1.339766000	-1.375801000
7	3.569464000	-1.757975000	-0.093708000
8	2.896380000	-2.049107000	-2.306847000
1	3.722266000	0.433479000	-2.331659000
1	4.191923000	2.658612000	0.316845000
1	1.755560000	-0.298205000	1.212028000
1	2.679977000	-0.829809000	2.641031000
1	5.181501000	0.711653000	-0.333572000
1	4.759365000	-0.838831000	1.388565000
7	-1.670308000	-0.540879000	2.187152000
6	-2.984623000	-1.258104000	2.105128000
6	-3.300027000	-1.744141000	0.688013000
7	-2.984910000	-0.715259000	-0.345440000
6	-3.923156000	0.450812000	-0.300347000
6	-3.211501000	1.803719000	-0.321468000
7	-2.174799000	1.935361000	0.742587000
6	-1.783997000	0.763435000	2.896038000
6	-2.661033000	1.753059000	2.134782000
6	-2.933683000	-1.335486000	-1.694916000
6	-1.901554000	-0.690335000	-2.584409000
7	-0.782602000	-0.262342000	-1.964644000
6	-2.033635000	-0.639595000	-3.971495000
6	-0.971468000	-0.151784000	-4.734420000
6	0.195339000	0.262629000	-4.088808000
6	0.247740000	0.193114000	-2.700418000
6	-0.614847000	-1.386159000	2.790928000
6	-0.127165000	-2.414651000	1.800645000
6	0.296239000	-3.685785000	2.182397000
6	0.767393000	-4.563634000	1.204521000
6	0.796554000	-4.144535000	-0.126685000
6	0.358628000	-2.858753000	-0.430753000
7	-0.089702000	-2.011875000	0.511729000
27	-0.967476000	-0.114734000	0.160543000
1	-3.769922000	-0.595934000	2.467789000
1	-2.978600000	-2.125273000	2.772686000
1	-4.353748000	-2.046531000	0.631560000
1	-2.686947000	-2.616444000	0.459668000
1	-4.554061000	0.357015000	0.583478000
1	-4.595659000	0.420833000	-1.163175000
1	-3.962262000	2.595967000	-0.210886000
1	-2.722070000	1.928390000	-1.285561000
1	-0.775027000	1.175052000	2.973831000
1	-2.182899000	0.620340000	3.909411000
1	-2.641519000	2.709222000	2.660950000
1	-3.697920000	1.427270000	2.101700000
1	-3.918768000	-1.339217000	-2.172027000
1	-2.626144000	-2.378780000	-1.571279000
1	-2.951395000	-0.982819000	-4.437488000
1	-1.052210000	-0.101667000	-5.816040000
1	1.050819000	0.634270000	-4.642338000
1	1.129163000	0.495364000	-2.151168000
1	-0.960217000	-1.866500000	3.713600000
1	0.227423000	-0.735773000	3.046328000
1	0.247031000	-3.977497000	3.226314000
1	1.099119000	-5.560745000	1.477533000
1	1.155894000	-4.792225000	-0.918641000
1	0.377580000	-2.480969000	-1.444838000
1	3.135115000	-2.604736000	0.250867000

1Bio_III

(G = -3404.54934) (Quadruplet)

6	-0.090085000	-2.629752000	-1.813891000
8	0.758818000	-2.416203000	-2.690510000
6	0.156958000	-3.622281000	-0.690356000
6	1.544177000	-4.282731000	-0.674986000
6	2.777772000	-3.357169000	-0.564743000
6	2.595619000	-2.151037000	0.391210000
6	2.556055000	-0.827638000	-0.381494000
1	-0.601496000	-4.412234000	-0.761996000
1	-0.037257000	-3.121252000	0.264400000
1	1.656708000	-4.908633000	-1.567641000
1	1.538709000	-4.966377000	0.183541000
1	3.033805000	-2.988639000	-1.562131000
1	3.626012000	-3.967131000	-0.234000000

1	3.391027000	-2.108476000	1.140516000
1	1.670173000	-2.275588000	0.954621000
16	1.595836000	0.532306000	0.445938000
6	2.291587000	1.707984000	-0.779812000
6	3.774740000	1.343124000	-0.912732000
6	3.941106000	-0.203500000	-0.689260000
7	4.886186000	-0.263419000	0.419544000
6	5.367268000	0.970178000	0.784009000
7	4.604319000	1.915339000	0.141017000
8	6.293636000	1.190208000	1.571021000
1	5.462802000	-1.077442000	0.581313000
1	4.955298000	2.861295000	0.072699000
1	2.048181000	-0.978819000	-1.336544000
1	2.136366000	2.737500000	-0.453541000
1	1.796785000	1.543617000	-1.738187000
1	4.353017000	-0.699651000	-1.572931000
1	4.130236000	1.652028000	-1.900773000
7	-1.582444000	1.146563000	-1.907743000
6	-3.073533000	1.301507000	-2.002687000
6	-3.757595000	1.032779000	-0.665166000
7	-3.179210000	-0.171996000	-0.015008000
6	-3.548548000	-1.426796000	-0.749414000
6	-2.418026000	-2.427588000	-0.979252000
7	-1.299468000	-1.964949000	-1.831223000
6	-1.031075000	0.268815000	-2.984609000
6	-1.579047000	-1.161932000	-3.033360000
6	-3.573222000	-0.244015000	1.414548000
6	-2.556321000	-1.002705000	2.229738000
7	-1.259207000	-0.765586000	1.924269000
6	-2.921926000	-1.835419000	3.285571000
6	-1.924544000	-2.426446000	4.061892000
6	-0.587974000	-2.156989000	3.763587000
6	-0.302362000	-1.321971000	2.688546000
6	-0.935578000	2.480343000	-1.973553000
6	-0.989479000	3.185431000	-0.640963000
6	-0.984390000	4.574312000	-0.520260000
6	-0.956828000	5.142323000	0.754056000
6	-0.942125000	4.308231000	1.875575000
6	-0.957205000	2.932112000	1.677484000
7	-0.978535000	2.388775000	0.446427000
27	-1.069667000	0.337574000	0.113523000
1	-3.456128000	0.636597000	-2.775994000
1	-3.323980000	2.316910000	-2.321359000
1	-4.839926000	0.924138000	-0.812949000
1	-3.589448000	1.873625000	0.009752000
1	-4.020009000	-1.151823000	-1.691645000
1	-4.313838000	-1.958288000	-0.174411000
1	-2.876694000	-3.321045000	-1.424280000
1	-2.013112000	-2.712020000	-0.010261000
1	0.048182000	0.217876000	-2.823424000
1	-1.213897000	0.732114000	-3.964881000
1	-1.095789000	-1.639931000	-3.889354000
1	-2.649160000	-1.186113000	-3.232076000
1	-4.574034000	-0.671418000	1.536369000
1	-3.597671000	0.780063000	1.801735000
1	-3.973004000	-2.011455000	3.488710000
1	-2.186769000	-3.082114000	4.886463000
1	0.222873000	-2.583520000	4.343672000
1	0.721468000	-1.082966000	2.433444000
1	-1.382050000	3.102461000	-2.757565000
1	0.113386000	2.342046000	-2.240376000
1	-1.001293000	5.190984000	-1.412732000
1	-0.951085000	6.221615000	0.871082000
1	-0.923311000	4.710584000	2.882320000
1	-0.951094000	2.229943000	2.505123000

1Bio_IV

(G = −3404.076347) (Quadruplet)

6	2.093179000	-1.194503000	-2.008067000
8	2.691093000	-0.330630000	-2.664949000
6	2.797711000	-2.009371000	-0.930095000
6	4.248824000	-1.609308000	-0.604083000
6	4.504890000	-0.138280000	-0.220964000
6	3.556701000	0.424036000	0.844190000
6	3.587410000	1.958594000	1.029521000
1	2.790520000	-3.061645000	-1.242679000
1	2.189067000	-1.971423000	-0.024260000
1	4.887943000	-1.852634000	-1.461773000
1	4.568474000	-2.268190000	0.214516000
1	4.401794000	0.464589000	-1.123598000
1	5.546560000	-0.039797000	0.115464000
1	3.762632000	-0.030406000	1.821269000
1	2.532901000	0.140365000	0.592707000
16	3.518903000	2.895076000	-0.570068000
6	1.753142000	2.390448000	-0.746315000
6	1.148989000	2.451408000	0.665606000
6	2.306051000	2.511012000	1.717741000
7	1.764812000	1.713270000	2.808250000
6	0.546902000	1.127470000	2.420662000
7	0.333086000	1.298627000	1.091078000
8	-0.169841000	0.500626000	3.228524000
1	1.838470000	2.051167000	3.759429000
1	4.496412000	2.275181000	1.551599000
1	1.718134000	1.379409000	-1.150522000
1	1.269027000	3.070526000	-1.449013000
1	2.498717000	3.537038000	2.040577000
1	0.543141000	3.366739000	0.739119000
7	-1.511487000	0.664501000	-2.003020000
6	-2.717764000	-0.093561000	-2.470589000
6	-3.218609000	-1.113193000	-1.442905000
7	-2.082110000	-1.784018000	-0.779299000
6	-1.396499000	-2.732629000	-1.711922000
6	0.133070000	-2.696843000	-1.756036000
7	0.753095000	-1.440475000	-2.229387000
6	-0.440212000	0.645860000	-3.034437000
6	0.138088000	-0.736493000	-3.365425000
6	-2.511573000	-2.469494000	0.456893000
6	-1.308372000	-2.774406000	1.314605000
7	-0.361457000	-1.816189000	1.334270000
6	-1.175579000	-3.961736000	2.034682000
6	-0.020790000	-4.165614000	2.791741000
6	0.963482000	-3.175717000	2.802158000
6	0.747812000	-2.014755000	2.063853000
6	-1.887488000	2.063055000	-1.683107000
6	-2.792085000	2.120485000	-0.471290000
6	-3.772014000	3.101358000	-0.310259000
6	-4.529768000	3.113721000	0.861490000

6	-4.291142000	2.144137000	1.839557000
6	-3.296381000	1.198985000	1.606305000
7	-2.570853000	1.189507000	0.476375000
27	-0.860209000	-0.029697000	0.104143000
1	-2.474406000	-0.596857000	-3.406258000
1	-3.531584000	0.600831000	-2.703643000
1	-3.878128000	-1.838113000	-1.941690000
1	-3.801026000	-0.613780000	-0.669737000
1	-1.800406000	-2.588829000	-2.713931000
1	-1.662867000	-3.759012000	-1.431698000
1	0.434280000	-3.520042000	-2.420200000
1	0.519678000	-2.919812000	-0.766349000
1	0.365975000	1.283885000	-2.679418000
1	-0.821228000	1.077267000	-3.973438000
1	0.900872000	-0.573578000	-4.131425000
1	-0.614426000	-1.387012000	-3.808608000
1	-3.080027000	-3.384997000	0.246208000
1	-3.165404000	-1.785038000	1.008591000
1	-1.957660000	-4.712467000	1.984626000
1	0.113429000	-5.085864000	3.352533000
1	1.883560000	-3.295184000	3.364278000
1	1.483883000	-1.222903000	2.043178000
1	-2.367595000	2.556430000	-2.538713000
1	-0.971820000	2.615198000	-1.450624000
1	-3.934803000	3.834413000	-1.093746000
1	-5.299331000	3.865774000	1.007131000
1	-4.860406000	2.117576000	2.762489000
1	-3.054648000	0.427284000	2.329324000

1Bio_V
(G = −3404.069320) (Quadruplet)

6	3.774335000	-0.374494000	-1.461525000
8	4.289373000	0.365673000	-2.317738000
6	4.452906000	-0.521566000	-0.107213000
6	4.889570000	0.853586000	0.435188000
6	3.793579000	1.928970000	0.357617000
6	2.421075000	1.490167000	0.890686000
6	1.471464000	2.665745000	1.074412000
1	5.328047000	-1.170458000	-0.235898000
1	3.806765000	-1.003127000	0.625296000
1	5.769234000	1.207194000	-0.112286000
1	5.195183000	0.713688000	1.479769000
1	3.686179000	2.254297000	-0.683260000
1	4.127569000	2.806954000	0.926207000
1	2.543721000	1.019506000	1.875975000
1	1.958608000	0.740957000	0.238383000
16	0.965784000	3.517716000	-0.503553000
6	-0.591816000	4.186028000	0.250473000
6	-0.705333000	3.644070000	1.705721000
6	0.181567000	2.390959000	1.819749000
7	-0.729826000	1.303083000	1.396453000
6	-1.960535000	1.690790000	1.856700000
7	-2.027245000	3.092830000	1.985876000
8	-2.934659000	0.971775000	2.145224000
1	1.994552000	3.422654000	1.672842000
1	-1.439122000	3.838111000	-0.344674000
1	-0.572712000	5.278270000	0.226722000
1	0.464212000	2.226908000	2.874822000
1	-0.430239000	4.417724000	2.425836000
7	-0.501915000	-0.149499000	-2.189495000
6	-1.026480000	-1.372847000	-2.882577000
6	-1.328332000	-2.531570000	-1.920676000
7	-0.404432000	-2.522464000	-0.772281000
6	0.970426000	-2.975946000	-1.162008000
6	2.136105000	-2.076383000	-0.735496000
7	2.583265000	-1.015638000	-1.676676000
6	0.760212000	0.317423000	-2.824070000
6	1.890172000	-0.713250000	-2.928851000
6	-0.927970000	-3.344369000	0.336840000
6	-0.243059000	-2.966966000	1.626010000
7	-0.019630000	-1.647837000	1.782420000
6	0.117200000	-3.891742000	2.605398000
6	0.720457000	-3.433079000	3.778246000
6	0.945084000	-2.063589000	3.935841000
6	0.555865000	-1.203859000	2.911786000
6	-1.511299000	0.940677000	-2.262510000
6	-2.787299000	0.491696000	-1.590489000
6	-4.052680000	0.773074000	-2.107308000
6	-5.175413000	0.256465000	-1.458704000
6	-4.998816000	-0.528216000	-0.317069000
6	-3.704720000	-0.740168000	0.150294000
7	-2.625319000	-0.242298000	-0.472152000
27	-0.564418000	-0.337214000	0.154239000
1	-0.305225000	-1.695604000	-3.630731000
1	-1.938802000	-1.131479000	-3.436239000
1	-1.273578000	-3.482462000	-2.470578000
1	-2.339317000	-2.438976000	-1.529199000
1	0.995554000	-3.177981000	-2.233555000
1	1.151889000	-3.942265000	-0.680666000
1	2.985818000	-2.743418000	-0.566399000
1	1.880579000	-1.618992000	0.221293000
1	1.109902000	1.181368000	-2.254301000
1	0.539345000	0.654363000	-3.849896000
1	2.633742000	-0.279188000	-3.597363000
1	1.562297000	-1.637107000	-3.402500000
1	-0.825083000	-4.420346000	0.142228000
1	-1.994623000	-3.123027000	0.445104000
1	-0.068665000	-4.948360000	2.442089000
1	1.015689000	-4.133972000	4.553253000
1	1.413730000	-1.664375000	4.828950000
1	0.699138000	-0.132098000	2.974397000
1	-1.713688000	1.226887000	-3.303602000
1	-1.098894000	1.812819000	-1.741452000
1	-4.146342000	1.363929000	-3.012613000
1	-6.170770000	0.449900000	-1.847685000
1	-5.842521000	-0.963587000	0.207785000
1	-3.511748000	-1.321688000	1.042405000
1	-2.563264000	3.457852000	2.764248000

1Bio_VI
(G = −3536.822856) (Quadruplet)

6	-2.610501000	0.582832000	-2.091632000
8	-3.532251000	-0.244908000	-2.092352000
6	-2.792061000	1.978918000	-1.508167000
6	-4.123421000	2.262050000	-0.788530000
6	-4.536529000	1.296299000	0.340699000

6	-3.430519000	0.951194000	1.346062000
6	-3.737265000	-0.257913000	2.257203000
1	-2.680836000	2.702606000	-2.326426000
1	-1.959706000	2.177896000	-0.831259000
1	-4.933571000	2.281600000	-1.527749000
1	-4.042237000	3.284310000	-0.395170000
1	-4.868601000	0.366989000	-0.123711000
1	-5.401429000	1.722746000	0.867611000
1	-3.211412000	1.811312000	1.993103000
1	-2.507306000	0.739695000	0.804881000
16	-4.261092000	-1.764690000	1.307371000
6	-2.518415000	-1.976147000	0.741479000
6	-1.614791000	-1.557131000	1.915781000
6	-2.495575000	-0.843014000	2.989315000
7	-1.522881000	0.066762000	3.562088000
6	-0.460007000	0.261834000	2.663038000
7	-0.552425000	-0.577553000	1.605562000
8	0.426304000	1.116245000	2.892972000
1	-1.817867000	0.874075000	4.097104000
1	-4.541563000	-0.021428000	2.962008000
1	-2.352002000	-1.334688000	-0.123160000
1	-2.381402000	-3.017114000	0.445398000
1	-2.853455000	-1.550909000	3.741597000
1	-1.160675000	-2.457475000	2.353805000
7	0.403527000	-2.095728000	-1.733743000
6	1.545044000	-2.045194000	-2.697986000
6	2.522053000	-0.902679000	-2.404956000
7	1.786554000	0.312285000	-2.003510000
6	1.049988000	0.894174000	-3.171112000
6	-0.406981000	1.321227000	-2.967590000
7	-1.377774000	0.261194000	-2.622756000
6	-0.891212000	-2.222638000	-2.447078000
6	-1.282023000	-1.026606000	-3.326408000
6	2.693247000	1.309951000	-1.403234000
6	1.873261000	2.354900000	-0.692729000
7	0.798866000	1.879632000	-0.030777000
6	2.186542000	3.712886000	-0.720010000
6	1.354643000	4.610530000	-0.049261000
6	0.234824000	4.118734000	0.622565000
6	-0.000789000	2.746105000	0.611719000
6	0.587462000	-3.225316000	-0.796402000
6	1.788142000	-3.009808000	0.099733000
6	2.590688000	-4.063359000	0.540959000
6	3.654536000	-3.792525000	1.402469000
6	3.892686000	-2.473590000	1.798169000
6	3.052160000	-1.476477000	1.314018000
7	2.030430000	-1.740521000	0.482531000
27	0.583423000	-0.314257000	-0.104674000
1	1.147215000	-1.941392000	-3.707575000
1	2.095025000	-2.992769000	-2.686225000
1	3.143498000	-0.720421000	-3.294239000
1	3.188269000	-1.170125000	-1.586213000
1	1.119795000	0.198225000	-4.006167000
1	1.575816000	1.798067000	-3.501654000
1	-0.711432000	1.791110000	-3.914461000
1	-0.444478000	2.087904000	-2.200873000
1	-1.666156000	-2.371496000	-1.698823000
1	-0.879020000	-3.115251000	-3.093489000
1	-2.260132000	-1.266491000	-3.751786000
1	-0.597444000	-0.910972000	-4.166013000
1	3.352941000	1.774568000	-2.148257000
1	3.322313000	0.798557000	-0.667828000
1	3.059899000	4.051419000	-1.267673000
1	1.571722000	5.674449000	-0.060395000
1	-0.449352000	4.778250000	1.145670000
1	-0.852420000	2.322920000	1.123454000
1	0.687890000	-4.180910000	-1.330073000
1	-0.300778000	-3.291845000	-0.162522000
1	2.381734000	-5.074594000	0.207412000
1	4.291801000	-4.597878000	1.755096000
1	4.711189000	-2.217996000	2.462354000
1	3.186618000	-0.435090000	1.583912000
7	5.279392000	1.661932000	1.154015000
6	4.382242000	2.061722000	1.776641000
6	3.246054000	2.542803000	2.546173000
1	2.380501000	1.884096000	2.405168000
1	3.506244000	2.566444000	3.608970000
1	2.982704000	3.552289000	2.218058000

1Bio_VII

(G = −3536.822633) (Quadruplet)

6	-3.469263000	1.328924000	-1.132656000
8	-3.753792000	1.013097000	-2.299277000
6	-4.344195000	0.857871000	0.019662000
6	-5.023245000	-0.498203000	-0.216011000
6	-4.056058000	-1.654692000	-0.558482000
6	-2.652539000	-1.494251000	0.045817000
6	-1.783707000	-2.748633000	0.035215000
1	-5.106550000	1.637584000	0.159110000
1	-3.790184000	0.818442000	0.955824000
1	-5.774517000	-0.410670000	-1.007524000
1	-5.565289000	-0.738358000	0.707014000
1	-3.952591000	-1.726037000	-1.647044000
1	-4.501920000	-2.598392000	-0.222058000
1	-2.736055000	-1.174217000	1.089929000
1	-2.118357000	-0.699872000	-0.482434000
16	-1.958493000	-3.817510000	-1.478490000
6	-0.547011000	-4.807212000	-0.850909000
6	0.480890000	-3.795143000	-0.314396000
6	-0.253405000	-2.491938000	0.164977000
7	0.248661000	-1.395741000	-0.682711000
6	1.031297000	-1.946405000	-1.653676000
7	1.353132000	-3.270289000	-1.349389000
8	1.481544000	-1.402276000	-2.681113000
1	-2.081771000	-3.396245000	0.870408000
1	-0.133887000	-5.428135000	-1.650606000
1	-0.894915000	-5.462394000	-0.044998000
1	-0.013245000	-2.294775000	1.209496000
1	1.059846000	-4.260981000	0.490509000
7	0.608772000	2.158140000	-1.912573000
6	1.059142000	3.497103000	-1.448017000
6	1.407756000	3.484106000	0.035276000
7	0.420275000	2.692333000	0.806884000
6	-0.903173000	3.407555000	0.849053000
6	-2.151154000	2.580911000	0.544955000
7	-2.404532000	2.153694000	-0.856778000
6	-0.638844000	2.217510000	-2.705914000

6	-1.836232000	2.874965000	-2.006208000
6	0.961996000	2.503590000	2.173881000
6	0.159614000	1.505773000	2.960772000
7	-0.143381000	0.354125000	2.325123000
6	-0.224164000	1.762998000	4.278684000
6	-0.944186000	0.796135000	4.980174000
6	-1.259171000	-0.395909000	4.330370000
6	-0.840988000	-0.567369000	3.011661000
6	1.694810000	1.508159000	-2.665947000
6	2.809159000	1.091151000	-1.736286000
6	4.155925000	1.140789000	-2.100349000
6	5.123630000	0.698359000	-1.197637000
6	4.721662000	0.222088000	0.053009000
6	3.361847000	0.210299000	0.347281000
7	2.432358000	0.635168000	-0.523821000
27	0.370045000	0.568046000	-0.089170000
1	0.287436000	4.237632000	-1.649871000
1	1.939559000	3.821149000	-2.014248000
1	1.460355000	4.514560000	0.414700000
1	2.384387000	3.027320000	0.191250000
1	-0.856640000	4.293759000	0.215844000
1	-1.055627000	3.784763000	1.866075000
1	-3.001404000	3.179619000	0.895390000
1	-2.098700000	1.683926000	1.160839000
1	-0.903776000	1.190255000	-2.969756000
1	-0.467813000	2.776787000	-3.641098000
1	-2.620053000	2.947941000	-2.763133000
1	-1.613254000	3.896479000	-1.700053000
1	1.018519000	3.459469000	2.710804000
1	1.980958000	2.116715000	2.068781000
1	0.036117000	2.712010000	4.735902000
1	-1.256579000	0.973660000	6.004883000
1	-1.820166000	-1.183515000	4.822278000
1	-1.079463000	-1.484589000	2.493897000
1	2.084385000	2.162342000	-3.458827000
1	1.306270000	0.589824000	-3.110429000
1	4.433285000	1.525143000	-3.076637000
1	6.176175000	0.730993000	-1.462952000
1	5.439394000	-0.129324000	0.786255000
1	2.986273000	-0.142085000	1.302331000
7	2.061210000	-2.501566000	3.233404000
6	2.784083000	-2.806355000	2.375477000
6	3.680180000	-3.179650000	1.290880000
1	3.935539000	-4.240400000	1.373553000
1	3.186813000	-3.004131000	0.328971000
1	4.594505000	-2.582577000	1.344499000
1	1.592205000	-3.863542000	-2.135260000

1Bio_VIII

(G = -3537.300424) (Quadruplet)

6	0.636847000	2.841451000	-1.257776000
8	0.007849000	2.737546000	-2.317925000
6	0.019996000	3.494758000	-0.026188000
6	-1.499094000	3.707523000	-0.122931000
6	-2.331588000	2.543774000	0.443712000
6	-2.078799000	1.162964000	-0.188508000
6	-2.538866000	0.995163000	-1.647252000
1	0.531361000	4.457974000	0.101914000
1	0.255842000	2.907570000	0.867435000
1	-1.772521000	3.907764000	-1.163653000
1	-1.756079000	4.607034000	0.447981000
1	-3.391706000	2.807350000	0.375154000
1	-2.110881000	2.456943000	1.515762000
1	-2.555245000	0.394496000	0.428959000
1	-1.004353000	0.950427000	-0.149915000
16	-1.656047000	-0.395132000	-2.489156000
6	-2.787086000	-1.628648000	-1.717490000
6	-4.174199000	-0.959429000	-1.655338000
6	-4.025702000	0.589083000	-1.850333000
7	-4.980748000	1.100205000	-0.877320000
6	-5.367401000	0.156709000	0.037790000
7	-4.811771000	-1.045280000	-0.341531000
8	-6.074671000	0.347797000	1.036015000
1	-5.082169000	2.083087000	-0.668070000
1	-5.260002000	-1.899222000	-0.035743000
1	-2.302746000	1.892746000	-2.220156000
1	-2.433741000	-1.873197000	-0.712846000
1	-2.787193000	-2.537758000	-2.322283000
1	-4.321008000	0.874523000	-2.862327000
1	-4.828826000	-1.374366000	-2.429022000
7	2.432419000	-0.539722000	-1.876716000
6	3.908863000	-0.678762000	-1.633639000
6	4.260812000	-0.678093000	-0.143621000
7	3.483045000	0.358436000	0.590979000
6	3.937741000	1.744615000	0.241556000
6	2.827541000	2.752996000	-0.060662000
7	1.938679000	2.389058000	-1.181254000
6	2.129708000	0.533531000	-2.869100000
6	2.544098000	1.946439000	-2.448853000
6	3.519810000	0.122645000	2.059489000
6	2.256489000	0.593797000	2.740079000
7	1.105598000	0.361978000	2.068626000
6	2.254609000	1.144638000	4.019829000
6	1.033151000	1.440251000	4.627733000
6	-0.151844000	1.170494000	3.940723000
6	-0.071212000	0.632889000	2.660040000
6	1.848765000	-1.820213000	-2.349739000
6	1.697904000	-2.802878000	-1.217046000
6	1.759354000	-4.184392000	-1.391692000
6	1.535796000	-5.014259000	-0.291851000
6	1.266285000	-4.442547000	0.954466000
6	1.229434000	-3.055940000	1.053864000
7	1.441319000	-2.260110000	-0.009759000
27	1.460257000	-0.183545000	0.073499000
1	4.426535000	0.129224000	-2.149726000
1	4.274516000	-1.610846000	-2.073942000
1	5.340462000	-0.525827000	-0.019188000
1	4.002701000	-1.642566000	0.295112000
1	4.630387000	1.679253000	-0.596998000
1	4.513335000	2.152216000	1.078634000
1	3.318008000	3.712902000	-0.272243000
1	2.221736000	2.882210000	0.832543000
1	1.050627000	0.526653000	-3.020927000
1	2.619566000	0.301714000	-3.825526000
1	2.223098000	2.617373000	-3.250927000
1	3.625722000	2.045162000	-2.370434000
1	4.404726000	0.576803000	2.515799000
1	3.581647000	-0.958575000	2.221092000
1	3.195981000	1.330508000	4.526283000
1	1.008452000	1.870967000	5.624023000
1	-1.122562000	1.374513000	4.379174000

1	-0.956748000	0.400582000	2.086054000
1	2.437881000	-2.252697000	-3.167046000
1	0.847710000	-1.605561000	-2.734644000
1	1.977045000	-4.593573000	-2.372706000
1	1.576460000	-6.093283000	-0.405168000
1	1.088589000	-5.053309000	1.832768000
1	1.025723000	-2.551789000	1.991935000
7	-2.004018000	-2.102563000	1.956668000
6	-3.064889000	-2.029650000	2.426165000
6	-4.395902000	-1.927970000	3.005880000
1	-4.935531000	-2.868209000	2.856030000
1	-4.317838000	-1.727269000	4.078760000
1	-4.949947000	-1.116518000	2.521694000

1Bio_IX

(G = -3404.545793) (Quadruplet)

6	-0.690013000	3.217688000	-1.013009000
8	-0.904044000	3.098969000	-2.230610000
6	-1.805778000	3.703204000	-0.090645000
6	-3.209406000	3.225166000	-0.494873000
6	-3.624692000	1.905875000	0.178334000
6	-2.615725000	0.752406000	0.045720000
6	-2.413390000	0.228925000	-1.385342000
1	-1.747302000	4.797533000	-0.174393000
1	-1.620139000	3.472450000	0.959179000
1	-3.257363000	3.140149000	-1.585140000
1	-3.938720000	3.992126000	-0.211236000
1	-4.606551000	1.606123000	-0.205514000
1	-3.758018000	2.089431000	1.252659000
1	-2.926739000	-0.064951000	0.696423000
1	-1.650450000	1.087339000	0.436920000
16	-0.718851000	-0.461755000	-1.697489000
6	-1.186145000	-2.230626000	-1.417682000
6	-2.716766000	-2.316045000	-1.496508000
6	-3.350650000	-0.935384000	-1.845657000
7	-4.616297000	-1.029165000	-1.135699000
6	-4.572288000	-1.952803000	-0.117227000
7	-3.360637000	-2.614397000	-0.215327000
8	-5.444876000	-2.148896000	0.731953000
1	-5.271942000	-0.261314000	-1.087591000
1	-3.316269000	-3.556226000	0.155323000
1	-2.487475000	1.056034000	-2.093459000
1	-0.816349000	-2.566795000	-0.448660000
1	-0.703709000	-2.818924000	-2.199092000
1	-3.510564000	-0.848806000	-2.921700000
1	-3.003698000	-3.058288000	-2.249849000
7	2.484414000	0.642633000	-1.395123000
6	3.764560000	1.001863000	-0.696984000
6	3.714752000	0.708736000	0.801881000
7	2.399697000	1.082891000	1.391347000
6	2.199247000	2.574219000	1.421740000
6	0.844285000	3.098526000	0.945513000
7	0.573056000	3.036640000	-0.511434000
6	1.983207000	1.774670000	-2.227184000
6	1.669596000	3.080313000	-1.490912000
6	2.252307000	0.487392000	2.747225000
6	0.842868000	0.046365000	3.060164000
7	0.146483000	-0.508464000	2.042149000
6	0.335875000	0.079404000	4.358739000
6	-0.900231000	-0.512144000	4.620285000
6	-1.587774000	-1.134780000	3.576689000
6	-1.031353000	-1.106708000	2.302924000
6	2.684714000	-0.539895000	-2.269620000
6	2.765639000	-1.812782000	-1.464941000
6	3.523001000	-2.913819000	-1.860934000
6	3.487354000	-4.073811000	-1.085811000
6	2.701805000	-4.101003000	0.069513000
6	1.980587000	-2.961546000	0.407221000
7	2.012302000	-1.846875000	-0.346630000
27	1.024802000	-0.109239000	0.181286000
1	3.986398000	2.053117000	-0.877673000
1	4.596510000	0.436547000	-1.126816000
1	4.537299000	1.229838000	1.309009000
1	3.840183000	-0.362225000	0.967517000
1	3.019129000	3.047724000	0.883544000
1	2.293339000	2.907891000	2.459337000
1	0.778244000	4.138434000	1.288813000
1	0.071892000	2.522628000	1.458262000
1	1.075536000	1.436781000	-2.727257000
1	2.728961000	2.009657000	-3.001096000
1	1.389965000	3.793688000	-2.270866000
1	2.552449000	3.491098000	-1.004775000
1	2.628662000	1.161435000	3.522627000
1	2.866407000	-0.418430000	2.779410000
1	0.912199000	0.552664000	5.146735000
1	-1.314152000	-0.496467000	5.623830000
1	-2.540858000	-1.627360000	3.735553000
1	-1.537604000	-1.572052000	1.466866000
1	3.574603000	-0.425221000	-2.899966000
1	1.823388000	-0.618060000	-2.941018000
1	4.128078000	-2.854399000	-2.759414000
1	4.070300000	-4.942668000	-1.375627000
1	2.651405000	-4.980919000	0.701285000
1	1.359635000	-2.915910000	1.295518000

1Bio_X

(G = -3537.296798) (Quadruplet)

6	0.984148000	-2.616233000	-1.178852000
8	1.975621000	-2.437648000	-1.890295000
6	1.063296000	-3.370933000	0.135692000
6	2.418517000	-4.023413000	0.442217000
6	3.668488000	-3.131660000	0.550447000
6	3.578115000	-1.925660000	1.512207000
6	3.070564000	-0.626447000	0.877809000
1	0.303494000	-4.160021000	0.133552000
1	0.771226000	-2.682257000	0.935537000
1	2.615034000	-4.793125000	-0.314413000
1	2.289321000	-4.554467000	1.394362000
1	3.955078000	-2.796044000	-0.448596000
1	4.482763000	-3.777392000	0.901960000
1	4.575168000	-1.726948000	1.920725000
1	2.934659000	-2.178791000	2.364734000
16	3.107305000	0.791552000	2.071268000
6	2.801928000	1.919898000	0.658940000
6	3.691449000	1.422069000	-0.489618000
6	3.858316000	-0.132862000	-0.359808000
7	5.303980000	-0.288547000	-0.244484000
6	5.990311000	0.886919000	-0.399065000
7	5.066115000	1.903034000	-0.403502000
8	7.218197000	1.013636000	-0.488340000
1	5.769198000	-1.167846000	-0.420045000
1	5.332587000	2.814376000	-0.750076000

1	2.025385000	-0.727156000	0.567279000
1	3.018869000	2.954885000	0.932874000
1	1.751077000	1.838595000	0.373420000
1	3.480917000	-0.654536000	-1.242623000
1	3.244570000	1.701756000	-1.449068000
7	-0.653114000	0.820235000	-2.126856000
6	-2.091229000	0.901883000	-2.544291000
6	-3.049556000	0.679512000	-1.370575000
7	-2.595428000	-0.446281000	-0.507292000
6	-2.732613000	-1.775864000	-1.185189000
6	-1.506146000	-2.664176000	-1.007974000
7	-0.251024000	-2.087103000	-1.560302000
6	0.146901000	-0.083362000	-3.002147000
6	-0.292686000	-1.544856000	-2.936327000
6	-3.277236000	-0.432191000	0.833349000
6	-4.790798000	-0.457268000	0.791389000
7	-5.384259000	-1.665713000	0.732211000
6	-5.525102000	0.735872000	0.808548000
6	-6.917693000	0.678038000	0.748727000
6	-7.534151000	-0.572209000	0.675327000
6	-6.724650000	-1.710599000	0.673000000
6	-0.024792000	2.164369000	-2.079231000
6	-0.478012000	2.929587000	-0.862707000
6	-0.609676000	4.315928000	-0.832027000
6	-0.955211000	4.933374000	0.371561000
6	-1.164623000	4.148725000	1.508772000
6	-1.022545000	2.769283000	1.399078000
7	-0.686062000	2.179637000	0.238663000
27	-0.589412000	0.112946000	-0.067790000
1	-2.270525000	0.167251000	-3.328697000
1	-2.298338000	1.882305000	-2.983079000
1	-4.058871000	0.499986000	-1.758400000
1	-3.087058000	1.568565000	-0.739235000
1	-2.961511000	-1.617493000	-2.237793000
1	-3.587047000	-2.312563000	-0.766836000
1	-1.712877000	-3.632335000	-1.481279000
1	-1.363363000	-2.826067000	0.059862000
1	1.182774000	-0.016324000	-2.664013000
1	0.097267000	0.259339000	-4.044751000
1	0.383463000	-2.120172000	-3.573273000
1	-1.295823000	-1.679235000	-3.335440000
1	-2.944774000	0.471887000	1.349752000
1	-2.902531000	-1.297239000	1.383129000
1	-5.007471000	1.687977000	0.868604000
1	-7.508177000	1.589510000	0.761673000
1	-8.614159000	-0.669480000	0.629023000
1	-7.169715000	-2.701951000	0.627506000
1	-0.217273000	2.731134000	-2.997093000
1	1.057067000	2.020860000	-1.991557000
1	-0.443054000	4.892508000	-1.735811000
1	-1.063466000	6.012535000	0.420334000
1	-1.435763000	4.591202000	2.460951000
1	-1.177725000	2.107001000	2.244059000
7	-0.209791000	-0.505500000	1.867029000
6	0.081892000	-0.804987000	2.944454000
6	0.459108000	-1.196719000	4.286250000
1	-0.361377000	-0.979176000	4.976438000
1	0.676007000	-2.269050000	4.300791000
1	1.350842000	-0.638713000	4.586626000

1Bio_XI

(G = -3537.294852) (Quadruplet)

6	-0.004419000	-1.836593000	2.734516000
8	0.417485000	-2.985276000	2.666154000
6	0.826660000	-0.693307000	3.288772000
6	2.332915000	-0.965233000	3.356633000
6	3.037923000	-1.049293000	1.992343000
6	2.735460000	0.145576000	1.073015000
6	3.558106000	0.140711000	-0.214073000
1	0.441220000	-0.494760000	4.298422000
1	0.639148000	0.216398000	2.714345000
1	2.516948000	-1.888444000	3.916622000
1	2.778319000	-0.146640000	3.935517000
1	2.749716000	-1.976181000	1.488061000
1	4.117753000	-1.116716000	2.173162000
1	2.913258000	1.085125000	1.610310000
1	1.674559000	0.133191000	0.797992000
16	3.024928000	1.481659000	-1.375257000
6	4.566351000	1.232966000	-2.342266000
6	5.689909000	0.993216000	-1.319343000
6	5.085151000	0.325864000	-0.031606000
7	5.444122000	1.273926000	1.014753000
6	6.229510000	2.304216000	0.570907000
7	6.260300000	2.232911000	-0.800605000
8	6.781983000	3.160330000	1.272933000
1	5.439990000	1.025823000	1.993853000
1	6.978877000	2.733544000	-1.305433000
1	3.409484000	-0.807246000	-0.742853000
1	4.768541000	2.108098000	-2.964270000
1	4.451816000	0.357484000	-2.989371000
1	5.537700000	-0.650683000	0.166104000
1	6.468932000	0.370163000	-1.770883000
7	-2.438991000	-2.273505000	-0.363104000
6	-3.803573000	-1.655279000	-0.324483000
6	-3.741203000	-0.124597000	-0.380484000
7	-2.713317000	0.387494000	0.566315000
6	-3.130985000	0.179187000	1.986272000
6	-1.981776000	-0.323931000	2.848725000
7	-1.312692000	-1.533090000	2.281555000
6	-2.219343000	-3.299392000	0.697706000
6	-2.210906000	-2.716426000	2.114558000
6	-2.314400000	1.808504000	0.292161000
6	-3.436794000	2.822225000	0.362439000
7	-3.665834000	3.397981000	1.559394000
6	-4.199924000	3.128475000	-0.772124000
6	-5.241844000	4.049724000	-0.661335000
6	-5.486816000	4.640114000	0.579800000
6	-4.670323000	4.283521000	1.655330000
6	-2.124490000	-2.808019000	-1.712436000
6	-1.741745000	-1.693814000	-2.659231000
6	-1.974396000	-1.754633000	-4.032815000
6	-1.524817000	-0.708626000	-4.840523000
6	-0.856721000	0.369188000	-4.254087000
6	-0.669186000	0.362120000	-2.874850000
7	-1.104566000	-0.645878000	-2.100997000
27	-0.982153000	-0.761375000	0.034865000
1	-4.309691000	-1.986518000	0.582084000
1	-4.401303000	-2.016206000	-1.166353000
1	-4.731660000	0.287355000	-0.153809000
1	-3.459525000	0.210111000	-1.379765000
1	-3.972568000	-0.511402000	2.007793000

1	-3.491085000	1.115996000	2.418488000
1	-2.353849000	-0.544264000	3.856212000
1	-1.243896000	0.470005000	2.922192000
1	-1.248263000	-3.755322000	0.499353000
1	-2.986995000	-4.082319000	0.643354000
1	-1.887787000	-3.508234000	2.793851000
1	-3.211966000	-2.417543000	2.420359000
1	-1.867551000	1.826009000	-0.704554000
1	-1.540834000	2.060395000	1.021056000
1	-3.974372000	2.651162000	-1.720400000
1	-5.847027000	4.303805000	-1.526691000
1	-6.283973000	5.364169000	0.715146000
1	-4.824579000	4.729816000	2.635214000
1	-2.959263000	-3.391690000	-2.115026000
1	-1.265454000	-3.479010000	-1.620105000
1	-2.501079000	-2.605089000	-4.453121000
1	-1.698361000	-0.732013000	-5.912054000
1	-0.492536000	1.201728000	-4.846248000
1	-0.161551000	1.172621000	-2.362519000
7	0.651737000	-2.023572000	-0.321866000
6	1.468066000	-2.767095000	-0.663258000
6	2.505255000	-3.690973000	-1.076207000
1	3.205373000	-3.841039000	-0.249010000
1	2.052861000	-4.648211000	-1.352512000
1	3.039019000	-3.277571000	-1.936895000

1Bio_XII

(G = -3537.292232) (Quadruplet)

6	-0.884181000	2.246499000	-2.395316000
8	-1.669120000	3.149505000	-2.657038000
6	0.551019000	2.481958000	-1.973387000
6	0.892114000	3.922031000	-1.540504000
6	1.716793000	3.930861000	-0.241619000
6	3.025504000	3.112740000	-0.326501000
6	3.398876000	2.387431000	0.965833000
1	1.196203000	2.160443000	-2.799012000
1	0.756349000	1.786134000	-1.152744000
1	-0.028935000	4.491893000	-1.383813000
1	1.440195000	4.430826000	-2.341850000
1	1.083605000	3.522637000	0.554452000
1	1.939948000	4.964237000	0.048504000
1	3.862155000	3.769911000	-0.598172000
1	2.958566000	2.363154000	-1.119947000
16	2.105809000	1.165932000	1.520295000
6	3.332147000	0.437475000	2.673527000
6	4.673874000	0.399382000	1.923043000
6	4.709901000	1.569910000	0.874525000
7	4.872356000	0.858414000	-0.389127000
6	5.064605000	-0.490778000	-0.230731000
7	4.817492000	-0.785941000	1.085465000
8	5.369514000	-1.296669000	-1.118815000
1	5.224309000	1.315451000	-1.218380000
1	5.110730000	-1.675637000	1.464505000
1	3.513164000	3.110301000	1.782781000
1	3.011820000	-0.561634000	2.978634000
1	3.413862000	1.069739000	3.563440000
1	5.555895000	2.243969000	1.045601000
1	5.499452000	0.470008000	2.638741000
7	-3.441160000	-0.153300000	-0.666491000
6	-3.493908000	-1.610571000	-1.018997000
6	-2.251557000	-2.368596000	-0.535246000
7	-1.013429000	-1.601322000	-0.840522000
6	-0.730521000	-1.551483000	-2.307599000
6	-0.320100000	-0.156547000	-2.761422000
7	-1.317692000	0.895993000	-2.391907000
6	-3.754877000	0.738815000	-1.820538000
6	-2.693464000	0.679666000	-2.922270000
6	0.176873000	-2.062245000	-0.050665000
6	0.632967000	-3.479822000	-0.321168000
7	1.609792000	-3.635998000	-1.236712000
6	0.055924000	-4.567016000	0.348540000
6	0.494329000	-5.857705000	0.051072000
6	1.500035000	-6.022278000	-0.903391000
6	2.026026000	-4.881792000	-1.514064000
6	-4.294072000	0.163726000	0.507059000
6	-3.626730000	-0.272243000	1.790512000
6	-4.333260000	-0.708873000	2.909956000
6	-3.626733000	-1.026050000	4.071578000
6	-2.235606000	-0.897594000	4.082902000
6	-1.600091000	-0.461708000	2.923781000
7	-2.283187000	-0.161105000	1.806809000
27	-1.453377000	0.339799000	-0.067453000
1	-3.597565000	-1.700088000	-2.100505000
1	-4.383024000	-2.070895000	-0.578190000
1	-2.231918000	-3.361348000	-0.999934000
1	-2.287257000	-2.504948000	0.546617000
1	-1.606665000	-1.904688000	-2.849013000
1	0.082889000	-2.234980000	-2.562280000
1	-0.172706000	-0.158298000	-3.847818000
1	0.627532000	0.086405000	-2.286443000
1	-3.798527000	1.757378000	-1.429483000
1	-4.734855000	0.489358000	-2.247365000
1	-2.926737000	1.452167000	-3.657718000
1	-2.713808000	-0.276832000	-3.440414000
1	-0.084042000	-1.951574000	1.004289000
1	0.988839000	-1.367088000	-0.273867000
1	-0.718433000	-4.397053000	1.089617000
1	0.062429000	-6.716536000	0.556508000
1	1.875715000	-7.005918000	-1.166854000
1	2.817311000	-4.969078000	-2.255292000
1	-5.291205000	-0.279480000	0.410768000
1	-4.412804000	1.251323000	0.548002000
1	-5.413379000	-0.800610000	2.863875000
1	-4.154580000	-1.373019000	4.954665000
1	-1.650818000	-1.134637000	4.965016000
1	-0.521925000	-0.352027000	2.868278000
7	-1.605179000	2.334934000	0.474031000
6	-1.694635000	3.441253000	0.796783000
6	-1.781200000	4.835457000	1.180176000
1	-2.290967000	5.396990000	0.391714000
1	-2.339184000	4.927723000	2.116452000
1	-0.769816000	5.231011000	1.313909000

1Bio_XIII

(G = -3537.291079) (Quadruplet)

6	-0.983268000	-1.857966000	-2.635202000
8	-1.241124000	-3.056480000	-2.777120000
6	-2.060088000	-0.807568000	-2.444414000
6	-3.464977000	-1.347552000	-2.129494000
6	-4.143681000	-0.505900000	-1.037586000
6	-4.503885000	0.926601000	-1.483561000
6	-4.648643000	1.978264000	-0.364555000
1	-2.069247000	-0.148233000	-3.319383000
1	-1.727455000	-0.194176000	-1.606109000

1	-3.387362000	-2.382803000	-1.786149000
1	-4.079771000	-1.369619000	-3.037729000
1	-3.476874000	-0.475266000	-0.169961000
1	-5.055952000	-1.012105000	-0.700086000
1	-5.441908000	0.891184000	-2.048941000
1	-3.750710000	1.309571000	-2.183467000
16	-5.488778000	1.320157000	1.162020000
6	-4.729416000	2.636088000	2.188242000
6	-3.312610000	2.838040000	1.653324000
6	-3.318704000	2.663441000	0.100856000
7	-2.102537000	1.886881000	-0.112780000
6	-1.610973000	1.359495000	1.028010000
7	-2.371799000	1.793191000	2.066875000
8	-0.622236000	0.594678000	1.141892000
1	-1.696367000	1.706515000	-1.018080000
1	-2.026817000	1.721045000	3.015107000
1	-5.283460000	2.787405000	-0.736997000
1	-4.731133000	2.334119000	3.238589000
1	-5.292554000	3.569204000	2.089162000
1	-3.233429000	3.623330000	-0.412151000
1	-2.937424000	3.823484000	1.950631000
7	2.099865000	-2.375947000	-0.374758000
6	3.398270000	-1.670670000	-0.626316000
6	3.332912000	-0.178778000	-0.286142000
7	2.056178000	0.428662000	-0.757882000
6	1.996397000	0.476130000	-2.257879000
6	0.674534000	-0.003543000	-2.847486000
7	0.331765000	-1.418046000	-2.565084000
6	1.689474000	-3.227341000	-1.527077000
6	1.364576000	-2.441879000	-2.797860000
6	1.834084000	1.787929000	-0.154484000
6	2.908007000	2.818590000	-0.433559000
7	2.751828000	3.584111000	-1.532096000
6	4.003555000	2.965498000	0.427810000
6	4.974268000	3.924573000	0.137548000
6	4.819224000	4.710830000	-1.005623000
6	3.692066000	4.503151000	-1.803769000
6	2.178626000	-3.217013000	0.845853000
6	2.213957000	-2.364996000	2.088023000
6	2.934149000	-2.718257000	3.228330000
6	2.874266000	-1.888902000	4.348974000
6	2.098354000	-0.728913000	4.294882000
6	1.410006000	-0.441530000	3.119851000
7	1.467866000	-1.242859000	2.041452000
27	0.583753000	-0.838521000	0.158970000
1	3.675483000	-1.808714000	-1.670706000
1	4.196501000	-2.128234000	-0.033899000
1	4.198741000	0.325638000	-0.730982000
1	3.378267000	-0.028861000	0.793300000
1	2.836449000	-0.083688000	-2.665267000
1	2.134383000	1.506144000	-2.593839000
1	0.719210000	0.154428000	-3.933312000
1	-0.115723000	0.630019000	-2.450334000
1	0.792705000	-3.767778000	-1.219057000
1	2.475680000	-3.961822000	-1.751098000
1	1.007393000	-3.157529000	-3.542958000
1	2.249226000	-1.964877000	-3.215013000
1	1.740752000	1.645545000	0.923542000
1	0.875594000	2.145965000	-0.533462000
1	4.085396000	2.338118000	1.309822000
1	5.830954000	4.057559000	0.791764000
1	5.545119000	5.472296000	-1.272629000
1	3.532289000	5.103154000	-2.696831000
1	3.044462000	-3.888954000	0.810691000
1	1.276615000	-3.836182000	0.883946000
1	3.532440000	-3.623324000	3.227444000
1	3.430192000	-2.140390000	5.247105000
1	2.028010000	-0.053486000	5.140656000
1	0.792990000	0.442793000	3.015539000
7	-0.932099000	-2.244185000	0.440693000
6	-1.846971000	-2.931989000	0.603115000
6	-2.998731000	-3.791296000	0.792235000
1	-3.048790000	-4.511410000	-0.029972000
1	-2.906938000	-4.326156000	1.742030000
1	-3.907074000	-3.181812000	0.799172000

1Bio_XIV

(G = -3404.533486) (Quadruplet)

6	-0.776280000	-3.072488000	1.055122000
8	-1.685466000	-2.997529000	1.890697000
6	-0.962057000	-3.786201000	-0.273396000
6	-2.370701000	-4.324195000	-0.558440000
6	-3.515521000	-3.293059000	-0.650099000
6	-3.153593000	-1.992458000	-1.410242000
6	-3.073491000	-0.799085000	-0.452222000
1	-0.255341000	-4.625973000	-0.299104000
1	-0.643591000	-3.118949000	-1.080515000
1	-2.634034000	-5.075330000	0.194765000
1	-2.299892000	-4.855113000	-1.516370000
1	-3.844340000	-3.037474000	0.361622000
1	-4.368065000	-3.779883000	-1.136816000
1	-3.883444000	-1.771683000	-2.193838000
1	-2.197145000	-2.111156000	-1.927948000
16	-1.957853000	0.555938000	-1.058700000
6	-2.687320000	1.700246000	0.188448000
6	-4.189504000	1.407149000	0.197910000
6	-4.430631000	-0.109972000	-0.133739000
7	-5.349126000	-0.041011000	-1.260529000
6	-5.706010000	1.238634000	-1.598579000
7	-4.905628000	2.091063000	-0.873128000
8	-6.562757000	1.566829000	-2.425622000
1	-5.942350000	-0.814713000	-1.524852000
1	-5.192872000	3.055284000	-0.768661000
1	-2.636298000	-1.115049000	0.497991000
1	-2.462588000	2.734301000	-0.075494000
1	-2.256770000	1.468637000	1.162121000
1	-4.889964000	-0.639102000	0.705565000
1	-4.597907000	1.677047000	1.177190000
7	0.847570000	0.406235000	2.256170000
6	2.337263000	0.508903000	2.396509000
6	3.033718000	0.548835000	1.033571000
7	2.426372000	-0.445930000	0.109043000
6	2.775936000	-1.842922000	0.526894000
6	1.619951000	-2.828387000	0.441298000
7	0.464901000	-2.514833000	1.313069000
6	0.245778000	-0.700029000	3.059182000
6	0.720045000	-2.112731000	2.707961000
6	2.785489000	-0.189874000	-1.326747000
6	4.268104000	-0.176771000	-1.638173000
7	4.832395000	-1.350612000	-1.984133000
6	5.006484000	1.010980000	-1.553833000
6	6.375630000	0.980434000	-1.819501000
6	6.964720000	-0.236970000	-2.165694000
6	6.150589000	-1.369541000	-2.237931000
6	0.203531000	1.692802000	2.625799000

6	0.418982000	2.718449000	1.541718000
6	0.542021000	4.083544000	1.792347000
6	0.697133000	4.956059000	0.714146000
6	0.731070000	4.439915000	-0.584133000
6	0.604292000	3.065710000	-0.756231000
7	0.448968000	2.229132000	0.285257000
27	0.340963000	0.150156000	0.152211000
1	2.696329000	-0.324920000	2.999020000
1	2.595416000	1.417917000	2.946697000
1	4.106124000	0.365201000	1.166257000
1	2.916565000	1.531929000	0.576181000
1	3.196748000	-1.816997000	1.530209000
1	3.569528000	-2.225843000	-0.119205000
1	2.013218000	-3.824362000	0.684869000
1	1.275735000	-2.846343000	-0.591396000
1	-0.832285000	-0.650229000	2.893999000
1	0.443798000	-0.529006000	4.126566000
1	0.178374000	-2.790569000	3.373600000
1	1.779828000	-2.248379000	2.918153000
1	2.351336000	0.776910000	-1.597713000
1	2.288528000	-0.965234000	-1.914232000
1	4.509797000	1.937506000	-1.283871000
1	6.968917000	1.888187000	-1.759682000
1	8.025440000	-0.311589000	-2.383271000
1	6.571663000	-2.333232000	-2.515400000
1	0.569583000	2.060261000	3.591106000
1	-0.871567000	1.514348000	2.726221000
1	0.521736000	4.446005000	2.814611000
1	0.797567000	6.023394000	0.885295000
1	0.857179000	5.083778000	-1.447440000
1	0.628557000	2.606639000	-1.739235000

1Bio_XV

(G = -3670.044603) (Quadruplet)

6	-0.231862000	-1.591493000	2.594104000
8	-0.855118000	-0.999140000	3.475526000
6	-0.893138000	-2.629613000	1.697953000
6	-2.396744000	-2.789115000	1.955427000
6	-3.253780000	-1.625776000	1.432170000
6	-3.445805000	-1.652688000	-0.094416000
6	-3.974678000	-0.326434000	-0.638389000
1	-0.386206000	-3.587629000	1.868072000
1	-0.699529000	-2.368121000	0.651869000
1	-2.557188000	-2.905755000	3.032065000
1	-2.726205000	-3.722760000	1.482045000
1	-2.789106000	-0.682521000	1.732416000
1	-4.234074000	-1.656495000	1.922765000
1	-4.129027000	-2.466193000	-0.366112000
1	-2.489012000	-1.866928000	-0.581651000
16	-4.218370000	-0.325151000	-2.475145000
6	-5.133412000	1.260504000	-2.317157000
6	-6.004588000	1.141562000	-1.052427000
6	-5.324359000	0.141413000	-0.050309000
7	-6.316506000	-0.922820000	0.065270000
6	-7.504201000	-0.615171000	-0.551643000
7	-7.293977000	0.510198000	-1.304396000
8	-8.559237000	-1.256089000	-0.466111000
1	-6.325877000	-1.553942000	0.854365000
1	-8.077792000	1.016800000	-1.691402000
1	-3.239831000	0.458368000	-0.430029000
1	-5.738332000	1.438738000	-3.209235000
1	-4.416895000	2.080577000	-2.205791000
1	-5.144852000	0.606483000	0.923546000
1	-6.139843000	2.132476000	-0.607140000
7	2.250037000	1.421852000	2.029043000
6	3.721802000	1.177380000	1.890192000
6	4.076849000	0.519655000	0.557013000
7	3.135978000	-0.587106000	0.234065000
6	3.292410000	-1.751048000	1.163089000
6	1.960097000	-2.305464000	1.653072000
7	1.126884000	-1.323154000	2.396817000
6	1.715693000	0.938989000	3.333490000
6	1.782054000	-0.579984000	3.499873000
6	3.248327000	-1.004393000	-1.204967000
6	4.633167000	-1.415963000	-1.659461000
7	4.982091000	-2.704798000	-1.475481000
6	5.500824000	-0.483966000	-2.244421000
6	6.773993000	-0.894459000	-2.640209000
6	7.141357000	-2.226247000	-2.439947000
6	6.210362000	-3.089258000	-1.857348000
6	1.929783000	2.858762000	1.839468000
6	1.966875000	3.236077000	0.378190000
6	2.328629000	4.506370000	-0.068049000
6	2.274782000	4.783210000	-1.434955000
6	1.864394000	3.782405000	-2.319323000
6	1.525074000	2.536787000	-1.800288000
7	1.576789000	2.274380000	-0.483164000
27	1.199643000	0.405309000	0.391092000
1	4.056229000	0.556556000	2.721010000
1	4.269290000	2.121155000	1.971479000
1	5.112606000	0.162252000	0.599683000
1	4.007659000	1.245527000	-0.254970000
1	3.931470000	-1.460596000	1.995004000
1	3.814512000	-2.562706000	0.650989000
1	2.162770000	-3.179689000	2.284980000
1	1.396259000	-2.636137000	0.781887000
1	0.670887000	1.246800000	3.385948000
1	2.258024000	1.410650000	4.164434000
1	1.283266000	-0.824631000	4.440813000
1	2.809894000	-0.927256000	3.585889000
1	2.904995000	-0.159254000	-1.806589000
1	2.551915000	-1.831548000	-1.348392000
1	5.175971000	0.542151000	-2.384652000
1	7.463057000	-0.190216000	-3.097274000
1	8.119576000	-2.594194000	-2.732866000
1	6.457301000	-4.136136000	-1.695507000
1	2.601277000	3.498728000	2.422814000
1	0.912785000	3.030149000	2.203371000
1	2.649379000	5.256473000	0.647247000
1	2.555206000	5.764644000	-1.805022000
1	1.812740000	3.956403000	-3.388493000
1	1.207731000	1.718069000	-2.437261000
7	-0.666668000	1.189493000	1.076973000
6	-1.635414000	1.719276000	1.420259000
6	-2.857758000	2.364342000	1.858515000
1	-3.433373000	1.664081000	2.470554000
1	-2.612798000	3.252632000	2.448409000
1	-3.449261000	2.653676000	0.985324000
7	0.169035000	-0.527273000	-1.176443000
6	-0.286559000	-1.088721000	-2.078960000
6	-0.837340000	-1.815943000	-3.204266000
1	-1.546685000	-2.563886000	-2.838598000
1	-1.353011000	-1.122982000	-3.873909000
1	-0.024145000	-2.314276000	-3.741035000

1Bio_XVI

(G = -3537.431323) (Triplet)

6	-0.391014000	-2.690242000	-1.228002000
8	-0.020018000	-2.543512000	-2.400347000
6	0.594025000	-3.068760000	-0.124445000
6	2.033146000	-3.234715000	-0.629504000
6	2.755910000	-1.902866000	-0.887837000
6	3.273941000	-1.245535000	0.403662000
6	3.639167000	0.223188000	0.201223000
1	0.249713000	-4.006353000	0.328463000
1	0.544417000	-2.314982000	0.670200000
1	2.015156000	-3.829067000	-1.548478000
1	2.596419000	-3.813486000	0.113856000
1	2.067638000	-1.224228000	-1.400717000
1	3.595154000	-2.069300000	-1.574140000
1	4.145303000	-1.797389000	0.775939000
1	2.504998000	-1.307370000	1.180022000
16	4.221509000	1.061828000	1.747624000
6	4.776493000	2.482848000	0.721911000
6	5.404945000	1.884608000	-0.550200000
6	4.741199000	0.492721000	-0.846733000
7	5.871649000	-0.426998000	-0.763458000
6	7.076914000	0.216539000	-0.637132000
7	6.811295000	1.537228000	-0.383481000
8	8.196680000	-0.305558000	-0.709557000
1	5.845409000	-1.341082000	-1.193561000
1	7.548483000	2.223855000	-0.461282000
1	2.745099000	0.767361000	-0.123097000
1	5.490681000	3.096367000	1.276052000
1	3.909320000	3.097855000	0.460182000
1	4.295750000	0.462861000	-1.845407000
1	5.275443000	2.581824000	-1.384342000
7	-3.358357000	-0.088125000	-1.695829000
6	-4.703223000	-0.402107000	-1.140104000
6	-4.753304000	-0.302999000	0.394153000
7	-3.556555000	-0.906384000	1.015275000
6	-3.544242000	-2.386271000	0.881894000
6	-2.209787000	-2.987816000	0.434251000
7	-1.720259000	-2.547411000	-0.891098000
6	-2.867785000	-1.112284000	-2.640595000
6	-2.667049000	-2.502258000	-2.021476000
6	-3.360166000	-0.467266000	2.409938000
6	-1.899056000	-0.495090000	2.802320000
7	-1.043229000	-0.030481000	1.860399000
6	-1.460591000	-0.914901000	4.057034000
6	-0.099104000	-0.837583000	4.365626000
6	0.780073000	-0.337695000	3.401868000
6	0.265105000	0.051210000	2.167403000
6	-3.317286000	1.262107000	-2.288614000
6	-3.392263000	2.332113000	-1.219546000
6	-4.084540000	3.529145000	-1.403607000
6	-4.072158000	4.487993000	-0.387113000
6	-3.369456000	4.211843000	0.788890000
6	-2.710791000	2.989111000	0.899940000
7	-2.717168000	2.063678000	-0.077091000
27	-1.866030000	0.162550000	-0.030052000
1	-4.996449000	-1.403407000	-1.459115000
1	-5.456639000	0.279162000	-1.553496000
1	-5.682855000	-0.773604000	0.751412000
1	-4.777154000	0.745799000	0.690896000
1	-4.343266000	-2.688049000	0.203817000
1	-3.782216000	-2.849489000	1.848351000
1	-2.326208000	-4.081125000	0.442849000
1	-1.457242000	-2.727818000	1.175610000
1	-1.903231000	-0.765319000	-3.016147000
1	-3.553198000	-1.224847000	-3.497647000
1	-2.290306000	-3.149922000	-2.818547000
1	-3.612294000	-2.929992000	-1.689594000
1	-3.960129000	-1.053172000	3.120104000
1	-3.691003000	0.574830000	2.474096000
1	-2.178586000	-1.296547000	4.776561000
1	0.265531000	-1.162958000	5.335320000
1	1.844996000	-0.256446000	3.592095000
1	0.905874000	0.434378000	1.380569000
1	-4.114712000	1.411573000	-3.031737000
1	-2.356789000	1.366804000	-2.804406000
1	-4.626616000	3.700105000	-2.328785000
1	-4.605088000	5.426287000	-0.508597000
1	-3.334168000	4.923318000	1.607726000
1	-2.158117000	2.722329000	1.796146000
7	-0.306303000	0.637972000	-1.134866000
6	0.536860000	0.960301000	-1.869456000
6	1.583916000	1.363499000	-2.795874000
1	2.100030000	0.478437000	-3.179972000
1	1.148411000	1.915414000	-3.635070000
1	2.311036000	2.002462000	-2.285690000

1Bio_XVII

(G = -3404.674588) (Triplet)

6	1.463634000	2.764873000	-1.184016000
8	1.033926000	3.139695000	-2.284023000
6	0.965157000	3.388752000	0.109573000
6	-0.232391000	4.334979000	-0.071018000
6	-1.495232000	3.730731000	-0.711417000
6	-2.025834000	2.482613000	-0.000929000
6	-3.332896000	1.953652000	-0.603928000
1	1.792990000	3.943796000	0.569599000
1	0.719002000	2.584604000	0.808300000
1	0.081360000	5.196923000	-0.671258000
1	-0.485390000	4.721895000	0.925068000
1	-1.287404000	3.491251000	-1.757019000
1	-2.281444000	4.498919000	-0.705479000
1	-2.210223000	2.727642000	1.052813000
1	-1.273303000	1.682952000	-0.013299000
16	-3.068626000	1.220831000	-2.299573000
6	-2.785005000	-0.423978000	-1.547498000
6	-3.914105000	-0.547976000	-0.519162000
6	-4.031548000	0.823326000	0.222904000
7	-3.407243000	0.516085000	1.507582000
6	-3.267018000	-0.834146000	1.721526000
7	-3.655115000	-1.483576000	0.569829000
8	-2.864576000	-1.370850000	2.759416000
1	-3.518507000	1.124417000	2.307353000
1	-4.029196000	2.786843000	-0.735490000
1	-1.808464000	-0.443715000	-1.054842000
1	-2.818050000	-1.200847000	-2.314478000
1	-5.083293000	1.090659000	0.366431000
1	-4.847141000	-0.793756000	-1.031376000

7	1.572549000	-0.964338000	-2.062936000
6	2.802563000	-1.788852000	-1.862088000
6	3.108257000	-2.083642000	-0.385686000
7	2.878860000	-0.902500000	0.471431000
6	3.873641000	0.182067000	0.253726000
6	3.279644000	1.583462000	0.060570000
7	2.387750000	1.741760000	-1.109971000
6	1.825663000	0.176780000	-2.971574000
6	2.821323000	1.197322000	-2.406464000
6	2.742684000	-1.262469000	1.895434000
6	1.871736000	-0.276818000	2.637958000
7	0.766557000	0.147353000	1.965535000
6	2.140814000	0.109003000	3.948782000
6	1.238616000	0.938458000	4.622162000
6	0.084332000	1.344026000	3.949622000
6	-0.109516000	0.928653000	2.634957000
6	0.446622000	-1.787615000	-2.546045000
6	-0.079296000	-2.693506000	-1.455015000
6	-0.558113000	-3.976759000	-1.713582000
6	-1.069048000	-4.741479000	-0.661286000
6	-1.075133000	-4.193950000	0.624581000
6	-0.576101000	-2.906643000	0.805507000
7	-0.086422000	-2.163061000	-0.207299000
27	0.831043000	-0.352300000	-0.015458000
1	3.649902000	-1.276027000	-2.318053000
1	2.707272000	-2.745379000	-2.389344000
1	4.142099000	-2.454822000	-0.306145000
1	2.443492000	-2.870281000	-0.026477000
1	4.507344000	-0.083142000	-0.593755000
1	4.543683000	0.248489000	1.120045000
1	4.122968000	2.283622000	-0.026509000
1	2.719582000	1.848483000	0.954849000
1	0.870864000	0.681015000	-3.134860000
1	2.201756000	-0.170702000	-3.947900000
1	2.910788000	2.009836000	-3.132601000
1	3.813825000	0.766649000	-2.288663000
1	3.715597000	-1.372689000	2.393976000
1	2.232992000	-2.231146000	1.937516000
1	3.047040000	-0.243204000	4.431967000
1	1.431011000	1.251959000	5.643688000
1	-0.659732000	1.974064000	4.426658000
1	-0.996054000	1.214244000	2.087335000
1	0.719259000	-2.380824000	-3.431294000
1	-0.357620000	-1.104911000	-2.839665000
1	-0.524912000	-4.367234000	-2.726083000
1	-1.446941000	-5.743452000	-0.840758000
1	-1.460576000	-4.747213000	1.474904000
1	-0.577249000	-2.431570000	1.780304000
1	-3.281532000	-2.406527000	0.387172000

1Bio_XVIII

(G = -3404.566553) (Triplet)

6	0.081975000	-2.623977000	-1.788438000
8	0.914156000	-2.390569000	-2.678871000
6	0.383984000	-3.592061000	-0.655171000
6	1.795040000	-4.198720000	-0.641032000
6	2.996558000	-3.230690000	-0.529045000
6	2.756566000	-1.999265000	0.380042000
6	2.655931000	-0.703787000	-0.436991000
1	-0.341347000	-4.413923000	-0.710444000
1	0.177671000	-3.089379000	0.295906000
1	1.930259000	-4.822159000	-1.532385000
1	1.813373000	-4.881707000	0.218139000
1	3.268143000	-2.884947000	-1.530875000
1	3.853933000	-3.804763000	-0.159012000
1	3.548611000	-1.896257000	1.127291000
1	1.839795000	-2.143906000	0.953389000
16	1.502598000	0.575501000	0.262078000
6	2.194677000	1.770124000	-0.950634000
6	3.710462000	1.547288000	-0.963697000
6	3.999361000	0.031227000	-0.669144000
7	4.864187000	0.097215000	0.504243000
6	5.193818000	1.380131000	0.861958000
7	4.403229000	2.227788000	0.125599000
8	6.026047000	1.711081000	1.715121000
1	5.489916000	-0.656741000	0.749911000
1	4.662104000	3.202570000	0.054853000
1	2.239358000	-0.934212000	-1.419987000
1	1.923722000	2.791483000	-0.677481000
1	1.791228000	1.535187000	-1.938660000
1	4.521357000	-0.451300000	-1.501262000
1	4.114524000	1.857375000	-1.932947000
7	-1.639966000	1.036494000	-1.954964000
6	-3.126614000	1.097425000	-2.010053000
6	-3.773047000	0.816257000	-0.650653000
7	-3.133136000	-0.336160000	0.011496000
6	-3.431474000	-1.611745000	-0.691772000
6	-2.232061000	-2.530757000	-0.919204000
7	-1.154751000	-2.019381000	-1.799396000
6	-1.063107000	0.204107000	-3.032231000
6	-1.499328000	-1.269820000	-3.019902000
6	-3.472492000	-0.396932000	1.444323000
6	-2.407749000	-1.111671000	2.240004000
7	-1.130213000	-0.759619000	1.947265000
6	-2.718883000	-2.025422000	3.245591000
6	-1.689636000	-2.587003000	4.005524000
6	-0.376549000	-2.197909000	3.734754000
6	-0.148081000	-1.287623000	2.705284000
6	-1.076027000	2.397530000	-1.953927000
6	-1.255816000	3.080812000	-0.613756000
6	-1.443949000	4.459507000	-0.508831000
6	-1.546071000	5.043536000	0.755874000
6	-1.468991000	4.220477000	1.883038000
6	-1.291005000	2.852353000	1.697228000
7	-1.181701000	2.285158000	0.479547000
27	-0.942469000	0.267173000	0.123701000
1	-3.491676000	0.387153000	-2.752245000
1	-3.455762000	2.085521000	-2.353409000
1	-4.854606000	0.660691000	-0.790889000
1	-3.642541000	1.678851000	0.003495000
1	-3.931667000	-1.394084000	-1.635886000
1	-4.150567000	-2.197297000	-0.104292000
1	-2.622642000	-3.472717000	-1.330017000
1	-1.795931000	-2.748375000	0.053175000
1	0.023371000	0.243874000	-2.923904000
1	-1.321512000	0.609172000	-4.025757000
1	-1.000154000	-1.745604000	-3.868422000
1	-2.569796000	-1.370401000	-3.194088000
1	-4.456897000	-0.853286000	1.620353000
1	-3.511320000	0.633785000	1.813581000

1	-3.756860000	-2.288367000	3.424736000
1	-1.909075000	-3.304780000	4.790109000
1	0.461378000	-2.590258000	4.301917000
1	0.858976000	-0.959965000	2.475405000
1	-1.510858000	3.020803000	-2.749629000
1	-0.007273000	2.323362000	-2.158268000
1	-1.509628000	5.061039000	-1.410360000
1	-1.690655000	6.114791000	0.858616000
1	-1.549635000	4.624604000	2.886978000
1	-1.232363000	2.167555000	2.537826000

1Bio_XIX

(G = -3405.089484) (Triplet)

C	-0.560331	-2.693761	-0.771374
O	-0.272739	-2.692498	-1.959044
C	0.4584153	-2.982582	0.3136848
C	1.8803838	-3.128137	-0.241765
C	2.5630186	-1.782376	-0.555415
C	3.2940857	-1.210544	0.6704905
C	3.8062565	0.2133043	0.4602990
H	0.1422076	-3.912417	0.8045904
H	0.4133444	-2.205222	1.0831720
H	1.8432043	-3.751329	-1.139943
H	2.4816272	-3.673648	0.4952953
H	1.8148602	-1.063340	-0.913008
H	3.2762222	-1.918163	-1.376615
H	4.1350409	-1.866368	0.9256642
H	2.6145090	-1.217418	1.5299346
S	4.6787502	0.8907858	1.9489601
C	5.2843801	2.2865600	0.9191914
C	5.6629938	1.6880277	-0.449583
C	4.8023262	0.3984243	-0.706402
N	5.8126882	-0.651924	-0.789951
C	7.0949653	-0.158863	-0.806263
N	7.0249178	1.1716244	-0.491429
O	8.1235385	-0.807219	-1.036219
H	5.6243581	-1.529238	-1.254988
H	7.8306178	1.7692030	-0.611604
H	2.9573662	0.8798999	0.2671817
H	6.1385871	2.7679460	1.4006717
H	4.4827717	3.0224690	0.8001322
H	4.2432453	0.4677279	-1.645107
H	5.5108344	2.4396619	-1.230850
N	-3.581854	-0.412873	-1.610164
C	-4.925656	-0.586305	-0.935122
C	-4.886000	-0.177331	0.5374309
N	-3.640453	-0.688091	1.1871316
C	-3.668231	-2.182246	1.3766848
C	-2.356906	-2.855005	0.9789179
N	-1.920243	-2.446857	-0.391314
C	-3.187710	-1.618732	-2.394832
C	-2.885374	-2.801529	-1.482270
C	-3.339226	0.0245015	2.4620832
C	-1.852518	0.1511123	2.6718921
N	-1.098225	0.1852171	1.5450674
C	-1.279656	0.3364195	3.9274784
C	0.0896249	0.5880731	4.0145982
C	0.8541491	0.6437229	2.8462671
C	0.2252671	0.4297021	1.6275424
C	-3.543291	0.8119815	-2.450962
C	-3.402738	2.0359908	-1.582994
C	-3.920517	3.2835014	-1.926451
C	-3.674422	4.3687473	-1.084556
C	-2.919876	4.1750547	0.0752235
C	-2.444496	2.8979936	0.3562394
N	-2.689429	1.8555897	-0.455321
Co	-2.138993	-0.172455	-0.124604
H	-5.228927	-1.627155	-1.038672
H	-5.676180	0.0158299	-1.454092
H	-5.778421	-0.548707	1.0546438
H	-4.867049	0.9088003	0.6228505
H	-4.500866	-2.583993	0.8018059
H	-3.870154	-2.415281	2.4253751
H	-2.481848	-3.942523	1.0283965
H	-1.577944	-2.567971	1.6819088
H	-2.288516	-1.359088	-2.952359
H	-3.983083	-1.889798	-3.099423
H	-2.465214	-3.606598	-2.087828
H	-3.791586	-3.185636	-1.019477
H	-3.824078	-0.456832	3.3160713
H	-3.740591	1.0397667	2.3823323
H	-1.904136	0.2925728	4.8133516
H	0.5554631	0.7404915	4.9832862
H	1.9199955	0.8412541	2.8721125
H	0.7635429	0.4367675	0.6893364
H	-4.427211	0.8780409	-3.092892
H	-2.657105	0.7475699	-3.089775
H	-4.503660	3.3920999	-2.834874
H	-4.068575	5.3504658	-1.328147
H	-2.706649	4.9914049	0.7566012
H	-1.861782	2.6900815	1.2463985
H	-1.020683	0.1775517	-1.022758

2Bio_I

(G = -4372.261249) (Quadruplet)

7	2.757127000	-0.784556000	-2.210338000
6	4.120640000	-1.404238000	-2.045570000
6	4.467283000	-1.796349000	-0.604408000
7	3.991338000	-0.819488000	0.412494000
6	4.780749000	0.440490000	0.478576000
6	4.515235000	1.412757000	-0.664386000
7	3.043046000	1.683845000	-0.829746000
6	2.818894000	0.456549000	-3.041362000
6	2.606292000	1.769236000	-2.256920000
16	2.679952000	3.207219000	-0.005042000
6	3.966648000	-1.446401000	1.758622000
6	2.844616000	-0.907584000	2.612266000
8	3.261093000	3.062692000	1.339586000
7	1.733771000	-0.515305000	1.955775000
6	2.904839000	-0.917309000	4.006052000
6	1.777954000	-0.538537000	4.735696000
6	0.619927000	-0.162102000	4.050651000
6	0.644411000	-0.159384000	2.660862000
6	1.791498000	-1.760437000	-2.774658000
6	1.418575000	-2.820012000	-1.764499000
6	1.053020000	-4.110143000	-2.151311000
6	0.682033000	-5.031493000	-1.171981000
6	0.708245000	-4.641979000	0.168789000
6	1.090329000	-3.339667000	0.473906000
7	1.421986000	-2.442887000	-0.470191000
27	1.963807000	-0.357615000	-0.146124000

8	3.132400000	4.315040000	-0.867218000
6	0.910406000	3.261835000	0.127194000
6	0.134257000	3.802289000	-0.902472000
6	-1.252794000	3.827988000	-0.779976000
6	-1.863199000	3.313029000	0.381123000
6	-1.058876000	2.806028000	1.422019000
6	0.321100000	2.780848000	1.299510000
7	-3.245804000	3.257447000	0.578472000
6	-4.281099000	3.640064000	-0.247932000
8	-4.108091000	4.174485000	-1.344501000
6	-5.665616000	3.305800000	0.285471000
6	-6.317781000	2.143997000	-0.503933000
6	-5.426407000	0.902872000	-0.663153000
6	-5.026347000	0.203534000	0.652933000
6	-3.681564000	-0.511627000	0.519349000
16	-3.126886000	-1.321808000	2.086183000
6	-1.828195000	-2.219050000	1.147073000
6	-2.387062000	-2.539281000	-0.257443000
6	-3.621888000	-1.621870000	-0.547507000
7	-4.735833000	-2.562103000	-0.477062000
6	-4.326215000	-3.872772000	-0.446917000
7	-2.954556000	-3.875540000	-0.389395000
8	-5.059391000	-4.868883000	-0.479132000
7	0.121464000	0.216984000	-0.934393000
6	-0.753168000	0.537563000	-1.619920000
6	-1.809810000	0.944085000	-2.523219000
1	4.866093000	-0.712928000	-2.431894000
1	4.189331000	-2.305589000	-2.663623000
1	5.553848000	-1.935948000	-0.527671000
1	3.990630000	-2.746828000	-0.367762000
1	5.854276000	0.210213000	0.508709000
1	4.510090000	0.934739000	1.412595000
1	4.891091000	1.045446000	-1.614117000
1	5.069900000	2.335286000	-0.468661000
1	2.040017000	0.421078000	-3.805468000
1	3.773292000	0.487460000	-3.570261000
1	3.133261000	2.575719000	-2.776863000
1	1.544281000	2.007329000	-2.243413000
1	4.931046000	-1.342728000	2.268329000
1	3.779097000	-2.516809000	1.631542000
1	3.820448000	-1.223711000	4.501328000
1	1.802312000	-0.539394000	5.821196000
1	-0.283135000	0.130904000	4.574801000
1	-0.220673000	0.141583000	2.083743000
1	2.184660000	-2.226696000	-3.686115000
1	0.882809000	-1.217496000	-3.046120000
1	1.065342000	-4.379694000	-3.202407000
1	0.387635000	-6.038963000	-1.449683000
1	0.437189000	-5.326251000	0.965324000
1	1.122869000	-2.988375000	1.498095000
1	0.600707000	4.198900000	-1.797340000
1	-1.860133000	4.231512000	-1.576730000
1	-1.524906000	2.421590000	2.324611000
1	0.935976000	2.398773000	2.104300000
1	-3.526781000	2.834522000	1.455880000
1	-6.280849000	4.204061000	0.174455000
1	-5.623433000	3.067779000	1.352350000
1	-6.585226000	2.507591000	-1.502562000
1	-7.254727000	1.880075000	0.001257000
1	-4.519819000	1.199748000	-1.202183000
1	-5.933584000	0.182208000	-1.315841000
1	-5.803269000	-0.508271000	0.954268000
1	-4.941489000	0.930729000	1.466740000
1	-2.916134000	0.229169000	0.261254000
1	-1.539315000	-3.121474000	1.688274000
1	-0.952050000	-1.580003000	1.042512000
1	-1.591210000	-2.391341000	-0.991895000
1	-3.563439000	-1.168146000	-1.541003000
1	-5.640886000	-2.336390000	-0.866911000
1	-2.461598000	-4.694732000	-0.059063000
1	-2.205675000	0.066595000	-3.041721000
1	-1.400906000	1.650027000	-3.252255000
1	-2.606235000	1.429935000	-1.957239000

2Bio_II

(G = −4239.495692) (Quadruplet)

7	-1.554278000	0.552343000	-2.270654000
6	-2.841929000	0.323778000	-3.017272000
6	-4.034520000	-0.035932000	-2.118099000
7	-3.679849000	-0.930263000	-0.983297000
6	-3.423247000	-2.347244000	-1.357232000
6	-2.064331000	-2.571764000	-2.010592000
7	-0.962465000	-1.988309000	-1.178156000
6	-0.409869000	-0.200749000	-2.870881000
6	0.125194000	-1.338380000	-1.978335000
16	-0.339346000	-3.249573000	-0.051775000
6	-4.715924000	-0.873629000	0.078752000
6	-4.110926000	-1.083635000	1.447815000
8	-0.975970000	-2.981880000	1.244840000
7	-2.844539000	-0.651274000	1.600907000
6	-4.833932000	-1.617074000	2.514979000
6	-4.232008000	-1.681063000	3.772212000
6	-2.923257000	-1.215437000	3.925957000
6	-2.261526000	-0.715347000	2.809565000
6	-1.255351000	1.999392000	-2.139153000
6	-2.219234000	2.666089000	-1.186547000
6	-2.659814000	3.977278000	-1.358625000
6	-3.495506000	4.541006000	-0.392986000
6	-3.875429000	3.773727000	0.710635000
6	-3.401874000	2.468443000	0.807154000
7	-2.585482000	1.929385000	-0.115630000
27	-1.866710000	-0.113111000	-0.174017000
8	-0.555440000	-4.563801000	-0.688251000
6	1.422653000	-2.997819000	0.086880000
6	2.267315000	-3.563398000	-0.874677000
6	3.639721000	-3.366062000	-0.761808000
6	4.161341000	-2.625882000	0.310770000
6	3.301498000	-2.126426000	1.300082000
6	1.923081000	-2.290477000	1.180720000
7	5.562731000	-2.433876000	0.396393000
6	6.263768000	-1.244635000	0.399485000
8	7.497436000	-1.270650000	0.432705000
6	5.486212000	0.051104000	0.273711000
6	4.936888000	0.240765000	-1.175229000
6	3.466539000	0.682848000	-1.276401000
6	3.170006000	2.177674000	-1.031437000
6	3.528381000	2.787818000	0.340703000

1	-2.683705000	-0.459065000	-3.755608000
1	-3.103866000	1.227289000	-3.577717000
1	-4.821661000	-0.485550000	-2.737794000
1	-4.437502000	0.874853000	-1.676032000
1	-4.211605000	-2.715470000	-2.027038000
1	-3.469626000	-2.931511000	-0.434618000
1	-2.008861000	-2.121038000	-2.995312000
1	-1.916308000	-3.642812000	-2.164886000
1	0.427849000	0.478649000	-3.043421000
1	-0.701974000	-0.588804000	-3.848019000
1	0.830388000	-0.925316000	-1.260390000
1	0.645213000	-2.060341000	-2.616986000
1	-5.524346000	-1.590045000	-0.107331000
1	-5.158058000	0.127083000	0.068753000
1	-5.847790000	-1.970034000	2.356206000
1	-4.774538000	-2.091388000	4.618559000
1	-2.419067000	-1.247512000	4.885748000
1	-1.237757000	-0.362544000	2.858882000
1	-1.264580000	2.502740000	-3.113269000
1	-0.249787000	2.095700000	-1.716816000
1	-2.351209000	4.538419000	-2.234567000
1	-3.849236000	5.561519000	-0.503514000
1	-4.527612000	4.171458000	1.480573000
1	-3.668354000	1.826807000	1.639699000
1	1.863301000	-4.131404000	-1.705290000
1	4.312025000	-3.771809000	-1.511235000
1	3.711733000	-1.610952000	2.161971000
1	1.251174000	-1.886804000	1.928537000
1	6.138375000	-3.249937000	0.208602000
1	6.175173000	0.852839000	0.544303000
1	4.671586000	0.068926000	0.997936000
1	5.027033000	-0.708457000	-1.715083000
1	5.577615000	0.953063000	-1.707895000
1	2.860342000	0.039348000	-0.635010000
1	3.129319000	0.477243000	-2.300503000
1	2.107462000	2.355536000	-1.236288000
1	3.726975000	2.745430000	-1.785410000
16	3.465469000	4.641375000	0.303136000
6	1.637714000	4.628167000	0.547235000
6	1.337312000	3.435347000	1.474345000
6	2.571549000	2.474240000	1.525539000
7	1.923057000	1.168193000	1.486053000
6	0.650312000	1.247489000	1.032490000
7	0.284931000	2.552019000	0.962130000
8	-0.042004000	0.248374000	0.709780000
1	2.440975000	0.308442000	1.388115000
1	-0.690686000	2.808087000	1.009287000
1	4.552699000	2.531101000	0.616461000
1	1.132289000	4.502467000	-0.413505000
1	1.333640000	5.581555000	0.983165000
1	3.120871000	2.598566000	2.459482000
1	1.079540000	3.783675000	2.478614000

2Bio_III

(G = −4239.486580) (Quadruplet)

7	-2.169337000	0.358429000	-2.291669000
6	-3.604644000	0.041869000	-2.627385000
6	-4.475379000	-0.260922000	-1.402504000
7	-3.767588000	-1.051292000	-0.360629000
6	-3.579221000	-2.488662000	-0.692037000
6	-2.457916000	-2.737532000	-1.690214000
7	-1.172794000	-2.067572000	-1.260886000
6	-1.214116000	-0.396452000	-3.160502000
6	-0.409984000	-1.478886000	-2.408957000
16	-0.213152000	-3.321091000	-0.394192000
6	-4.450272000	-0.925123000	0.948961000
6	-3.480869000	-1.142686000	2.084668000
8	-0.785938000	-3.355762000	0.958354000
7	-2.204776000	-0.752375000	1.870554000
6	-3.895005000	-1.672497000	3.306613000
6	-2.970640000	-1.795943000	4.342769000
6	-1.652466000	-1.394268000	4.120007000
6	-1.313128000	-0.887498000	2.870876000
6	-1.929147000	1.819380000	-2.336938000
6	-2.564155000	2.517052000	-1.158425000
6	-3.039674000	3.825422000	-1.240425000
6	-3.545839000	4.434566000	-0.092204000
6	-3.576366000	3.712033000	1.102971000
6	-3.098322000	2.405975000	1.101444000
7	-2.594563000	1.823410000	-0.001186000
27	-1.832659000	-0.170427000	-0.161806000
8	-0.249045000	-4.541525000	-1.223168000
6	1.487662000	-2.796076000	-0.323648000
6	2.303269000	-3.009603000	-1.443893000
6	3.658921000	-2.740614000	-1.348327000
6	4.220791000	-2.301697000	-0.132556000
6	3.396484000	-2.146253000	0.993135000
6	2.023769000	-2.369066000	0.893776000
7	5.617751000	-2.130070000	-0.110073000
6	6.457146000	-1.192636000	0.460707000
8	7.671374000	-1.316200000	0.268246000
6	5.923603000	0.006558000	1.216217000
6	5.732723000	1.229203000	0.279732000
6	4.455149000	1.210588000	-0.574797000
6	3.188777000	1.287019000	0.287774000
6	1.881953000	1.389241000	-0.519054000
1	-3.624421000	-0.796580000	-3.319242000
1	-4.048645000	0.889998000	-3.158156000
1	-5.385743000	-0.779725000	-1.729437000
1	-4.775003000	0.676144000	-0.934072000
1	-4.510682000	-2.916868000	-1.084322000
1	-3.335628000	-3.004139000	0.239049000
1	-2.704834000	-2.376139000	-2.682157000
1	-2.316260000	-3.814398000	-1.804346000
1	-0.484358000	0.292095000	-3.591043000
1	-1.756750000	-0.839187000	-3.996824000
1	0.488655000	-1.028722000	-1.988634000
1	-0.110162000	-2.250663000	-3.125688000
1	-5.298416000	-1.615077000	1.027025000
1	-4.845653000	0.090990000	1.033865000
1	-4.926618000	-1.984858000	3.431306000
1	-3.271429000	-2.206006000	5.301962000
1	-0.893194000	-1.478950000	4.889850000
1	-0.293698000	-0.591592000	2.655616000
1	-2.281324000	2.256500000	-3.278365000
1	-0.850880000	1.976296000	-2.278621000
1	-3.007930000	4.349612000	-2.189825000

1	-3.916162000	5.454352000	-0.130507000
1	-3.966851000	4.143712000	2.017998000
1	-3.105324000	1.798578000	1.999923000
1	1.889635000	-3.379932000	-2.374426000
1	4.299076000	-2.882665000	-2.213619000
1	3.819962000	-1.877095000	1.952551000
1	1.389491000	-2.249881000	1.764191000
1	6.119912000	-2.730039000	-0.759663000
1	6.690302000	0.246126000	1.957015000
1	5.003234000	-0.207681000	1.757163000
1	6.612523000	1.319056000	-0.367787000
1	5.716908000	2.125746000	0.911613000
1	4.418807000	0.305092000	-1.194164000
1	4.490533000	2.059788000	-1.266201000
1	3.264871000	2.140754000	0.970024000
1	3.134864000	0.396064000	0.913553000
16	0.490316000	0.648899000	0.467400000
6	0.340833000	2.191643000	1.451049000
6	0.564405000	3.350651000	0.463564000
6	1.391695000	2.843561000	-0.774807000
7	2.434112000	3.844227000	-0.873800000
6	2.417417000	4.768785000	0.133617000
7	1.404951000	4.414030000	1.006227000
8	3.179161000	5.732918000	0.256001000
1	3.122028000	3.878299000	-1.611736000
1	0.999819000	5.142429000	1.580117000
1	1.949096000	0.824606000	-1.452823000
1	1.121844000	2.178149000	2.214323000
1	-0.631944000	2.219964000	1.938650000
1	0.774054000	2.848851000	-1.672887000
1	-0.399991000	3.743857000	0.133726000

2Bio_IV

(G = −4372.193255) (Quadruplet)

7	-0.958734000	1.184379000	2.151200000
6	-1.522739000	2.525369000	2.468406000
6	-2.612615000	2.964409000	1.468240000
7	-2.418111000	2.422144000	0.098303000
6	-1.490651000	3.205038000	-0.756680000
6	-0.144224000	3.614775000	-0.190299000
7	0.900494000	2.514922000	-0.009495000
6	0.522209000	1.125776000	2.139915000
6	1.300831000	2.227215000	1.418090000
16	2.426831000	3.141266000	-1.061264000
6	-3.724813000	2.360870000	-0.611788000
6	-3.672507000	1.408163000	-1.779031000
8	1.914287000	2.990172000	-2.421041000
7	-2.896873000	0.320566000	-1.600549000
6	-4.417179000	1.598493000	-2.942437000
6	-4.364724000	0.626636000	-3.942575000
6	-3.568082000	-0.503880000	-3.749127000
6	-2.848380000	-0.615273000	-2.563604000
6	-1.458483000	0.146253000	3.087938000
6	-2.918468000	-0.146688000	2.858735000
6	-3.798823000	-0.457541000	3.893893000
6	-5.110840000	-0.816808000	3.578907000
6	-5.504891000	-0.843160000	2.239397000
6	-4.569705000	-0.498555000	1.266731000
7	-3.308410000	-0.158101000	1.569956000
27	-1.765076000	0.334850000	0.218442000
8	2.675714000	4.448574000	-0.458631000
6	3.759255000	2.047693000	-0.734848000
6	4.621492000	2.344034000	0.334086000
6	5.655286000	1.463225000	0.611628000
6	5.816403000	0.298039000	-0.159514000
6	4.998163000	0.072194000	-1.280381000
6	3.949116000	0.934949000	-1.565459000
7	6.814444000	-0.623090000	0.202077000
6	6.672380000	-1.971152000	0.497934000
8	7.674824000	-2.609539000	0.824887000
6	5.288485000	-2.589160000	0.523113000
6	4.491723000	-2.165067000	1.798999000
6	3.234621000	-1.311604000	1.555118000
6	2.053235000	-2.036883000	0.856407000
6	1.653465000	-1.473178000	-0.524935000
1	-0.719706000	3.256395000	2.515228000
1	-1.968305000	2.516912000	3.467972000
1	-2.676394000	4.060087000	1.448293000
1	-3.573622000	2.585915000	1.815135000
1	-1.969578000	4.158195000	-1.024614000
1	-1.334438000	2.642745000	-1.681862000
1	-0.213392000	4.152580000	0.750406000
1	0.253322000	4.326654000	-0.914028000
1	0.781021000	0.166307000	1.695162000
1	0.921265000	1.144468000	3.165039000
1	2.327701000	1.860786000	1.404056000
1	1.296675000	3.182456000	1.940491000
1	-4.048324000	3.357413000	-0.936279000
1	-4.470458000	1.984484000	0.092865000
1	-5.021694000	2.492617000	-3.054542000
1	-4.935239000	0.751020000	-4.857925000
1	-3.502105000	-1.286773000	-4.496865000
1	-2.222738000	-1.474611000	-2.360300000
1	-1.271942000	0.434115000	4.130248000
1	-0.914329000	-0.780392000	2.878132000
1	-3.456282000	-0.422588000	4.922959000
1	-5.814153000	-1.068426000	4.367024000
1	-6.512999000	-1.118075000	1.948332000
1	-4.825659000	-0.492635000	0.212820000
1	4.470963000	3.226116000	0.945811000
1	6.315162000	1.647878000	1.452943000
1	5.185697000	-0.781826000	-1.919407000
1	3.303957000	0.755638000	-2.417977000
1	7.690465000	-0.226245000	0.531850000
1	5.451787000	-3.668375000	0.515865000
1	4.718285000	-2.350111000	-0.374902000
1	5.154906000	-1.617233000	2.479872000
1	4.197618000	-3.074203000	2.335443000
1	3.499446000	-0.410886000	0.996113000
1	2.893914000	-0.957068000	2.535268000
1	1.175276000	-1.958406000	1.504024000
1	2.262342000	-3.108426000	0.774866000
16	2.481832000	-2.334031000	-1.939268000
6	1.259001000	-3.721909000	-1.818594000
6	-0.074931000	-3.098698000	-1.361536000
6	0.153675000	-1.624460000	-0.925017000
7	-0.800950000	-1.387229000	0.150161000

6	-1.186269000	-2.600074000	0.642864000
7	-0.621741000	-3.638631000	-0.119890000
8	-1.919120000	-2.821071000	1.624581000
1	-1.162551000	-4.494979000	-0.151555000
1	1.920297000	-0.416149000	-0.582009000
1	1.611794000	-4.458257000	-1.091303000
1	1.187197000	-4.203063000	-2.796095000
1	-0.022547000	-0.933287000	-1.754343000
1	-0.811308000	-3.160691000	-2.173057000
7	-6.195783000	-2.245794000	-1.719252000
6	-5.269774000	-2.835272000	-1.336650000
6	-4.104249000	-3.555906000	-0.847966000
1	-3.293288000	-3.484255000	-1.578115000
1	-3.770561000	-3.123561000	0.100397000
1	-4.356490000	-4.609261000	-0.693156000
1	0.599494000	1.643852000	-0.473412000

2Bio_V

(G = −4239.033427) (Quadruplet)

7	2.150189000	1.266203000	-1.812617000
6	3.231754000	2.264108000	-1.587278000
6	4.051977000	1.985336000	-0.312877000
7	3.292951000	1.288934000	0.758562000
6	2.442022000	2.167532000	1.619854000
6	1.585136000	3.252162000	0.974911000
7	0.345859000	2.813943000	0.251508000
6	0.823340000	1.875679000	-2.084316000
6	0.382561000	3.053008000	-1.218152000
16	-1.029479000	3.579342000	0.969145000
6	4.248705000	0.577047000	1.650846000
6	3.622889000	-0.591286000	2.370336000
8	-0.906241000	3.353892000	2.422289000
7	2.681174000	-1.260070000	1.679095000
6	4.072352000	-1.034480000	3.615100000
6	3.555037000	-2.221849000	4.133537000
6	2.608557000	-2.934362000	3.391694000
6	2.194714000	-2.413746000	2.170029000
6	2.477431000	0.362954000	-2.940460000
6	3.590217000	-0.585792000	-2.588487000
6	4.575017000	-0.971101000	-3.498182000
6	5.522956000	-1.919178000	-3.109551000
6	5.462856000	-2.447864000	-1.818298000
6	4.458031000	-2.000913000	-0.964171000
7	3.542666000	-1.092284000	-1.340023000
27	2.049345000	-0.265381000	-0.104227000
8	-1.139928000	4.973086000	0.481424000
6	-2.476763000	2.693314000	0.397186000
6	-3.015974000	2.931727000	-0.873643000
6	-4.147670000	2.235940000	-1.273506000
6	-4.794847000	1.335118000	-0.402277000
6	-4.303162000	1.192566000	0.906213000
6	-3.133140000	1.843530000	1.290766000
7	-5.934511000	0.690337000	-0.914179000
6	-6.561320000	-0.521540000	-0.683245000
8	-7.489222000	-0.833165000	-1.436588000
6	-6.156350000	-1.429867000	0.459938000
6	-6.041441000	-2.904164000	0.030715000
6	-4.771581000	-3.261936000	-0.770035000
6	-3.503783000	-3.529923000	0.073094000
6	-2.779261000	-2.284935000	0.587178000
1	2.806309000	3.262728000	-1.559241000
1	3.925003000	2.262782000	-2.434823000
1	4.487462000	2.921524000	0.061104000
1	4.876152000	1.322846000	-0.578585000
1	3.107428000	2.705708000	2.310592000
1	1.803312000	1.510573000	2.217307000
1	2.177320000	3.891978000	0.319075000
1	1.298473000	3.887583000	1.815043000
1	0.093539000	1.068810000	-1.996584000
1	0.792317000	2.253503000	-3.118707000
1	-0.621623000	3.270577000	-1.573814000
1	0.963084000	3.957306000	-1.426749000
1	4.721511000	1.266906000	2.360448000
1	5.041057000	0.158570000	1.023225000
1	4.818523000	-0.460462000	4.154908000
1	3.889087000	-2.588956000	5.099259000
1	2.190795000	-3.868127000	3.752238000
1	1.449573000	-2.911538000	1.558853000
1	2.723220000	0.932975000	-3.846413000
1	1.595575000	-0.254694000	-3.139748000
1	4.591565000	-0.532295000	-4.490503000
1	6.298428000	-2.235379000	-3.800755000
1	6.180026000	-3.184308000	-1.471947000
1	4.375457000	-2.368072000	0.052922000
1	-2.575653000	3.653044000	-1.551168000
1	-4.545091000	2.395603000	-2.271682000
1	-4.824999000	0.595910000	1.640719000
1	-2.752230000	1.708779000	2.295969000
1	-6.304944000	1.126470000	-1.755199000
1	-6.949994000	-1.323782000	1.211159000
1	-5.236107000	-1.104007000	0.929353000
1	-6.927553000	-3.156628000	-0.560446000
1	-6.078814000	-3.525673000	0.933708000
1	-4.571803000	-2.487948000	-1.523843000
1	-4.981116000	-4.181081000	-1.330543000
1	-2.791971000	-4.108918000	-0.526024000
1	-3.785030000	-4.161705000	0.925282000
16	-1.440943000	-2.684658000	1.809987000
6	-0.856316000	-0.950632000	1.648191000
6	-0.910983000	-0.616019000	0.149766000
6	-2.096174000	-1.413533000	-0.496592000
7	-1.411103000	-2.181944000	-1.521448000
6	-0.062489000	-1.839895000	-1.613274000
7	0.288212000	-1.015422000	-0.597217000
8	0.675833000	-2.279925000	-2.521994000
1	-3.469194000	-1.640077000	1.133904000
1	0.146377000	-0.834045000	2.057337000
1	-1.532825000	-0.300094000	2.209293000
1	-2.845027000	-0.744860000	-0.932811000
1	-1.050847000	0.463500000	0.047666000
1	-1.889740000	-2.455705000	-2.368633000

2Bio_VI

(G = −4372.193255) (Quadruplet)

7	-0.958734000	1.184379000	2.151200000
6	-1.522739000	2.525369000	2.468406000

6	-2.612615000	2.964409000	1.468240000
7	-2.418111000	2.422144000	0.098303000
6	-1.490651000	3.205038000	-0.756680000
6	-0.144224000	3.614775000	-0.190299000
7	0.900494000	2.514922000	-0.009495000
6	0.522209000	1.125776000	2.139915000
6	1.300831000	2.227215000	1.418090000
16	2.426831000	3.141266000	-1.061264000
6	-3.724813000	2.360870000	-0.611788000
6	-3.672507000	1.408163000	-1.779031000
8	1.914287000	2.990172000	-2.421041000
7	-2.896873000	0.320566000	-1.600549000
6	-4.417179000	1.598493000	-2.942437000
6	-4.364724000	0.626636000	-3.942575000
6	-3.568082000	-0.503880000	-3.749127000
6	-2.848380000	-0.615273000	-2.563604000
6	-1.458483000	0.146253000	3.087938000
6	-2.918468000	-0.146688000	2.858735000
6	-3.798823000	-0.457541000	3.893893000
6	-5.110840000	-0.816808000	3.578907000
6	-5.504891000	-0.843160000	2.239397000
6	-4.569705000	-0.498555000	1.266731000
7	-3.308410000	-0.158101000	1.569956000
27	-1.765076000	0.334850000	0.218442000
8	2.675714000	4.448574000	-0.458631000
6	3.759255000	2.047693000	-0.734848000
6	4.621492000	2.344034000	0.334086000
6	5.655286000	1.463225000	0.611628000
6	5.816403000	0.298039000	-0.159514000
6	4.998163000	0.072194000	-1.280381000
6	3.949116000	0.934949000	-1.565459000
7	6.814444000	-0.623090000	0.202077000
6	6.672380000	-1.971152000	0.497934000
8	7.674824000	-2.609539000	0.824887000
6	5.288485000	-2.589160000	0.523113000
6	4.491723000	-2.165067000	1.798999000
6	3.234621000	-1.311604000	1.555118000
6	2.053235000	-2.036883000	0.856407000
6	1.653465000	-1.473178000	-0.524935000
1	-0.719706000	3.256395000	2.515228000
1	-1.968305000	2.516912000	3.467972000
1	-2.676394000	4.060087000	1.448293000
1	-3.573622000	2.585915000	1.815135000
1	-1.969578000	4.158195000	-1.024614000
1	-1.334438000	2.642745000	-1.681862000
1	-0.213392000	4.152580000	0.750406000
1	0.253322000	4.326654000	-0.914028000
1	0.781021000	0.166307000	1.695162000
1	0.921265000	1.144468000	3.165039000
1	2.327701000	1.860786000	1.404056000
1	1.296675000	3.182456000	1.940491000
1	-4.048324000	3.357413000	-0.936279000
1	-4.470458000	1.984484000	0.092865000
1	-5.021694000	2.492617000	-3.054542000
1	-4.935239000	0.751020000	-4.857925000
1	-3.502105000	-1.286773000	-4.496865000
1	-2.222738000	-1.474611000	-2.360300000
1	-1.271942000	0.434115000	4.130248000
1	-0.914329000	-0.780392000	2.878132000
1	-3.456282000	-0.422588000	4.922959000
1	-5.814153000	-1.068426000	4.367024000
1	-6.512999000	-1.118075000	1.948332000
1	-4.825659000	-0.492635000	0.212820000
1	4.470963000	3.226116000	0.945811000
1	6.315162000	1.647878000	1.452943000
1	5.185697000	-0.781826000	-1.919407000
1	3.303957000	0.755638000	-2.417977000
1	7.690465000	-0.226245000	0.531850000
1	5.451787000	-3.668375000	0.515865000
1	4.718285000	-2.350111000	-0.374902000
1	5.154906000	-1.617233000	2.479872000
1	4.197618000	-3.074203000	2.335443000
1	3.499446000	-0.410886000	0.996113000
1	2.893914000	-0.957068000	2.535268000
1	1.175276000	-1.958406000	1.504024000
1	2.262342000	-3.108426000	0.774866000
16	2.481832000	-2.334031000	-1.939268000
6	1.259001000	-3.721909000	-1.818594000
6	-0.074931000	-3.098698000	-1.361536000
6	0.153675000	-1.624460000	-0.925017000
7	-0.800950000	-1.387229000	0.150161000
6	-1.186269000	-2.600074000	0.642864000
7	-0.621741000	-3.638631000	-0.119890000
8	-1.919120000	-2.821071000	1.624581000
1	-1.162551000	-4.494979000	-0.151555000
1	1.920297000	-0.416149000	-0.582009000
1	1.611794000	-4.458257000	-1.091303000
1	1.187197000	-4.203063000	-2.796095000
1	-0.022547000	-0.933287000	-1.754343000
1	-0.811308000	-3.160691000	-2.173057000
7	-6.195783000	-2.245794000	-1.719252000
6	-5.269774000	-2.835272000	-1.336650000
6	-4.104249000	-3.555906000	-0.847966000
1	-3.293288000	-3.484255000	-1.578115000
1	-3.770561000	-3.123561000	0.100397000
1	-4.356490000	-4.609261000	-0.693156000
1	0.599494000	1.643852000	-0.473412000

2Bio_VII

(G = −4371.767289) (Quadruplet)

7	1.019668000	1.207608000	-2.099495000
6	1.621011000	2.530822000	-2.427271000
6	2.641298000	3.003696000	-1.369898000
7	2.355804000	2.497944000	-0.005048000
6	1.360186000	3.299278000	0.760761000
6	0.074553000	3.729676000	0.071017000
7	-0.977220000	2.672680000	-0.128485000
6	-0.467954000	1.174973000	-2.144679000
6	-1.253778000	2.350396000	-1.555294000
16	-2.379325000	3.243739000	0.717412000
6	3.605215000	2.457545000	0.794920000
6	3.462478000	1.546838000	1.987799000
8	-1.995369000	3.265269000	2.141747000
7	2.712725000	0.443333000	1.786970000
6	4.114339000	1.786947000	3.196584000
6	3.998944000	0.849697000	4.224026000
6	3.238468000	-0.300481000	4.007147000

6	2.614417000	-0.463497000	2.773699000
6	1.546934000	0.150117000	-2.996278000
6	3.001456000	-0.128295000	-2.714453000
6	3.917896000	-0.460059000	-3.711036000
6	5.222214000	-0.797044000	-3.343559000
6	5.573432000	-0.782360000	-1.991975000
6	4.604803000	-0.418661000	-1.059751000
7	3.352409000	-0.096333000	-1.414394000
27	1.751784000	0.388786000	-0.141214000
8	-2.854353000	4.506419000	0.107091000
6	-3.676691000	2.032333000	0.489295000
6	-4.590762000	2.209080000	-0.556366000
6	-5.614517000	1.282174000	-0.721230000
6	-5.731486000	0.199422000	0.162408000
6	-4.860285000	0.085893000	1.253998000
6	-3.816781000	0.995862000	1.414246000
7	-6.748637000	-0.763897000	-0.059767000
6	-6.588940000	-2.093741000	-0.386872000
8	-7.589296000	-2.774729000	-0.638869000
6	-5.187739000	-2.663366000	-0.485840000
6	-4.443290000	-2.215095000	-1.782822000
6	-3.166237000	-1.381253000	-1.576968000
6	-1.986869000	-2.095262000	-0.863678000
6	-1.632322000	-1.547614000	0.536400000
1	0.831830000	3.265379000	-2.559552000
1	2.138098000	2.476071000	-3.390283000
1	2.701068000	4.100319000	-1.377872000
1	3.624994000	2.621362000	-1.642252000
1	1.847670000	4.233732000	1.077291000
1	1.104813000	2.733934000	1.660683000
1	0.262487000	4.234023000	-0.877012000
1	-0.322966000	4.508971000	0.725015000
1	-0.762842000	0.258625000	-1.632755000
1	-0.805953000	1.103233000	-3.189908000
1	-2.290601000	2.025149000	-1.649394000
1	-1.160507000	3.253164000	-2.168112000
1	3.913482000	3.462827000	1.109238000
1	4.399759000	2.051371000	0.162738000
1	4.697437000	2.693500000	3.321964000
1	4.495441000	1.014304000	5.175566000
1	3.128853000	-1.061824000	4.771859000
1	2.026810000	-1.345465000	2.557007000
1	1.394410000	0.412952000	-4.051225000
1	0.999255000	-0.773665000	-2.784319000
1	3.608596000	-0.458728000	-4.751222000
1	5.952775000	-1.065272000	-4.100894000
1	6.573134000	-1.043475000	-1.661862000
1	4.822590000	-0.388895000	0.002618000
1	-4.492661000	3.045107000	-1.239483000
1	-6.309433000	1.377848000	-1.549439000
1	-4.994127000	-0.718758000	1.967787000
1	-3.132226000	0.905228000	2.250114000
1	-7.678658000	-0.401563000	-0.249886000
1	-5.310994000	-3.748020000	-0.472891000
1	-4.600343000	-2.404244000	0.395184000
1	-5.127551000	-1.640341000	-2.419237000
1	-4.184324000	-3.113142000	-2.355272000
1	-3.408957000	-0.457038000	-1.047385000
1	-2.830141000	-1.067823000	-2.572956000
1	-1.094649000	-1.973404000	-1.484560000
1	-2.168594000	-3.174078000	-0.812536000
16	-2.450768000	-2.448685000	1.932502000
6	-1.184921000	-3.795729000	1.815335000
6	0.135874000	-3.121720000	1.395675000
6	-0.135909000	-1.652781000	0.962880000
7	0.834328000	-1.373361000	-0.088232000
6	1.267951000	-2.567918000	-0.580077000
7	0.728353000	-3.632914000	0.163253000
8	2.018850000	-2.760886000	-1.556772000
1	1.298099000	-4.470220000	0.197663000
1	-1.934979000	-0.502222000	0.604686000
1	-1.499034000	-4.529054000	1.067372000
1	-1.117449000	-4.292736000	2.785271000
1	-0.005115000	-0.962112000	1.800157000
1	0.854921000	-3.162898000	2.224064000
7	5.252314000	-2.573268000	1.918941000
6	5.013593000	-3.217694000	0.981029000
6	4.707141000	-4.009913000	-0.200097000
1	4.449422000	-5.031085000	0.097565000
1	3.859911000	-3.564378000	-0.736808000
1	5.580368000	-4.039476000	-0.858808000

2Bio_VIII

(G = −4239.019366) (Quadruplet)

7	1.418149000	0.635405000	-2.078932000
6	2.188882000	1.830559000	-2.525017000
6	3.264446000	2.259192000	-1.505290000
7	2.912670000	1.931498000	-0.100992000
6	2.028000000	2.923963000	0.572817000
6	0.807289000	3.450543000	-0.167420000
7	-0.375243000	2.528529000	-0.291407000
6	-0.059549000	0.795841000	-2.149399000
6	-0.681841000	2.116423000	-1.688311000
16	-1.693617000	3.353598000	0.479074000
6	4.146912000	1.811016000	0.715657000
6	3.905888000	1.012132000	1.971473000
8	-1.334713000	3.415292000	1.908664000
7	3.014765000	0.007368000	1.857496000
6	4.609942000	1.242927000	3.153401000
6	4.398175000	0.395730000	4.241338000
6	3.489098000	-0.657027000	4.113206000
6	2.817976000	-0.812827000	2.903917000
6	1.802516000	-0.568865000	-2.857097000
6	3.210048000	-1.000555000	-2.533194000
6	4.082271000	-1.525420000	-3.485663000
6	5.335273000	-1.983113000	-3.073168000
6	5.680433000	-1.894033000	-1.722708000
6	4.759098000	-1.337636000	-0.838222000
7	3.556915000	-0.897446000	-1.236195000
27	2.021439000	-0.068536000	-0.048158000
8	-1.966207000	4.628507000	-0.223318000
6	-3.150289000	2.332023000	0.290296000
6	-3.990127000	2.548877000	-0.809339000
6	-5.122367000	1.756055000	-0.961515000
6	-5.420579000	0.767963000	-0.011466000
6	-4.622609000	0.630175000	1.131991000
6	-3.471007000	1.401254000	1.280289000

7	-6.541255000	-0.075049000	-0.221633000
6	-6.536805000	-1.437302000	-0.440042000
8	-7.601957000	-2.005523000	-0.705095000
6	-5.217509000	-2.184105000	-0.410747000
6	-4.364237000	-1.945652000	-1.696557000
6	-2.996032000	-1.275455000	-1.481065000
6	-1.965292000	-2.081033000	-0.644802000
6	-1.574615000	-1.445239000	0.708474000
1	1.502461000	2.646909000	-2.731593000
1	2.691305000	1.619073000	-3.474206000
1	3.475445000	3.331033000	-1.617264000
1	4.183648000	1.716562000	-1.726713000
1	2.630219000	3.816154000	0.801074000
1	1.708697000	2.486625000	1.522460000
1	1.064231000	3.842423000	-1.152004000
1	0.512724000	4.328497000	0.412038000
1	-0.476668000	-0.018119000	-1.557899000
1	-0.397339000	0.667426000	-3.189043000
1	-1.751804000	1.926892000	-1.775564000
1	-0.459382000	2.936855000	-2.378530000
1	4.567576000	2.795393000	0.957024000
1	4.892435000	1.273108000	0.123647000
1	5.308588000	2.071465000	3.209834000
1	4.932942000	0.554661000	5.172892000
1	3.296606000	-1.343693000	4.930454000
1	2.107492000	-1.615327000	2.753844000
1	1.680462000	-0.398090000	-3.934567000
1	1.138363000	-1.385537000	-2.555723000
1	3.778644000	-1.576630000	-4.526252000
1	6.031840000	-2.399546000	-3.794715000
1	6.642462000	-2.238960000	-1.358982000
1	4.979227000	-1.235368000	0.219961000
1	-3.751078000	3.307924000	-1.545425000
1	-5.762204000	1.878015000	-1.829734000
1	-4.898461000	-0.088177000	1.895104000
1	-2.840330000	1.284760000	2.154458000
1	-7.401676000	0.383053000	-0.508231000
1	-5.479865000	-3.239637000	-0.316737000
1	-4.639946000	-1.923766000	0.476755000
1	-4.934594000	-1.337080000	-2.409029000
1	-4.206367000	-2.912763000	-2.187550000
1	-3.134789000	-0.286559000	-1.038386000
1	-2.572360000	-1.093224000	-2.476123000
1	-1.046334000	-2.172025000	-1.231724000
1	-2.320244000	-3.105181000	-0.489955000
16	-2.573032000	-2.066084000	2.140419000
6	-1.533534000	-3.597287000	2.203306000
6	-0.107317000	-3.176224000	1.797881000
6	-0.128588000	-1.733780000	1.216945000
7	0.909506000	-1.710750000	0.194895000
6	1.185905000	-3.001109000	-0.152157000
7	0.449143000	-3.891903000	0.654209000
8	1.942493000	-3.401378000	-1.055406000
1	0.875864000	-4.798986000	0.800358000
1	-1.711882000	-0.364315000	0.657752000
1	-1.932126000	-4.337626000	1.504033000
1	-1.584364000	-4.008513000	3.213731000
1	0.080326000	-0.992303000	1.993598000
1	0.559182000	-3.241951000	2.667594000

2Bio_IX

(G = -4371.773971) (Quadruplet)

7	1.829941000	1.434064000	-1.934371000
6	2.692468000	2.646217000	-1.877258000
6	3.582636000	2.689347000	-0.622145000
7	2.989685000	2.017625000	0.564169000
6	1.997796000	2.829673000	1.332880000
6	0.939919000	3.622738000	0.577443000
7	-0.207799000	2.851958000	-0.012926000
6	0.407265000	1.732494000	-2.234763000
6	-0.260313000	2.895197000	-1.501004000
16	-1.655424000	3.487881000	0.692051000
6	4.081113000	1.645930000	1.505333000
6	3.714803000	0.497501000	2.409261000
8	-1.486315000	3.339824000	2.150544000
7	2.945079000	-0.457980000	1.851413000
6	4.255887000	0.354437000	3.687025000
6	4.029015000	-0.832120000	4.385429000
6	3.282499000	-1.844693000	3.778689000
6	2.755165000	-1.613114000	2.511830000
6	2.324077000	0.477397000	-2.953086000
6	3.603925000	-0.182125000	-2.517118000
6	4.652054000	-0.460643000	-3.394702000
6	5.783161000	-1.121839000	-2.913701000
6	5.836894000	-1.480570000	-1.565314000
6	4.753002000	-1.165512000	-0.751381000
7	3.660507000	-0.534129000	-1.215548000
27	2.065966000	0.148634000	-0.020331000
8	-1.911192000	4.843652000	0.152676000
6	-3.027460000	2.456858000	0.184244000
6	-3.644725000	2.671149000	-1.055389000
6	-4.768858000	1.931930000	-1.391018000
6	-5.338767000	1.023881000	-0.475135000
6	-4.771797000	0.905942000	0.803761000
6	-3.595970000	1.586638000	1.117437000
7	-6.500805000	0.357217000	-0.904383000
6	-7.061886000	-0.884768000	-0.673669000
8	-8.058732000	-1.187208000	-1.339224000
6	-6.509664000	-1.872142000	0.334746000
6	-6.032339000	-3.182707000	-0.340604000
6	-4.553474000	-3.209725000	-0.771918000
6	-3.553732000	-3.357796000	0.406086000
6	-2.962938000	-2.033221000	0.904978000
1	2.073974000	3.536599000	-1.938789000
1	3.349074000	2.680664000	-2.752963000
1	3.847257000	3.729860000	-0.390466000
1	4.507340000	2.154526000	-0.840607000
1	2.554401000	3.580128000	1.912830000
1	1.509641000	2.155898000	2.042709000
1	1.384090000	4.254064000	-0.192427000
1	0.555532000	4.319144000	1.325618000
1	-0.149297000	0.818495000	-2.025302000
1	0.291880000	1.966248000	-3.305173000
1	-1.296759000	2.828953000	-1.824678000
1	0.101371000	3.865625000	-1.855414000
1	4.417822000	2.511902000	2.087930000
1	4.932066000	1.301313000	0.909402000
1	4.852826000	1.154681000	4.112278000

1	4.439731000	-0.969158000	5.381248000
1	3.104577000	-2.793599000	4.273133000
1	2.176454000	-2.366139000	1.994062000
1	2.452983000	0.968196000	-3.927109000
1	1.577706000	-0.318222000	-3.049395000
1	4.577677000	-0.156805000	-4.433729000
1	6.611081000	-1.347389000	-3.579029000
1	6.696071000	-1.993369000	-1.146703000
1	4.744262000	-1.419791000	0.301953000
1	-3.270571000	3.413678000	-1.750117000
1	-5.230023000	2.071579000	-2.364520000
1	-5.248593000	0.310403000	1.570316000
1	-3.152700000	1.468644000	2.099406000
1	-6.965623000	0.813701000	-1.685800000
1	-7.355682000	-2.094814000	0.993944000
1	-5.725335000	-1.453606000	0.955851000
1	-6.676089000	-3.379767000	-1.204630000
1	-6.199452000	-4.007771000	0.361697000
1	-4.319344000	-2.317844000	-1.368868000
1	-4.422435000	-4.065733000	-1.444525000
1	-2.727369000	-4.017497000	0.122160000
1	-4.068675000	-3.847157000	1.241135000
16	-2.134366000	-2.196368000	2.571035000
6	-0.482916000	-1.734710000	1.932104000
6	-0.709062000	-0.816537000	0.714179000
6	-1.951769000	-1.352148000	-0.048574000
7	-1.286600000	-2.229836000	-1.007467000
6	0.011184000	-1.755007000	-1.238492000
7	0.392488000	-0.902348000	-0.256231000
8	0.679172000	-2.115430000	-2.233938000
1	-3.771586000	-1.329429000	1.074614000
1	0.054080000	-2.634147000	1.622735000
1	0.077276000	-1.237107000	2.725465000
1	-2.464412000	-0.532720000	-0.568660000
1	-0.858824000	0.213491000	1.047074000
7	3.404506000	-4.422289000	0.632887000
6	3.312786000	-4.278799000	-0.517446000
6	3.183715000	-4.080884000	-1.952725000
1	2.988044000	-5.040410000	-2.441394000
1	2.351699000	-3.391303000	-2.145844000
1	4.110441000	-3.656625000	-2.349545000
1	-1.795670000	-2.521003000	-1.833476000

2Bio_X
(G = -4372.243991) (Quadruplet)

7	-2.681993000	1.260490000	-0.557333000
6	-4.079154000	1.445883000	-0.037568000
6	-4.213942000	0.925915000	1.387155000
7	-3.609564000	-0.420732000	1.577466000
6	-4.368699000	-1.546695000	0.969542000
6	-4.265648000	-1.625156000	-0.546992000
7	-2.829842000	-1.549492000	-1.010295000
6	-2.673420000	0.838040000	-1.987946000
6	-2.667679000	-0.706414000	-2.240728000
16	-2.301165000	-3.228056000	-1.362556000
6	-3.408011000	-0.695248000	3.022962000
6	-2.076462000	-1.347917000	3.294766000
8	-2.789442000	-4.017894000	-0.221458000
7	-1.106017000	-1.122842000	2.387588000
6	-1.823362000	-2.060578000	4.466952000
6	-0.529903000	-2.519693000	4.714714000
6	0.480326000	-2.245992000	3.788753000
6	0.148200000	-1.546700000	2.635561000
6	-1.850845000	2.488872000	-0.309938000
6	-2.217451000	3.715190000	-1.119619000
6	-1.552018000	4.002811000	-2.319033000
6	-1.919102000	5.135041000	-3.047189000
6	-2.938196000	5.949607000	-2.551634000
6	-3.537304000	5.596408000	-1.340041000
7	-3.190668000	4.510490000	-0.631486000
27	-1.698505000	-0.342152000	0.550835000
8	-2.748851000	-3.564811000	-2.724386000
6	-0.531769000	-3.178705000	-1.310275000
6	0.212947000	-2.974062000	-2.474934000
6	1.602300000	-2.900914000	-2.399215000
6	2.242303000	-3.025472000	-1.149773000
6	1.473049000	-3.286269000	0.002259000
6	0.092815000	-3.360063000	-0.071403000
7	3.615967000	-2.863346000	-0.952443000
6	4.616762000	-2.586523000	-1.859476000
8	4.437879000	-2.576530000	-3.078075000
6	5.952270000	-2.230388000	-1.227797000
6	6.262644000	-0.723946000	-1.406847000
6	5.133866000	0.221298000	-0.967144000
6	4.808010000	0.204481000	0.539265000
6	3.408169000	0.758159000	0.808792000
16	2.938100000	0.773879000	2.598853000
6	1.464505000	1.788581000	2.171115000
6	1.903293000	2.776898000	1.070861000
6	3.156315000	2.200742000	0.324149000
7	4.211406000	3.130308000	0.708110000
6	3.751813000	4.214243000	1.409025000
7	2.398702000	4.052035000	1.576518000
8	4.427650000	5.170642000	1.809522000
7	0.024875000	-0.103430000	-0.625951000
6	0.688598000	0.178373000	-1.531188000
6	1.457575000	0.559514000	-2.697115000
1	-4.776987000	0.957103000	-0.710567000
1	-4.342217000	2.506256000	-0.045808000
1	-5.271241000	0.927306000	1.684055000
1	-3.671458000	1.601017000	2.053240000
1	-5.428070000	-1.489027000	1.254260000
1	-3.949420000	-2.464494000	1.384541000
1	-4.809594000	-0.831392000	-1.047825000
1	-4.736275000	-2.555382000	-0.876020000
1	-1.769571000	1.233530000	-2.448334000
1	-3.522666000	1.288937000	-2.507935000
1	-3.444548000	-0.967840000	-2.962787000
1	-1.704834000	-0.965006000	-2.680254000
1	-4.226524000	-1.295431000	3.434335000
1	-3.412584000	0.255749000	3.563347000
1	-2.630266000	-2.240563000	5.169805000
1	-0.311718000	-3.077977000	5.620078000
1	1.503083000	-2.568369000	3.949025000
1	0.885812000	-1.316419000	1.878189000
1	-0.817488000	2.220582000	-0.518695000
1	-1.933319000	2.709578000	0.756902000

1	-0.756766000	3.351188000	-2.667597000
1	-1.415891000	5.377511000	-3.978697000
1	-3.258048000	6.842071000	-3.080033000
1	-4.325304000	6.214530000	-0.915655000
1	-0.280608000	-2.859012000	-3.433684000
1	2.184541000	-2.724359000	-3.291654000
1	1.967978000	-3.404771000	0.961607000
1	-0.493761000	-3.546224000	0.819774000
1	3.903721000	-2.870773000	0.019565000
1	6.724488000	-2.818719000	-1.733242000
1	5.968517000	-2.503205000	-0.168479000
1	6.473770000	-0.539051000	-2.466150000
1	7.183480000	-0.500054000	-0.854612000
1	4.226976000	-0.029758000	-1.530144000
1	5.398573000	1.241410000	-1.270191000
1	5.558165000	0.781231000	1.092769000
1	4.847012000	-0.819972000	0.924450000
1	2.679968000	0.112956000	0.306899000
1	1.092745000	2.304570000	3.059710000
1	0.672056000	1.138093000	1.788495000
1	1.068970000	2.941324000	0.384966000
1	3.013912000	2.200953000	-0.760067000
1	5.091381000	3.181584000	0.214153000
1	1.916273000	4.561599000	2.304857000
1	1.693570000	1.626178000	-2.645353000
1	0.858098000	0.358351000	-3.590601000
1	2.380017000	-0.022409000	-2.744080000

2Bio_XI

(G = -4239.477515) (Quadruplet)

7	-1.466827000	1.766111000	-1.113232000
6	-2.763634000	2.320779000	-1.631734000
6	-3.945522000	1.960168000	-0.740011000
7	-3.955438000	0.527212000	-0.338811000
6	-4.223419000	-0.455141000	-1.425957000
6	-3.021350000	-0.736432000	-2.327636000
7	-1.773799000	-1.006834000	-1.530381000
6	-0.645540000	1.154464000	-2.206068000
6	-0.541397000	-0.380018000	-2.116060000
16	-1.581993000	-2.795000000	-1.318194000
6	-4.897364000	0.309743000	0.788745000
6	-4.379314000	-0.739832000	1.742597000
8	-2.210061000	-3.101797000	-0.026112000
7	-3.039648000	-0.859083000	1.815395000
6	-5.224213000	-1.501354000	2.549838000
6	-4.661790000	-2.390019000	3.466219000
6	-3.270534000	-2.499085000	3.544564000
6	-2.495068000	-1.721227000	2.692460000
6	-0.705600000	2.772025000	-0.304368000
6	-0.221055000	4.008405000	-1.034376000
6	-0.923402000	5.218486000	-0.964539000
6	-0.430238000	6.332552000	-1.646721000
6	0.751624000	6.202885000	-2.376669000
6	1.392425000	4.960809000	-2.383221000
7	0.929179000	3.886598000	-1.727893000
27	-1.969270000	0.160396000	0.340357000
8	-2.094820000	-3.442936000	-2.539274000
6	0.171909000	-3.106262000	-1.225014000
6	0.877648000	-3.339743000	-2.410958000
6	2.247695000	-3.566185000	-2.342001000
6	2.902613000	-3.568922000	-1.099795000
6	2.164366000	-3.397909000	0.080919000
6	0.795779000	-3.142875000	0.023314000
7	4.301626000	-3.792186000	-1.067958000
6	5.296015000	-2.963876000	-0.584417000
8	6.475978000	-3.303177000	-0.710240000
6	4.898711000	-1.629339000	0.014718000
6	4.431710000	-0.626573000	-1.083903000
6	3.180378000	0.199292000	-0.740965000
6	3.366062000	1.388430000	0.225666000
6	3.847347000	1.132523000	1.671274000
1	-2.925242000	1.959724000	-2.644222000
1	-2.712680000	3.409978000	-1.706233000
1	-4.881792000	2.233673000	-1.244774000
1	-3.875594000	2.534284000	0.187247000
1	-5.064379000	-0.120773000	-2.047389000
1	-4.517190000	-1.387895000	-0.938832000
1	-2.805657000	0.093690000	-2.991449000
1	-3.259965000	-1.581883000	-2.976556000
1	0.373667000	1.537373000	-2.155310000
1	-1.043891000	1.459126000	-3.175146000
1	0.278824000	-0.632272000	-1.447577000
1	-0.325164000	-0.779028000	-3.112565000
1	-5.899707000	0.051233000	0.429612000
1	-4.984589000	1.246513000	1.346721000
1	-6.299791000	-1.393176000	2.454908000
1	-5.299289000	-2.993154000	4.105559000
1	-2.793040000	-3.180663000	4.240085000
1	-1.413440000	-1.784982000	2.684644000
1	0.160507000	2.253825000	0.103387000
1	-1.354300000	3.057784000	0.527805000
1	-1.835160000	5.282686000	-0.378652000
1	-0.956895000	7.281484000	-1.605025000
1	1.176690000	7.040133000	-2.921091000
1	2.322368000	4.824612000	-2.931030000
1	0.371695000	-3.325249000	-3.369608000
1	2.820031000	-3.723851000	-3.250726000
1	2.660204000	-3.469531000	1.043026000
1	0.225587000	-2.983836000	0.930130000
1	4.646916000	-4.525882000	-1.680490000
1	5.774599000	-1.254130000	0.546299000
1	4.115114000	-1.778033000	0.756615000
1	4.210008000	-1.181677000	-2.002309000
1	5.264142000	0.043216000	-1.329561000
1	2.390476000	-0.477905000	-0.407464000
1	2.811122000	0.638508000	-1.676716000
1	2.425091000	1.948132000	0.257710000
1	4.101680000	2.060543000	-0.230740000
16	4.270391000	2.728502000	2.517395000
6	2.496209000	3.033702000	2.927009000
6	1.871015000	1.650777000	3.194531000
6	2.829427000	0.525833000	2.678557000
7	1.879274000	-0.430390000	2.115234000
6	0.706065000	0.175019000	1.814521000
7	0.660306000	1.383891000	2.408867000
8	-0.165188000	-0.338086000	1.060558000
1	2.177358000	-1.223074000	1.566181000
1	-0.204835000	1.898804000	2.509551000
1	4.762574000	0.537106000	1.669744000
1	1.997774000	3.528766000	2.089997000
1	2.446332000	3.685526000	3.800923000
1	3.379465000	0.075481000	3.505185000
1	1.660949000	1.522198000	4.260160000

2Bio_XII
(G = -4504.989257) (Quadruplet)

7	-2.951308000	0.955957000	-0.822881000
6	-4.367994000	1.009042000	-0.337546000
6	-4.450489000	0.866055000	1.184850000
7	-3.606983000	-0.236276000	1.733179000
6	-4.175538000	-1.602521000	1.570247000
6	-4.269377000	-2.085160000	0.135134000
7	-2.970787000	-1.924519000	-0.622331000
6	-2.807207000	0.173080000	-2.076501000
6	-3.177070000	-1.317463000	-1.978777000
16	-2.202848000	-3.498955000	-0.733677000
6	-3.332231000	-0.022971000	3.176967000
6	-2.064136000	-0.726432000	3.598810000
8	-2.365365000	-4.095903000	0.603431000
7	-1.129639000	-0.885703000	2.641022000
6	-1.831502000	-1.109399000	4.920107000
6	-0.588217000	-1.642294000	5.260354000
6	0.387684000	-1.776018000	4.269418000
6	0.072978000	-1.387021000	2.971790000
6	-2.384657000	2.336657000	-1.004253000
6	-2.870988000	3.089951000	-2.225298000
6	-2.117320000	3.095254000	-3.406982000
6	-2.597774000	3.788770000	-4.518044000
6	-3.819193000	4.456733000	-4.414252000
6	-4.499837000	4.406093000	-3.195491000
7	-4.044052000	3.744995000	-2.119724000
27	-1.741799000	-0.126333000	0.726108000
8	-2.742616000	-4.213800000	-1.906590000
6	-0.472056000	-3.188028000	-0.999315000
6	0.048576000	-3.012401000	-2.284215000
6	1.420622000	-2.833636000	-2.454527000
6	2.274856000	-2.846707000	-1.334117000
6	1.729868000	-3.039885000	-0.048981000
6	0.365853000	-3.211860000	0.119476000
7	3.662073000	-2.684173000	-1.401835000
6	4.488677000	-2.481378000	-2.485474000
8	4.077169000	-2.404936000	-3.644505000
6	5.958640000	-2.323686000	-2.125991000
6	6.444562000	-0.861363000	-2.274143000
6	5.550928000	0.177968000	-1.581132000
6	5.424382000	0.033261000	-0.047789000
6	4.051743000	0.500251000	0.437102000
16	3.789223000	0.303798000	2.257452000
6	2.261285000	1.315530000	2.111383000
6	2.540489000	2.424031000	1.074425000
6	3.718688000	1.977621000	0.144737000
7	4.786585000	2.898822000	0.517084000
6	4.367967000	3.897848000	1.358434000
7	3.045714000	3.667233000	1.645343000
8	5.052659000	4.841049000	1.774638000
7	-0.051491000	0.033791000	-0.461570000
6	0.679224000	0.269526000	-1.326232000
6	1.539079000	0.580465000	-2.448814000
1	-4.945683000	0.242721000	-0.845142000
1	-4.825202000	1.961855000	-0.614989000
1	-5.497776000	0.737660000	1.486802000
1	-4.079995000	1.788439000	1.636600000
1	-5.178031000	-1.642468000	2.018041000
1	-3.526340000	-2.283801000	2.122909000
1	-5.039537000	-1.554460000	-0.415581000
1	-4.586886000	-3.130788000	0.155604000
1	-1.766414000	0.268265000	-2.383095000
1	-3.422811000	0.600744000	-2.876758000
1	-4.214512000	-1.485649000	-2.274911000
1	-2.565214000	-1.836676000	-2.716046000
1	-4.180125000	-0.339451000	3.795766000
1	-3.184725000	1.048120000	3.342148000
1	-2.613243000	-0.982204000	5.661945000
1	-0.382992000	-1.944856000	6.282689000
1	1.372436000	-2.173372000	4.490003000
1	0.794611000	-1.467236000	2.168402000
1	-1.300348000	2.237017000	-1.052697000
1	-2.632849000	2.901304000	-0.106114000
1	-1.173928000	2.559406000	-3.447492000
1	-2.031116000	3.807114000	-5.444480000
1	-4.235324000	5.010271000	-5.250046000
1	-5.448804000	4.923731000	-3.074086000
1	-0.598266000	-3.024485000	-3.154143000
1	1.830037000	-2.691110000	-3.443993000
1	2.384603000	-3.056601000	0.817649000
1	-0.046986000	-3.382273000	1.105165000
1	4.128089000	-2.719794000	-0.502750000
1	6.527174000	-2.962034000	-2.809576000
1	6.144629000	-2.685646000	-1.110875000
1	6.495881000	-0.615450000	-3.340988000
1	7.468526000	-0.807817000	-1.884840000
1	4.553919000	0.119993000	-2.032799000
1	5.922798000	1.181302000	-1.820084000
1	6.214570000	0.603374000	0.453336000
1	5.557045000	-1.009614000	0.257029000
1	3.284212000	-0.110608000	-0.051563000
1	1.985191000	1.723842000	3.085943000
1	1.446446000	0.685572000	1.753237000
1	1.626241000	2.611054000	0.503990000
1	3.464795000	2.090620000	-0.912514000
1	5.593569000	3.045806000	-0.073454000
1	2.622154000	4.092194000	2.459376000
1	1.719224000	1.658499000	-2.481563000
1	1.045132000	0.260319000	-3.370899000
1	2.486272000	0.049471000	-2.341730000
7	-1.165897000	1.756091000	1.656405000
6	-0.811416000	2.710444000	2.205041000
6	-0.357481000	3.910088000	2.883315000
1	0.412446000	3.644988000	3.613742000
1	0.060145000	4.606435000	2.150277000
1	-1.200414000	4.382316000	3.396299000

2Bio_XIII
(G = -4372.226191) (Quadruplet)

7	-1.450810000	1.427873000	-1.419924000
6	-2.750470000	1.700661000	-2.130792000
6	-3.975447000	1.160898000	-1.389955000
7	-3.787950000	-0.217726000	-0.861440000
6	-3.734108000	-1.291088000	-1.892442000
6	-2.399399000	-1.385524000	-2.621424000

7	-1.250317000	-1.421191000	-1.656483000
6	-0.415430000	0.863523000	-2.347220000
6	-0.071094000	-0.615601000	-2.105933000
16	-0.805144000	-3.140300000	-1.344776000
6	-4.830446000	-0.553265000	0.142094000
6	-4.298349000	-1.531769000	1.164573000
8	-1.492556000	-3.525107000	-0.105819000
7	-2.975072000	-1.469761000	1.399916000
6	-5.127142000	-2.396650000	1.879968000
6	-4.566534000	-3.192701000	2.879368000
6	-3.194148000	-3.106765000	3.130402000
6	-2.431902000	-2.235621000	2.358883000
6	-0.945567000	2.645545000	-0.701088000
6	-0.488231000	3.806371000	-1.562478000
6	-1.337060000	4.886750000	-1.839677000
6	-0.869087000	5.936308000	-2.632444000
6	0.437061000	5.878494000	-3.119725000
6	1.220641000	4.772488000	-2.780178000
7	0.780406000	3.760374000	-2.018506000
27	-1.918327000	-0.134271000	0.144780000
8	-1.085798000	-3.903953000	-2.576491000
6	0.960943000	-3.170949000	-1.084550000
6	1.798773000	-3.333050000	-2.193408000
6	3.175019000	-3.361397000	-1.995500000
6	3.705098000	-3.238785000	-0.702017000
6	2.845338000	-3.136848000	0.401753000
6	1.465208000	-3.083168000	0.213987000
7	5.113760000	-3.261148000	-0.534420000
6	5.928506000	-2.261764000	-0.041921000
8	7.152239000	-2.423733000	-0.041207000
6	5.282250000	-0.969033000	0.415502000
6	4.767180000	-0.128250000	-0.792955000
6	3.377902000	0.507839000	-0.615897000
6	3.293449000	1.761293000	0.279108000
6	3.681938000	1.642281000	1.768640000
1	-2.700606000	1.286177000	-3.134780000
1	-2.894009000	2.775599000	-2.260007000
1	-4.846314000	1.207607000	-2.057409000
1	-4.176996000	1.797416000	-0.526817000
1	-4.538745000	-1.154233000	-2.626385000
1	-3.913804000	-2.235311000	-1.372905000
1	-2.240002000	-0.547884000	-3.290670000
1	-2.407632000	-2.273331000	-3.257277000
1	0.519242000	1.409943000	-2.220913000
1	-0.727712000	1.024634000	-3.380988000
1	0.665848000	-0.679245000	-1.308916000
1	0.366708000	-1.017666000	-3.026307000
1	-5.737545000	-0.939132000	-0.336723000
1	-5.104677000	0.364057000	0.670879000
1	-6.188002000	-2.436135000	1.654628000
1	-5.190561000	-3.872316000	3.451853000
1	-2.719552000	-3.707757000	3.898600000
1	-1.359406000	-2.142213000	2.487875000
1	-0.109021000	2.321415000	-0.082268000
1	-1.747657000	2.974123000	-0.040959000
1	-2.342485000	4.905261000	-1.430761000
1	-1.509934000	6.783431000	-2.859123000
1	0.847724000	6.670996000	-3.737294000
1	2.249214000	4.699732000	-3.126958000
1	1.386985000	-3.418978000	-3.192492000
1	3.845899000	-3.460740000	-2.842930000
1	3.257447000	-3.106063000	1.404882000
1	0.795224000	-2.984002000	1.059597000
1	5.613400000	-3.976098000	-1.055862000
1	6.041547000	-0.426185000	0.980554000
1	4.467336000	-1.191436000	1.104649000
1	4.716271000	-0.772131000	-1.677939000
1	5.505992000	0.647579000	-1.025409000
1	2.675201000	-0.264552000	-0.295932000
1	3.031720000	0.826987000	-1.607536000
1	2.278668000	2.167677000	0.204631000
1	3.955691000	2.516978000	-0.158684000
16	3.821467000	3.315717000	2.557030000
6	1.995113000	3.397589000	2.805350000
6	1.537628000	1.957504000	3.103600000
6	2.668193000	0.945939000	2.721454000
7	1.893045000	-0.149132000	2.143144000
6	0.663003000	0.265924000	1.756415000
7	0.436532000	1.502740000	2.250685000
8	-0.108992000	-0.410892000	1.025987000
1	2.323932000	-0.937430000	1.683326000
1	-0.500166000	1.876659000	2.309942000
1	4.664318000	1.178226000	1.871785000
1	1.509822000	3.775016000	1.901770000
1	1.782479000	4.079583000	3.630583000
1	3.201201000	0.605529000	3.609744000
1	1.264435000	1.849874000	4.157524000
7	-2.622409000	1.338033000	1.601802000
6	-3.210136000	1.971092000	2.373523000
6	-3.949662000	2.767519000	3.333470000
1	-5.012796000	2.749611000	3.074697000
1	-3.812475000	2.352640000	4.336453000
1	-3.586167000	3.799043000	3.311020000

2Bio_XIV

(G = -4372.379902) (Triplet)

7	-2.833148000	0.786326000	-2.167231000
6	-4.186047000	1.361765000	-1.918536000
6	-4.486975000	1.673337000	-0.441264000
7	-3.904208000	0.705596000	0.513208000
6	-4.618160000	-0.589978000	0.584739000
6	-4.442130000	-1.522680000	-0.613537000
7	-3.007466000	-1.847582000	-0.873386000
6	-2.888715000	-0.439087000	-3.000140000
6	-2.538423000	-1.759076000	-2.282984000
16	-2.591637000	-3.355874000	-0.170805000
6	-3.838865000	1.295880000	1.868344000
6	-2.718857000	0.710154000	2.697722000
8	-3.185738000	-3.350420000	1.180610000
7	-1.581348000	0.410996000	2.028164000
6	-2.823492000	0.577137000	4.083097000
6	-1.712448000	0.153582000	4.815443000
6	-0.527338000	-0.124206000	4.129940000
6	-0.511887000	0.012723000	2.744739000
6	-1.905893000	1.792321000	-2.724583000
6	-1.603741000	2.895083000	-1.732737000
6	-1.428734000	4.220498000	-2.134186000
6	-1.120834000	5.190844000	-1.177851000
6	-1.021392000	4.804017000	0.161005000
6	-1.216927000	3.463385000	0.481720000
7	-1.486345000	2.518748000	-0.438458000
27	-1.794676000	0.477397000	-0.070735000
8	-2.949371000	-4.463919000	-1.085575000
6	-0.817653000	-3.330486000	-0.013563000
6	-0.005414000	-3.828116000	-1.034710000

6	1.380715000	-3.813777000	-0.887635000
6	1.952231000	-3.296329000	0.290103000
6	1.113542000	-2.823818000	1.319495000
6	-0.264719000	-2.839068000	1.170672000
7	3.331479000	-3.196587000	0.512611000
6	4.390507000	-3.543706000	-0.295333000
8	4.255699000	-4.092829000	-1.391005000
6	5.753021000	-3.146225000	0.251171000
6	6.348827000	-1.947598000	-0.528310000
6	5.396851000	-0.751264000	-0.679539000
6	4.973836000	-0.075523000	0.640974000
6	3.608533000	0.600443000	0.510097000
16	3.028580000	1.385819000	2.079980000
6	1.704996000	2.256341000	1.147242000
6	2.256747000	2.594344000	-0.256011000
6	3.516912000	1.713737000	-0.550371000
7	4.604689000	2.684445000	-0.476731000
6	4.157494000	3.983054000	-0.446127000
7	2.787222000	3.946493000	-0.384937000
8	4.861740000	5.000099000	-0.481054000
7	-0.105281000	-0.136193000	-0.852741000
6	0.753825000	-0.468038000	-1.565006000
6	1.763995000	-0.871146000	-2.529787000
1	-4.938296000	0.678342000	-2.310147000
1	-4.306159000	2.295466000	-2.482981000
1	-5.578736000	1.747437000	-0.315552000
1	-4.061643000	2.645679000	-0.193980000
1	-5.697474000	-0.419472000	0.727965000
1	-4.242858000	-1.114191000	1.465579000
1	-4.858489000	-1.102531000	-1.523693000
1	-5.028727000	-2.425849000	-0.415689000
1	-2.178143000	-0.356888000	-3.828274000
1	-3.877602000	-0.526048000	-3.459480000
1	-2.948086000	-2.578137000	-2.887720000
1	-1.455038000	-1.868773000	-2.251224000
1	-4.796785000	1.212344000	2.400828000
1	-3.621435000	2.362339000	1.753847000
1	-3.763521000	0.809624000	4.574298000
1	-1.770969000	0.044322000	5.894240000
1	0.368465000	-0.448586000	4.649673000
1	0.382556000	-0.209588000	2.175666000
1	-2.292138000	2.230881000	-3.657112000
1	-0.967692000	1.280957000	-2.960022000
1	-1.536864000	4.483060000	-3.182173000
1	-0.974750000	6.226382000	-1.470189000
1	-0.797516000	5.520983000	0.944342000
1	-1.150836000	3.112701000	1.506207000
1	-0.445506000	-4.223421000	-1.943473000
1	2.015169000	-4.184149000	-1.679330000
1	1.550968000	-2.429273000	2.232048000
1	-0.905791000	-2.474957000	1.963312000
1	3.582911000	-2.761317000	1.392650000
1	6.414152000	-4.011138000	0.139334000
1	5.691002000	-2.915912000	1.318733000
1	6.635198000	-2.290586000	-1.529102000
1	7.271246000	-1.641060000	-0.020168000
1	4.500843000	-1.089781000	-1.212207000
1	5.864316000	-0.005063000	-1.333301000
1	5.729125000	0.656358000	0.949637000
1	4.909502000	-0.812669000	1.447618000
1	2.865985000	-0.160937000	0.246154000
1	1.404131000	3.152190000	1.692904000
1	0.838320000	1.602659000	1.042282000
1	1.467016000	2.424562000	-0.991438000
1	3.469407000	1.263856000	-1.546286000
1	5.513482000	2.485542000	-0.872438000
1	2.270079000	4.752847000	-0.060122000
1	2.144410000	0.007704000	-3.059243000
1	1.321493000	-1.561349000	-3.255264000
1	2.592323000	-1.373696000	-2.026711000

2Bio_XV

(G = -4239.605454) (Triplet)

7	-1.582594000	0.625682000	-2.264742000
6	-2.884482000	0.435223000	-2.968241000
6	-4.065353000	0.068152000	-2.045578000
7	-3.702948000	-0.835562000	-0.935875000
6	-3.463903000	-2.241634000	-1.326453000
6	-2.133712000	-2.493056000	-2.037214000
7	-0.970166000	-2.010285000	-1.235535000
6	-0.471870000	-0.141474000	-2.874782000
6	0.087294000	-1.272440000	-1.990732000
16	-0.346239000	-3.316529000	-0.249061000
6	-4.685264000	-0.772725000	0.167838000
6	-4.048897000	-1.137258000	1.493720000
8	-1.002692000	-3.229003000	1.064880000
7	-2.769727000	-0.726839000	1.658394000
6	-4.746962000	-1.807208000	2.498256000
6	-4.117608000	-2.046209000	3.723354000
6	-2.799448000	-1.613745000	3.894917000
6	-2.164703000	-0.969676000	2.836048000
6	-1.258212000	2.056106000	-2.087603000
6	-2.225254000	2.716761000	-1.135798000
6	-2.728325000	3.997703000	-1.339358000
6	-3.578338000	4.567707000	-0.383313000
6	-3.901572000	3.812540000	0.750778000
6	-3.369826000	2.534900000	0.884022000
7	-2.542774000	1.975574000	-0.034497000
27	-1.920837000	0.045730000	-0.052018000
8	-0.485613000	-4.589008000	-0.997129000
6	1.410989000	-3.023673000	-0.050974000
6	2.290435000	-3.566508000	-0.994064000
6	3.658032000	-3.363801000	-0.837460000
6	4.141748000	-2.638036000	0.261531000
6	3.248946000	-2.153567000	1.227289000
6	1.874333000	-2.325752000	1.064409000
7	5.542373000	-2.442475000	0.392467000
6	6.241388000	-1.254035000	0.392828000
8	7.475290000	-1.276818000	0.447850000
6	5.462635000	0.040793000	0.257671000
6	4.862817000	0.208998000	-1.172331000
6	3.398950000	0.679171000	-1.229653000
6	3.143323000	2.184145000	-1.006855000
6	3.540261000	2.817977000	0.344187000
1	-2.765964000	-0.330325000	-3.734232000
1	-3.158350000	1.354931000	-3.501131000
1	-4.869493000	-0.357665000	-2.666891000
1	-4.451157000	0.979522000	-1.587274000
1	-4.277089000	-2.609104000	-1.972250000
1	-3.478882000	-2.837264000	-0.409715000
1	-2.098529000	-2.004223000	-3.004354000
1	-2.053028000	-3.563348000	-2.246960000
1	0.374926000	0.521530000	-3.079402000
1	-0.782870000	-0.541174000	-3.843918000
1	0.746095000	-0.839792000	-1.239938000

1	0.673237000	-1.936172000	-2.639737000
1	-5.566261000	-1.402502000	-0.022024000
1	-5.030562000	0.263312000	0.240575000
1	-5.766861000	-2.133746000	2.317977000
1	-4.642126000	-2.563140000	4.521464000
1	-2.265830000	-1.781039000	4.825396000
1	-1.134134000	-0.638274000	2.903775000
1	-1.237770000	2.596816000	-3.045773000
1	-0.258659000	2.109018000	-1.642975000
1	-2.454371000	4.540809000	-2.239143000
1	-3.977612000	5.567612000	-0.521727000
1	-4.558154000	4.203984000	1.521729000
1	-3.597309000	1.912389000	1.743761000
1	1.914215000	-4.127535000	-1.841990000
1	4.355855000	-3.754667000	-1.571460000
1	3.631372000	-1.644105000	2.105881000
1	1.175579000	-1.925285000	1.788101000
1	6.123995000	-3.260473000	0.234672000
1	6.160976000	0.845961000	0.491514000
1	4.675620000	0.072690000	1.011622000
1	4.915312000	-0.752272000	-1.694950000
1	5.496414000	0.897631000	-1.743703000
1	2.799969000	0.063940000	-0.554905000
1	3.022515000	0.460590000	-2.237330000
1	2.082015000	2.382663000	-1.195293000
1	3.698925000	2.724056000	-1.782373000
16	3.461695000	4.670391000	0.260787000
6	1.639163000	4.651436000	0.562655000
6	1.362373000	3.454441000	1.492796000
6	2.624669000	2.535281000	1.569742000
7	2.013212000	1.213876000	1.633050000
6	0.740059000	1.227117000	1.134209000
7	0.356415000	2.526957000	0.973936000
8	0.069466000	0.214065000	0.864819000
1	2.557379000	0.367861000	1.561898000
1	-0.630984000	2.743547000	0.967121000
1	4.574919000	2.571732000	0.591832000
1	1.103509000	4.532800000	-0.382479000
1	1.351048000	5.603357000	1.012540000
1	3.194915000	2.736806000	2.478003000
1	1.082247000	3.803753000	2.492132000

2Bio_XVI

(G = -4239.604508) (Triplet)

7	-2.271917000	0.370417000	-2.279737000
6	-3.717257000	0.083635000	-2.508715000
6	-4.508721000	-0.230258000	-1.226935000
7	-3.749864000	-1.018309000	-0.237148000
6	-3.578645000	-2.445172000	-0.577378000
6	-2.526181000	-2.726892000	-1.646109000
7	-1.191766000	-2.118662000	-1.312775000
6	-1.381120000	-0.404934000	-3.174545000
6	-0.502553000	-1.450849000	-2.457596000
16	-0.221892000	-3.375487000	-0.591244000
6	-4.342454000	-0.889244000	1.108293000
6	-3.329366000	-1.222042000	2.178551000
8	-0.770901000	-3.585487000	0.759166000
7	-2.061507000	-0.806286000	1.943518000
6	-3.692654000	-1.894385000	3.345957000
6	-2.728386000	-2.138803000	4.325541000
6	-1.421723000	-1.706246000	4.091023000
6	-1.137806000	-1.055166000	2.893457000
6	-1.991242000	1.815927000	-2.313352000
6	-2.601375000	2.539583000	-1.134207000
6	-3.113696000	3.832606000	-1.248313000
6	-3.611856000	4.473860000	-0.111913000
6	-3.596625000	3.787205000	1.105275000
6	-3.079177000	2.494840000	1.133756000
7	-2.579737000	1.878033000	0.045811000
27	-1.786931000	-0.054266000	-0.036139000
8	-0.183222000	-4.538408000	-1.510340000
6	1.461904000	-2.784328000	-0.472040000
6	2.295870000	-2.915596000	-1.589857000
6	3.645485000	-2.624181000	-1.463624000
6	4.184930000	-2.245221000	-0.218800000
6	3.341227000	-2.147401000	0.897848000
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2Bio_XVII

(G = -4240.04142) (Triplet)

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H	-1.498355	-2.862025	1.4625322
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H	-1.222165	-1.811701	-1.088420
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3.NMR SPECTRA

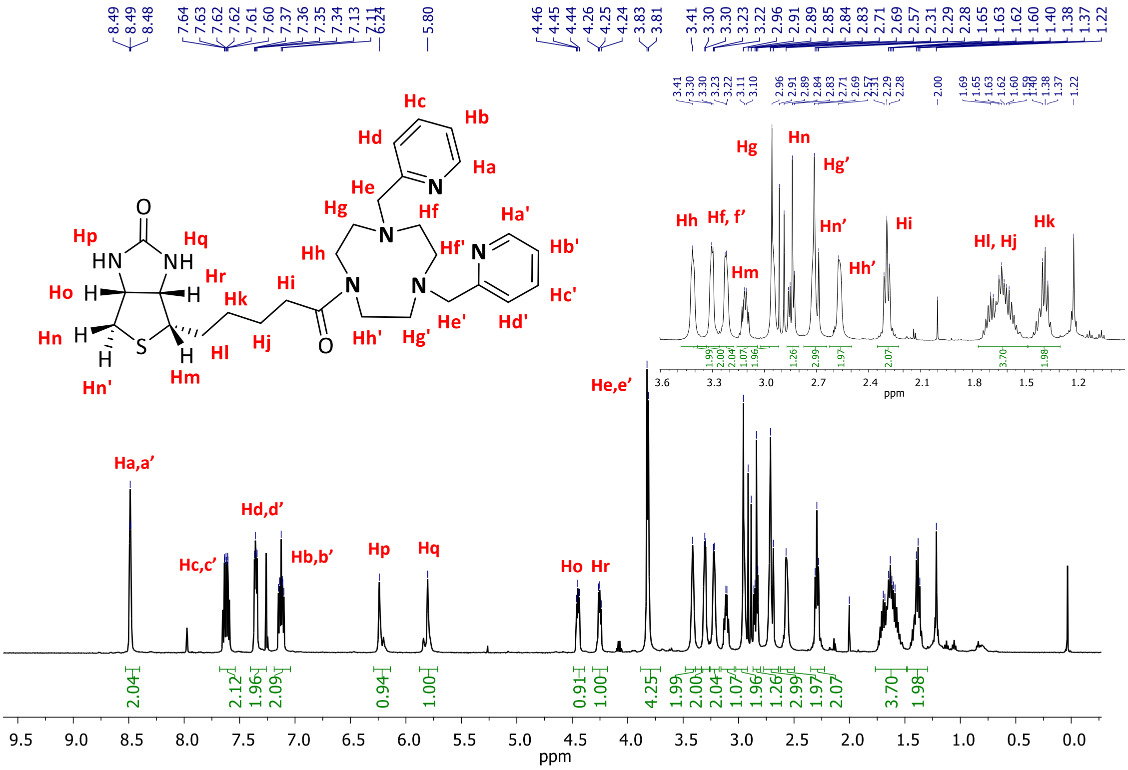

Figure S88. ^{1}H NMR ($CDCl_3$, 500 MHz, 300 K) spectrum of **$^{Bio}Py_2tacn$**.

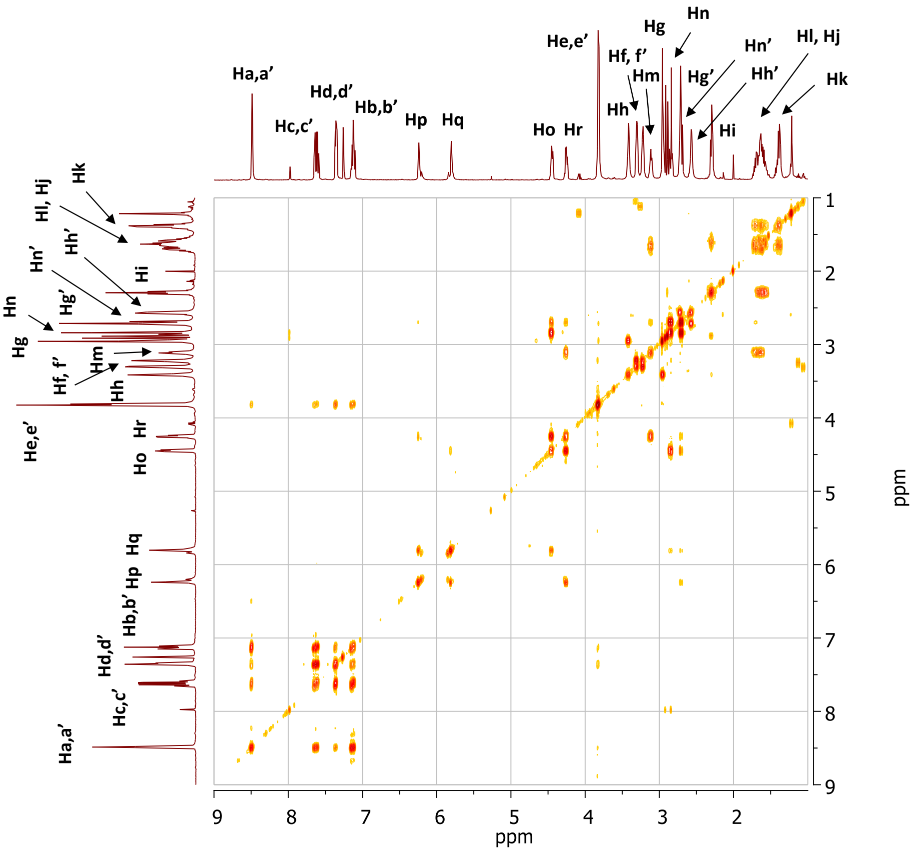

Figure S89. ^{1}H-^{1}H COSY ($CDCl_3$, 500 MHz, 300 K) spectrum of **$^{Bio}Py_2tacn$**.

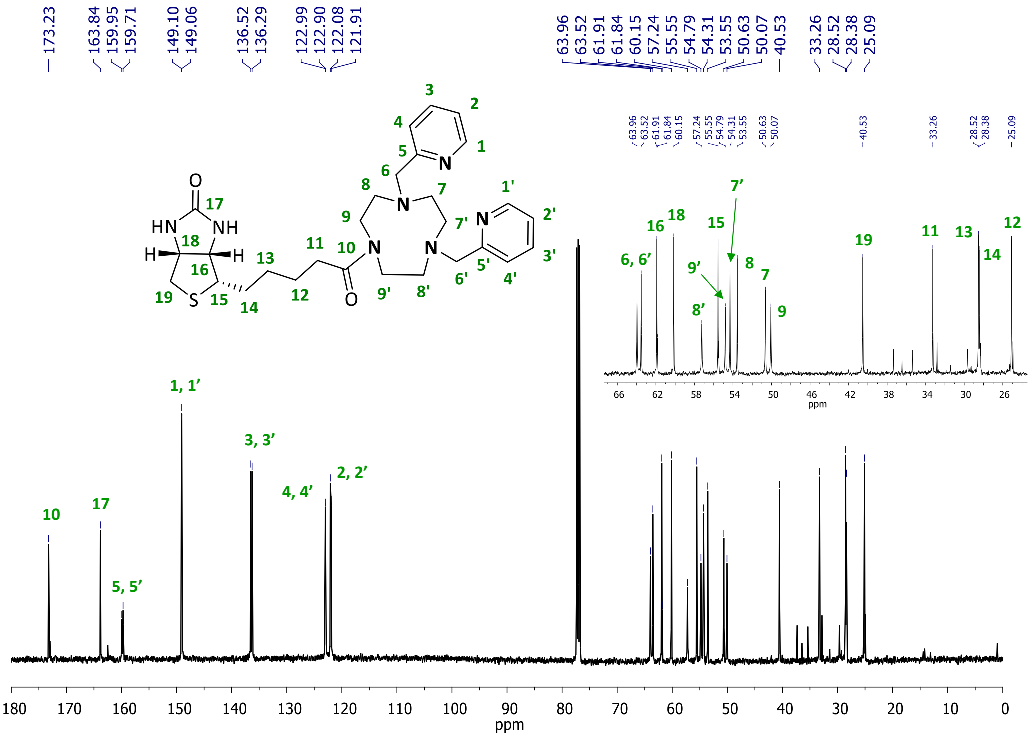

Figure S90. ^{13}C NMR ($CDCl_3$, 125 MHz, 300 K) spectrum of **$^{Bio}Py_2tacn$**.

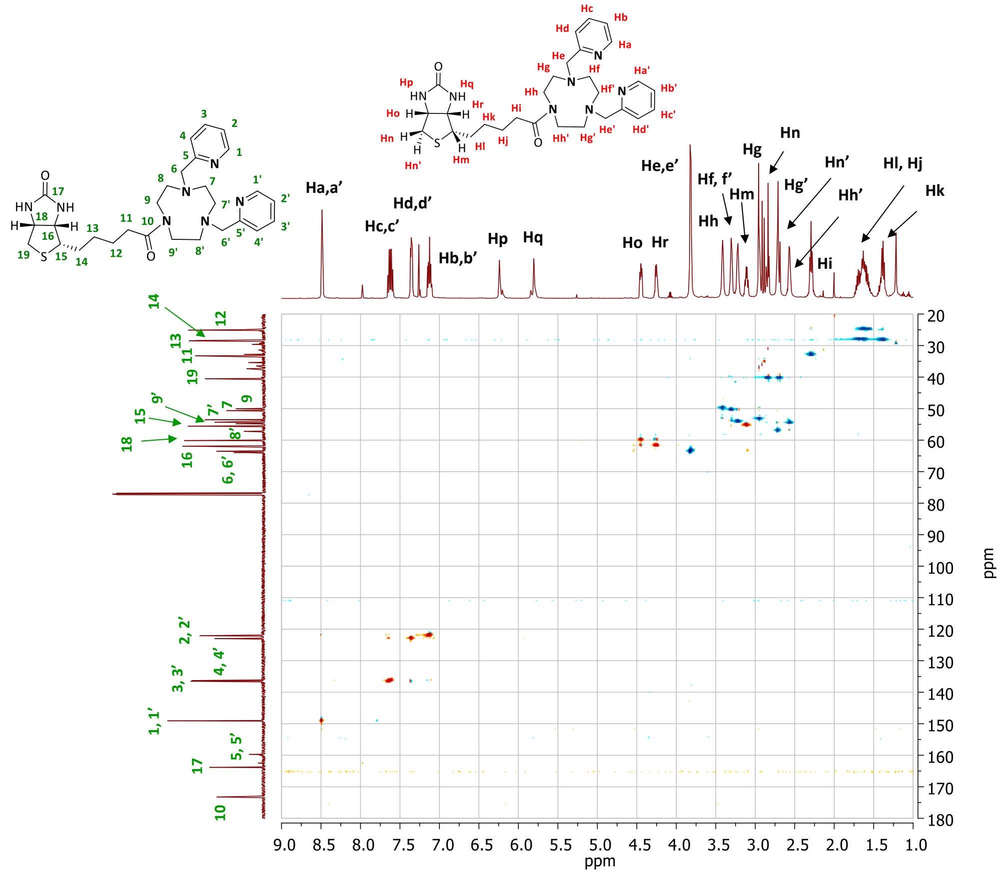

Figure S91. ^{1}H- ^{13}C HSQC ($CDCl_3$, 500 MHz, 300 K) spectrum of ^{Bio}**Py$_2$tacn**.

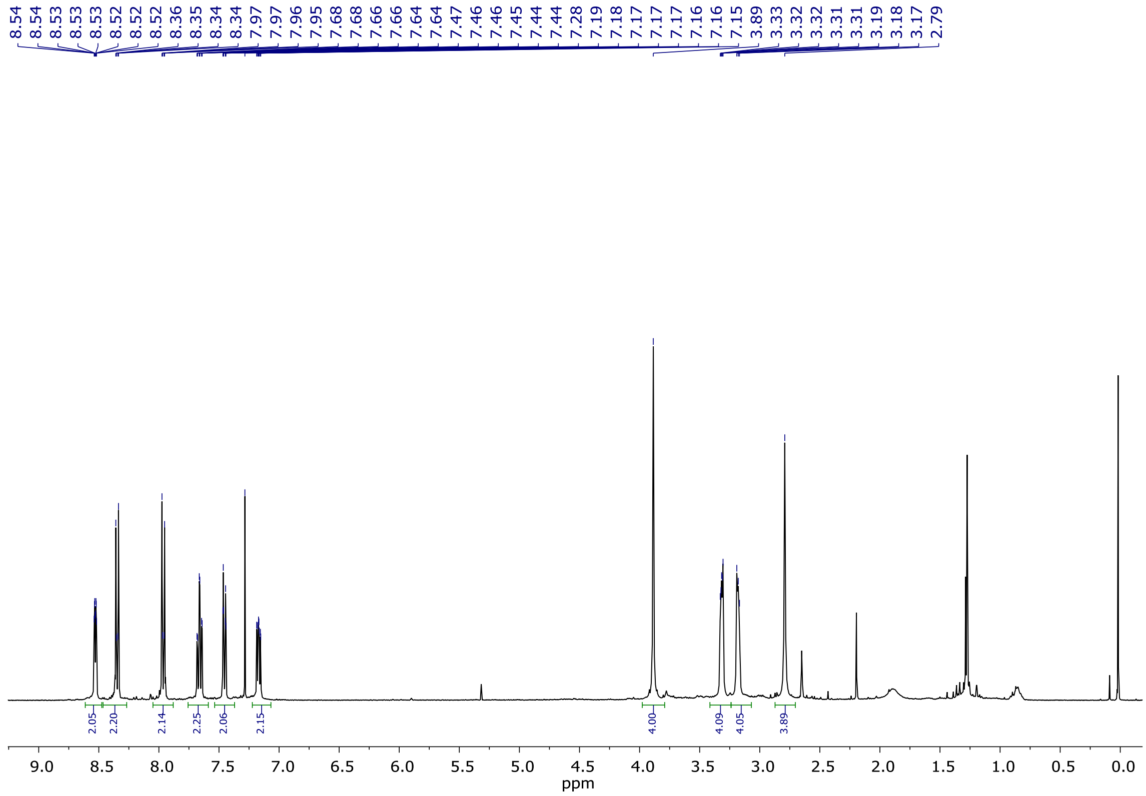

Figure S92. ^{1}H NMR ($CDCl_3$, 400 MHz, 300 K) spectrum ^{NO2}**Py$_2$tacn**.

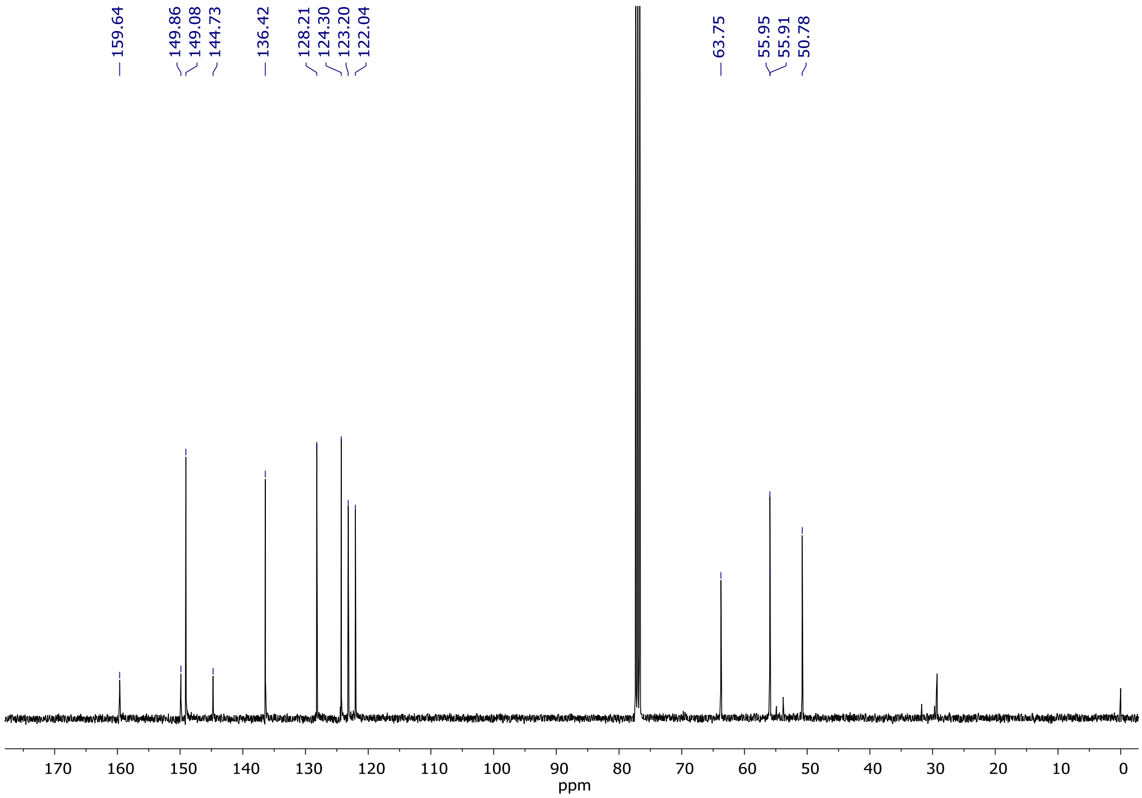

Figure S93. ^{13}C NMR ($CDCl_3$, 101 MHz, 300 K) spectrum $^{\mathbf{NO2}}$**Py$_2$tacn**.

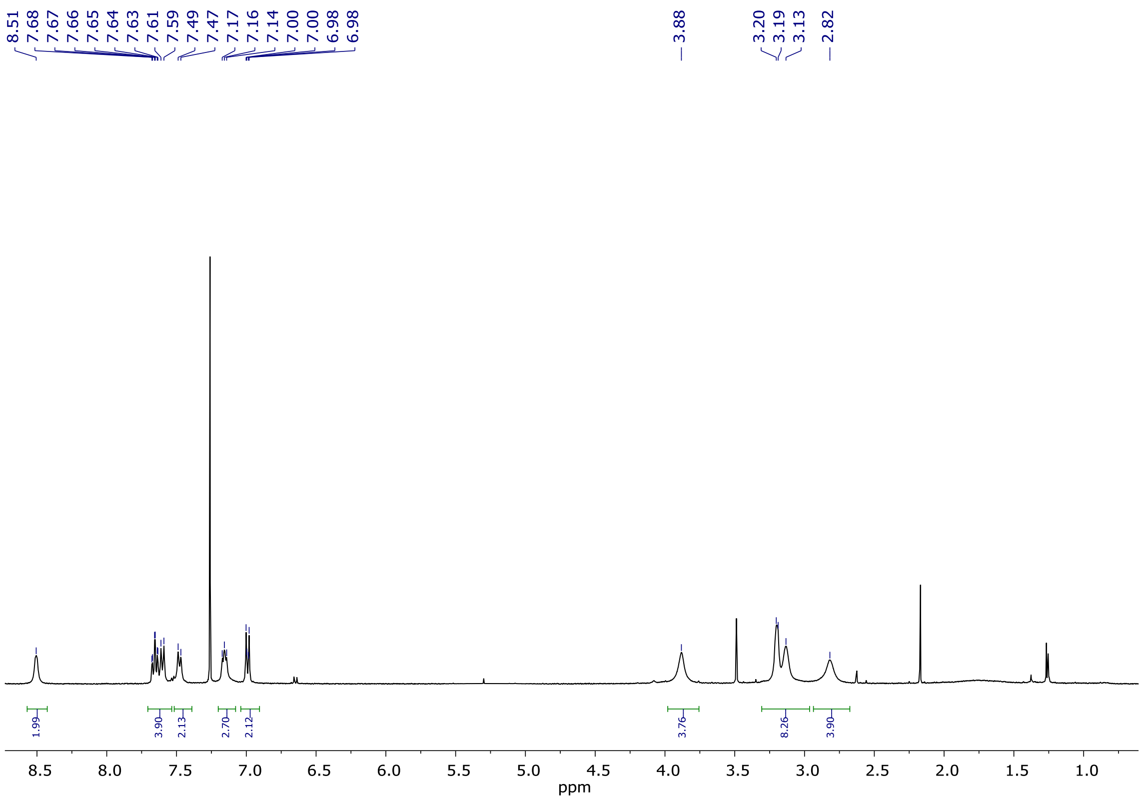

Figure S94. ^{1}H NMR ($CDCl_3$, 400 MHz, 300 K) spectrum $^{\mathbf{NH2}}$**Py$_2$tacn**.

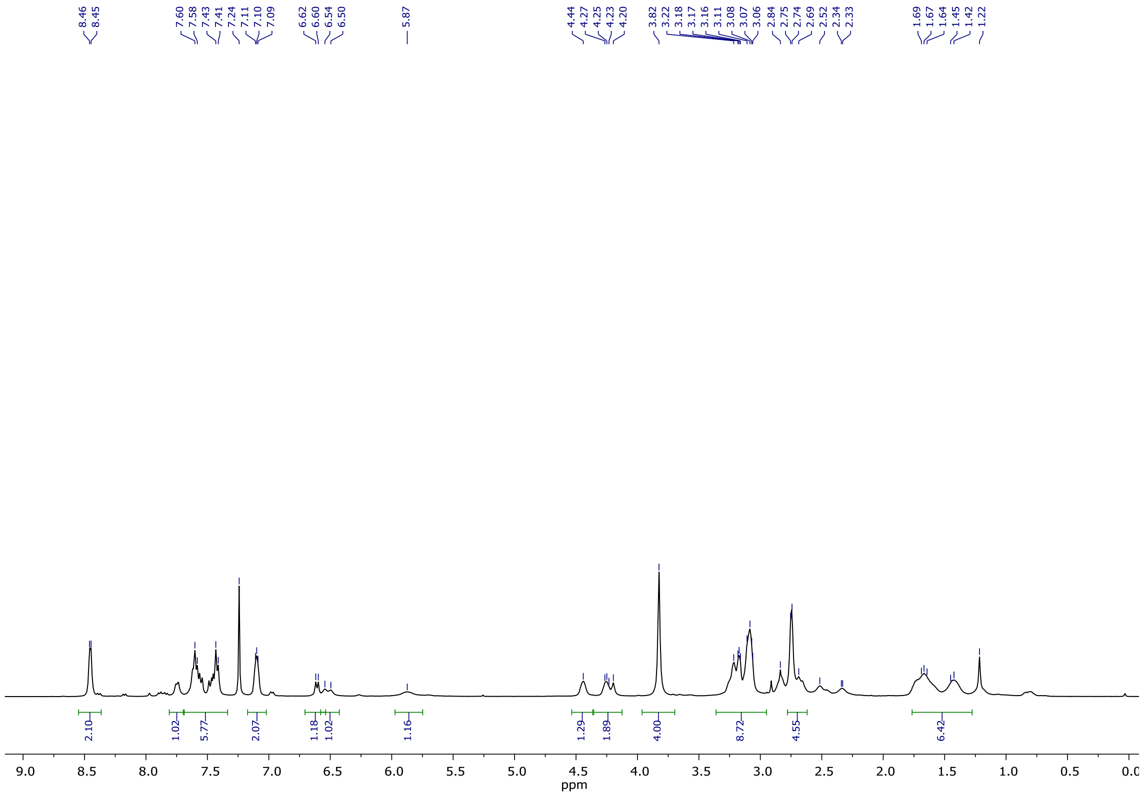

Figure S95. ^{1}H NMR ($CDCl_3$, 500 MHz, 300 K) spectrum of $^{\textbf{Bio-SP}}$**Py$_2$tacn**

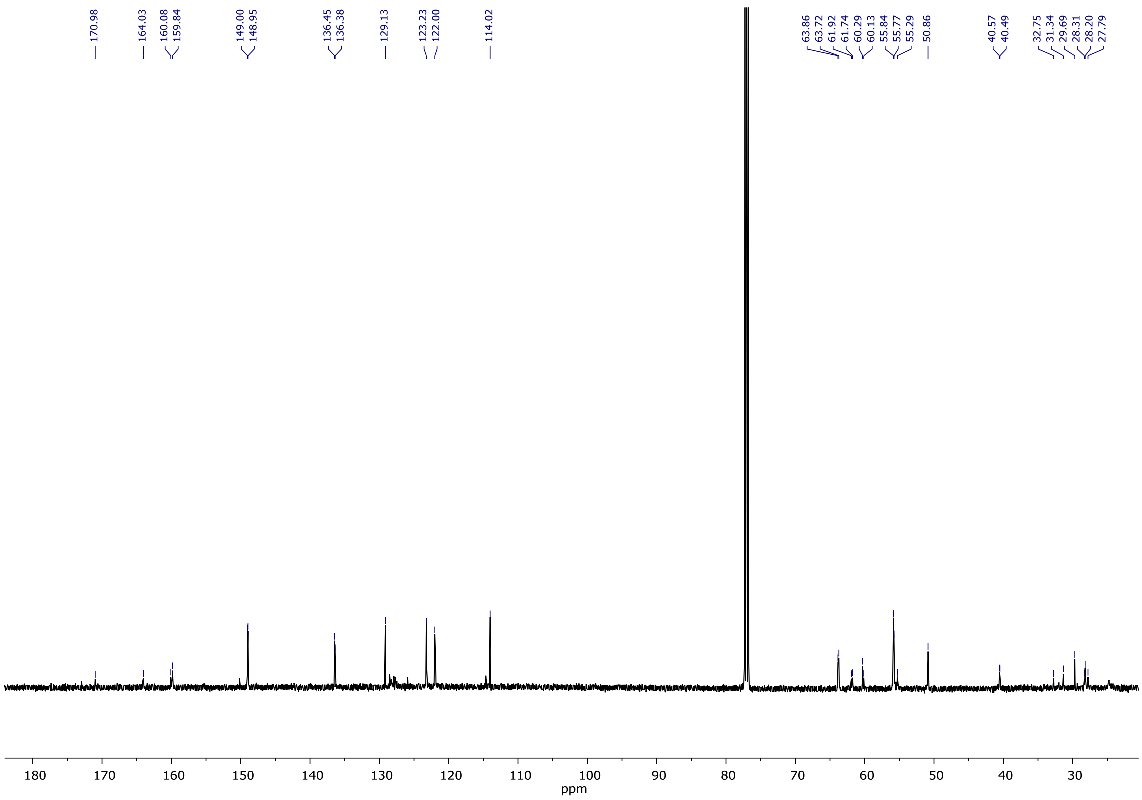

Figure S96. ^{13}C NMR ($CDCl_3$, 101 MHz, 300 K) spectrum $^{\textbf{Bio-SP}}$**Py$_2$tacn**

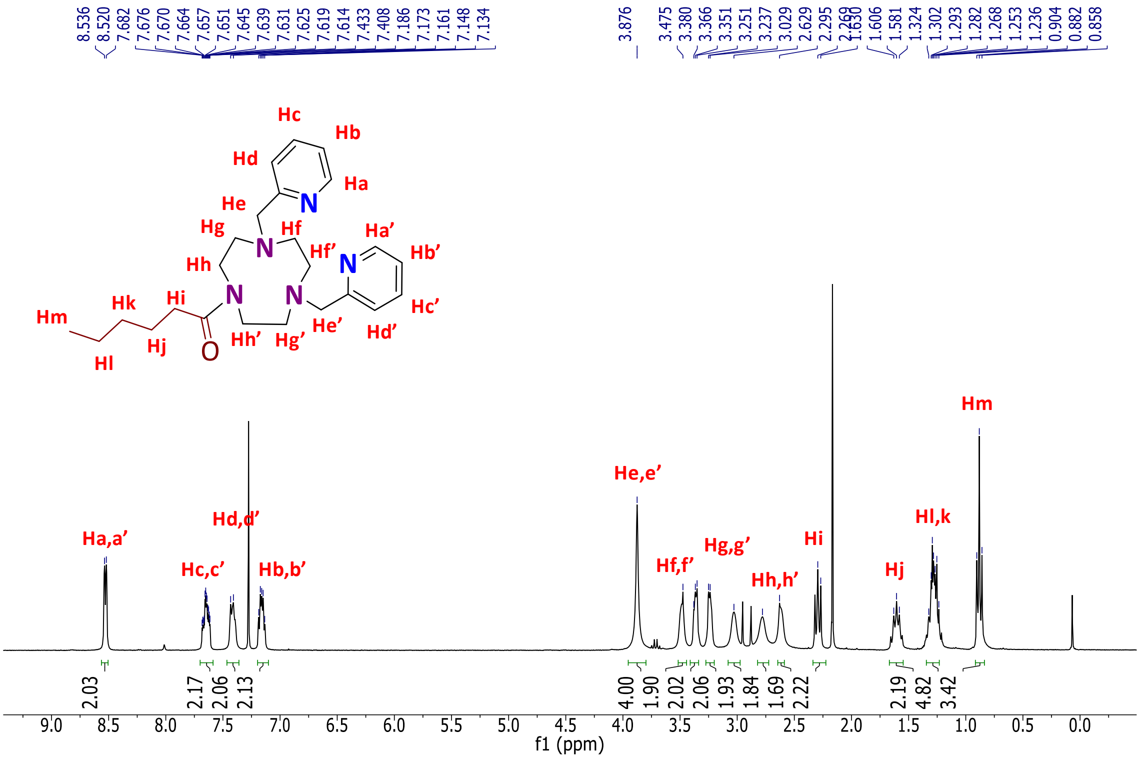

Figure S97. ^{1}H NMR ($CDCl_3$, 500 MHz, 300 K) spectrum of **^{Amide}Py$_2$tacn**.

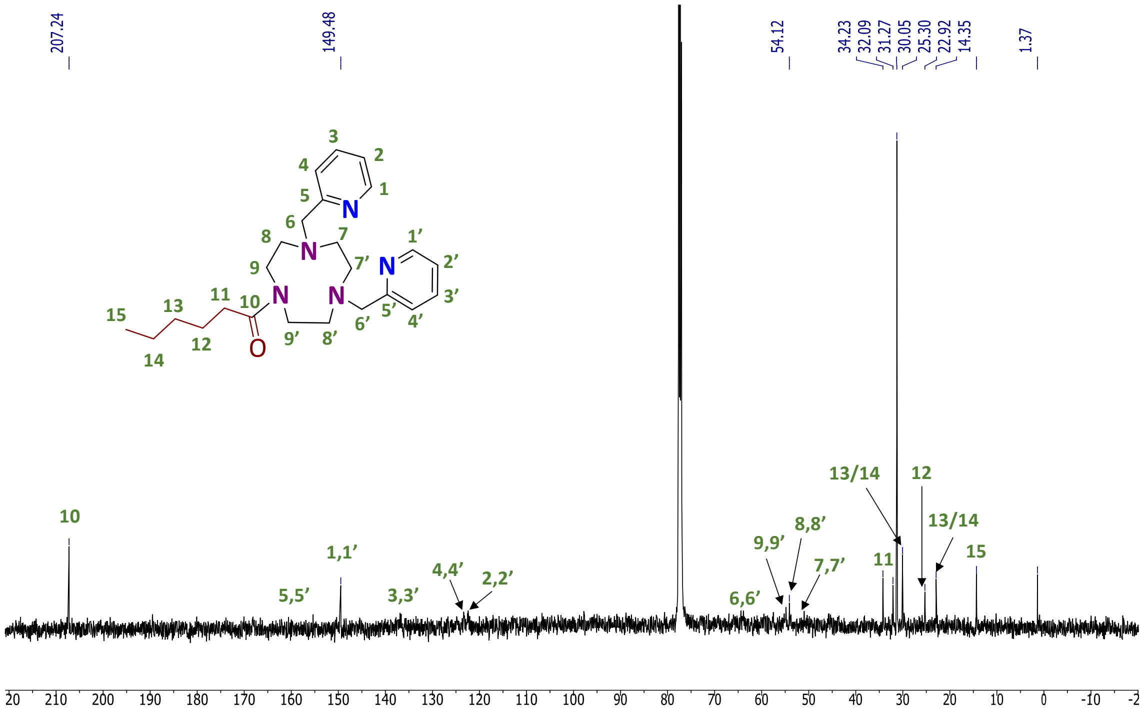

Figure S98. ^{13}C NMR ($CDCl_3$, 101 MHz, 300 K) spectrum of **^{Amide}Py$_2$tacn**.

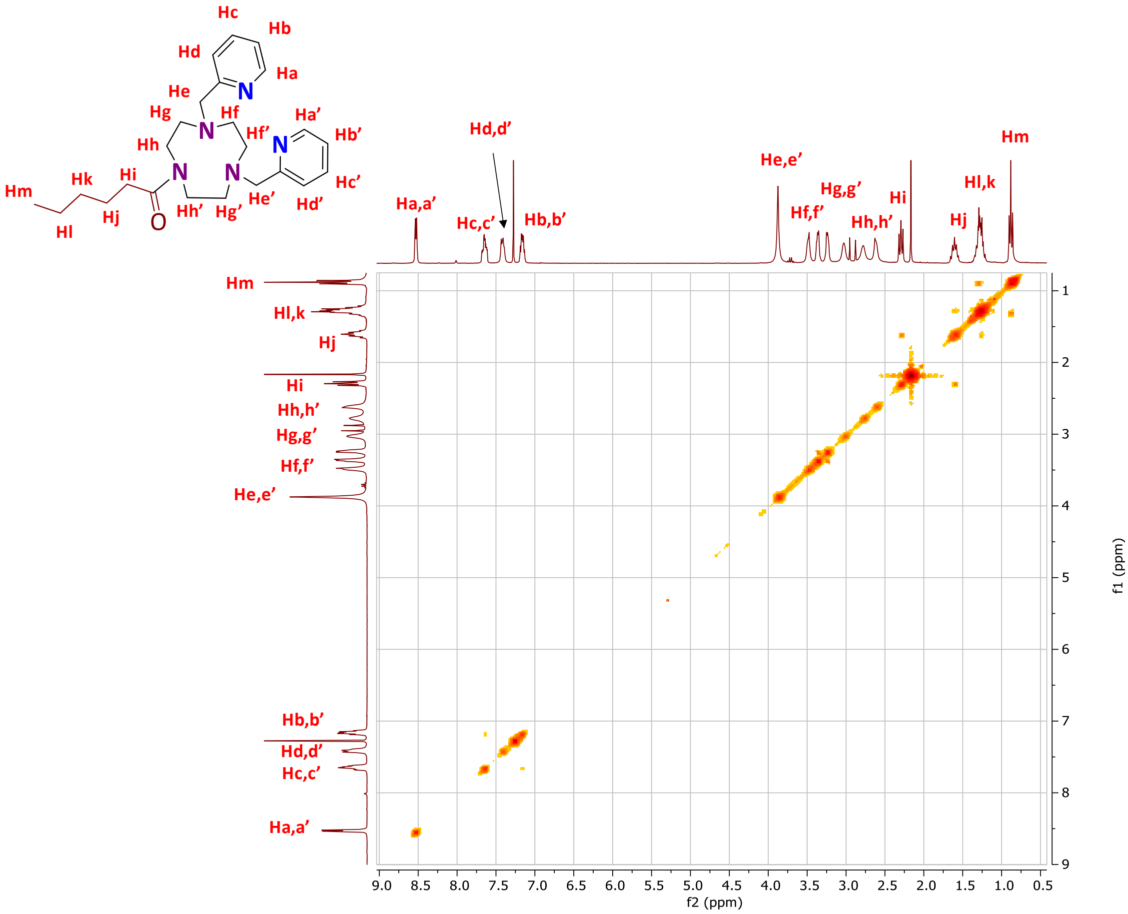

Figure S99. ^{1}H-^{1}H COSY ($CDCl_3$, 500 MHz, 300 K) spectrum of ^{Amide}**Py$_2$tacn**.

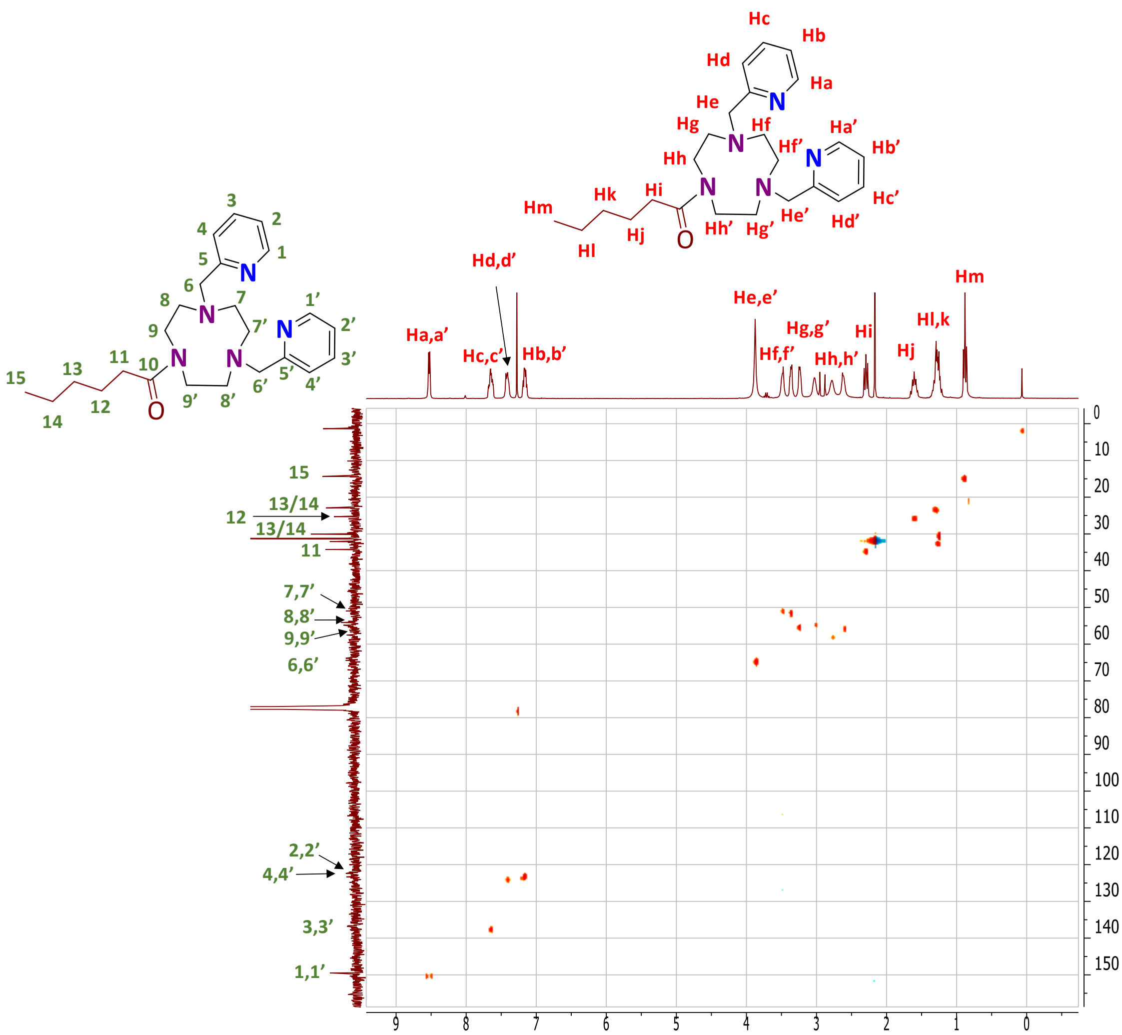

Figure S100. ^{1}H- ^{13}C HSQC ($CDCl_3$, 500 MHz, 300 K) spectrum of $^{\mathbf{Amide}}\mathbf{Py_2tacn}$.

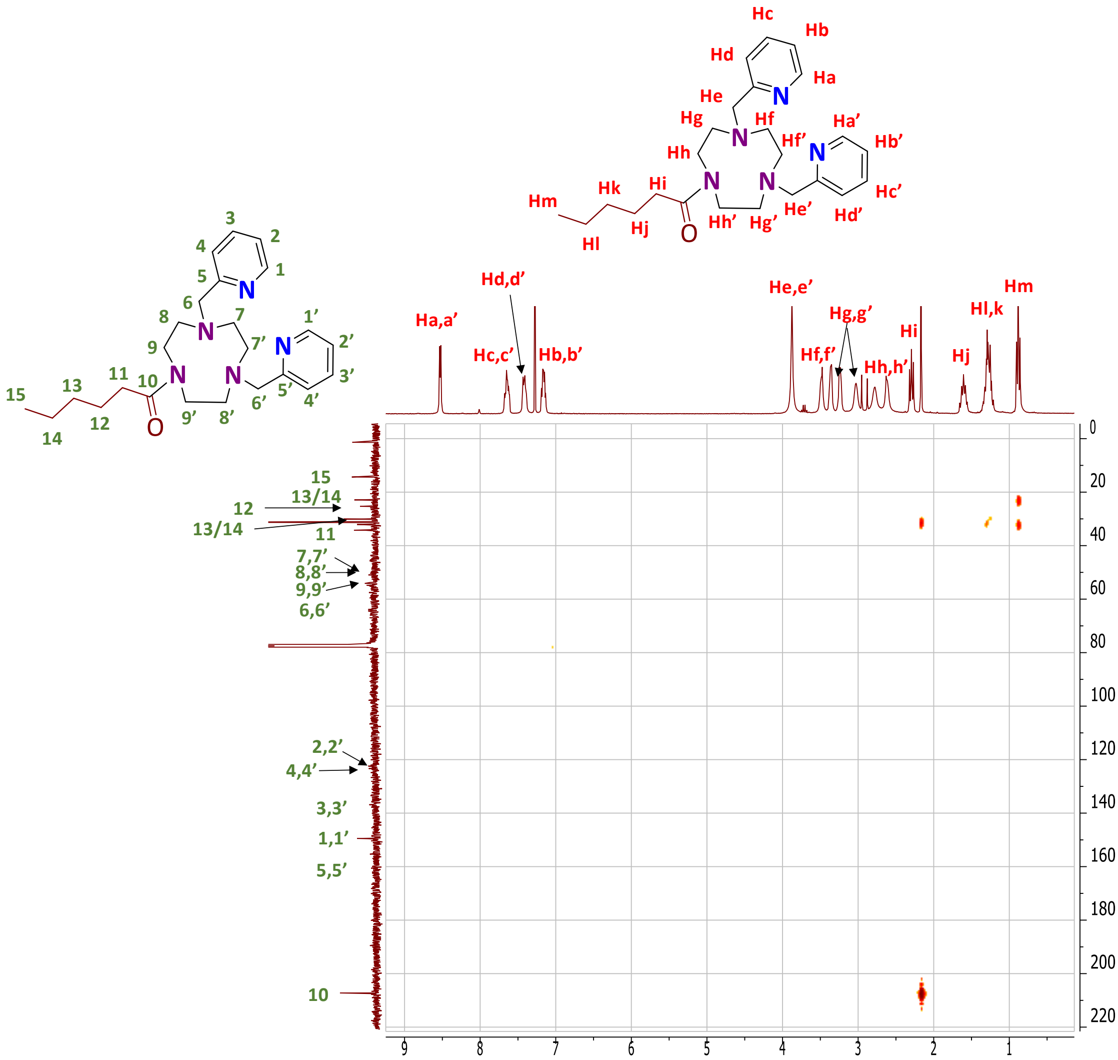

Figure S101. ^{1}H- ^{13}C HMBC ($CDCl_3$, 500 MHz, 300 K) spectrum of ^{Amide}**Py$_2$tacn**.

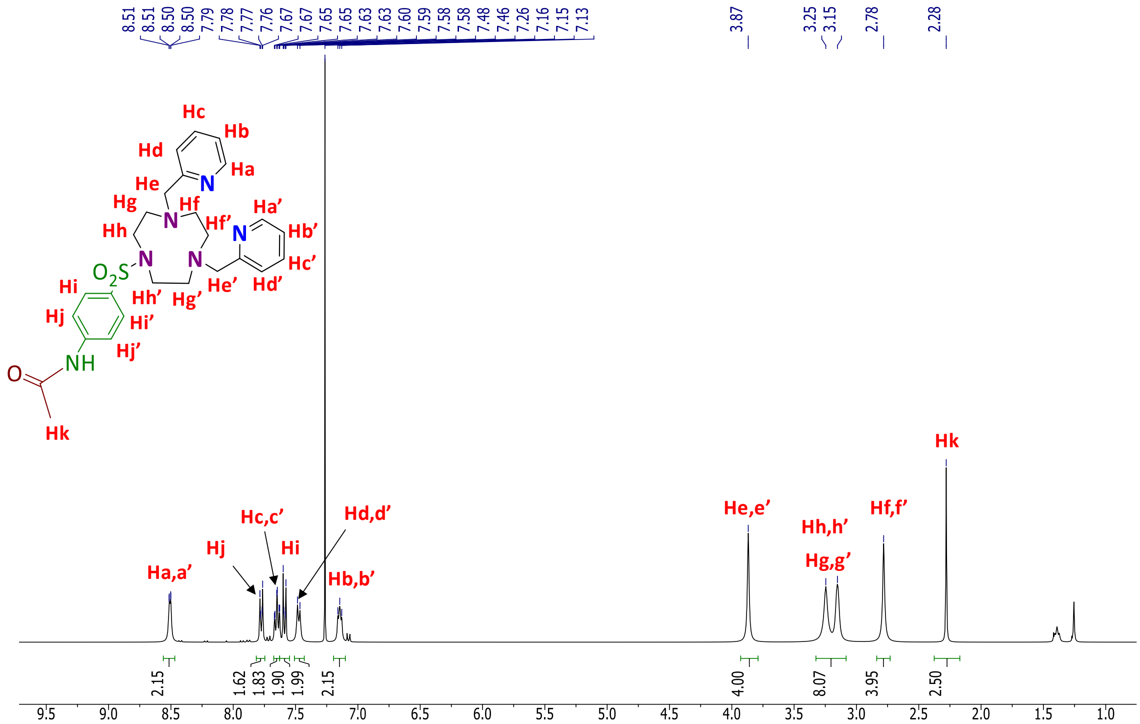

Figure S102. ^{1}H NMR ($CDCl_3$, 400 MHz, 300 K) spectrum of $^{\text{Amide-SP}}$**Py$_2$tacn**.

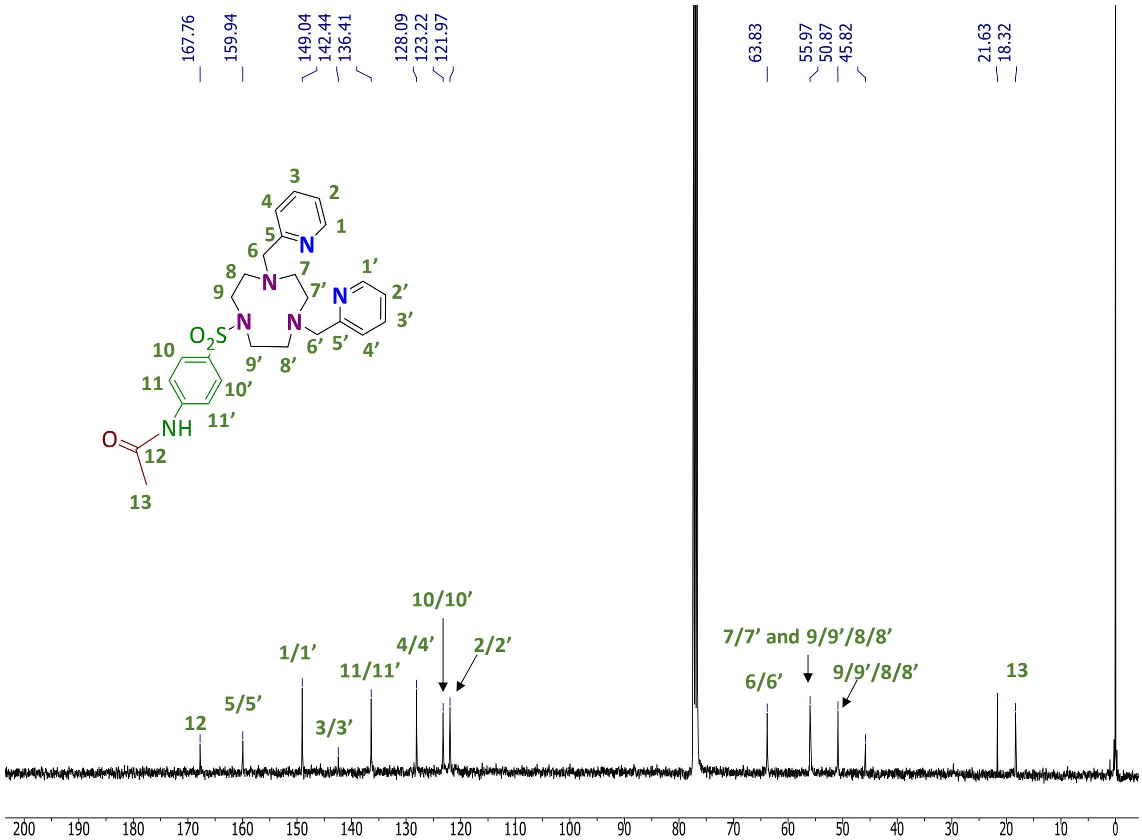

Figure S103. ^{13}C NMR ($CDCl_3$, 101 MHz, 300 K) spectrum of $^{\text{Amide-SP}}$**Py$_2$tacn**.

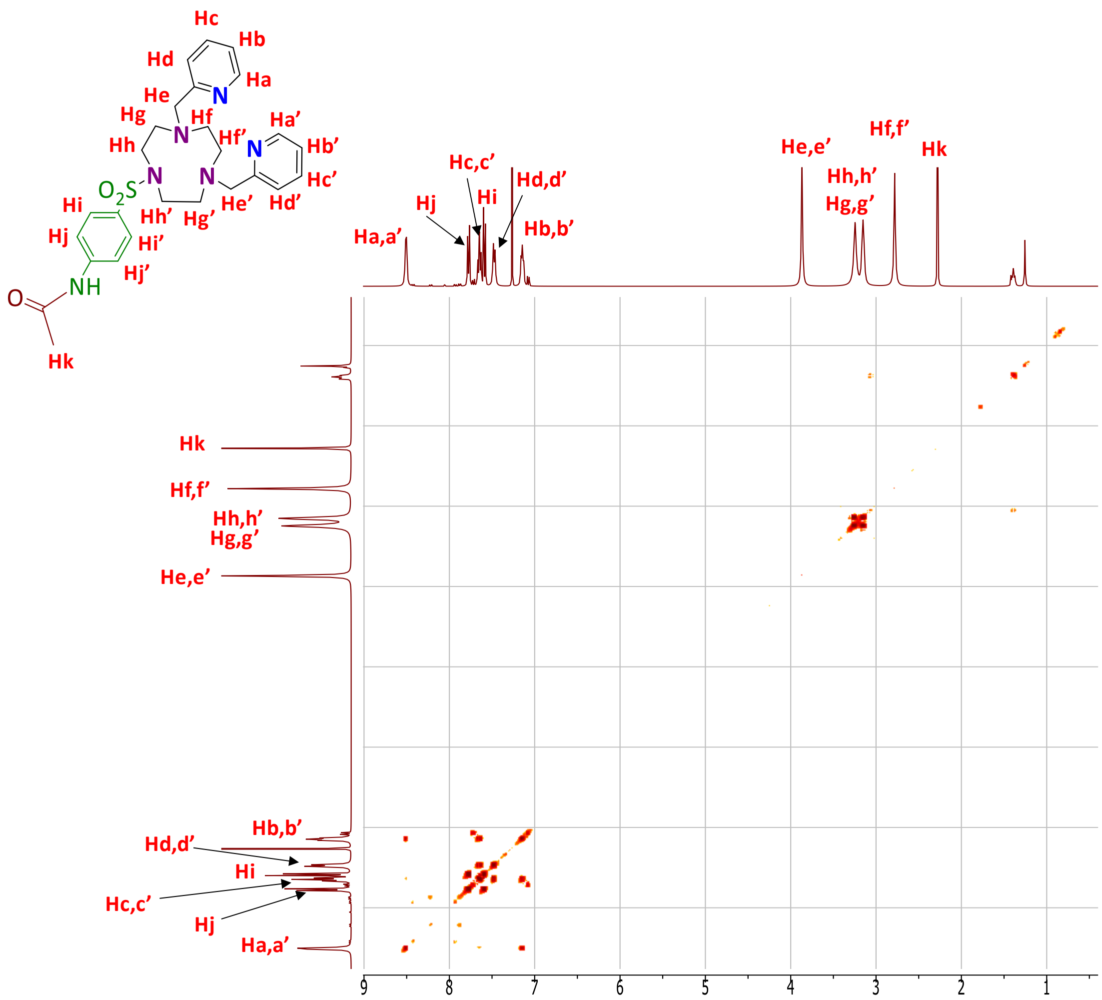

Figure S104. ^{1}H-^{1}H COSY ($CDCl_3$, 400 MHz, 300 K) spectrum of $^{Amide\text{-}SP}$**Py$_2$tacn**.

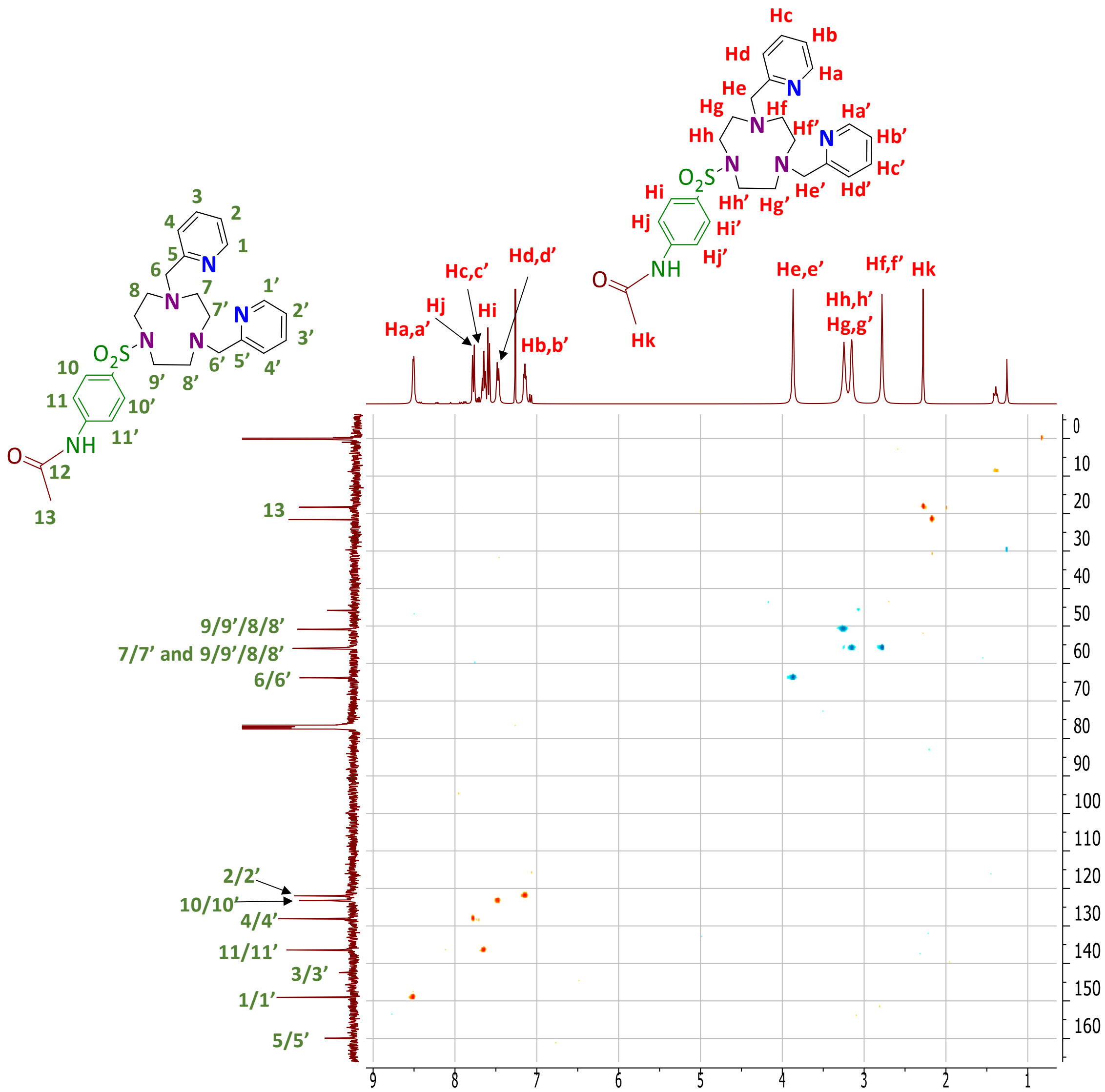

Figure S105. ^{1}H- ^{13}C HSQC ($CDCl_3$, 400 MHz, 300 K) spectrum of $^{Amide\text{-}SP}$**Py$_2$tacn**.

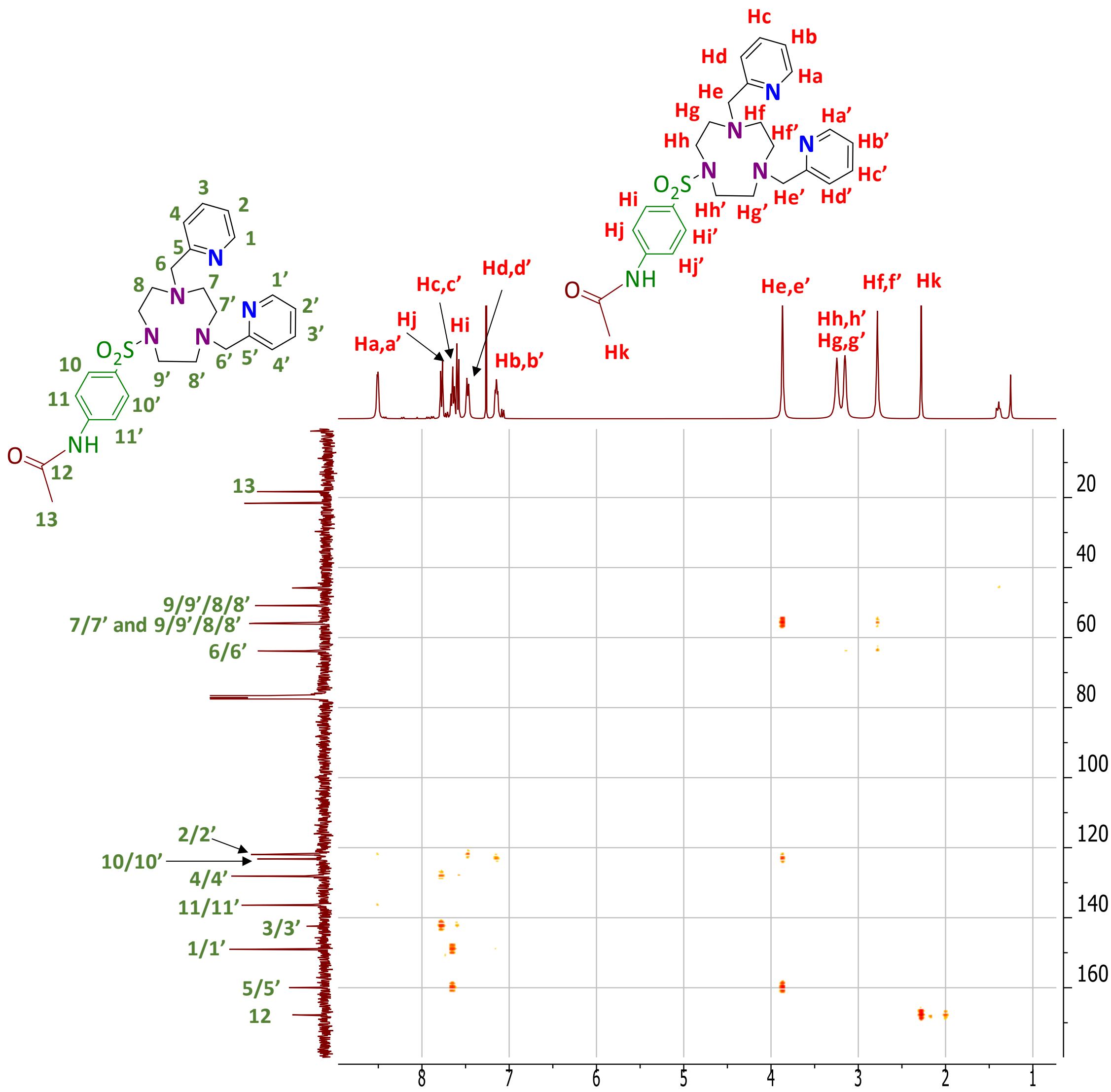

Figure S106. ^{1}H- ^{13}C HMBC ($CDCl_3$, 400 MHz, 300 K) spectrum of $^{\text{Amide-SP}}$**Py$_2$tacn**.

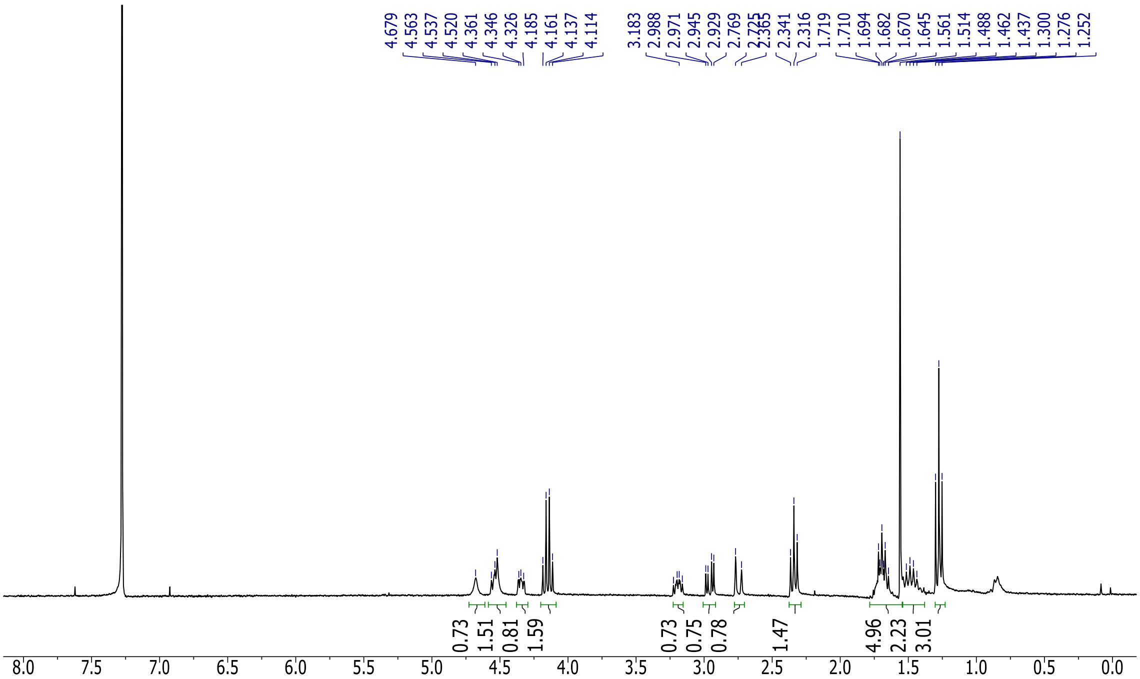

Figure S107. ^{1}H NMR ($CDCl_3$, 400 MHz, 300 K) spectrum of $^{\mathbf{COOEt}}$**Biotin**.

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