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A Stereodynamic encapsulation complex containing a Cu(II) center within square-pyramidal ligand field provided by *tris*-quinolinyl basket

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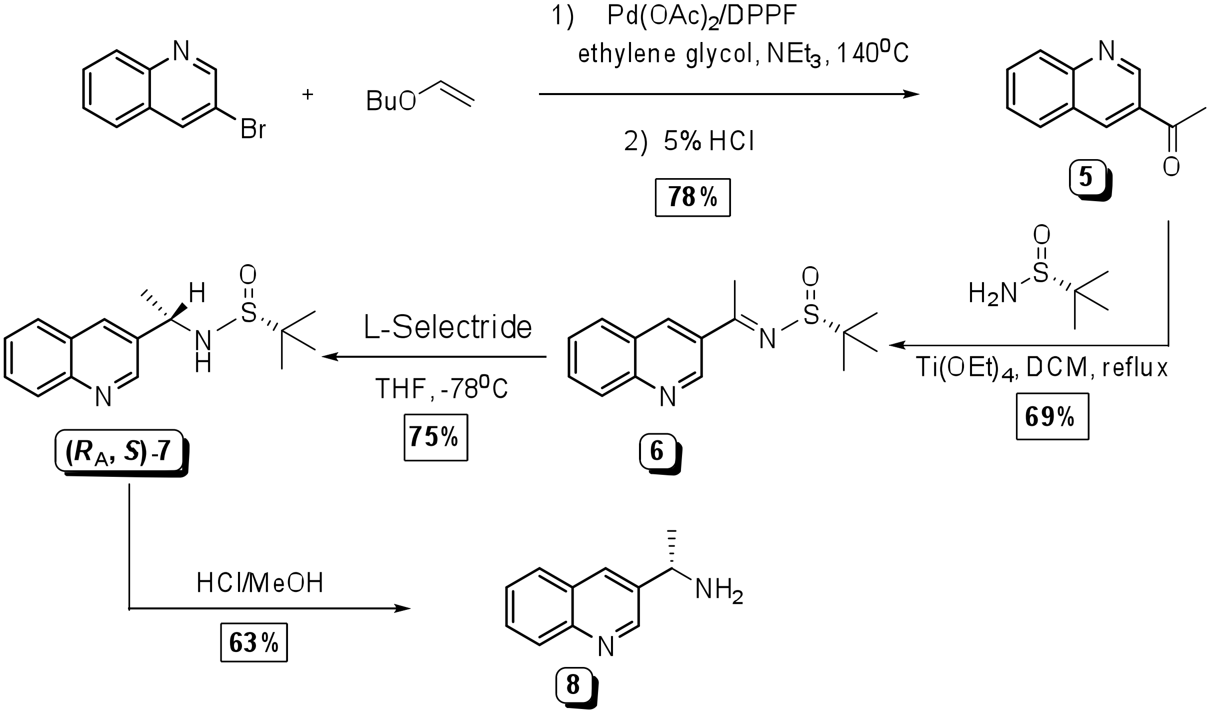
Supplementary Information

General

All chemicals were purchased from commercial sources, and used as received unless stated otherwise. All solvents were dried prior to use according to standard literature protocols. Chromatography purifications were performed using silica gel 60 (Sorbent Technologies 40-75µm, 200 x 400 mesh). Thin-layer chromatography (TLC) was performed on silica-gel plate w/UV254 (200µm). ^{1}H and ^{13}C NMR spectra were recorded, at 400 MHz and 100 MHz respectively, on a Bruker DPX-400 spectrometer unless otherwise noted. The NMR spectra were referenced using solvent residual signal as an internal standard. NMR samples were prepared with $CDCl_3$ and CD_3CN solvents that were purchased from Cambridge Isotope Laboratories. The chemical shift values are expressed as δ values (ppm) and the couple constants (*J*) are given in Hertz (Hz). The following abbreviations were used for signal multiplicities: s, singlet; d, doublet; t, triplet; m, multiplet; and br, broad.

Synthetic Procedures and Characterization



Scheme S1: Synthetic scheme for the preparation of (*S*)-1-(quinolin-3-yl)ethanamine **8**.

Compound 5: Oven dried, two-necked flask was charged with 3-bromoquinoline (2.081 g, 10 mmol), $Pd(OAc)_2$ (70 mg, 0.3 mmol), DPPF (250 mg, 0.6 mmol) and ethylene glycol (20 ml) under nitrogen and at room temperature. The solvent was degassed three times upon the addition of vinylbutyl ether (2 g, 20 mmol) and NEt_3 (2.02 g, 20 mmol). The flask was subsequently placed in an oil-bath and the mixture was stirred and heated at 140^0C for two hours under argon. After the completion of the reaction (TLC), water was added and the aqueous phase extracted with dichloromethane (3 x 100 mL). The organic extract was evaporated and the crude mixture dissolved in tetrahydrofuran (30mL). Aqueous HCl (5%, 50 ml) was added and the mixture stirred for additional 30 min. The mixture was then treated with saturated solution of Na_2CO_3 (30 mL) and extracted with dichloromethane (3 x 50 mL). The combined organic layer was dried with Na_2SO_4, filtered and concentrated in vacuo. The crude product was purified with chromatography (SiO_2, ethyl acetate: hexanes=1:4) to afford 1.335 g of compound **5** (yield 78%). ^{1}H NMR (500 MHz, $CDCl_3$, 298 K): δ = 9.46 (s, 1H), 8.74 (s, 1H), 8.19 (d, *J*=8.3 Hz, 1H), 7.98 (d, *J*=8.3 Hz, 1H), 7.87 (t, *J*=7.6 Hz, 1H), 7.66 (t, *J*=7.6 Hz, 1H), 2.77 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$, 298 K): δ = 196.68, 149.80, 149.19, 137.40, 132.07, 129.48, 129.38, 129.33, 127.62, 126.88, 26.83 ppm; HRMS ESI: *m*/*z* calcd for $C_{11}H_9NO$: 172.0762 $[M + H]^+$, found: 172.0758.

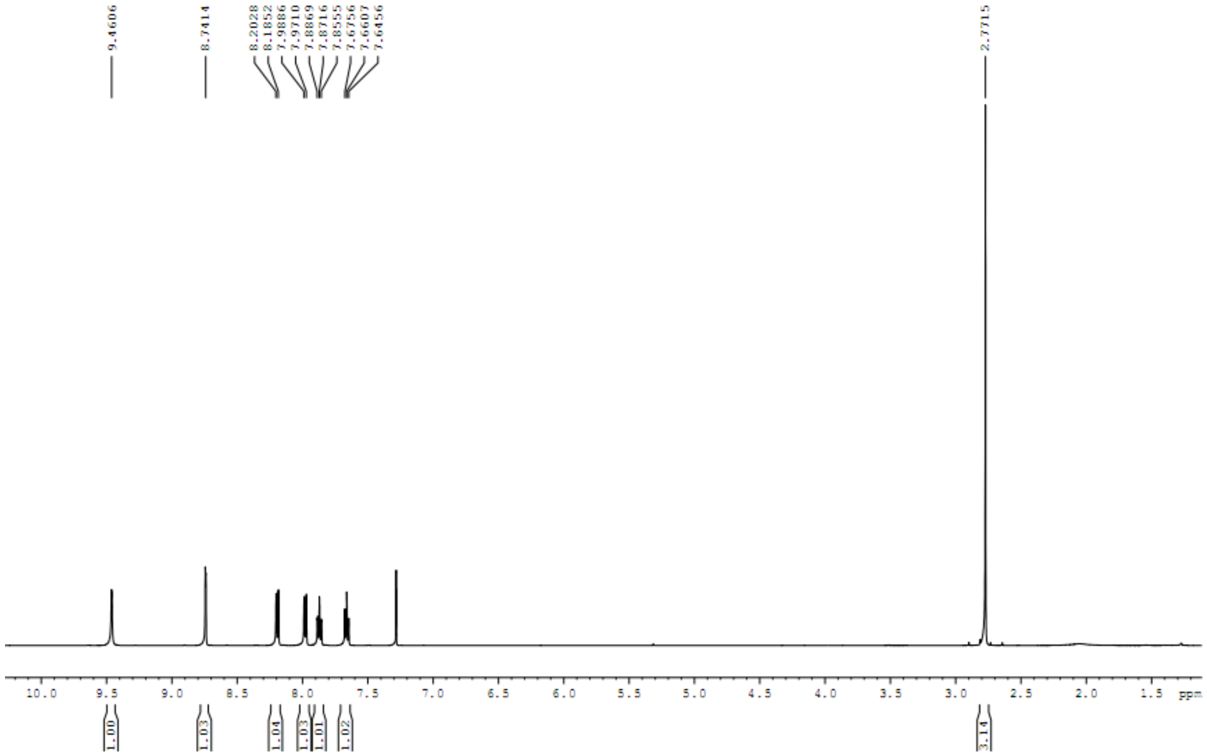


Figure S1: ^{1}H NMR spectrum (500 MHz) of compound **5** in $CDCl_3$ at 298 K.

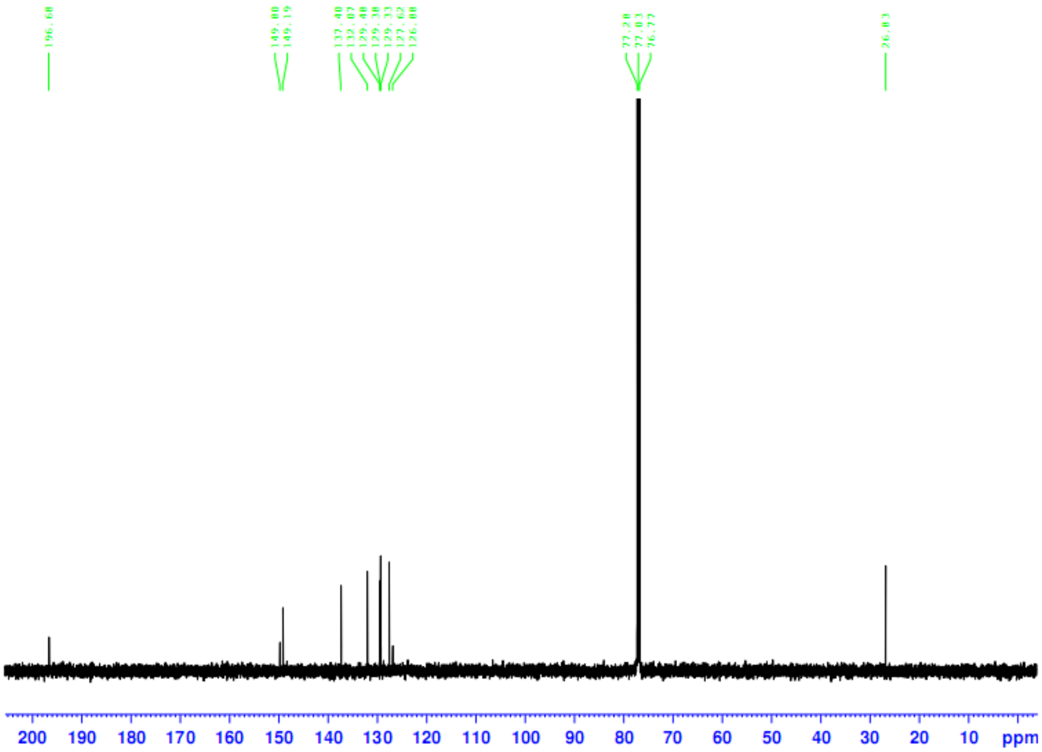


Figure S2: ^{13}C NMR spectrum (125 MHz) of compound **5** in $CDCl_3$ at 298 K.

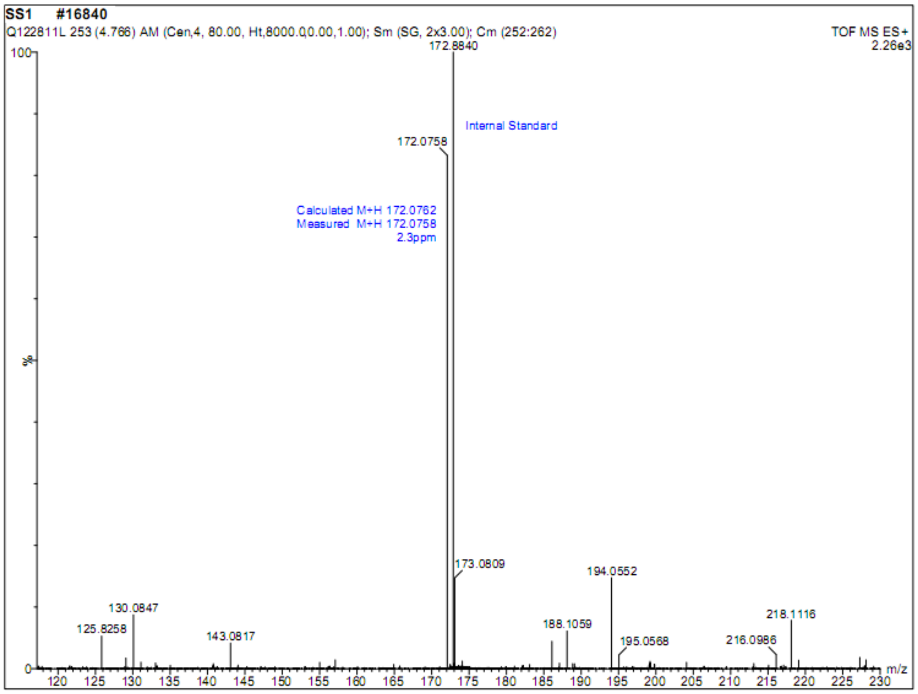


Figure S3: High resolution MS (ESI) spectrum of compound **5** showing a strong signal at 172.0758 corresponding to its $(M+H)^+$ ion.

Compound 6: To a solution of 3-acetylquinoline **5** (1 g, 5.84 mmol) and compound (*R*)-2-methylpropane-2-sulfinamide (640 mg, 5.3 mmol) in dry tetrahydrofuran (16 mL), $Ti(OEt)_4$ (2.24 mL, 10.6 mmol) was added. The resulting mixture was stirred at reflux for 60 h and under an atmosphere of nitrogen. After cooling to room temperature, the solvent was removed under vacuum and the residue extracted with ethyl acetate (2 x 40 mL). After addition of brine (16 mL), the mixture was filtered through a pad of Celite. The organic phase was dried with $MgSO_4$ and the solvent evaporated in vacuum to give a solid residue. The residue was purified with flash chromatography (SiO_2, ethyl acetate: hexanes=7:1) to give 999 mg of compound **6** (yield 69 %). ^{1}H NMR (500 MHz, $CDCl_3$, 298 K): δ = 9.47 (d, *J*=2.3 Hz, 1H), 8.52 (d, *J*=2.3 Hz, 1H), 8.14 (d, *J*=8.3 Hz, 1H), 7.92 (d, *J*=8.3 Hz, 1H), 7.80 (dt, *J*=7.7, 1.5 Hz, 1H), 7.62 (dt, *J*=7.7, 1.5 Hz, 1H), 2.90 (s, 3H), 1.37 (s, 9H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$, 298 K): δ = 174.15, 149.04, 148.94, 135.02, 131.32, 131.16, 129.37, 128.94, 127.46, 126.92, 57.96, 22.62, 19.51 ppm; HRMS ESI: *m*/*z* calcd for $C_{15}H_{18}N_2OS$: 297.1038 $[M + Na]^+$, found: 297.1026.

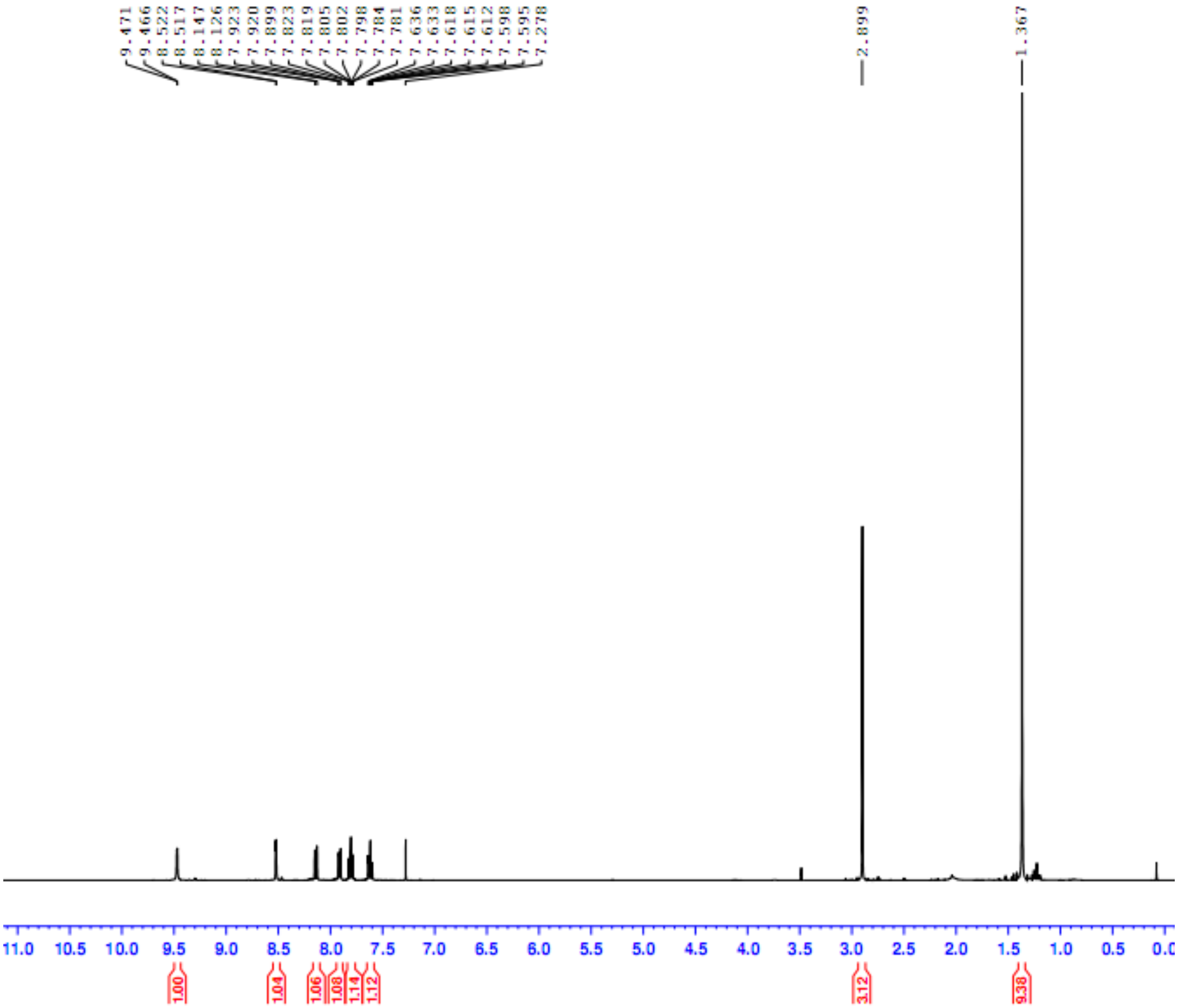


Figure S4: ^{1}H NMR spectrum (500 MHz) of compound **6** in $CDCl_3$ at 298 K.

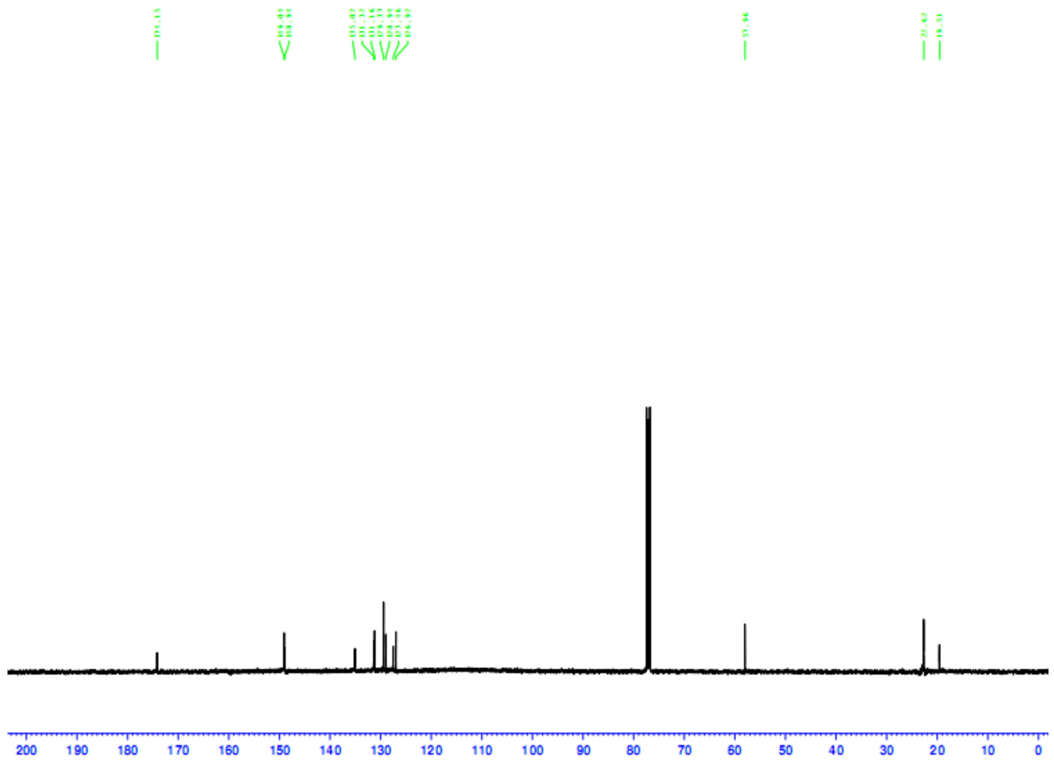


Figure S5: ^{13}C NMR spectrum (125 MHz) of compound **6** in $CDCl_3$ at 298 K.

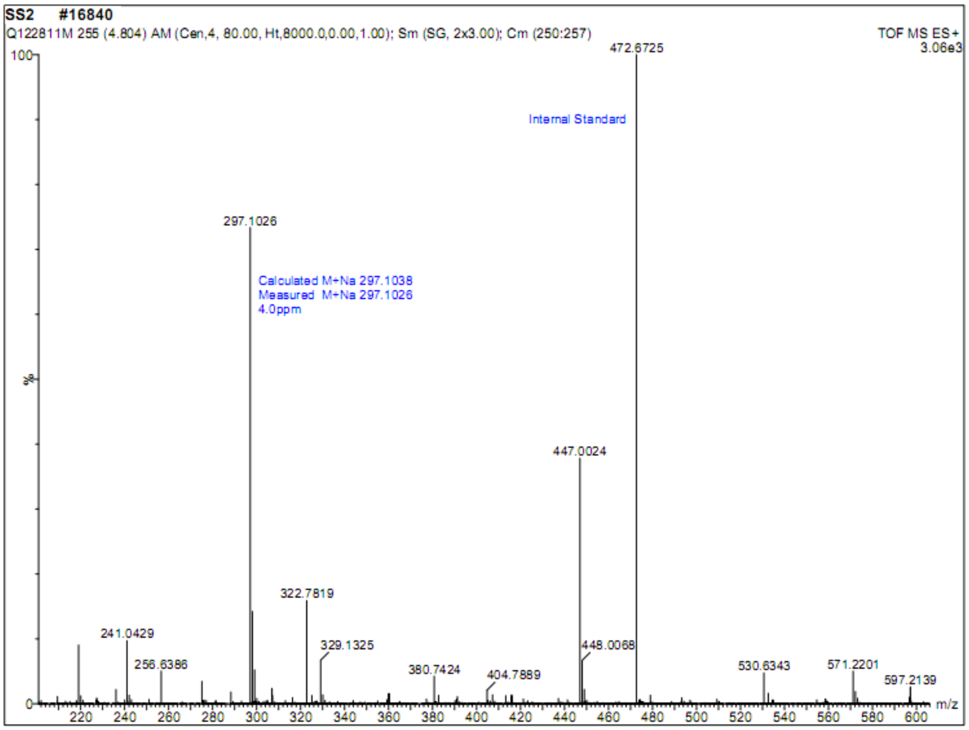


Figure S6: High resolution MS (ESI) spectrum of **6** showing a strong signal at 297.1026 corresponding to its $(M+Na)^+$ ion.

<u>Compound (R_A,S)-7</u>: To a solution of compound **6** (553 mg, 2.01 mmol) in dry tetrahydrofuran (20 mL) at -78^0 C was slowly added 1.0 M solution of *L*-Selectride (2.0 mL, 2.01 mmol). After 6 h, the reaction mixture was quenched with saturated NH_4Cl (30 mL) and then extracted with of ethyl acetate (2 x 30 mL). The organic phase was dried over $MgSO_4$ and the solvent evaporated under reduced pressure. The solid residue was purified with flash chromatography (SiO_2, dichloromethane:methanol=9:1) to exclusively give 418 mg of (R_A,S)-**7** diastereomer (yield 75 %). Importantly, we did not observe the formation of (R_A, R)-**7** diastereomer, which is in accord with our earlier study (*Chem. Sci.* **2011**, *2*, 752). ^{1}H NMR (500 MHz, $CDCl_3$, 298 K): δ = 8.94 (d, *J*=2.3 Hz, 1H), 8.11 (d, *J*=8.7 Hz, 1H), 8.08 (d, *J*=2.3 Hz, 1H), 7.82 (d, *J*=8.7 Hz, 1H), 7.72 (dt, *J*=7.7, 1.5 Hz, 1H), 7.57 (dt, *J*=7.7, 1.5 Hz, 1H), 4.81 (dq, *J*=6.5, 3.4 Hz, 1H), 3.52 (d, *J*=3.4, NH), 1.68 (d, *J*=6.5, 3H), 1.23 (s, 9H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$, 298 K): δ = 150.22, 147.61, 135.82, 133.86, 129.48, 129.20, 127. 78, 127. 72, 126.97, 55.83, 52.90, 24.70, 22.55 ppm; HRMS ESI: *m*/*z* calcd for $C_{15}H_{20}N_2OS$: 299.1194 [M + Na]$^+$, found: 299.1194.

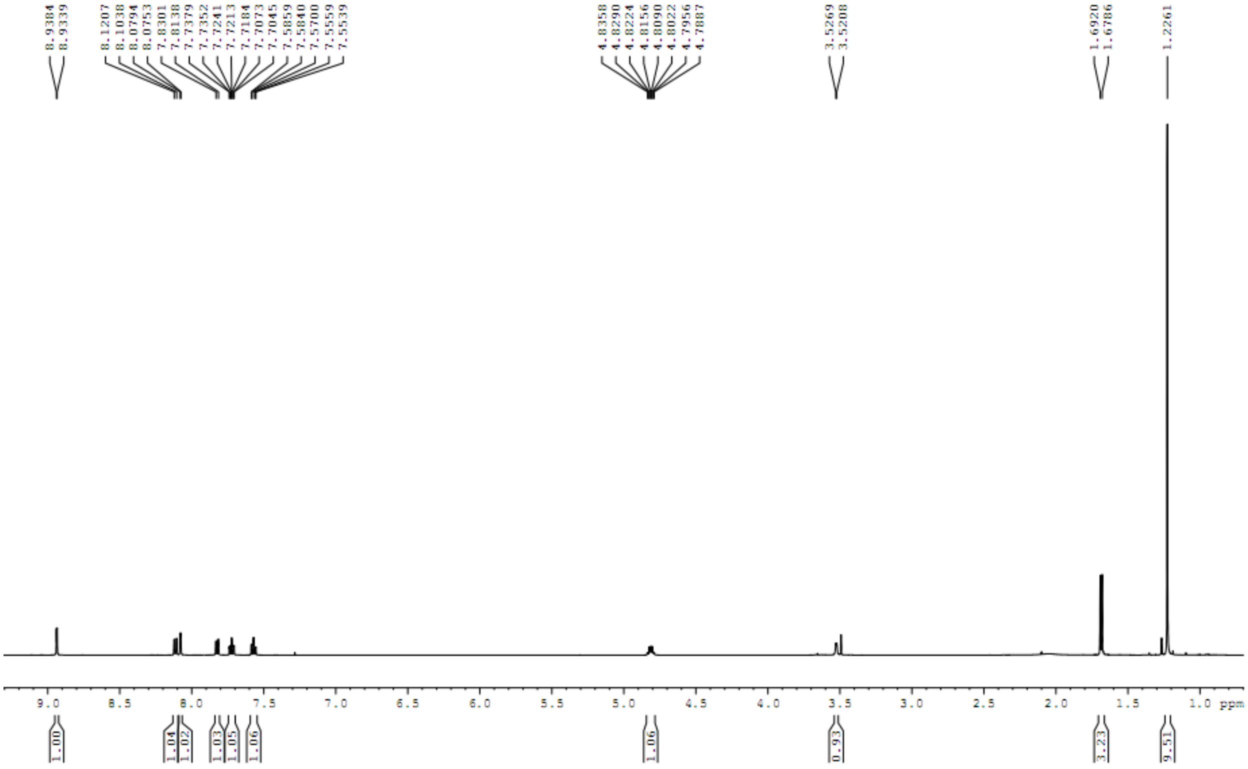


Figure S7: ^{1}H NMR spectrum (500 MHz) of compound (R_A,S)-**7** in $CDCl_3$ at 298 K.

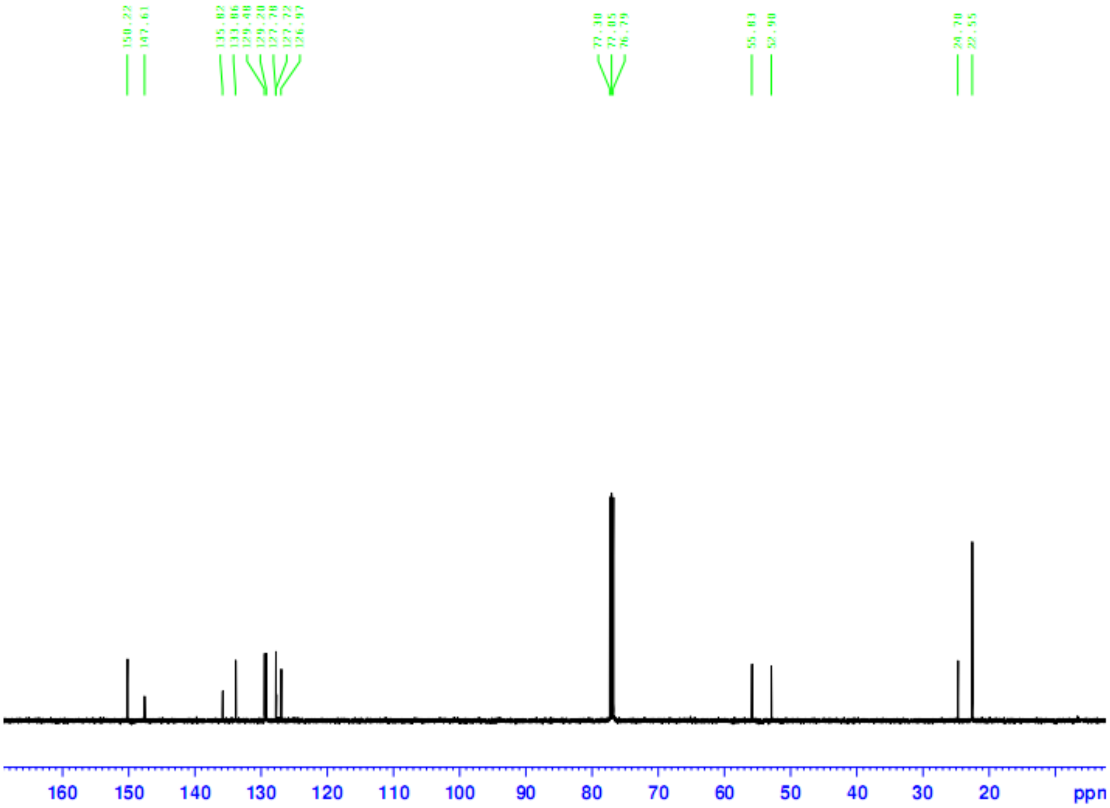


Figure S8: ^{13}C NMR spectrum (125 MHz) of compound (*R*$_A$,*S*)-**7** in CDCl$_3$ at 298 K.

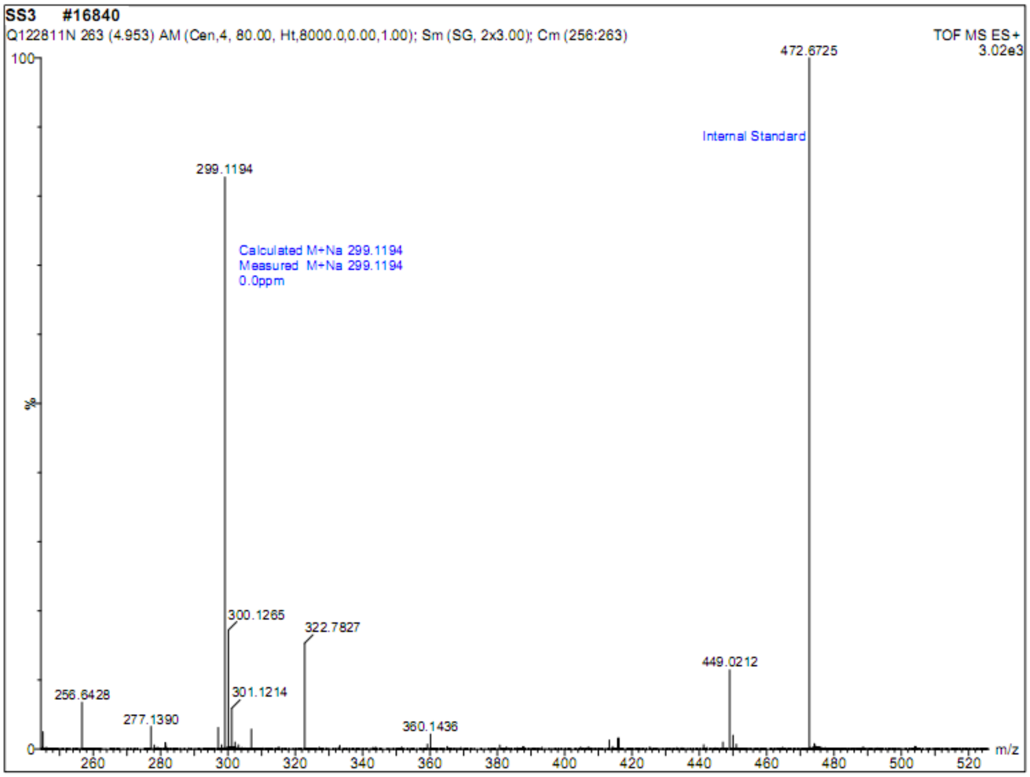


Figure S9: High resolution MS (ESI) spectrum of compound (*R*$_A$,*S*)-**7** showing a strong signal at 299.1194 corresponding to its (M+Na)$^+$ ion.

Compound 8: Compound (*R_A,S*)-**7** (142 mg, 0.514 mmol) was dissolved in 10 mL of methanol after which 10 ml of 4 M HCl (in methanol) was added. The reaction mixture was stirred at room temperature for one hour. Methanol was evaporated under reduced pressure and 10 ml of H_2O was added. Upon the extraction of aqueous solution with diethyl ether (3 x 20 mL), 2 M NaOH was added dropwise to have pH~12. The organic layer was extracted with dichloromethane (3 x 20 mL) and dried with $MgSO_4$. The solvent was evaporated under reduced pressure to give 55.6 mg of (*S*)-1-(quinolin-3-yl)ethanamine **8** (yield 63%). ^{1}H NMR (500 MHz, $CDCl_3/CD_3OD$, 298 K): δ = 8.96 (d, *J*=2.3 Hz, 1H), 8.42 (d, *J*=2.3 Hz, 1H), 7.95 (d, *J*=8.7 Hz, 1H), 7.83 (d, *J*=8.7 Hz, 1H), 7.65 (dt, *J*=7.7, 1.5 Hz, 1H), 7.50 (dt, *J*=7.7, 1.5 Hz, 1H), 4.65 (q, *J*=6.9 Hz, 1H), 1.75 (d, *J*=6.9, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3/CD_3OD$, 298 K): δ = 149.18, 147.40, 135.28, 131.16, 130.47, 128.39, 128.28, 127.53, 127.39, 20.19 ppm (one signal is hidden under the solvent peak at 49 ppm); HRMS ESI: *m*/*z* calcd for $C_{11}H_{12}N_2$: 173.1079 $[M + H]^+$, found: 173.1071.

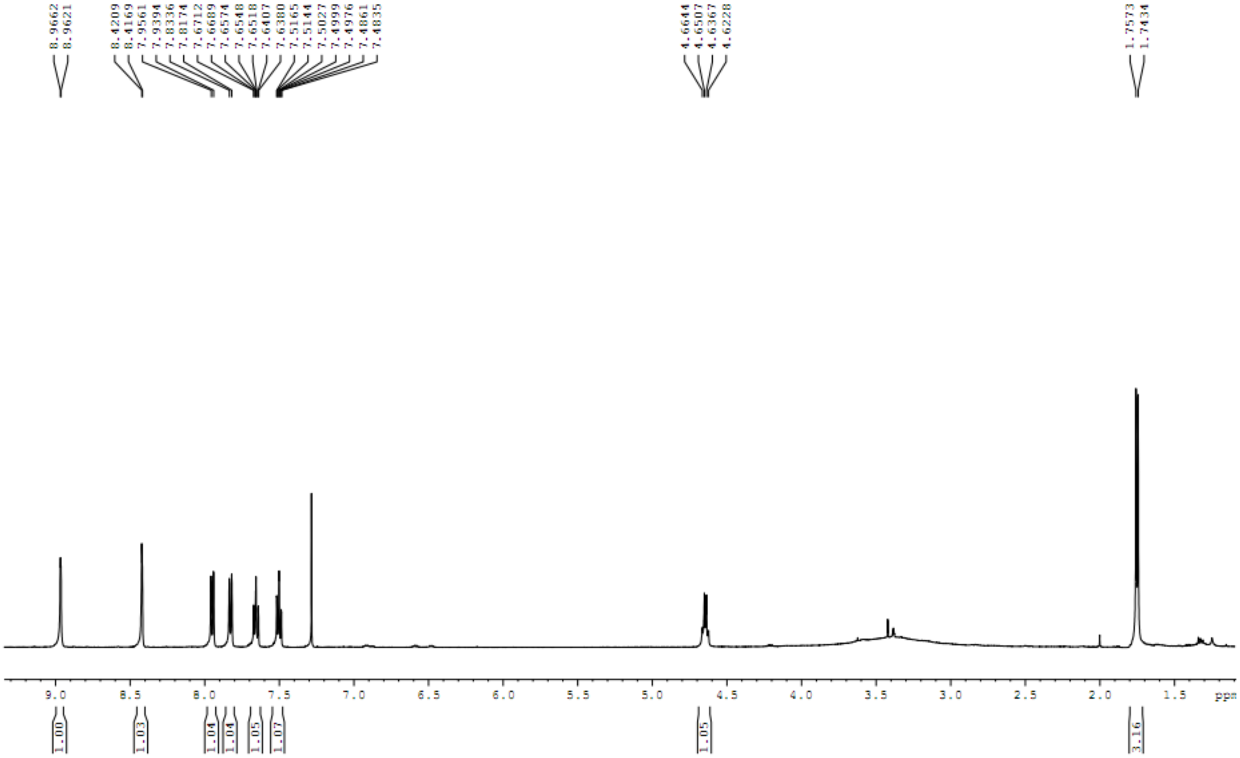


Figure S10: ^{1}H NMR spectrum (500 MHz) of compound **8** in $CDCl_3/CD_3OD$ at 298 K.

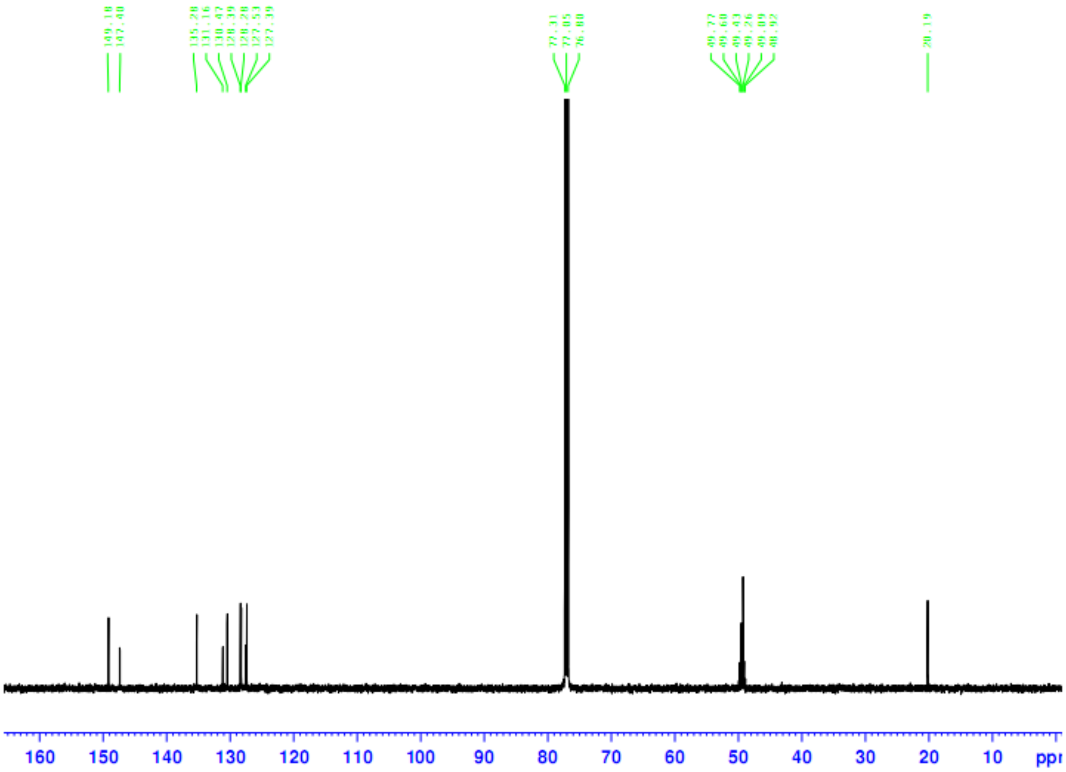


Figure S11: ^{13}C NMR spectrum (125 MHz) of compound **8** in $CDCl_3/CD_3OD$ at 298 K.

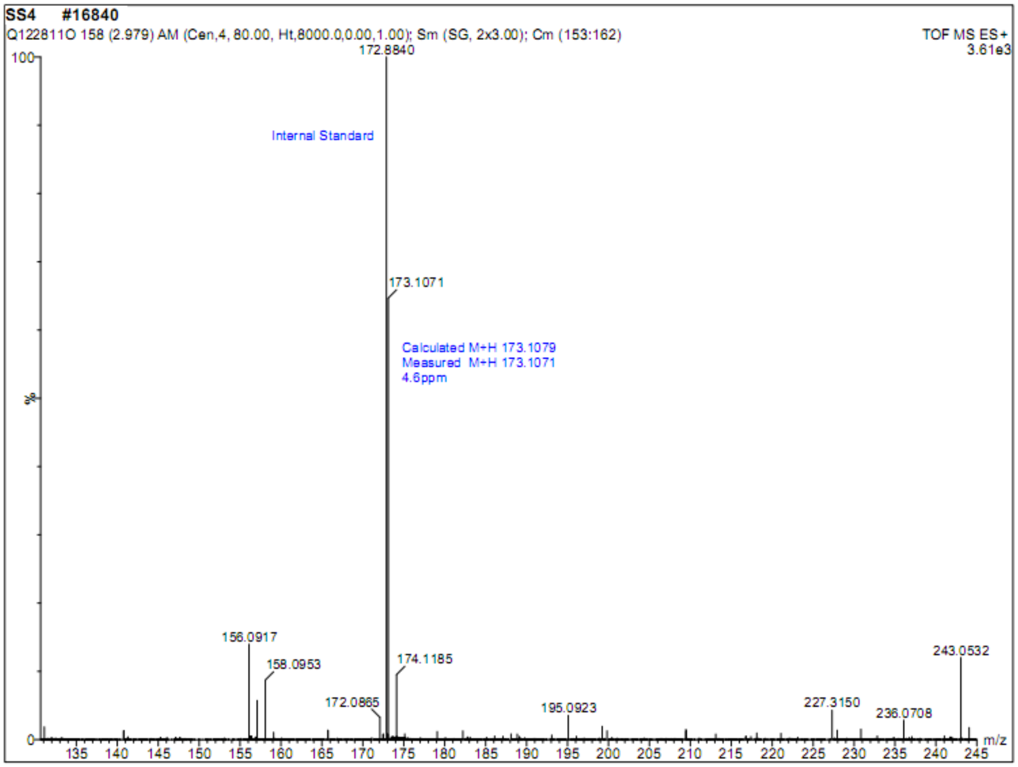
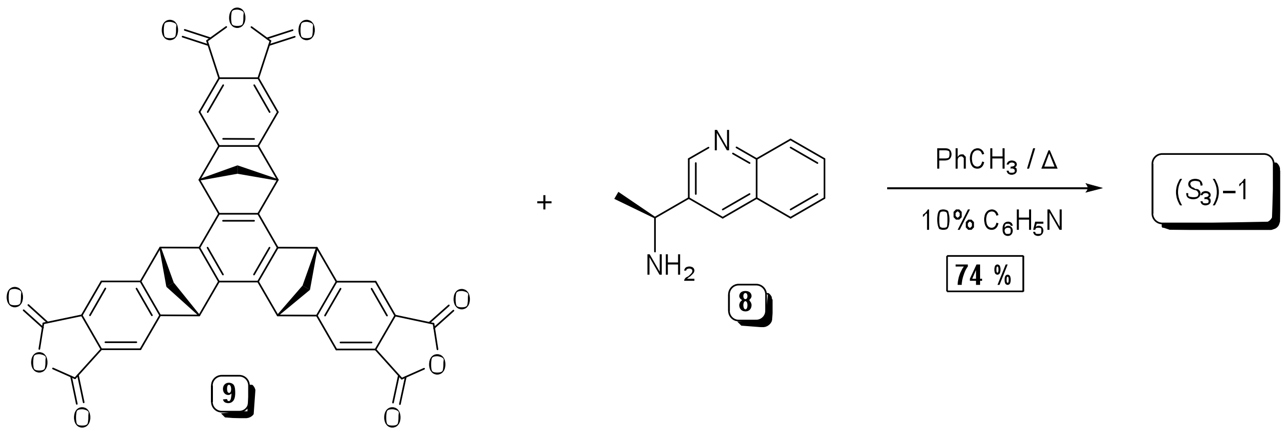


Figure S12: High resolution MS (ESI) spectrum of compound **8** showing a strong signal at 173.1071 corresponding to its $(M+H)^+$ ion.



Scheme S2: Synthesis of molecular basket **(S_3)–1.**

Basket (S_3)–1: Compound **8** (2.7 mg, 0.0158 mmol) was added to a solution of *tris*-anhydride **9** (2.0 mg, 0.00317 mmol) in 2 mL of toluene. The solution was heated to reflux and stirred for 1 h upon which 200 μL of neat pyridine was added. The resulting mixture was stirred for additional 24 h and then cooled down to room temperature. The mixture was concentrated under reduced pressure and the residue purified with thin-layer chromatography (SiO_2, dichloromethane:methanol=9:1) to yield 2.56 mg of basket (S_3)-**1** (74%). ^1H NMR (500 MHz, $CDCl_3$, 298 K): δ = 8.91 (s, 3H), 8.21 (s, 3H), 8.03 (d, *J*=8.3, 3H), 7.79 (d, *J*=8.3, 3H), 7.65 (t, *J*=7.6, 3H), 7.50 (t, *J*=7.6, 3H), 7.49 (s, 3H), 7.45 (s, 3H), 5.61 (q, *J*=7.3 Hz, 3H), 4.48 (d, *J*=3.7 Hz, 6H), 2.57 (s, 6H), 1.82 (d, *J*=7.3 Hz, 9H); ^{13}C NMR (125 MHz, $CDCl_3$, 298 K): δ = 167.73, 167.71, 156.85, 156.77, 150.48, 147.46, 137.86, 134.34, 132.99, 130.45, 130.21, 129.44, 129.06, 128.03, 127.63, 126.76, 116.10, 116.00, 65.72, 49.09, 47.18, 17.28 ppm; note that both ^1H and ^{13}C NMR spectra of (S_3)–**1** are in agreement with the formation of enantiopure compound, since the presence of other diastereomers would give rise to more complicated spectra. HRMS ESI: *m*/*z* calcd for $C_{72}H_{48}N_6O_6$: 1115.3533 $[M + Na]^+$, found: 1115.3521.

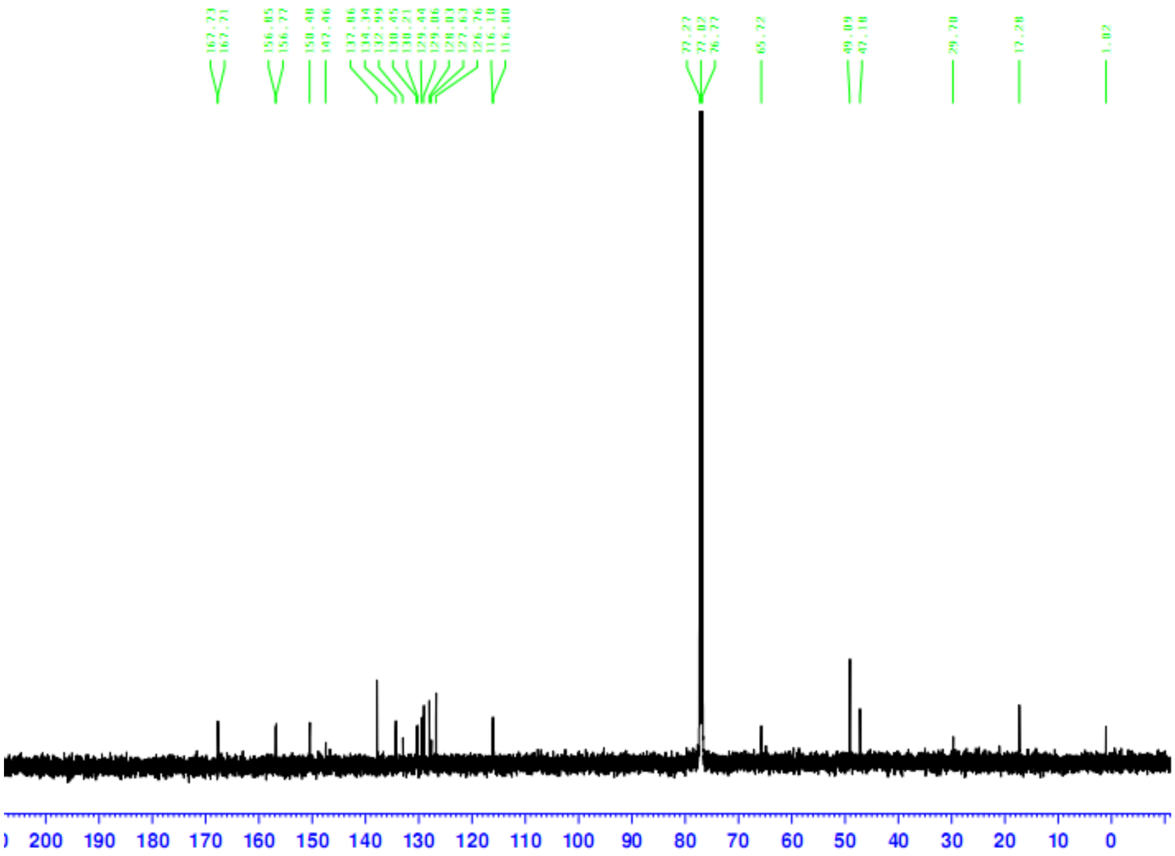


Figure S13: ^{13}C NMR spectrum (125 MHz) of basket (S_3)-**1** in $CDCl_3$ at 298 K.

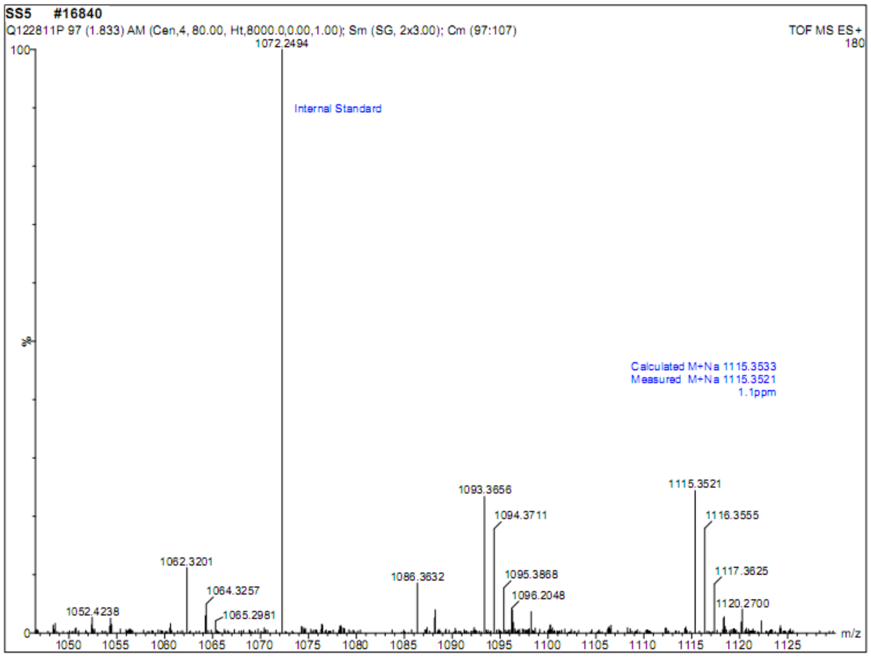


Figure *S*14: High resolution MS (ESI) spectrum of basket (S_3)-**1** showing a signal at 1115.3521 corresponding to its $(M+Na)^+$ ion.

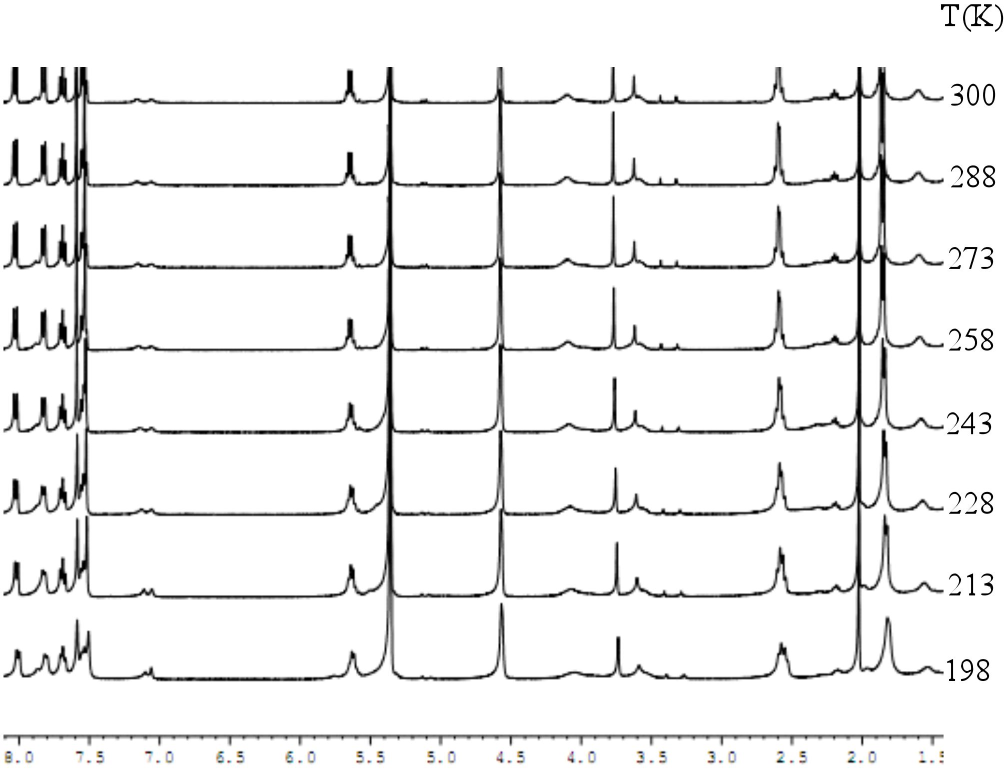


Figure S15: Variable temperature ^{1}H NMR (400 MHz) spectra of 1.1 mM solution of (S_3)–**1** in CD_2Cl_2.

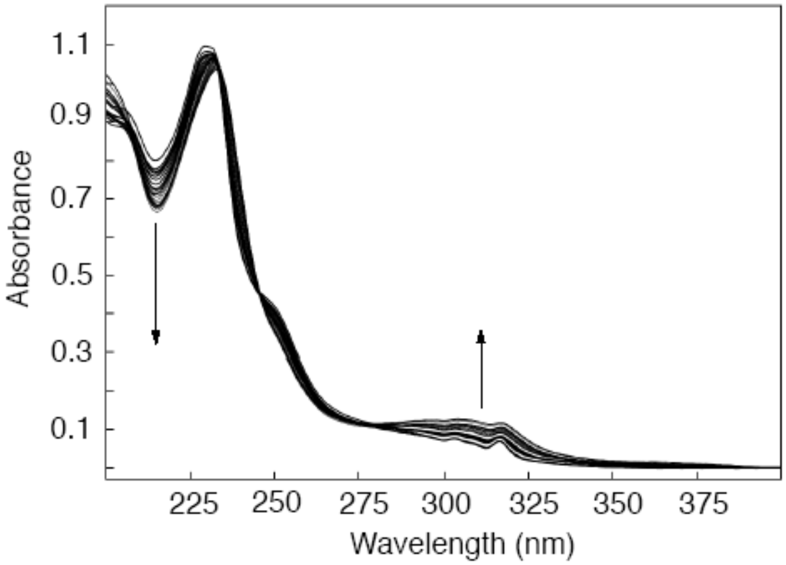


Figure S16: UV-Vis spectra of (S_3)–**1** (2.63 μM) obtained upon incremental addition (0.1-4.0 molar equivalents) of $Cu(BF_4)_2$ x $6H_2O$ (0.121 mM) in acetonitrile at 298 K.

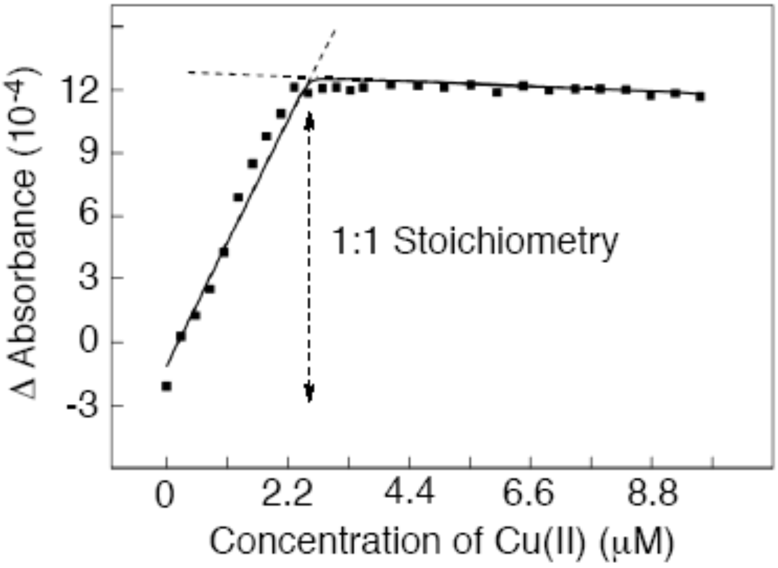


Figure S17: Experimental and theoretical CD binding isotherms (ReactLab software) showing the change in absorbance of (*S*$_3$)**–1** (2.63 μM) at 230 nm as a function of added Cu(BF$_4$)$_2$ x 6H$_2$O (0.1-4.0 molar equivalents) in acetonitrile at 298 K.

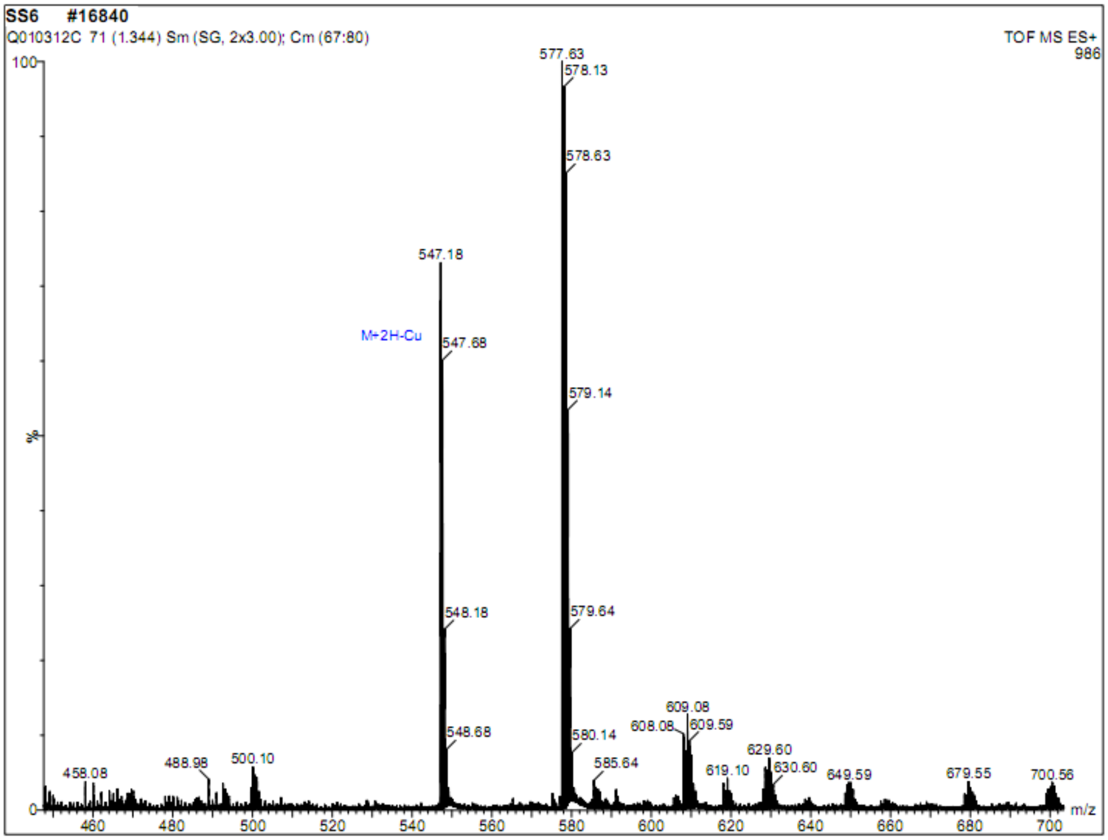


Figure S18: High resolution MS (ESI) spectrum of Cu(II)-(*S*$_3$)-**1** (compound **3**) showing a strong signal at 577.63 corresponding to ((*S*$_3$)-**1**-Cu)$^{2+}$ ion.

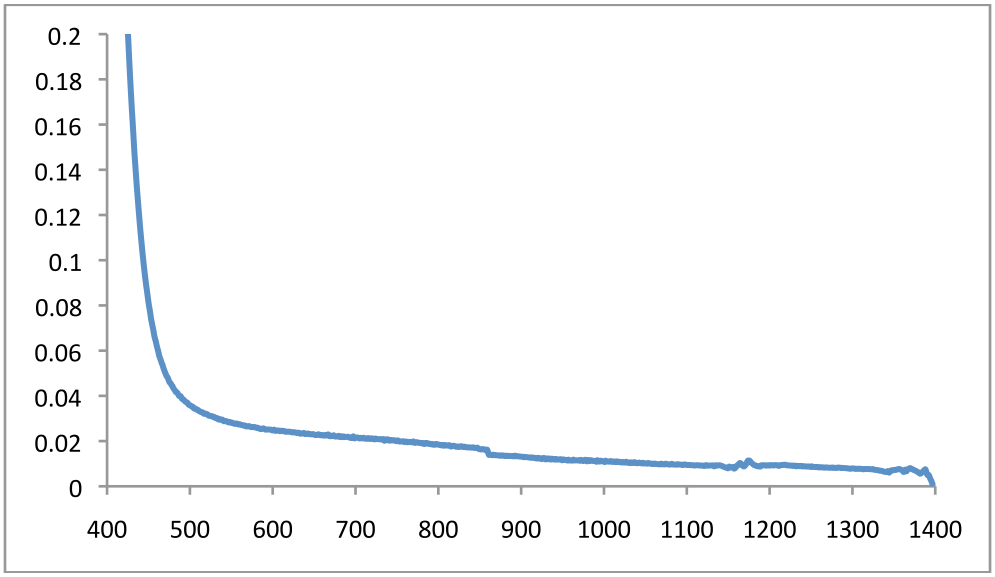


Figure S19: UV-Vis spectrum of Cu(II)–(*S₃*)-**1** (compound **3**, 0.59 mM) in acetonitrile at 298 K.

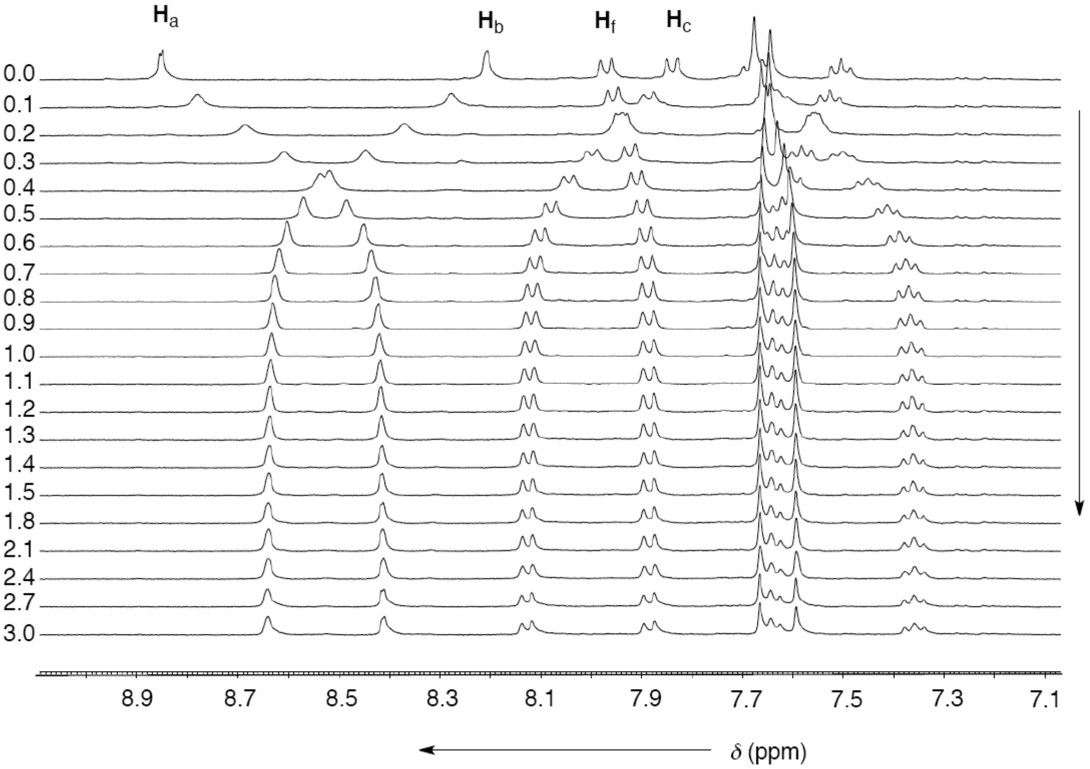


Figure S20: A series of ^{1}H NMR spectra (400 MHz, CD_3CN, 298.0 K) recorded on the addition of 45.25 mM standard solution of $[Cu(CH_3CN)_4]PF_6$ (molar equivalents are shown on the left) to 0.6 mM solution of (*S₃*)–**1**.

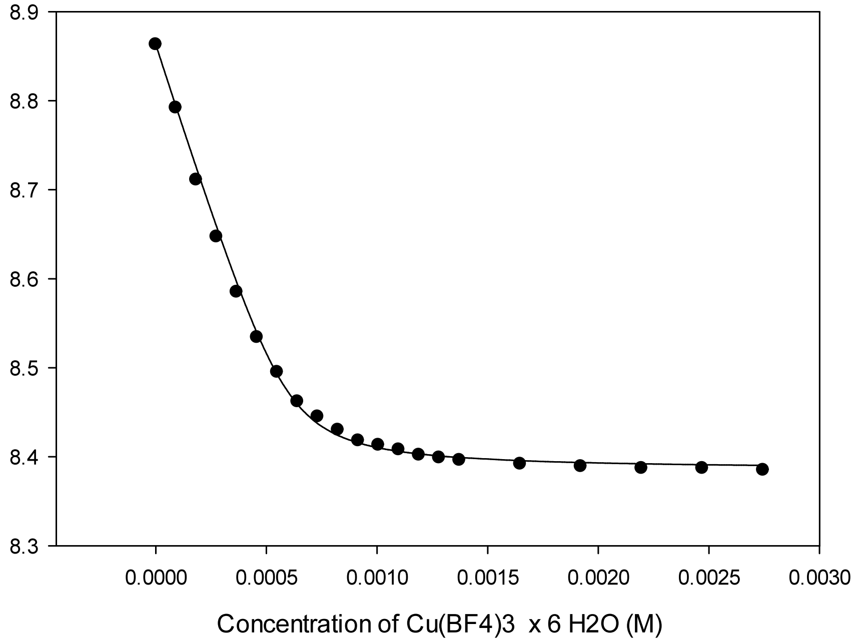


Figure S21: Nonlinear least-square fitting (SigmaPlot 12.0) of ^{1}H NMR (400 MHz, CD_3CN, 298.0 K) chemical shifts of **H**$_a$ in (*S*$_3$)–**1** (0.6 mM), obtained upon the incremental addition of $[Cu(CH_3CN)_4]PF_6$, gave $K_a = 4.1 \pm 0.3 \cdot 10^4$ M^{-1} for the formation of complex **4**.

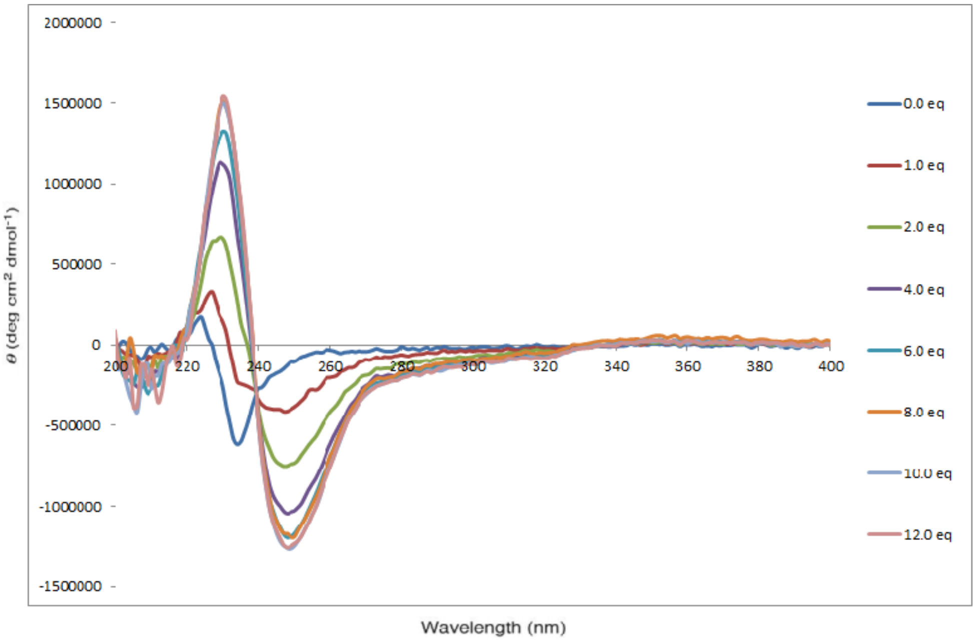


Figure S22: CD spectra obtained upon incremental addition of 0.0, 1.0, 2.0, 4.0, 6.0, 8.0, 10.0, 12.0 molar equivalents of $[Cu(CH_3CN)_4]PF_6$ (0.99 mM) to (*S*$_3$)-**1** (1.65 μM) dissolved in CH_3CN.

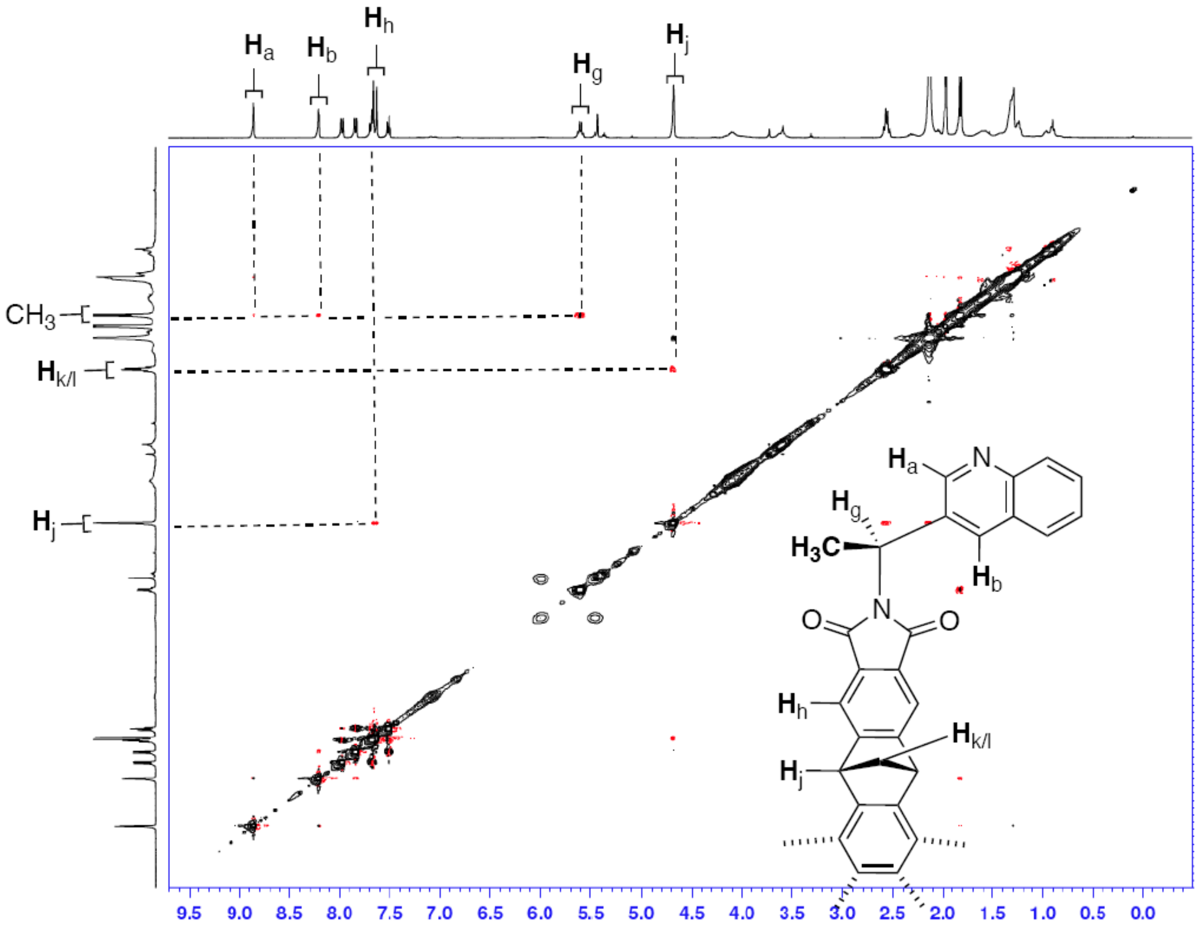


Figure S23: ^{1}H-^{1}H NOESY NMR spectrum (400 MHz, 298 K) of 1.83 mM solution of (S_3)-**1** in CD_3CN.

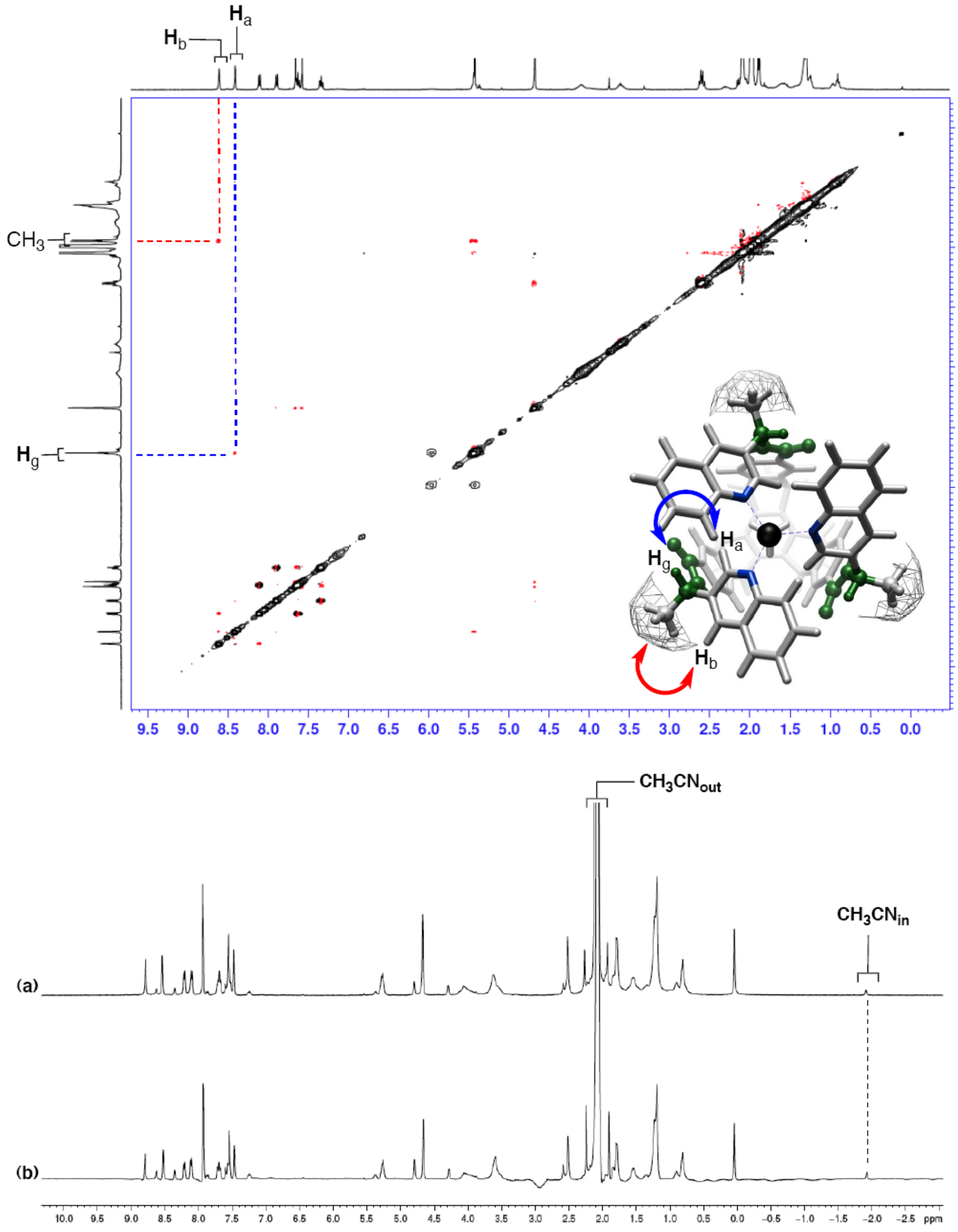


Figure S24: (Top) ^{1}H-^{1}H NOESY NMR spectrum (400 MHz, 298 K) of compound **4** (1.83 mM) in CD_3CN. (Bottom) Variable temperature ^{1}H NMR spectra of compound **4** (xx mM, $CDCl_3$:CD_3COCD_3 = 5:3) at xxx K and containing 100 (a) and 500 (b) molar equivalents of CH_3CN.

Electron Paramagnetic Resonance (EPR) Spectroscopy

EPR spectra were recorded with a Bruker ESP 300E spectrometer (Bruker Bioscience, Billerica, Massachusetts) operating at X-band with 100 kHz modulation frequency and a TM_{110} cavity as described previously (M. Velayutham et al., Free Radical Biology and Medicine, **2007**, *43*, 1076-1085). The instrument was also equipped with a proton probe gaussmeter and a microwave frequency counter to enable precise calibration of magnetic field and microwave frequency.

For low temperature (77 K) EPR experiment, the sample was placed in quartz tube and frozen at 77 K. The frozen sample was placed into the finger Dewar containing liquid nitrogen and positioned within the EPR spectrometer cavity. EPR spectrum was recorded with the following spectrometer conditions: microwave frequency 9.4363 GHz, modulation amplitude 2 G, receiver gain 5×10^3, time constant 163 ms, scan time 120 s, microwave power 20 mW, number of scan 1.

Cyclic Voltammetry (CV) Experiments

Additional electrochemistry data, in support of the assignments of the cyclic voltammetry (CV) made in the main text, are presented here. During addition of 0.1, 0.2, 0.5 and 1.0 eq. of Cu(II), the peaks assigned as **a** and **d** in the main text are observed to grow in, while the peaks for the phthalimide walls of the basket (**b** and **c**) remain relatively unchanged (Figure S25). When the same titration CVs were clipped prior to the phthalmide reduction, the same trends are observed (Figure S26). A comparison of the two CVs clipped before and after phthalimide (Figure S27) show modest differences. The CVs recorded at faster scan rates, e.g., 0.2, 0.5 and 1 V s^{-1} show the loss of intensity of peaks **a** and **d** (Figure S28). This behavior persisted up to 20 V s^{-1} (data not shown).

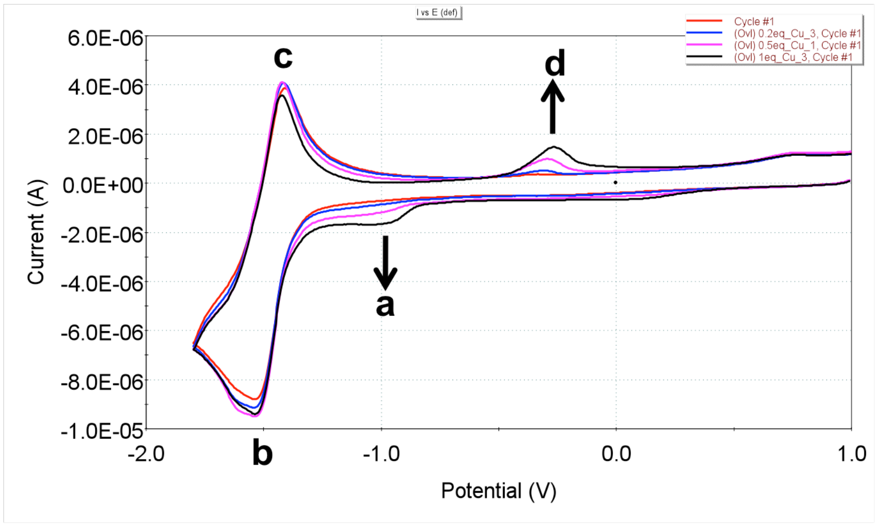


Figure S25. CVs generated of basket (S_3)**–1** (1.0 mM) upon addition of Cu(II): 0.1 eq. (red), 0.2 eq. (blue), 0.5 eq. (magenta) and 1.0 eq. (black). Conditions: 0.2 V s^{-1}, degassed CH_3CN, 0.1 *n*-$BuNPF_6$, glassy carbon working electrode, Ag/AgCl ref.

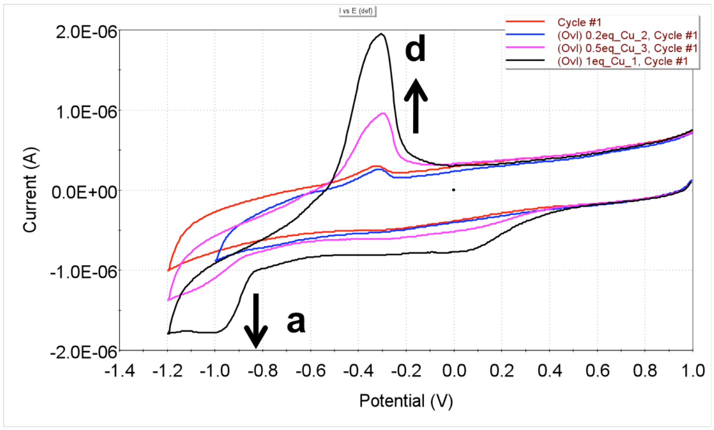


Figure S26. CVs generated during the same titration as Figure S1 but clipped at –1.2 V.

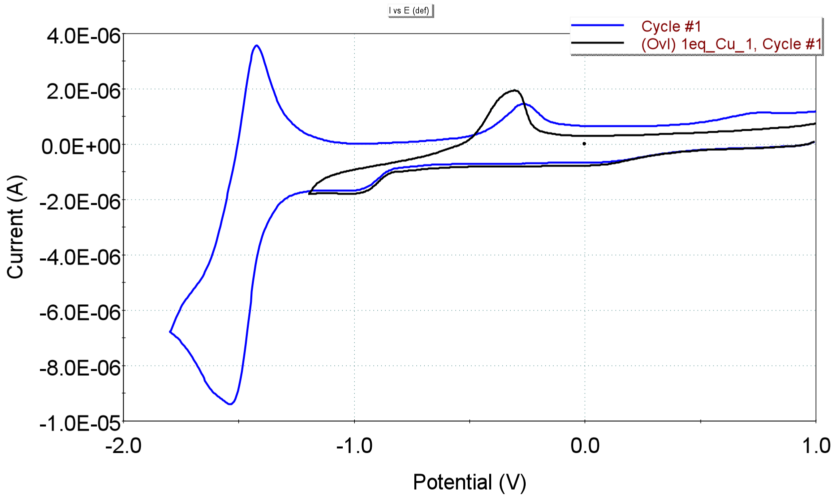


Figure S27. Comparison CVs generated of the complex (1.0 mM) when clipped before (black) and after (blue) the phthalimide reduction. Conditions: 0.2 V s^{-1}, degassed CH$_3$CN, 0.1 *n*-BuNPF$_6$, glassy carbon working electrode, Ag/AgCl ref.

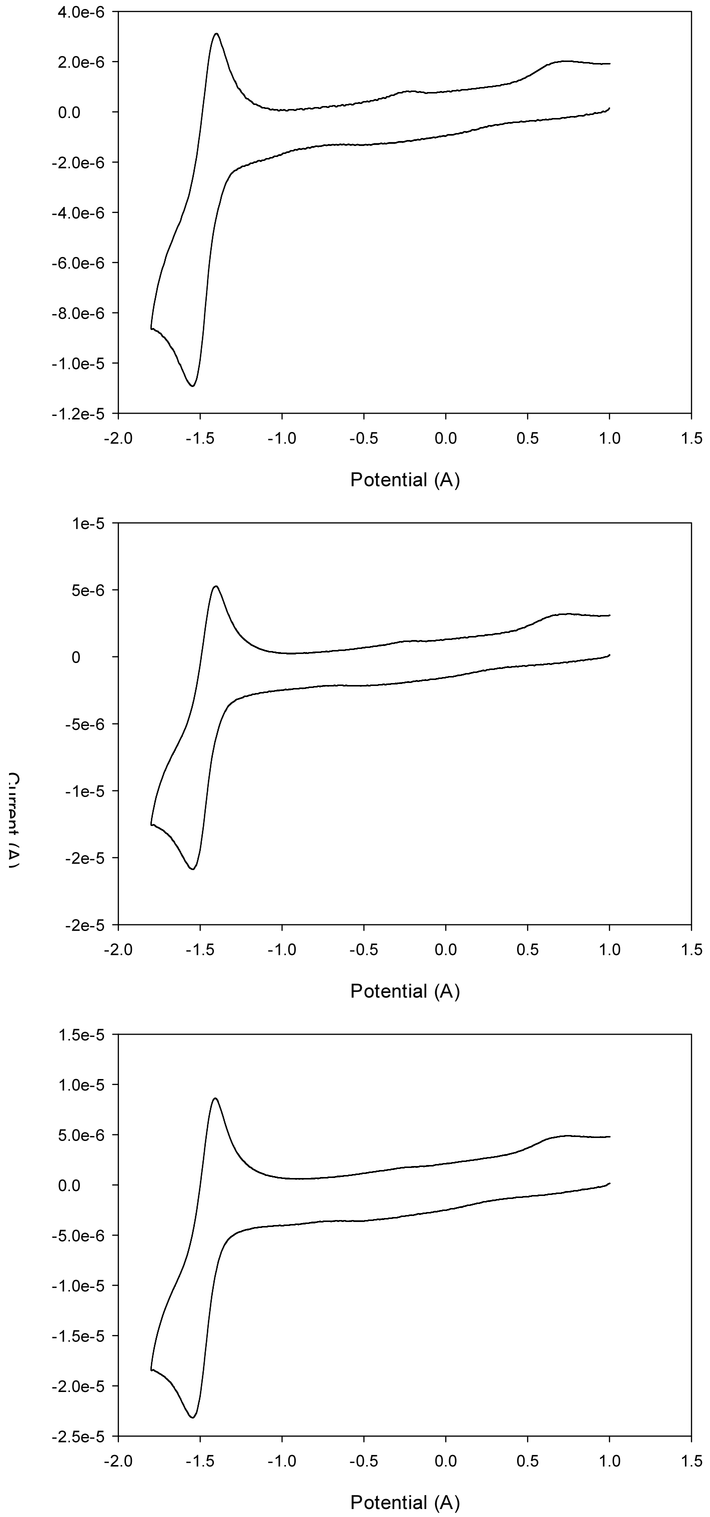


Figure S28: CVs of compound **3** (1.0 mM in CH_3CN) were obtained at scanning rates of 0.5, 1.0 and 2.0 V/s (top to bottom); Conditions: 0.2 V s^{-1}, degassed CH_3CN, 0.1 *n*-$BuNPF_6$, glassy carbon working electrode, Ag/AgCl ref..

Computational Studies

The Turbomole 6.3.1 software package was employed for all of the computational work in the manuscript.[i] Using the *jobex* module,[ii] geometry optimizations of trigonal bipyramidal complex **2** and square-pyramidal complex **3** were performed using density functional theory (DFT), with the BHLYP[iii] functional. In order to accurately represent the electronic structure of copper(II), the TZVP basis set[iv] was used, while the SV(P) basis set[v] was selected for all other atoms. Additionally, the resolution-of-the-identity (RI) approximation[vi] was utilized in order to decrease the computational cost of the system, while maintaining computational accuracy. In the manuscript, RI-BHLYP/TZVP,SV(P) is written as a shorthand to represent the entire methodology of the calculations. The Cartesian coordinates and bottom-of-the-well energies for both conformers are listed at the end of this document. Each stationary point was confirmed to be a minimum on the potential energy surface by computation of the analytical second derivatives, using the *aoforce* module,[ii] at the same level of theory.

Excited state calculations of complex **3** were performed using the shared-memory parallelization[vii] (SMP) version of the *escf* module[viii] in Turbomole 6.3.1. The newly developed version of *escf* made it possible to compute the first 185 excited states of the entire CD and UV spectra using 8 processors simultaneously. Time-dependent density functional theory was employed (TD-BHLYP/TZVP,SV(P)) for the excited state calculations.[ix] A uniform 0.3 eV Gaussian line broadening was applied to the oscillator strengths (for the UV spectrum) and rotatory strengths (for the CD spectrum) in order to properly simulate the observed spectra. A redshift of 0.7 eV was applied to the excitation energy values. Based on previous work on simulating UV and CD spectra, including our own, a phase shift value of –0.7 eV was chosen to align the theoretical UV spectrum with experiment at 233 nm.[x] In Figure 5 of the manuscript, the oscillator and rotatory strengths were normalized to fit on the same graph as the experimental spectra. The unshifted and –0.7 eV shifted excitation values (in eV and nm), as well as oscillator strengths and rotatory strengths obtained directly from the *escf* module are listed at the end of this document.

For the excited states of interest, electron density difference plots of complex **3** were calculated using the SMP version of the *egrad* module[xi] in Turbomole 6.3.1. The plots for fourteen excited states (S40, S42, S47, S58, S100, S107, S108, S156, S157, S160, S161, S165, S168, S171) were computed based on their dominant contributions to significant peaks on the computed spectra. The depletion of electron density from the ground state to the excited state of interest is shown in red, whereas the accumulation of electron density in the excited state is shown in green. The contour values for the plots ranged from ±0.001 to 0.002 au. The specific contour values for each plot are listed in Figure S30.

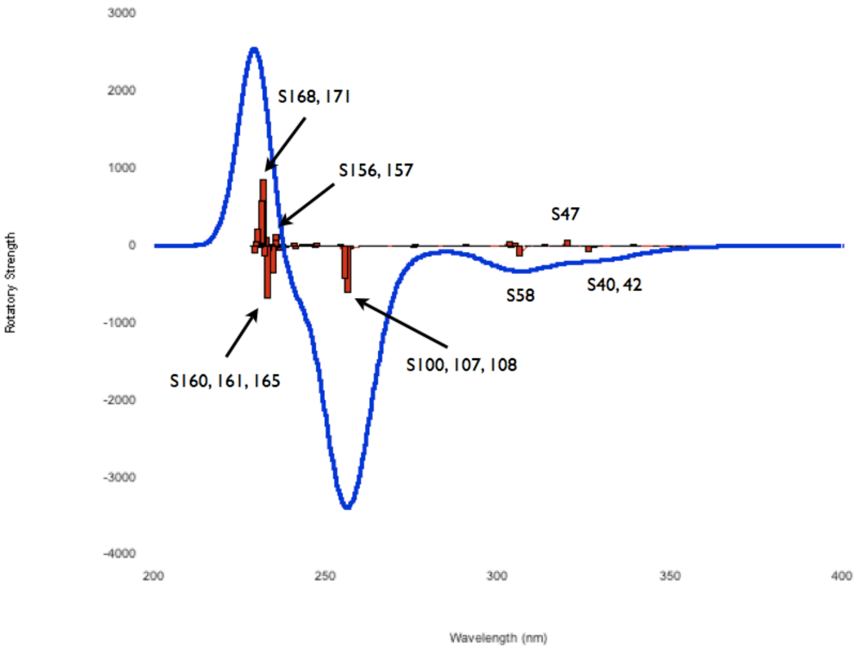
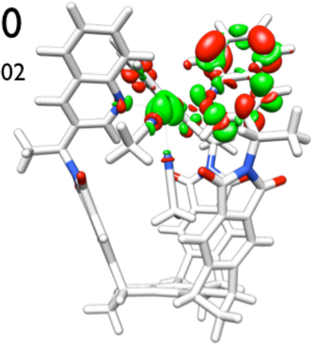
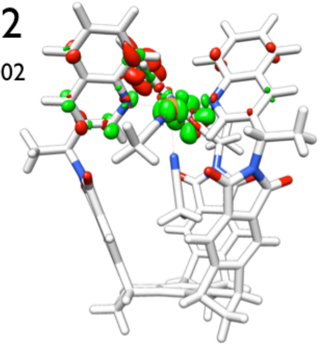


Figure S29. Density functional theory (TD-BHLYP/TZVP,SV(P)) computed CD spectra of complex **3**. For the excited states listed, electron density difference plots were computed and are shown in Figure S28.

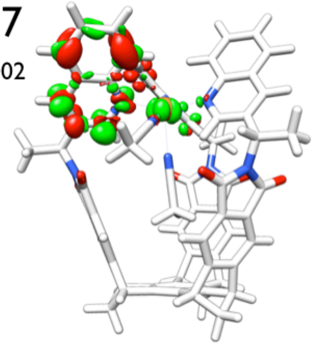
S40
±0.002



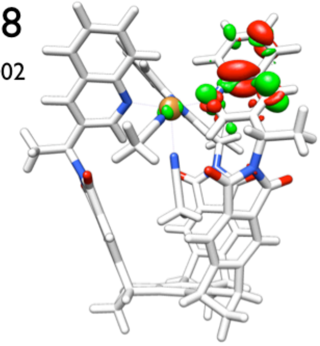
S42
±0.002



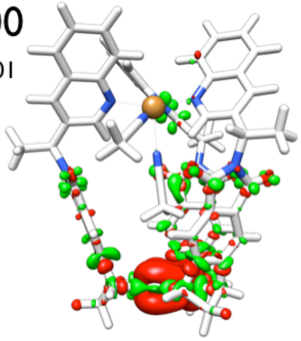
S47
±0.002



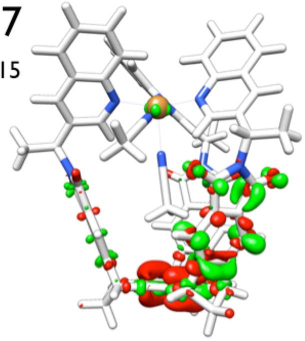
S58
±0.002



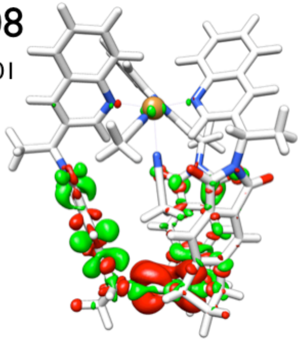
S100
±0.001



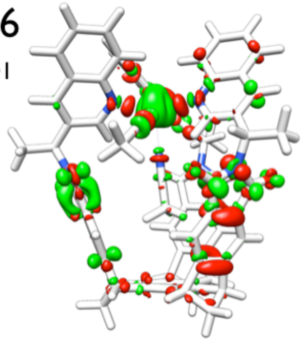
S107
±0.0015



S108
±0.001



S156
±0.001



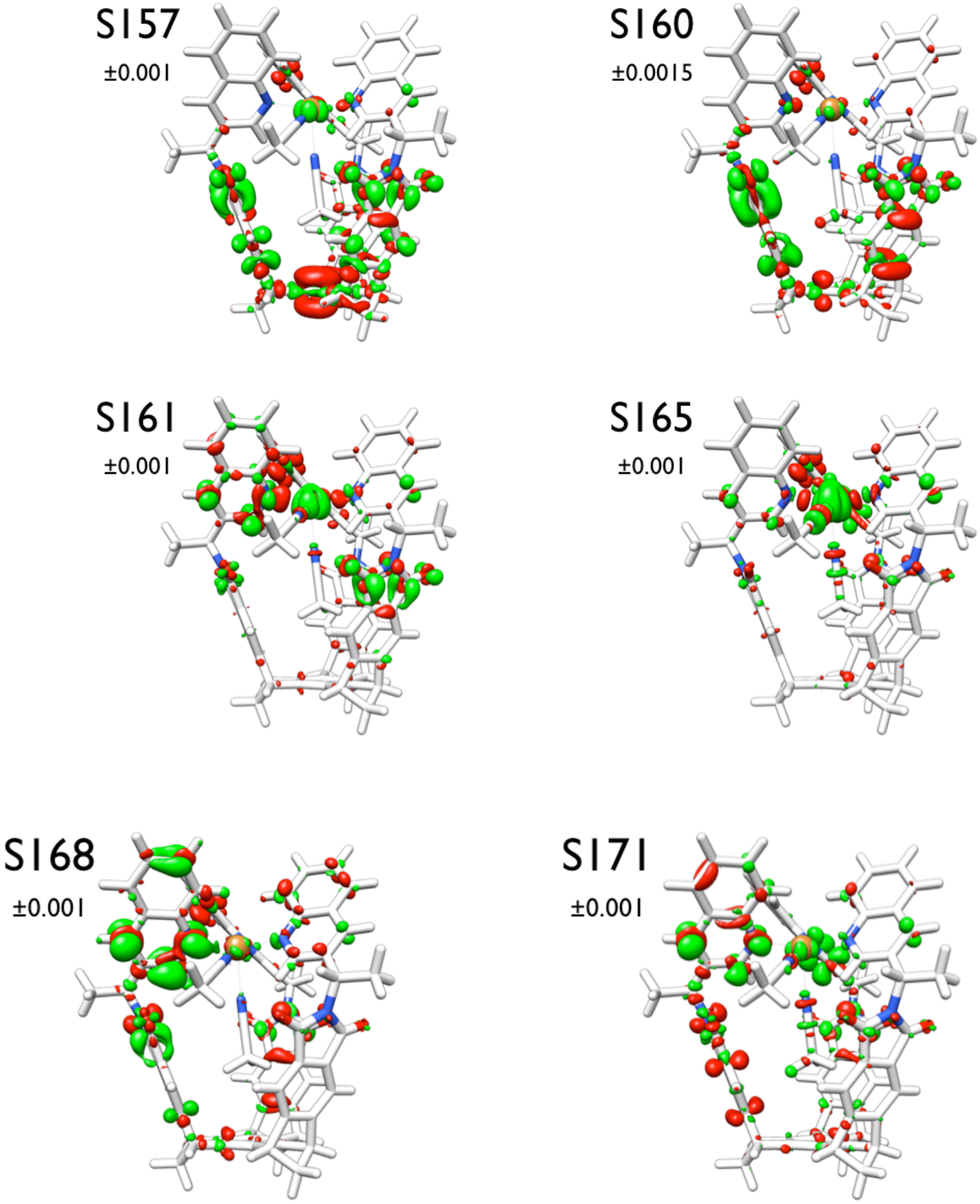
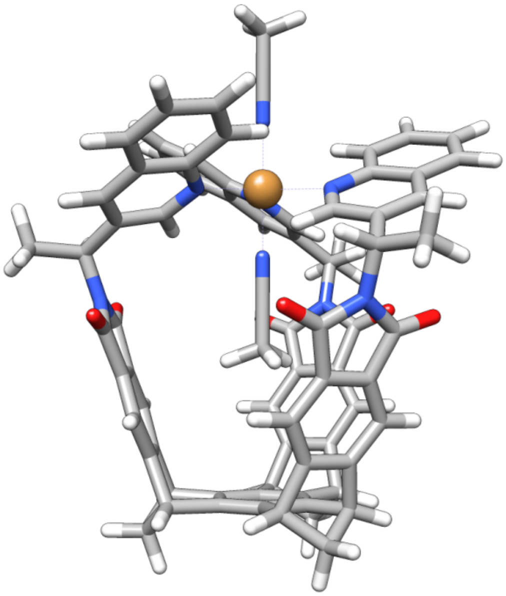


Figure S30. Electron density difference plots of notable transitions observed in the computed UV or CD spectra pf complex **3**. The calculations were performed using the *egrad* module in Turbomole 6.3.1. The red color represents the depletion and green represents the accumulation of electron density between the ground state configuration and desired excited state configuration. Contour values (in au) are listed beside each plot.

Complex **2**



RI-BHLYP/TZVP,SV(P)

E_{bw} = -5453.050730741 hartrees

C	-0.3940761	-1.3361808	-5.7044742
C	-1.7032712	2.3408493	-5.6868692
C	0.5088953	2.8447367	-5.6319284
C	2.8788706	0.3046515	-5.6868692
C	-1.4343886	2.9260892	-4.3126472
C	-0.0567303	3.2202944	-4.2671869
C	-2.7604916	-1.6592771	-4.2671869
C	-1.8168733	-2.7052616	-4.3126472
C	2.8172219	-1.5610173	-4.2671869
C	3.2512619	-0.2208276	-4.3126472
C	-2.2689732	3.1523033	-3.2344077
C	0.9362703	-1.0303621	-5.6950200
C	0.5413521	3.7151014	-3.1219366

C	-3.4880483	-1.3887260	-3.1219366
C	-1.5954881	-3.5411400	-3.2344077
C	2.9466961	-2.3263754	-3.1219366
C	3.8644613	0.3888368	-3.2344077
C	-1.6621912	3.6656913	-2.0954560
C	-0.3021205	3.9233378	-2.0347845
C	4.0056774	-0.3933459	-2.0954560
C	3.5487705	-1.7000249	-2.0347845
C	-3.2466499	-2.2233129	-2.0347845
C	1.3542046	0.3268105	-5.7044742
C	-2.3434862	-3.2723454	-2.0954560
C	0.0133714	4.4070870	-0.6649171
C	-2.2651225	4.0268559	-0.7859593
C	4.6199208	-0.0517744	-0.7859593
C	3.8099636	-2.2151234	-0.6649171
C	-2.3547983	-3.9750816	-0.7859593
C	-3.8233350	-2.1919636	-0.6649171
C	-1.3393426	4.9021999	1.3911731
C	4.9151009	-1.2911952	1.3911731
C	-3.5757583	-3.6110047	1.3911731
C	0.4241846	1.3260149	-5.6950200
C	-2.4127079	-2.2170649	-6.5157797
C	3.1263885	-0.9809339	-6.5157797
C	-0.7136806	3.1979988	-6.5157797
C	-1.6644389	-4.6031611	2.7718068
C	-2.3176068	-3.5257264	2.2369485
C	-1.7416508	-2.2608776	2.4545138

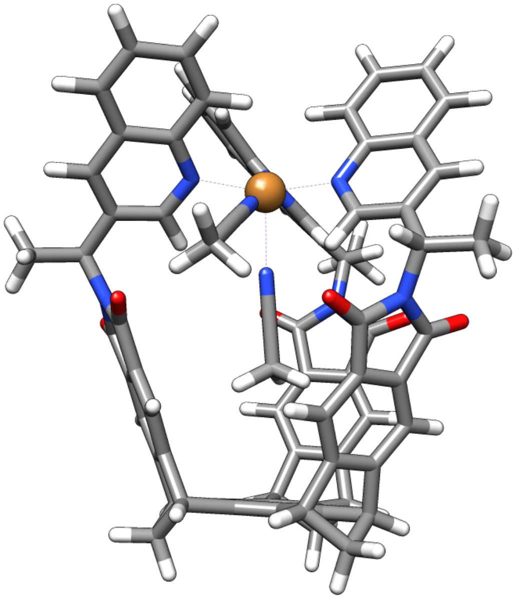
C	2.6766862	1.5809877	3.6693647
C	4.0678340	1.8013226	3.5067058
C	-0.9601284	1.0093703	-5.7044742
C	4.8186739	0.8601342	2.7718068
C	4.2121720	-0.2442432	2.2369485
C	2.8288028	-0.3778751	2.4545138
C	-2.7075186	1.5275845	3.6693647
C	-1.0871520	2.6387527	2.4545138
C	-1.8945652	3.7699695	2.2369485
C	-3.1542350	3.7430269	2.7718068
C	-1.3604549	-0.2956528	-5.6950200
C	2.2091666	-1.8630846	-5.6319284
C	-1.1755994	-2.6455008	-5.6868692
C	-2.7180619	-0.9816521	-5.6319284
H	2.1158939	-2.9174896	-5.8870976
H	-3.3349246	2.9538205	-3.2623689
H	-4.2151118	-0.5858409	-3.0620585
H	-0.8906213	-4.3650397	-3.2623689
H	-3.2129861	-2.9625232	-6.5047261
H	-2.1656105	-1.9512217	-7.5467876
H	4.1721134	-1.3012660	-6.5047261
H	2.7726128	-0.8998629	-7.5467876
H	-0.6364999	-3.5382163	-6.0004735
H	-0.9591273	4.2637892	-6.5047261
H	-0.6070023	2.8510845	-7.5467876
H	-2.0413293	-5.6092171	2.6296047
H	-2.2398338	-1.3885198	2.0376385

H	5.8783892	1.0367655	2.6296047
H	2.3224103	-1.2454931	2.0376385
H	-0.0825765	2.6340129	2.0376385
H	-3.8370598	4.5724516	2.6296047
H	-3.5845671	-0.3736730	-5.8870976
H	-2.7459352	2.3203333	-6.0004735
H	1.4686732	3.2911627	-5.8870976
H	3.3824352	1.2178830	-6.0004735
H	2.6149090	-3.3574734	-3.0620585
H	4.2255459	1.4112191	-3.2623689
H	1.6002028	3.9433144	-3.0620585
N	-3.2579855	-3.2748854	0.0111542
N	-1.2071412	4.4589409	0.0111542
N	4.4651267	-1.1840555	0.0111542
N	-0.6334502	-2.0434266	3.1258146
N	2.0863844	0.4731293	3.1258146
N	-1.4529342	1.5702973	3.1258146
O	1.0740565	4.6638906	-0.1807685
O	-3.4057765	3.9584070	-0.4391701
O	5.1309693	0.9702854	-0.4391701
O	3.5020195	-3.2621056	-0.1807685
O	-1.7251928	-4.9286924	-0.4391701
O	-4.5760760	-1.4017851	-0.1807685
C	1.3923282	-5.3120451	4.7583800
H	1.9321674	-6.1516801	5.1819108
C	1.8928245	-4.0035661	4.9186849
H	2.8169987	-3.8507795	5.4665638

C	0.0308324	-3.1085721	3.6693647
C	-0.4739259	-4.4235089	3.5067058
C	1.2318408	-2.9263917	4.3901648
H	1.6299740	-1.9285001	4.5202124
C	0.2322823	-5.5152846	4.0655065
H	-0.1619208	-6.5166529	3.9281784
C	-3.5939082	2.6221863	3.5067058
C	-5.2965301	1.4502310	4.7583800
H	-6.2935949	1.4025340	5.1819108
C	-4.4136021	0.3625490	4.9186849
H	-4.7433723	-0.5142027	5.4665638
C	-3.1502500	0.3963904	4.3901648
H	-2.4851170	-0.4473488	4.5202124
C	-4.8925178	2.5564799	4.0655065
H	-5.5626265	3.3985540	3.9281784
C	3.9042019	3.8618141	4.7583800
H	4.3614275	4.7491461	5.1819108
C	2.5207777	3.6410171	4.9186849
H	1.9263735	4.3649822	5.4665638
C	1.9184092	2.5300013	4.3901648
H	0.8551431	2.3758489	4.5202124
C	4.6602354	2.9588047	4.0655065
H	5.7245473	3.1180989	3.9281784
Cu	0.0000000	0.0000000	3.1994534
C	-2.1063106	6.2128944	1.4927914
H	-1.5851718	6.9846626	0.9192118
H	-3.1206610	6.1202232	1.0963829

H	-2.1602083	6.5464856	2.5339510
C	6.4336796	-1.2823287	1.4927914
H	6.8414811	-2.1195323	0.9192118
H	6.8605993	-0.3575399	1.0963829
H	6.7495270	-1.4024475	2.5339510
C	-4.3273690	-4.9305657	1.4927914
H	-5.2563094	-4.8651303	0.9192118
H	-3.7399382	-5.7626833	1.0963829
H	-4.5893187	-5.1440381	2.5339510
H	-4.2451772	-2.8086209	1.7104085
H	-0.3097484	5.0807418	1.7104085
H	4.5549257	-2.2721209	1.7104085
C	0.0000000	0.0000000	6.3874324
N	0.0000000	0.0000000	5.2468010
C	0.0000000	0.0000000	7.8397387
H	0.0912633	-1.0267105	8.2070696
H	0.8435257	0.5923915	8.2070696
H	-0.9347890	0.4343189	8.2070696
C	0.0000000	0.0000000	-0.0114947
N	0.0000000	0.0000000	1.1304907
C	0.0000000	0.0000000	-1.4643866
H	-0.8756455	-0.5449139	-1.8320023
H	-0.0340865	1.0307881	-1.8320023
H	0.9097320	-0.4858743	-1.8320023

Complex **3**



RI-BHLYP/TZVP,SV(P)

E_{bw} = -5453.053912725 hartrees

C	-5.5740189	-1.5946922	-0.3551154
C	-5.3933097	-0.9402457	2.3510735
C	-5.9616417	-0.3050061	0.0935968
C	-5.1479187	-2.5276945	0.5475316
C	-5.0832113	-2.2021214	1.9291915
C	-5.8549412	0.0212749	1.4140889
C	-6.3746075	0.4762248	-1.1464364
H	-6.9828205	1.3642571	-0.9819269
C	-5.7258223	-1.5741045	-1.8721615
H	-5.7445092	-2.5400612	-2.3746282
C	-4.6787110	-0.5854376	-2.3704979
C	-5.0873512	0.6872153	-1.9223376

C	-6.9842556	-0.6762834	-1.9832997
H	-7.8669467	-1.1210747	-1.5170654
H	-7.2134432	-0.3839096	-3.0119168
C	-4.3496888	1.8282183	-2.1794949
H	-4.6565191	2.8153667	-1.8512339
C	-3.5108064	-0.7583124	-3.0904271
H	-3.1851282	-1.7270474	-3.4537530
C	-3.1805616	1.6434648	-2.9060767
C	-2.7730700	0.3944791	-3.3438280
C	-5.2757717	-0.2072813	3.6845032
H	-5.2095862	-0.8234982	4.5797224
C	-6.0293486	1.3210879	2.1862172
H	-6.6455391	2.0892021	1.7214322
C	-4.1342837	0.7805461	3.4641323
C	-4.6038540	1.7230812	2.5274175
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H	-7.4383397	0.2403320	3.5104021
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H	-2.4570155	0.1073416	4.6709268
C	-3.7878594	2.7133358	2.0140961
H	-4.1283560	3.4397903	1.2841004
C	-2.0187972	1.8141195	3.4181819
C	-2.4792497	2.7224750	2.4790535
C	-4.6663536	-3.9688672	0.4305268
H	-4.8999136	-4.4855115	-0.4993627
C	-4.6040620	-3.4608923	2.6419400

H	-4.7874749	-3.5100251	3.7140719
C	-3.1640680	-3.6532125	2.2080312
C	-3.1955979	-3.9555398	0.8311381
C	-5.2725200	-4.5319381	1.7421355
H	-4.9394602	-5.5487519	1.9685812
H	-6.3642656	-4.4846534	1.7601373
C	-2.0336356	-4.1659306	0.1084980
H	-2.0385577	-4.4081043	-0.9488544
C	-1.9795837	-3.5772685	2.9144852
H	-1.9389354	-3.3725040	3.9787751
C	-0.8417861	-4.0781382	0.8243191
C	-0.8223607	-3.8057044	2.1819951
C	-0.5780344	2.0987816	3.6689691
C	-1.3455785	3.5914647	2.0757306
C	-1.4865411	0.5605930	-4.0636783
C	-2.1782586	2.6461863	-3.3550813
C	0.5653153	-4.2526057	0.3686403
C	0.5854805	-3.8457545	2.6449689
O	-2.1514952	3.8195566	-3.1585687
O	-0.7685720	-0.2863191	-4.5216974
O	-1.3224694	4.4758634	1.2757907
O	0.1751329	1.5588970	4.4214387
O	0.9760664	-4.4321530	-0.7434195
O	1.0245858	-3.6796700	3.7390328
N	1.3551383	-4.1184081	1.5056250
N	-0.2431201	3.1428451	2.8066301
N	-1.2119815	1.9212426	-4.0667053

C	-0.0804547	2.5031553	-4.7750101
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C	2.7814566	-4.3927819	1.6030636
H	3.0359461	-4.0747865	2.6184969
C	1.0282516	3.8491131	2.7945051
H	0.9406923	4.5259963	1.9407429
C	2.1899442	2.9137184	2.5073602
C	4.3384482	1.3294693	1.7118930
C	3.2200946	2.6982172	3.3811770
C	2.2586828	2.2422909	1.2709826
N	3.2496735	1.4664305	0.8859683
C	4.3271654	1.9127105	3.0040609
H	3.2186261	3.1488806	4.3662541
H	1.4378877	2.3585860	0.5706656
C	1.0480679	2.8803010	-3.8278835
C	3.2937645	3.1730169	-2.1991193
C	1.7941828	4.0242013	-3.9210739
C	1.4417001	1.9510748	-2.8484934
N	2.4980893	2.0627630	-2.0758673
C	2.9334548	4.2031652	-3.1057748
H	1.5448218	4.7993534	-4.6363940
H	0.8522152	1.0528921	-2.7244404
C	3.5712579	-3.5304279	0.6384901
C	4.8667210	-1.7978293	-1.1100862
C	4.6317033	-3.9878070	-0.0953556
C	3.2191955	-2.1750605	0.4718808
N	3.8106505	-1.3570917	-0.3613632

C	5.3212351	-3.1299204	-0.9802391
H	4.9576742	-5.0185702	-0.0228457
H	2.3871424	-1.7686303	1.0384819
C	5.5046590	0.6541872	1.2946732
H	5.5660839	0.2525690	0.2956077
C	5.4386887	1.7416060	3.8628508
H	5.4024911	2.1811157	4.8539903
C	6.5769696	0.5256871	2.1382851
H	7.4677506	0.0117189	1.7927503
C	6.5429118	1.0549863	3.4433323
H	7.3968610	0.9323018	4.1001137
C	5.5166455	-0.9369628	-2.0202782
H	5.1730389	0.0862503	-2.1405081
C	6.4234698	-3.5652985	-1.7531081
H	6.7669866	-4.5888615	-1.6455706
C	7.0442318	-2.7102407	-2.6211351
H	7.8904330	-3.0468389	-3.2098863
C	6.5822561	-1.3847044	-2.7556011
H	7.0768320	-0.7136297	-3.4498442
C	4.4849858	3.3099466	-1.4557488
H	4.7877798	2.5250465	-0.7768438
C	3.7478001	5.3555637	-3.2096552
H	3.4562087	6.1397257	-3.9002792
C	5.2606600	4.4316385	-1.5893713
H	6.1752819	4.5205255	-1.0127928
C	4.8877255	5.4716255	-2.4643124
H	5.5115416	6.3543039	-2.5504426

C	1.1962272	4.6986284	4.0477647
H	1.2158436	4.0847230	4.9526810
H	0.3576294	5.3965492	4.1252318
H	2.1159183	5.2894240	3.9980154
C	3.0648918	-5.8853850	1.4947300
H	2.4501434	-6.4244689	2.2208017
H	4.1101500	-6.1045620	1.7308153
H	2.8385204	-6.2650527	0.4936874
C	-0.5063880	3.6105563	-5.7295159
H	-0.8498641	4.4996244	-5.1970799
H	-1.3208633	3.2515299	-6.3650385
H	0.3252374	3.8806813	-6.3867908
N	2.2570496	-0.8347786	-2.4975323
C	1.8297430	-1.6750988	-3.1426313
C	1.2612671	-2.7597792	-3.9203587
H	1.0148976	-3.5809328	-3.2372396
H	0.3611458	-2.3896090	-4.4212043
H	1.9848716	-3.1040176	-4.6650511
N	0.6753423	0.0162906	-0.1826106
C	-0.4294021	-0.1518923	0.0634327
C	-1.8339665	-0.3579910	0.3717922
H	-2.0793846	0.1228996	1.3226335
H	-2.0422212	-1.4289103	0.4454779
H	-2.4519414	0.0735866	-0.4206340
Cu	2.8613711	0.3986378	-0.8802277

Table S1. Excitation values, oscillator strengths (for the UV spectrum) and rotatory strengths (for the CD spectrum) from the excited state calculation of square-pyramidal complex **3**. Values were obtained using the *escf* module in Turbomole 6.3.1. Excitation values that are bolded indicate that an electron density difference plot was calculated (and is provided below).

Excitation	**Unshifted Excitation Values**		**–0.7 eV Shift**		**Oscillator (UV) Values**	**Rotatory (CD) Values**
	eV	**nm**	**eV**	**nm**		
1	1.12	1104.52	0.42	2930.56	0.000	-2.29
2	1.41	882.44	0.71	1757.21	0.001	-5.08
3	1.52	814.72	0.82	1507.67	0.000	2.49
4	1.58	782.97	0.88	1402.43	0.000	3.11
5	2.37	523.05	1.67	742.00	0.000	0.01
6	2.38	522.17	1.68	740.22	0.000	0.00
7	2.38	521.42	1.68	738.72	0.000	-0.01
8	2.64	470.01	1.94	639.60	0.000	0.00
9	2.69	461.28	1.99	623.53	0.000	0.00
10	2.70	460.24	2.00	621.65	0.000	0.00
11	3.01	412.83	2.31	538.17	0.000	0.00
12	3.67	338.13	2.97	417.84	0.000	0.01
13	3.68	337.05	2.98	416.19	0.000	-0.01
14	3.69	335.88	2.99	414.40	0.000	0.00
15	4.06	305.78	3.36	369.52	0.000	0.03
16	4.06	305.34	3.36	368.88	0.000	0.00
17	4.07	304.91	3.37	368.26	0.000	0.00
18	4.08	303.96	3.38	366.87	0.000	0.00
19	4.08	303.81	3.38	366.66	0.000	0.00
20	4.10	302.40	3.40	364.60	0.000	0.00
21	4.11	302.23	3.41	364.35	0.000	0.02

22	4.12	300.86	3.42	362.37	0.000	0.00
23	4.13	300.34	3.43	361.61	0.000	0.00
24	4.14	299.66	3.44	360.63	0.000	0.00
25	4.18	296.94	3.48	356.69	0.000	0.00
26	4.19	295.94	3.49	355.24	0.000	0.00
27	4.22	293.99	3.52	352.44	0.000	0.00
28	4.24	292.40	3.54	350.16	0.000	0.00
29	4.28	289.59	3.58	346.13	0.001	-13.15
30	4.34	285.78	3.64	340.71	0.000	0.00
31	4.36	284.80	3.66	339.32	0.007	11.04
32	4.36	284.38	3.66	338.72	0.000	0.00
33	4.37	283.84	3.67	337.95	0.000	0.00
34	4.40	282.27	3.70	335.74	0.000	0.00
35	4.40	282.09	3.70	335.48	0.000	0.01
36	4.40	281.72	3.70	334.96	0.000	0.42
37	4.41	281.63	3.71	334.83	0.000	-0.17
38	4.42	280.97	3.72	333.90	0.000	0.02
39	4.47	277.89	3.77	329.55	0.019	3.24
40	**4.48**	**276.89**	**3.78**	**328.15**	**0.078**	**-23.23**
41	4.50	275.90	3.80	326.76	0.000	-0.08
42	**4.50**	**275.67**	**3.80**	**326.44**	**0.105**	**-74.09**
43	4.52	274.64	3.82	324.99	0.000	0.00
44	4.55	272.97	3.85	322.65	0.000	-0.01
45	4.56	272.18	3.86	321.55	0.003	-4.04
46	4.56	271.89	3.86	321.14	0.000	0.01
47	**4.58**	**271.17**	**3.88**	**320.14**	**0.102**	**72.15**
48	4.60	269.74	3.90	318.16	0.001	-14.37
49	4.61	269.17	3.91	317.36	0.003	0.78

50	4.61	268.90	3.91	316.98	0.006	-6.59
51	4.62	268.80	3.92	316.85	0.004	-0.27
52	4.62	268.42	3.92	316.32	0.019	-12.76
53	4.65	266.57	3.95	313.76	0.003	20.65
54	4.67	265.78	3.97	312.67	0.000	-0.02
55	4.67	265.74	3.97	312.61	0.000	-0.14
56	4.68	264.87	3.98	311.40	0.000	0.00
57	4.72	263.11	4.02	308.98	0.021	-11.30
58	**4.75**	**261.22**	**4.05**	**306.37**	**0.026**	**-139.99**
59	4.75	261.03	4.05	306.10	0.023	-12.41
60	4.77	260.25	4.07	305.03	0.013	31.39
61	4.78	259.54	4.08	304.06	0.052	-25.46
62	4.79	259.22	4.09	303.62	0.056	52.37
63	4.82	257.69	4.12	301.52	0.003	-3.11
64	4.88	254.43	4.18	297.06	0.052	-6.40
65	4.88	254.33	4.18	296.93	0.000	-0.03
66	4.91	252.76	4.21	294.80	0.002	-3.44
67	4.93	251.84	4.23	293.54	0.000	0.00
68	4.94	251.07	4.24	292.49	0.003	-6.20
69	4.94	251.02	4.24	292.43	0.011	-7.24
70	4.97	249.89	4.27	290.91	0.010	7.38
71	4.99	248.84	4.29	289.48	0.002	0.00
72	5.01	247.80	4.31	288.07	0.007	3.22
73	5.03	246.55	4.33	286.39	0.000	0.25
74	5.03	246.49	4.33	286.30	0.000	0.02
75	5.06	245.43	4.36	284.87	0.037	-3.45
76	5.10	243.06	4.40	281.69	0.000	1.51
77	5.11	242.87	4.41	281.43	0.002	-5.28

78	5.11	242.69	4.41	281.19	0.000	0.02
79	5.12	242.22	4.42	280.56	0.000	0.84
80	5.15	241.06	4.45	279.00	0.000	-0.55
81	5.15	240.79	4.45	278.64	0.001	0.34
82	5.17	239.84	4.47	277.37	0.003	0.36
83	5.18	239.62	4.48	277.07	0.000	2.91
84	5.18	239.53	4.48	276.96	0.002	-5.17
85	5.20	238.79	4.50	275.97	0.002	3.69
86	5.20	238.45	4.50	275.51	0.005	-17.40
87	5.21	238.20	4.51	275.17	0.012	-8.77
88	5.22	237.73	4.52	274.55	0.001	-1.17
89	5.22	237.69	4.52	274.50	0.002	3.02
90	5.23	237.43	4.53	274.16	0.002	0.60
91	5.25	236.18	4.55	272.48	0.003	-0.27
92	5.26	235.88	4.56	272.08	0.001	0.33
93	5.29	234.65	4.59	270.45	0.000	-0.04
94	5.29	234.46	4.59	270.20	0.002	-0.62
95	5.35	232.08	4.65	267.04	0.000	0.11
96	5.35	231.80	4.65	266.68	0.004	0.11
97	5.37	231.16	4.67	265.83	0.003	-2.28
98	5.37	230.87	4.67	265.45	0.000	0.12
99	5.38	230.49	4.68	264.94	0.002	-0.80
100	**5.42**	**229.13**	**4.72**	**263.14**	**0.111**	**-13.03**
101	5.43	228.60	4.73	262.45	0.004	-3.23
102	5.44	227.94	4.74	261.58	0.000	-0.04
103	5.46	227.19	4.76	260.58	0.001	-6.97
104	5.46	227.14	4.76	260.53	0.000	-0.43
105	5.52	224.73	4.82	257.35	0.005	-44.26

106	5.52	224.66	4.82	257.27	0.002	-2.53
107	**5.54**	**224.05**	**4.84**	**256.47**	**0.197**	**-614.57**
108	**5.55**	**223.51**	**4.85**	**255.76**	**0.149**	**-420.15**
109	5.58	222.53	4.88	254.47	0.007	4.88
110	5.59	221.92	4.89	253.68	0.001	-2.32
111	5.60	221.77	4.90	253.48	0.001	1.17
112	5.62	220.84	4.92	252.26	0.003	2.28
113	5.64	220.05	4.94	251.24	0.005	2.71
114	5.66	219.15	4.96	250.07	0.006	1.15
115	5.68	218.38	4.98	249.07	0.000	-0.76
116	5.69	218.11	4.99	248.71	0.002	0.71
117	5.69	217.99	4.99	248.56	0.001	1.85
118	5.70	217.61	5.00	248.06	0.000	0.03
119	5.71	217.27	5.01	247.62	0.042	35.94
120	5.72	217.03	5.02	247.32	0.016	-0.13
121	5.72	216.89	5.02	247.13	0.003	1.56
122	5.72	216.74	5.02	246.94	0.015	-24.16
123	5.73	216.70	5.03	246.89	0.016	-27.97
124	5.75	215.94	5.05	245.89	0.017	10.29
125	5.76	215.42	5.06	245.23	0.002	-0.67
126	5.77	215.16	5.07	244.88	0.045	17.59
127	5.77	214.95	5.07	244.61	0.009	1.12
128	5.78	214.81	5.08	244.43	0.001	0.90
129	5.78	214.57	5.08	244.12	0.000	0.04
130	5.79	214.30	5.09	243.76	0.001	1.36
131	5.79	214.25	5.09	243.71	0.001	0.62
132	5.79	214.18	5.09	243.61	0.007	-0.93
133	5.79	214.14	5.09	243.56	0.010	-9.32

134	5.80	214.02	5.10	243.41	0.002	-1.27
135	5.80	213.96	5.10	243.33	0.010	1.71
136	5.80	213.88	5.10	243.23	0.058	14.86
137	5.82	213.27	5.12	242.44	0.000	0.00
138	5.84	212.37	5.14	241.28	0.096	-48.69
139	5.85	212.16	5.15	241.00	0.001	3.82
140	5.85	212.07	5.15	240.89	0.022	38.76
141	5.86	211.64	5.16	240.33	0.001	0.14
142	5.87	211.49	5.17	240.15	0.000	0.24
143	5.88	211.11	5.18	239.65	0.001	-0.69
144	5.89	210.76	5.19	239.20	0.010	-7.88
145	5.90	210.39	5.20	238.72	0.004	-9.66
146	5.91	210.03	5.21	238.26	0.019	-32.03
147	5.91	209.85	5.21	238.03	0.005	-22.59
148	5.92	209.73	5.22	237.87	0.010	-19.96
149	5.92	209.51	5.22	237.59	0.007	4.37
150	5.93	209.39	5.23	237.44	0.019	-3.73
151	5.93	209.33	5.23	237.37	0.020	16.82
152	5.94	208.91	5.24	236.82	0.030	-56.58
153	5.94	208.86	5.24	236.76	0.004	-6.44
154	5.94	208.74	5.24	236.60	0.010	-12.28
155	5.95	208.58	5.25	236.40	0.004	-18.17
156	**5.96**	**208.08**	**5.26**	**235.75**	**0.248**	**132.79**
157	**5.97**	**207.97**	**5.27**	**235.61**	**0.141**	**68.70**
158	5.97	207.87	5.27	235.48	0.091	-16.61
159	5.98	207.51	5.28	235.02	0.007	-39.13
160	**5.98**	**207.45**	**5.28**	**234.95**	**0.018**	**-106.70**
161	**5.99**	**207.32**	**5.29**	**234.78**	**0.066**	**-351.40**

162	6.00	206.88	5.30	234.22	0.001	5.09
163	6.01	206.37	5.31	233.57	0.039	-28.15
164	6.01	206.34	5.31	233.52	0.014	-56.17
165	**6.02**	**206.10**	**5.32**	**233.22**	**0.275**	**-673.87**
166	6.03	205.71	5.33	232.71	0.107	108.77
167	6.04	205.42	5.34	232.34	0.095	-131.03
168	**6.05**	**205.06**	**5.35**	**231.88**	**0.467**	**842.66**
169	6.05	204.94	5.35	231.73	0.054	150.52
170	6.06	204.85	5.36	231.62	0.010	-5.76
171	**6.06**	**204.68**	**5.36**	**231.39**	**0.581**	**582.28**
172	6.06	204.61	5.36	231.31	0.017	13.53
173	6.07	204.51	5.37	231.18	0.095	37.37
174	6.07	204.46	5.37	231.11	0.013	-14.65
175	6.08	204.24	5.38	230.83	0.031	12.58
176	6.08	204.21	5.38	230.80	0.049	-18.77
177	6.08	204.09	5.38	230.65	0.011	12.53
178	6.09	203.88	5.39	230.38	0.235	-13.03
179	6.09	203.78	5.39	230.25	0.273	206.93
180	6.09	203.71	5.39	230.16	0.021	34.22
181	6.10	203.52	5.40	229.92	0.044	21.54
182	6.10	203.46	5.40	229.84	0.029	4.75
183	6.10	203.37	5.40	229.73	0.039	52.10
184	6.11	203.09	5.41	229.37	0.087	-90.06
185	6.12	202.84	5.42	229.05	0.010	1.97

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[i] TURBOMOLE V6.3.1 2011, a development of University of Karlsruhe and Forschungszentrum Karlsruhe GmbH, 1989-2007, TURBOMOLE GmbH, since 2007; available from http://www.turbomole.com.

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