Controlled Supramolecular Assemblies of Luminescent Tridentate Cyclometalated Alkynyl Gold (III) Amphiphiles in Aqueous Media

Supporting Information

Experimental details, supporting figures, and copies of spectra

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1. General

NMR spectra were recorded at 20.0 °C on Bruker AVANCE III 600 NMR spectrometer (^{1}H: 600 MHz, ^{13}C: 151 MHz) or Bruker AVANCE III 400 NMR spectrometer (^{1}H: 400 MHz, ^{13}C: 101 MHz). Chemical shifts (δ) are expressed relative to the resonances of the residual nondeuterated solvent for ^{1}H [$CDCl_3$: ^{1}H(δ) = 7.26 ppm, CD_3OD: ^{1}H(δ) = 3.31 ppm, CD_3SOCD_3: ^{1}H(δ) = 2.50 ppm] and ^{13}C [$CDCl_3$: ^{13}C(δ) = 78.0 ppm, CD_3OD: ^{13}C(δ) = 49.15 ppm]. Absolute values of the coupling constants are given in Hertz (Hz), regardless of their sign. Multiplicities are abbreviated as singlet (s), doublet (d), doublet of doublets (dd), triplet (t), triplet of doublets (td), quartet (q), multiplet (m), and broad (br). High-resolution mass spectrometry (HRMS) was performed on Agilent 6540 UHD Accurate-Mass Q-TOF LC/MS system with ESI ionization.

2. Supporting Figures

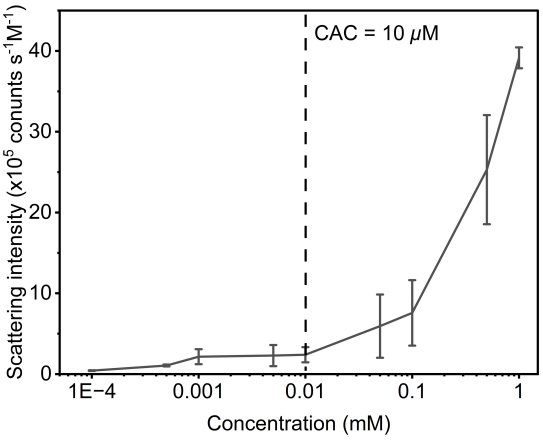

Figure S1: The critical aggregation concentration of aqueous solution of **GA**.

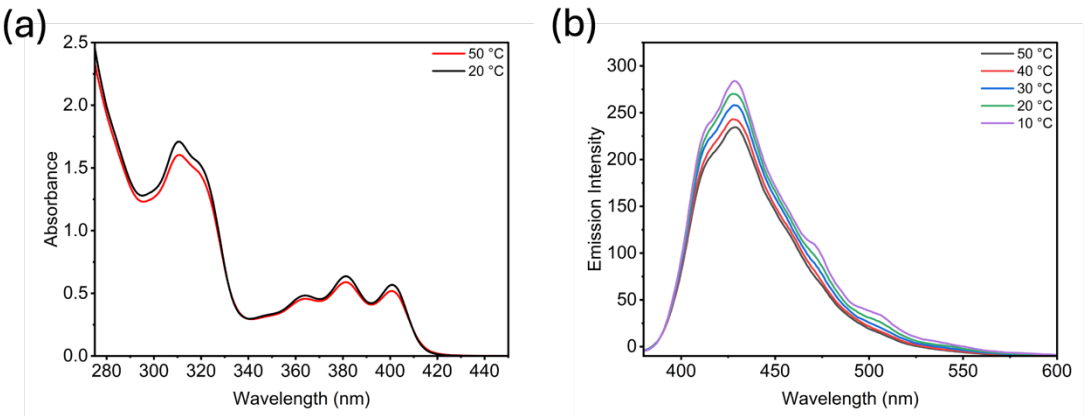

Figure S2: (a) UV-vis absorption spectra of **GA** (200 μM) in methanol was cooled from 50.0 °C (red-line) to 20.0 °C (black-line) at a rate of 1.0°C/min. (b) Emission spectra of **GA** (200 μM) in methanol upon decreasing temperature from 50.0 °C to 10.0 °C.

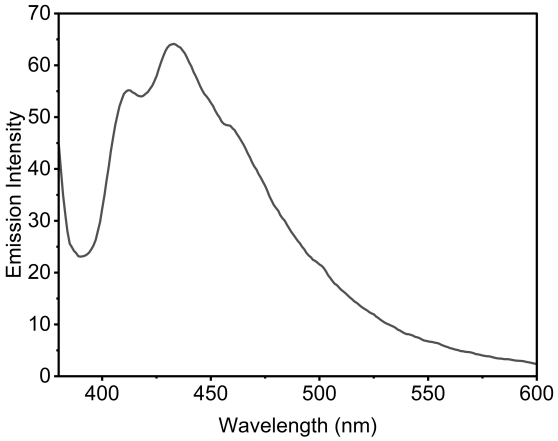

Figure S3: Emission spectrum of the cyclometalated gold (III) complex **2** in dichloromethane (200 μM).

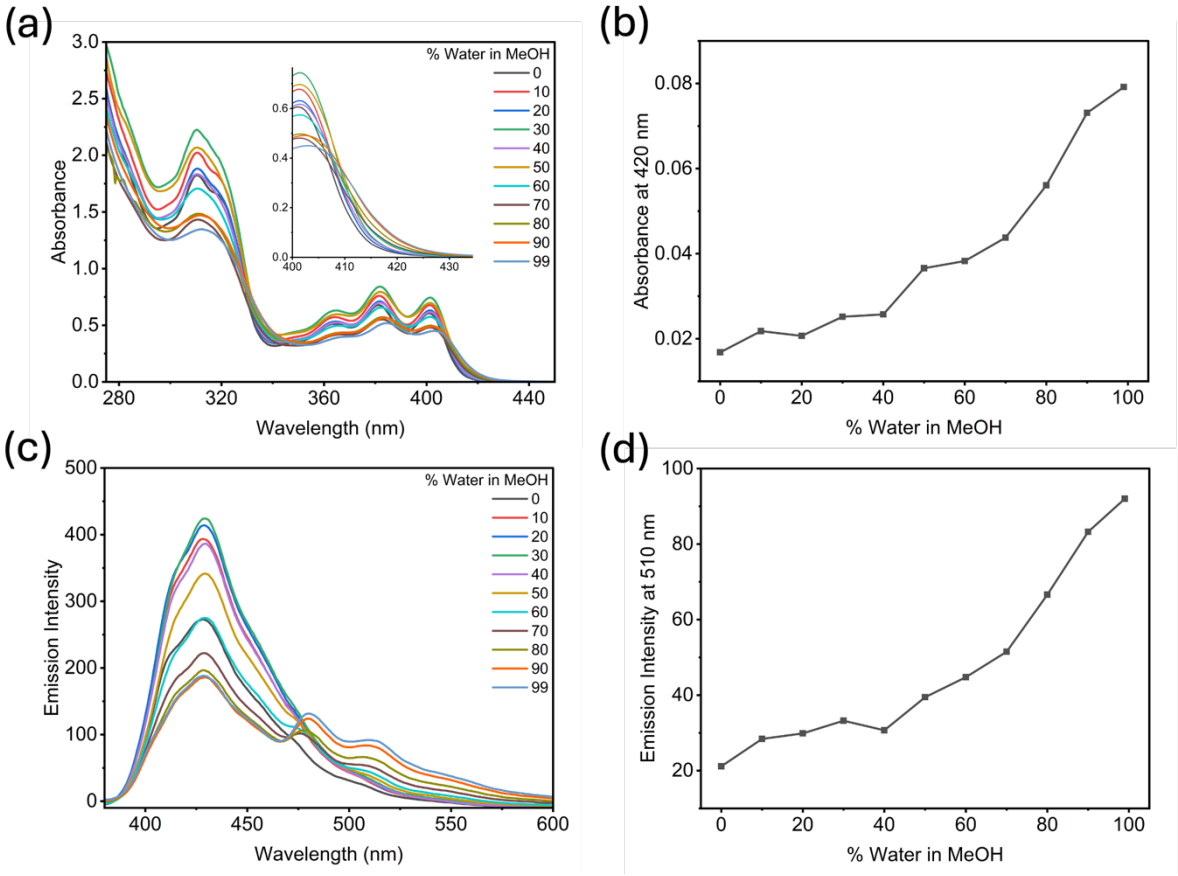

Figure S4: (a) UV-vis absorption spectra of **GA** (200 μM) in methanol at 20.0 °C upon increasing water content. (b) A plot of absorbance at 420 nm against water fraction of methanol. (c) Emission spectra of **GA** (200 μM) at 20.0 °C upon increasing water content. (d) A plot of emission at 430 nm and 510 nm against water fraction of methanol.

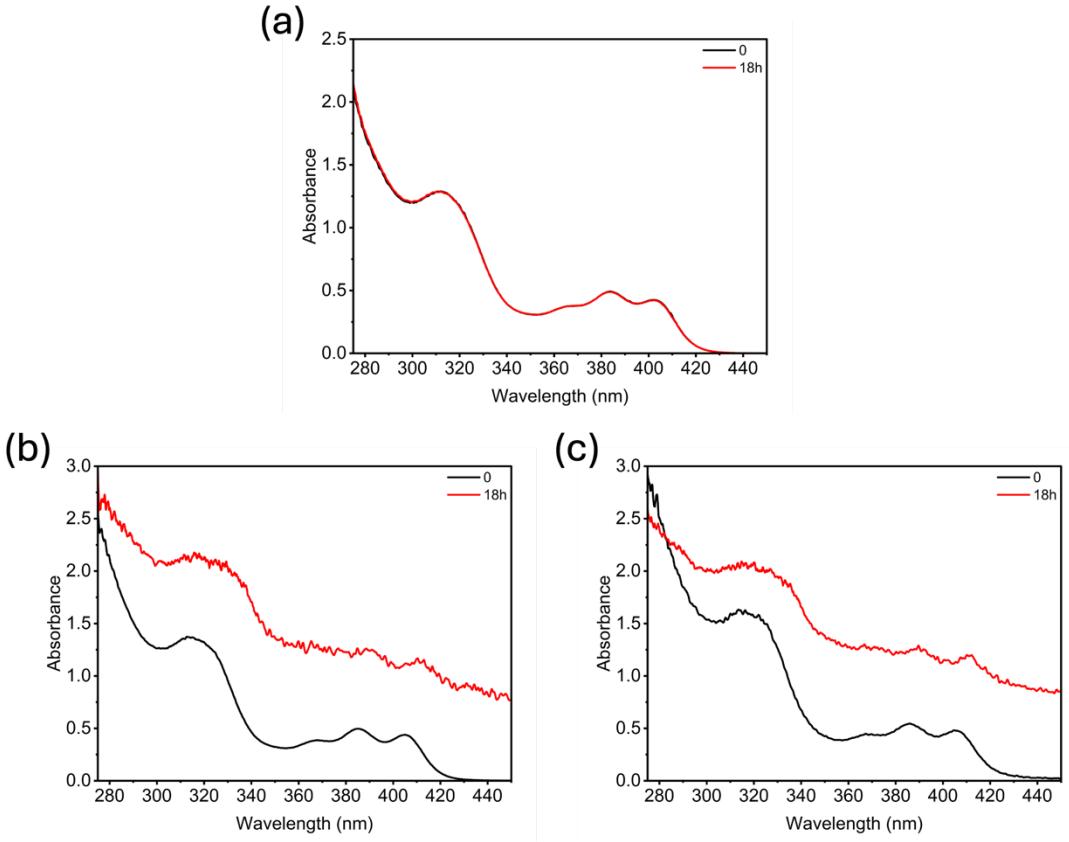

Figure S5: Time-dependent UV-vis adsorption spectra of **GA** (200 μM) (a) without the addition of with sodium tosylate, with the addition of (b) 2.0 equiv. and (c) 4.0 equiv. of sodium tosylate in MQ water at 20.0 °C.

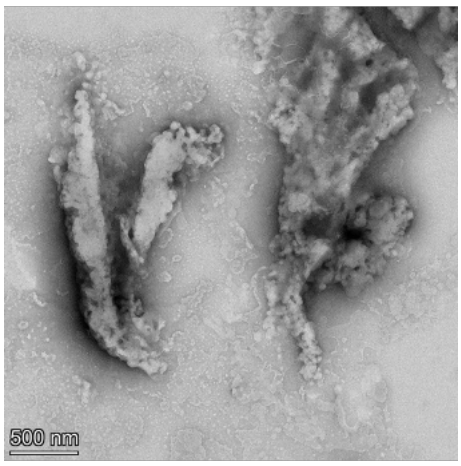

Figure S6: TEM image of thermal annealed **GA** solution (2.68 mM) with the addition of 4.0 equiv. of sodium tosylate obtained at 18 h.

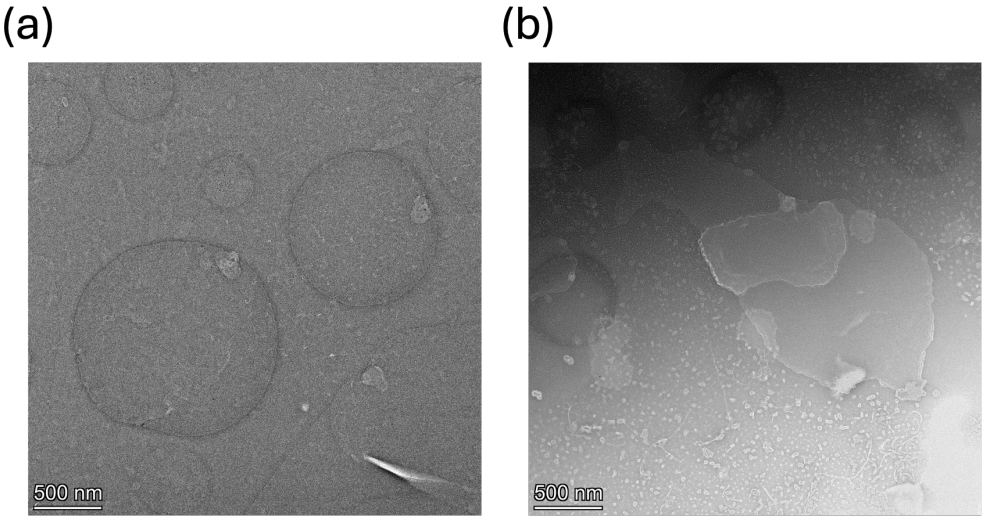

Figure S7: TEM images of thermal annealed solution of **GA** (2.68 mM) after addition of (a) 1.0 equiv. and (b) 2.0 equiv. of sodium bromide as further counterion exchange.

3. Compound Characterization

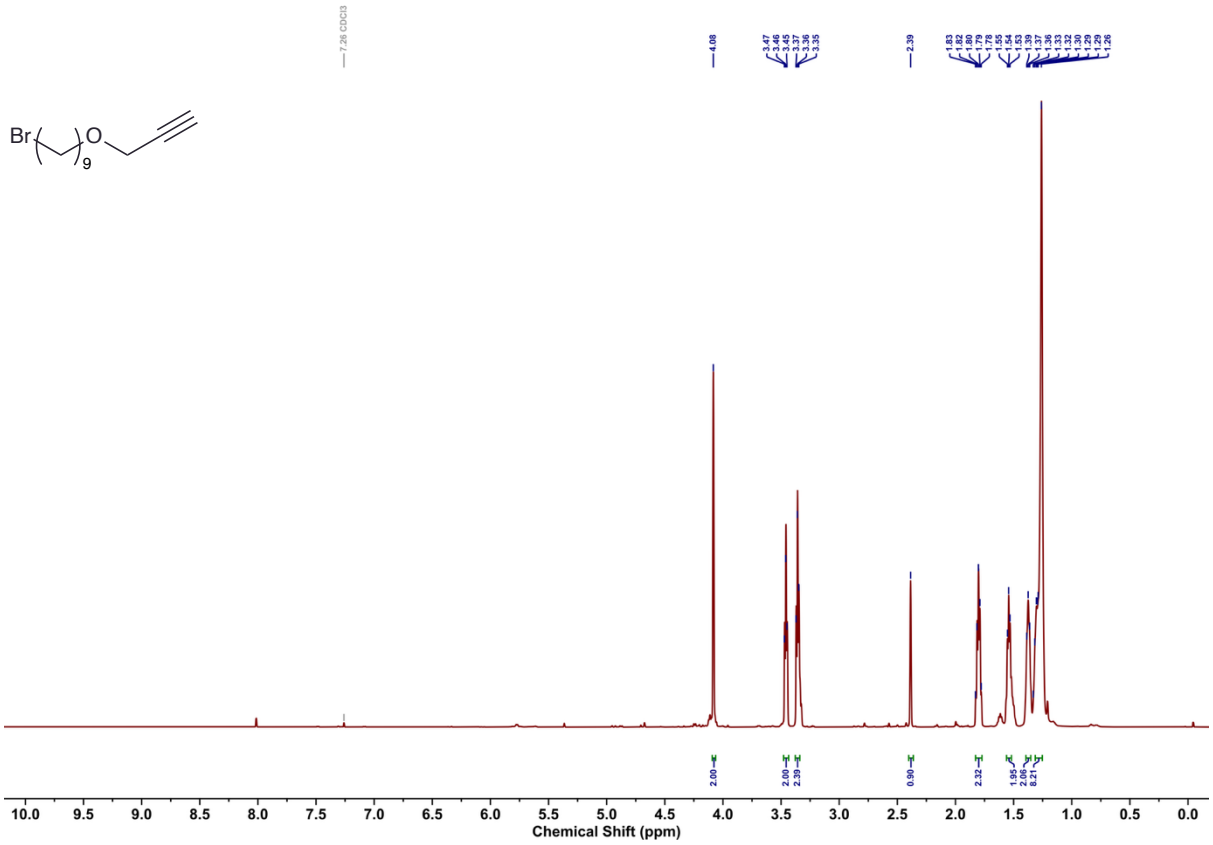

Figure S8: ^{1}H NMR spectrum (600 MHz) of compound **1** in $CDCl_3$ at 20.0 °C.

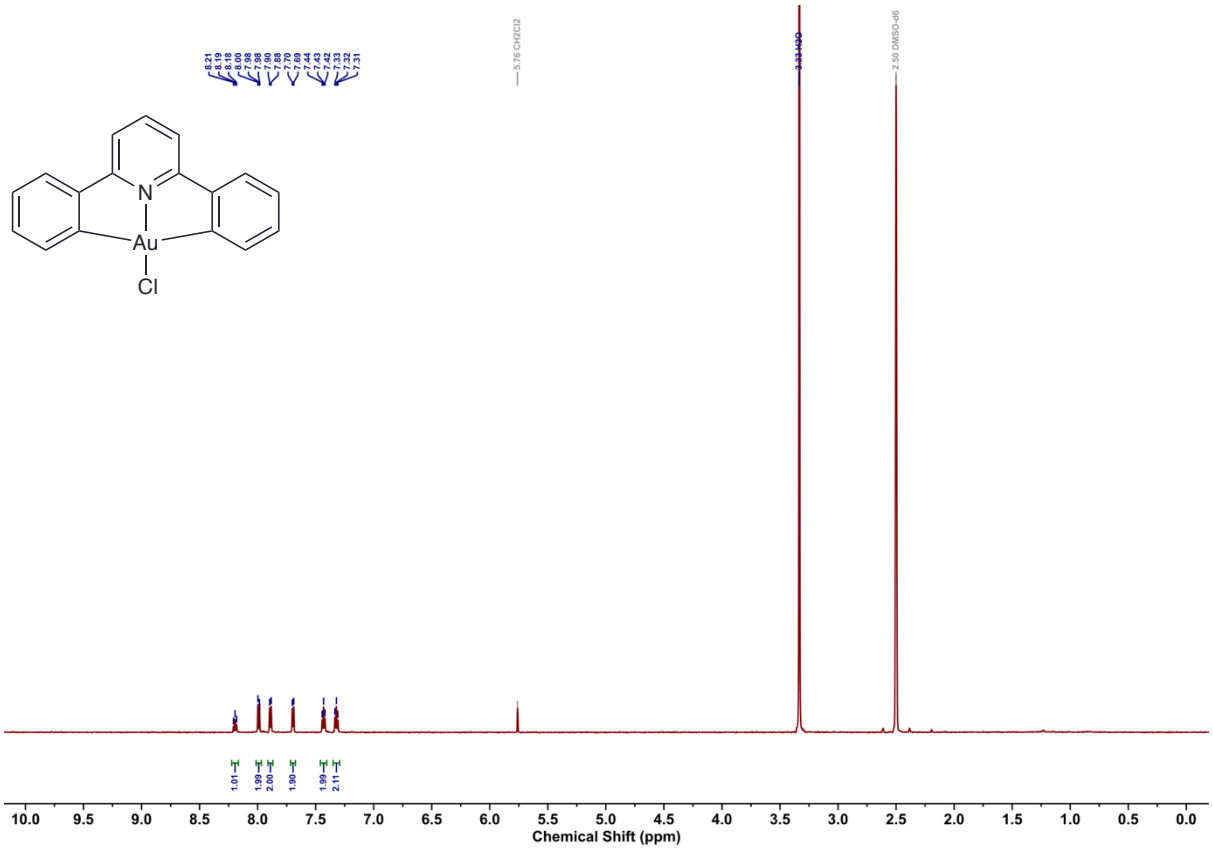

Figure S9: ^{1}H NMR spectrum (600 MHz) of compound **2** in CD_3SOCD_3 at 20.0 °C.

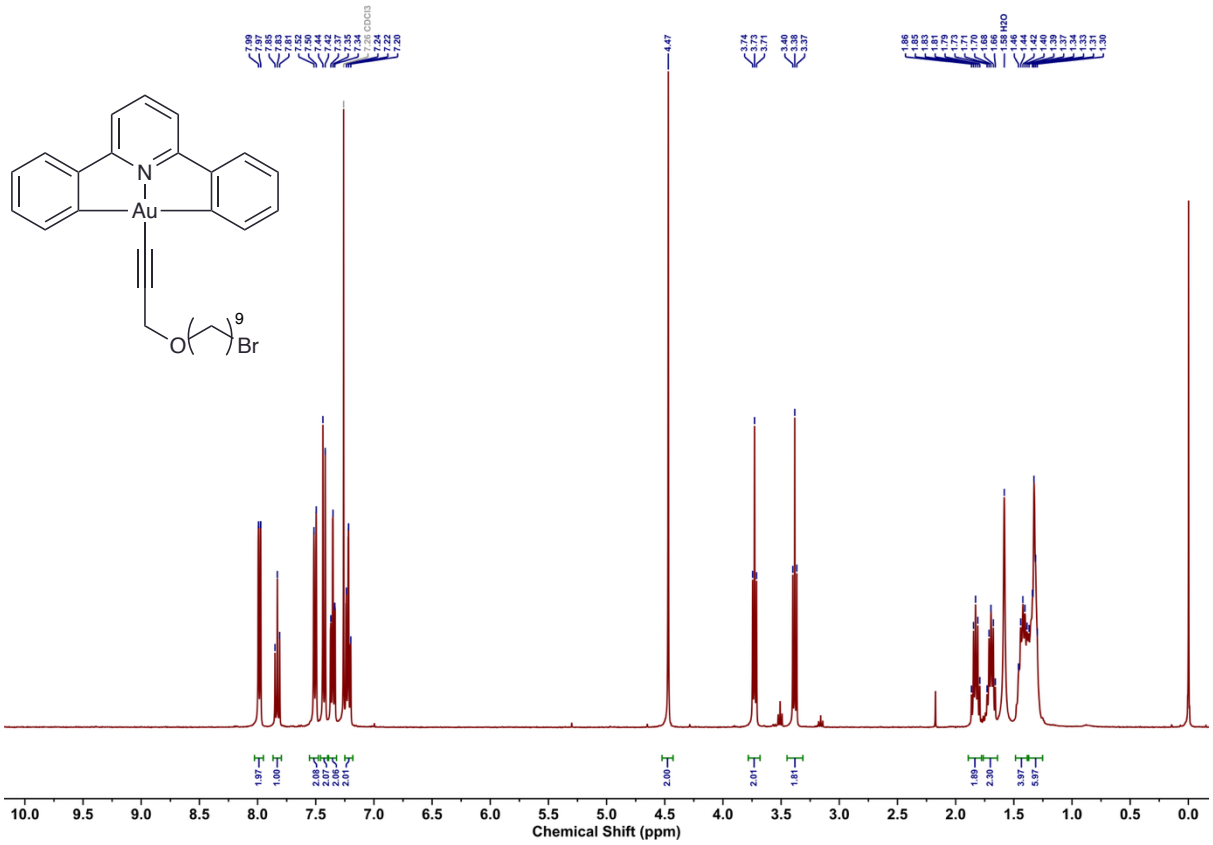

Figure S10: ^{1}H NMR spectrum (400 MHz) of compound **3** in $CDCl_3$ at 20.0 °C.

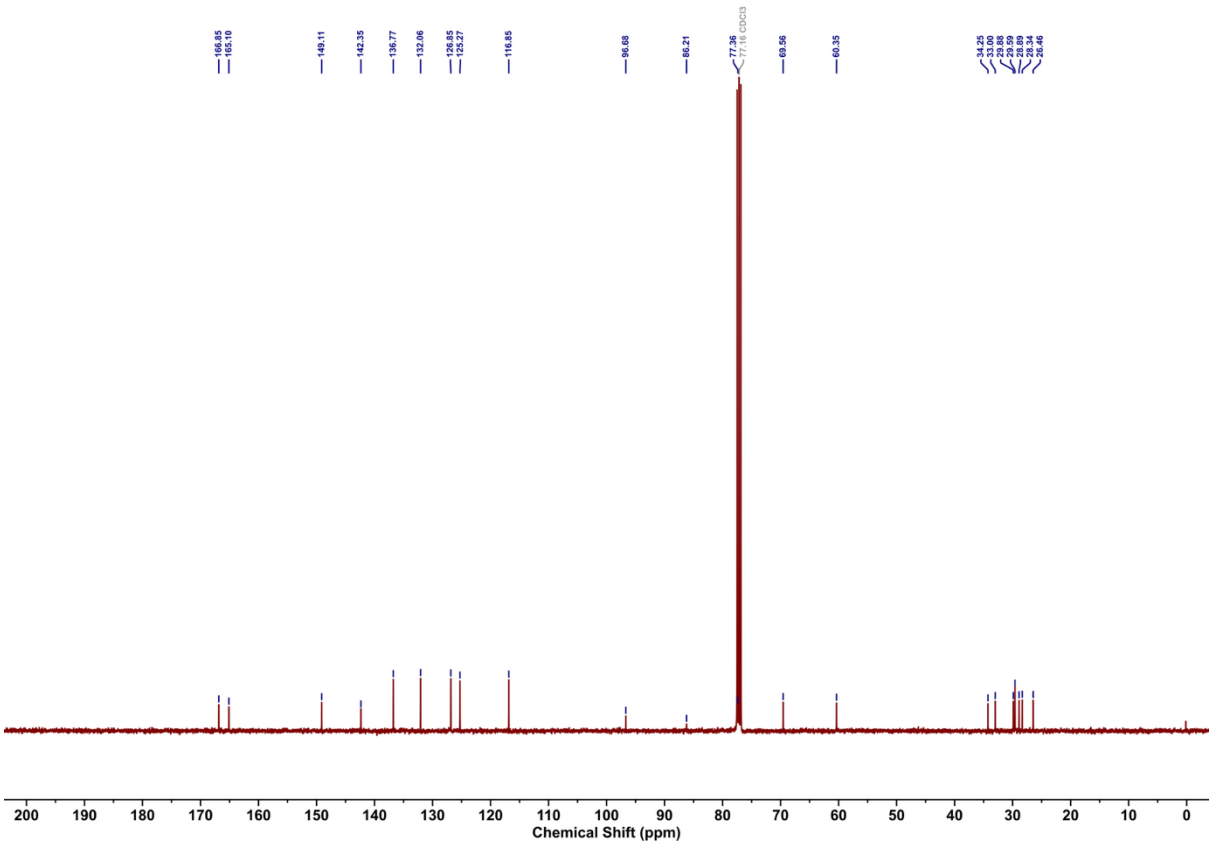

Figure S11: ^{13}C NMR spectrum (101 MHz) of compound **3** in $CDCl_3$ at 20.0 °C.

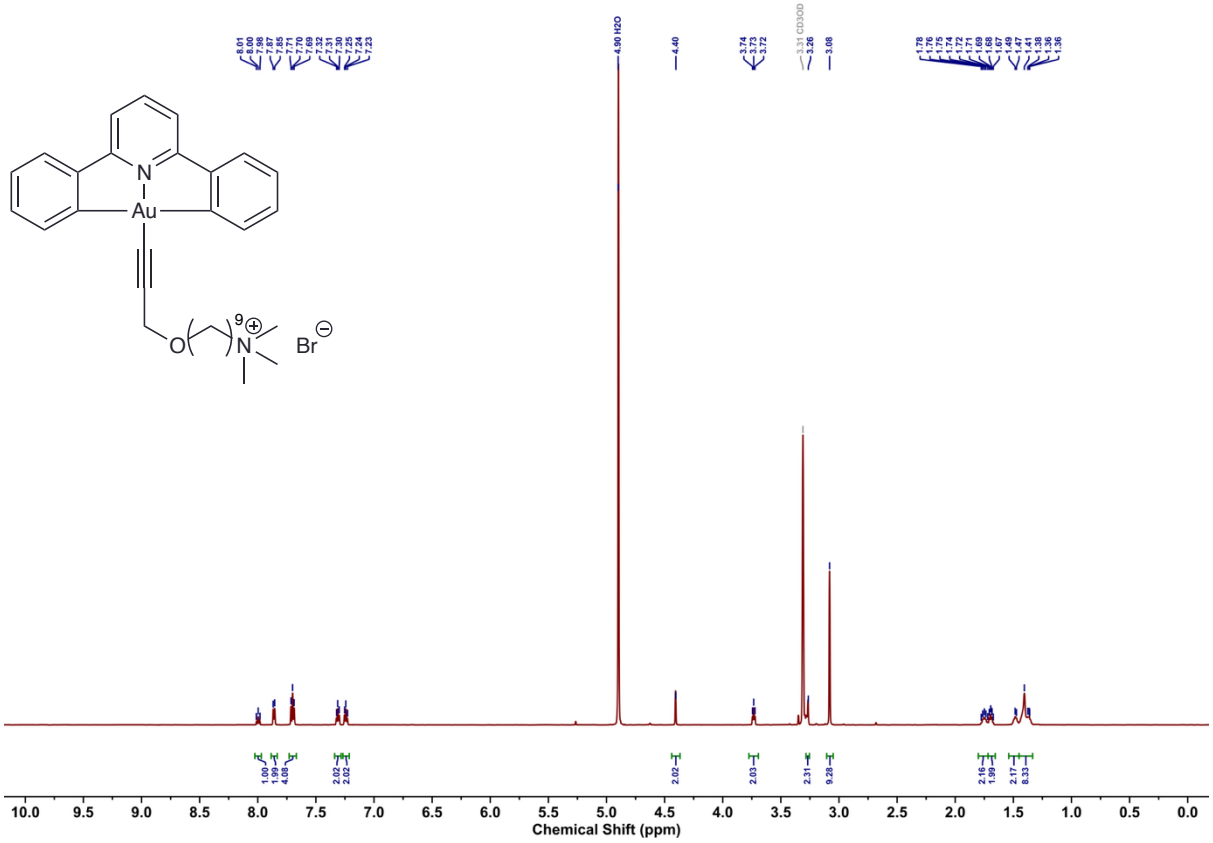

Figure S12: ^{1}H NMR spectrum (600 MHz) of **GA** in CD_3OD at 20.0 °C.

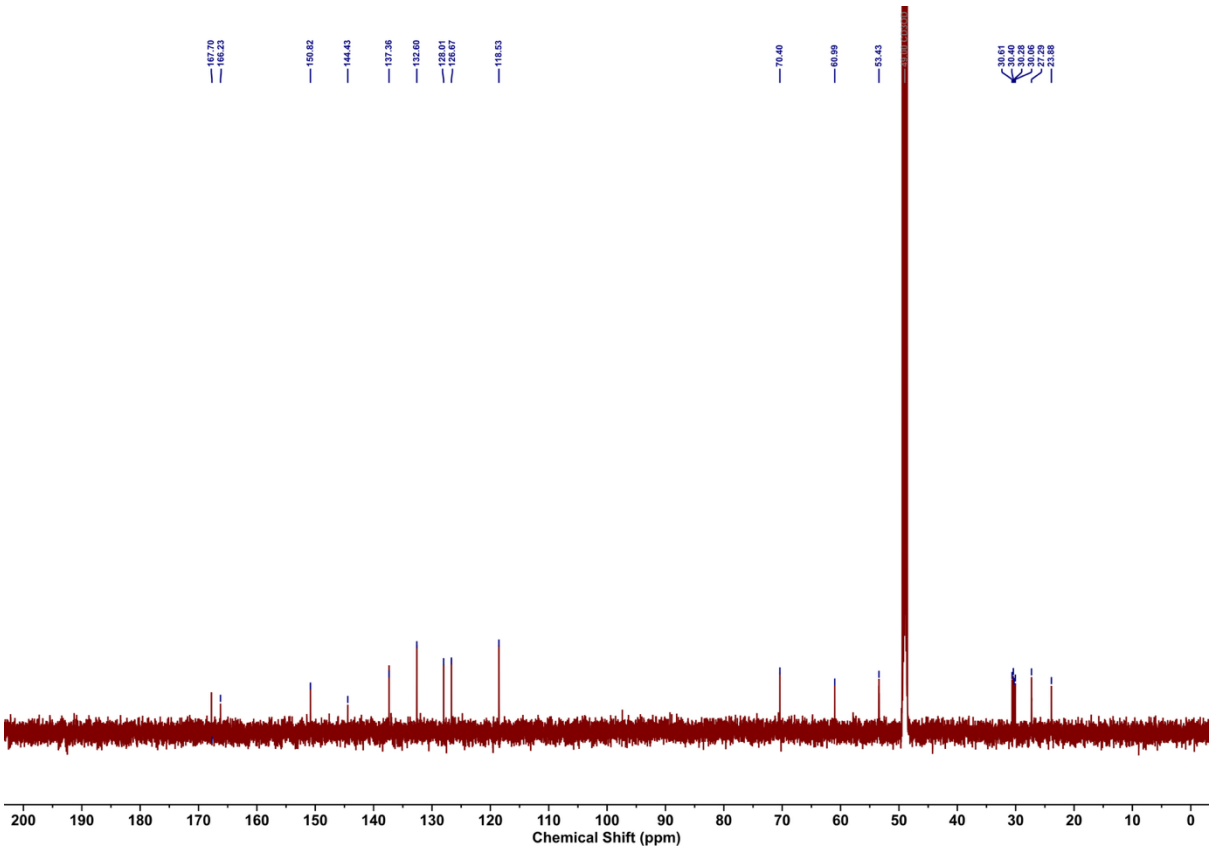

Figure S13: ^{13}C NMR spectrum (151 MHz) of **GA** in CD_3OD at 20.0 °C.