

# Supporting Information

for

## Selective anticancer and antimicrobial metallodrugs based on gold(III) dithiocarbamate complexes

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### Table of Contents

**Figure S1.** <sup>1</sup>H-NMR spectra of **C1-6** complexes, and APT spectra for **C3**, **C5-C6**.

**Figure S2.** Comparison of the theoretical and experimental MS spectra of complexes **C2**, **C3** and **C6** (from left to right). The software used to predict the theoretical isotopic distribution of the complexes was Bruker Compass Data Analysis 4.0.

**Figure S3.** UV-Vis spectra of **C1-6** complexes recorded at different times for 24 h in PBS at 37°C.

**Figure S4.** UV-Vis spectra of **C1-6** complexes recorded at different times for 24 h in PBS at 37°C in presence of GSH (0-50 μM).

**Figure S5.** UV-Vis spectra of **C1-6** complexes recorded at different times for 24 h in PBS at 37°C in presence of AsA (0-20 μM).

**Figure S6.** Fluorescence emission spectra of BSA at 298 K in the presence of increasing amounts of the gold(III) complexes.

**Figure S7.** Cell viability of tumor Caco-2 cells (5 days after seeding) treated with **C1-6** gold(III) complexes for 72h. All the results are expressed as mean ± SEM (n ≥ 12 experiments). \*P<0.05; \*\*P<0.01; \*\*\*P<0.001 vs. control.

**Figure S8.** Cell viability of normal Caco-2 cells (15 days after seeding) treated with **C1-6** gold(III) complexes for 72h. All the results are expressed as mean ± SEM (n ≥ 12 experiments). \*P<0.05; \*\*P<0.01; \*\*\*P<0.001 vs. control.

**Figure S9.** Fluorescence histograms of the distribution of cell populations in different stages: necrosis (B+-), living cells (B--), late apoptosis (B++) and early apoptosis (B+-), in control (DMSO) and gold(III) complexes (20 μM, 24 h) treated Caco-2/TC7 cells.

**Figure S10.** Fluorescence histograms obtained by flow cytometry of the cell populations in different phases of the cell cycle after 24 h of incubation of the cells with DMSO (control) and gold(III) complexes **1** and **5-6** (20 μM).

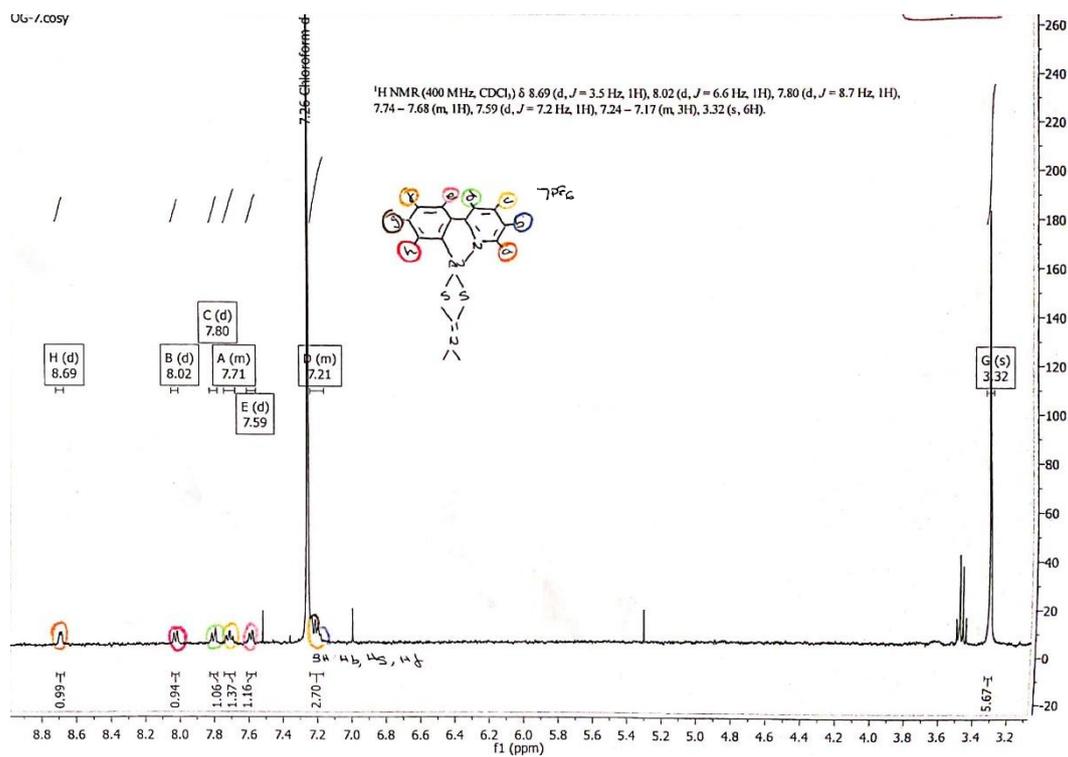
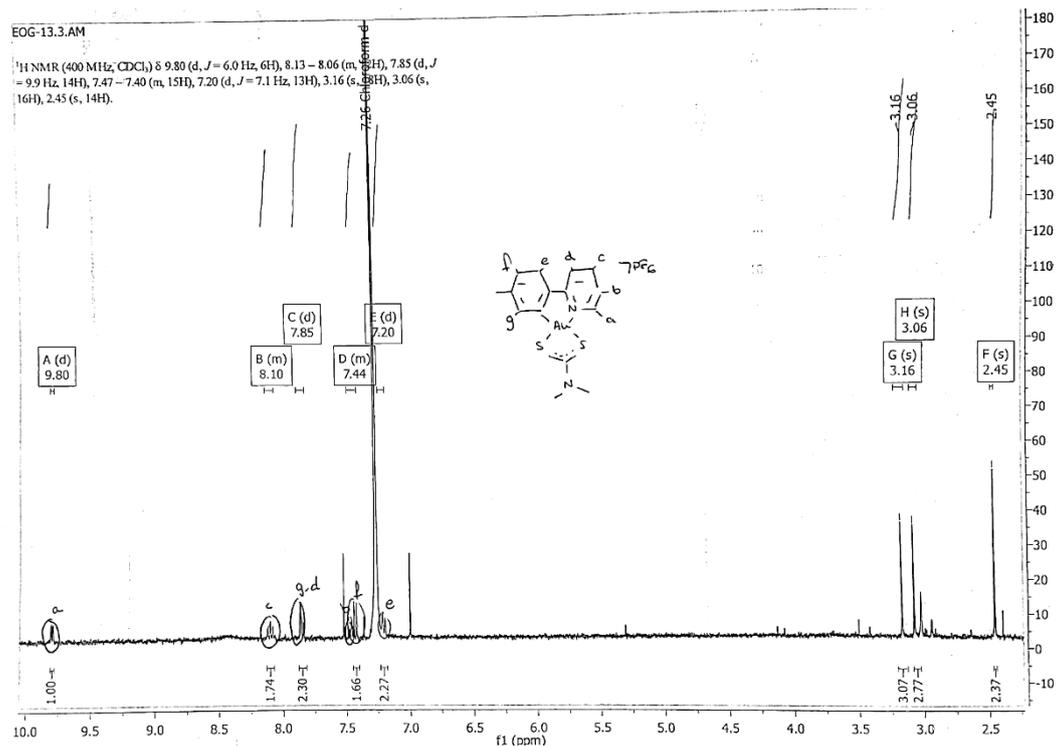


Figure S1a. <sup>1</sup>H-NMR spectra of C1 (above) and C2 (bottom) complexes in chloroform-d.

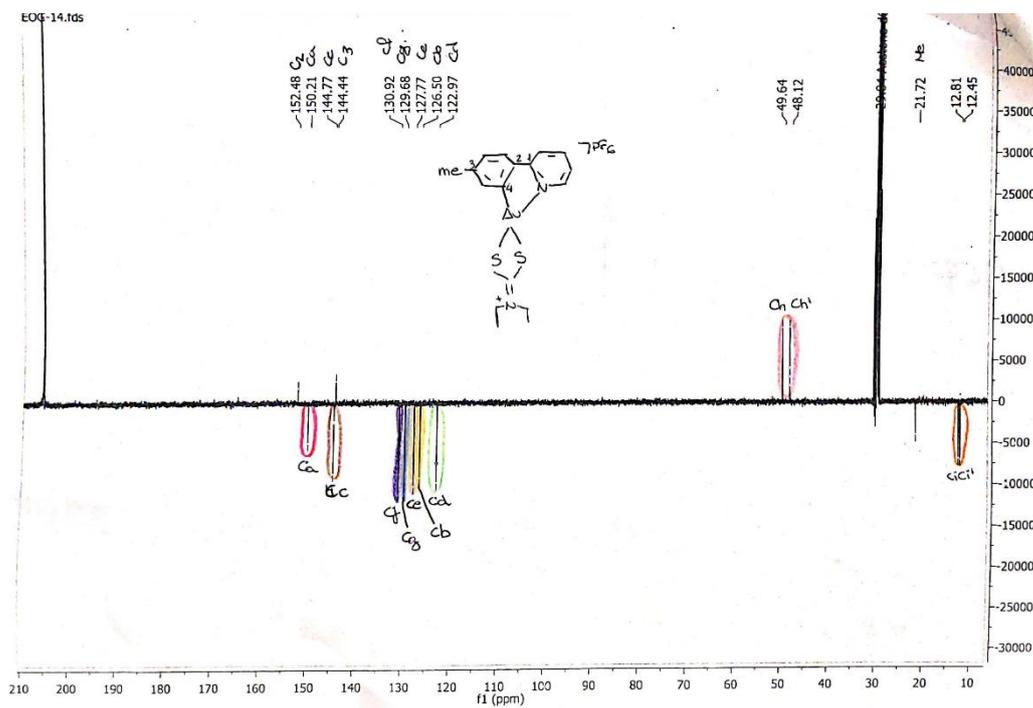
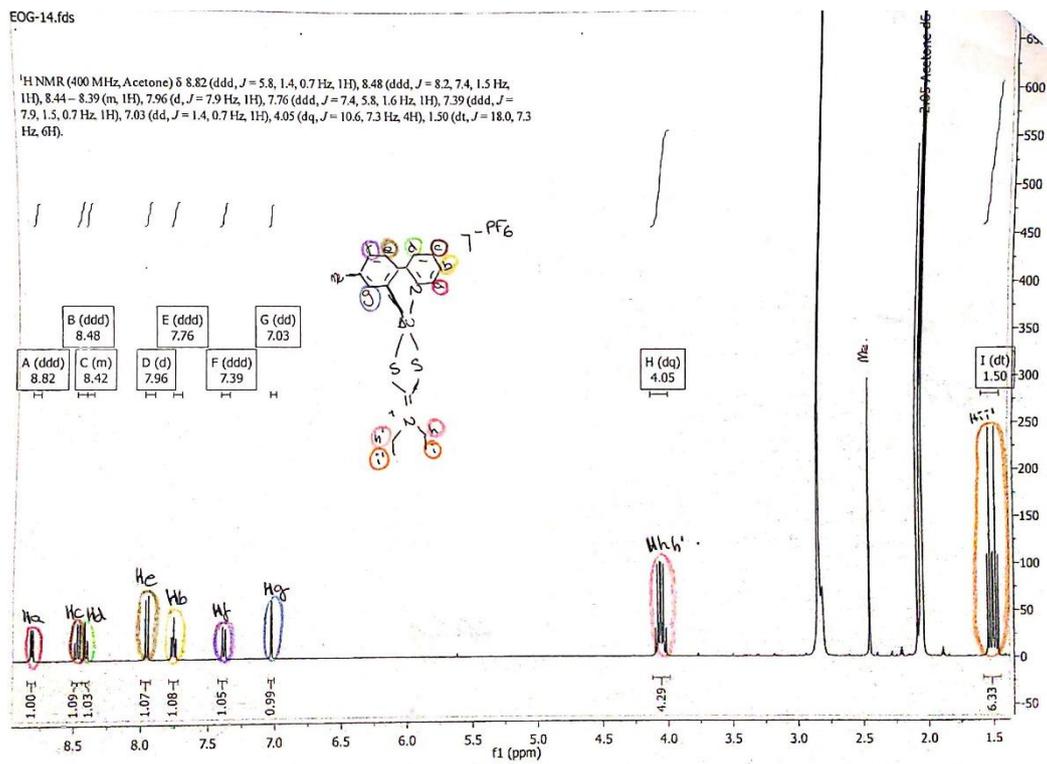


Figure S1b. <sup>1</sup>H-NMR and APT-NMR spectra of **C3** in acetone-*d*<sub>6</sub>.

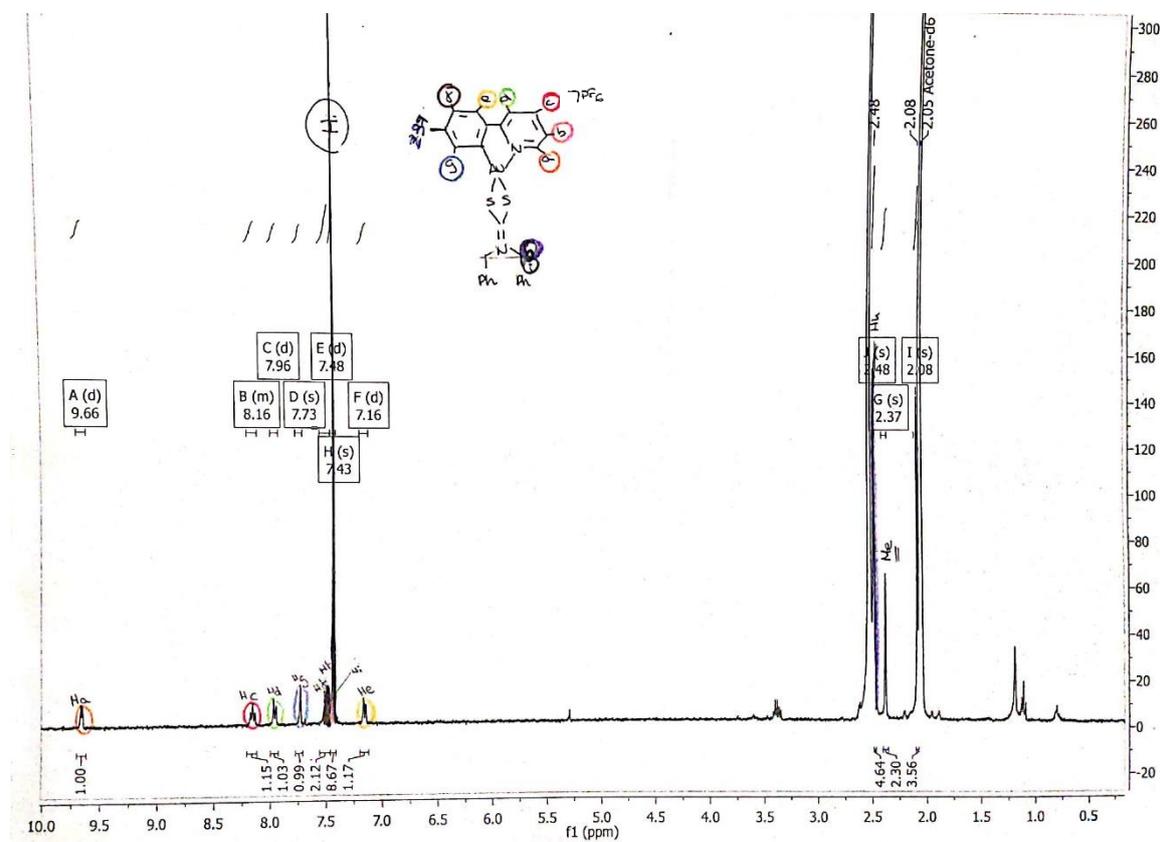
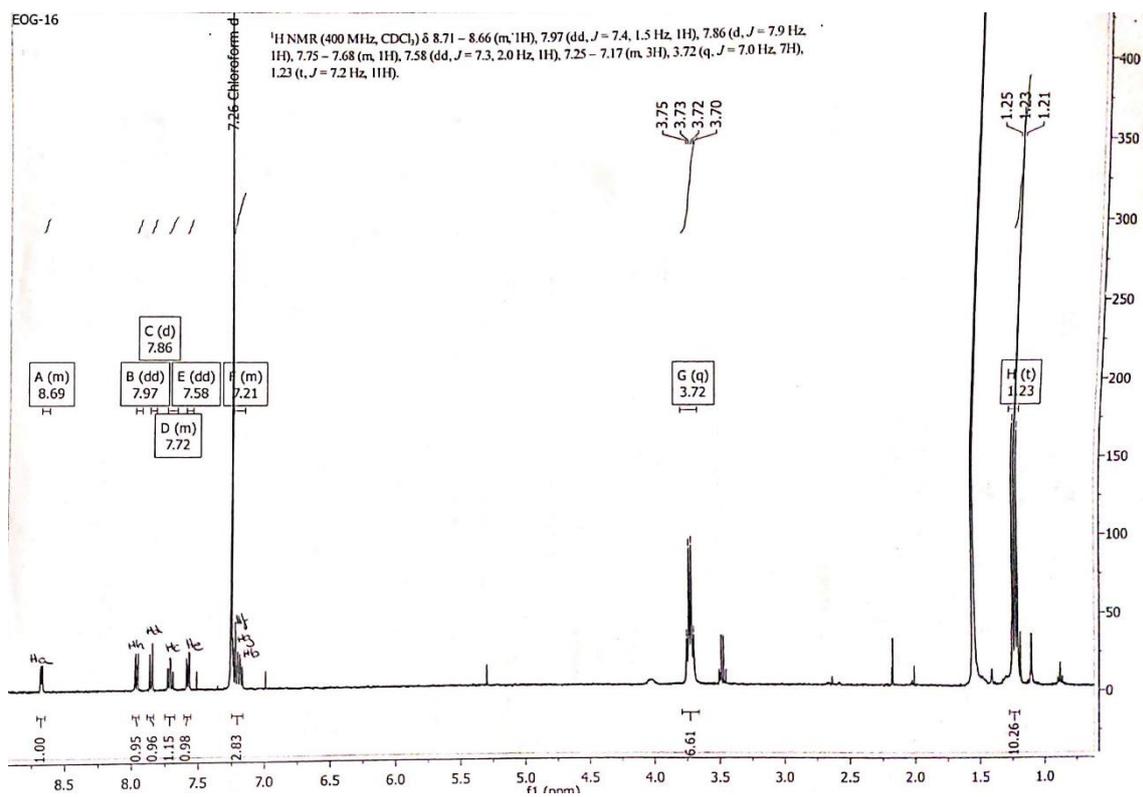


Figure S1c. <sup>1</sup>H-NMR spectra of **C3** in chloroform-*d* (above), and **C4** in acetone-*d*<sub>6</sub> (bottom) complexes.

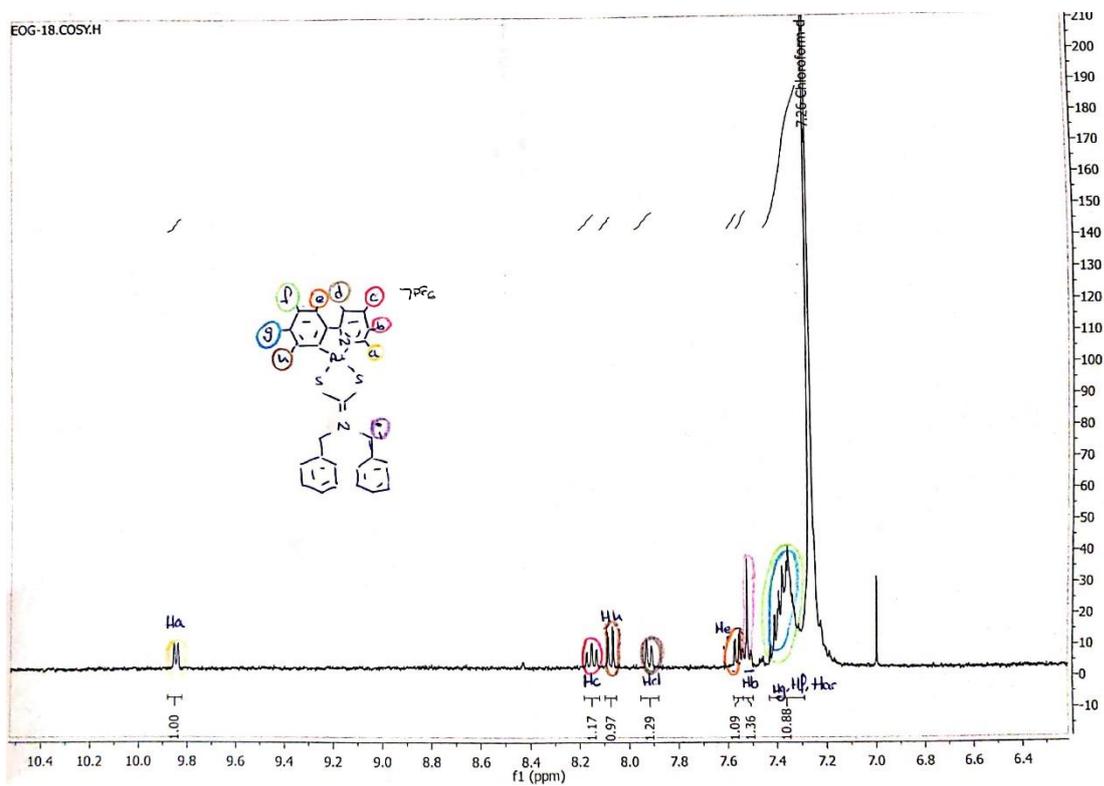
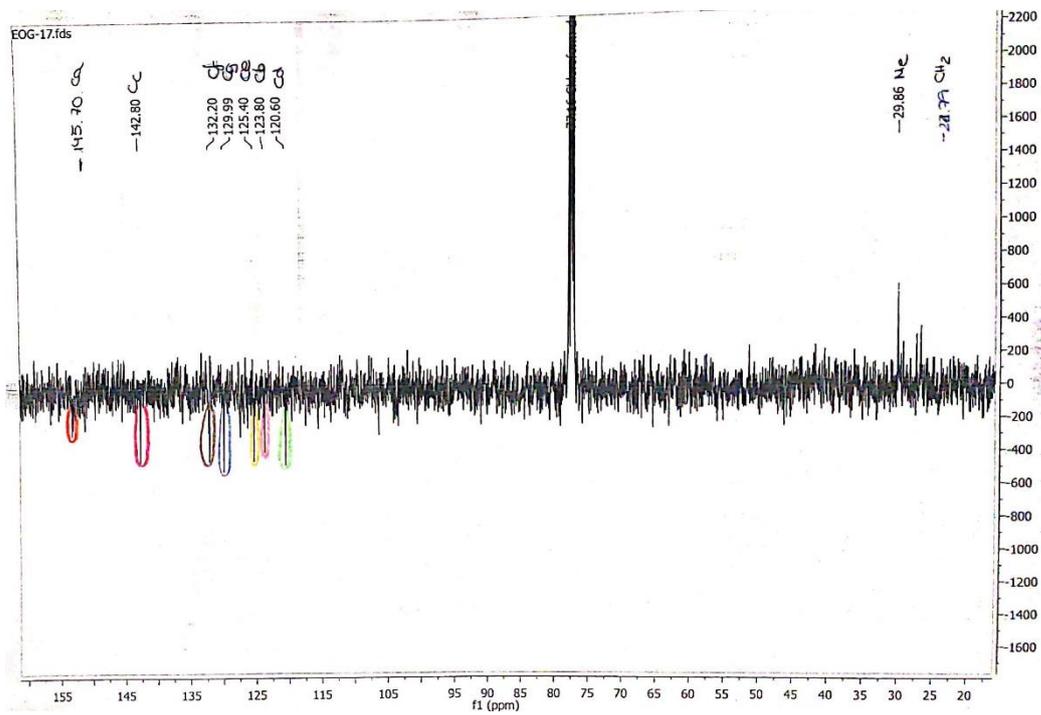


Figure S1d. APT-NMR spectrum of C4 in acetone-d<sub>6</sub> (above) and <sup>1</sup>H-NMR spectrum of C3 in chloroform-d (bottom).

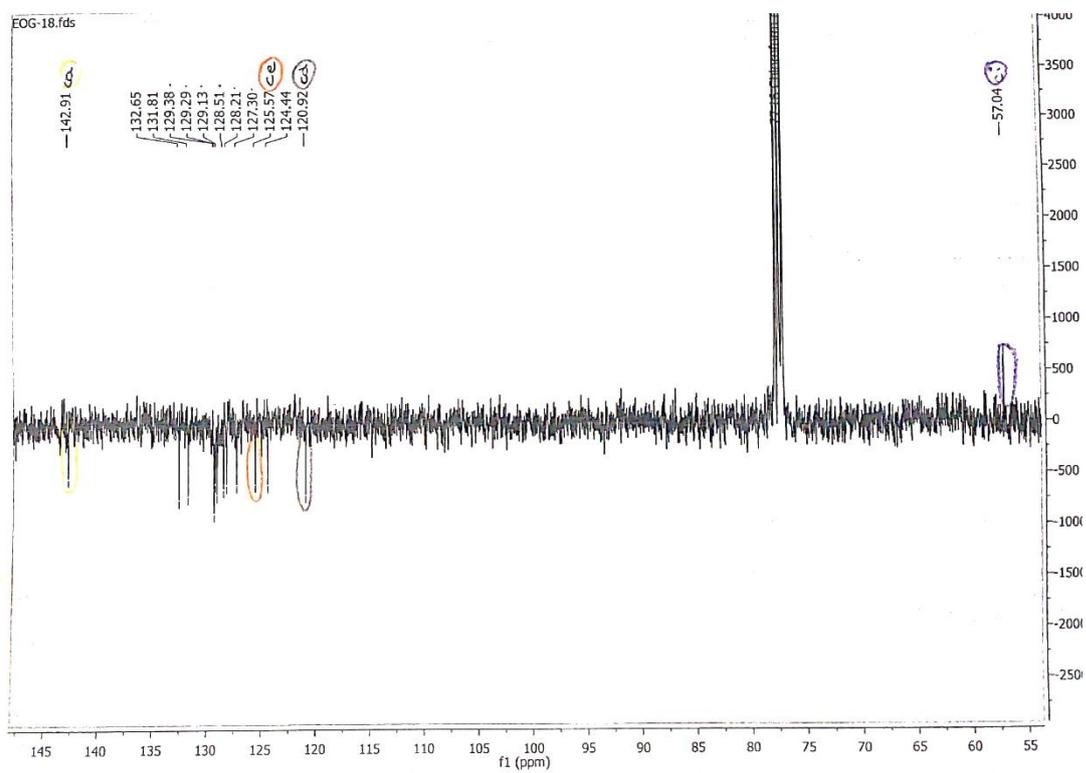
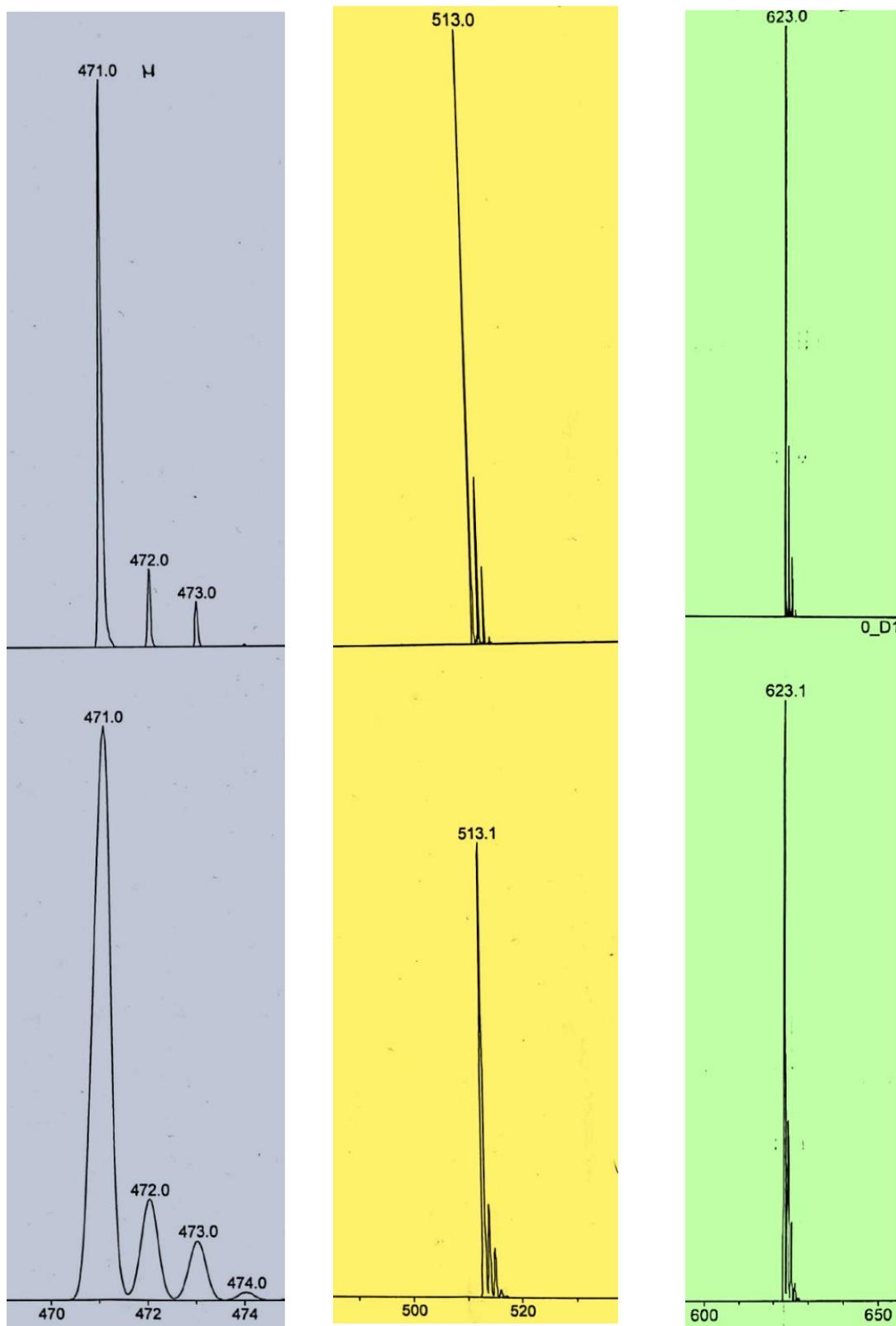
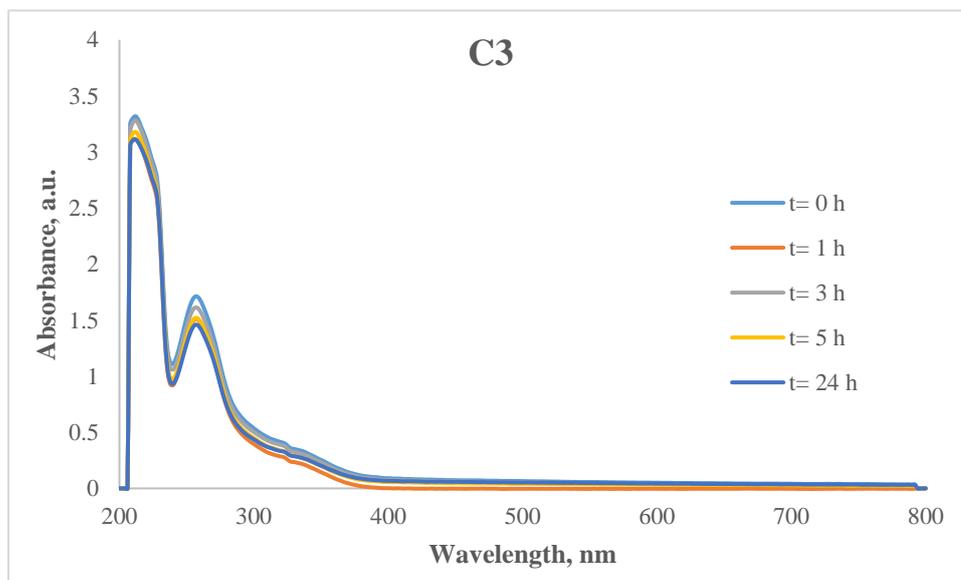
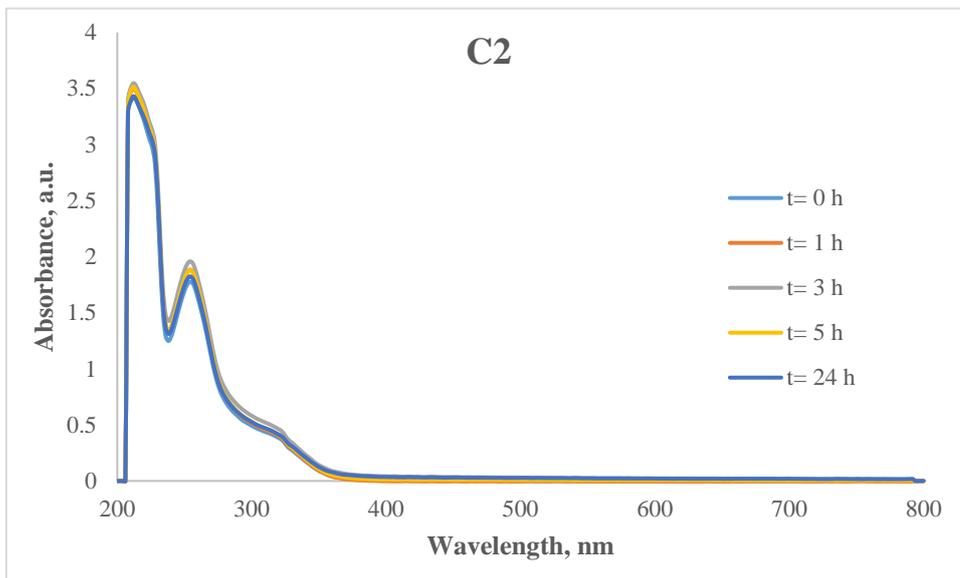
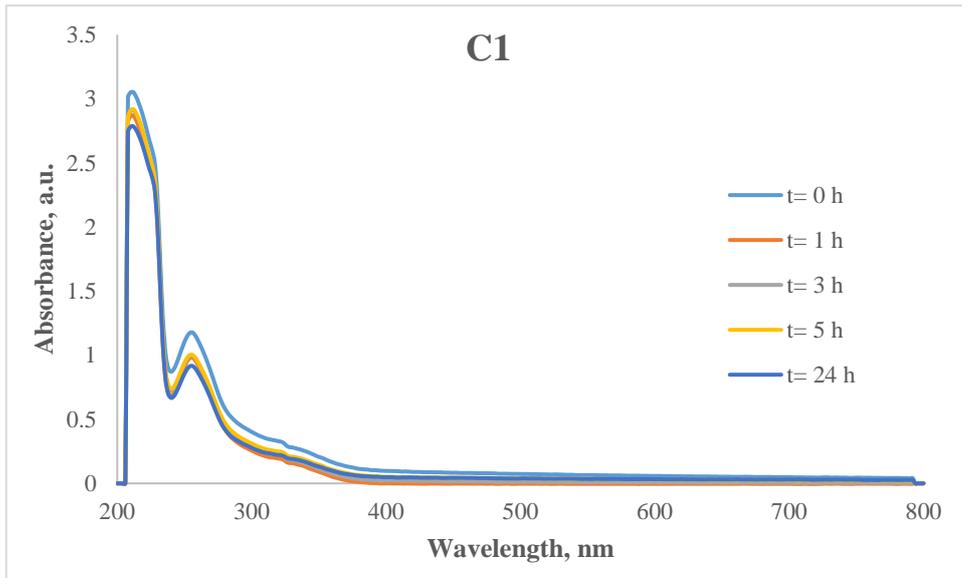
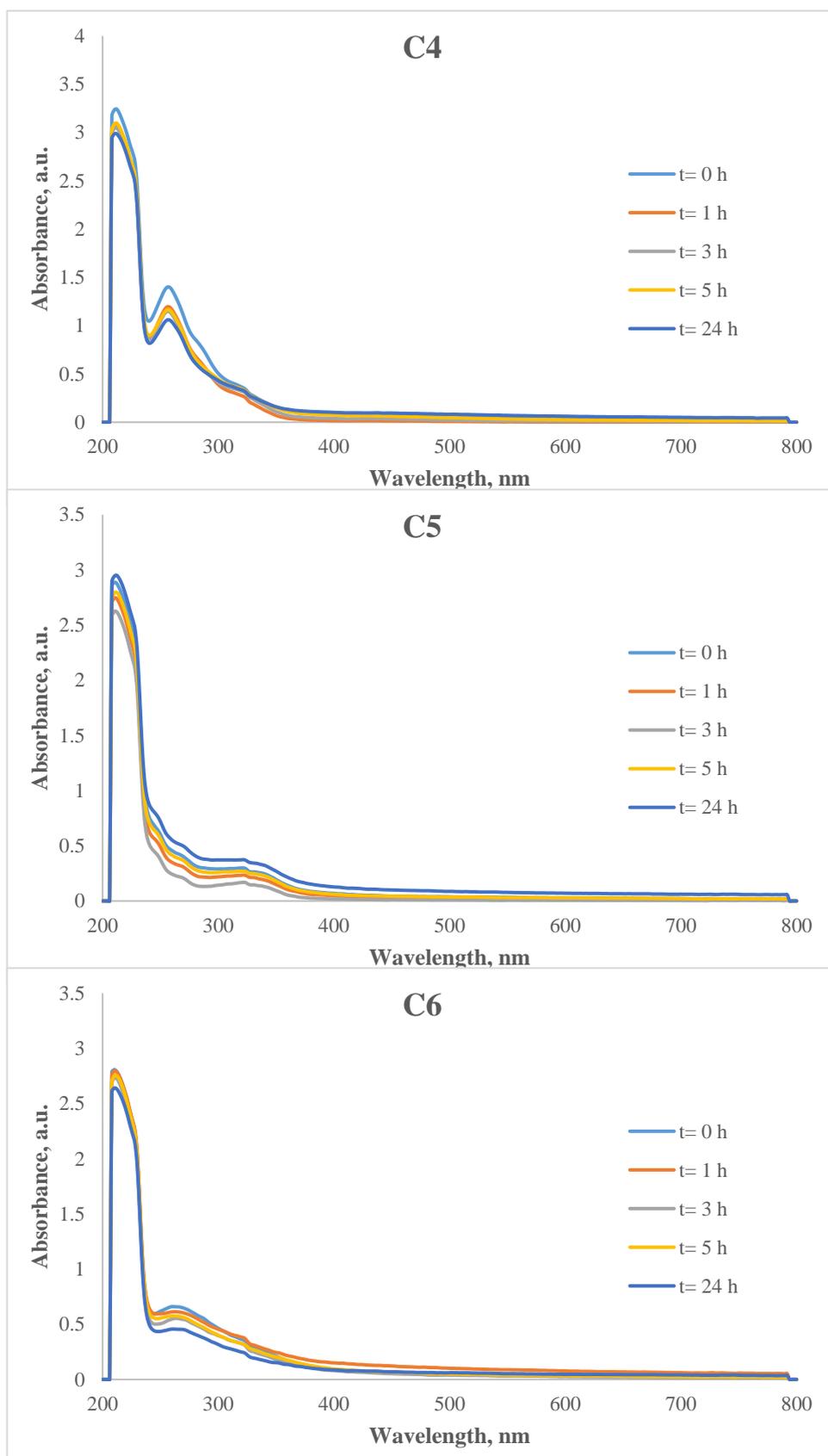


Figure S1e. APT-NMR spectrum of **C3** in chloroform-d.

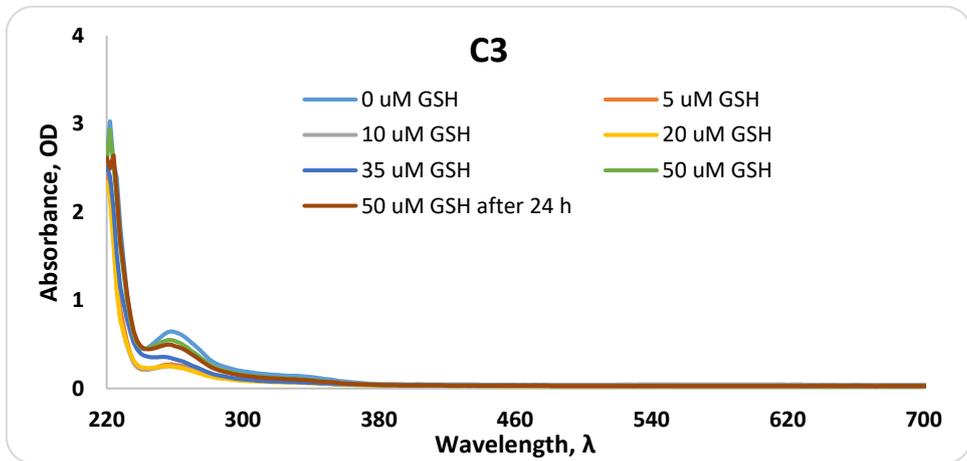
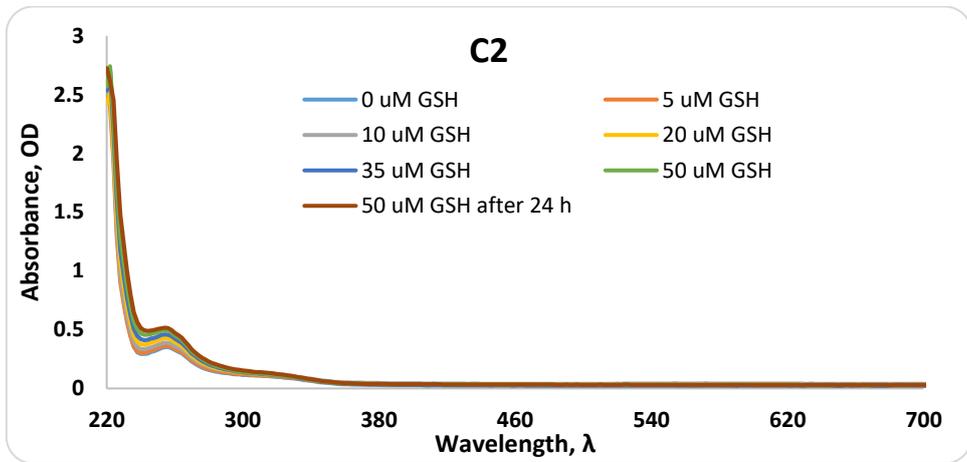
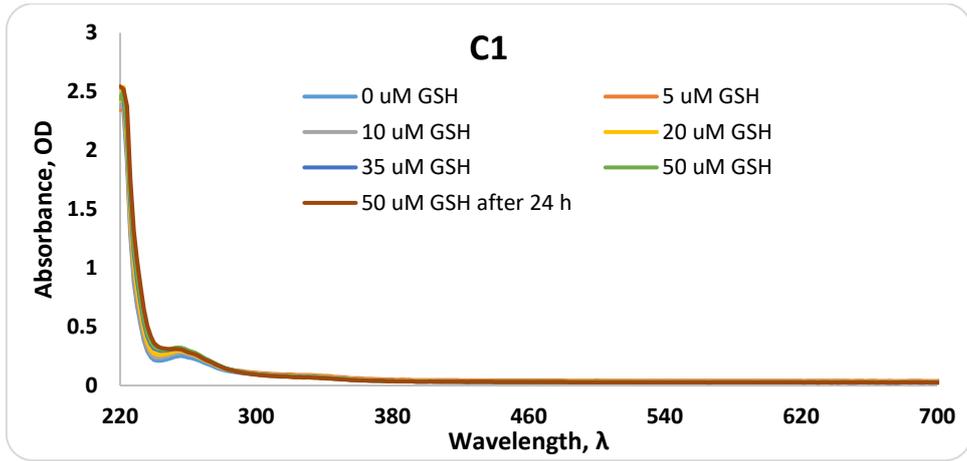


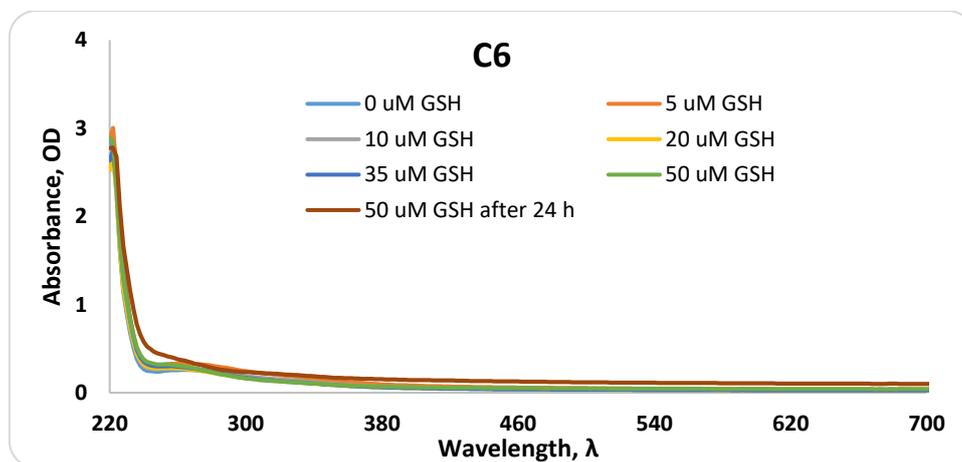
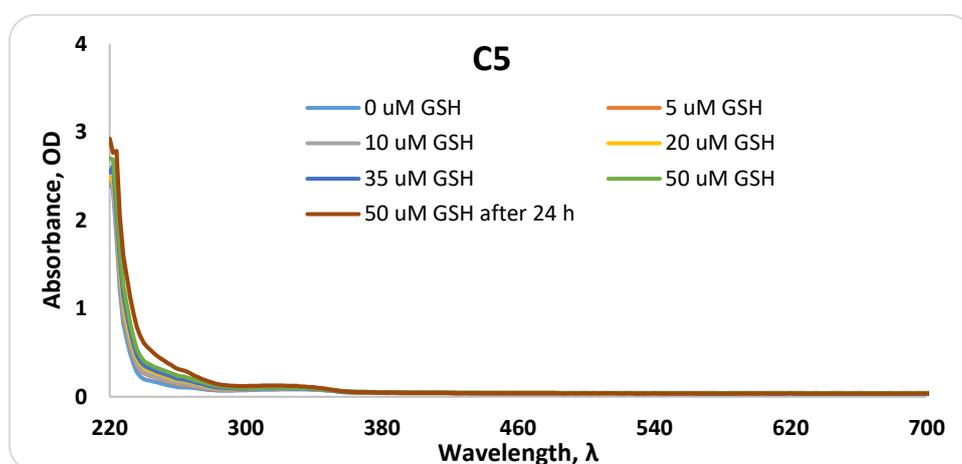
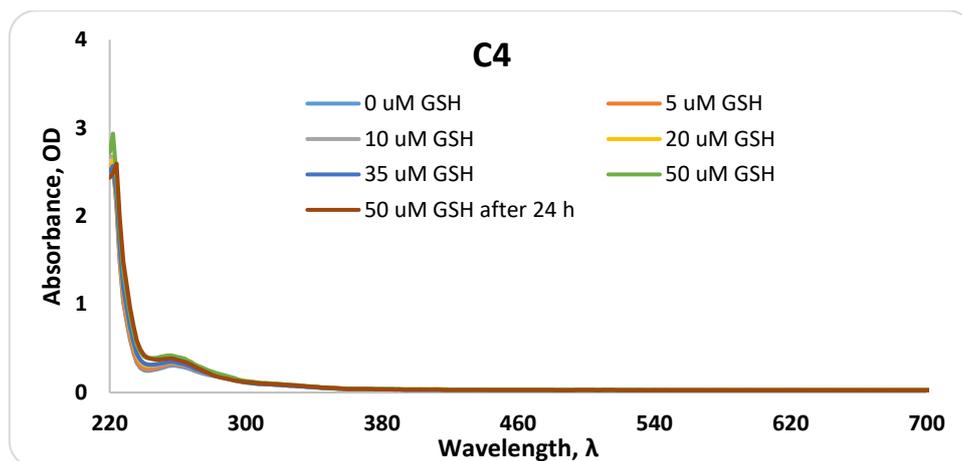
**Figure S2.** Comparison of the theoretical and experimental MS spectra of complexes **C2**, **C3** and **C6** (from left to right).



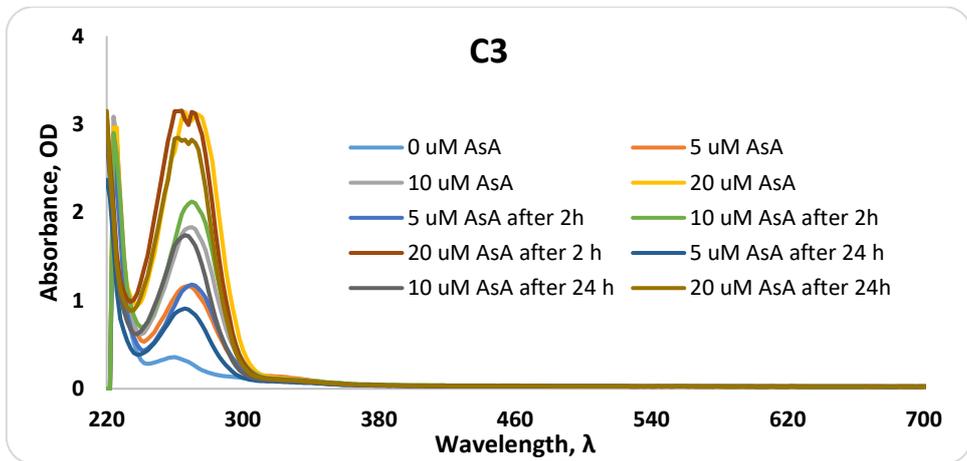
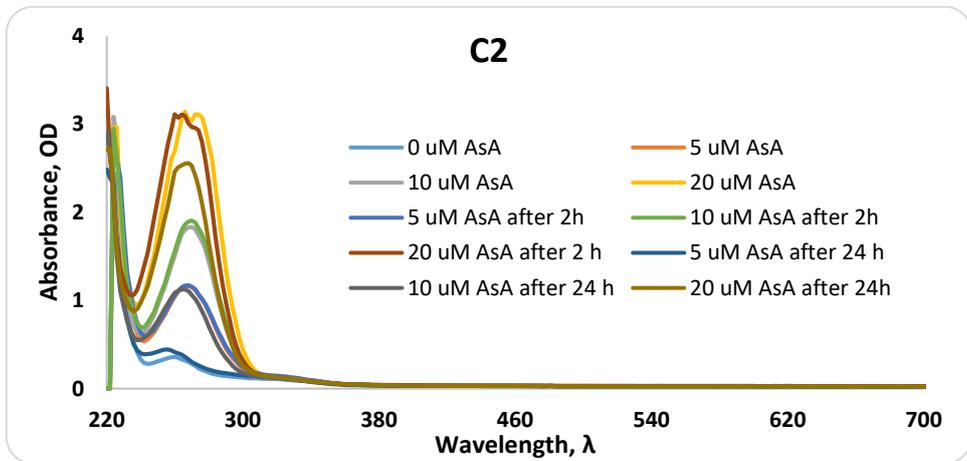
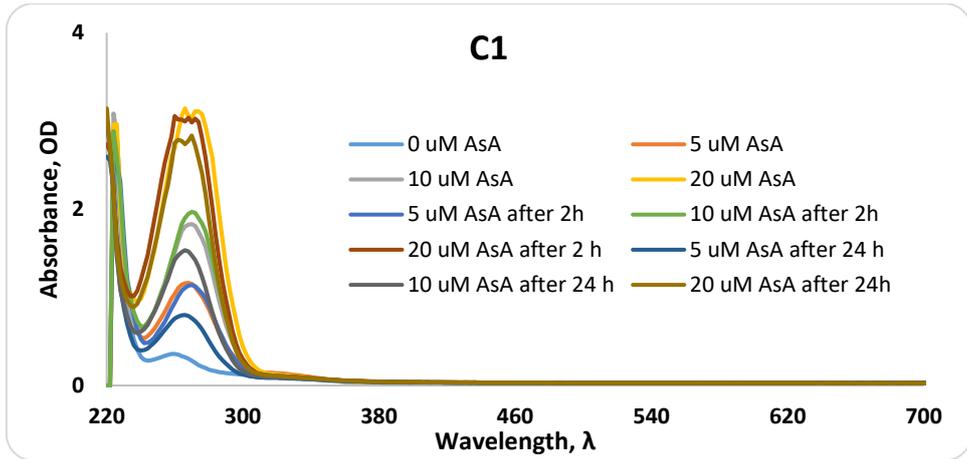


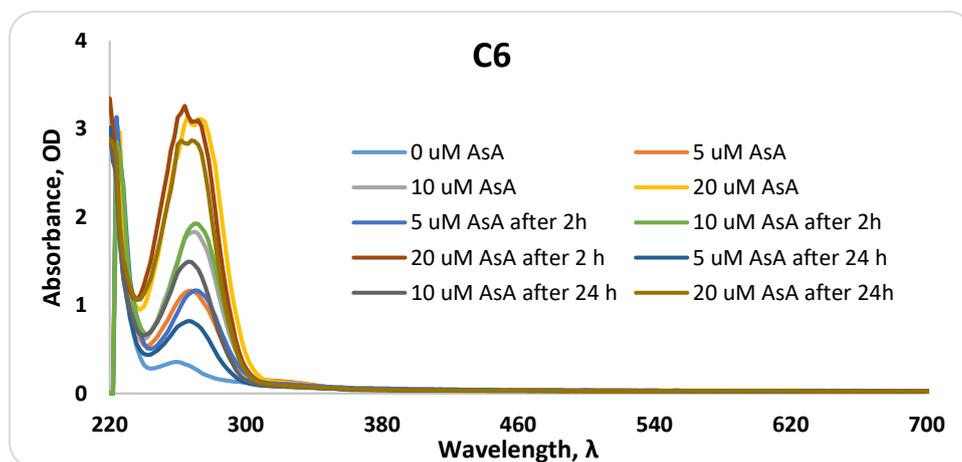
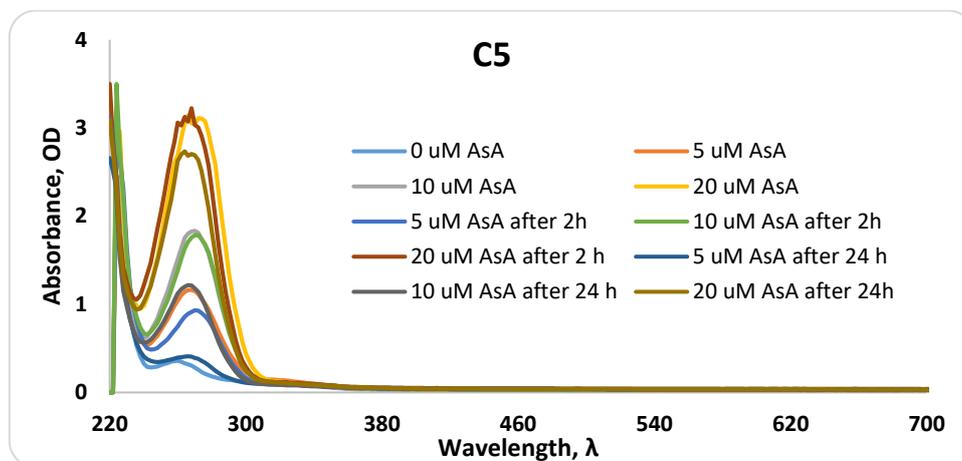
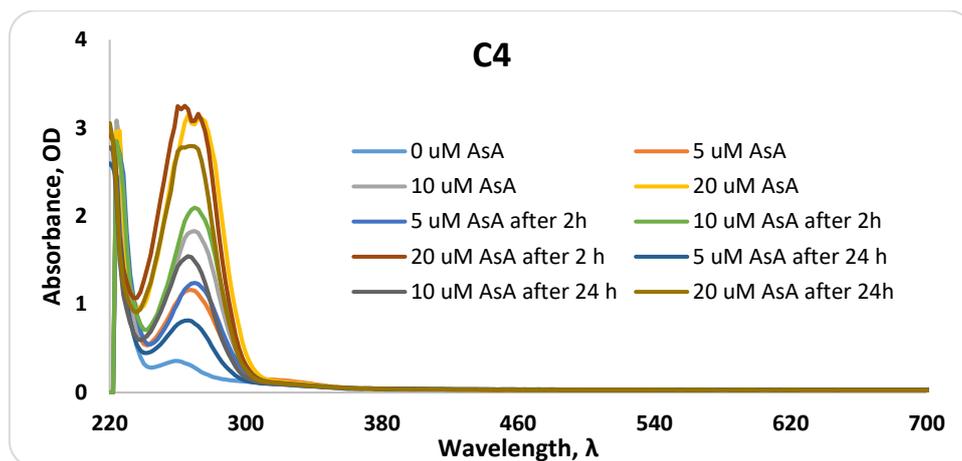
**Figure S3.** UV-Vis spectra of **C1-6** complexes recorded at different times for 24 h in PBS at 37°C.



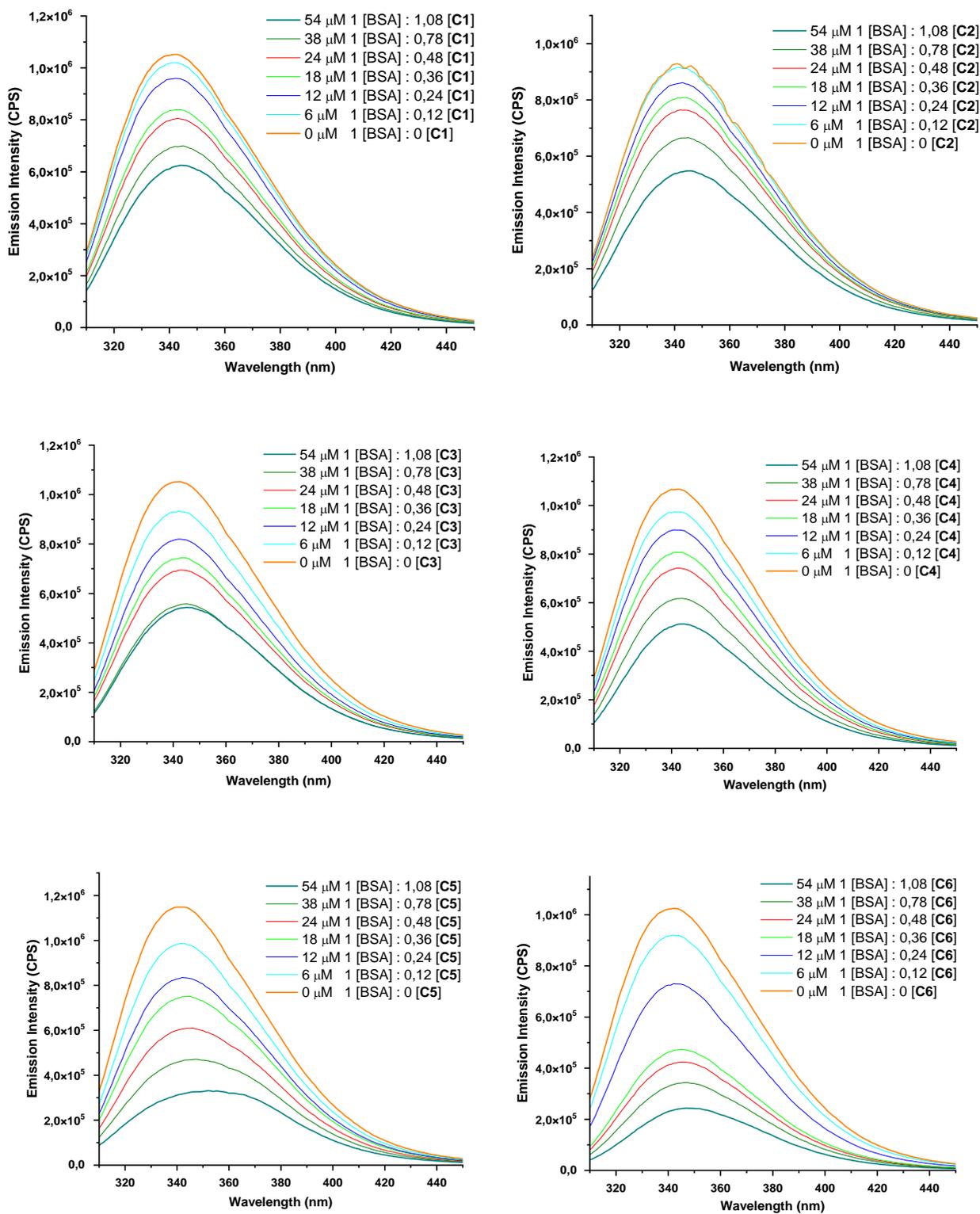


**Figure S4.** UV-Vis spectra of **C1-6** complexes recorded at different times for 24 h in PBS at 37°C in presence of GSH (0-50  $\mu$ M).

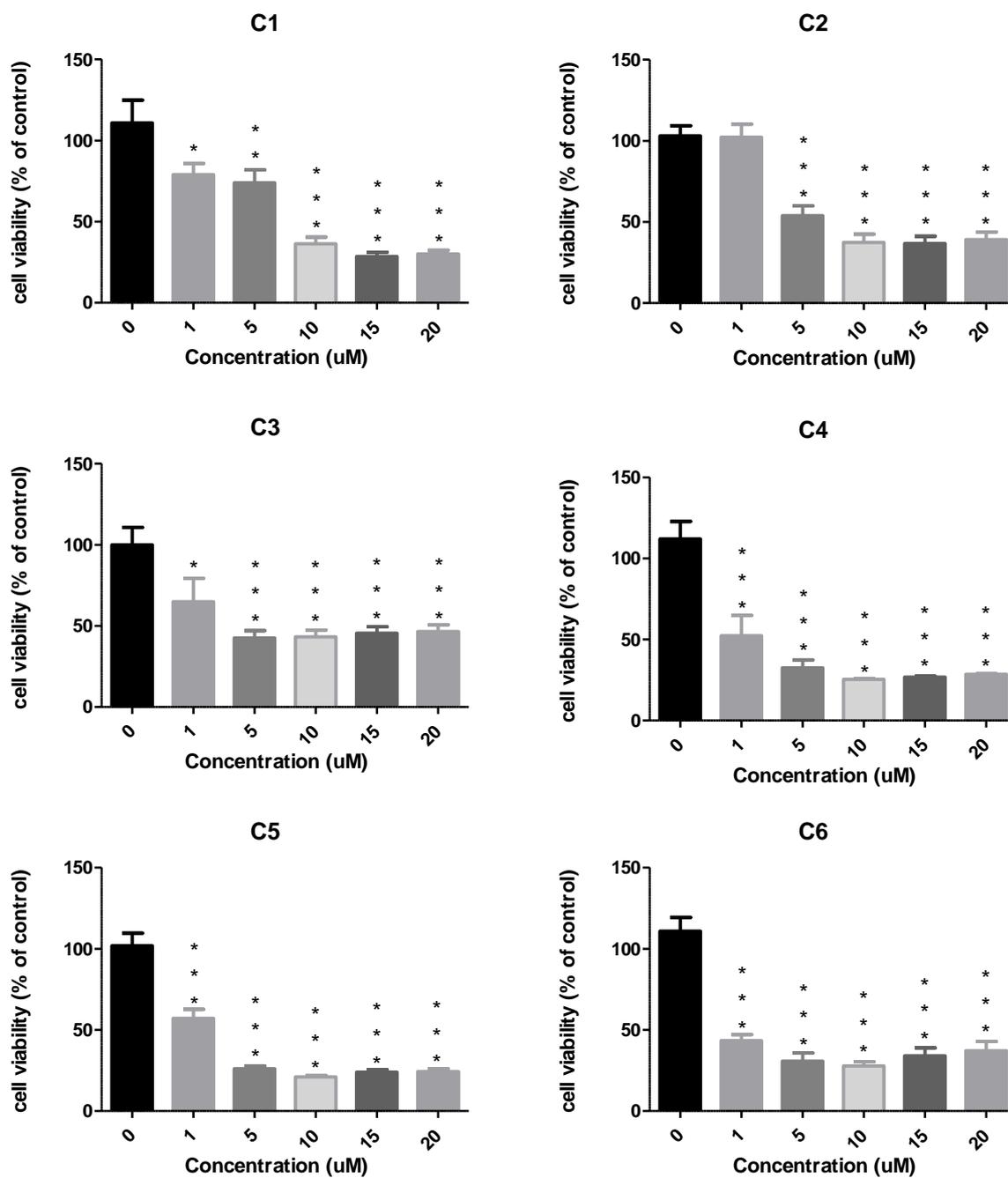




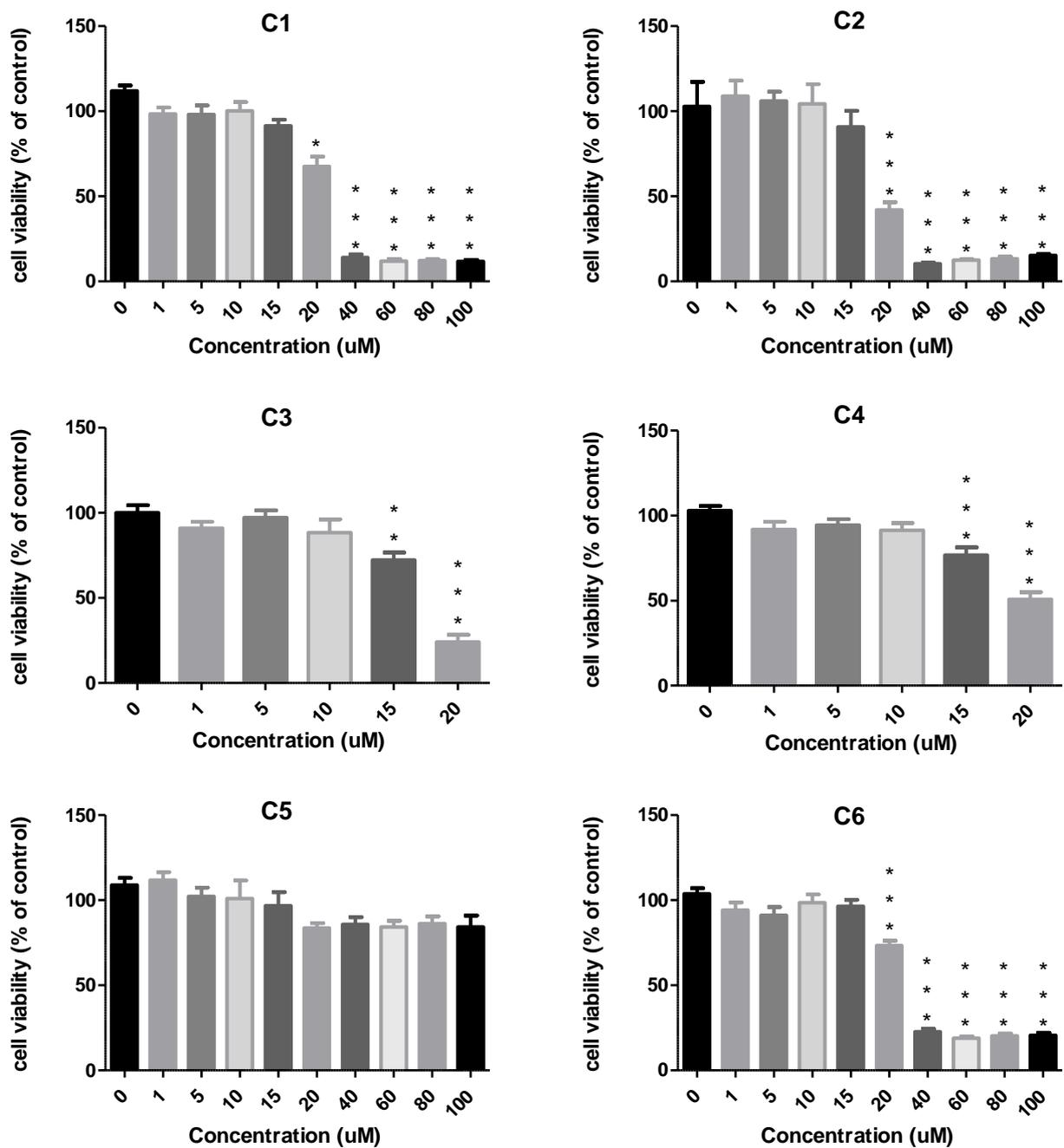
**Figure S5.** UV-Vis spectra of C1-6 complexes recorded at different times for 24 h in PBS at 37°C in presence of AsA (0-20  $\mu\text{M}$ ).



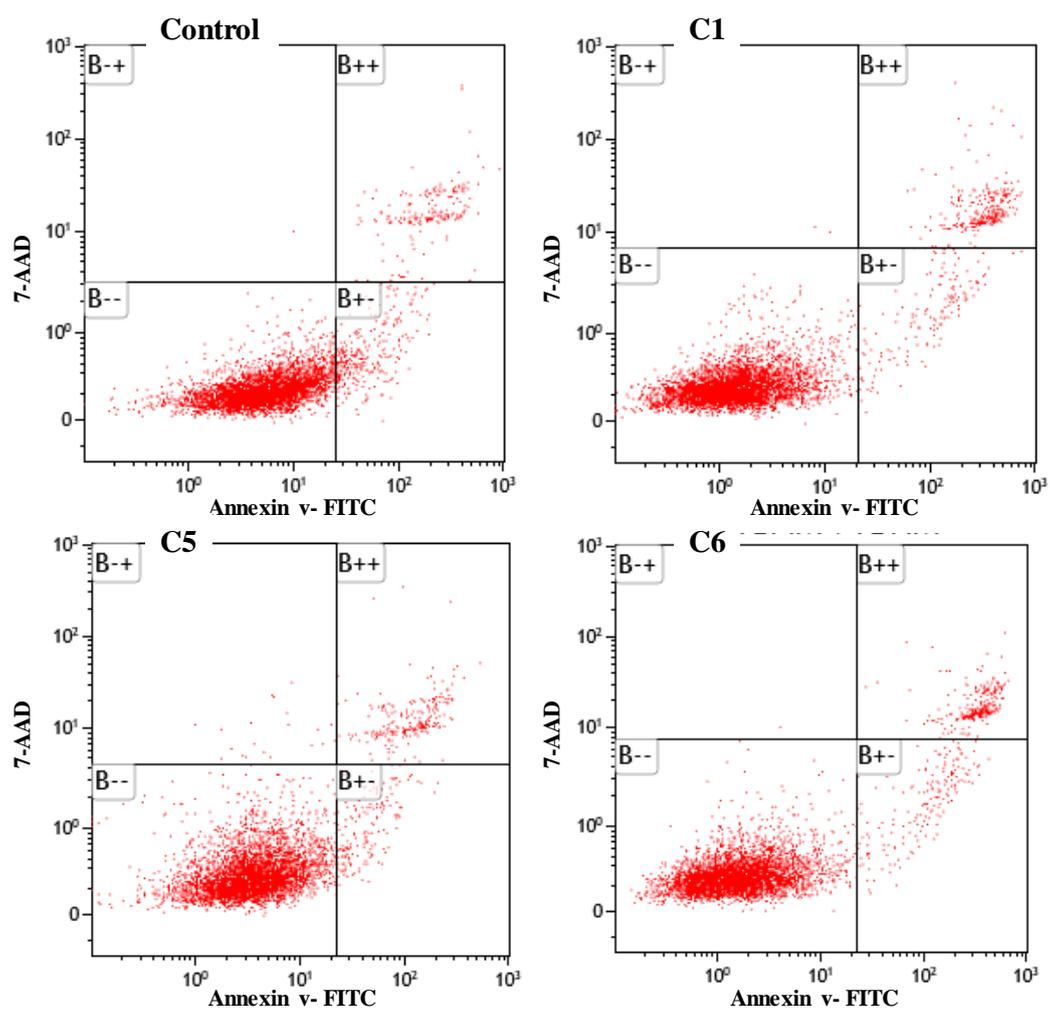
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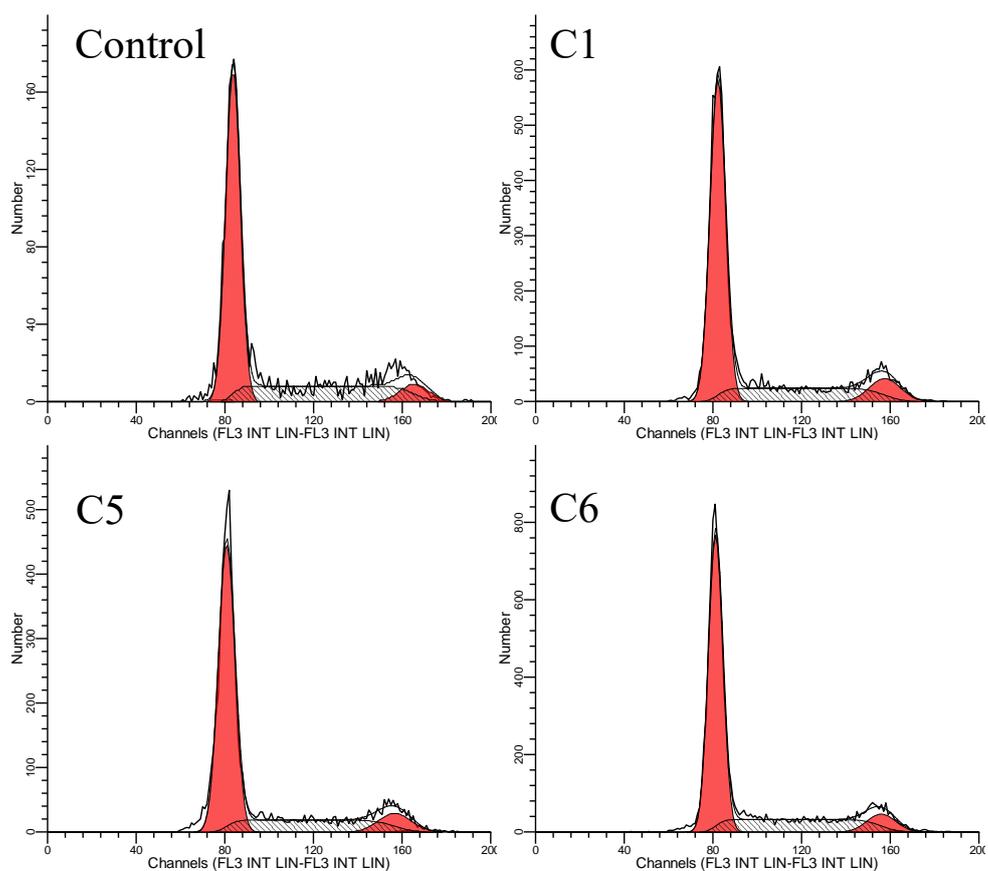
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