

Inclusion Complex of Gold(I) Organometallics in β -Cyclodextrin: Advancing Therapeutic Applications

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Since ancient times, gold has been used to treat various diseases. Gold thiolates were one of the first FDA-approved class of gold-based drugs used to treat rheumatoid arthritis, and later they showed potential anticancer activity¹. Researchers then explored other gold compounds with various types of ligands. In our research group, we study gold(I) complexes containing different classes of ligands, including N-heterocyclic carbenes, as drug candidates for the treatment of neglected tropical diseases such as *leishmaniasis*², arboviruses infections (*Zika*, *Chikungunya*)³, and various types of tumor cell lines (ovarian, prostate, thyroid). The organometallic Au(I)IBnCl (1,3-benzyl-1H-imidazol-2-ylidene, Figure 1), studied by our group, exhibited EC₅₀ values of 1.65 ± 0.16 for *L. amazonensis* and 1.70 ± 0.42 for *L. braziliensis*, with a CC₅₀ of 18.52 ± 1.08 for BMDM macrophages², consequently having selectivity index of 11.2 and 10.9 for *L. amazonensis* and *L. braziliensis*, respectively. One of the main characteristics of gold(I) compounds is their speciation (ligand exchange) and reduction in biological media⁴. If controlled, this speciation can be advantageous for developing pro-drugs. Our group is investigating methodologies to control this speciation, and one of them is the formation of inclusion complexes with β -cyclodextrin. Recent research has shown that including a gold(I) complex with dithiocarbamates selectively killed cancer cells⁵. In this work, we successfully encapsulated Au(I)IBnCl in β -CD. The ¹H NMR shows the 1:2 encapsulation and NOESY suggests the benzyl groups are the guests into the cavity of two units of β -cyclodextrin (Figure 1). The elemental analysis and ICP-OES confirm the 1:2 complex: β -CD ratio.

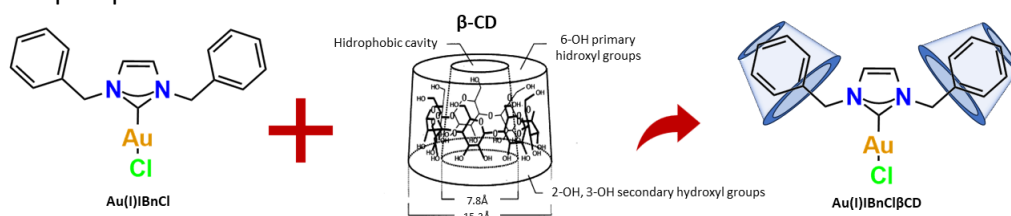


Figure 1. Structure and inclusion of gold(I) complex Au(I)IBnCl and β -CD.

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References

- [1] S. J. Berners-Price, *et al.*, *Metallomics*, **3**, 863–873 (2011).
- [2] L. B. Rosa *et al.*, *Journal of Inorganic Biochemistry*, **15**, 1030 (2022).
- [3] R. L. Aires, *et al.*, *Metallomics*, **14** (2022).
- [4] G. R. Clauss, *et al.*, *New Journal of Chemistry*, **48**, 2040 (2024)
- [5] M. Morgen, *et al.*, *Chemistry a European Journal*, **27**, 12156-12165 (2021).