Frontiers in Bioinorganic Chemistry: Metal-based Molecules for Biomedical Applications

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One of the challenges of modern inorganic chemistry is translating the potential of metal catalysts to living systems to achieve controlled non-natural transformations. To this aim, transition metal catalysts offer an opportunity of modulating bio-processes through reactions that are complementary to enzymes. In this context, gold complexes, both coordination and organometallics, have emerged as promising tools for bio-orthogonal transformations, endowed with excellent reactivity and selectivity, compatibility within aqueous reaction medium, fast kinetics of ligand exchange reactions and mild reaction conditions. [1] This lecture will summarize recent findings from our group on Au(III)-catalyzed reductive elimination in aqueous media, providing the proof-of-concept for the use of organogold compounds – cyclometalated Au(III) C’N complexes - for the efficient modification of proteins through C-atom transfer, enabling chemoproteomic studies (e.g. profiling of cysteine residues) and novel therapeutic approaches.[2] Furthermore, the obtained mechanistic insights have allowed to extend the cross-coupling concept to other substrates, to enable C–P and C–C bond formation under mild conditions.[3-4]

As a second topic, the application of discrete supramolecular metal-based structures, specifically self-assembled metallacages, as potential new generation *theranostic* agents will be introduced. The robustness and modular composition of such supramolecular metal-based molecules allows for the incorporation of different functionalities in the same scaffold to enable imaging in cells via different modalities, but also active tumor targeting and stimuli-responsiveness. In this context, examples of metallacages as targeted drug delivery systems for anticancer chemotherapeutics and radioactive imaging agents will be presented.[5] Certainly, the myriad of possible metallacage-structures and their almost limitless modularity and tunability suggest that the biomedical applications of such complex chemical entities will continue along this already promising path.

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