MedChem & CADD-2013
2nd International Conference on
Medicinal Chemistry & Computer Aided Drug Designing
October 15-17, 2013 Las Vegas, USA

Design and synthesis of metal containing molecular therapeutics

Tulay A. Atesin

The University of Texas-Pan American, USA

Abstract

Metal complexes have long been known for their therapeutic effects against diseases such as hypertension, arthritis, cancer and hypercalcemia. Their mechanism of action, however, is not always entirely understood. The potential for metals to contribute more widely in the treatment and control of diseases has increased research efforts to develop novel metal-based drugs. Basic research on coordination complexes and enzyme active sites can lead to rational design of new drugs, and we use this approach to find metal complexes that bind tightly and selectively to specific amino-acid residues known to play critical roles in target enzymes and proteins. We then improve the molecular targeting based on detailed understanding of the interactions between metal complexes and amino acid residues. The structural diversity of metal complexes, their rich geometric possibilities together with the possibility of secondary interactions with the pendant groups make them attractive drug candidates. The *activity* and *selectivity* towards amino acid residues are determined by studying the *kinetics* and *thermodynamics* of the reaction. Computational modeling is used to predict the relative stability of interactions between the metals with different amino acid residues and these predictions will be further tested experimentally.

Biography

Dr. Tulay A. Atesin received her Ph. D. in 2007 from the University of Rochester under the supervision of Professor William D. Jones working on the mechanisms of strong bond activation reactions. After her postdoctoral research at the University of Wisconsin-Madison from 2007 to 2009 and Northwestern University from 2009 to 2011, she taught at the University of Wisconsin-Whitewater from 2011 to 2013. She is currently an assistant professor in the Chemistry Department at The University of Texas-Pan American, working on the synthesis and characterization of ligands, metal complexes and nanoparticles, studying reaction mechanisms using experimental and computational methods. She received a 2008 Young Investigator Award from the ACS Division of Inorganic Chemistr.