OMICS Group Conferences
Accelerating Scientific Discovery

2nd International Conference on
Medicinal Chemistry & Computer Aided Drug Designing

October 15-17, 2013 Hampton Inn Tropicana, Las Vegas, NV, USA

# Metalloenzymes: Cytochrome P450s and others

**Joshua Pottel**
McGill University, Canada

Metalloenzymes are ubiquitous proteins, some of which take advantage of the Lewis acidic properties of zinc ions including proteases and deacetylases, while others are taking advantage of the redox properties of metals such as oxidases, critical for the breakdown of xenobiotics. These two classes both have pharmaceutical relevance and can be significant for modelling studies; the first includes drug targets for many diseases including cancer while the second class determines the fate of drugs while absorbed. We have taken new approaches to modelling these metalloenzymes and report herein our efforts to better parameterize the metal coordination process as well as predict sites of metabolism. We have implemented our findings into two computational tools, namely FITTED (Flexibility Induced Through Targeted Evolutionary Description) and IMPACTS (*In-silico* Metabolism Prediction by Activated Cytochromes and Transition States). Both software packages have been validated and their significance described.

## Biography

Joshua Pottel received his B.Sc. from McGill University (Montreal, Quebec, Canada) and is pursuing his Ph.D. with Prof. Nicolas Moitessier in the field of computational chemistry. He obtained an honours degree in chemistry and concurrently completed a minor degree in computer science. He has just finished his second year of studies and his current projects involve the further development of software tools ranging from small-scale quantum mechanical parameterization to large-scale metabolism predictions as well as the design of new *in-silico* biocatalyst engineering software. He has published 3 papers in reputed journals and has presented his work at various conferences.

joshua.pottel@mail.mcgill.ca