



Gino DiLabio

Department Head
Chemistry
Univ. of BC, Okanagan

Host: Hicham Fenniri
h.fenniri@neu.edu

“Cool quantum effects revealed through mutagenesis & simulation studies of omithine 4,5-aminomutase”

Wednesday, May 13
135 Shillman
11:45am – 1:00pm

Refreshments will be served

ABSTRACT Aminomutases catalyze the reversible transfer of amino groups between adjacent carbons on amino acid substrates using free radical mechanisms. Two cofactors, adenosylcobalamin (AdoCbl; coenzyme B12) and pyridoxal-5'-phosphate (PLP) are utilized by aminomutases to facilitate this energetically challenging reaction. The former cofactor acts as "radical repository" while the latter forms an imine linkage to the migrating amino group of the substrate. To date, there is a lack of spectroscopic evidence for numerous radical intermediates that form during the course of the catalytic cycle, presumably due to their short lifetimes. Moreover, the contribution of the protein and cofactors towards lowering of the energy barrier associated with many steps of the mechanism is not well understood. The results of the application of a novel density-functional theory simulation method on a model of aminomutase containing the PLP cofactor will be presented. Experimental data show, and modeling results help to explain, how modifications made to the amino acid residues of the enzyme in the vicinity of the PLP cofactor affect the kinetics of PLP transformation. It will be demonstrated that several different quantum mechanical phenomena are at play in the PLP chemistry that occurs within the aminomutase model.

BIOGRAPHY Gino DiLabio is the Head of the Department of Chemistry at the Okanagan Campus of the University of British Columbia. His research centres on the behaviour of radicals at interfaces, including the damaging effects radicals on biological materials, and on the development of computational tools to simulate these systems. Prior to joining UBC, Professor DiLabio was an associate director and senior research scientist with the National Institute for Nanotechnology in Edmonton, Alberta, an Institute to which he remains affiliated through a fellowship appointment. He has published more than 120 papers, patents, and book chapters related to free-radical chemistry, nanotechnology, computational methodologies and organic chemistry.