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POMÈS LAB

Computational Biophysics: Biomacromolecular Structure, Function, and Dynamics



Rowan Henry

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Education:

- B.Sc. Honours, Computational Science, Biochemistry Option; University of Waterloo, Waterloo, ON (2006)

Research Experience:

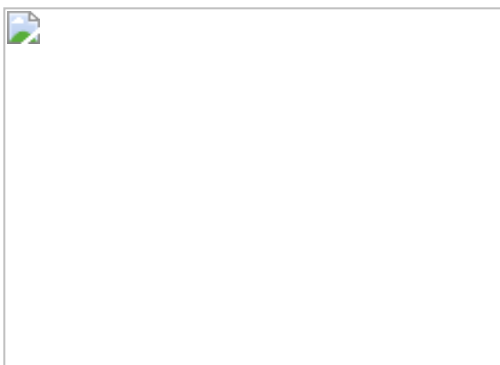
- Research Assistant, Radiation Laboratory, University of Notre Dame, Notre Dame, IN (2003)
Stochastic modelling of the chemistry induced by high energy particles travelling through various liquid mediums.
- Research Intern, J. J. Slaon Group, University of Waterloo Chemistry Department, Waterloo, ON (2003)
Aerosol spectra extraction from satellite spectroscopic data.

Research Interests:

- **Proton Uptake in the D Channel of Cytochrome c Oxidase**
Cytochrome c oxidase is a membrane protein involved in respiration. Its role is to utilize the energy liberated by the reduction of molecular oxygen to water to pump protons against an electrochemical gradient. The resulting proton-motive force drives the synthesis of ATP from ADP. Although several high-resolution three-dimensional structures of the enzyme are known, the molecular mechanism of redox-coupled proton movement is unknown. I use molecular dynamics simulations to examine the relay and delivery of protons to the active site of the enzyme. In particular, I combine free energy calculations with large-scale simulation methods developed recently in our laboratory (Rodinger et al., J. Chem. Theory and Comput. 2, 725-731, 2006) to study the thermodynamic basis of proton movement.

Publications:

- R. M. Henry, C-H. Yu, T. Rodinger, and R. Pomès, "Functional Hydration and Conformational Gating of Proton Uptake in Cytochrome c Oxidase", J. Mol. Bio., 387, 1165-1185 (2009).



Group - Alumni

- [Aditi Ramesh](#) - MSc
- [Adrian Levine](#) - Researcher
- [Ana Nikolic](#) - Researcher
- [Ching-Hsing Yu](#) - Researcher
- [Chris Madill](#) - PhD
- [Chris Neale](#) - PhD
- [David Caplan](#) - MSc
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- [Grace Li](#) - Ph.D.
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- [Kethika Kulleperuma](#) - PhD
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- [Marty Kurylowicz](#) - PhD
- [Nick Wang](#) - Researcher
- [Nilu Chakrabarti](#) - Postdoctoral Fellow
- [Nisha Patel](#) - Researcher
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- [Tom Rodinger](#) - PhD
- [Zhuyi Xue](#) - MSc

Contact

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- [Canadian Institutes of Health Research](#)
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