

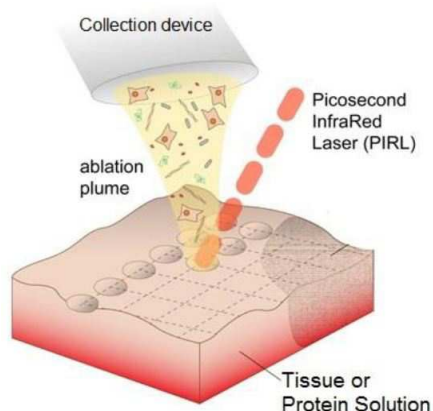
Development of AI & Numerical Modeling in PIRL-DIVE-MS process

Prof. R. J. Dwayne Miller

<http://lphys.chem.utoronto.ca/>

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The Picosecond InfraRed Laser (PIRL) was developed based on the new insights gained from the group discoveries in strongly driven phase transitions and in energy redistribution in the hydrogen bond network of liquid water [1, 2]. The laser-matter interaction of biological tissue with PIRL radiation occurs under the condition of Desorption by Impulsive Vibrational Excitation (DIVE). PIRL excites the OH vibrational stretch mode of water at $3\mu\text{m}$. This vibrational energy is then transferred directly into translational motion on an ultrafast time scale (100 fs) through the strong hydrogen bond network within the water [2]. The water acts as a propellant to drive biomolecules and proteins within the absorption volume into the gas phase completely intact, faster than nucleation formation, and without cavitation-induced shock waves. PIRL-DIVE is the first method by any means capable of scar free surgery at the fundamental single cell limit.



Schematics of tissue being ablated by PIRL and the plume being directed to a mass spectrometer.

A remarkable feature of PIRL's tissue ablation is that the ablated tissue remains undamaged on a molecular level such that entire proteins, from weakly bound proteins to protein complexes up to Mega-Dalton (MDa) ranges and viruses are ejected perfectly intact into the gas phase without any trace of thermal fragmentation and with complete retention of biological activity [4, 5].

The ablated tissue can be detected via the most general and sensitive method of spatially resolved Mass Spectrometry (MS). The Miller group has carried extensive work on PIRL-DIVE-MS with many different biological samples and the method has been advanced to detect very small sample volumes down to attomole level with exceptionally good signal-to-noise ratio.

This project has several components and is suited for a 3rd or 4th year undergraduate Physics student familiar with and interested in numerical modeling. The project components are:

- Development of artificial intelligence (AI) for identification of molecules in samples ablated by PIRL. The AI platform will use the large molecular data base to train the available machine learning algorithms.
- Numerical modeling of space-charge screening using General Particle Tracer (GPT) code to optimize ion collection efficiency in a new generation of mass spectrometer.
- Software development to superimpose optical and MS images to determine and display location of m/z values within the sample.

References

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