



Proudly Operated
by **Battelle** Since 1965

Battelle Number(s):

16720-E

Available for licensing in all fields

Available Technologies

Instrument Control and Data Visualization Software for Integrated Liquid Chromatography/Ion Mobility/Mass Spectrometry (LC\IMS\MS) Systems

SUMMARY

Integrated analytical systems, such as LC\IMS\MS systems, require seamless integration of the various instruments and processes if the analytical benefits of these integrated systems are to be realized. In association with the development of state-of-the-art LC\IMS\MS systems, PNNL has developed software capable of controlling and managing these systems and visualizing the data outputs from the systems. The software includes three major functionalities as follows:

- * Instrument settings/controls that prepare the instrument for data acquisition and actively control voltages/waveforms during experiments.
- * Multithreaded data acquisition, processing and storage that retrieves signals from the TOFMS detector and is capable of handling both Time to Digital Converter (TDC) and ADC acquisition boards. This function provides a highly optimized, multi threaded application to acquire, process, and save data.
- * Graphical data visualization that provides common objects used by the instrument settings/controls and data acquisition functionalities to tune the instrument, monitors instrumental parameters, calibrates and visualizes raw data, and performs data processing and reduction procedures.

Though data transfer between the three functionalities makes them interdependent, they are self sufficient, making parallel development and upgrade of each functionality relatively straightforward. The software has been programmed using C# .NET 2.0 and C++.

This software has been fully deployed and demonstrated in PNNL's integrated LC\IMS\MS systems. It is available for immediate deployment and use by interested external parties desiring to avoid the costs and time required to develop similar software on their own.



Technology Portfolio(s)

- » Mass Spectrometry Data Analysis and Control Software

Potential Industry Applications

- » Chemicals
- » Healthcare, Pharma, Biotech & Medical
- » Professional Services
- » Security

Bruce J. Harrer
Pacific Northwest National Laboratory
(509) 375-6958
bruce.harrer@pnnl.gov
<http://availabletechnologies.pnnl.gov>



Proudly Operated by **Battelle** Since 1965