Report as of FY2006 for 2006ME84B: "Identification of Disinfection Byproducts by High Resolution Gas Chromatography Fourier Transform Ion Cyclotron Resonance Mass Spectrometry"

Publications

- Conference Proceedings:
  - Solouki, T.; Szulejko, J. E.; Silwal, I.; Heffner, C., Experimental and Theoretical Approaches: Identification of Disinfection Byproducts in Drinking Water with multidimensional GC/FT-ICR MS, Proceedings of the 54th ASMS Conference on Mass Spectrometry and Allied Topics, 2006, Seattle, Washington.
  - Touradj Solouki, Indira Silwal, John M. Peckenham, Jayendran C. Rasaiah, and Caleb Heffner, Emerging Technologies for Sample-printing and Identification of Disinfection By-Products in Drinking Water: Multidimensional GC/FT-ICR MS and Theoretical Calculations Gordon Conference, August 2006.
  - Touradj Solouki, Abdullah Alfdeilat, Caleb Heffner, Indira Silwal, Remote Sampling and Emerging Mass Spectral Technologies for Analysis of Complex Environmental Samples: Collective Performance Characteristics, Wellington, New Zealand, EnviroAnalysis Conference 7-10 February 2007.
  - Touradj Solouki, Caleb Heffner, Indira Silwal, John M.Peckenham, Emerging Technologies for Comprehensive Analyses of Complex Environmental Samples: Theoretical Modeling Combined with ESI and GC/FT-ICR Mass Spectrometry MICROPIOL & ECOHAZARD: 5th IWA Specialised Conference on Assessment and Control of Micropollutants / Hazardous Substances in Water, Frankfurt, Germany, June 2007.
- Other Publications:
  - Caleb Heffner, Applications of Emerging Analytical Technologies in Environmental Analysis: A Multidimensional Approach, Department of Chemistry, University of Maine, May 2nd, 2007.
- Articles in Refereed Scientific Journals:
  - Caleb Heffner, Indira Silwal, John M. Peckenham, Touradj Solouki Emerging Technologies for Identification of Disinfection By-Products: GC/FT-ICR MS Characterization of Solvent Artifa cts, in press, Environmental Science & Technology, 2007.

Report Follows

I- Reporting (& Performance) Period: 03/01/2006 – 04/01/2007

This annual report contains the research activities for the USGS funding period (*i.e.*, 03/01/2006 – 04/01/2007).

II- Personnel Directly Involved with the Research:

1. **Touradj Solouki (PI)**: Funding was not requested for the PI but he contributed time to support the overall project. The PI was involved in all aspects of the research, teaching and training activities. During the USGS funding period, the PI, developed mass spectral methods, collected data, presented data in various conferences and meetings, prepared and submitted proposals and manuscripts. In addition, Dr. Solouki supervised an undergraduate student and a graduate student who were directly involved with the USGS supported activities.

2. **John Peckenham (Co-PI):** Funding was not requested for the Co-PI but he was involved in sample preparation, data interpretations, and various significant aspects of the research activities (*e.g.*, proposal and manuscript preparation).

3. **Indira Silwal (Ph.D. Candidate):** Indira is a graduate student in the PI's group and she was supported during the funding period. She was initially a Master's of Science (MS) student in Chemistry. However, her accomplishments with the research activities and successful completion of the comprehensive examinations during the funding period have allowed her to become a Ph.D. candidate. Indira has completed a significant portion of her thesis work, written and successfully defended an NSF style proposal titled "MALDI-TOF MS Study of Identification of the Molecular Content of RBL (Rat Basophilic Leukemia) at a Single Cell level". The anticipated completion date for Indira's thesis work is December 2007. Indira has co-authored a manuscript that has been accepted and is in press (Environmental Science and Technology); moreover, she is in process of finishing another manuscript titled "Determination of Gas Phase Basicities, and Proton

Affinities Using Gas Chromatography/Fourier Transform Ion Cyclotron Resonance Mass Spectrometry (GC/FT-ICR MS) and Ab- initio Calculations".

4. **Caleb Heffner (Undergraduate Research and Thesis)**: Caleb is an undergraduate student in the Chemistry Department (Bachelor of Science, BS) who has been quite prolific with his research activities. Based on his research work, Caleb submitted a proposal titled "Identification of Disinfection By-Products in Drinking Water Using Multi-Dimensional GC/FT-ICR MS and Theoretical Calculations" to Pfizer. In addition, he was the first author on a paper that was submitted to the Environmental Science and Technology. This manuscript was reviewed and accepted for publication. Moreover, based on his research conducted under the USGS funding, Caleb has been selected as the ***Recipient of 2007 J. Morris Student Innovation Award*** *(only two of these awards are given annually university wide)*. Caleb's undergraduate thesis is titled *"Applications of Emerging Analytical Technologies in Environmental Analysis"* and he will be defending it in May 2007.

III- Budget: Budget was adequate to fulfill the initially proposed USGS tasks. Additional budgetary details are available upon request. The major portion of the funding was for the student support and cryogens for normal operation of the superconducting 7 tesla magnet (*i.e.*, FT-ICR mass spectrometer and sample preparation).

V- Other Invited Oral Presentations Acknowledging The USGS Support:

1. Touradj Solouki, "National Science Foundation & Azerbaijan National Academy of Sciences– "Collaborative Research Opportunities - Civilian Research Development & Foundation (CRDF)", formal meetings with the President of ANSF ANAS, *Baku Azerbaijan*, January **2007**.

2. Touradj Solouki, "Fourier Transform Ion Cyclotron Resonance MS– Surpassing World Record Mass Resolving Power in Gas Chromatographic Analyses of Complex Mixtures", *University of Sharif*, May, **2006**.

3. Touradj Solouki, "Analytical Challenges in X-omics and Emerging Fourier Transform Ion Cyclotron Resonance Mass Spectrometry Capabilities for Complex Sample Characterization", Bilkent University, Ankara Turkey, March 16, **2007**.

4. Touradj Solouki, "Ongoing Improvements to Ionization Techniques and Fourier Transform Ion Cyclotron Resonance Mass Spectrometry Capabilities: Unraveling Nature's Complexities", *Ankara, Turkey METU University*, March 17, **2007**.

7. Touradj Solouki, "Emerging & High Performance Instrumentation for Sampleprinting in Forensic and Bioanalytical Sciences", *University North Texas*, April, **2006**.

VI - Theses Prepared / Under Preparation:

1. Undergraduate Student Thesis:
    a. Caleb Heffner, ""*Applications of Emerging Analytical Technologies in Environmental Analysis"*, three chapters written and reviewed. Will be defended in May **2007**.

2. Graduate Student Thesis (Ph.D.):
    a. Indira Silwal, *"Experimental and Theoretical Approaches to Determine Thermodynamical Parameters for Multidimensional Mass Spectrometry"*, in preparation.

VII - Proposals Prepared Based On The Data Acquired From This Project:

PI:	Touradj Solouki
Title:	Multidimensional GC/FT-ICR MS: Characterization of Environmental Contaminants and Cancer Biomarkers at a High Level of Confidence"
Source of Support:	NSF
Total Award Amount:	$ 384694
Total Award Period:	06/01/06- 05/31/09
Status:	Pending

PI:	John Peckenham
Co-PI:	Gail Lipfert, Touradj Solouki, Andy Tolman
Title:	"The influence of chloride and natural organic matter gradients on disinfection by-product formation in Maine"
Source of Support:	USGS
Total Award Amount:	~ $ 45000
Total Award Period:	04/01/07- 03/31/09
Status:	Funded

PI:	Touradj Solouki
Title:	"Early Detection of Epithelial Ovarian Cancer Using Exhaled Breath Markers: GC/FT-ICR Mass Spectrometry and Canine Olfaction"
Source of Support:	DOD
Total Award Amount:	$ 473549
Total Award Period:	02/01/07- 01/31/09
Status:	Funded