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February Meeting

Tuesday, February 21, 2006

The February 2006 meeting will be held at the Technology Institute at Northwestern University, located at the Technology Institute, 2145 Sheridan Road, Evanston IL, 60208. See the map on the following page.

Setup: 5:00 - 6:30 PM **Posters: 5:30 - 8:30 PM** **Awards: 8:30 PM**

Poster Session on Spectroscopy

1) **Rapid Detection of an Anthrax Biomarker by Surface-Enhanced Raman Spectroscopy** -- *Poster by Xiaoyu Zhang (Northwestern University)*

2) **Real-Time Glucose Sensing by Surface-Enhanced Raman Spectroscopy: In Vitro Plasma and In-Vivo Rat Models** -- *Poster by Nilam C. Shah (Northwestern University)*

3) **Isomerization Kinetics of Desmethylxanthohumol (DMX) by qHNMR** -- *Poster by Shao-Nong (UIC)*

4) **Localized Surface Plasmon Resonance** -- *Poster by Jing Zhao (Northwestern University)*

5) **Tip-Enhanced Raman Spectroscopy for Applications in Nanotribology and High Spatial Resolution Chemical Analysis** -- *Poster by Matthew A. Young (Northwestern University)*

6) **Novel Methodologies in Enhanced Raman Spectroscopy** -- *Poster by Jon A. Dieringer (Northwestern University)*

7) **Comparison of FT-Based and Dispersive Vibrational Circular Dichroism (VCD). Development of a New Dispersive VCD** -- *Poster by Ahmed Lakhani (UIC)*

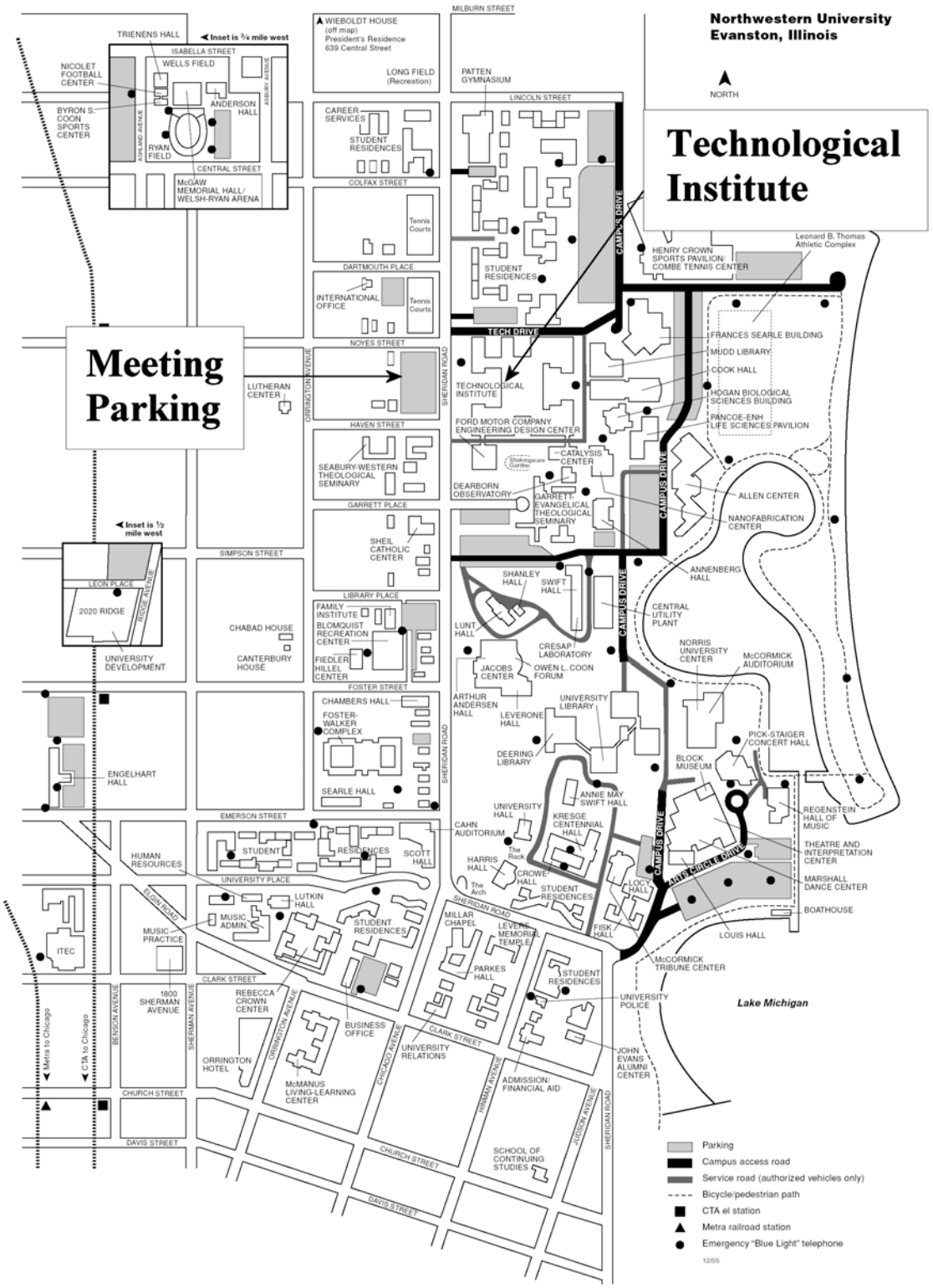
8) **Conformational States and Thermodynamics of Alpha-Lactalbumin: A Model Study using Spectroscopy** – *Poster by Ning Ge (UIC)*

9) **Bringing FT-IR and CD Spectroscopies Together for Structural Studies of Proteins** – *Poster by Daniell Kelly (Elmhurst College)*

Look for future announcements about the Workshop on Chemometrics scheduled for May 16, 2006 in Naperville, IL. Featuring presentations by Dr. Barry Lavine (Oklahoma State University) and Dr. Gary Small (The University of Iowa).

Directions and Parking

- For maps and directions to Northwestern University's Evanston Campus go to www.northwestern.edu/visiting/maps.
- After 4 pm, parking is free in the lot across from the Technological Institute on Sheridan Road.
- Posters will be in the Technological Institute Lobby.



1) Rapid Detection of an Anthrax Biomarker by Surface-Enhanced Raman Spectroscopy

Poster by Xiaoyu Zhang

Chemistry Department; Northwestern University

Xiaoyu Zhang and Richard P. Van Duyne

A rapid detection protocol suitable for use by first-responders to detect anthrax spores using a low-cost, battery powered, portable Raman spectrometer has been developed. *Bacillus subtilis* spores, harmless simulants for *Bacillus anthracis*, were studied using surface enhanced Raman spectroscopy (SERS) on silver film over nanosphere (AgFON) substrates. Calcium dipicolinate (CaDPA), a biomarker for bacillus spores, was efficiently extracted by sonication in nitric acid and rapidly detected by SERS. AgFON surfaces optimized for 750-nm laser excitation have been fabricated and characterized by UV-vis diffuse reflectance spectroscopy and SERS. The SERS signal from extracted CaDPA was measured over the spore concentration range 10^{-14}-10^{-12} M to determine the saturation binding capacity of the AgFON surface and calculate the adsorption constant (Kspore = 1.7×10^{13} M^{-1}). At present, an 11-minute procedure is capable of achieving a limit of detection (LOD) of ~ 2.6×10^{3} spores, below the anthrax infectious dose of 10^{4} spores. The data presented herein also demonstrate that the shelf life of pre-fabricated AgFON substrates can be as long as 40 days prior to use. Finally, these sensing capabilities have been successfully transitioned from a laboratory spectrometer to a fieldportable instrument. Using this technology, 10^{4} bacillus spores were detected with a five-second data acquisition period on a one-month-old AgFON substrate. The speed and sensitivity of this SERS sensor indicate that this technology can be used as a viable option for the field analysis of potentially harmful environmental samples.

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2) Real-Time Glucose Sensing by Surface-Enhanced Raman Spectroscopy: In Vitro Plasma and In-Vivo Rat Models

Poster by Nilam C. Shah

Department of Chemistry, Northwestern University

Nilam C. Shah[1], Olga Lyandres[2], Chanda R. Yonzon[1], Matthew Glucksberg[2], Joseph T. Walsh[2], Richard P. Van Duyne[1]

1)Department of Chemistry, Northwestern University; 2) Biomedical Engineering Department, Northwestern University

This work represents our recent significant progress towards developing a minimally invasive, continuously monitoring glucose sensor based on surface-enhanced Raman spectroscopy (SERS). An Ag film over nanosphere (FON) functionalized with a self- assembled monolayer (SAM) is used as the substrate to allow for direct detection of glucose using SERS. The sensor has been evaluated in vitro for reversibility, real-time detection, quantitative measurement, and long-term stability. The 1/e time constant was calculated to be 28 s for partitioning and 25 s for departitioning in bovine plasma. Multivariate analysis was used to quantitate physiological levels of glucose in bovine plasma as well as in a solution of 1 mM lactate and 2.5 mM urea. Bovine plasma closely mimics the in vivo environment. The experiments yielded root-mean-square error of prediction (RMSEP) of 83.16 mg/dl (4.62 mM) with 85% of the validation points falling within the acceptable detection range. The sensor has also been evaluated in vivo in a rat model for quantitative detection. This resulted in an RMSEP of 53.42 mg/dl with 100 % of the validation points falling within the acceptable detection range.

3) Isomerization Kinetics of Desmethylxanthohumol (DMX) by qHNMR

Poster by Shao-Nong Chen

Dept. Medical Chemistry and Pharmacognosy; College of Pharmacy, UIC

Shao-Nong Chen[1], Lucas R. Chadwick[1], Birgit U. Jaki[2], David Lankin[1] and Harry H.S. Fong[1], Norman R. Farnsworth1, Guido F. Pauli[1]*

1) UIC/NIH Center for Botanical Dietary Supplements Research and Department of Med. Chemistry and Pharmacognosy, and 2) Institute for Tuberculosis Research, College of Pharmacy, University of Illinois at Chicago, 833 S. Wood Street, Chicago, Illinois 60612, USA

The resinous inflorescences of the twining vine Humulus lupulus L. (Cannabaceae) commonly known as hops, is one of the plants investigated in the UIC/NIH Center for Botanical Dietary Supplements Research. The plant exhibits very potent in vitro estrogenic activity, and the prenylated flavanone, 8-prenylnaringenin (8PN), was identified as the active principle, representing one of the most potent non-steroidal estrogen known from the plant kingdom. In addition to 8PN, congeneric isoflavanones and chalcone derivatives also contribute to the overall estrongic activity of hops extracts. For example, the chalcone precursor of 8PN, desmethylxanthohumol (DMX), demonstrated weak estrogenic activity in vitro. However, from a long-term kinetic quantitative 1H NMR (qHNMR) study, we were able to demonstrate that DMX itself is inactive. The observed activity is due to minute amounts of 8PN, representing a prominent impurity in DMX samples. The qHNMR experiments indicated that DMX isomerizes to 8PN and 6-prenylaringenin (6PN) in relatively short periods of time, even under stringent storage condition. The isomerization rate slows down with time. Using newly established 13C-decoupled qHNMR methodology, the observations underline the relevance of purity determination and stability for an important group of estrogens from hops. Moreover, the findings potentially have a broader impact in the analysis of bioactive herbal constituents.

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4) Localized Surface Plasmon Resonance

Poster by Jing Zhao

Department of Chemistry, Northwestern Univeristy

"Localized Surface Plasmon Resonance (LSPR) is one of the feature optical characteristics of nobel metal nanoparticles. The extreme sensitivity of LSPR to the surrounding environment makes nanoparticle arrays and single nanoparticles excellent bio/chemical sensors. This poster presents the study of short and long range distance dependence of the LSPR sensors. In addition, the interaction of molecular resonance with LSPR has been demonstrated. The nanoparticles synthesized by nanosphere lithography on substrate can be released into solution. The LPSR sensors have been used to detect streptavidin and ADDls related to Alzheimer's disease. Moreover, the nanoparticle array based sensor is transitioned to a single nanoparticle based LSPR sensor."

5) Tip-Enhanced Raman Spectroscopy for Applications in Nanotribology and High Spatial Resolution Chemical Analysis

Poster by Matthew A. Young

Department of Chemistry, Northwestern University

Matthew A. Young, Peter C. Stair, and Richard P. Van Duyne

In this work, we present our efforts toward developing tip-enhanced Raman spectroscopy (TERS) in order to combine the high sensitivity and rich chemical information of surface-enhanced Raman spectroscopy (SERS) with the excellent spatial resolution provided by scanning probe microscopies (SPM). TERS can provide Raman spectra with a spatial resolution equal to the radius of curvature of the SPM tip, which is a significant improvement on diffraction limit. Tips made of or coated with Ag or Au have been shown to enhance the Raman scattering cross section of molecules very near the tip (but not adsorbed to the tip) by 3 to 6 orders of magnitude. We demonstrate high quality TERS spectra of self-assembled monolayers (SAMs) using an AFM mounted on an inverted microscope. TERS is a relatively new technique and its substantial potential is largely untapped. One area where TERS is well suited for application is nanotribology, the study of friction, wear, and pressure at the nanoscale. Atomic force microscopy (AFM) provides an excellent technique for probing tip-sample interactions at the nanoscale. In our work, we extend the information available from AFM by using TERS for probing the tribological properties of alkyl SAMs on surfaces. This represents the first time TERS has been employed in the direction of solving problems in nanotribology. We report initial TERS spectra acquired using Ag-coated AFM tips and discuss the results in terms of molecular events (molecular bending or tilt) and localized heat generation. The AFM tip is used to create very high local pressures (>10 GPa) and fast sliding speeds. TERS spectra are acquired in contact mode with (1) the tip held stationary in the x-y plane to probe pressure dependence and (2) dynamic sliding (tip scanning) situations to probe molecular events.

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6) Novel Methodologies in Enhanced Raman Spectroscopy

Poster by Jon A. Dieringer

Department of Chemistry, Northwestern University

Jon A. Dieringer and Richard P. Van Duyne

Surface-enhanced Raman spectroscopy (SERS) has seen a resurgence of interest due to recent developments such as tip enhanced Raman spectroscopy, the observation of single molecule SE RS and nanoparticle plasmonics. This poster describes recent advances made in the above fields. First, a preliminary experiment shows that the signal intensity of benzenethiol adsorbed to a thin gold surface is modulated by a gold STM tip brought into and out of tunneling position. Second, the distance decay of the electromagnetic field enhancement is measured by depositing sub nanometer alumina layers via Atomic Layer Deposition (ALD) on a SERS active. The SERS spectrum of pyridine was taken at different distances from the SERS surface. The signal was attenuated by two orders of magnitude over 5 nanometers and the decay profile fits a theoretical model previously published. Finally, two dimensional correlation is applied to SERS data, which offers evidence of single molecule SERS behavior. In addition, isotopically labeled resonant molecules are used in conjunction with two dimensional correlation to study single molecule SERS.

7) Comparison of FT-Based and Dispersive Vibrational Circular Dichroism (VCD). Development of a New Dispersive VCD

Poster by Ahmed Lakhani

Department of Chemistry, University of Illinois at Chicago, 845 West Taylor Street, Chicago, Illinois, USA.

Ahmed Lakhani, Peter Malon, Vladimir Setnicka, Rong Huang, and Timothy A. Keiderling

In this poster, we will present a comparison of FT-based and new dispersive vibrational circular dichroism (VCD) spectrometers. Additionally, the optical and electronic schematic design, plus current performance characteristics of a new dispersive VCD purpose built for peptide and protein studies will be described. Vibrational circular dichroism is the differential absorption of left and right circularly polarized light via vibrational transitions of chiral molecules in the infrared region. Dispersive VCD instruments utilize a monchromator to scan through the selected frequency range. Fourier transform (FT) VCD uses a Michelson interferometer to encode the optical wave numbers as a function of the moving mirror position, resulting in an interferogram and yielding the well-known FT advantages. Dispersive VCD for single broad bands in a biopolymer can negate the FT multiplex and through put advantages. To compare three instruments, the performance in measuring VCD for the same sample (a protein or polypeptide) in the same total time is shown.

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8) Conformational States and Thermodynamics of Alpha-Lactalbumin: A Model Study using Spectroscopy

Poster by Ning Ge

Department of Chemistry, University of Illinois at Chicago

Ning Ge, Xiuqi Zhang, Timothy A. Keiderling

Alpha-Lactalbumin (BLA) has been studied as a model membrane protein which has measurable different conformations under different conditions, thus deepens our knowledge of the behavior of amphitropic proteins. In this poster, the conformational changes of BLA in solution under various conditions, such as pH, temperature and medium, has been investigated using various spectroscopic methods, such as CD, fluorescence. In addition, we also investigated the association of the protein with lipid bilayers composed of different lipids, such as POPA and POPC, at pH 2.5, under conditions where the protein adopts a molten globule-like state. The conformational changes of molten globule-like states of the protein upon binding the lipids were studied.

9) Bringing FT-IR and CD Spectroscopies Together for Structural Studies of Proteins

Poster by Daniell Kelly

Elmhurst College, 190 Prospect Ave., Elmhurst, IL 60126, USA.

Daniell Kelly[1], Jasmine Nguyen[1], Peter King[2], David Gregson[2] and Rina K. Dukor[3]

1) Elmhurst College, 190 Prospect Ave., Elmhurst, IL 60126, USA; 2) Applied Photophysics Ltd, 203-205 Kingston Rd., Leatherhead KT22 7PB, UK; 3) BioTools, Inc. 950 N. Rand Rd., Unit 123, Wauconda, IL 60084, USA

Proteins play a vital role in the development of new biotechnology drugs and pharmaceuticals. Characterization of proteins is required at all stages of development – from R&D to formulation to manufacturing. The two most common techniques used for such studies are Circular Dichroism in the UV region (UV-CD) and FT-IR. The techniques are complementary and as has been shown by Keiderling and co-workers (1) probe the secondary structure to a different degree of local order. Thus, CD is usually much better in predicting the helical content while FT-IR and other vibrational techniques are more sensitive to -sheet and turns. Although both techniques are now used extensively in the biopharmaceutical industry, a significant difference in spectral analysis exists, primarily due to the history of the application developments. CD has been used for protein structural studies for over 30 years and many databases of protein CD spectra exist in the literature. In addition, many different algorithms have been proposed for structure elucidation. The most common method of analysis is the use of an online database (3), which allows for reference protein and algorithm selectivity. This is not a problem in an academic environment but creates a confidentiality problem for pharmaceutical companies. FT-IR spectroscopy, although over 25 years old, has only been used for protein structural characterization in industry for the past 10 years, due to the efforts of BioTools and their first commercial system for protein structure – PROTA. PROTA comes with an algorithm based on the work of Keiderling and co-workers (2) and its own extensive database of proteins. Although a few free databases exist in literature and on the internet, the commercial product allows companies to contain results in house. Here in lies a problem: comparison of CD and FT-IR is done against different databases and different algorithms introducing an inherent uncertainty due to incompatibility in approach. The goal of this study is to build a large, unified database of protein UV-CD and FT-IR spectra that contains structures of proteins used extensively in biopharmaceutical development including antibodies, hormones and growth factors. This database would be internally consistent with respect to the proteins, sampling conditions to the degree possible, and algorithms for analysis. In addition, for the first time, a CD database and algorithm will be available for confidential use within a research laboratory or pharmaceutical company.

(1) Dukor, R. K. and T. A. Keiderling. *Biopolymers* 1991, 31(14), 1747.
(2) Pancoska, P., Yasui, S.C., and T. A. Keiderling. *Biochemistry* 1991, 20, 5089.
(3) Whitmore, L. and B. A. Wallace. *Nucleic Acids Research* 2004, 32, W668.

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