SAS-Chicago

November Meeting

Tuesday, November 13, 2007

The November 2007 meeting will be held at the Wellington Restaurant, located at 2121 S Arlington Heights Rd, Arlington Heights, IL 60005. See the map on the following page.

Social Hour: 5:30 PM **Dinner: 6:30 PM** **Speaker: 7:30 PM**

NMR Outside Of The Box

by

Gary Martin, Ph.D.
Schering Plough

Hyphenated 2D NMR experiments such as GHSQC-TOCSY and related experiments have sensitivity losses associated with them that significantly offset the benefits of the information-rich spectra that these experiments provide. The recent development of covariance NMR methods provides a potential high-sensitivity alternative to access what would otherwise be low sensitivity or impossible to acquire 2D NMR correlation data. Given two coherence transfer experiments, A• B and A• C, it is possible to indirectly determine B• C coherence without ever performing the experiment. The application of unsymmetrical indirect covariance processing methods to generate GHSQC-COSY and GHSQC-NOESY data from more readily acquired GCOSY, NOESY, and ^{1}H-^{13}C GHSQC 2D NMR spectra will be shown. Further examples of the derivation of ^{13}C-^{15}N heteronuclear shift correlation data will also be shown, these data derived *via* the unsymmetrical indirect covariance coprocessing of ^{1}H-^{13}C GHSQC and ^{1}H-^{15}N GHMBC or IMPEACH spectra. Various indole alkaloids will be used to illustrate the application of the unsymmetrical indirect covariance processing technique. Finally, methods of 'forecasting' the location of potential artifacts in various types of spectra calculated using indirect covariance processing methods will also be discussed.

Please make your dinner reservations for the upcoming meeting by email at **sas.chicago@bigfoot.com**, by using the form on our web page < **http://www.sas-chicago.org/Online%20Registration%20at%20Wellington.htm**> or by calling Slav Stepanovich at **847-421-2056**. Leave **your name**, **company affiliation**, a **telephone number,** the **number of reservations** and **your choice of entree**. Please call by **noon Friday, November 9th**, so that proper arrangements can be made with the restaurant. If you can't attend, cancel by Friday noon: SAS is charged for no-shows.

Entree choices: London Broil with Bordelaise Sauce, Breast of Chicken with Teriyaki Sauce, or Vegetarian Fettuccine.

The dinner wine will be provided by Marty Marek of Varian Inc.

VARIAN

Dinner Cost Members: $25 **Students and Unemployed Members: $10** **Non-members: $30**

Biography of Gary Martin

Gary received a B.S. Pharmacy from the University of Pittsburgh in 1972 and a Ph.D. in 1975 from the University of Kentucky in the combined areas of solid-phase synthesis and NMR studies of reaction mechanisms. He was a Professor at the University of Houston from 1975-1989, leaving there to assume responsibility for NMR spectroscopy with Burroughs Wellcome, Co. in the US from 1989-1995. From 1996 through early 2006, he headed a group at Upjohn/Pharmacia/Pfizer responsible for the isolation and structural characterization of impurities and degradation products or pharmaceuticals. In March 2006, he joined Chemical & Physical Sciences at Schering-Ploughs, Summit, NJ facility where he continues to work on the characterization of impurities and degradation products of pharmaceuticals and the development of new NMR methods and applications.

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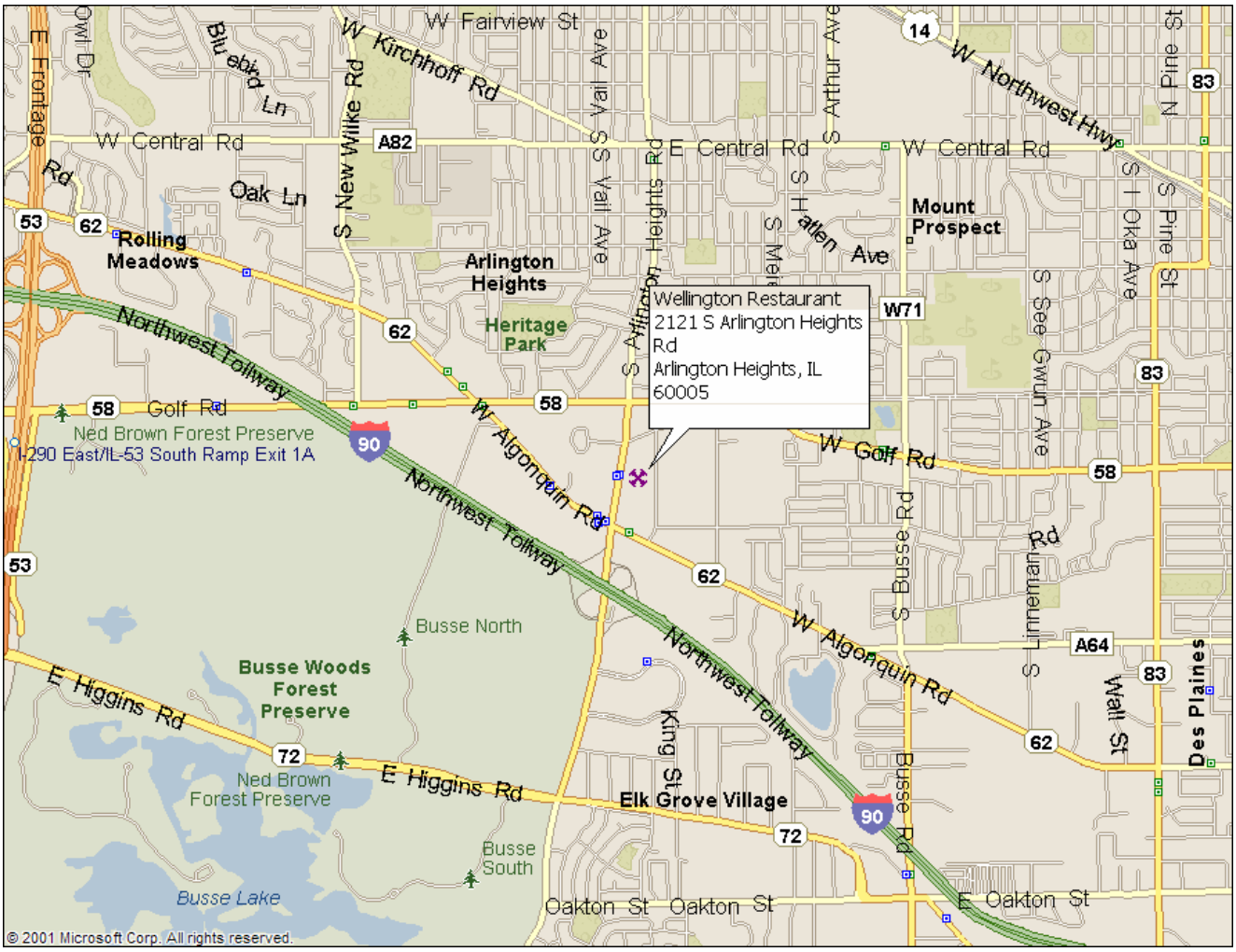
DIRECTIONS TO THE WELLINGTON RESTAURANT

From Chicago: Take Interstate 90 (Northwest Tollway) west to Arlington Heights Road exit. Proceed north to the restaurant.

From the southwest: Take 355 north to Route 53 north and exit at Algonquin Road east. Go to Arlington Heights Road. Turn left (north) and proceed to the restaurant.



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September Meeting Highlights

Wanda K. Hartmann, *Freelance Science Writer*

Professor Julie Jessop studies light activated polymerization reactions like the one that occurs when your tooth filling hardens with UV light at the dentist office. Dr. Jessop, a professor at the University of Iowa, spoke on October 9 for the Chicago SAS in Arlington Heights on her research on "Investigation of Inhibition Effects in Acrylate/Epoxide Hybrid Systems Using Raman Spectroscopy." The term hybrid refers to two types of reactions occurring in the same polymer matrix, cationic and free radical reactions. Her group studies the influence of oxygen and water during polymer formation, the presence of which is detrimental to polymerization. Using confocal microscopy and Raman spectroscopy at wavelengths away from fluorescence (785 nm), she examines chemical reactions at different depths of the polymer layers and unravels the processes going on. Interestingly, in the dark no free radical polymerization occurs, however the cationic reaction keeps going. One of many end goals of Jessop's current research is to determine why high moisture makes it more difficult for hybrid polymerization to occur, a process that is more complex to understand than oxygen inhibited polymerization.