



Spectroscopy Society of Pittsburgh September Meeting

Duquesne University – Mellon Hall of Science (Laura Falk Hall)

Wednesday – September 17, 2008

Technology Forum Speaker's Presentation **5:30PM**

Social Hour **6:00PM**

Dinner in the City View Café (6th Floor) **6:30PM**

Business Meeting **8:00PM**

Technical Program Speaker's Presentation **8:15PM**

Deadline for Dinner Reservations **9/12/08**

Carolyn Benga crbssp@yahoo.com or (412) 487-0915

TECHNOLOGY FORUM - 5:30 PM

Richard F. Rosenberger

"Long Rifles of Western PA"

Richard F. Rosenberger and Charles Kaufmann have written the definitive work on the guns and gunsmiths of Allegheny & Westmoreland counties, with an emphasis on the golden age of 1785-1815. Rick's discussion will present a brief history of the longrifle, aka Kentucky rifle, and introduction to its manufacture and use in western PA. The evolution of the American longrifle, from its European ancestry, is discussed, along with its importance on the frontier and settlers and their ability to survive in the wilderness. Rick has documented western PA as an important site in the longrifle development.



Bio

Born in 1938 and grew up in Scott Twp, when it was still a rural area, Rick found the area ideal, as a youngster, for small game hunting with the bow and arrow. His love of Geometry led to employment as a Designer in the Iron, steel and glass industry and hunting led to a lifelong interest in firearms and the outdoors.

Hunting adventures peaked, in 1968, with a honeymoon trip to India for a tiger hunt. Family responsibilities put an end to hunting trips, but his interest in guns and history combined into an attraction to antique rifles. While it was known that the American longrifle (aka Kentucky rifle) was made and used in Western PA, no one had documented this industry.

In the early 70's, Rich worked from home, as an independent contractor, which afforded flexibility in pursuing his interest in history and the longrifle. His efforts included research of census, tax, deed and newspaper records.

Fellow collector C. Kaufmann and Rick accumulated and studied sufficient data to prove that an original school of long rifle design had developed in the area. The University of Pittsburgh agreed with the importance of their study and in 1993 "Longrifles of Western PA: Allegheny and Westmoreland Counties" was published.

Rick is past president and was a board member of the Fort Pitt Museum Associates. He is also called upon to authenticate ancient artifacts. Retired now, and relocated to Butler Co, Rick keeps busy with volunteer work and his hobbies.



TECHNICAL PROGRAM - 8:15PM

Dr. Rina K. Dukor - BioTools, Inc.

"Application of FT-IR and Vibrational Circular Dichroism to Problems of Pharmaceutical Interest: from Proteins to Chiral Drugs"

Proteins play a vital role in the development of new biotechnology drugs and pharmaceuticals. New protein sequences and existing protein based products require rapid, cost-effective methods of characterization. Infrared spectroscopy, such as Fourier Transform Infrared (FT-IR) and vibrational circular dichroism (VCD) are ideally suited for this purpose. The main advantage of infrared techniques is that the protein sample can be studied in any state: liquid, solid, powder, fibrils or suspension. In the past decade, FT-IR and VCD techniques have been shown useful in applications such as developing formulations for stabilizing proteins, drug design, mutation studies, environmental effects and secondary structure prediction for membrane proteins and globular proteins.

The production of chiral pharmaceutical molecules that have known absolute configuration and enantiomeric excess is becoming increasingly important. In order to determine these properties in all types of chiral compounds, improved methods for the routine measurement of absolute configuration and enantiomeric excess are needed. In the past few years, vibrational circular dichroism (VCD) has become increasingly valuable in a variety of applications of pharmaceutical interest. In cases where chromatographic separation of enantiomers is difficult or too time-consuming, VCD can be used instead since the VCD spectrum scales proportionately in size with the percent enantiomeric excess. In cases where the absolute configuration of a chiral substance is needed, and where X-ray crystallography is either impractical due to problems with crystal growth or accessibility to needed instrumentation, VCD offers an alternative for solution-state measurements. Here, the results of VCD measurements can be compared to the results of ab initio calculations for an unambiguous determination of absolute configuration. In addition, VCD spectral measurements and ab initio calculations can be used together to determine solution-state conformation of chiral molecules that can be useful as a basis for molecular modeling studies.

In this presentation, we will discuss and demonstrate the sensitivity and advantages of FT-IR and VCD spectroscopy to protein structural studies and chiral molecule analysis.

Bio

Rina Dukor is the President of BioTools, a company she co-founded with Professor Laurence Nafie in 2000.

Rina received a Ph.D. in physical chemistry from the University of Illinois, Chicago in 1991. Her thesis explored Vibrational Circular Dichroism (VCD) of biological molecules. Upon graduation, Rina joined Amoco (currently Vysis, a subsidiary of Abbott) where she established a spectroscopy laboratory focused on proteins and nucleic acids. While in industry, she pioneered the introduction of aqueous infrared spectroscopy to the biopharmaceutical industry through the development of instrumentation, sampling techniques and software for protein secondary structure determination. Her methodology, commercialized as PROTA, is now used by over 60 of the leading biopharmaceutical companies. She has pioneered the development of reflection infrared micro-spectroscopy for cancer diagnostics. And by bringing VCD to the market, Rina helped cement the use of VCD by major pharmaceutical companies for the determination of absolute configuration of chiral pharmaceuticals which has truly become one of the most-talked about techniques for chiral analysis.

Rina has co-authored over 35 peer-reviewed papers; several review chapters and is a holder of four patents. Dr. Dukor is a recipient of the prestigious Williams-Wright Award that was presented at Pittcon 2008.

Dinner Reservations:

Please email Carolyn Benga at crbssp@yahoo.com or call (412) 487-0915 to make dinner reservations NO LATER THAN FRIDAY, September 12, 2008. This month's entrée will be Herb Crusted Roast Tenderloin Beef. Dinner will cost \$8 and checks can be made out to the SSP. If you have dietary restrictions, please let Carolyn know when you RSVP.

Parking Instructions:

The Duquesne University Parking Garage is located on Forbes Avenue. Upon entering the garage, receive parking ticket and drive to upper floors. Pick up a parking chit at the dinner or meeting. If any difficulties arise, contact Dr. Mitch Johnson at Duquesne University.