

CINTACS



Newsletter of the Cincinnati Section of the American Chemical Society December, 2002
Vol. 40, No. 4

Calendar

Wednesday, December 11 Dr. Harold Schueler
at Xavier University
with: **Analytical Discussion Group
Resume Preparation Workshop**

New online registration!

Thursday, Jan. 16, 2003 Dr. Steven D. Ittel
at P&G HCRC

Wednesday, February 12 Dr. Paul Lahti
at Vernon Manor

Wednesday, March 12 Cincinnati Chemist
at Givaudan

Wednesday, April 9 Mr. Frederick Wallace
at Northern Kentucky

Friday, May 16 Party Night!
Robert Mondavi

December Monthly Meeting

“Death: A Postmortem Toxicological Approach”

Dr. Harold Schueler

Chief Toxicologist
Broward County Medical
Examiner’s Office



Abstract

The most esoteric cause of death usually encountered by a Coroner or Medical Examiner involves the absence or presence of clinically significant toxic substances found within a deceased person’s body. A forensic toxicologist’s role is to assist the pathologist in determining the cause and manner of death using chemical and analytical methods to detect and quantify these toxic

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About the Speaker

Dr. Schueler is currently the Chief Toxicologist with the Broward County Medical Examiner’s Office in Fort Lauderdale, Florida where he supervises a forensic toxicology laboratory that conducts analyses on Medical Examiner, law enforcement, drug court and drug rehabilitation cases. He has testified as an expert witness in numerous court cases involving postmortem toxicology in death investigations and antemortem toxicology in driving under the influence (DUI) traffic investigations. He has authored several peer-reviewed journal articles and lectured many times to law enforcement, attorneys, laboratory and medical professionals, and

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THE CINTACS NEWSLETTER**Vol. 40, No. 4 December, 2002**

Editor.....Bruce S. Ault
 Advertising.....Ed Hunter

CINTACS is published nine times a year (September through May) by the Cincinnati Section of the American Chemical Society. The submission deadline will be approximately December 19 for the February, 2003 issue. Electronic submission is strongly preferred, except for original photos. All materials should be sent to:

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from the Chair

If you have not looked at the Section's web site recently, I strongly urge you to do so. In the past, I have mentioned the new pictures, the up-dated list of officers and committee chairs, and a few other changes. Kim now has the meeting-registration-form up and working on the web. A few of you already have used on-line registration for the Oesper banquet. I strongly urge all of you to use this method of registering for the December meeting. Even if you type as slowly as I do, it takes only about a minute and you get a confirmation that your registration has been received. If you have any problems, please let me know and I will pass them on to Kim.

The December meeting, which will be at Xavier University, is sponsored by Bob Laughlin. Bob has been a long time member of the Cincinnati Section and a past Chemist of the Year Award winner. This is the second year in a row in which Bob has sponsored a meeting. On behalf of the Cincinnati Section, I would like to thank Bob very much for his generosity. In addition, I would like to thank Dan McLoughlin for taking care of all the arrangements for this meeting. All I have to do is show-up. The after-dinner speaker will be Harold Schueler, who obtained his Ph.D. from UC about a decade ago. Harold is now Chief Toxicologist for the Broward County Florida Medical Examiner's Office. He will discuss a number of case studies. (This is not quite "CSI-Miami", but it is close.) In addition, at the December meeting there will be an analytical discussion group and a resume preparation workshop.

In this statement, I would like to say something about the

(Continued on page 5)

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**December Monthly Meeting
December 11, 2002
Conaton Board Room, Room 201 Schmidt Hall
Xavier University**

Sponsored by Dr. Robert Laughlin

Featured Speaker

Dr. Harold Schueler, Chief Toxicologist
Broward County Medical Examiner's Office

Program

- 5:30 – 6:30 Board Meeting, Schmidt Hall, President's Conference Room,
Mary Virginia Sullivan Room, Room 204
Analytical Discussion Group – Albers Hall, Room 107—see page 5 for details
Resume Preparation Workshop – Linder Hall, Room 101—see page 6 for details
- 5:30 – 7:00 Registration, Conaton Board Room, 2nd Floor, Schmidt Hall
- 6:00 – 7:00 Social (Cash Bar), Conaton Board Room
- 7:00 – 8:00 Dinner, Conaton Board Room (\$20.00, half price for students, emeritus,
unemployed and new members)

Dinner Menu

Pan Seared Chicken Breast with Hunter Sauce
Garden Greens Salad with Italian Vinaigrette
Wild Rice Pilaf

(Continued on page 4)

**Reservation Information, Directions and Parking Pass
follow on Page 4**

Please cut out parking pass and display on passenger
side of dashboard

(Continued from page 3)

Fresh Seasonal Vegetable Medley
Fresh Baked Bread
Chocolate Mousse with Raspberry Sauce, Whipped Cream and Chocolate Shavings
Coffee, Tea.

Vegetarian Entrée Available upon Request when making reservations

8:00 – 9:00 Dr. Harold Schueler
“*Death: A Postmortem Toxicological Approach*”

Reservations: New! A meeting reservation form is now online at: <http://www.che.uc.edu/acs/cinacs.html>. This is the best and easiest way to register. As a lesser alternative, you may send your reservations to Kim.Carey@uc.edu <Kim.Carey@uc.edu>. If absolutely impossible to make reservations via the internet, telephone 513-556-0293. Deadline for reservations is Friday, December 6, 2002. Include your name, affiliation, and state if you're in one of the 1/2 price categories. As a reminder, if you decide you must miss a meeting after you have made reservations, please call to cancel. If you do not cancel, the Section will have to charge you because it will have been charged by the University.

Directions:

The Xavier University Conaton Presidential Board Room is located on the second floor of Schmidt Hall. Parking is provided free **with the enclosed Parking Pass (see below)** at the F&W Center on Dana Avenue across the street from Schmidt Hall.

I-71: Exit at Dana Avenue exit. Proceed west on Dana Avenue past Ledgewood Drive. As the road begins a slight turn, the F&W parking area will be on the left before you reach Victory Parkway.

I-75: Exit at Mitchell Avenue. Proceed east on Mitchell Avenue, crossing over Reading Road. Continue to Dana Avenue and turn left. Just after crossing Victory Parkway, the entrance to F&W parking area will be on the right.

Rt. 562: Exit the Norwood Lateral at Reading Road. Continue in the left lane of Reading Road to Victory Parkway. Merge left onto Victory Parkway at the light. Continue to Dana Avenue. Turn left onto Dana Avenue. The entrance to F&W parking area will be on the right in about half a block.

Cut here

XAVIER UNIVERSITY
Conaton Presidential Board Room
Second floor Schmidt Hall

Temporary Reserved Parking Permit

Valid for American Chemical Society Meeting
F&W PARKING AREA
December 11, 2002

CARD MUST BE DISPLAYED ON PASSENGER SIDE OF DASHBOARD

(Continued from page 1)

substances. The breadth of analytes tested for include drugs of abuse, alcohol, poisons, prescription medications, inhalants, pesticides and many other readily available chemicals. These toxic substances can be isolated from complex biological matrices, for example blood, urine, liver, brain, vitreous and bile using an arsenal of solid phase and liquid-liquid extraction procedures. The final extracts from these procedures can be analyzed by GC, GC/MS, HPLC and UV/Vis to determine the identities and concentrations of toxic substances within the postmortem specimens.

The interpretation of postmortem toxicology findings is often as difficult as the actual analyses, particularly when establishing the cause and manner of death. Evaluating drug concentrations requires consideration of many pharmacological parameters, including the volume of distribution, half-life and drug interactions, as well as other factors such as post-mortem mechanisms and the specimen origin and integrity. References to actual Medical Examiner cases will also be presented.

(Continued from page 1)

civic groups regarding various aspects of forensic toxicology.

Previously, Dr. Schueler earned his B.A. in Chemistry from Kenyon College and his M.S. and Ph.D. in Biochemistry from the University of Cincinnati. After graduate school, he became a toxicologist and subsequently the Chief of Toxicology at the Hamilton County Coroner's Office in Cincinnati, Ohio. He holds active membership in the Society of Forensic Toxicologists (SOFT) and the American Chemical Society (ACS).

(Continued from page 2)

Oesper Banquet/Symposium and about National Chemistry Week, but due to the lead-time required for Cintacs, at the time of this writing, those events have not been held. Thus, in the January Cintacs, I will have some information for you. The January meeting will be held at P&G HCRC. The speaker will be Steve Ittel from duPont, who was an undergraduate student at Miami University.

Analytical Discussion Group

Dr. Heather Allen, Assistant Professor Chemistry
The Ohio State University

"From surface structure of solutions and particles to nonlinear optics: Application to analytical chemistry and the atmosphere"

Abstract

To understand the molecular-level chemistry at an interface, state-of-the-art nonlinear optical technologies that utilize ultra-fast femto and picosecond laser pulses are necessary. Thus, surface vibrational sum frequency generation (SFG) spectroscopy, broadband and scanning technologies, are used to elucidate interfacial chemistry. SFG is inherently surface-selective in the dipole-approximation and provides molecular-level surface information that includes relative orientation and structure of the surface species, i.e. the surface signature. In addition, an array of analytical tools is incorporated to fully understand the heterogeneous chemical processes at an environmental interface (e.g. mass spectrometry, GC, microscopy and Raman Spectroscopy). Examples of a few chemical systems that we are investigating include: the surface orientation of straight chain and poly-aromatic hydrocarbons, in addition to simple alcohols. These chemical systems are important to the understanding of aerosol growth and chemistry in urban regions. We are studying supercooled liquids, ice, and clathrate formation.

About the Speaker

Professor Allen received her B.S. degree in Chemistry (1993) and Ph.D. in Physical Chemistry (1997) at University of California Irvine. Her undergraduate advisor was Professor F. S. Rowland (1995 Nobel Laureate), and her graduate advisor and co-advisor were Professors J. C. Hemminger and B. J. Finlayson-Pitts, respectively. She received several fellowships, Fannie and John Hertz, EPA, and NSF Traineeship fellowships. Dr. Allen worked as a NOAA Post-Doctoral Fellow in Climate and Global Change, which was awarded for her proposal based upon the use of nonlinear spectroscopy to study surfaces relevant to aerosol chemistry. Dr. Allen was awarded the Research Innovation Award from Research Corp. in 2001, OSU-OMA Distinguished Professional Mentor Award in 2001, and an NSF CAREER Award in 2002.

Resume Preparation Workshop

New to the work force? Getting ready for a career change? Haven't updated your resume since the Nixon administration? Then you should attend the discussion group sponsored by the Career Services Committee! In these days the definition of job security is the ability to find a new job. The first step in finding a rewarding position is an effective resume. Richard Cordero from Aerotek Scientific will make a presentation on writing a winning resume at the *December meeting*. After his presentation, there will be plenty of time for discussion with a question and answer period. So come on out and learn how to put some polish on your resume.

Industrial/Individual Section Meeting Sponsorship

We now have one individual and two industrial sponsors for our 2002-2003 meeting's schedule. Recall this sponsorship entails a \$1000 commitment to cover speaker, meeting, and ancillary expenses.

This is a relatively inexpensive way to show support for your Section and its programs. It's good for the Section, the individual, the company, and for Chemistry in general.

Please consider this opportunity and call me with questions or sign-up. We need 2-3 more sponsors.

Ted J. Logan, Chair, Solicitations Committee,
and Councilor
Tel.: 513-385-8856
E-mail: TJLOGANCIN@AOL.COM

Chemical Information Update: Searching the Web

Edlyn Simmons

Chair, Chemical Information Discussion Group

My friend Bob, a very bright guy, complained that he wasn't able to read his professional society's newsletter online. His browser never found the right URL when he keyed the society's name into the search box in his browser. What was he doing wrong?

Bob was making the common mistake of assuming that web search engines actually search the World Wide Web. They don't, or at least they don't do it directly. The search engine on your browser searches a database that contains information about websites that's been collected by a software tool called a "web crawler." There are lots of web search engines, and each one has its own rules for collecting websites and its own rules for indexing the information on the websites and displaying results when a search is requested.

Some engines search for new or changed websites frequently, while others do not. Some search engines index only the information provided as metadata or only the text of the home page, while others index the text of some following pages. Not all websites are indexed. Web crawlers can be discouraged from indexing a website by adding a "don't index" flag to the metadata, and web crawlers normally don't access and index web pages protected by a password. Most search engines offer an opportunity to have a URL displayed early in the list of search results or to have your site's indexing refreshed more often by paying a fee.

If you use Internet Explorer, clicking on the Search button or entering keywords into the Address box at the top of the screen brings up MSN Search, the Microsoft web search engine. If you use Netscape, keywords entered into the Netsite box are searched using Google. If you click on Netscape's Search button, you're given a choice of five search engines, Net-

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National Chemistry Week 2002

This article was written on Mole Day (celebrated at 6:02, 10/23), marking the midpoint for NCW 2002. Over 125 volunteers from P&G, Cincinnati Specialties LLC, HG Consulting, Cognis Corporation, Bayer Corporation, Girindus, Waytek Corporation, Wright Patterson's Air Force Research Laboratory, The Cincinnati Museum Center, The Public Library of Cincinnati and Hamilton County, Xavier University, College of Mount St. Joseph, Miami University, University of Cincinnati, Northern Kentucky University, Wilmington College, Summit Country Day High School, Seven Hills High School, and Oak Hills High School provided NCW programs for over 40 local library branches, schools, colleges, and the Cincinnati Museum Center.

The Cincinnati Museum Center hosted the National Chemistry Week 2002 kickoff on October 20th. Dr. Barbara J. Slatt, Procter and Gamble's Manager of Corporate Research and Development and External Relations, read the proclamation from the city declaring the week officially NCW in Cincinnati, cut the NCW ribbon, and shared P&G's role in how "Chemistry Keeps Us Clean" started with candles.

Milli Mole (Dr. Susan Hershberger, Miami University) worked the crowd the entire afternoon, getting into photos and passing out balloons, coloring pages, and temporary tattoos to over 500 happy kids. Several NCW volunteers came decked out in their NCW t-shirts, including students from Oak Hills High School, Wilmington College, and the University of Cincinnati. Six Boy Scouts from Ft. Hamilton district's Troop 956 volunteered as gophers and "barkers" (announcing in the rotunda and all 3 museums that the demos were about to begin). Four 30-minute chemistry demonstrations in the Cincinnati Museum Center's Newsreel Theater, led by P&G's Ed VonBargen, capped off the day.



Wilmington College student Dan Tener and Ed VonBargen share the magic of chemistry, 10/20/2002.

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scape (i.e., Google), Ask Jeeves, LookSmart, Lycos and Overture. The same search terms will give different results with the six search engines.

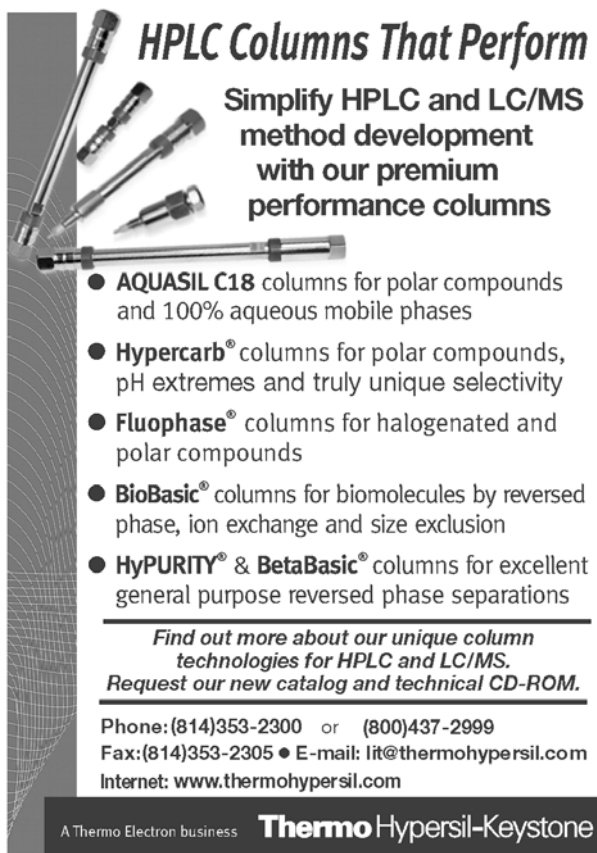
A search for "American Chemical Society", for example, brings up Chemistry.org as the first of 983000 answers when searched in the Netscape default Google engine. (My friend Bob obviously isn't a chemist). Adding Cincinnati to your search brings up the Cincinnati section as the first of 27900 websites.

In Ask Jeeves, Chemistry.org is the first website listed for "American Chemical Society," but when you add Cincinnati to the search, the Cincinnati Section URL is preceded by a box offering travel reservations through Expedia and another box recommending the Cincinnati Bell Yellow Pages, as a "sponsored result." The second real answer to the search is the 1997-8 Section committee chair listing from an archive site. Ask Jeeves offers some additional (and irrelevant) suggestions for additional searches, including one for the Cincinnati riots.

LookSmart's "American Chemical Society" search results begin with a list of sponsored listings that begins with "Sleepless Society – Select Comfort." Following that list, Chemistry.org is the first of only 76 answers. When Cincinnati is added to the search, the first of 68 answers is the site of the Tri-State German American Society School of Cincinnati. The Cincinnati Section doesn't show up until you reach a third list of answers, identified as the first of 1000 sites identified by Inktomi, a partner of LookSmart.

The Lycos search for "American Chemical Society" shows Chemistry.org as the first of 2,789,993, answers. Adding Cincinnati brings up the Cincinnati Section in second place behind a page from the ACS Division of Chemical Health and Safety that announces Diane Schmidt's election to the ACS Board. Overture showed those sites at the top of its list, but the following listings were a lot different from those selected by the other engines.

In Internet Explorer, MSN Search shows Chemistry.org as a "featured site" when you search for "American Chemical Society". The search for "American Chemical Society and Cincinnati" brought up the Cincinnati Section homepage first,



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the CHAS announcement of Diane's election to the Board second, and a meeting announcement for the Cincinnati Section's October, 1998, meeting third.

The ACS wants people to find it on the web – it has carefully indexed its homepage so it can be found. The Cincinnati Section has also done a good job of making our webpage accessible. But searches for other website aren't likely to be so efficient. Even if a site is retrieved, it might be buried in a list of 2 million websites!

The solution to Bob's problem is simple: don't search. If you know the URL of the site you want to access, enter it directly. Try guessing the URL of the site you want, e.g., www.acs.org brings up the Chemistry.org homepage. For a specialized topic, do your search at a directory website; e.g., the Virtual Library site at www.vlib.org. Most important, once you find a site you like, add it to your bookmarks or favorites list.

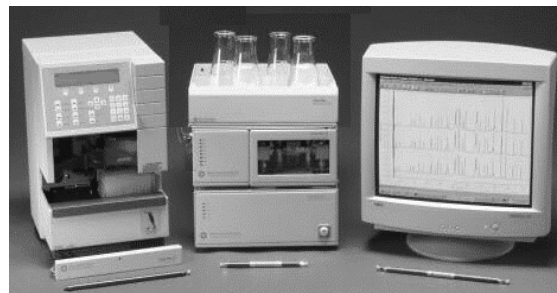


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Everyone who came that day had to opportunity to register to win two gift baskets of goodies from The American Chemical Society and The Procter and Gamble Company (to be raffled off at the last Cincinnati Museum Center demo of NCW, Oct. 26, 2002). MediaBridges taped the kickoff event and will play it on a Cincinnati local access cable channel in the near future.

Kathleen Gibboney and Gloria Story organized a donation of \$8,000 from P&G, matched by the National ACS, to fund NCW activities, especially the Cincinnati Enquirer's "Newspapers In Education" program. Check out the content on the NIE website, <http://cincinnati.com/nie/chemistry/>. Publicity for NCW was spread throughout the area by the Enquirer, local access cable, the Hamilton County libraries website and flyers, the Cincinnati Museum Center's Museum of Natural History and Science website and Mosaic magazine, and the local ACS section's website

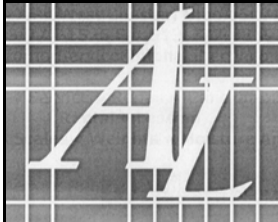
and flyers produced by Gwen Baumann, the local section's media relations chair. Richard Sunberg (head honcho of the local section's NCW elementary school contest) organized this year's "Chemistry Keeps Us Clean" poster contest for grades K-12. Winners will be invited to receive their awards in a future section meeting. Our website summarizes all the section's NCW activities, <http://www.che.uc.edu/acs/ncw/ncw02.html>.

Thanks to P&G's Pharmaceutical, Analytical, and Organic Chemistry groups, Cascade, Bounty, Dawn, and PuR brands for donating cash, products, packages, and dry ice for this year's demonstrations. Thanks to VWR's Linda Tobeson for her efforts in providing demo items from VWR, Corning, Rubbermaid, and Nalgene for this year's demonstrations.



Mike Hardy and crew helped Dr. Slatt share a few fun experiments during the opening celebration, 10/20/2002




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