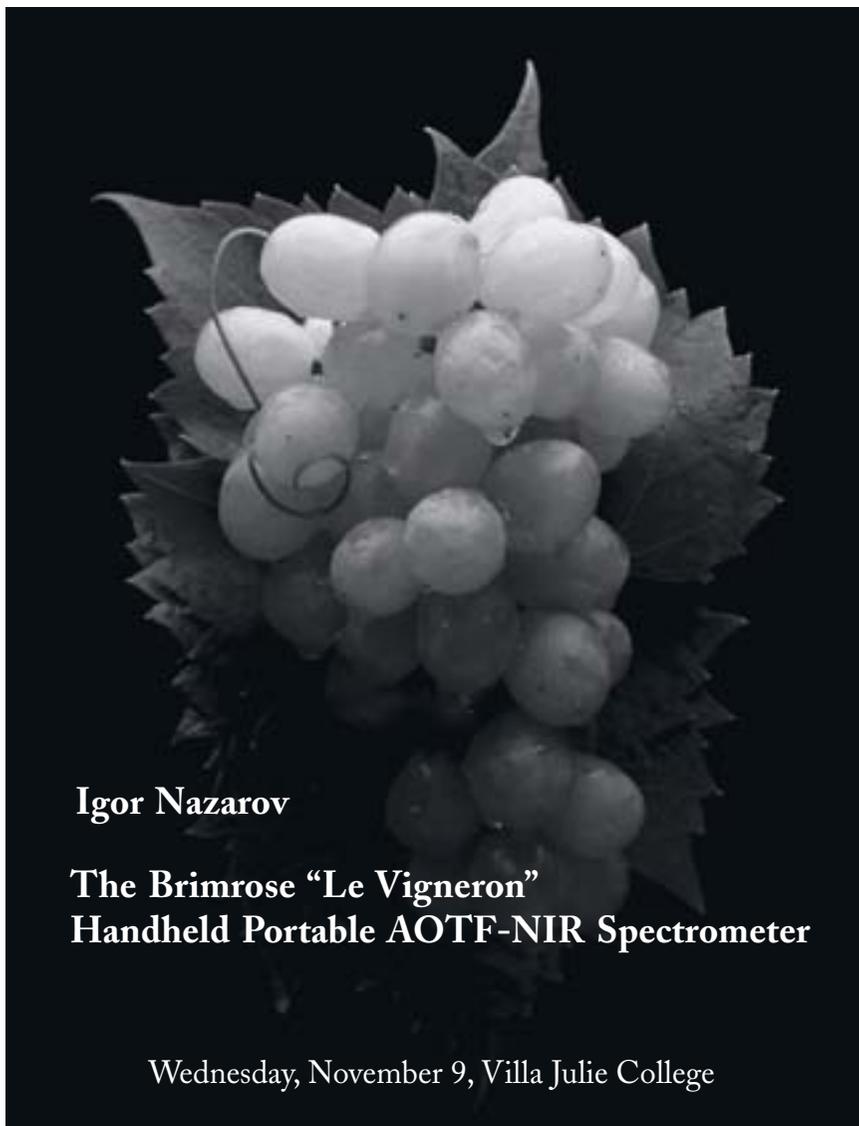


Chesapeake Chemist

*Maryland Section
American Chemical
Society*



Igor Nazarov

**The Brimrose “Le Vigneron”
Handheld Portable AOTF-NIR Spectrometer**

Wednesday, November 9, Villa Julie College

Powerful substance search enhancements launched by SciFinder

SciFinder 2006 marks decade of innovation by launching powerful substance search enhancements

Building upon a decade of innovation, the new SciFinder 2006 advances SciFinder's reputation as an essential information tool and "part of the process" of chemical and pharmaceutical research. For the first time, scientists exploring the CAS Registry of 26 million organic and inorganic chemical substances can retrieve "similar substances" to foster new ideas and directions in drug discovery and other fields of scientific inquiry. "Similarity Searching" is only one of several new features adding new power and depth to SciFinder this year. CAS launched SciFinder 2006 and SciFinder Scholar 2006 at the ACS National Meeting in Washington, D.C. in August.

In honor of SciFinder's tenth year, Nobel Laureate, Dr. K. Barry Sharpless, W. M. Keck Professor of Chemistry at the Scripps Research Institute, shared his reflections regarding the significance of this research tool:

"We were using SciFinder at Scripps even before SciFinder Scholar was invented," said Dr. Sharpless. "I am a big user and don't see how any researcher could hope to excel without daily, round-the-clock access. In the old days, you could be forgiven for not knowing about a certain paper, but now there is no excuse. The speed and scope of its search power is amazing, and the answer to 'what aspect is most helpful for you?' could be as diverse as the users. In my case, SciFinder enhances my reactivity insights, making it easier to 'see' those ill-defined boundaries where important new phenomena are lurking."

New features of SciFinder 2006 include a number of enhancements for substance information, as well as ease-of-use improvements:

- Similarity Searching – as a complement to SciFinder substructure searching, similarity searching permits new options for identifying substances of interest via precise statistical analysis using the Tanimoto algorithm;
- Structure Query Tools – to identify substances more precisely, new tools permit drawing a variable attachment point and a repeating group;
- Reaction Searching – finding reaction information has been enriched with new content and features; these include reaction conditions and identifying intermediate reactions in a multi-step reaction. Scientists also can click any substance in the reaction display to find additional information, including retro-synthetic pathways;
- Navigation & Usability – improvements include duplicate detection and removal for more efficient combined searching of the CAplusSM and MEDLINE® databases. A new Locate feature permits quick access to journal

Continued on page 5

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Chair: Alan C. Samuels, 410-436-5874
alan.samuels@sbccom.apgea.army.mil

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410-306-0679
skyoung@arl.army.mil

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301-975-6448
stephanie.watson@nist.gov

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lryzhkov@towson.edu

Treasurer: Angela Sherman, 410-532-5713
CND of MD
4701 North Charles Street
Baltimore, MD 21210
asherman@ndm.edu

Councilors

Merle I. Eiss 410-484-0521 meiss32@aol.com	Donald Jones 202-364-2740 djones@erols.com
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David Roswell 410-617-2458 droswell@loyola.edu	Charles Rowell 410-647-9452 rowell@toad.net
--	---

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gfarrant@ccbcmd.edu

Remsen Award (May/June): Lev Ryzhkov

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Maryland Chemist Award (December):
Shekhar Munavalli, 410-436-2819
Shekar.munavalli@sbccom.apgea.army.mil

Maryland Service Award:
Shree Iyengar, 410-541-2266

Maryland Section on the Web: <http://mdchem.org>

Webmaster: Sandy Young
(chemists4fun@yahoo.com)
Paul Smith, pjsmith@umbc.edu

Programs

Archives: Ernie Silversmith, 443-885-3214

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Earth Day: Paul Smith & Sandy Young

Environmental Issues:
Shirish Shah, 410-704-2720
sshah@towson.edu
Sandy Young

Finance Committee:
Jan Kolakowski,
410-436-2755, jan.kolakowski@us.army.mil

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Shirish Shah & Robert von Tersch

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Alfred Amah, 410-602-7164,
f-amah@mail.vjc.edu

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Shirish Shah & Walter Roy,
Walter_Roy@mccormick.com

Retired Chemists: Alvin Bober, 410-581-5321

Women Chemists/Younger Chemists:
Sara Narayan, 410-602-7326
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Chemistry Olympiad/Chem-a-Thon:
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Mike_Zapf@mccormick.com

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Kids & Chemistry/Chemistry-in-the-Library:
Sue Procell, 410-436-4604,
suzanne.procell@us.army.mil
Sandy Young

National Chemistry Week (NCW):
Shirish Shah & Sandy Young

Chesapeake Chemist Editor: cakvt@hotmail.com

Cindy Kronman
734 Benfield Road
Severna Park, MD 21146

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November Dinner Meeting

Wednesday, November 9, 2005, Villa Julie College

4:45-5:30 pm	Chemistry Magic Show, Knott Hall, Room 23
6:00-6:45 pm	Registration and Networking, Glass Pavilion
7:00-7:45 pm	Dinner
8:00-8:50 pm	Igor Nazarov, "The Brimrose "Le Vigneron" Handheld Portable AOTF-NIR Spectrometer "

Cost for the dinner is \$20.00 for members; \$15.00 for spouses, retired chemists and guests, and \$10.00 for students. For reservations please contact Shirish Shah at 410-323-0803(H) or by email at dr.shah@juno.com.

Directions to Villa Julie College: From the beltway (695), take Falls Road north. At the light (approximately a mile), turn left on to Green Spring Valley Road. Cross the Green Spring Avenue intersection. From there, the college is approximately 2 miles on the left side. The gate for Villa Julie College is soon after the Sisters of Notre Dame Community gate. There will be signs for parking.

The Brimrose "Le Vigneron" Handheld Portable AOTF-NIR Spectrometer

The Brimrose Corporation of Baltimore, Maryland, has developed a portable handheld solid-state spectrometer with no moving parts for use in the wine industry. The unit, dubbed *Le Vigneron* is based on AOTF-NIR (acousto-optic tunable filter, near-infrared) technology, backed up by powerful chemometrics-based statistical analysis. Rather than performing chemical analysis of grapes, it compares the spectrum of a sample with a mathematical model of pre-calibrated spectra from the same materials, in this case grapes.

Brimrose has initially focused on developing applications for monitoring ripening grapes in the vineyard. The unit uses NIR spectroscopy and statistical analysis to predict brix, pH and total acidity (TA) in individual berries. The unit, which is battery powered, contains an on-board computer with wireless Ethernet capability. When the user is sampling a vineyard block, all data are automatically downloaded and stored on a remote laptop or a desktop computer. It then computes the resulting averages and reports them numerically and graphically.



Le Vigneron's system combines physics and statistical analysis to perform its function. The first step in creating the applications was to acquire a database of the spectra of ripening grapes and known values for their brix, pH and TA. This database is the foundation of the statistical model that drives the predictions. As the model acquires more and more data points from the field, it will become more and more robust.

Based on the experience of NIR technology in wine and related fields, Brimrose developed further applications for *Le Vignerone*. In the vineyard, leaf study looks to be a promising area for research. Viticulturists familiar with *Le Vignerone* have suggested scanning growing leaves, in place on the vine, for moisture content, as an indicator of water use or drought stress in the vine. Other attributes, such as nutrient utilization and photosynthetic activity, may also be measured this way.

Brimrose has created a separate probe for work in the cellar. This stainless steel “transflectance” probe is used for measurements of aging wine. Brimrose is actively requesting wineries to share samples that are being sent out for laboratory analysis along with their results so that a database can be built to support these important applications. *Le Vignerone* is used in the cellar to monitor aging wine on a barrel by barrel basis, obtaining results on the spot in real time. The successful development of cellar applications offers substantial cost-benefit rewards.

About the speaker. Igor Nazarov has a master’s degree in system, electronics engineering from the National Aviation University in Kiev, Ukraine. He has been working at the Brimrose Corporation for more than 12 years in the Near Infra-red Division as a system designer, application engineer, and division manager. Mr. Nazarov was involved in the design of AOTF-NIR Analyzers, a system including electronics, optics, software, and applications. For the last few years, he has managed the NIR Spectrometer Division, including sales, marketing, applications, and support. He is personally involved in the management of various projects, providing near infrared solutions for different industries, including pharmaceutical, chemical, and agricultural.

SciFinder 2006 continued

and patent documents by entering journal titles, author names and other partial bibliographic information.

While announcing the release of SciFinder 2006 for Windows, CAS revealed that a native MAC OS X version of SciFinder will appear in fourth quarter 2005.

SciFinder was created in 1995 to provide scientists easy, point-and-click access to chemical information. The new intelligent research tool – a client-server product for the desktop – was an immediate hit with chemists, assisting them and other researchers worldwide with access to the multidisciplinary CAS databases. More information about SciFinder 2006 can be found on the web at <http://www.cas.org/SCIFINDER/scicover2.html>.

Upcoming meetings and events:

Wednesday, December 7, Maryland Chemist Award, Berkshire Marriott Conference Hotel, Towson

November Historical Events in Chemistry

by Leopold May, The Catholic University of America, Washington, D.C.

- November 3, 1921 American Association of Textile Chemists and Colorists was founded.
- November 7, 1878 Lise Meitner, who explained nuclear fission and discovered protactinium in 1917, was born on this day.
- November 11, 1925 Discovery of cosmic rays was announced in Madison, WI.
- November 13, 1867 Kristian Birkleland and S. Eyde performed the first industrial fixation of nitrogen. KB was born on this date.
- November 15, 1280 St. Albertus Magnus discovered arsenic in 1250 and was the first to use affinity in the sense of chemical reactions. He died on this date.
- November 18, 1906 George Wald, who did research in the field of chemistry of vision, was born on this date. In 1967, he shared the Nobel Prize in Medicine with Ragner Granit and Haldan Keffer for their discoveries concerning the primary physiological and chemical visual processes in the eye.
- November 20, 1873 William W. Coblentz, who was born on this date, was a pioneer in infrared spectroscopy. He founded the radiometry section of National Bureau of Standards now NIST, and headed the section for 40 years.
- November 21, 1824 Hieronymus T. Richter, who co-discovered indium with Ferdinand Reich in 1863, was born on this date.
- November 24, 1833 This is the birthday of Alexandre P. Borodin, a chemist-composer, who was a researcher on organofluorine compounds and the Borodin-Hunsdieker reaction and a composer of classical music. (Some celebrate his birthday on November 12.)*
- November 26, 1817 Birthdate of C. Adolphe Wurtz, who discovered the method of synthesis of hydrocarbons (Wurtz Reaction) in 1855. He also isolated methyl and ethylamines in 1849, phosphorous oxychloride in 1846, and glycol in 1856.
- November 27, 1903 Lars Onsager, a researcher in thermodynamics of irreversible reactions, received the Nobel Prize (1968) for the discovery of the reciprocal relations bearing his name, which are fundamental for the thermodynamics of irreversible processes.

Continued next page

Advancing diversity in the chemical sciences

The American Chemical Society Committee on Minority Affairs is pleased to announce a Call for Nominations for the Stanley C. Israel Regional Award For Advancing Diversity in the Chemical Sciences

The American Chemical Society Committee on Minority Affairs is pleased to announce a Call for Nominations for the Stanley C. Israel Regional Award For Advancing Diversity in the Chemical Sciences

Purpose: To recognize individuals and/or institutions that have advanced diversity in the chemical sciences and significantly stimulated or fostered activities that promote inclusiveness within the region.

Nature: The award consists of a medal and a \$1,000 grant to support and further the activities for which the award was made. The award also will include funding to cover the recipient's travel expenses to the ACS regional meeting at which the award will be presented.

Rules of Eligibility: Individuals nominated for the award may come from any professional setting: academia, industry, government, or other independent facility. Nominees may also be organizations, including ACS local sections and divisions. The awardees will have increased the participation and leadership of persons from diverse or underrepresented minority group(s), persons with disabilities, or women.

To Nominate: For nomination of individuals, a letter of nomination of no more than three pages and a CV or resume is required. For institutions or corporations, a brief description of the institution or organization must be included. Nominations may also include up to two supporting letters of no more than three pages and up to five different samples of program materials.

Send nominations to:

Committee on Minority Affairs
American Chemical Society
1155 16th Street NW
Washington, DC 20036

For information regarding the award, contact Stephanie Allen, 800/227-5558 ext. 6262, or e-mail: s_allen@acs.org.

Deadline for receipt of nominations is January 13, 2006

November 29, 1849 Georg E. E. Wagner was born on this date. He was a researcher in terpene chemistry, permanganate hydroxylation of alkenes, and Wagner-Meerwein rearrangements.

November 30, 1901 On this date, Monsanto Chemical Co. was organized.

*A symposium on chemist-composers will be held at the next ACS National Meeting in Atlanta in March 26-30, 2006.

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ACS Leadership Conference - Baltimore, Md.

If you are a new ACS leader—whether leading a local section, a division, or a national committee; running a regional meeting; serving as a career consultant; or emerging as a leader as a younger chemist—plan to attend the ACS Leaders Conference scheduled for January 27 – 29, 2006, at the Baltimore, MD, Marriott Waterfront Hotel. Learn how to plan, organize, and inspire your constituency and how to make a difference for the Society and the profession of chemistry! Get further information by calling ACS at (800) 227-5558 and requesting to speak with the office working with the group with which you are affiliated: Local Sections, ext. 6149; Technical Division Advancement, ext. 4064; national committees, ext. 6070; regional meetings, ext. 6264; career consultants, ext. 6076; and younger chemists, ext. 6243.



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