

Conference Call

Chemistry for Agriculture

by Adam Pawelczyk

The XXXI International Conference on "Chemistry for Agriculture" was held 6–9 December 2005 at the famous health resort called Priessnitz, located in Jeseník, Czech Republic. Since 1999, the conference has been held in this scenic spot in the Sudetan Mountains that straddle the Polish-Czech border.

The conference was attended by 197 participants from who presented 141 posters and gave a number of lectures. Attendees included chemists, fertilizer specialists, environmental protection specialists, and representatives of scientific institutions, industry, veterinary medicine, agriculture, and local government.

The main topics of oral and poster presentations were as follows:

- technology of mineral fertilizers, feed phosphates, and other additives
- agricultural chemistry—how fertilizer nutrients and pesticides change in the environment, nutrient availability
- phosphorus and nitrogen problems in the environment
- ecotoxicology
- development in the production of chemical agents for agriculture
- new methods for applying agricultural chemicals
- impact of chemical products on plant and animal production
- harmful substances in agriculture and the environment

The conference was inaugurated by Zbigniew Dobrzanski from Wroclaw University of Agriculture who

recalled the long history of meetings of specialists of various disciplines and discussed the current state of science and agriculture in Poland. The scientific program of the introductory session included the following lectures:

- Henryk Górecki, "New Chances for Financing Scientific Research from Public Means"
- Pawel Kafarski, "On the Borderline of Biology and Chemistry—Four Stories with a Moral"
- Hennie van de Coevering, Barbara Kozłowska, "Life Cycle Analysis (LCA), a Sustainable Perspective from Cradle to Grave. An Example from Agriculture: Maize Corn Production"
- Adam Pawelczyk, "Organic Waste—EU Legislative Constraints and Future Prospects"

In his lecture, Górecki discussed new opportunities and prospects for government funding of scientific research. He encouraged scientists to put more effort into gaining grants from state entities and preparing new applications for financial support.

Kafarski presented a very interesting lecture on the frontiers of biology and chemistry in which he used four examples based on old myths and legends: He connected Santa Claus with Amanita mushrooms, showed why druids from Galia were considered dangerous by Romans, rationalized vampires from a chemical point of view, and showed how it is possible to create zombies.

Van de Coevering and Kozłowska delivered a joint lecture about life cycle analysis of products and their impact on the environment. The analysis/assessment includes the entire life cycle of the product, process, or activity, encompassing extraction and processing of raw materials, manufacturing, transportation, distribution, use, maintenance, recycling, and final disposal.

Pawelczyk focused his lecture on the recycling of nutrients from organic waste for use in agriculture. He pointed out the legislative and economical ways of promoting organic waste recycling that have been developed and implemented in Europe during the last 30 years.

For the past two years, "Chemistry for Agriculture" has been sponsored by IUPAC. In 2005, the conference



The XXXIst Conference was inaugurated by Prof. Z. Dobrzanski (Poland).



A discussion during a poster session.

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Prof. Hennie van de Coevering (Netherlands) addresses the audience.

was organized by the AGROPHOS Scientific Research Center of Chemistry, Agrochemistry, and Environment Protection, Wrocław, Poland, and the Czech-Pol-Trade Company, Jeseník, Czech Republic, on behalf of Wrocław University of Technology; Institute of Mineral Fertilizers, Pulawy, Poland; Institute of Inorganic Chemistry, Gliwice, Poland; and the University of Agriculture, Wrocław, Poland.

Evening social events, such as dances and a gala dinner, provided opportunities for attendees to talk about scientific issues with

new acquaintances. On one evening, participants were enchanted by the recital of the famous opera singer Anna Bernacka.

The next XXXII conference will be held at Priessnitz in December 2006.

Adam Pawelczyk <adam.pawelczyk@pwr.wroc.pl> has been the chairman of the organizing committee since 1998. He is an academic teacher at the Wrocław University of Technology.

Photodynamics

by Jesus Rubayo Soneira

The **Fourth International Meeting on Photodynamics** was held in Havana from 6–10 February 2006. Approximately 100 scientists from 19 countries met to discuss a range of experimental and theoretical viewpoints on the physical and chemical processes related to environmental and biological systems.

The conference was sponsored by the Cuban Ministry of Science and Technology, the Cuban Physical Society, IUPAC,* and the Abdus Salam International Center for Theoretical Physics.

The international scientific committee consisted of Vincenzo Aquilanti (Italy), Majed Chergui (Switzerland), Gerardo Delgado-Barrio (Spain), Antonio Varandas (Portugal), Julian Echave (Argentina), Annick Suzor-

Editor's note: this event also benefited from IUPAC's financial support via the program for Conferences in Scientifically Emerging Regions. For more information, see <www.iupac.org/symposia/support.html>.

Weiner (France), and Jesús Rubayo-Soneira (Cuba, chairman).

Prior to the conference, a seminar was held from 1–4 February 2006 that focused on a new generation of young researchers from Cuba and Latin American countries, as well as the rest of the world. Fifty students attended the following short courses, which were given by professors with excellence in both teaching and research:

- "Some Elements on Theoretical and Statistical Approaches of Elementary Reactions" (Jean Claude Rayez)
- "Van der Waals Clusters" (Gerardo Delgado Barrio)
- "Wavepacket Dynamics, Photochemistry, and Coherent Control" (David J. Tannor)
- "Molecular Science at the Nanoscale" (Vincenzo Aquilanti)
- "Lepton Chemistry: Molecular Processes and Reactions Induced by Low-Energy Electrons and Positrons" (Franco A. Gianturco)

The meeting, which featured 30 plenary lectures, 12 oral communications, and 43 poster presentations, covered the following topics: structure and energetics of molecular systems, dynamics and reactivity of isolated molecular species, dynamics of molecular species embedded in small and large clusters, dynamics of molecules in the condensed phase (liquid, solid) and at surfaces, control of chemical reactions, and collisions with surfaces.

The purpose of the meeting was to stimulate discussion about the structure and dynamics of molecular systems among scientists working in the chemical-physics. Keynote lectures were given by Peter Hering (Düsseldorf, Germany), Gustav Gerber (Wuerzburg, Germany), Osman Atabek (Paris, France), Reinhard Nesper (Zurich, Switzerland), and William Jackson (California, USA), among others.

In particular the conference provided a timely opportunity for scientific exchange among outstanding scientists and young researchers from all over the world. Based on the scientific success and interest in the Havana meeting, the participants agreed that this kind of meeting should be held again in the near future.

The seminar and meeting took place at the National Capitol, the main building of the Cuban Academy of Sciences, which is located in the heart of Old Havana.

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Green/Sustainable Chemistry

by M. Kidwai

The IUPAC-sponsored **Second International Symposium on Green/Sustainable Chemistry**, held in Delhi, India, from 10–13 January 2006, was a showcase for green chemistry innovations from all over the world. Green chemistry can be challenging, but it is fundamental to the future of chemical production, especially in the pharmaceutical and agricultural fields. The conference's 550 attendees from 22 countries took stock of recent advances in environmentally friendlier chemistry.

The organizing committee made a strong effort to help participants from economically less developed countries attend the event. The Third World Academy of Sciences gave USD 2000 to fellows from countries such as Ghana and Bangladesh so they could attend the conference.

The conference, which offered 8 plenary lectures, 31 main lectures, and 44 invited lectures featuring eminent scientists, focused on the vital role played by chemists in designing green methods of chemistry and how to widen the use of green technology.

A number of prominent speakers shared the results of their cutting-edge research. In his plenary lecture, E.J. Thomas from the University of Manchester, UK, discussed alternatives to allyl stannanes for remote stereo chemical control and encouraged the use of fictionalized ionic liquids. Pietro Tundo, from Ca' Foscari University, Italy, lectured about the tunable reactivity and selectivity towards C and N methylation in dimethyl carbonate chemistry using basic and acidic catalysts. Arthur C. Watterson from the University of Massachusetts, USA, discussed the chemo-enzymatic green synthesis of polymeric materials, which is an environmentally benign technique for medical, imaging, and other applications. John C. Warner, from the same university, discussed using entropic control in materials design.

In addition, there were 33 oral presentations by upcoming postdoctoral and Ph.D. fellows who shared their experiences with green chemistry. The poster presentations showcased the most up-to-date research in the areas of synthesis of bioactive compounds, green, use of biomaterials, nanotechnology, biomimetic processes, microwave technology, ionic liquids, and the edges of physical chemistry, including computational methods. Five awards were presented for best poster presentations.

Among the attendees were representatives of 28 chemical and pharmaceutical industries, a number of whom were inspired by green industrial methods described in lectures. Industries represented included Matrix Laboratories Ltd., Pfizer Global Research & Development, Emcure Pharma Ltd., Merck Research Laboratories, and Bristol-Myers Squibb Company.

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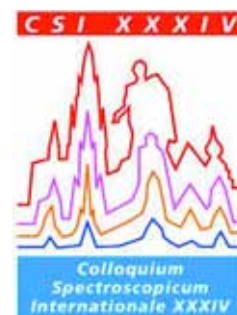
Analytical Spectroscopy

by René Van Grieken

The **34th Colloquium Spectroscopicum Internationale (CSI-XXXIV)**, held in Antwerp, Belgium, from 4–9 September 2005, was hosted by the University of Antwerp. Since the first CSI conference, organized in Paris, France, in 1949, this prestigious series of biannual conferences has established itself as the premier forum for presentation and discussion of new developments in all branches of analytical spectroscopy. While many conference series decline after 20–30 years, the CSI series is still vigorous, probably because it is a truly international series of conferences. In Antwerp, as in previous conferences, there were participants from about 40 countries and from all continents.

The most recent CSI conferences took place in Granada, Spain (2003), Pretoria, South Africa (2001) and Ankara, Turkey (1999). The next one will be organized in Xiamen, China, from 24–28 September 2007, while in 2009, the event will take place in Budapest, Hungary. The conference alternates, in principle, between Europe and other parts of the world.

Following the tradition of the preceding CSI conferences, emphasis was placed on new developments and applications of spectroscopy in all branches of analytical chemistry. At this conference there were almost 300 participants, and more than 300 abstracts were received for oral and poster contributions. The topics included new research of various spectroscopic techniques and methodologies (such as atomic plasma spectrometry, molecular spectroscopy, organic and inorganic mass spectrometry, X-ray spec-



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trometry, hybrid techniques, laser spectroscopy, imaging techniques, quality control, and chemometrics), as well as applications of spectroscopy in, among others, micro-, surface and interface analysis, speciation, proteomics, environmental and geochemical analysis, and archaeometry and cultural heritage.

The program included 5 invited plenary lectures (by Y. Baba, M. Blades, D. Günther, G.M. Hieftje, and R. Niessner), 8 invited keynote lectures (by A. de Juan Capdevilla, M. Höhn, J. Kolar, A. Laskin, N. Omenetto, C. Gruening, K. Shimizu, and F. Vanhaecke), 120 oral contributions in 20 parallel sessions introduced by the invited speakers, and 3 poster sessions. Two vendor sessions were arranged as well.

During the opening ceremony, the CSI-XXXIV Award was given to Yoichi Gohshi, whose professional career has been of impressive relevance both to X-ray spectrometry and to analytical science in Japan. Gohshi retired recently from the National Institute for Environmental Studies in Tsukuba, Japan, and earlier from the University of Tokyo. This award was sponsored by Wiley, publisher of scientific books and of the journal *X-Ray Spectrometry*, for which Gohshi served for many years as editor for Japan. The laudation for the award was given by Jun Kawai from Kyoto University, one of Gohshi's famous students. After receiving his award, Gohshi highlighted some of his research over the decades.

Furthermore, at the conference dinner, three poster prizes, sponsored by Elsevier, were awarded to Kouichi Tsuji (Osaka City University, Japan), David De Muynck (Ghent University, Belgium) and Gerardo Gamez (Indiana University, USA), and their coworkers.

Besides the interesting scientific contributions, the participants of the CSI-XXXIV conference did find opportunities to sample some of Antwerp's cultural and historical treasures and some of its gastronomy and lifestyle. The city of Antwerp, in addition of hosting one of the most important harbors, the second largest petrochemical complex, and the most important diamond center in the world, also has a unique late medieval historical center, the home of Rubens, and numerous fine museums. The conference itself was held in the medieval "Elzenveld" conference center, which was originally a hospital when built in 1238. It was given to the city of Antwerp by Napoleon was turned into a conference center in 1989. The CSI participants enjoyed the quiet environment and beautiful gardens of the complex, which were especially attractive in the nice summer weather.

The homepage of CSI-XXXIV, including its detailed scientific program, can still be viewed at <www.csixxiv.ua.ac.be>. The Website of the next conference in China in 2007 is already in place at <www.csixxv.org>.

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ThermoML: New IUPAC Standard for Thermodynamic Data Communications

by Michael Frenkel

A one-day symposium on **ThermoML: Purpose, Structure, and Applications** was held on 27 March 2006 in Atlanta, Georgia, USA, as part of the 231st National Meeting of the American Chemical Society. Speakers from the USA, Canada, UK, Germany, Netherlands, and New Zealand represented all components of the global data delivery process based on ThermoML (Markup Language for Thermodynamics).

Introductory remarks for the symposium were given by Bryan R. Henry, IUPAC president (University of Guelph, Canada); Daniel Friend, acting chief of the Physical and Chemical Properties Division, U.S. National Institute of Standards and Technology; and Catherine T. Hunt, president elect of ACS (Rohm and Haas Company). The announcement of ThermoML as a new IUPAC standard was made on 27 March 2006 by IUPAC President Bryan R. Henry during a special "ThermoML" reception co-sponsored by IUPAC, NIST, FizChemie Berlin (Germany), and Elsevier (Netherlands).

Thermodynamic property data represent a key resource for development and improvement of all chemical process technologies. However, rapid growth



Michael Frenkel, conference organizer, opens the ThermoML symposium. Seated at the table (from left) are Catherine Hunt, Bryan Henry, and Daniel Friend.

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Bryan Henry (left), IUPAC president, announces ThermoML as a new IUPAC standard for thermodynamic data communications during the "ThermoML" reception. He is joined by Michael Frenkel.

in the number of custom-designed software tools for engineering applications has created an interoperability problem between the formats and structures of thermodynamic data files and required input/output structures for the software applications. Establishment of efficient means for thermodynamic data communications is absolutely critical for provision of solutions to such technological challenges as elimination of data processing redundancies and data collection process duplication, creation of comprehensive data storage facilities, and rapid data propagation from measurement to data-management system and from data-management system to engineering application. Taking into account the diversity of thermodynamic data and numerous methods of their reporting and presentation, standardization of thermodynamic data communications is very complex.

In 2002, IUPAC approved project 2002-055-3-024, "XML-Based IUPAC Standard for Experimental and Critically Evaluated Thermodynamic Property Data Storage and Capture," and established a task group to carry out the project. Michael Frenkel, USA, was the chair of this group, whose members included John Dymond, UK; Erich Königsberger, Australia; Kenneth Marsh, New Zealand; Stephen Stein, USA; and William Wakeham, UK. This project was completed with the establishment of the new IUPAC standard for ThermoML. The full description of ThermoML was published in the March 2006 issue of *Pure and Applied Chemistry*, and the ThermoML namespace has been established on the IUPAC Website.

Michael Frenkel <frenkel@boulder.nist.gov> acted as symposium organizer; for details on the session program see <www.iupac.org/symposia/2006/ThermoML-symposium.html>. For more information on this project see <www.iupac.org/namespaces/ThermoML>.

Advanced Materials and Polymer Characterization

by Michael Hess

The 14th POLYCHAR Conference—Annual World Forum on Advanced Materials was held in Nara, Japan, from 17–21 April 2006 during the Japanese cherry blossom season. One day prior to the main conference, a Short Course on Polymer Characterization was held, which was an educational project of the IUPAC Polymer Division (IV). The organization committee was led by Masaru Matsuo, Nara Women University, chair, and co-chairs Kohji Tashiro, Toyota Technical Institute, Tokyo, and Yoshiyuki Einaga, Nara Women's University.

The annual POLYCHAR conferences have been IUPAC-sponsored for several years and are well-known among scientists interested in the properties and characterization of polymers and the synthesis, processing, and manufacturing of novel polymers. The conference was subdivided into 10 sections:

- Predictive Methods
- Synthesis
- Nanomaterials and Smart Materials
- Mechanical Properties and Performance
- Dielectric and Electrical Properties
- Surfaces, Interfaces, and Tribology
- Rheology, Solutions, and Processing
- Biomaterials and Tissue Engineering
- Natural and Biodegradable Materials and Recycling
- Characterization and Structure—Property Relationships

Due to the high number of participants, two parallel sessions had to be organized for the conference. This is usually not the case with POLYCHAR conferences.



Paul J. Flory Laureate Koichi Hatada (right) receiving his award from Moshe Narkis.

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However, this event attracted 240 participants from 35 countries, who presented about 270 contributions (oral and 2 poster sessions). Many students also attended the presentations. It is not so much the intention of the conference to have a high number of participants and parallel sessions but rather to attract young scientists and advanced and graduate students and give them the opportunity to meet with colleagues and well-known scientists to exchange experiences, make contacts and present their results to the scientific community.



Paul J. Flory Laureate Witold Brostow (right) receiving his award from Moshe Narkis.

The conference is also the platform for the prestigious Paul J. Flory Research Award, which that was jointly awarded to Witold Brostow, University of North Texas, Denton—for his work on the prediction of long-term reliability of viscoelastic materials and discoveries in tribology—and Koichi Hatada, Fukui University of Technology—for his spectroscopy and other research presented in 390 publications, and also for his efforts to encourage interest among children in materials science and engineering.

Although encouraged by the organizers to present oral contributions, many students' presentation were found in the two poster sessions comprising 136 excellent contributions. Of these presentations, three were

recipients of the IUPAC Student Poster Awards:

- Steven Lamoriniere, Imperial College London (advisor Alexander Bismarck), for his work on composites reinforced with carbon nanotubes
- Kyota Miyamoto, Kyushu University, Fukuoka (advisor Atsushi Takahara), for results on surface and interface structures of blend thin films
- Yumiko Nakano, Nara Women's University (advisors Yuezhen Bin and Masaru Matsuo), for her results on carbonization of poly(vinyl alcohol) films containing carbon fillers and metal dioxides

It is difficult to select particular contributions from the multitude of excellent oral and poster contributions from universities, research institutes, and industry without overlooking important contributions. The full conference program is available at www.nara-wu.ac.jp/polychar-14/index.html.

The Short Course on Polymer Characterization has been an integral part of the conference from the very beginning and is held the day before the conference. The course offers condensed presentations by well-known specialists who provide basic information for students and newcomers in the field and who update participants on popular characterization techniques. A nice feature of the course is that the lecturers are available to participants during the whole conference. Due to the support of the IUPAC Polymer Division, it was possible to waive the fee for the 40 participants.

POLYCHAR-15 will be held in April 2007 in Rio de Janeiro, Brazil. POLYCHAR-16 will be held in Lucknow, India, in January 2008.

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After conference excursion of the POLYCHAR 14 participants to the cherry blossoms in the Yoshino mountain area.

Food and Drug Administration—100 Years of Service

by *Laure Joumel*

On 16 May 2006, the Food and Drug Administration's (FDA) tour of the United States in celebration of its 100th anniversary stopped by the Chemical Heritage Foundation in Philadelphia. Around 250 people came to celebrate and hear speakers from the FDA and the industry consider the history of the administration. Dr. Andrew von Eschenbach, acting commissioner of the FDA, presented his vision for the agency.

The FDA's centennial provides a good opportunity to reflect on its history. The agency, part of the U.S. Department of Health and Human Services, regulates food, drugs, cosmetics, medical devices, dietary supplements, biologics, and blood products.

Suzanne White Junod, FDA historian, provided some perspective on FDA's past, and Peter Barton Hutt, senior counsel for the law firm Covington and Burling and former legal counsel for the FDA, considered "the 10 most important turning points in FDA history."

According to the speakers, the beginnings of drug regulation in the United States can be traced to an 1862 meeting between President Abraham Lincoln and the chemist Charles Wetherill that led to the creation of the Division (later Bureau) of Chemistry within the Department of Agriculture. This year's centennial celebrates the anniversary of the 1906 Food and Drugs Act, signed by President Theodore Roosevelt, which according to Hutt, marked the birth of premarket drug approval. The act also became known as the Wiley Act for the chief chemist's long-standing efforts to secure a law.

In 1927, the bureau was divided into two parts: the Food, Drug, and Insecticide Administration and the Bureau of Chemistry and Soils. Three years later, the

word "Insecticide" was dropped and the Food and Drugs Administration gained its present name.

The 1906 act was extended in 1938 after a health

scandal. A raspberry-flavored sulfa elixir that was not tested before being launched on the market caused the death of more than 100 people. The elixir was mostly composed of diethyl glycol—now known to be poisonous. Due to public outrage, the FDA obtained the right to control every new drug. A second scandal would reinforce the power of the FDA. In 1962, the drug Thalidomide caused an international scare when it was found to cause deformities in babies whose mothers had used it during their pregnancy. After this event, pharmaceutical companies have had to prove to the FDA the safety as well as efficacy of all products they produce.

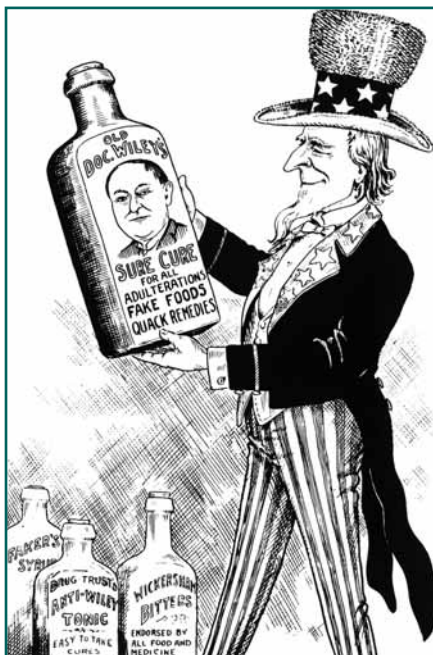
Recent developments in U.S. food and drug regulation include the 1990 requirement that all food packaging have nutrition labeling and health claims. The FDA has introduced measures to allow faster approval for some drugs

and its staff has increased. The Prescription and User Fees Act of 1992 asked companies to pay fees for every new drug application. More recently, government pressure on the FDA to help consumers choose heart-healthy food, resulted in a 2003 measure requiring food producers to note the presence of "trans fat" in their products.

In the realm of drug advertising, the agency has seen its regulatory power reduced despite the vision of the FDA. Since 1997, companies have been able to spend less ad time or space reviewing the side effects of the drugs they market. It is interesting to note that in most countries in Europe and in Asia advertising for prescription drugs is forbidden.

To Better Communication

Since the Prescription and User Fees Act of 1992, the FDA has been financially dependent on the drug



J.F. McPhee's 1906 cartoon reflected public expectations concerning the "Wiley Act." The new law, it was hoped, would put a stop to food adulteration and the marketing of quack remedies. Courtesy FDA History Office.

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industry. During this same period, public suspicion of the drug regulation system has seemed to grow after drugs with dangerous side effects were approved by the FDA. In particular, the Vioxx controversy has Americans asking for more transparency. “We want more information” hears Steven Galson, director of the FDA center for Drug Evaluation and Research.

In 1999, Merck received authorization to sell rofecoxib (Vioxx), a nonsteroid anti-inflammatory drug. In April 2000, a study requested by Merck revealed an increase of myocardial infarcts among people taking the drug. Despite this, Vioxx was still prescribed by doctors. In 2001, *The Journal of the American Medical Association* published a meta analysis that pointed out the risk of infarcts. In response, the FDA warned Merck that their ads were untrue and in 2002 cautioned doctors against the use of Vioxx for patients with coronary disease. However, it was not until 2004 that the drug was withdrawn from the market.

Could another “Vioxx situation” occur? “This controversy about Vioxx has already resulted in large changes” said Galson. “We need to improve FDA communication about emerging drugs,” he said and added, “Even with perfect information and improved analysis there will be disagreement.”

Toward Individualized Prescriptions

One of the goals of FDA and industry is to better envisage drugs’ side effects. “We want to be able to predict if this drug is or is not for you” said Ronald Krall, senior vice president of worldwide development for GlaxoSmithKline. The aim is to establish a bridge between a study conducted on a sample of the population before commercialization and the real-market population. “By now, we can predict the side effects. We can tell, in some cases, this drug might [cause] nausea or somnolence or sweating,” said Krall. But the goal is to target the patient. Predicting if this patient, in particular, is going to have this side effect and not another one, is the aim, he said. And in the future, companies will correlate one side effect with the other, according to Krall, so the prescription will be individualized.

Food Issues

Robert Brackett, director of the FDA’s Center for Food Safety and Applied Nutrition, reminded the audience that “76 millions food-borne illnesses, 325 000 hospi-



Courtesy FDA History Office.

talizations, and 5 000 deaths” occur each year in the United States because of food intoxication. He explained how the role of FDA changed after the Pasteurized Milk Ordinance of 1924 because the philosophy of the public changed. Today, we are more aware about nutrition and labeling, but new diseases and ways of transmission have been introduced. New products on the market, like mangos or bean-sprouts, call for new ways of controlling food-borne pathogens.

Acting Commissioner von Eschenbach—who was named one of the 100 most influential people in the world in a May 2006 issue of *Time* magazine—concluded the anniversary day by summarizing his wishes for the future of the FDA and introducing The Oncology Biomarker Qualification Initiative. This collaboration among the FDA, National Cancer Institute, and the Center for Medicare and Medicaid Services is intended to provide modern tools to define biomarkers. According to Eschenbach, these biomarkers will allow the creation of a healthcare and healthcare delivery system in the United States in which medicine will be personalized.

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www.chemheritage.org/events/fda
www.fda.gov/centennial

An article by John P. Swann titled “How Chemists Pushed for Consumer Protection—the Food and Drugs Act of 1906” was published in *Chemical Heritage*, 24:2, summer 2006, p. 6.