I. General Aspects

1. Optimizing Therapy by Analogues (J. Fischer, C.R. Ganellin, E.M. Alapi)
2. Analogues and Standalone Drugs (J. Fischer, C.R. Ganellin, A. Ganesan, J. Proudfoot)
3. Lead and Drug Optimization (J. Fischer, C.R. Ganellin, and J. Proudfoot)
4. Molecular Modeling in ABDD (G. Ferenczy)
5. The Impact of Natural Products upon Modern Drug Discovery (A. Ganesan)
6. Monoterpenoid Indole Alkaloids (A. Nemes)
7. Paclitaxel Analogue (P. Erhardt and M. El-Dakdouki)
8. Issues for Patenting of Analogues (S. Smith)

II. Analogue Classes

1. Beta2 Agonists (G. Gaviraghi)
2. M3 Muscarinic Antagonists (M. Grauert, P. Casarosa, M.P. Pieper)
3. SSRIs (D. Rotella and W.E. Childers)
4. Progestogens (Z. Tuba , S. Maho, J. Csorgei, and C. Molnar)
5. DPP-IV Inhibitors (J.U. Peters, P. Mattei)
6. PDE5 Inhibitors (H. Haning, E. Bischoff)
7. Serotonin and Norepinephrine Reuptake Inhibitors (M. Abou-Gharbia and W. Childers)
8. Anthracyclines (F.A. Arcamone)
9. Rifampicin analogues (E. Selva and G. Lancini)

III. Case Studies

1. Eplerenone (J. Kalvoda and M. De Gasparo)
2. Lapatinib (K. Lackey)
3. Dasatinib (J. Das and J.C. Barrish)
4. Conazoles (J. Heeres, P. Lewi, L. Meerpoel)
5. Clevudine (C.K. Chu)
6. Rasagiline (M. Youdim)
7. Liraglutide (L.B. Knudsen)
8. Tipranavir (S. Thaisrivongs, J. Strohbach, S. Turner)
9. Rilpivirine (J. Guillemont and J. Heeres)

The second volume will discuss a broad spectrum of discoveries of anticancer, antifungal, antiviral, cardiovascular, CNS, diuretic, hormonal, respiratory, and diabetes type 2 drugs. The majority of the authors, who come from 10 different countries, were also involved as inventors. This IUPAC project started in May 2008. According to the planned contents, 42 authors will participate.

For further information and comments, contact János Fischer <j.fischer@richter.hu> or C. Robin Ganellin <c.r.ganellin@ucl.ac.uk>.

www.iupac.org/web/ins/2008-013-1-700

Frontiers of Chemical Sciences: Research and Education in the Middle East

Building on the tremendous success of the first, second, and third Malta conferences (see projects 2002-061-1-020, 2004-030-1-020, and 2006-035-1-020, respectively), the Executive Committee has recently approved a project to be known as Malta IV. The objectives are as follows:

- to use science as a bridge to peace in the Middle East by bringing together top scientists from 14 Middle East countries (Bahrain, Egypt, Israel, Iran, Iraq, Jordan, Kuwait, Lebanon, Libya, the Palestinian Authority, Qatar, Saudi Arabia, Turkey, the United Arab Emirates) for a five-day conference
- to give scientists the unique opportunity to develop cross-border collaborations to solve regional problems involving the environment, water, and energy, and to design a unified chemical education curriculum
- to attempt, via this conference and workshops, to generate trust among scientific communities—despite the hostility that some of the governments have toward each other—on ways that chemistry can address the problems of the region

The chemical sciences occupy a central position in the world economy, offering the possibility to cultivate mutual understanding through joint research projects and economic development. A general desire to improve the quality of life and political stability in the Middle East is being fulfilled by identifying unique opportunities for network creation and collaboration among chemical scientists to solve chemical, environmental, and educational problems.

The American Chemical Society, the German Chemical Society, the Royal Society of Chemistry, UNESCO, and IUPAC will cosponsor this fourth conference. It will include 70 around representatives, primarily from 14 Middle Eastern nations as well as from Canada, France, Germany, Norway, Switzerland, Taiwan, UK, and USA.

During the five-day conference, six Nobel Laureates will deliver plenary lectures and act as catalysts in the following workshops: Environment; Air and Water Quality; Science Education and Green Chemistry; Alternative Energy Sources; Medicinal and Natural Products; and Nanotechnology and Material Science.

A principal goal of this conference will be to continue to capture the attention of national governments

by inviting the best qualified chemical scientists from those countries to discuss how chemistry can address the problems of the region and contribute to the stability and prosperity of the Middle East.

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Investigating Out-of-Specification Test Results of Chemical Composition Based on Metrological Concepts

By the current good manufacturing practice in pharmaceutical industry, out-of-specification (OOS) test results are results that fall outside the specifications or established acceptance criteria. Identifying OOS test results is described in FDA Guidance for Industry "Investigating OOS Test Results for Pharmaceutical Production" (2006). By analogy, measurement/test results obtained in other industries and such fields as environmental analysis, which do not comply with regulatory or specification limits, can be named also as OOS test results. When the compliance assessment is made on the basis of a measurement result accompanied by information on the uncertainty associated with the result, the rules developed in the EURACHEM/CITAC Guide "Use of Uncertainty Information in Compliance Assessment" (2007) are applicable.

After identification of the OOS test result it is important to determine its root causes: to ensure that another OOS test result is not possible or even inevitable. The FDA Guidance mentioned above formulates general rules for investigation an OOS test result, including production review, additional laboratory testing, reporting testing results, and determining the cause. Thus, it establishes an organizational approach to the full-scale investigation and decisions which can be accepted at the different stages of this investigation.

Another approach, outlined in the this new IUPAC project, is based on metrological concepts and includes assessment of the measurement process used for the test, from sampling to chemical analysis of a test portion. The project results will be formulated as a guide. In particular, the following should be addressed in a future development of the guide:

- assessment of validation data of the measurement process, including sampling, sample preparation, and chemical analysis
- use of the validation data for evaluation of the measurement uncertainty components
- assessment of traceability chains important for measurement parameters and environmental conditions influencing the test results

The project will be carried out in collaboration with the Cooperation on International Traceability in Analytical Chemistry. The planned IUPAC/CITAC guide will be helpful for full-scale investigations of OOS test results in pharmaceutical industry (in addition to the FDA Guidance) and in other fields of testing.

For more information and comments, contact the Task Group Chair Ilya Kuselman <ilya.kuselman@moital.gov.il>.

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Young Ambassadors for Chemistry in Taipei, Taiwan, and Mauritius

by Lida Schoen, Mei-Hung Chíu, Erica Steenberg

The Young Ambassadors for Chemistry (YAC) project is a partnership of IUPAC's Committee on Chemistry Education (CCE) and Science Across the World (SAW), designed to facilitate the flow of ideas between chemistry and society using young people as mediators.

After five years of holding successful programs around the world—in Argentina, Bulgaria, Egypt, Jordan, Korea, Lithuania, Russia, South Africa, Taiwan—CCE submitted a new project proposal titled Research-Based Evaluation of the Young Ambassadors for Chemistry Project. This project was designed to

Students in Taipei produce a 30-second TV commercial.