

## BIOLOGICAL MODELING SPECIALTY SECTION (BMSS)

### ANNUAL REPORT: 2010 – 2011

May 1, 2010 – April 30, 2011

#### I. Officers/Comittees:

##### Officers:

President:

Vice President:

Vice President-Elect:

Secretary/Treasurer:

Councilors:

Past President

Postdoctoral Representative:

Graduate Student Representative:

##### 2009-2010

Richard A. Corley

Robert S. Dewoskin

James V. Bruckner

Hisham El-Masri

Jerry Campbell

Michael J. Bartels

Jeffrey Schroeter

Craig M. Zwicki

Susan E. Crowell

Christopher Carosino

##### 2010 – 2011

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Susan E. Crowell

#### II. Activities

The **2011 SOT Annual Meeting Reception** was held Wednesday, March 9, at the Walter E. Washington Convention Center in Washington, DC. Approximately 70 - 90 people were in attendance.

Rob Dewoskin called the meeting to order at 6:00 pm on March 9<sup>th</sup>. Rob described key activities of the specialty section in 2010 – 2011. He also named and introduced the retiring and the new BMSS Council members. Rob then discussed ways section members could participate in BMSS activities, including: volunteering to be a candidate for the Council; assisting the Council; actively using ToxChange, on which members can vote to choose reception activities, vote for the year's best modeling paper, and post announcements on courses, special journal issues and papers, etc. Jean Domoradzki was given special thanks for working to identify and screen candidates for the best paper award. A PubMed search using the key words "PBPK" and "Physiologically Based Pharmacokinetic" yielded 128 papers in 2010, a substantial increase over the last 25 years.

A series of speakers gave short presentations and answered questions about their topics and on-going research. Hugh Barton of Pfizer Inc. discussed the current role of PBPK modeling in pharmaceutical industry research and development programs. He was followed by Jeff Fisher, who described a number of in silico activities at the Division of Biochemical Toxicology at NCTR/FDA. These activities included: development of QSAR and SAR endocrine disruptor and liver toxicity databases; utilization of 3-D drug-protein and QSADockingR computations; development of PBPK models for bisphenol A, methylphenidate and isoflavones; and construction of BBDR modeling of the maturing thyroid axis. George Loizou of the United Kingdom Health and Safety Laboratory spoke about global sensitivity analysis of PBPK models. He introduced application of a new computational approach (eFAST using acsIX Libro) to produce Lowry plots to assess the influences of individual model parameters, interactions between parameters, and interactions between parameters and non-linear processes. Annie Jarabek, Lyle Burgoon, John Wambaugh and Nicole Kleinstreuer of the U.S.EPA described several new risk assessment initiatives involving modeling

at their agency, including: the Global to Genome (G2G) project; the Advancing to the Next Generation (NexGen) of Risk Assessment project, that aims to create a less expensive but more robust risk assessment process and incorporates new knowledge about molecular and systems biology; the Virtual Liver project; new Virtual Embryo Tools and Models; and Developmental Toxicology (DevTox) Predictive Modeling strategy. Harvey Clewell of the Hamner Institutes for Health Sciences spoke about their planned work on the P53 DNA-damage toxicity pathway, involving protein activation and cell cycle perturbations in response to chemicals.

**Awards:** There were many good papers dealing with biological modeling published in 2010. A BMSS Council working group evaluated some 40 papers, selected 10 finalists and posted them on ToxChange to be voted upon by the BMSS membership. The votes were very close. Nicholas Luke, Reeder Sams, Mike DeVito, Rory Conolly and Hisham El-Masri won the BMSS Best Paper Award for 2010 for their published work entitled “Development of a Quantitative Model Incorporating Key Events in a Hepatotoxic Mode of Action to Predict Tumor Incidence.”

This year’s winner of the Perry J. Gehring Student Award for Excellence in Biological Modeling is Anne Loccisano for her research project entitled “Development of Human Gestation and Lactation Models for Perfluorooctanoate (PFOA) and Perfluorooctanesulfonate (PFOS).” Anne is a postdoctoral fellow working at the Hamner Institutes under the direction of Mel Andersen and Harvey Clewell. They and John Hutenhoff were coauthors.

## **2011 SOT Annual Meeting Courses/Sessions:**

**Sponsored:**

PBPK Model Use in Risk Assessment: Why Being Published is Not Enough (workshop)

**Endorsed:**

Best Practices for Developing, Characterizing and Applying Physiologically Based Pharmacokinetic Models in Risk Assessment (CE course)

Using Mode of Action Data to Guide Quantitative Cancer Risk Assessment: A Case Study of Hexavalent Chromium in Drinking Water (workshop)

Understanding Structural and Physical Drivers of Drug Toxicity: Utility and Translatable Value (workshop)

Approaches for Incorporating Non-Chemical Stressors into Cumulative Risk Assessments (workshop)

Vascular Developmental Toxicity: Identification, Prioritization and Application (symposium)

The Use of Epidemiological Data and PBPK Modeling in a Risk Assessment for Manganese that Considers its Essentiality (symposium)

## **BMSS Contribution to the SOT Time Capsule**

BMSS contributed three items to the 50<sup>th</sup> Anniversary Time Capsule. These included: (1) the BMSS Best Paper Award manuscript by Luke et al. (2010); (2) examples of the M-file programming code used by Luke et al. (2010); and (3) the 2011 Perry J. Gehring Student award abstract by Loccisano et al.

**Membership and Financial:**

Currently, there are 129 BMSS members. Net financial assets, as of 5-31-11, were \$9,512. The success of the awards program and our specialty section has been advanced by the generous support of our sponsors Aegis Technologies and Lhasa Limited.

**Newsletters:**

Volume 3, No. 1

Volume 3, No. 2

These issues are available for download from the BMSS Specialty Section of ToxChange.