

NAME OF SPECIALTY SECTION Biological Modeling

ANNUAL REPORT: 2015-2016

May 1, 2015 to April 30, 2016

I. Officers/Committees:

<u>Officers</u>	<u>2014-2015</u>	<u>2015-2016</u>
President:	Harvey Clewell	Paul Hinderliter
Vice President:	Paul Hinderliter	Eva D McLanahan
Vice President-Elect:	Eva D McLanahan	Jeffery M. Gearhart
Secretary/Treasurer:	Stephen Edwards	Stephen Edwards
Past President	Cecilia Tan	Harvey Clewell
Councilors:	Miyoung Yoon Qiang Zhang	Qiang Zhang Annie Lumen
PDA Representative:	Martin Phillips	Christopher D. Ruark
GSLC Representative:	Todd Zurlinden	Rachel Worley

Committees:

The BMSS 2015 Best Paper Award committee was formed by the officers from volunteers among the specialty section members and chaired by Eva McLanahan (BMSS Vice President). Committee members were Eva McLanahan (ATSDR, Chair), Jeff Gearhart (Jackson Foundation), Jeff Fisher (FDA), and Zhoumeng Lin (KS State). Papers published either electronically or in hard copy from January to December 2015 were considered. The review process included an initial screening of hundreds of abstracts obtained by electronic searching and nominations from BMSS members followed by reading and ranking of the top papers resulting in one winning paper and four with an honorable mention.

II. Activities:

2016 SOT Annual Meeting Reception was held in New Orleans, Louisiana on March 14, 2016.

Approximately 85 people were in attendance.

Dr. Hinderliter called the meeting to order at 6:15 PM.

Meeting Minutes:

Paul Hinderliter welcomed the attendees and briefed the audience on the status of the specialty section. Jeff Gearhart announced Rachel Worley as the recipient of the 2016 Perry L. Gehring award for best presentation on biological modeling for her work on the impact of kidney transporters on renal absorption. Eva McLanahan briefed the audience on the selection process for the best paper award. The honorable mentions and best paper award were then recognized. Paul Hinderliter highlighted Mel Andersen as the recipient of the SOT Merit Award, which honors “distinguished contributions to toxicology throughout an entire career in areas such as research, teaching, regulatory activities, consulting and service to the Society.” Stephen Edwards provided the budget update. Paul Hinderliter thanked outgoing officers and congratulated the new incoming officers. He then led a short discussion on the future of the BMSS webinar series

on computational tools to support biological modeling. To encourage more interaction among the specialty section members, Eva McLanahan and Rachel Worley led everyone in a networking game where teams competed to rank themselves based on the criteria provided by the master of ceremonies. Members then mingled and congratulated Mel Andersen on his outstanding accomplishment.

Awards:

BMSS 2016 Perry J. Gehring Award

Rachel Rogers Worley

Agency for Toxic Substances and Disease Registry, Division of Community Health Investigations

“Application of Physiologically-Based Pharmacokinetic Modeling to Explore the Role of Kidney Transporters in Renal Reabsorption of Perfluorooctanoic Acid in the Rat”

BMSS 2015 Best Paper Award

1st place

Richard A. Corley, Senthil Kabilan, Andrew P. Kuprat, James P. Carson, Richard E. Jacob, Kevin R. Minard, Justin G. Teeguarden, Charles Timchalk, Sudhakar Pipavath, Robb Glenny, and Daniel R. Einstein, “Comparative Risks of Aldehyde Constituents in Cigarette Smoke Using Transient Computational Fluid Dynamics/Physiologically Based Pharmacokinetic Models of the Rat and Human Respiratory Tracts”, *Toxicological Sciences*, (2015) **146**(1):65-88.

BMSS 2015 Best Paper Honorable Mentions

Sehan Lee, et al., “Development of 3D-QSAR Model for Acetylcholinesterase Inhibitors Using a Combination of Fingerprint, Molecular Docking, and Structure-Based Pharmacophore Approaches.” *Toxicological Sciences* (2015) **148**(1):60-70.

Zhoumeng Lin, et al., “A physiologically based pharmacokinetic model for polyethylene glycol-coated gold nanoparticles of different sizes in adult mice.” *Nanotoxicology* (2016) **10**(2):162-172, early online in 2015.

Marc-André Verner, et al., “Associations of Perfluoroalkyl Substances (PFAS) with Lower Birth Weight: An Evaluation of Potential Confounding by Glomerular Filtration Rate Using a Physiologically Based Pharmacokinetic Model (PBPK).” *Environmental Health Perspectives* (2015) **123**(12):1317-1324.

Barbara A. Wetmore, et al., “Incorporating High-Throughput Exposure Predictions with Dosimetry-Adjusted In Vitro Bioactivity to Inform Chemical Toxicity Testing.” *Toxicological Sciences*, (2015) **148**(1):121-136.

2016 SOT Annual Meeting Courses/Sessions:

This year, BMSS sponsored eight annual meeting proposals, including one Continuing Education course, one roundtable, four symposium sessions, and two workshops. Out of these eight proposals, five were accepted by the SOT Program Committee (the type of session was changed in several cases):

CE course: “Exploring Chemical Space in the New Toxicity Testing Paradigm: From Data Curation to Computational Simulations”

Workshop: “Moving Beyond Prioritization towards True In Vitro-Based Safety Assessment”, “Safety Assessment of Topically Exposed Cosmetic Ingredients: Lessons Learned”, “Advanced Techniques in PBPK Modeling to Improve Quantitative Risk Assessment for Infants and Children”

Informational Session: “Tox21 Challenge To Build Predictive Models of Nuclear Receptor and Stress Response Pathways As Mediated by Exposure to Environmental Toxicants and Drugs”

Endowment Fund Details:

Perry J. Gehring BMSS Endowment Fund

Balance as of December 31, 2015 = \$43,722 (an increase of \$870 over the past year)

BMSS Webinar Series:

The BMSS hosted a series of two webinars to discuss mathematical modeling languages and software with specific emphasis on physiologically-based pharmacokinetic (PBPK) model applications. The webinars were widely attended.

1. Thursday, February 4, 2016 11:00 AM EST - R modeling language.
 - a. Dr. Chris Ruark (ScitoVation)
“Introduction to the R Project and RStudio”
 - b. Dr. Woodrow Setzer (US Environmental Protection Agency)
“MCSim and the R package deSolve”
 - c. Dr. George Loizou (Health & Safety Laboratory)
“Using RVis to run PBPK models coded in R and C++”
2. Friday, March 4, 2016 10:00 am, EST - Developing PBPK models in MATLAB and SimBiology
 - a. Dr. Fulden Buyukozturk (MathWorks) and Mr. Ricardo Paxson (MathWorks)
“SimBiology as a platform for PBPK modeling”
 - b. Drs. Robin McDougall (Astra Zeneca) and Martin Philips (Minnesota Department of Health)
“How to translate an acslX PBPK model into the MATLAB language”

More webinars are planned for the 2016-2017 year.