

NAME OF SPECIALTY SECTION _____ Biological Modeling _____

ANNUAL REPORT: 2016-2017

May 1, 2016 to April 30, 2017

I. Officers/Committees:

<u>Officers</u>	<u>2016-2017</u>	<u>2017-2018</u>
President:	Eva D McLanahan	Jeffery M Gearhart
Vice President:	Jeffery M Gearhart	Jeffrey William Fisher
Vice President-Elect:	Jeffrey William Fisher	Brad Reisfeld
Secretary/Treasurer:	Martin B Phillips	Martin B Phillips
Past President	Paul M Hinderliter	Eva D McLanahan
Councilors:	Annie Lumen	Anne Loccisano
	Andy Nong	Andy Nong
PDA Representative:	Christopher Daniel Ruark	Miao Li
GSLC Representative:	Rachel Worley	Axelle Marchand

Committees:

The BMSS 2016 Best Paper Award committee was formed by the officers from volunteers among the specialty section members and chaired by Jeff Gearhart (BMSS Vice President). Committee members were Miao Li (Kansas State), Marie-Emilie Willemin (FDA), and Colin North (Exxon Mobile). Papers published either electronically or in hard copy from January to December 2016 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 nine with an honorable mention.

II. Activities:

2017 SOT Annual Meeting Reception

was held in Baltimore, Maryland on March 14, 2017. Approximately 75 people were in attendance. Dr. McLanahan called the meeting to order at 6:15PM on March 14, 2017. Meeting minutes are included in Attachment I.

Awards:

- **Biological Modeling Best Paper Award for Publication Year 2016:** Sluka JP, Fu X, Swat M, Belmonte JM, Cosmanescu A, Clendenon SG, Wambaugh, JF, and Glazier, JA. (2016) A Liver-Centric Multiscale Modeling Framework for Xenobiotics. PLoS ONE 11(9): e0162428. doi:10.1371/journal.pone.0162428.
- **Biological Modeling Best Paper Honorable Mention (see Attachment I for listing)**
- **2017 Perry J. Gehring Biological Modeling Endowment Award:** Marie-Emilie Willemin, FDA
- **2017 Melvin E. Andersen Trainee Award:** Jeremy Leonard, EPA
- **BMSS Student Travel Support:** Anteneh Assefa, EU JRC

2017 SOT Annual Meeting Courses/Sessions Endorsed by BMSS:

This year, BMSS sponsored six accepted annual meeting sessions, including one Continuing Education course, three workshops, and 2 symposia.

CE Course

“Read Across: Case Studies, New Techniques, and Guidelines for Practical Application,”
Dr. Sullivan, Dr. Cronin

Workshops

“Using Bioinformatics Tools to Accelerate Data Analysis and Hypothesis Generation” (ID 92)
Susan Bello, Marc Gillespie, Elissa Chesler, Sean Watford, Jing Yuan

“Fit for Purpose: Using Computational Models for Risk” (ID 54)

John Wambaugh, Jon Arnot, Lesa Aylward, Hugh Barton, Nisha Sipes, Ryan Hansen

“Evolution of Chemical-Specific Adjustment Factors (CSAFs) based on Recent International Experience; Increasing Utility and Facilitating Regulatory Acceptance” (ID 38),
Richard Brown, Bette Meek, John Lipscomb, Alan Boobis, Virunya Bhat, Mathieu Valcke

Symposia

“Increasing Confidence in Safety Assessment Decisions – The Inclusion of Metabolism in Toxicity Testing Strategies” (ID 147)

Miyoung Yoon, Cecilia Tan, Stephen Ferguson, Bas Blaauboer, Emanuela Testai

“Novel In Vitro and In Silico Platforms for Modeling Developmental and Reproductive Toxicity” (ID 169)

Teresa Woodruff, Nicole Kleinstreuer, Randolph Ashton, Thomas Knudsen, George Daston

Endowment Fund Details:

Andersen/Clewell Trainee Award fund as of March 31, 2017: Balance \$50,780 (a new fund)
Perry J. Gehring Biological Modeling Student Award fund as of March 31, 2017: Balance \$47,286 (includes donations of \$1,000, investment gain of \$3,564, and award given of \$500)

Webinars:

The BMSS hosted a series of webinars to discuss mathematical modeling. The webinar coordinator was Dr. Christopher Ruark. The webinars were widely attended by SOT members across the organization.

1. Date: Thursday, February 16th, 2017
Title: Understanding Dermal Drug Disposition Using TCAT—A Novel PBPK Model.
Presenters: Anu Krishntry, Valeriu Damian, and Jessica Spires
Number of Attendees: ~150
2. Date: Tuesday, October 25th, 2016
Title: Application of Physiologically-Based Pharmacokinetic Modeling to Explore the Role of Kidney 2 Transporters in Renal Reabsorption of Perfluorooctanoic Acid in the Rat

Presenters: Rachel Worley
Number of Attendees: ~ 125

3. Date: Friday, July 22, 2016
Title: PharmML-Exchange Format for Models Used in Quantitative System Pharmacology and Pharmacometrics
Presenters: Maciej J Swat
Number of Attendees: ~40

4. Date: Thursday, June 16, 2016
Title: Saying I do to the QSAR/PBPK marriage in GastroPlus to predict chemical exposure for safety evaluation
Presenters: John DiBella, Fagen Zhang, and Leah Luna
Number of Attendees: ~150

More webinars are planned for 2017-2018 and the new webinar coordinator is Ms. Sandrine Chebekoue.

Attachment I - 2017 Annual meeting – Minutes

1. Buffet / Meet & Greet
2. Welcome –Eva McLanahan (Pres)
3. Presentation of Student awards - Jeff Fisher (VP-Elect)
 - 2017 Perry J. Gehring Award for Biological Modeling – **Marie-Emilie Willemin** (FDA)
 - 2017 Trainee Award, made possible from a generous donation from Melvin E. Andersen – **Jeremy Leonard** (EPA)
 - Student travel support – **Anteneh Assefa** (EU JRC)
4. Best paper award - Jeff Gearhart (VP)
 - Recognize committee participants and acknowledge process
 - Honorable Mentions:
 - **Martin B. Phillips:** A Workflow to Investigate Exposure and Pharmacokinetic Influences on High-Throughput in Vitro Chemical Screening Based on Adverse Outcome Pathways.
 - **Patricia Ruiz:** A Systems Biology Approach Reveals Converging Molecular Mechanisms that Link Different POPs to Common Metabolic Diseases.
 - **Jingtao Lu:** Developing a Physiologically-Based Pharmacokinetic Model Knowledgebase in Support of Provisional Model Construction
 - **Hisham El-Masri:** Integration of Life-Stage Physiologically Based Pharmacokinetic Models with Adverse Outcome Pathways and Environmental Exposure Models to Screen for Environmental Hazards
 - **Jeremy A. Leonard:** Evaluating the Impact of Uncertainties in Clearance and Exposure When Prioritizing Chemicals Screened in High Throughput Assays.
 - **Allison Franzen** A global human health risk assessment for Decamethylcyclopentasiloxane (D5).
 - **Torka Poet:** Using physiologically based pharmacokinetic modeling and benchmark dose methods to derive an occupational exposure limit for N-methylpyrrolidone.
 - **Charles Breckenridge:** PBPK-Based Probabilistic Risk Assessment for Total Chlorotriazines in Drinking Water
 - **Marije Strikwold:** Integrating in vitro data and physiologically based kinetic (PBK) modelling to assess the in vivo potential developmental toxicity of a series of phenols.
 - WINNER: **JP Sluka et al.** *A Liver-Centric Multiscale Modeling Framework for Xenobiotics* (John Wambaugh accepted as co-author)
5. New Joint Award with RASS/Endowment Award – Eva McLanahan
 - Andersen/Clewell Trainee Award Fund – forms available in person or donate online
 - Thanked Hugh Barton for his efforts to establish the fund. Will alternate between RASS and BMSS being responsible for selecting winner and presenting at SOT annual meeting. RASS will give first award.
 - The collaboration of Melvin E. Andersen and Harvey J. Clewell III has been significant in the history of toxicology for the development and application of biological modeling in risk assessment. Melvin E. Andersen's focus was on the development of physiologically based pharmacokinetic (PBPK) models and then biologically based dose-response models. Harvey J. Clewell III collaborated in the development of these models and then explored their implementation for risk assessment of chemicals. These approaches

directly incorporated scientific knowledge into interspecies extrapolation, route-to-route extrapolation, characterizing human variability, and use of metabolic and mechanistic information in biologically informed analyses.

Established in November 2016, the goal of the Andersen/Clewell Trainee Award Fund is to encourage the education and training of toxicologists in biological modeling and risk assessment. The proceeds of the fund will be used to provide annually one or more award stipends given to domestic or international graduate students or postdoctoral scholars demonstrating interest and expertise in the development of biologically based models or their application in risk assessment. The awards will carry the designation “Andersen/Clewell Biological Modeling and Risk Assessment Award.” The first award(s) from the fund will be given once the Fund has assets in excess of \$50,000.

6. Treasurer's report – Martin Phillips

- Fiscal Year 16 (ending June 30, 2016) showed positive growth in both funds overseen by BMSS.
 - In our general fund, we had revenues of \$5,685 and expenses of \$4,674, with a net gain of \$1,010 to end at \$13,484. Major sources of revenue include membership dues (\$2,645) and our share of registration fees (\$1,235) from SOT. We also received \$1000 in donations. The major expense, as usual, was the cost of the annual reception (\$4,269) for the meeting in New Orleans in March 2016.
 - In our endowment fund, we had revenues of \$1,200 and expenses of \$500, with a net gain of \$700 to end at \$43,222. Revenue was from member contributions (which SOT matches), while the only expense was the graduate student travel award paid out of this fund.
- Fiscal Year 17 (to end June 30, 2017) has been stable based on the reports available so far.
 - In the general fund, there have been no revenues or expenditures, so the current balance is \$13,484 as of December 31, 2016 (latest available).
 - In the endowment fund, there have been revenues of \$1,035 from gains on investments, to end the fund at \$44,257 as of Sept 30, 2016 (latest available).
- In all, BMSS is in good financial health. To help improve the health of our specialty section, be sure to recruit your friends and colleagues to join! The more members, the more dues we collect to help support students and young scientists, as well as promote the use of biological modeling within the Society and in the scientific community at large!

7. Thank outgoing Officers – Eva McLanahan

- Annie Lumen - Councilor
- Chris Ruark – Postdoc representative
- Rachel Worley – Graduate student representative
- Paul Hinderliter – Past-President

8. Election results: Introduction of new Officers Term Begins May 1 – Eva McLanahan

- Brad Reisfeld (Colorado State) – VP Elect
- Anne Loccisano (Exponent) – Councilor
- Miao Li (Kansas State Univ) – Postdoctoral Representative
- Axelle Marchand (University of Montreal) – Graduate student representative

9. Future BMSS Webinars

- New webinar coordinator: Sandrine Chebekoue (PhD Candidate at Univ Montreal)
- Send any ideas to BMSS leadership or Ms. Chebekoue (chebs81@yahoo.fr)

10. Presentations from GastroPlus (John DiBella) and Scitovation/EPA (Harvey Clewell)
11. Reminder about mentoring lunch for those that have RSVP'd and closing remarks, Q&A for BMSS leadership – Eva
 - Wednesday, March 15, Noon, Kona Grill, 1 E Pratt St – Thanks Andy!
12. Team Trivia – Andy, Eva, Rachel