Biological Modeling Specialty Section Newsletter

Volume 9
February 2024

President's message

Dear Biological Modeling Specialty Section (BMSS) members,

I am honored to lead our Biological Modeling Specialty Section (BMSS) this year. With approximately 134 members across many disciplines, we are a strong and vital Specialty Section, focused on being your go-to biological modeling professional resource. Our dedicated BMSS volunteer leaders, a group of sponsors, and our volunteers make this all possible.

We provide our BMSS membership with several opportunities yearly with a set of activities. Our BMSS leaders shape these activities specifically for you, and I have always been impressed with the quality of our efforts, together with our increased focus on collaboration, empowerment, and diversity.

In all our efforts as the BMSS leadership, we attempt to actively engage with you, our members—through networking, mentoring, webinars, and other events. Having a strong professional network that you can count on with a difficult question or help you improve your career journey is very important if a job/career/project change is on the horizon.

All BMSS initiatives focus on enriching your experience as members, so we are always open to feedback on our current opportunities and how we can better serve you.

Feel free to contact us or any of our BMSS leaders if you have ideas or would like to get involved.

Thank you, members, for your continued support, participation, and enthusiasm in our professional community. Finally, I'd like to give a special shout-out of appreciation to our BMSS leaders for their hard work and the support they provide.

Wishing you a good and successful rest of 2024 and looking forward to seeing you soon in Salt Lake City.

Stay well,

Zhoumeng Lin

BMSS President 2023-2024

BMSS Officers 2023-2024

President
Zhoumeng Lin

Vice President
John Wambaugh

Vice President-Elect
Stephen W. Edwards

Secretary-Treasurer
Dustin Kapraun

Past President
Patricia Ruiz

Councilors
Sudin Bhattacharya
Wei-Chun Chou

Postdoctoral Representative
Qiran Chen

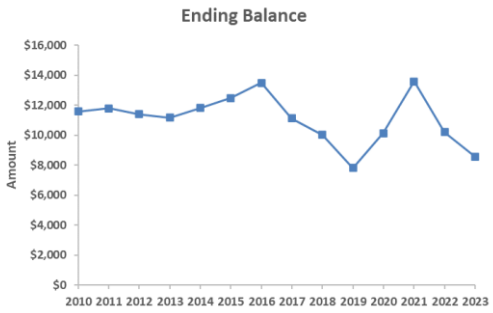
Student Representative
David Umbaugh

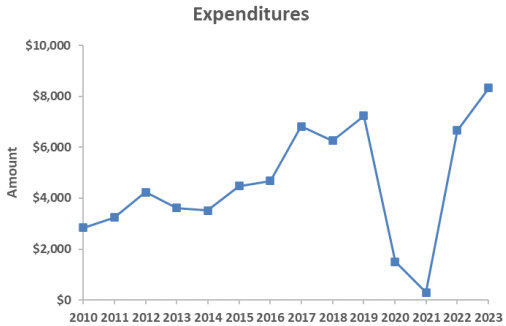
Treasurer's Report

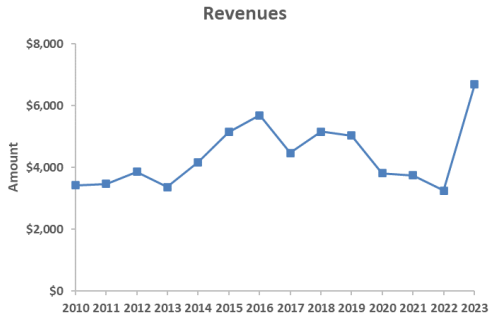
Treasurer's Report for 2023 – Dustin Kapraun, BMSS Secretary-Treasurer

BMSS General Operating Fund

- Between January 2023 and December 2023, BMSS had revenues (credits) of $6,689 and expenditures (debits) of $8,331, resulting in a net loss of $1,641. (This represents an improvement over 2022, in which BMSS had a net loss of $3,415.)
- The balance as of December 2023 is $8,566.
- The major sources of revenue this year were BMSS membership dues ($2,470) and a **generous donation from EsqLABS GmbH** ($2000). The major expenses were costs associated with the BMSS reception ($5,311) and the BMSS mentoring event ($2,058), which both occurred at the SOT Annual Meeting in Nashville in March 2023.
- Revenues were considerably higher in 2023 ($6,689) than in 2022 ($3,253). Recognizing that revenues had declined in 2020 through 2022 (primarily because SOT ended its policy of sharing revenues from Annual Meeting registration fees with Specialty Sections in 2019), BMSS officers developed and implemented strategies to increase revenue. These strategies included recruiting sponsors and requesting donations from members.
- In August 2023, **EsqLABS GmbH made a BMSS sponsorship donation of $2000**.
- In October and November, **three BMSS members made donations to BMSS totaling $550**.
- BMSS officers also noticed that there was an erroneous charge ($700) to the general operating fund and worked with SOT staff to ensure that this money was credited back to BMSS.
- Expenses were significantly greater in 2022 and 2023 than in the previous two years. In 2020, the SOT Annual Meeting was canceled, and in 2021, the SOT Annual Meeting was completely virtual; therefore, BMSS did not host a reception in either of those years. Our major operating expense each year has typically been the cost of the BMSS reception, and that expense returned in 2022 and 2023 when there were in-person SOT Annual Meetings!







Treasurer's Report

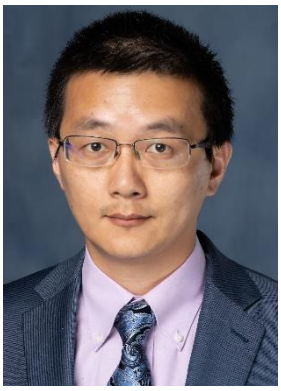
Treasurer's Report for 2023 – Dustin Kapraun, BMSS Secretary-Treasurer

Accounting summaries for the Andersen/Clewell Trainee Award Fund and the Perry J. Gehring Biological Modeling Student Award Fund can be found in the "Endowments" section of this newsletter.

Summary

- Overall, the financial health of BMSS might be described as "moderate but improving." For the 2024 Annual Meeting, we have estimated that the total expenses to be debited from the general operating fund will be about $7000. (This includes expenses associated with the Annual Meeting reception and the mentoring luncheon.) If total revenue (from SOT member dues, interest, sponsorships, and donations) for 2024 is comparable to revenue for 2023, there will be a net decrease in our general operating fund again in 2024. Consider recruiting your friends and colleagues to join BMSS—member dues are a major source of revenue and allow us to maintain the quality of events such as the mentoring luncheon and the annual reception! You might also consider making a donation to BMSS or to one of the award funds. Inquire with Dustin Kapraun or any of the other BMSS officers for details.

Meet our BMSS officers!



President – Zhoumeng Lin

Dr. Zhoumeng Lin is an Associate Professor in the Department of Environmental and Global Health at College of Public Health and Health Professions at the University of Florida. He has joint appointments in Department of Pharmaceutics at College of Pharmacy and Department of Physiological Sciences in College of Veterinary Medicine. He is a member of the Center for Environmental and Human Toxicology (CEHT) and the Center for Pharmacometrics and Systems Pharmacology (CPSP). He received a BMed in Preventive Medicine from Southern Medical University in China in 2009 and a PhD in Toxicology from the University of Georgia in 2013. He completed his postdoctoral training in the Institute of Computational Comparative Medicine at Kansas State University in 2016.

He was an Assistant Professor from 2016 to 2021 and then an Associate Professor from March to May 2021 at Kansas State University, prior to joining the University of Florida as an Associate Professor in May 2021. Dr. Lin's research is focused on the development and application of computational technologies, especially physiologically based pharmacokinetic (PBPK) modeling, quantitative structure-activity relationship (QSAR) modeling, machine learning, and artificial intelligence approaches, to study nanomedicine, food safety, nanoparticle and chemical risk assessment. He is a co-author of more than 100 peer-reviewed publications. Dr. Zhoumeng Lin teaches two graduate level courses entitled "Physiologically Based Pharmacokinetic Modeling in Toxicology and Risk Assessment" and "Artificial Intelligence in Environmental and Global Health" at the University of Florida. Dr. Lin is a co-editor and a co-author of five chapters of the textbook entitled "Physiologically Based Pharmacokinetic (PBPK) Modeling: Methods and Applications in Toxicology and Risk Assessment".

Vice President – John Wambaugh

Dr. John Wambaugh is a Research Physical Scientist with the Center for Computational Toxicology and Exposure at the US Environmental Protection Agency (US EPA). John's areas of active research include high throughput methods for chemical exposure, toxicokinetics, and toxicology. He co-leads the US EPA "exposure forecasting" or "ExpoCast" project. John develops and evaluates predictive models using mathematics, machine learning, Bayesian methods, and other applied statistics techniques. John collaborates on the design of new experiments to refine models and reduce uncertainty in chemical risk assessment. A primary focus of John's research is *in vitro-in vivo* extrapolation (IVIVE), including the development of high throughput toxicokinetics (HTTK).

Meet our BMSS officers

Vice President-Elect – Stephen W. Edwards

Stephen Edwards is director of the Scientific Computing and Data Curation Division within the Center for Computational Toxicology and Exposure (CCTE) at the US Environmental Protection Agency. This division is responsible for curating and managing CCTE data resources and developing web tools such as the CompTox Chemicals Dashboard. Dr. Edwards received his Bachelor of Science in chemistry from the University of North Carolina at Chapel Hill and his doctorate in pharmacology from Vanderbilt University Medical Center.

In addition to the US EPA, Dr. Edwards worked for RTI International examining the combined impact of genetic and environmental factors on disease manifestation to better support both precision medicine and public health protection. He also has experience in pharmaceutical target discovery where he led a team focused on identifying potential diabetes targets for the Merck high throughput screening program based upon computationally derived disease networks.

Secretary-Treasurer – Dustin Kapraun

Dustin Kapraun, PhD, is a Physical Scientist at the US Environmental Protection Agency (US EPA) Office of Research and Development (ORD) Center for Public Health and Environmental Assessment (CPHEA) and an expert in physiologically based pharmacokinetic (PBPK) models and their applications in chemical risk assessment.

He develops and applies PBPK models and other mathematical and statistical models to support chemical risk assessments, including Integrated Risk Information System (IRIS) toxicological reviews, and he has a special interest in pharmacokinetic models for gestation and the early post-natal period. Dr. Kapraun also serves as Co-Chair of the CPHEA Pharmacokinetics Workgroup (PKWG) and is an Adjunct Associate Professor in the Department of Mathematics at North Carolina State University. He enjoys teaching and mentoring postdoctoral researchers and graduate students and leading workshops and training sessions on PBPK modeling and related topics.

Past President – Patricia Ruiz

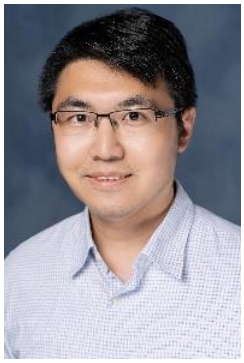
Patricia Ruiz, PhD., is an accomplished scientific leader/mentor. She currently is the chief Simulation Science Section at the Office of Innovation and Analytics/ the Agency of Toxic Substances and Disease Registry.

Dr. Ruiz received her doctoral degree from Georgia State University. Patricia also holds a BS in Pharmaceutical Sciences from the University of Cartagena in Cartagena, Colombia. She has 25 years of experience developing and applying computational modeling in government and academia.

Meet our BMSS officers!

Senior Councilor – Sudin Bhattacharya

Dr. Sudin Bhattacharya is an Associate Professor in the Departments of Biomedical Engineering and Pharmacology & Toxicology at Michigan State University, where he conducts research at the interface of computation and biology. Sudin's lab uses quantitative tools to study the signaling and transcriptional networks that regulate cell fate and the perturbation of these networks by environmental pollutants. His current interests include dynamical and deep generative modeling of single-cell fate choice under environmental perturbation.



Junior Councilor – Wei-Chun Chou

Dr. Wei-Chun Chou is an Assistant Professor in the Department of Environmental Sciences in the College of Natural & Agricultural Sciences at the University of California, Riverside (UCR). He received his PhD in Biomedical Engineering and Environmental Sciences from the National Tsing-Hua University in 2013 and furthered his expertise through postdoctoral training at the Institute of Computational Comparative Medicine at Kansas State University, completing it in 2021. Before his current position at UCR, Dr. Chou was a Research Assistant Professor in the Department of Environmental and Global Health at the University of Florida from Mary 2021 to December 2023. Chou's lab focuses on advancing computational technologies, particularly in physiologically based pharmacokinetic (PBPK) modeling, machine learning, and artificial intelligence applications in nanomedicine, nanoparticles, and chemical risk assessment, aiming to elucidate their effects on the environment and human health.

Postdoctoral Representative – Qiran Chen

Dr. Qiran Chen is a postdoctoral fellow at the Department of Environmental and Global Health and a member of the Center for Environmental and Human Toxicology at the University of Florida, where she is to advance the human risk assessment of environmental chemicals and nanoparticles using machine learning and other computational methodologies. She received a doctorate in environmental health from Indiana University Bloomington in 2020. Her doctoral research focused on the improvement of dose-response analysis in chemical risk assessment. Qiran is also the author/co-author of 10 peer-reviewed articles. She became a member of SOT in 2020. Her relevant work was recognized by the Society of Toxicology and awarded Andersen-Clewell Trainee Award (2020), Perry J. Gehring Award (2022), and the Best Postdoctoral Publication Award (2023). In 2023, Qiran was elected as the Treasurer of the Postdoctoral Assembly Executive Board and the Postdoctoral Representative of the Biological Modeling Specialty Section.

Student Representative – David Umbaugh

David is a 5th year graduate student in the Department of Pharmacology, Toxicology and Therapeutics at the University of Kansas Medical Center. David's ongoing doctoral research is aimed at understanding the signaling network between cells in liver injury and disease, using insights from single-cell RNAseq data to guide wet lab experiments and identify novel therapeutic strategies that enhance the liver's innate capacity for repair. To explore this, he integrates molecular and systems biology approaches, including data mining, single-cell transcriptomics, FACs (in combination with RNAseq), and a battery of assays *in vivo* and *in vitro* with pharmacologic and genetic manipulation.

Thanking our outgoing BMSS officers

Patricia Ruiz (past president):

Dr. Ruiz acted as the Past President this past year after serving as the President in 2022-2023, Vice President in 2021-2022, and Vice President-Elect in 2020-2021, and she leaves us with the following message:

What a pleasure! I want to start by saying that it has been a great privilege for me to have been allowed to serve the BMSS. In retrospect, the last four years have been an exceptionally busy time. We have had to deal with many important events and situations still unfolding. Indeed, for me, it has been a most eventful period, at times challenging but a most rewarding experience. BMSS is constantly working to strengthen, improve, and maintain our activities and efforts to give our members a fantastic space to network and promote collaboration and personal development on many levels. As my tenure ends, I have no doubt that BMSS is in a strong position to succeed; we have a team committed to serving and members passionate about contributing. BMSS is a great SOT Specialty Section. I intend to stay involved!

Constant progress is being made in the fields of toxicology, risk assessment, and biological modeling, but I'm confident that we're getting closer to seeing more significant advancements than we have in the past due to AI, NAMs, and other advances in science and technology. There are numerous ways that we can influence toxicological and biological modeling. I can never express how much I appreciate your passion, commitment, and constant support. Together, we have made a difference. I hope to see the BMSS continue to grow and succeed, so please continue to support BMSS with your finances, time, and expertise.

Sudin Bhattacharya (Senior Councilor):

Dr. Sudin Bhattacharya served as BMSS councilor from 2022-2024, and he leaves us with the following message:

I would like to thank my fellow officers and the membership of BMSS for the opportunity to serve in the capacity of councilor. As we enter what we might cautiously and optimistically term the post-COVID era, it has been gratifying to observe the return to largely in-person attendance of SOT members at the Annual and Regional Meetings, and the accompanying opportunity for increased social interactions, which can foster collaborations and friendships in a way that is difficult to achieve online.

These are exciting times for the field of toxicology and biological modeling. Technologies like artificial intelligence and single-cell omics are transforming the availability of biological data and the opportunity to mine and analyze it for extraction of mechanistic hypotheses and predictive modeling for risk assessment. The Generative AI revolution will also transform the entire scientific research enterprise in coming years in ways we are only beginning to fathom. Biological modelers will be at the forefront of this transformation, and newer generations of students, postdocs, and investigators will be urgently needed to address the accompanying scientific challenges. It is incumbent on us as current practitioners of biological modeling to encourage the next generation of scientists into this field.

2023 SOT Annual Meeting BMSS Events

2023 BMSS Mentoring Event:

March 20, 2023, Venue: Broadway Ballroom K, Omni Hotel. Nashville, TN

2023 BMSS Reception

March 20, 2023, Venue: Broadway Ballroom H, Omni Nashville Hotel. Nashville, TN

2024 BMSS Reception and Mentoring Event Information

Biological Modeling Specialty Section Mentoring Event

Where: Salt Lake Ballroom D, Hyatt Regency

When: Wed, March 13, 2024, 5:00 - 6:00 PM Mountain time

&

Biological Modeling Specialty Section Meeting/Reception

Where: Salt Lake Ballroom D, Hyatt Regency

When: Wed, March 13, 2024, 6:00 - 7:30 PM Mountain time

Visit the Online Planner to add these to your schedule!

BMSS Endowments

Andersen-Clewell Trainee Award Fund

- The balance at the beginning of 2023 was $66,302.
- There were $200 in contributions in 2023.
- There was no net gain from investments in 2023.
- There was a disbursement of $1,500 (for a cash award) in 2023.
- The balance was $65,002 as of October 2023.

Perry J. Gehring Biological Modeling Award Fund

- The balance at the beginning of 2023 was $63,535.
- There were no contributions in 2023.
- There was no net gain from investments in 2023.
- There was a disbursement of $2,000 (for two cash awards) in 2023.
- The balance was $61,535 as of October 2023.

To make a donation to our operating fund, please use SOT's online donation form which will walk you through the whole process. Please select "Biological Modeling Specialty Section" as the designated Specialty Section. Once submitted, it will be processed by SOT and an invoice will be emailed to you.

BMSS would like to acknowledge the generous donation of $2,000 from esqLABS GmbH (Saterland, Germany) to the BMSS General Operating Fund.

esqLABS
WE EMPOWER HEALTH CARE

BMSS-Sponsored Continuing Education Courses and Sessions

BMSS Endorsed Continuing Education Courses
AM04: High-Throughput *In Vitro—In Vivo* Extrapolation for Predictive Toxicology
Sun, Mar 10
8:15 am - 12:00 pm (Mountain)

PM08: Benchmark Dose Modeling and Its Applications in Drug, Food, and Chemical Safety Evaluation and Assessment
Sun, Mar 10
1:15 pm - 5:00 pm (Mountain)

BMSS Endorsed Research Sessions
Use of PBPK and Novel Pharmacokinetic Approaches for the Quantitative Prediction of Tissue Residue and Withdrawal Times for Human Food Safety Assessment
Mon, Mar 11
Room 250 D, Salt Palace Convention Center
9:15 am - 12:00 pm (Mountain)

New Approach Methodology and Kinetic Modeling Approaches to Support Read-Across
Tue, Mar 12
Grand Ballroom E, Salt Palace Convention Center
8:00 am - 10:45 am (Mountain)

The Ties That Bind: Evaluating the Impact of PFAS Protein Binding and Transport on Persistence and Tissue Distribution
Tue, Mar 12
Grand Ballroom A, Salt Palace Convention Center
8:00 am - 10:45 am (Mountain)

Overcoming Barriers to More Scalable Environmental Health Science Research via Harmonized Language
Tue, Mar 12
Grand Ballroom J, Salt Palace Convention Center
1:00 pm - 2:30 pm (Mountain)

In Vitro to *In Vivo* Extrapolation to Predict Developmental Toxicity Potential
Tue, Mar 12
Grand Ballroom E, Salt Palace Convention Center
3:00 pm - 4:30 pm (Mountain)

Call for **2025** BMSS session proposals

Dear BMSS Members,

We hope you enjoy the 2024 SOT Annual Meeting in Salt Lake City and are excited for next year in Orlando. To prepare for next year's meeting, we would like to solicit ideas for session proposals related to biological modeling in toxicology. The SOT deadline for proposals is **May 15** for the guidelines on proposal development and session types.

If you are planning to submit proposals, we would like to encourage you to submit draft session proposals to Stephen Edwards (edwards.stephen@epa.gov) for pre-review by **May 6, 2024**. The BMSS review committee will review and provide feedback (**May 10, 2024**) to help strengthen the proposals before you submit your session on the SOT website (**May 15, 2024**).

Thank you!

BMSS Executive Committee.

BMSS Webinars

Can you suggest anyone that you think would be an excellent candidate to present during our BMSS webinars?

You are welcome to nominate yourself and anyone else who is actively involved in biological modeling, pharmacokinetics, or other innovative and cutting-edge modeling subjects.

Please submit your nominations via email to John Wambaugh (wambaugh.john@epa.gov) or Stephen Edwards (edwards.stephen@epa.gov) with the subject line "BMSS webinars".

BMSS social media accounts info

Find us online at:

(https://www.toxicology.org/groups/ss/BMSS/)

Follow us on:

(https://twitter.com/sotbmss)

(https://www.linkedin.com/in/sotbmss)