SPRING 2023 NEWSLETTER

Sustainable Chemicals through Contemporary Toxicology
Specialty Section

PRESIDENT'S LETTER

Dear Sustainable Chemicals through Contemporary Toxicology Members,

Spring is near, and that means the **SOT Annual Meeting** is right around the corner! Please make sure to reserve time on your Annual Meeting Planner to attend the **SCCT Annual Meeting and lunch**.

Please join us!
When: Monday, March 20th
Where: Room 104C, Music City Center
Time: 12 Noon to 1:30 PM

The Irish poet William Butler Yeats said long ago, "*there are no strangers here, only friends you haven't yet met.*" I like to think that Yeats' quote describes the SCCT specialty section meeting! Please stop by and share your ideas on advancing sustainable chemistry within our specialty section.

This issue of the newsletter has two great contributions from Rick Becker of the ACC where he presents the ACC's recent work on QSURS, as well as Chris Bartlett of ChemFORWARD who discusses ChemFORWARD's pivotal work establishing hazard assessment frameworks for botanicals. We applaud their accomplishments.

I look forward to seeing each of you at the SOT meeting!
Sincerely,

Meg Whittaker, PhD, MPH, CBiol, FRSB, ERT, DABT

SCCT President

IN THIS ISSUE

62nd Annual Meeting & ToxExpo • Nashville, TN
March 19–23, 2023

GRAD STUDENT & POSTDOCS SIGN UP FOR THE JOINT MENTORING EVENT

When: Monday March 20th 7:30 PM
Where: Omni Hotel Legends Ballroom C

Come meet 4+ mentors in careers matching your interests in a mixer-style event. Food and two drink tickets are included! See you there!

SCCT RESOURCES CORNER

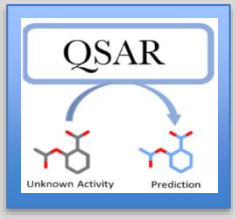
New to SCCT? New to sustainable research? Not new but looking for some resources? You have come to the right place! Check out our links to the **SCCT website** and a **resource list** that captures tools, learnings, and organizations in the field of sustainable toxicology. AND **SCCT is now on LinkedIn**!

SCCT Website Resources Page LinkedIn

FOLLOW US ON LINKEDIN!!

We want to support the SCCT community by re-sharing your event or your newest publication in the realm of sustainable chemicals and contemporary toxicology. To build our membership community and to show non-members the cutting-edge research in this field, we want to highlight you on our LinkedIn page. Send your responses to the following questions to Monika Roy (monika_roy@uml.edu) & Lauren Brown (lbrown@toxstrategies.com).

- Name, job title, company/organization
- Why did you get involved with SCCT?
- How does sustainable chemistry/chemicals connect to your work in toxicology?
- What has been exciting to you about this specialty section and/or what are you hoping to get out of this specialty section?



COMING SOON:

A REPORT ON THE NOVEMBER 2022 "QUANTITATIVE STRUCTURE USE RELATIONSHIP (QSUR) SUMMIT"

By Rick Becker, PhD DABT

The United States Environmental Protection Agency (US EPA) developed the concept of Quantitative Structure Use Relationships (QSURs), wherein the chemical structure is used to estimate the function of a chemical within a formulated product or an industrial process. QSURs are currently applied to help inform predictive tools for exposure assessment. In the absence of knowledge on the specific composition of a formulated product, QSURs can be used to estimate weight fractions of specific chemical components, and thus be used as input parameters for exposure modeling. To help advance the science in QSUR development and application, an invited expert QSUR Summit was convened. Scientists from Canada, Finland, France, the UK, and the USA, representing government, industry, and academia, with expertise in exposure science, chemical engineering, risk assessment, formulation chemistry, and machine learning participated in the Summit. Dr. Joel Tickner and Dr. Pamela Spencer participated in the Summit and led the discussion of potential utility of QSURs in alternatives assessment.

Since maintenance (or enhancement) of a chemical's function within a formulated product by substitution with an alternative, lower risk substance(s) with similar functionality is central to alternatives assessment, the QSUR concept and models have the potential to be particularly useful in the alternatives analyses. The QSUR Summit was hosted by the Long-Range Research Initiative of the American Chemistry Council, and a report and article summarizing the meeting presentations and discussions are being developed for public release. The report includes ideas on additional work and further research to improve and expand QSURs.

This concept will allow for the continued development of collaborative approaches to risk assessment. The SCCT will keep membership up to date on these endeavors! If you have any questions, please feel free to reach out or visit https://lri.americanchemistry.com/.

2022-2023 SCCT EXECUTIVE COMMITTEE

Meet the SCCT Executive Committee Members

Congratulations to the newly elected officers who will assume responsibility as officers starting May 1st, 2023.

Vice President-Elect: Damani Parran and Councilor: Monica Roy

Postdoctoral Representative Position remains open!

If you know of someone or if you are interested in joining our team, reach out to Past President Pam Spencer (PJSpencer@ANGUS.com).
We will hold a special election for this position once candidates have been received.

2023 SCCT Best Abstract Graduate Student Award

Award Sponsor: The Institute for In Vitro Sciences (IIVS)

Like many other SS and SIGs within SOT, SCCT offers a "*Best Abstract Award*" to a graduate student or postdoctoral scholar who is engaged in research that is relevant to sustainable toxicology, green toxicology, and/or New Approach Methodologies (NAMs). The research topics can include alternatives assessment, circular economy, sustainable design, and informed substitution, among others.

We are proud to introduce this year's winner!

Kelly Rivenbark, Texas A&M University

Abstract Title: *Using Green-engineering to Develop Sorbents for the Remediation of Benzene and Hazardous Environmental Samples*

4360: Poster Board: P226; Wednesday March 22nd @ 10:45 AM - 12:30 PM

Kelly Rivenbark is a graduate student at Texas A&M – Interdisciplinary Faculty of Toxicology and the Department of Veterinary Physiology and Pharmacology. She has been selected for her cutting-edge research that moves the needle in the field of sustainable toxicology. Congrats to Kelly, job well done!

THANK YOU for your sponsorship IIVS! Your contribution made it possible for us to acknowledge work that advances the sustainable toxicology and new approaches agenda.

Please consider applying for a SCCT graduate student or post-doc award,
more information can be found here: SCCT Awards.

Thank You to our Sponsors

Thank you to the generosity of our sponsors – We couldn't do what we do without you!

Consider Contributing to SCCT

By: A.J. Cuevas, PhD, DABT, MPH, MS

2020 did not just bring Covid, it also brought about SCCT's inaugural year! And now in 2023 SCCT remains a young SOT Specialty Section in need of your continued support and membership. The purpose of SCCT is to address the broader impact of toxicological research to inform decisions as we transition to safer chemistry throughout the product lifecycle, leading to a safer and healthier world. **We** as **toxicologist**, despite our specialty, **must stay committed to** a cleaner, **more sustainable future** regarding leading the charge for **chemical alternatives** and **alternative testing methodologies**.

We hope **you will continue** this journey with us by **renewing your membership in SCCT** and by inviting your colleagues and friends to join too!

Your **monetary support can provide an award(s)** to graduate students and post-doctoral fellows to acknowledge their novel, fit for purpose safety evaluation methodologies of green/sustainable toxicology. It can also be used to help provide support for SOT programs that foster sharing of best practices and cutting-edge knowledge related to the various cross functional areas that touch sustainable toxicology.

To donate – please visit the SCCT website: SCCT support or for more information, send an email to SOT Headquarters.

New Botanicals Methodology Helps Fill Data Gaps and Improve Decision Making for Natural Ingredients

Year-long multi-stakeholder collaboration develops a method for assessing botanical materials

By: Lauren Heine, PhD and Chris Bartlett, PhD

ChemFORWARD is science based non-profit organization based in Washington, DC.

ChemFORWARD, has posted a Botanicals Assessment Methodology v1.0 based on multi-stakeholder input and over 12-months of development, testing, and feedback. The methodology was developed to create an efficient, comprehensive way to characterize the hazard profiles of botanical ingredients and to allow for comparison to other chemicals, including non-botanical chemicals, in the product design process. This comparative methodology helps users to identify and select the safest alternatives.

While restricted substance lists (RSLs) are effective at eliminating chemicals that are known to have hazards of high concern, companies are moving toward using comprehensive chemical hazard assessments (CHAs) to inform proactive chemical management and avoid regrettable substitution. CHA is a systematic process of assessing, classifying hazards across a spectrum of human health and environmental endpoints and are essential to ensure safety. This comprehensive approach is key since it takes more information to prove the inherently safety of chemicals verses the data used to prove that it is toxic. For example, just knowing that a chemical is a carcinogen or that it causes skin sensitization can be enough to rule it out as a good candidate for product applications. But to be sure that it is inherently benign for its intended use means that data gaps must be filled across multiple human health and environmental endpoints. A lack of hazard data does not mean that a chemical is inherently benign.

ChemFORWARD aims to fill data gaps on botanical ingredients and substantiate clean beauty claims.

Selecting chemicals that are well characterized is critical to avoiding regrettable substitutions. ChemFORWARD hosts an online repository for chemical hazard assessments designed to aid users in identifying and selecting safer alternatives. The established methods for hazard classification such as the Globally Harmonized System for Classification and Labeling of Chemicals (GHS) and Cradle to Cradle Certified Material Health Methodology provide guidance for the classification of hazards on 24 human health and environmental impacts. These methods work well for traditional chemicals, but challenges remain in addressing other classes of chemicals, specifically polymers and botanicals.

Uncharacterized Botanicals

Many beauty and personal care brands are formulating with botanical ingredients as natural, safer alternatives, and driving safety and sustainability claims. However, the use of new plant-derived substances is growing much faster than industry's capacity to understand the impact on the health and safety of workers, consumers, and the natural environment.

In contrast to synthetic conventional chemicals, botanicals often contain dozens of compounds, which can vary with the source and influenced by seasons, geography, and extraction processes. This magnifies the complexity of assessing these materials.

A standardized approach to assessing botanical materials that is comparable to how conventional chemicals are assessed is imperative to allow for the evaluation of safer substitutions. Especially because the lack of hazard data for many botanicals creates the potential for regrettable substitution and risk to clean beauty claims.

Botanicals are often assumed to be safer than traditional chemicals, but that is not always the case. Botanical materials can be potent skin sensitizers, carcinogens, and endocrine disruptors. With this new botanical assessment method ChemFORWARD aims to fill data gaps on botanical ingredients, substantiate clean beauty claims, and standardize those claims and consumer expectations.

The Method

The method was developed to create an efficient, yet comprehensive way to characterize the hazard profile of botanical ingredients and allow for comparison to other chemicals in the product design process, while looking for potential safer alternatives.

The distinguishing features of the method include:

- Guidance to determine botanical composition prior to the safety assessment - identifying the constituents in a complex mixture
- Comprehensive approach to evaluate individual hazard endpoints for botanical materials as complex mixtures
- Comparability with hazard assessments used for synthetic conventional chemicals
- A refined approach to drawing insight from a history of safe use that is applied for specified exposure routes and concentrations

Pilot Results

After finalizing the botanical method ChemFORWARD piloted the approach with seven commonly used botanicals. Assessments were conducted byNSF International (one of ChemFORWARD's qualified assessors), see Table 1 for results.

Table 1: Summary of Pilot Results

INCI Name	Assessment Type	1. Empirical Data	2. History of Safe Use Relevant Exposure	3. Constituent Analysis	C2CC Rating	CF Hazard Band*
Redacted	Trade name	No	No	No	gray	U
Maltol	Generic	Yes	N/A	N/A	x/c-CMR(2)	C
Lavender Oil	Generic	Incomplete	No	Yes	x/c	C
Rosemary Extract	Generic	Yes	No	Yes	x/c	C
Green Tea Extract	Generic	Yes	N/A	N/A	x/c-CMR(2)	C
Catechins	Generic	Yes	N/A	N/A	x/c-CMR(2)	C
Jojoba Oil	Generic	Incomplete	Yes	N/A	b	B

**See Table 2 for a hazard band key*

One novel botanical material (redacted to protect confidential information) had insufficient data on the botanical material (whole and constituents) to generate hazard ratings. Maltol, green tea, catechins had enough empirical data on the botanical material as a whole to classify endpoints and generate a hazard band. Hazard band ratings are assigned according to the ChemFORWARD Program Description (See Table 2).

There other ingredients, jojoba oil, lavender oil, and rosemary extract, had data gaps on the botanical material as a whole and were therefore evaluated for hazards associated with their individual constituents. Lavender oil and rosemary extract have well characterized constituents, many of which are also well characterized toxicologically. Therefore, constituent analysis could be used to fill in data gaps. For jojoba oil, the assessor was able to fill in some data gaps with a well characterized dermal route of exposure history of safe use. Fulfilling those dermal endpoints provided enough information to rate jojoba oil.

The results indicated Cradle to Cradle Certified (C2CC) ratings of x/c or x/c CMR(2) for five of the six scored substances, indicating a moderate to high hazard and moderate risk. Two of them (lavender and rosemary were yellow for endocrine activity) showing the importance of characterizing the hazards and their relevance to the intended use of the ingredient. Jojoba oil was rated the best among screened substances, with an overall CF hazard band of B (indicating a moderate hazard and low risk).

Table 2: Hazard Band Key

Harmonized Hazard Band	Implications
A	Low hazard and low risk
B	Some moderate hazards, low risk
C	Moderate to high hazards and moderate risk; or uncertainty that could result in moderate risk
F	High hazards and high risk in most scenarios
U	CHA completed with excessive data gaps, rating is not possible
?	Request a CHA to inform a decision

As shown in Table 2, ChemFORWARD uses an algorithm that considers 24 human health and environmental endpoints to provide a roll-up score or hazard band (A, B, C, F, ?) for each chemical based on the endpoint inputs.

Uncharacterized chemicals (hazard band or U) have always posed a risk due to uncertainty with data gaps. Before the new method was developed, when botanicals were assessed using traditional hazard assessment methods, they were resulting in a hazard band of U — meaning excessive data gaps. The new Botanicals Hazard Assessment Method is enabling more data gaps to be filled thereby improving decision making for material selection.

Generic vs Trade Name Assessments

As with synthetic conventional chemicals, generic hazard assessment information can be used to point toward potentially safer alternatives. But it is more reliable to assess substances by trade name because that includes accurate characterization of constituents and impurities. The ChemFORWARD SAFER™ program was designed to obtain full disclosure of constituents and impurities in tradename materials as part of the ChemFORWARD material assessment process. Once a generic botanical material has been identified as a potential safer alternative, suppliers can quickly and easily have their trade name ingredients evaluated through the SAFER program to provide a third-party verification that all substances in the ingredient are safe as formulated.

The v1 Botanical Hazard Assessment Methodology is publicly available on the ChemFORWARD website. Work will continue with brand and retailer partners in the coming months to establish a minimum dataset for botanicals and further refine the assessment approach.

Call for Volunteers – Lots of Opportunities!

Your feedback is important - share your ideas for webinars, newsletter content, furthering communications (social media, blogs, etc.), award judging. Contact President Meg Whittaker (Mwhittaker@toxservices.com).