



Clustering and Classification Workshop:

Applications to Investigate Adverse Effects of Chemicals on Human Health and Environment

October 3-4, 2022

AGENDA

(All times EDT)

Day 1: Monday, October 3, 2022

8:30 a.m. Welcome

Kamel Mansouri, Ph.D., National Institute of Environmental Health Sciences (NIEHS)
Vicki Sutherland, Ph.D., NIEHS
Brian Berridge, D.V.M., Ph.D., NIEHS

8:45 - 11:45 a.m. Session 1: Chemicals and Similarity: Structures and Bioactivity

Chairs: Gloria Jahnke, D.V.M., DABT, and Vicki Sutherland, Ph.D., NIEHS

José Medina-Franco, Ph.D., FRSC, Universidad Nacional Autónoma de México

Molecular Similarity and Activity Cliffs

Esther Kellenberger, Ph.D., Université de Strasbourg

Similarity Between Bioactive Molecules From a Structural Bioinformatics Perspective

Andrea Mauri, Ph.D., Alvascience

Molecular Descriptors and Fingerprints as a Way to Represent Molecular Structures

Roundtable Discussion

Moderators: Kamel Mansouri, Ph.D., and Fred Parham, Ph.D., NIEHS

Discussants:

- Alexandre Varnek, Ph.D., Université de Strasbourg
- Cathy Lester, Ph.D., The Procter & Gamble Company
- Huixiao Hong, Ph.D., U.S. Food and Drug Administration, National Center for Toxicological Research

11:45 a.m. Lunch Break

**12:30 – 3:30 p.m. Session 2: Supervised and Unsupervised Approaches**

Chairs: Jui-Hua Hsieh, Ph.D., and Suril Mehta, Dr.P.H., MPH, NIEHS

Andreas Bender, Ph.D., University of Cambridge

Molecular Similarity – In the Eye of the Beholder, and Why Tailoring It to a Problem Is Necessary to Make It Meaningful

Davide Ballabio, Ph.D., Università degli Studi di Milano-Bicocca

Univariate vs. Multivariate for Clustering and Classification

Denis Fourches, Ph.D., Oerth Bio

Supervised vs. Unsupervised Approaches: Why One Typically Needs Both Anyway

Roundtable Discussion

Moderators: Kamel Mansouri, Ph.D., and Stephen Ferguson, Ph.D., NIEHS

Discussants:

- Tom Luechtefeld, Ph.D., Insilica
- Alexander Sedykh, Ph.D., Sciome LLC
- Elena Fioravanzo, Ph.D., ToxNavigation

3:30 p.m. Day 1 Wrap-Up

Vicki Sutherland, Ph.D., NIEHS

Day 2: Tuesday, October 4, 2022**8:30 a.m. Day 2 Welcome**

Kamel Mansouri, Ph.D., NIEHS

8:45 – 11:45 a.m. Session 3: How and When to Apply the Different Approaches

Chairs: Stephen Ferguson, Ph.D., and Vicki Sutherland, Ph.D., NIEHS

Alexander Tropsha, Ph.D., University of North Carolina at Chapel Hill

Similia Similibus Toxicus?

Alessandra Roncaglioni, Ph.D., Istituto Mario Negri

Analogues Selection for Read-Across: Combination of Supervised and Unsupervised Selection Methods

Todd Martin, Ph.D., U.S. Environmental Protection Agency

Best Practices on How to Select, Apply, and Interpret Supervised and Unsupervised Clustering and Classification Approaches

Roundtable Discussion

Moderators: Nicole Kleinstreuer, Ph.D., and Scott Auerbach, Ph.D., NIEHS

Discussants:

- Gilles Marcou, Ph.D., Université de Strasbourg
- Arianna Bassan, Ph.D., Innovatune
- Tomasz Sobanski, Ph.D., European Chemicals Agency



11:45 a.m. Lunch Break

12:30 – 3:30 p.m. **Session 4: Applications and Examples**

Chairs: Rachel Frawley and Amy Wang, Ph.D., NIEHS

Andrea Gissi, Ph.D., European Chemicals Agency

Chemical Similarity Under the EU REACH Regulation

Grace Patlewicz, Ph.D., U.S. Environmental Protection Agency

Practical Perspectives on the Development, Evaluation, and Application of In Silico NAMs for Predicting Toxicity

Andrew Rooney, Ph.D., and Suril Mehta, Dr.P.H., MPH, NIEHS, and Charles Bevington, MPH, U.S. Consumer Product Safety Commission

Class-Based Approaches to Evaluating Exposure, Hazard, and Risk: The Case for Taking Action on Organohalogen Flame Retardant Subclasses Using the NAS Roadmap

Roundtable Discussion

Moderators: Kyla Taylor, Ph.D., and Cynthia Rider, Ph.D., NIEHS

Discussants:

- Lauren Zeise, Ph.D., California Office of Environmental Health Hazard Assessment
- Louis (Gino) Sarcano, Ph.D., U.S. Environmental Protection Agency
- Patra Volarath, Ph.D., U.S. Food and Drug Administration, Center for Drug Evaluation and Research
- William Bisson, Ph.D., Inotiv

3:30 p.m. **Wrap-Up and Adjourn**

Kamel Mansouri, Ph.D., and Vicki Sutherland, Ph.D., NIEHS