

# ecetoc heatDB

## ECETOC launches a public directory of exposure data sources and exposure tools

The Human Exposure Assessment Tools Database (heatDB) is a resource for risk assessors to use to quickly search and locate human exposure tools and data available in the public domain.

Available sources of exposure data have been gathered, structured and categorised into a harmonised system. Additionally, available tools for exposure assessment were gathered and categorised into the same system. This allows risk assessors to quickly review what data sources and tools are available for given purposes and to have guidance on their appropriate use using a tiering system.

In parallel with this database, ECETOC Technical Report no. 126 provides analysis, discussion and case studies demonstrating different uses of some of the different tools and data sources (available on the main ECETOC website at <http://bit.ly/ecetoc-tr126>). There are hundreds of identified

sources of human exposure data and tools in heatDB. Thanks to Crème Global for the development and hosting of the database. Users can register for free, login and use the database as required at <https://heatdb.cremeglobal.com/>

For more information on events listed in this newsletter, please contact the ECETOC Secretariat by email: [info@ecetoc.org](mailto:info@ecetoc.org) or tel. +32 2 675 3600.

### In This Issue

#### Front page

- ECETOC launches a public directory of exposure data sources and exposure tools

#### Page 2

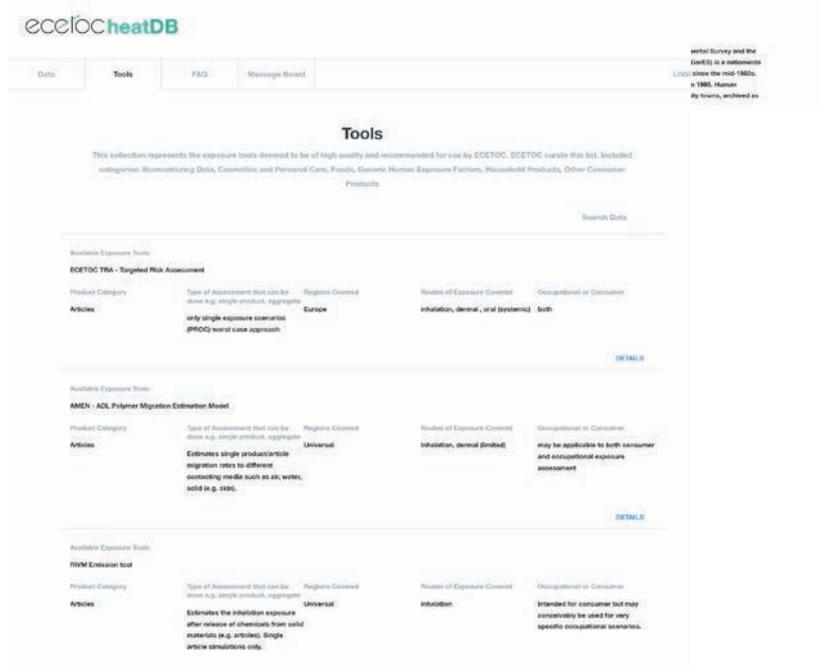
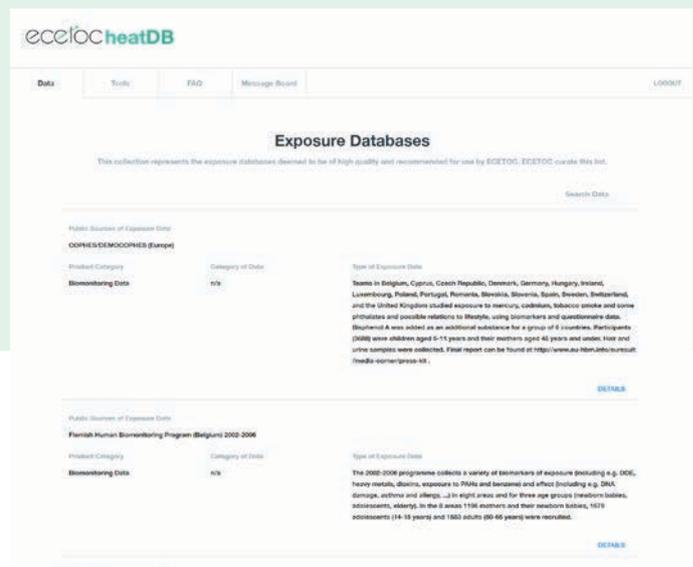
- News from the Scientific Committee and Secretariat

#### Page 3

- News from the Scientific Committee and Secretariat (Continued)
- Recent Events:
  - Advances in high tier environmental exposure modelling

#### Page 4

- Recent Events (Continued)
- Upcoming events:
  - When Omics Meet Regulations
  - ECETOC 2018 AGM & 40<sup>th</sup> Anniversary Celebrations
- Publications



# News from the Scientific Committee and Secretariat



## ECETOC at 40

2018 will mark 40 years since the founding of ECETOC and celebrations will kick-off at a special reunion and celebration for new and old members of the ECETOC network following the Annual General Meeting on 21 March, 2018 in Brussels. The meeting will review the impact of ECETOC during the past 40 years, look forward to what can be achieved during the next 40 and will also be the opportunity to meet the incoming Secretary General, Olivier de Matos.

## ECETOC Membership

ECETOC is delighted to introduce The Lubrizol Corporation as its latest Member Company effective May 2017. Headquartered in Wickliffe, Ohio, USA, Lubrizol, a subsidiary of Berkshire Hathaway, provides specialty chemicals for the transportation, industrial and consumer sectors. See the full Member Company list at <http://www.ecetoc.org/ecetoc-membership/member-companies>



## Board Membership

Board members have a two-year mandate and are responsible for the overall policy and finance of ECETOC as well as appointing the members of the Scientific Committee.

2 new Board Members have recently been proposed: Dr Chantal Smulders (Shell International) and Dr Volker Soballa (Evonik industries). They will attend ECETOC Board Meetings as guests until approved by members at the 2018 Annual General Meeting. See the full Board list at <http://www.ecetoc.org/about-ecetoc/board-of-administration/>

## Secretariat staffing

Please join us in welcoming Mr Olivier de Matos who will take over the position of Secretary General in September 2017 on the retirement of Dr Alan Poole. Leadership of ECETOC is an important role and Olivier as a graduate in International Law with 15 years of experience at Burson-Marsteller brings a wealth of expertise to understanding and solving science policy issues. Olivier is currently working with Alan Poole to ensure a smooth transition of responsibilities.

During his 5 year tenure, Dr Poole has streamlined and globalised ECETOC and refocused it on providing maximum value for its Members and bringing best scientific practices to the industry and the global regulatory community in the area of chemical risk assessment and the international harmonisation of chemical regulation. The Board, Scientific Committee and Secretariat thank him for his leadership over the last 5 years and wish him well in his retirement.

## New Expert Group

Initiative launched to improve the standardisation of metabolomics assays in regulatory toxicology

ECETOC has launched a new initiative which will accelerate the use of metabolomics technology to improve safety assessment of chemicals. Metabolomics is the study of the myriad of small molecules which sustain life, by generating energy, or building larger molecules such as DNA.

This technology has the potential to transform chemical risk assessment by providing a deeper view of the molecular events underpinning toxicity than is currently possible. However, because it is so new, scientists do not yet have standard procedures for applying metabolomics or reporting its findings, both of which are needed for chemical risk assessment.

The METabolomics standaRds Initiative in Toxicology (MERIT) brings together a team of international experts to address this problem by defining best practices and minimum reporting requirements when metabolomics is used in regulatory toxicology. It comprises partners from industry, government agencies, regulators and academia, from across Europe and the USA, including EFSA, US EPA, US FDA, BASF, Syngenta and Unilever.

Alan Poole, Secretary General of ECETOC explains that "Omics has enjoyed a great deal of success in research. Nevertheless, the use of omics data in regulatory assessment has been hindered by the different approaches to the acquisition and processing of the data which can lead to different outcomes, even from identical studies. By focusing on gene expression and metabolic phenotyping, we can gather significant complementary information on regulatory processes and downstream function – both critical to understanding mechanisms of toxicity".

Mark Viant, co-chair of the new group states "We need to address all the roadblocks to translating this highly effective technology of metabolomics into mechanism based safety science. The MERIT project is a critical step towards that goal".

For further details, or to express your interest in commenting upon the best practices and reporting requirements, please contact the MERIT co-Chairs, Dr Tim Ebbels ([t.ebbels@imperial.ac.uk](mailto:t.ebbels@imperial.ac.uk)) or Professor Mark Viant ([m.viant@bham.ac.uk](mailto:m.viant@bham.ac.uk)).

## New Expert Group

Equivalent Level of Concern (ELOC)

REACH Article 57f offers the possibility to identify chemicals which raise equivalent level of concern (ELOC) to CMRs and PBTs (so-called SVHC – substance of very high concern). CARACAL and the JRC proposed to compare different health outcomes by the following aspects:

- Type of possible health effects
- Irreversibility
- Delay of health effects
- Quality of life affected
- Societal concern
- Ability to derive a 'safe concentration'

Concept papers discussing potential criteria exist on these aspects, but no scientific discussion has taken place and no clear scientific criteria were established.

To date Endocrine Disrupting, Respiratory and Strong Skin Sensitizing chemicals have been identified as possible ELoC requiring further review although eMSCAs and ECHA have indicated that other human health endpoints may be included. The objective is to identify effects endpoints that are of ELOC to CMRs and PBTs and to propose science-based criteria for

the identification of candidate chemicals. This project has broad benefits to industry and society on the basis that:

- This focusses regulatory and industry resources to substances of real concern
- Lack of specificity in applying criteria for ELoC will undermine the credibility of the regulatory program.
- The activity should catalyse
- Expert discussion about how to compare the severity of impact of different diseases
- The development of appropriate science-based criteria for identifying substances that are ELoC across different toxicological endpoints.

## New Task Force

### DNEL Derivation Guidance

The ECETOC DNEL Derivation Guidance (2010) – which provides the technical underpinnings by which many/most of industry DNELs (derived no-effect levels) were developed in 2010 and post-2010 – are using guidance factors that differ from those in ECHA REACH guidance and Member States and ECHA generally challenge these when used.

A problem is that in many cases, the ECETOC guidance

factors have been applied but with insufficient supporting documentation (only citation to ECETOC report, rather than substance specific data to support). There is a need to provide scientific underpinnings for the values suggested by ECETOC 2010.

The joint ECHA RAC and SCOEL Task Force on 'Scientific aspects and methodologies related to the exposure of chemicals at the workplace' stated that the multiplication of default or specific AFs/UFs was a broadly supported and well-developed approach; the defaults are only used when there are no robust substance specific data available, with which to work. The overall recommendations from the Task Force were for the RAC "to assess the need to review ECHA Guidance on IR&CSA Chapter R8, to better reflect workplace risk assessment needs" and for the SCOEL "to explain and clarify how uncertainties have been taken into account in recommendations for OELs".

Thus, this ECETOC DNEL Task Force is in a good position to develop a language that can be included into REACH dossiers with the scientific basis of factors applied to the DNELs, including examples of chemical specific data, and an evaluation of current state of sciences to further support or refine ECETOC DNEL Derivation Guidance (2010) with possible probability data inclusion.

## Recent Events

### Advances in high tier environmental exposure modelling: Bridging the gaps between research and practical application

ECETOC Workshop, 04-05 May 2017, Brussels, Belgium

Assessing environmental exposure of chemicals used in commerce is a challenging, but critical part of assessing environmental risk. Approaches to assess exposure can vary between regulatory bodies. For instance, in Europe differences in estimating PECs vary between general chemicals, regulated under REACH, plant protection products (PPP), as defined by the PPP regulation (EC) No 1107/2009, and pharmaceuticals, regulated by the European Medicines Agency. Nonetheless, a common objective is to ensure the assessment is transparent, robust, and utilizes the latest advances in scientific developments, while at the same time providing a reasonable level of conservatism, necessary to account for associated uncertainties and natural variance in the environment that might influence the reliability of the exposure assessment.

During the last three decades, exposure models have played an important role in the assessment process, and when coupled with empirical data, provide reliable information regarding the exposure of chemicals to humans and the environment. An important group of models that have evolved and used within regulatory applications are the Mackay-type fugacity multimedia environmental fate models. During this time, there have been several opportunities that have enabled timely reflections of the state-of-the-art, regarding the use of exposure models. Beginning in 1994, a workshop was organised by the Society of Environmental Toxicology and Chemistry (SETAC) at Leuven, Belgium, 14-16 April, 1994 and then again at Denver, Colorado, 4-5 November, 1994, which brought together 28 model users and developers to discuss the application of the models, to evaluate their performance, to provide guidance on their use, and to make recommendations on how the models could be improved in an effort to strengthen the broader acceptability

and use of environmental fate models (Cowan, C.E, et al.<sup>1</sup>). Then in Ottawa, Canada, 29-31 October, 2001, an OECD/ UNEP Workshop was organised to assess the use of multimedia models for estimating overall environmental persistence and long-range transport in the context of POPs/PBTs Assessment, and which led to the publication of a number of studies (Fenner, K., et al.<sup>2</sup>) (Wegmann, F., et al.<sup>3</sup>). Then in 2010, MacLeod et al. (MacLeod, M., et al.<sup>4</sup>) published a feature article that reflected on the state-of-the-art in multimedia modelling at that time.

It is also notable that a number of related projects funded by CEFIC have also aimed at advancing the application of exposure models in risk assessment, specifically, ECO3A-UTA, ECO3A-DELFT, ECO4-RIVO, ECO13, ECO21, ECO26-RAD, ECO31, EEM6-INTE, EEM6-UCCRA, and EEM6-TECH. Furthermore, ECETOC have published several technical reports in which the use of models features prominently, including TR-29, 50, 61, 67, 73, 74, 76, 82, 90, 98, 111, 112, and 123, as well as three related workshop reports that primarily addressed persistence, WR-24, 10, and 01, which addressed the availability, interpretation, and use of environmental monitoring data. Lastly, industry specific workshops on the development and application of exposure models associated with the use of biocidal ingredients used in agricultural practices represent important events that bring together users and developers to address the state-of-the-art.

While there has clearly been a great deal of resource directed towards activities aimed at advancing the use and application of exposure models, the time is ripe to reflect on the use of exposure models used across the different industry sectors and regulatory bodies.

Attended by sixty international scientific experts from industry, academia and regulatory agencies, this 2-day workshop provided an opportunity to bring together users and developers of environmental fate models used in assessing exposure, with an emphasis on the following key themes:

1. Review recent advances in exposure models, with

a particular emphasis targeting tools that help to better quantify uncertainties associated with both information gaps and the variance in environmental properties and emission scenarios generally understood as being key parameters requiring refinement necessary to strengthen confidence in PEC estimates.

2. Identify and assess feasibility of models and research capable of being representative of harmonised approaches for assessing exposure between the different industry sector groups, and which build on the strengths of the various approaches.

3. Address applicability domain challenges, including chemical, spatial, and temporal. To this end, research aimed at novel methods used towards improving estimates of emissions, developments in the handling of polar, ionised, and other chemicals with properties outside the applicability domain of existing exposure models, advances in tools aimed at integrating environmental fate models with ecological and/or effects models, either as screening-level or high-tiered tools.

4. Discuss and capture advances related to the exposure assessment of chemical mixtures as well as tools capable of addressing the exposure of both the parent chemical and transformation products.

5. Identify best practices for addressing the influence of non-chemical stressors on chemical exposure.

A Workshop Report is currently being prepared for publication in the Autumn and a number of papers in peer-reviewed journals are anticipated.

### References

1. Cowan, C.E., et al., The Multi-Media Fate Model: A vital tool for predicting the fate of chemicals. 1995, Pensacola, FL: SETAC Press.
2. Fenner, K., et al., Comparing Estimates of Persistence and Long-Range Transport Potential among Multimedia Models. *Environmental Science & Technology*, 2005. 39(7): p. 1932-1942.
3. Wegmann, F., et al., The OECD software tool for screening chemicals for persistence and long-range transport potential. *Environmental Modelling & Software*, 2009. 24(2): p. 228-237.
4. MacLeod, M., et al., The State of Multimedia Mass-Balance Modeling in Environmental Science and Decision-Making. *Environmental Science & Technology*, 2010. 44(22): p. 8360-8364.

In addition, the ECETOC Technical and Workshop Reports referred to are freely available at the ECETOC website.

## Upcoming Events



### When Omics Meet Regulations

ECETOC Workshop Session at EUROTOX 2017, 11 September 2017, Bratislava, Slovakia

The robust and reproducible production, storage, analysis and application of omic data in regulatory decision making will require the validation and standardisation of best laboratory practices and use of standardised frameworks. This Workshop will look to begin establishing guidelines and best practices

for attaining, analysing and applying omic data in regulatory decision making. The acceptance and establishment of standardised practices and guidelines will provide confidence for regulators and registrants to interpret and apply omic data in regulatory decision making.

For more detailed information, visit the EUROTOX 2017 website: <http://www.eurotox2017.com/monday/>

### ECETOC AGM and 40<sup>th</sup> Anniversary Reunion

21 March 2018, Brussels, Belgium

See page 2 for more details.

## Publications

### Publications since the last newsletter in April 2017

The following publications are currently in press and will be available in the coming months.

- Set of Papers reporting the outcome of the ECETOC Workshop on Applying 'omics technologies in chemicals risk assessment, held 10-12 October 2016, Madrid, Spain

- Technical Report: Sufficiency of aquatic hazard information for environmental risk assessment

- Technical Report: Exploring community-based environmental hazard assessment of mixtures based on mode-of-action (MOA)-based approaches

The full catalogue of ECETOC publications can be downloaded at <https://goo.gl/aAhiS>



ECETOC reports are freely available from the ECETOC website: [www.ecetoc.org/publications](http://www.ecetoc.org/publications)

Newsletter graphics: Thanks to anamontreal on Flickr: <https://www.flickr.com/photos/30236331@N06/5927216681> Under the CC BY-SA 2.0 licence - <http://creativecommons.org/licenses/by/2.0/>

## EUROPEAN CENTRE FOR ECOTOXICOLOGY AND TOXICOLOGY OF CHEMICALS

Avenue E. Van Nieuwenhuyse 2 Bte. 8, B-1160 Brussels, Belgium  
Tel: +32 2 675 3600 Fax: +32 2 675 3625 VAT: BE 0418344469

Visit [www.ecetoc.org](http://www.ecetoc.org) or e-mail [info@ecetoc.org](mailto:info@ecetoc.org) for more information about ECETOC and to download ECETOC reports free of charge