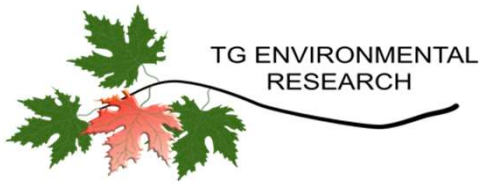


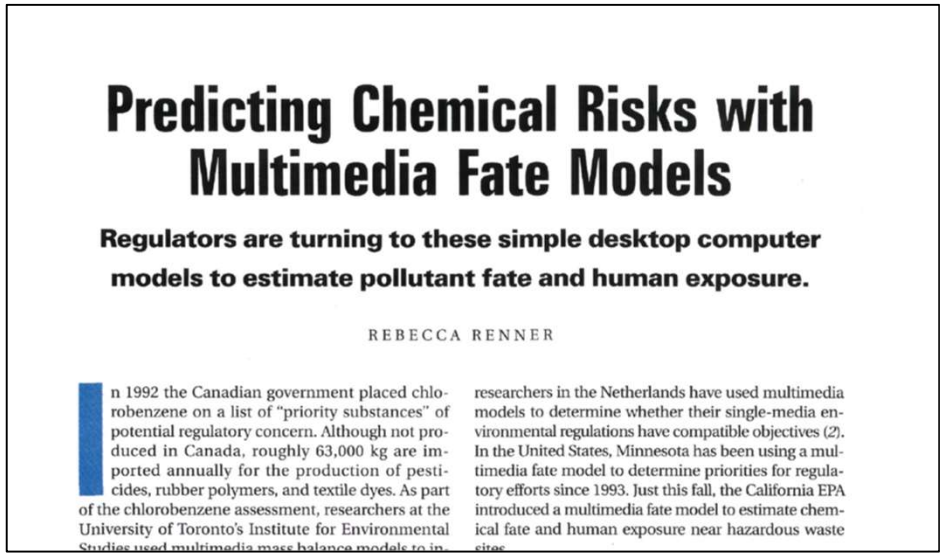
Exposure modelling in environmental risk assessment

Exposure Assessment

- In its most basic form assessing the exposure of chemicals involves quantifying the mass of chemical present relative to the exposure medium of interest (i.e. air, water, soil, sediment, biota)
- Quantifying the mass of chemical requires information on its use and release in commerce
  - i.e. Characterization and assessment of all uses and releases
- Quantifying the mass of chemical present in a specific environmental matrix requires an understanding of its fate and behaviour within the environmental
  - i.e. degradation and partitioning properties
- Standardized tests are typically used to characterize degradation and partitioning properties, which are then used as input into an environmental fate/exposure model

The role of environmental fate models

- >2 decades of use in assessing exposure within regulatory frameworks



Predicting Chemical Risks with Multimedia Fate Models

Regulators are turning to these simple desktop computer models to estimate pollutant fate and human exposure.

REBECCA RENNER

In 1992 the Canadian government placed chlorobenzene on a list of "priority substances" of potential regulatory concern. Although not produced in Canada, roughly 63,000 kg are imported annually for the production of pesticides, rubber polymers, and textile dyes. As part of the chlorobenzene assessment, researchers at the University of Toronto's Institute for Environmental Studies used multimedia mass balance models to in-

researchers in the Netherlands have used multimedia models to determine whether their single-media environmental regulations have compatible objectives (*2*). In the United States, Minnesota has been using a multimedia fate model to determine priorities for regulatory efforts since 1993. Just this fall, the California EPA introduced a multimedia fate model to estimate chemical fate and human exposure near hazardous waste sites

Renner, R. (1995). "Predicting chemical risks with multimedia fate models." Environ Sci Technol **29(12): 556A-559A.**

TABLE 1

Leading multimedia fate models

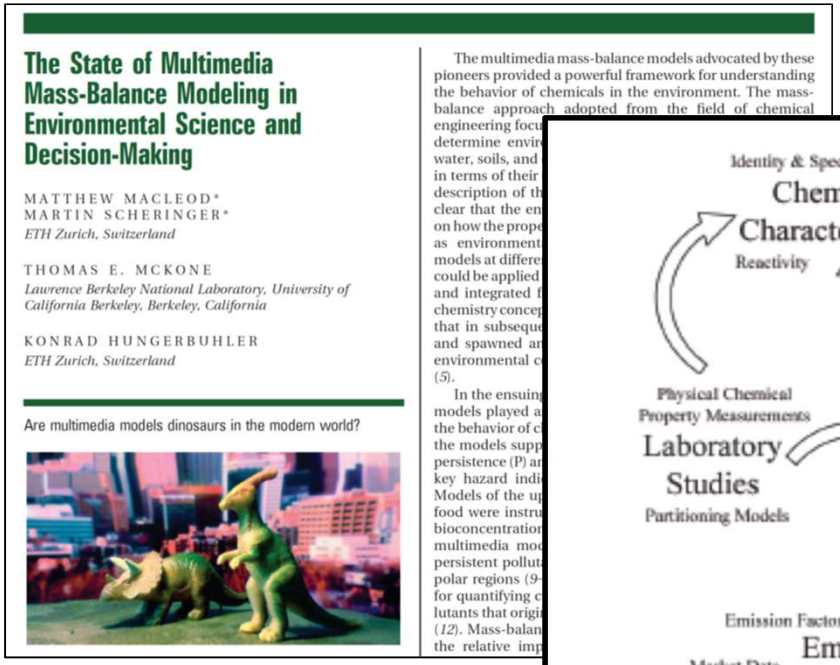
These four models were the subject of recent round-robin evaluations to address concerns of researchers and regulators that different models did not consistently produce comparable results. The models can be used to evaluate fates of chemicals that partition into all media and those soluble in water, but not metals, minerals, polymers, or speciating chemicals.

Model name	Description	Developer
CalTOX	Fugacity model combining a soil-layer model with a four-compartment Level III model; includes terrestrial vegetation compartment but not aquatic biota. Numerical solution method: Excel. Default environments: residential, commercial, and industrial landscapes in California.	Tom McKone, Lawrence Livermore National Laboratory, University of California–Davis
ChemCAN	Level III model with four main compartments and numerous subcompartments; vegetation included in add-on indirect exposure model. Numerical solution method: analytical solution. Default environments: 24 Canadian regions plus generic areas.	Donald Mackay, University of Toronto–Ontario
HAZCHEM	Level III model with four compartments; vegetation included in add-on indirect exposure model. Numerical solution method: matrix inversion routine. Default environments: 10 European regions and generic European.	European Center for Ecotoxicology and Toxicology of Chemicals, Brussels, Belgium
SimpleBOX	Level III model with six compartments (including aquatic biota, suspended solids as separate compartments); vegetation included in add-on indirect exposure model. Numerical solution method: compiled Lotus 1-2-3 spreadsheet.	Dik van de Meent, National Institute of Public Health and Environmental Protection, Bilthoven, the Netherlands

Source: Reference 1.

Cowan, C. E., et al. (1995). The Multi-Media Fate Model: A vital tool for predicting the fate of chemicals. Pensacola, FL, SETAC Press.

Repositories of knowledge and conceptual understanding



The State of Multimedia Mass-Balance Modeling in Environmental Science and Decision-Making

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Are multimedia models dinosaurs in the modern world?

The multimedia mass-balance models advocated by these pioneers provided a powerful framework for understanding the behavior of chemicals in the environment. The mass-balance approach adopted from the field of chemical engineering focu
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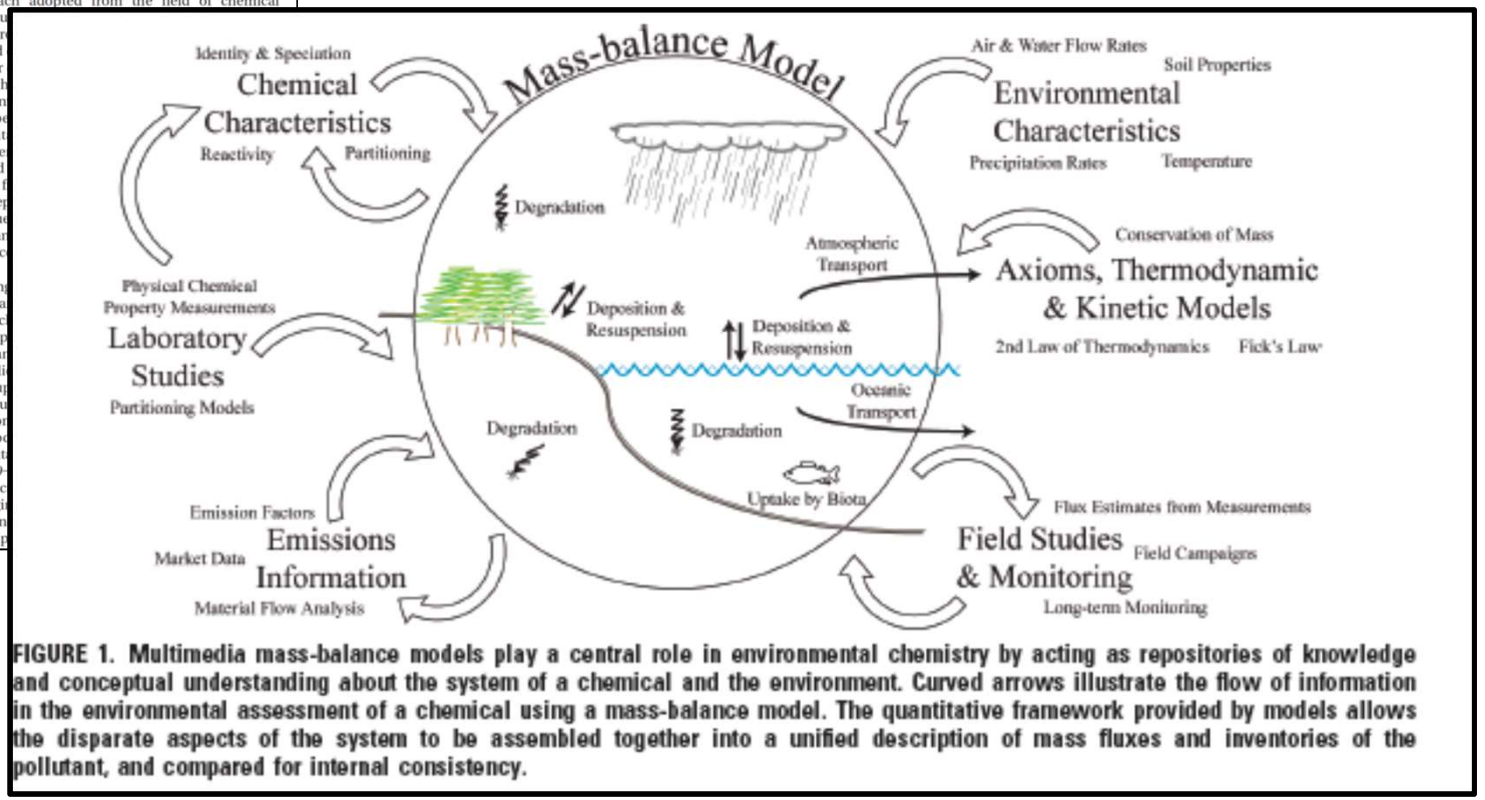


FIGURE 1. Multimedia mass-balance models play a central role in environmental chemistry by acting as repositories of knowledge and conceptual understanding about the system of a chemical and the environment. Curved arrows illustrate the flow of information in the environmental assessment of a chemical using a mass-balance model. The quantitative framework provided by models allows the disparate aspects of the system to be assembled together into a unified description of mass fluxes and inventories of the pollutant, and compared for internal consistency.

MacLeod, M., Scheringer, M., McKone, T. E., & Hungerbuhler, K. (2010). The State of Multimedia Mass-Balance Modeling in Environmental Science and Decision-Making. *Environmental Science & Technology, 44(22), 8360-8364.*

The role of models in the decision making process

- **Archives** of contemporary knowledge
- Enable the **interpretation** of links between health and environmental harm due to environmental releases
- Provide the practical **tools** necessary for prospective and perspective analysis to support the decision making process
- Enable the **communication** of complex relationships to the general public
- Provide **guidance** towards addressing gaps in contemporary knowledge.

Continuing challenges

- Often recognized as a weak point in both environmental and human health risk assessment
  - i.e. high level of uncertainty in assessing exposure can greatly impact decision-making process.
- Some of the key challenges include:
  - Poor understanding of use/tonnage and release of chemicals used in commerce
  - Widespread use of over-conservative ‘worst-case’ scenarios
  - Lack of integrated approaches for addressing combined stressors
  - Provides estimates of external environmental concentrations that are poorly linked to internal biological concentrations
  - Lack of identification of key exposure drivers
- In an effort to address existing challenges, tiered approaches are often used with a heavy reliance on models to prioritize and guide the decision making process

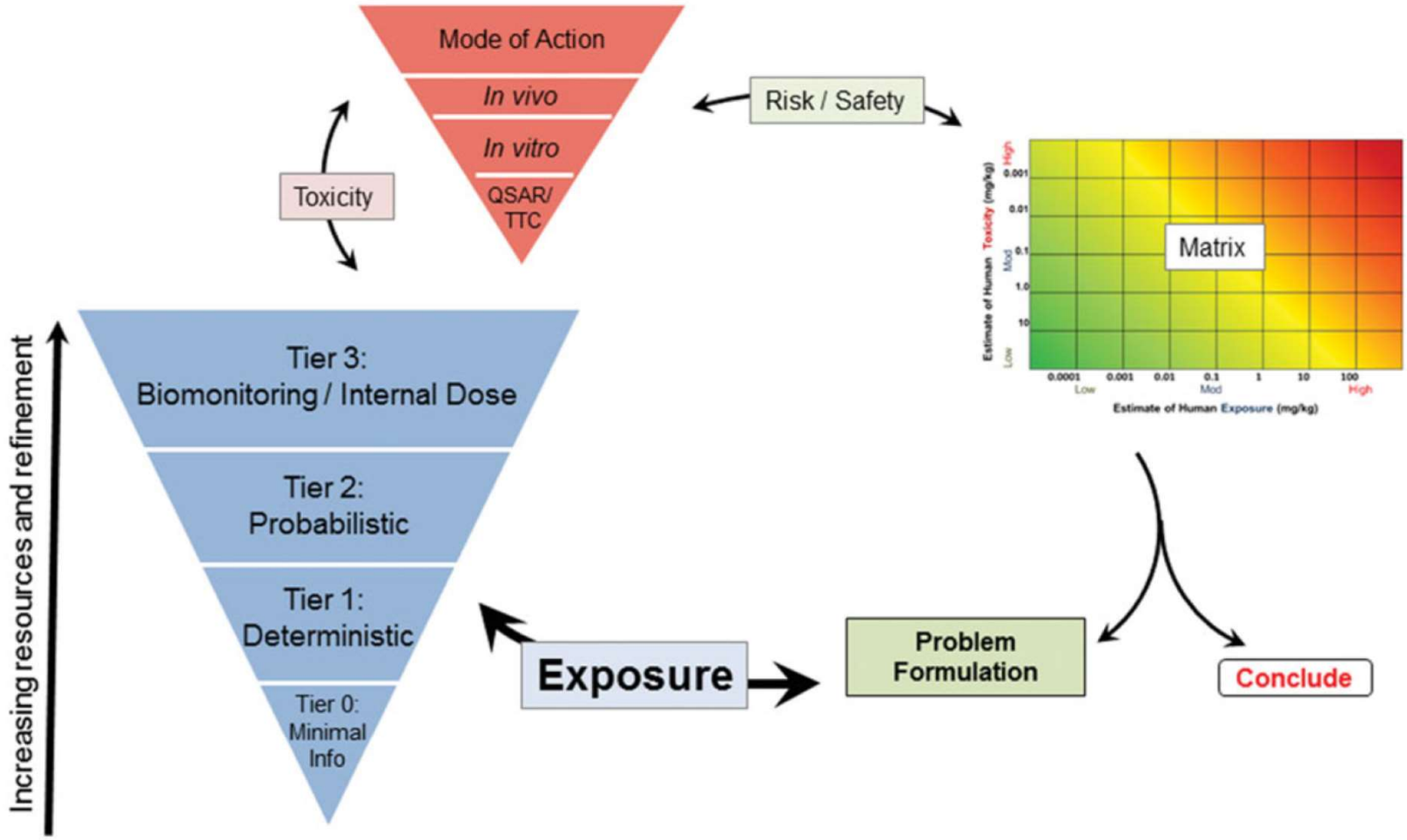
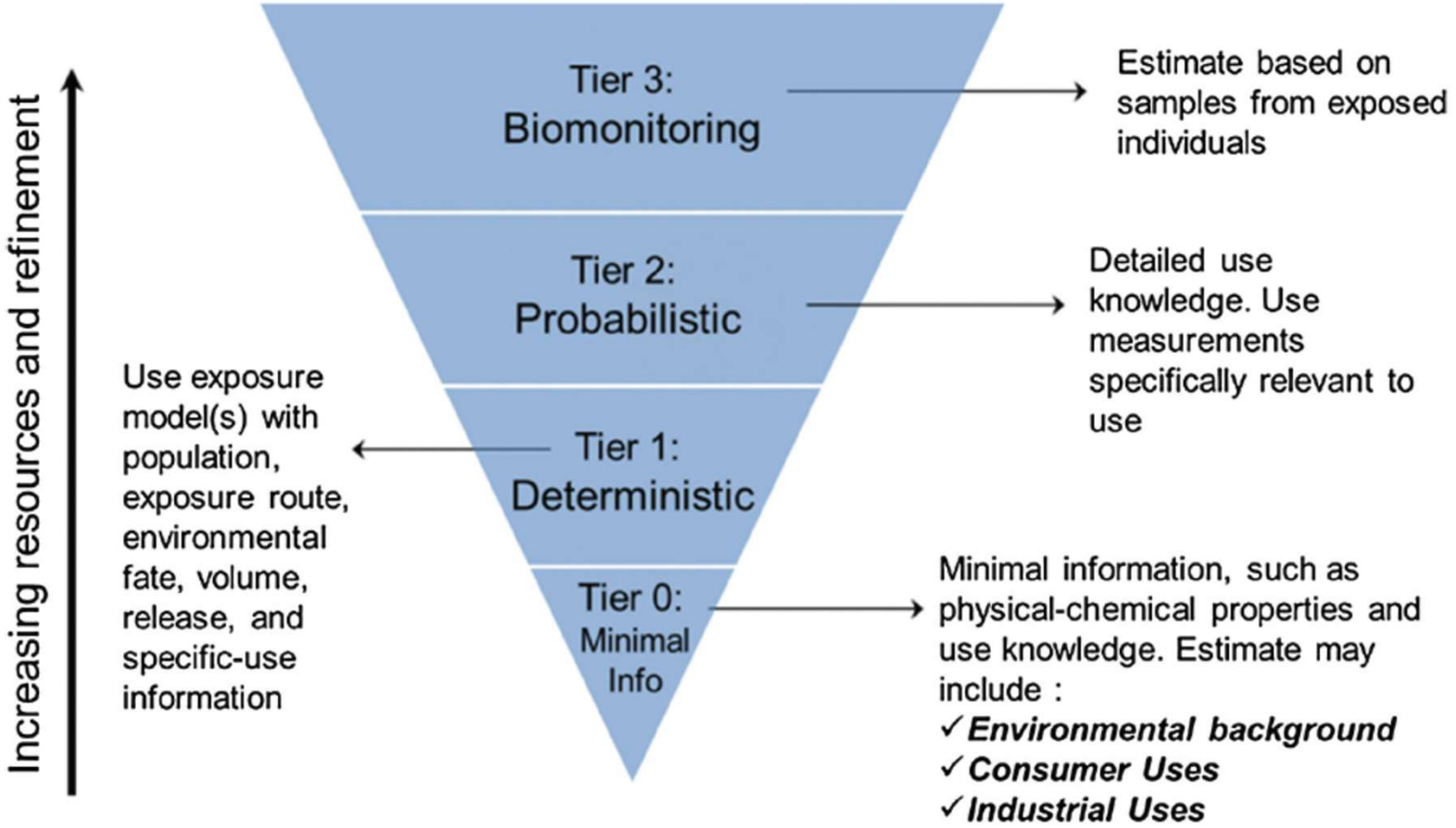


Figure 1. RISK21 tiered exposure assessment framework in the context of the RISK21 framework.

Embry, M. R., Bachman, A. N., Bell, D. R., Boobis, A. R., Cohen, S. M., Dellarco, M., . . . Doe, J. E. (2014). Risk assessment in the 21st century: roadmap and matrix. *Crit Rev Toxicol, 44 Suppl 3, 6-16.*


Increasing resources and refinement
Tier 3:
Biomonitoring
Estimate based on samples from exposed individuals
Tier 2:
Probabilistic
Detailed use knowledge. Use measurements specifically relevant to use
Use exposure model(s) with population, exposure route, environmental fate, volume, release, and specific-use information
Tier 1:
Deterministic
Tier 0:
Minimal Info
Minimal information, such as physical-chemical properties and use knowledge. Estimate may include :
✓Environmental background
✓Consumer Uses
✓Industrial Uses

Differences between industry sectors

- Regulatory requirements for estimating environmental exposure can differ depending on the use of a chemical as a pharmaceutical, plant protection product, or as a general chemical
- Chemicals used as pharmaceuticals or plant protection products can be characterized as being biologically active, whereas the majority of general chemicals are estimated to be baseline toxicants.
- Differences in inherent toxicity and use patterns has led to differences in the exposure assessment
  - General Chemicals as regulated under REACH, TSCA, the Canadian Environmental Protection Act (CEPA) 1999, etc.
  - Plant Protection Products as regulated in EU under Regulation (EC) No 1107/2009, US EPA Office of Pesticide Programs, the Canadian Pest Management Regulatory Agency (PMRA), etc.
  - Pharmaceuticals as regulated by European Medicines Agency, US Food and Drug Administration, Health Canada, etc.

Some useful links

- US EPA ExpoBox Tool
  - https://www.epa.gov/expobox
- OECD Environmental Risk Assessment Toolkit
  - http://envriskassessmenttoolkit.oecd.org/
- ECHA Information Toolkit
  - https://echa.europa.eu/en/support/information-toolkit
- CHEmical Safety Assessment and Reporting tool (chesar)
  - https://chesar.echa.europa.eu/
- CEFIC-LRI Toolbox
  - http://cefic-lri.org/lri-toolbox/
- Pesticide fate models
  - http://www.pfmodels.org/links.html
    - FOCUS DG Sante
      - http://esdac.jrc.ec.europa.eu/projects/focus-dg-sante
- Environmental risk assessment of pharmaceuticals
  - http://www.ema.europa.eu/ema/index.jsp?curl=pages/regulation/general/general_content_001004.jsp&mid=WC0b01ac0580a4aa6a
- MERLIN Exposure model
  - http://4funproject.eu/
- USETOX
  - http://www.usetox.org/
- RAIDAR
  - http://www.arnotresearch.com/#!/page_RAIDAR_DL
- Human consumer exposure to chemicals
  - http://www.rivm.nl/en/Topics/C/Consumer_exposure_to_chemical_substances