LRI TOOLBOX

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YOUR ONLINE SOLUTION TO CHEMICAL RISK ASSESSMENT

The LRI Toolbox provides European and national regulatory agencies, industry and academia with a selection of state-of-the-art, easy-to-use tools for better research, analysis and visualisation purposes, for use in risk assessment and toxicity testing of chemicals.

They can be used both in preparation of regulatory filings such as REACH (Registration, Evaluation, Authorisation and Restriction of Chemicals) and GHS (Globally Harmonized System of Classification and Labelling of Chemicals), as well as for research and development purposes.

LRI Long-Range Research Initiative

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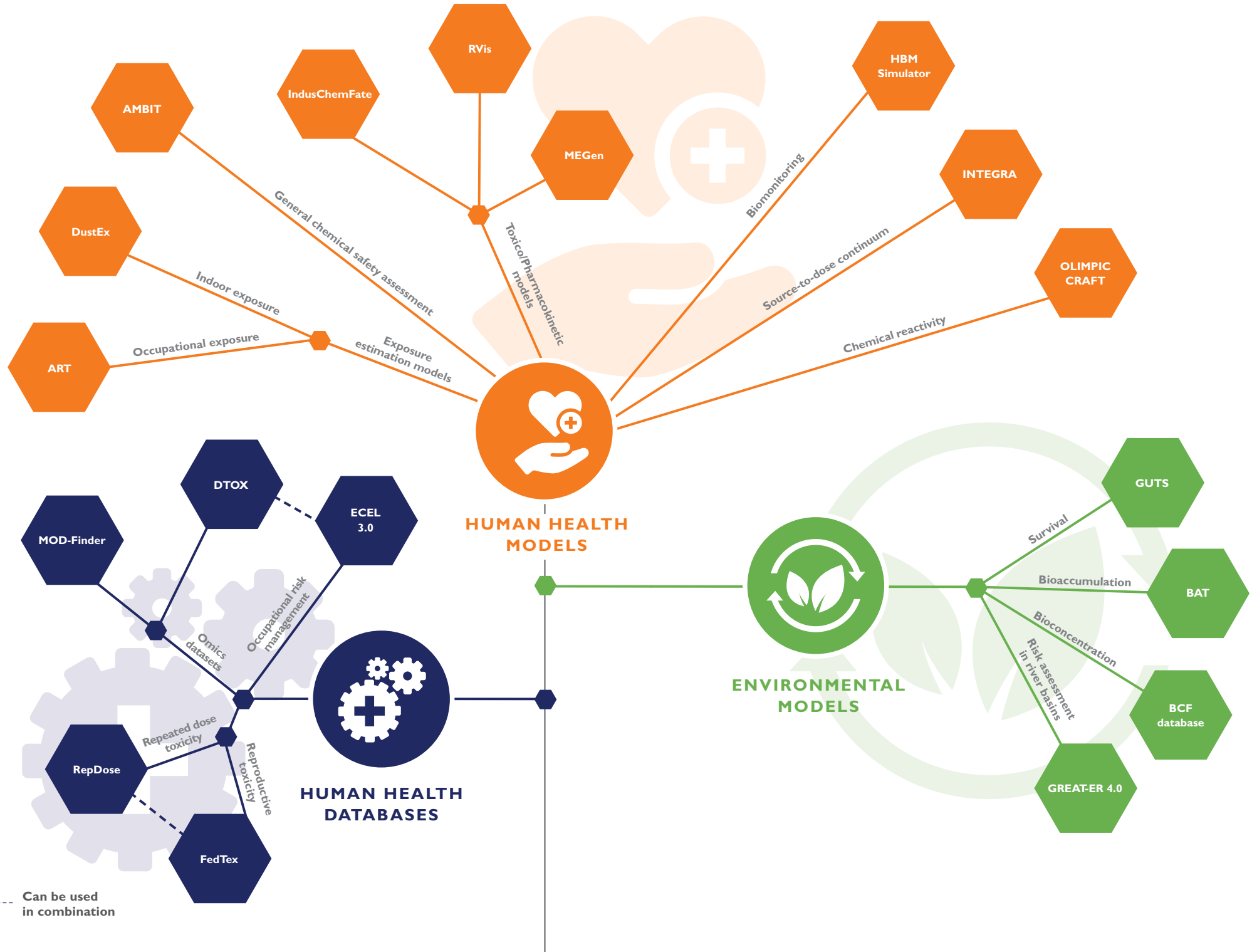
AMBIT
IndusChemFate
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ART
General chemical safety assessment
Toxico/Pharmacokinetic models
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Survival
Bioaccumulation
BAT
Bioconcentration
BCF database
Risk assessment in river basins
GREAT-ER 4.0
Can be used in combination

HUMAN HEALTH DATABASES

DTOX

Demonstrating chemical, physical and toxicological properties for a compound and its structural or biological analogues

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The DIAMONDS' Toxicity Toolbox (DTOX) helps strengthen traditional read-across techniques by providing tools to combine structural similarities with similarities based on biological responses (e.g. processed transcriptomics data).

ECEL 3.0

Assessing the effectiveness of control measures

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ECEL 3.0 is a searchable library of occupational and environmental Risk Management Measures (RMM) that provides information on the quantitative effectiveness of control measures.

REPDOSE

Performing analyses on repeated dose toxicity

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RepDose is a relational database on experimental NOEL and LOEL values for various repeated dose toxicity endpoints. The content and structure of the database RepDose provides a sound basis to perform analyses on repeated dose toxicity.

FEDTEX

Assessing fertility and developmental toxicity in experimental animals

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FedTex enables the evaluation of reproductive toxicity data on fertility and developmental effects of 100 chemicals. Affected parameters and effects are documented in relation to the development stage, gender and generation. FedTex addresses reproductive toxicity including one-, two- and three-generational studies.

MOD-FINDER

Finding compound-related multi-omics datasets in public databases

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The Multi-Omics Dataset Finder (MOD-Finder), an R Shiny application, was developed to efficiently search for compound-related omics datasets (transcriptome, proteome, metabolome) in an automated manner. Several publicly available databases are automatically queried for datasets with relation to a user specified compound or toxicant. The MOD-Finder application works as an easy-to-use webservice.

ENVIRONMENTAL MODELS

BAT

A quantitative weight of evidence framework to aid bioaccumulation assessment

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The accumulation of chemical substances in living organisms is a complex process, and one of increasing interest to regulatory agencies. The Bioaccumulation Assessment Tool (BAT) facilitates the systematic and transparent integration of information in a consistent framework to inform bioaccumulation assessment decision-making.

GREAT-ER 4.0

Environmental risk assessment and management of chemicals in river basins

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GREAT-ER (Geo-referenced Regional environmental Exposure Assessment Tool for European Rivers) is an advanced environmental exposure model for environmental risk assessment and management of chemicals in river basins, for use in the European chemicals risk assessment process (REACH), and in the EU Water Framework Directive (WFD).

BCF DATABASE

Deriving bioconcentration factor values

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The classical approach to derive bioconcentration values (using the OECD 305 bioconcentration test) is labour intensive, costly and requires a lot of test animals. BCF is a gold standard database allowing the derivation of bioconcentration factor values from existing information.

GUTS

Modelling survival of organisms through time under time-variable exposure to chemicals

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Making sense of organism survival after exposure to toxicants requires mechanism-based models, known as toxicokinetic-toxicodynamic (TKTD) models. For mortality, almost all published TKTD models can now be viewed as members of an over-arching framework: the General Unified Threshold model of Survival (GUTS). The GUTS software is a user-friendly, robust, freely-available and open-source software for standard GUTS applications.

HUMAN HEALTH MODELS

AMBIT

Facilitating chemical safety assessment

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The AMBIT system consists of a database including more than 450 000 chemical structures and REACH datasets for 14 570 substances, for which access was given to Cefic-LRI by ECHA. Users can search and access a wide range of existing information (structures, substructures, IUCLID6 data, etc.) and predictions (read-across, category formation, data analysis and exchange, etc.) about a specified chemical. This process makes the tool both unique and powerful, particularly for data-poor small and medium-sized enterprises and contributes to a reduction in testing and innovation costs.

DUSTEX

Estimating human exposure to substances released from products and articles in the indoor environment

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The DustEx model is used to assess exposure to semi-volatile substances (SVOCs) in products that are introduced into the indoor environment. The typical products considered are solid material products (e.g. flooring, wall covering, electronic devices) from which substances are released into indoor air and subsequently transported into different indoor compartments, airborne particles, indoor surfaces and dust. Exposures take place from inhalation, dermal absorption and oral ingestion.

ART

Estimating inhalation exposure

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The Advanced REACH Tool (ART) incorporates a mechanistic model of inhalation exposure and a statistical facility to update exposure estimates with the user's own data. This combination of model estimates and data produces more refined estimates of exposure and reduced uncertainty.

HBM SIMULATOR

Investigating the representativeness of spot biomonitoring samples

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HBM Simulator was developed to allow researchers and regulators to quickly investigate the representativeness of spot biomonitoring samples in relation to different exposure patterns and chemical-related properties, including half-life, and to estimate how this is affected by creatinine correction or multiple sampling strategies. This tool also provides reverse dosimetry calculations that estimate an individual's likely exposure given their measured biomarker concentration.

HUMAN HEALTH MODELS

INDUSCHEMFATE

Estimating the level of a chemical in various body tissues and body fluids following exposure

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IndusChemFate can be used to estimate the level of a chemical substance in various body tissues and body fluids following inhalation, oral intake or dermal exposure, according to user-defined exposure scenarios. It is regarded as a first tier or screening tool.

MEGEN

Generating and analysing PBPK models

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The MEGen (Model Equation Generator) software is a 'proof of concept' intuitive user interface for the rapid generation and analysis of physiologically-based pharmacokinetic (PBPK) models.

RVIS

Modelling biologically-based and quantitative risk assessment of chemicals

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RVis provides an intuitive, freely available modelling platform for biologically based, quantitative safety and risk assessment of chemicals. It allows the prediction of human in vivo doses from alternative-to-animal testing systems.

INTEGRA

Assessing the source-to-dose continuum for the entire life cycle of chemical substances

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INTEGRA brings together all available information within a coherent methodological framework for assessing the source-to-dose continuum for the entire life cycle of substances covering an extensive chemical space. The major component of INTEGRA is a unified computational platform that integrates environmental fate, exposure and internal dose dynamically in time.

OLIMPIC CRAFT

Evaluating chemical reactivity and fate

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CRAFT is a software suite for the evaluation of chemical reactivity to support scientists working in the area of product safety and hazard assessment. It has been designed to assist toxicologists to interactively evaluate the chemical reactivity, persistence, biodegradation and fate of chemical compounds in the environment.

ABOUT CEFIC-LRI:

The Long-range Research Initiative (LRI) programme of the European Chemical Industry Council (Cefic) serves to increase understanding of the potential impact of chemicals on human health and the environment, and to improve methods for risk assessment. Over the past two decades, the LRI Programme has funded more than 250 research projects through its grants and Innovative Science Award. These projects aim to provide proactive scientific advice on which the entire industry and regulatory bodies draw to respond more quickly and accurately to societal concerns.

Check out the Cefic-LRI tools at:

http://cefic-lri.org/lri-toolbox

cefic

European Chemical Industry Council - Cefic aisbl
www.cefic.org
EU Transparency Register n° 64879142323-90

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