Laboratory of Mathematical Chemistry

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http://oasis-lmc.org/

Solutions for present and future emerging pollutants in land and water resources management
29-31 October 2013, Leipzig

SOLUTIONS

SP T (Tools) — (Lead: UFZ)

T2 - Chemical analytical tools (CAT) — T2.3 Design of a streamlined non-target screening workflow (Lead: Eawag. Contributor: **LMC**); T2.4 Set of interacting compound identification tools (Lead: IPB. Contributors: Eawag, **LMC,** UFZ).

T3 - Effect-directed analysis (EDA) — T3.2 Higher Tier EDA (Lead: UFZ). Integration of structure elucidation approaches for toxicant identification into the EDA workflow (UFZ, IPB, **LMC**).

SP M (Models) — (Lead: Deltares)

M1 - Integrated Models — M1.1 Risk modelling framework (Lead: Deltares. Contributors: all partners in SP Models); M1.2 Europe-wide integrated risk modelling (Lead: Deltares. Contributors: RIVM, SU, **LMC**, Brunel, Mermayde); M1.3. Substances modelling information flows (Lead: RIVM. Contributors: Deltares, Mermayde, **LMC**, UFZ, Mermayde).

M2 - Sources and emission model — M2.1. Collect use information (Lead: RIVM. Contributors: Mermayde, Deltares); M2.2. Emission estimation model (Lead: RIVM. Contributors: Mermayde, Deltares, IVL).

M4 - Substance Metabolism and Properties Modeling (Lead: LMC) — M4.1 Identification of appropriate substance properties modelling approaches and identification of gaps (Lead: UFZ. Contributor: **LMC**); M4.2 Development of models for the prediction of fate-related partition parameters for compounds that are not covered by conventional models (Lead: UFZ. Contributors: UU, **LMC**); M4.3 Assessment and increase of the level of confidence of model predictions (Lead: UFZ. Contributor: **LMC**); M4.4 Structure-based prediction of properties, toxicity and transformation products (Lead: **LMC**. Contributor: UFZ).

SP C (Cases) — (Lead: EI)

C1 - Danube River Basin case study — C1.4. Identification of effect-based site specific toxicants (Lead: UFZ. Contributors: INERIS, NJU, **LMC**, UOB, NIVA, UQ, Brunel, UNS, MAXX, EI, ICPDR).

RESEARCH

Molecular Modeling

Substance identity (discrete substances, tautomers, mixtures, UVCB materials), computational methods (pattern recognition, conformer generation, applicability domain), and databasing (QA of chemical identity, search engine, databases of fate, (eco)toxicity and metabolism data).

Environmental Fate and Ecotoxicity

Models for predicting abiotic and biotic degradation (hydrolysis, autoxidation, Catabol, CATALOGIC 301 B, C and F models), bioconcentration (BCF base-line, half-life in fish) and acute aquatic toxicity (algae, crustaceans, fish).

Human Health Hazard

Models for predicting receptor mediated toxicity (ER, AR and AhR binding affinity, Aromatase inhibition), skin sensitization, in vitro (Ames, chromosomal aberration) and in vivo (liver, bone marrow MNT) genotoxicity.

Metabolism

Simulation of prokaryotic and eukaryotic metabolism - subcellular (micronucleous), cellular (rat liver S9) and in vivo and their implementation in fate and toxicological models (CATALOGIC and TIMES platforms).

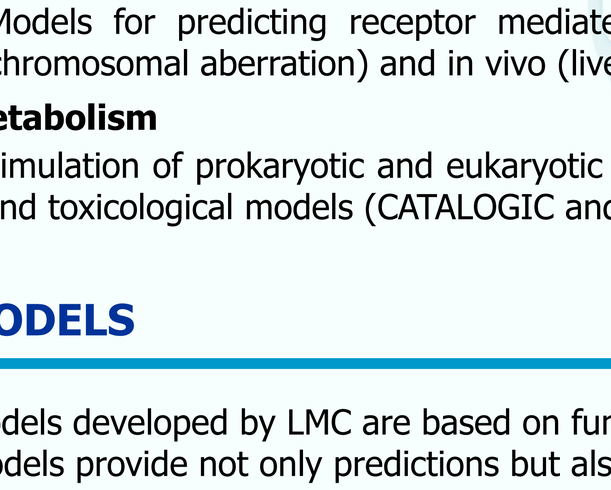
MODELS

Models developed by LMC are based on fundamental understanding of the physics, chemistry and biology governing the modeled phenomena. Our models provide not only predictions but also their mechanistic justification.

BCF base-line model

- Maximum potential for bioaccumulation (log BCF_{MAX})
- Mitigating factors

$$\log BCF = \log\left(\prod_i F_i \frac{{K_{OW}}^n}{(aK_{OW}+1)^{2n}} + F_W F_{WS}\right)$$



F_i – mitigating factors

Mitigating factors
- Metabolism
- Ionization
- Molecular size
- Water solubility

Skin sensitization model

- Metabolic activation of chemicals
  - Pre-electrophilic activation (autoxidation)
  - Pro-electrophilic activation (Phase I and Phase II reactions)
  - Interaction with macromolecules (Protein binding reactions)
- COREPA models for reactivity