

## Toxicology Reports by OntoChem IT Solution

Supporting Bioprofiling,  
Compound Registration,  
Environmental Risk  
Assessment, etc.

Based on our outstanding OCMiner® data and knowledge extraction technology we support you with comprehensive Toxicology & Bioprofile Reports for your chemical compounds, saving your human and financial resources you would otherwise spend for elaborative inquiries and research.

Our Toxicology Reports are ideally suited to assist you in compiling.



### REACH

registration dossiers<sup>1</sup>



### ENVIRONMENTAL RISK

Assessment of medicinal products<sup>2</sup>



### MARKET MONITORING

Post-market surveillance

Our **Toxicology Ontology** knowledge base (OntoToxBase) – validated by an interdisciplinary team of chemists, pharmacists, biochemists and bioinformation scientists – provides an expert background enables us to extract toxicological facts and relationships from virtually all Big Data sources, such as:

- Data bases of regulatory authorities (e.g. ECHA, EFSA, EMA, FDA, EPA etc.)
- Scientific publications
- Books
- Patents
- World Wide Web
- etc.

As of January 2015, our OntoToxBase comprises more than 1,200 validated concepts related to toxic effects, and assigned to toxicity concepts like: Carcinogenicity, Mutagenicity, Phototoxicity, Skin sensitization, Inhalation toxicity, Prenatal development toxicity, and many more.

# ontochem

These concepts meet, for instance, the OECD Guidelines for Testing of Chemicals, and go far beyond that supplying you the most relevant toxicology data for your compound.

As the underlying ontologies comprise human and animal toxicity terms our Toxicology Reports address the impact of your chemical compound on human health as well as environmental aspects. Toxicology Reports are also very helpful for market monitoring, e.g. for the post-market surveillance of medical devices.<sup>3</sup>

Toxicology Reports can be modularly customized:

## HUMAN TOX

Human health aspects in REACH (e.g. DNEL etc. for Chemical Safety Assessment accord. to (EC) No. 1907/2007 Art. 10b, Annex I; CLP Regulation (EC) No. 1272/2008)

- Preparation of IND and IMPD dossiers
- Cosmetics regulations<sup>4</sup>
- Market monitoring<sup>5</sup>

## ENVIRONMENTAL/ ANIMAL TOX

Environmental/animal aspects in REACH (e.g. PNEC, PBT/vPvB properties etc. for Chemical Safety Assessment accord. to (EC) No. 1907/2007 Art. 10b, Annex I; CLP Regulation (EC) No. 1272/2008; identifying data of recent vertebrate studies relevant for registration).

- Environmental Risk Assessment (e.g. of medicinal products accord. to Directive 2001/83/EC) etc.

Additionally, our toxicology prediction module is implementable in the Toxicology Reports. This Onto-ToxPredict module for so far untested chemical compounds is based on Big Data statistical analysis of ontological relations between chemical structures and data and evidences collected for related and similar structures.

Thus, the OntoToxPredict module supports:

- Toxicological pre-evaluation of compound libraries
- Avoiding resource-wasting aberrations in API development
- Avoiding animal trials
- Identifying less harmful alternatives of distinct compounds (e.g. „Substances of Very High Concern’ according to REACH Art. 57)
- Supporting data waiving for REACH annex XI

The format of our Toxicology Reports can be customized according to your needs as they are template-based, for instance pre-filled templates support completion and evaluation of REACH registration dossiers, Environmental Risk Assessment reports etc.

SAVING YOUR  
HUMAN, TIME  
AND FINANCIAL  
RESOURCES.

<sup>1</sup> according to Regulation (EC) No. 1907/2006 including Chemical Safety Assessment

<sup>2</sup> according to Directive 2001/83/EC

<sup>3</sup> according to Directive 2007/47/EC

<sup>4</sup> according to Regulation (EC) No. 1223/2009 on cosmetic products

<sup>5</sup> post-market surveillance of medicinal devices according to Directive 2007/47/EC