CADASTER

CAse studies on the Development and Application of in-Silico Techniques for Environmental hazard and Risk assessment

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Collaborative Project

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Chemical Structures and Molecular Descriptors Database

Due date of deliverable: June 30, 2009
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Start date of project: 1 January 2009 Duration: 4 years

Lead Contractor: National Institute of Public Health and the Environment (RIVM), Laboratory for Ecological Risk Assessment
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Deliverable no: 3.1 (Chemical Structures and Molecular Descriptors Database)
Nature: Prototype

Project co-funded by the EU Commission within the Seventh Framework Programme		
Dissemination Level		
PU	Public	X
RE	Restricted to a group specified by the consortium (including the Commission Services)	
CO	Confidential, only for members of the consortium (including the Commission Services)	

CADASTER

WP 3: Development and validation of QSARs

Work Package Leader: Paola Gramatica (Partner 3: University of Insubria)

Task 3.1- Chemical Structures and molecular descriptors database (Deliverable 3.1)

Overview

With regard to the database on chemical structures and molecular descriptors, two basically different activities may be distinguished:

1 – Design of the database: taking into account future usage needs foreseen at this stage, whilst still being flexible.

2 – Filling of the database and subsequent supplementing of descriptor values in the database upon inclusion of new chemicals.

In agreement with the CADASTER-planning, the design of the database was completed in June 2009 (i.e. within the first 6 months of the project). The database is made available via the project website CADASTER.eu. Thereupon, the database is filled with the relevant information on molecular descriptors (as specified below) for chemicals belonging to the four classes of interest for the CADASTER project for which at least one experimental data was available or are structurally related or for their specific usage (for example: the set of 240 flame retardants is composed of 209 congeneric PBDE's plus 31 chemicals with different structures that are also flame retardants).

Activity 2 is a continuous activity which was performed for the chemicals currently in the database. This activity will be continued for all new chemicals that will be introduced in the database during the course of the project.

Deliverable 3.1, consisting of chemical structures and DRAGON Descriptors in pdf files, is thus available for use.

Activities performed

Chemicals of the four classes of interest were collected from the literature and the ChemIDplus database (http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp). The majority of the corresponding experimental data have already been uploaded in the web-prototype 'New-Tox' (for WP2).

The drawing, the conformational analysis and geometry minimization of chemicals were done by the semi-empirical method AM1 in the software package Hyperchem (rel. 7.03 for Windows, 2002. Hypercube, Inc., Florida, USA). The files *.hin and *.mol have been saved in the attached zip files and sent to HMGU (partner 6 of CADASTER) for uploading in the web-prototype.

DRAGON descriptors (ver. 5.5 for Windows, Talete srl., 2007) have been calculated starting from the x,y,z coordinates of the chemical structure .

Deliverable 3.1, consisting of chemical structures and DRAGON Descriptors in pdf files, is thus available for use within the Project Partners. The consistency of the database is, so far, as following:

- **Flame retardants, including PBDEs: 240 structures and 1403 molecular descriptors**
- **PolyFluorinated chemicals, including their transformation products: 366 structures and 1862 molecular descriptors**
- **Fragrances: 79 structures and 1429 molecular descriptors**
- **Triazoles and Benzotriazoles: 279 structures and 1879 molecular descriptors**

The appendix to this report contains the chemical structures and the molecular descriptors calculated for each of the chemicals. The appendix is arranged according to the four classes of chemicals identified within CADASTER.

The other partners involved in WP3 (Partners 4, 5, 6, 7) will supplement the database, in the next months, with additional chemical structures and/or molecular descriptors.

In particular, it can be previewed that, following contacts with RIFM and Dupont, fragrances and PFAS chemicals will be implemented.

APPENDIX

Chemical structures and molecular descriptors calculated for all chemicals for which at least one experimental data was available or are structurally related or for their specific usage. The chemicals and additional information are arranged according to the four classes of chemicals identified within CADASTER:

1 - Flame retardants, including PBDEs: 240 structures and 1403 molecular descriptors

2 - PolyFluorinated chemicals, including their transformation products: 366 structures and 1862 molecular descriptors

3 - Fragrances: 79 structures and 1429 molecular descriptors

4 - Triazoles and Benzotriazoles: 279 structures and 1879 molecular descriptors