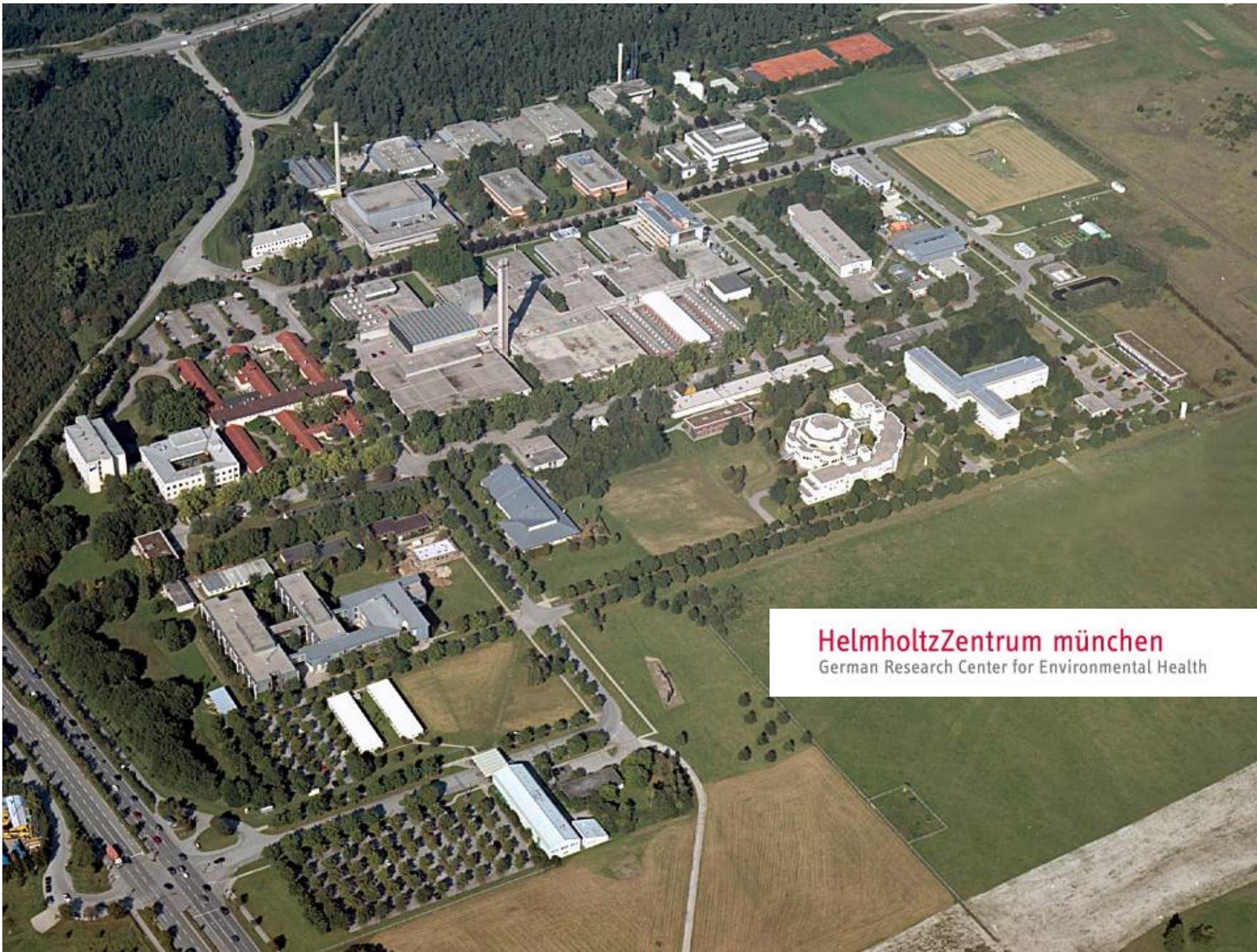


# CADASTER & MC ITN ECO

***Igor V. Tetko***

Chemoinformatics group, IBIS, Helmholtz Zentrum München &  
eADMET GmbH (Germany)

***SPRING workshop, Beijing, July 2-3, 2011***



**HelmholtzZentrum münchen**

German Research Center for Environmental Health

# Helmholtz Zentrum München

- Part of Helmholtz Association (17 centers, €3.3 billion, 33000 people)
- Leading center for Environmental Health in Germany
- 25 institutes (1879 people, 607 scientists & 307 PhD students)
- >70 contracts with EU (2 MC ITN, "ECO" and "GOODWATER")
- Disciplines
  - Biology 41%
  - Chemistry/biochemistry 14%
  - Physics 10%
  - Medicine 7%
- Chemoinformatics group, Institute for Bioinformatics & Systems Biology
  - 10 peoples, strong expertise in *in silico* data analysis, machine learning methods, chemoinformatics software development, data dissemination

# REACH

Registration, Evaluation, Authorisation and  
Restriction of Chemical substances



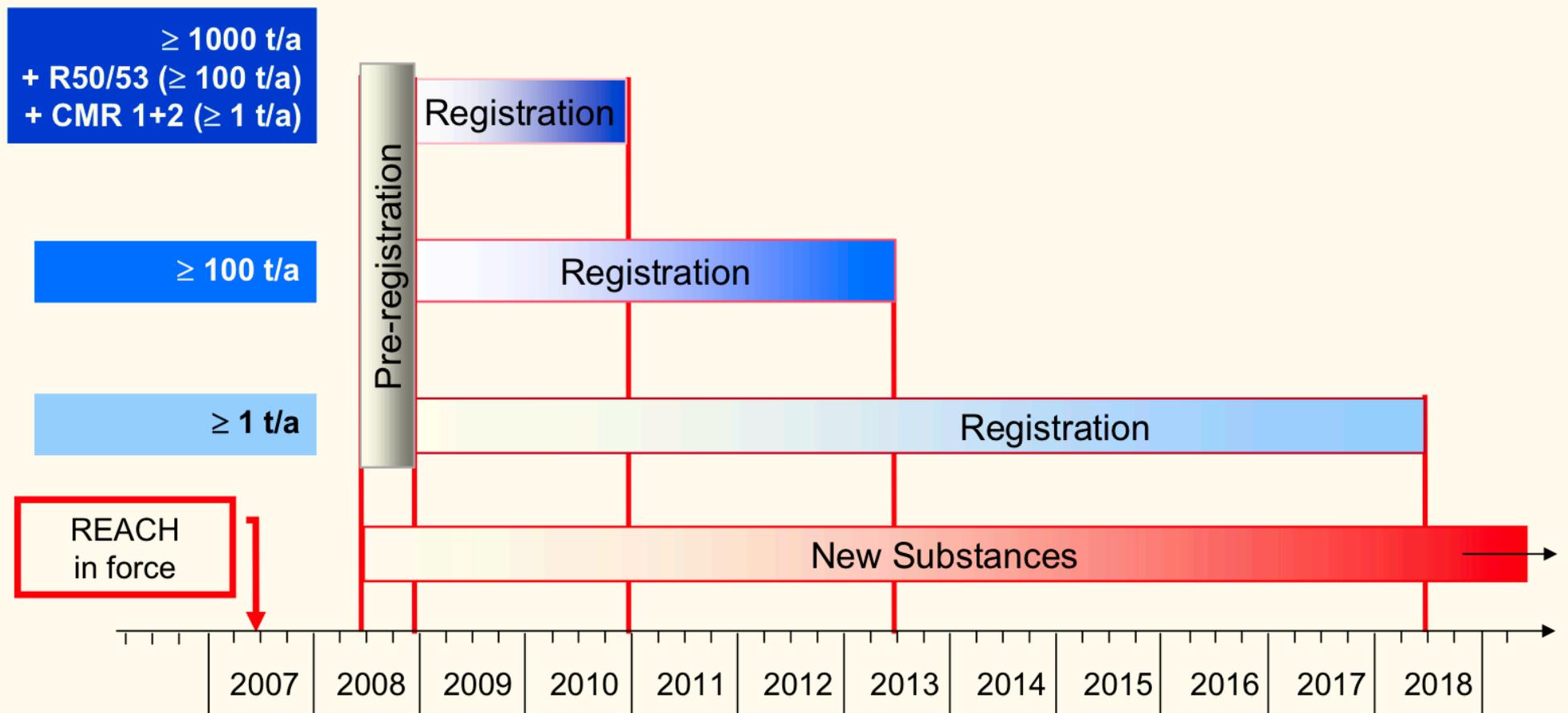
European Chemicals Agency (ECHA) in Helsinki



# What is the REACH Timetable?

**S/U/C/C/e/s/s**  
Added Value through Sustainability

**BASF**  
The Chemical Company

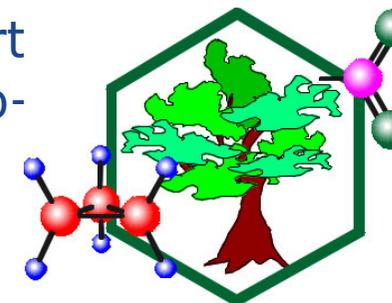


# REACH and Environmental Chemoinformatics

European Chemical Agency (ECHA) has to evaluate and register >140,000 chemicals

Testing cost up to 200k€/chemical (in total up to €6 billion)

REACH article 25: "Vertebrate testing is the last resort Existing information has to be gathered on physico-chemical, toxicological and ecotoxicological properties of a substance, including information generated by QSARs"



# CAsE studies on the development and application of in-silico techniques for environmental hazard and risk assessment

www.CADASTER.eu

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- TRISK is now open for application
- Challenge on [www.CADASTER.eu](http://www.CADASTER.eu)
- We are online !!!



### About CADASTER

Implementation of REACH requires demonstration of the safe manufacture and use of chemicals. REACH aims to achieve a proper balance between societal, economic and environmental objectives, and attempts to efficiently use the scarce and scattered information available on the majority of substances. Thereupon REACH aims to reduce animal testing by optimized use of in silico and in vitro information on related compounds.

The REACH regulation advocates the use of non-animal testing methods, but guidance is needed on how these methods should be used. The procedures include alternative methods such as chemical and biological read-across, in vitro results, in vivo information on analogues, (Q)SARs, and exposure-based waiving. The concept of Intelligent Testing Strategies for regulatory endpoints has been outlined to facilitate the assessments. Intensive efforts are needed to translate the concept into a workable, consensually acceptable, and scientifically sound strategy.

CADASTER aims at providing the practical guidance to integrated risk assessment by carrying out a full hazard and risk assessment for chemicals belonging to four compound classes. A Decision Support System (DSS) will be developed that will be updated on a regular basis in order to accommodate and integrate the alternative methods mentioned above.

# CADASTER Goals

- Exemplify the integration of information, models, strategies for safety-, hazard-, risk assessment for large numbers of substances
- Carry out “real” risk assessment for several classes of chemical substances according to the basic philosophy of REACH: < costs, animal testing, time
- Exemplify how to increase non-testing information whilst quantifying and reducing uncertainty

# CADASTER Aims

Provide full environmental hazard and risk assessment according to the REACH philosophy for chemicals belonging to 4 classes of emerging chemicals:

- 1. Polybrominated diphenylethers (PBDE)**, hydrophobic chemicals that pose a threat to man and the environment.
- 2. Perfluoroalkylated substances** and their transformation products, like perfluoroalkylated sulfonamides, alkanolic acids, sulfonates. Persistent hydrophilic compounds that may be toxic for man and environment.
- 3. Substituted musks/fragrances:** a heterogenic group of chemicals of varying composition like substituted benzophenones, polycyclic musks, terpene derivatives. Common emission pattern in the environment.
- 4. Triazoles/benzotriazoles:** increasingly used as pesticides and anti-corrosives.

# CADASTER Activities

- Collection of experimental data according to Screening Initial Data Set Dossier (SIDS)
- Development of Quantitative Structure-Activity and Structure-Property Relationship Studies (QSAR/QSPR)
- Generation of new data essential for validation and proper hazard/risk assessment
- Integration of QSARs within hazard and risk assessment
- Dissemination of information: web site, data & models

<http://www.cadaster.eu>

<http://www.qspr-thesaurus.eu>

- 1<sup>st</sup> Workshop on the use of the QSAR tools for the risks assessments in REACH (September 2011, <http://cmtpi-2011.si>)
- 2<sup>nd</sup> Workshop on the development and the use of QSAR models in REACH (2012, to be announced)

# Training activities



<http://www.eco-itn.eu>

# Overview of ECO

## Aims and Goals:

- Training of environmental chemoinformatics
- Education both in computational and experimental parts
- Provide expertise with respect to
  - Use of QSAR/QSPR models in environmental studies
  - Registration of new chemicals
  - Evaluation of chemicals before they enter the production chain

## Resources:

- Seven partners
- Twelve associated partners

## Training:

- 11 PhD positions (36 months)
- 37 short-term fellowships (3-12 months) - **Several fellowships are available**
- Six summer and winter schools
- Internship within partners and associated partners

## First ECO school at UFS Schneefernerhaus, Zugspitze



# Valorization and exploitation of project results

Support and further development of scientific findings after the end of projects

Commercial exploitation of project results

Our experience:



Company will support and extend activities after the end of the CADASTER project (2013+).



# eADMET R&D Pipeline: *in vitro* – *in vivo* correlations



# Collaboration

## **CADASTER:**

Data for analyzed chemical classes

Scientific expertise with respect to QSAR/QSPR model development for the registration of chemical compounds

## **ECO:**

Training in environmental chemoinformatics (STR are available)

## **eADMET GmbH:**

Collection, integration and application of chemical data and models in environmental chemistry, chemical industry and drug discovery

Use of *in vitro* to *in vivo* correlations; data analysis and interpretation



EU project partners

My team:

Eva Schlosser  
Vlad Kholodovych  
Iurii Sushko  
Ahmed Abdelaziz  
Stefan Brandmaier  
Jacques Ehret  
Robert Körner  
Sergii Novotarskyi  
Wolfram Teetz

