HelmholtzZentrum münchen
German Research Center for Environmental Health

eADMET
THE REFERENCE IN CHEMOINFORMATICS

CADASTER & MC ITN ECO

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SPRING workshop, Beijing, July 2-3, 2011

HELMHOLTZ
ASSOCIATION


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, chemoinfomatics software development, data dissemination

REACH

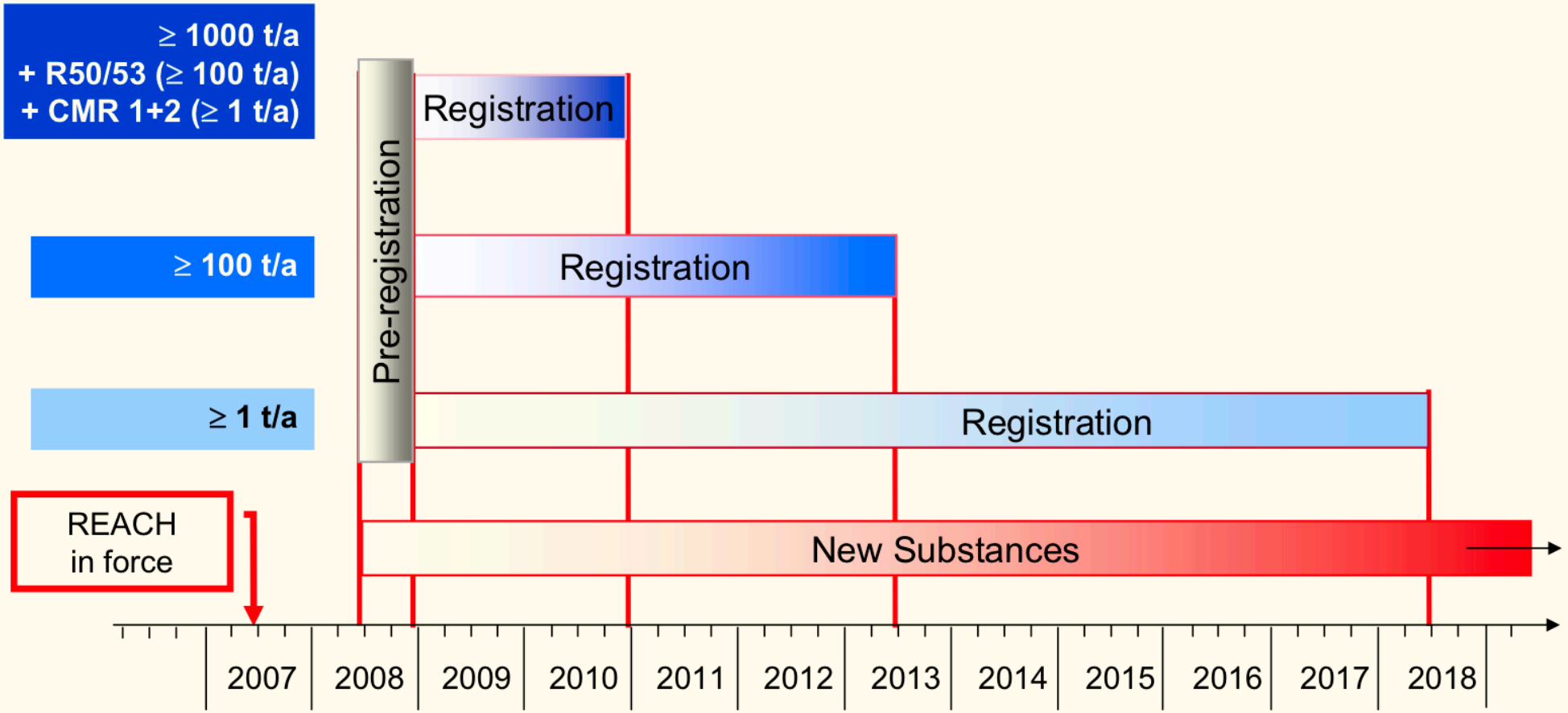
Registration, **E**valuation, **A**uthorisation and Restriction of **Ch**emical substances

European **Ch**emicals **A**gency (ECHA) in Helsinki

What is the REACH Timetable?

success
Added Value through Sustainability

BASF
The Chemical Company



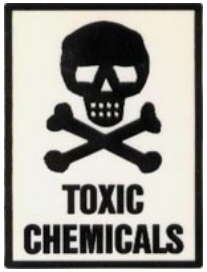
http://www.basf.com/group/corporate/en/sustainability/management-and-instruments/success-added-value

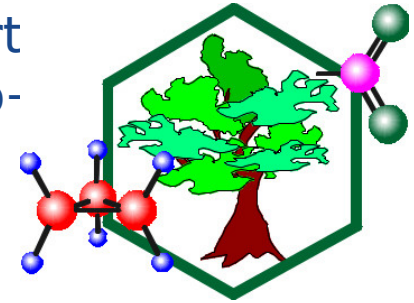
REACH and Environmental Chemoinformatics

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

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, alkanoic 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

  - 1st Workshop on the use of the QSAR tools for the risks assessments in REACH (September 2011, http://cmtpi-2011.si)
  - 2nd 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

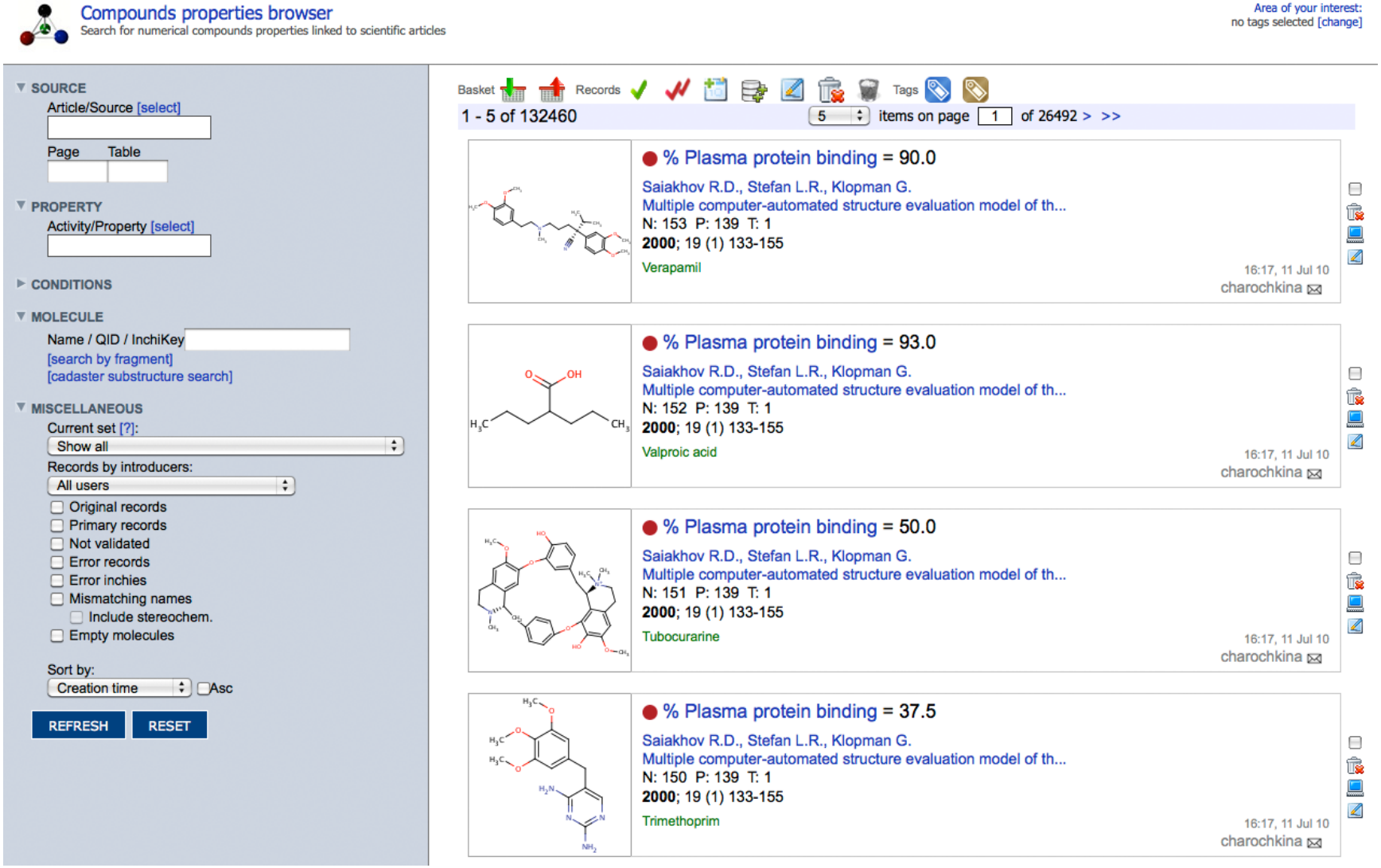
Support and further development of scientific findings after the end of projects

Commercial exploitation of project results

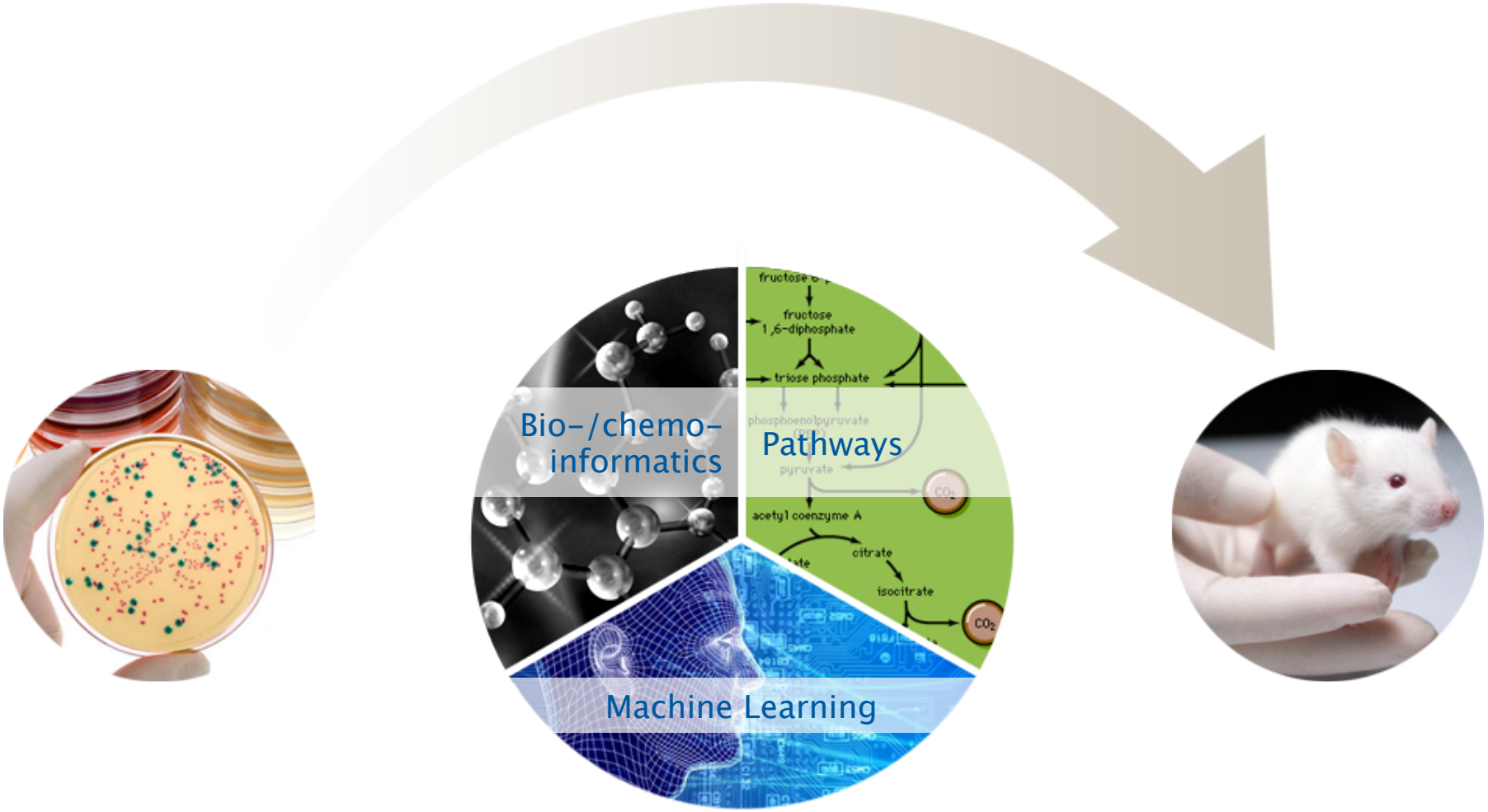
Our experience:

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

OCHEM – On-line Chemical Modeling Environment
http://ochem.eu



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



in-vitro ***in-silico*** ***in-vivo***

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 *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