

**HelmholtzZentrum münchen**

German Research Center for Environmental Health

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**Igor V. Tetko & Karl-Werner Schramm**

Helmholtz Zentrum München - German Research Center for Environmental Health (GmbH)

Munich, 26/10/2009





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# Helmholtz Zentrum München - as an Organization

- Previous name (before 2008): GSF
- Part of Helmholtz Network (2.8 Billiards Euro, 28000 people, 15 centers)
- Leading center for Environmental Health in Germany
- 25 institutes (1956 people, ca 700 scientists, ca 260 PhD students)\*
- 70 contracts with EU (GOODWATER MC ITN)
- Strong IPR and management support
  
- Institute for Bioinformatics & Systems Biology
  - 50 peoples, strong expertise in *in silico* data analysis, machine learning methods, software development, data dissemination (Web, Internet)

\*January 2009

# Chemoinformatics group

9 people + visiting scientists

- GO-Bio grant (ADMET properties prediction using neural networks)
- Germany-Ukraine collaboration grant on CYP450 modeling
- CADASTER (Case studies on the development and application of *in-silico* techniques for environmental hazard and risk assessment)



# *In silico* expertise of the group

## □ Main interests

- Methodology development for QSAR/QSPR studies
  - Accuracy estimation of models
  - Data integration
- Physico-chemical properties predictions
  - Lipophilicity, solubility, pK<sub>A</sub>
  - DMSO solubility; prediction of chromatography retention times
- Biological and toxicological properties prediction
  - CYP450 inhibition
  - AMES test
  - Blood-Brain barrier

## □ 15 years of expertise in data analysis

- QSAR/QSPR (2D, 3D)
- linear (regression, PCA, PLS)
- non-linear (SVM, neural networks, genetic algorithms ...)
- unsupervised methods (grouping approaches, clustering)

## □ Dissemination of models and results (QSAR web tools)

- Virtual Computational Chemistry Laboratory <http://www.vcclab.org>
- On-line chemical database & modeling environment <http://qspr.eu>

# Ecotoxicological Impact and Indicators



## Karl-Werner Schramm

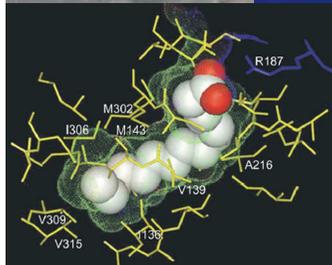
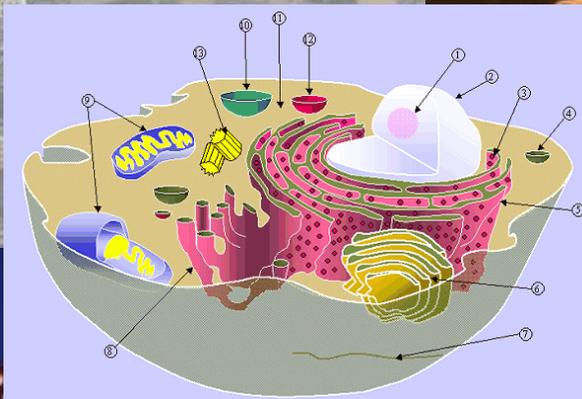
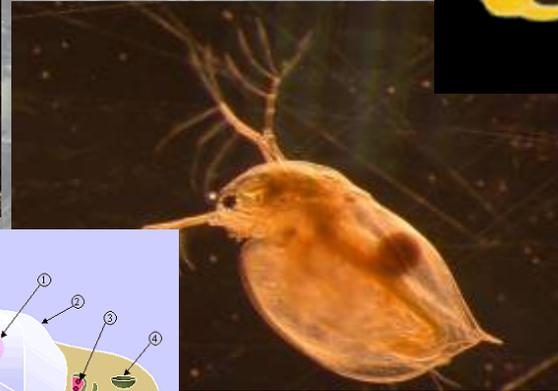
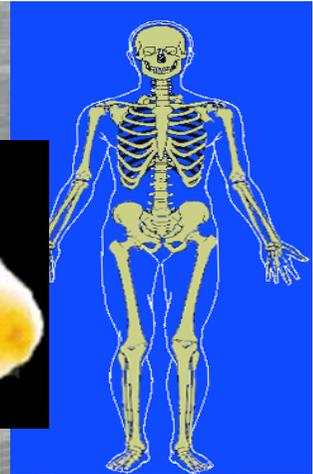
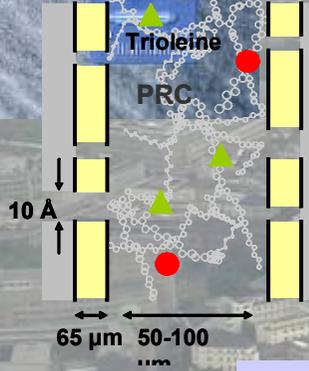
**HMGU- Deutsches Forschungszentrum für  
Gesundheit und Umwelt,  
Institut für Ökologische Chemie  
Ingolstädter Landstr. 1,  
D-85764 Neuherberg, Germany**

TUM – Technische Universität München,  
Wissenschaftszentrum Weihenstephan für Ernährung und  
Landnutzung, Department für Biowissenschaftliche  
Grundlagen, Weihenstephaner Steig 23, 85350 Freising,  
Germany

[schramm@helmholtz-muenchen.de](mailto:schramm@helmholtz-muenchen.de)

[schramm@wzw.tum.de](mailto:schramm@wzw.tum.de)

# ECOTOXICOLOGY Impact & Indicators



# Ecotoxicological Impact and Indicators

## SCOPES

Regulators across scales with chemical impact on environment and health

Regulators and their indicator scale expressed as multiple effects

Biogeosystems at different scales (nm, mm, m, km)

Environmental molecular signalling (endogenous vs. exogenous)

Regulatome

cell-tissue-organism-system

zoo-, phyto- and their nano-spheres

## **IMPACT**

Persistent hydrophilic and super-hydrophobic,  
low-molecular molecules

## **INDICATOR**

High biological activity such as hormones

## **BIOGEOSYSTEMS**

Nanospheres and Cells

## **TOOLBOX (quantitative)**

Cellular Ecotoxicology

Bio-molecular diagnostics (Bioassays, Reporter-Assays, Protozoa)

Molecular Modelling (semiepirical – ab initio)

Hyphenated instrumental chemical analysis for ultra-trace regulators

# Homeostasis of Regulatome

