Dissemination of information in CADASTER project

Igor V. Tetko
Helmholtz Zentrum München, Germany

CADASTER workshop on a use of alternative methods in REACH
Maribor, September 2nd, 2011

Dissemination of information

- Web site
  - http://www.cadaster.eu
  - http://www.qspr-thesaurus.eu
  - http://mopac.cadaster.eu
- Dissemination of developed models by web and standalone tools; integration with OECD QSAR toolbox
- Publications and presentations of results to conferences
- Newsletter
- Workshops

Project web site
http://www.cadaster.eu

- In function since April 2009
- Portal for news; forum
- All participants have their own pages
- More than > 2000 unique visits per month
- Access to deliverables; articles; posters & oral reports
- Environmental toxicity prediction challenge
  (in collaboration with ICANN)

try another color: try another fontsize: 60% 70% 80% 90%

www.CADASTER.eu

Home | REACH | CHALLENGE | Partners | WP | Meetings | News | Forum | Login

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Latest news

- CADASTER Workshop on the use of QSAR models in REACH

Home

FIRST CADASTER NEWSLETTER IS ONLINE to read it, please click here

FIRST CADASTER WORKSHOP IN MARIBOR to learn more, please click here

QSPR-Thesaurus is online go here

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

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- CADASTER Workshop on the use of QSAR models in REACH

Publications

Research Papers

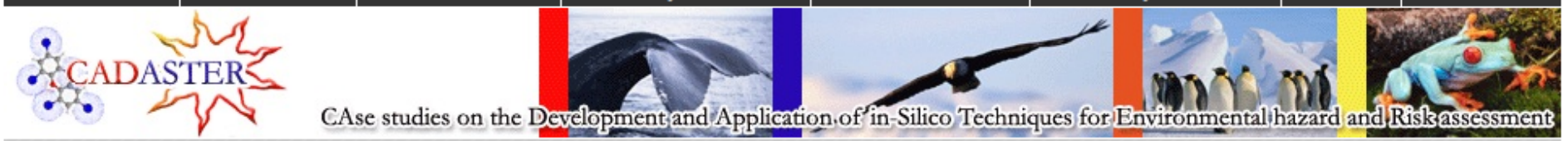
• Roy, P.P.; Kovarich, S.; Gramatica, P. QSAR model reproducibility and applicability: a case study of rate constants of hydroxy radical reaction models applied to Polybrominated Diphenyl Ethers and (Benzo-)Triazoles *J. Computational Chem.*, **2011**, online first

• Kovarich, S.; Papa, E.; Gramatica, P. QSAR classification models for the prediction of endocrine disrupting activity of brominated flame retardants *J. Hazard. Mater.*, **2011**, 190 (1-3), 106-112

• Papa E.; Kovarich, S.; Gramatica, P. On the use of local and global QSARs for the prediction of Physico-Chemical Properties of Polybrominated Diphenyl Ethers *Molecular Informatics*, **2011**, 30, 232–240

• Bhhatarai, B.; Teetz, W.; Liu, T.; Öberg, T.; Jeliazkova, N.; Kochev, N; Pukalov, O.; Tetko, I.; Kovarich, S.; Papa, E.; Gramatica, P. CADASTER QSPR Models for Predictions of Melting and Boiling Points of Perfluorinated Chemicals *Molecular Informatics*, **2011**, 30, 189-203

• Sushko I.; Novotarskyi S.; Körner R.; Pandey A.K.; Cherkasov A.; Li J.; Gramatica P.; Hansen K.; Schroeter T.; Müller K.R.; Xi L.; Liu H.; Yao X.; Öberg T.; Hormozdiari F.; Dao P.; Sahinalp C.; Todeschini R.; Polishchuk P.; Artemenko A.; Kuz'min V.; Martin T.M.; Young D.M.; Fourches D.; Muratov E.; Tropsha A.; Baskin I.; Horvath D.; Marcou G.; Muller C.; Varnek A.; Prokopenko V.V.; Tetko I.V. Applicability domains for classification problems: benchmarking of distance to models for ames mutagenicity set. *J Chem Inf Model*, **2010**, 50, 2094-2111



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Latest news

- CADASTER Workshop on the use of QSAR models in REACH

Environmental Toxicity Prediction Challenge

Organizers

This challenge is organized by ICANN'09: International Conference on Artificial Neural Networks, European Neural Network Society (ENNS) and CADASTER project.

Goals of this study

- Develop in silico models to predict environmental toxicity of molecules against T. pyriformis using data from [1].
- Estimate the prediction intervals for new compounds.

More detailed introduction can be found here, data can be downloaded at this page and results submitted here.

Important key dates

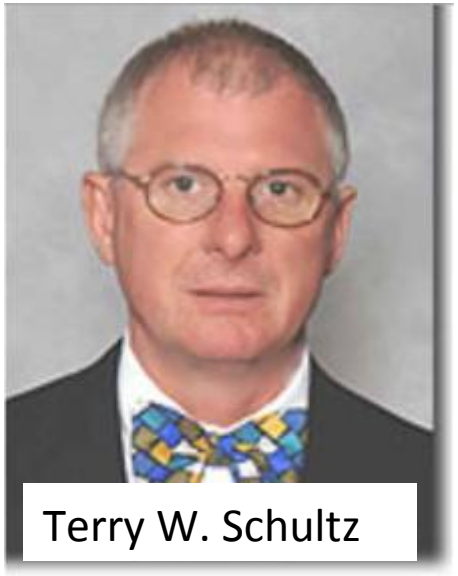
- **June 1** The submission of results is open.
- ~~**August 31** The submission of results is closed.~~
- ~~**September 10** New submission deadline~~
- **September 12** New submission deadline
- **September 14-17 2009** The winner will be announced at the ICANN'09 conference.
- **September 15 Final results are available here and experimental values can be downloaded here.**

The winner will be identified according to the criteria defined below and (s)he will receive a prize. It is expected that the winner as well as other participants will submit articles describing their methodological approaches for publication in a peer-reviewed journal (under discussion). Information on how you can participate can be found here.

Grand prize for the competition-winners is 1.000 € !

Challenge committee


Igor V. Tetko


Terry W. Schultz


Wlodzislaw Duch

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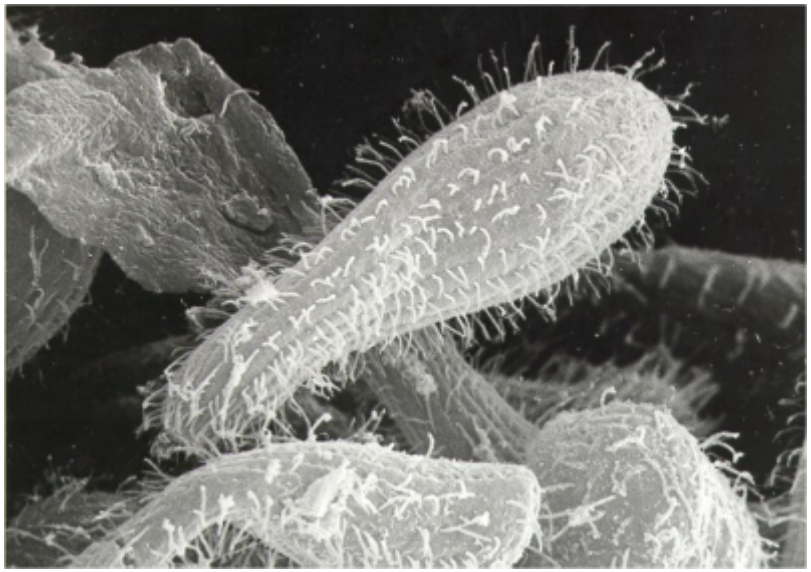
Estimation of toxicity against *T. pyriformis*

- Training set:
  n=644 molecules[1,2]

- Known set:
  n=449 molecules[1,2]

- Blind set:
  n=120 molecules[1,3]

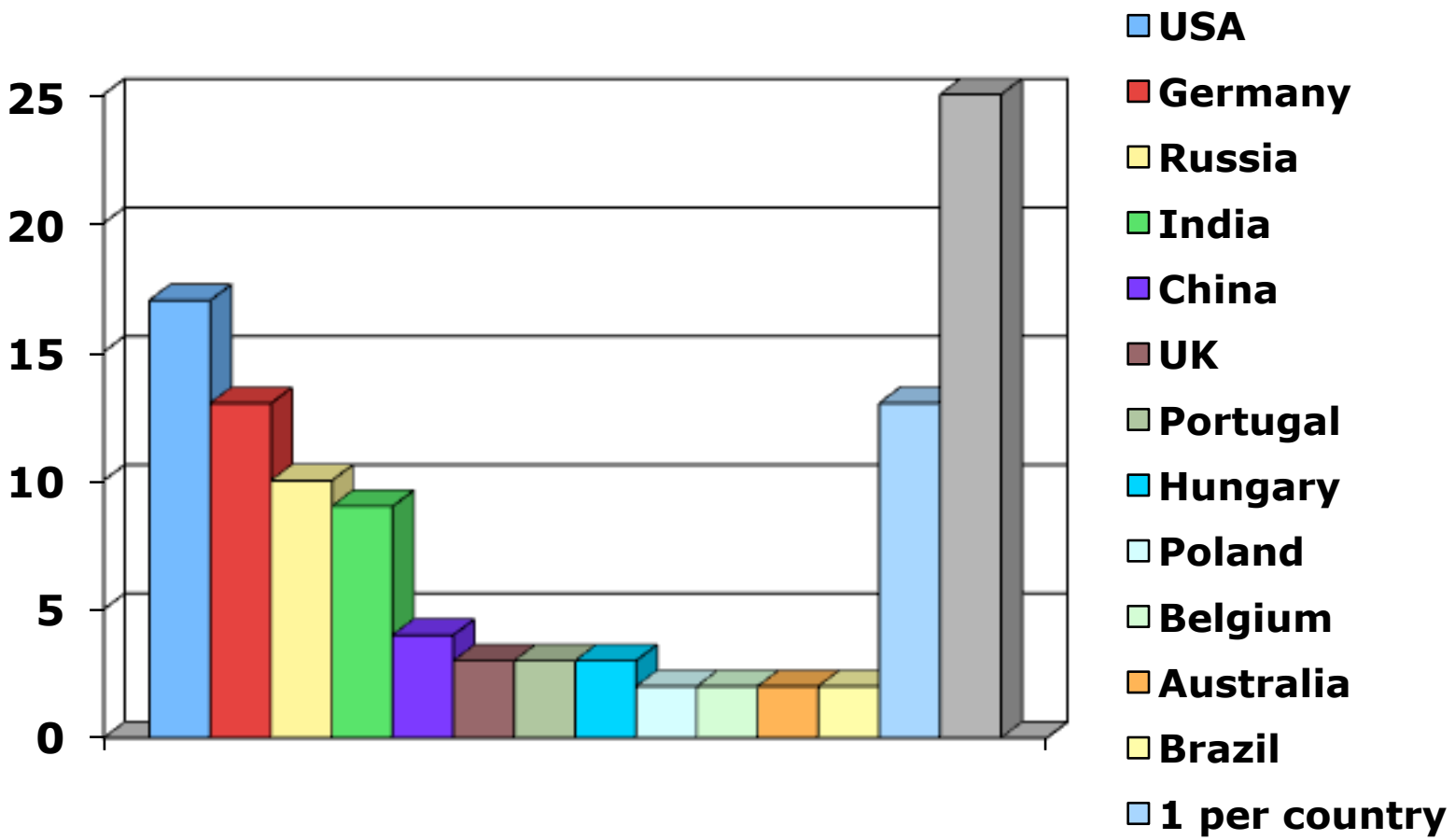


http://science.bard.edu/biology/ferguson/

The overall goal is to predict and to assess the reliability of predictions toxicity against T. pyriformis for chemicals directly from their structure.

[1]All experimental values were measured in laboratory of Prof. T.W. Schultz.
[2]Sets as described in Zhu et al, *J. Chem. Inf. Comput. Sci*, **2008**, 48, 766.
[3]Blind set was provided by Prof. T.W. Schultz at the end of the competition.

Country of participants



514 submission by 108 participants from > 25 countries

Final winners

- Dr Gavin C. Cawley
- School of Computing Sciences
- University of East Anglia
- Norwich, NR4 7TJ, U.K.

- Lowest RMSE for the Blind set

- Dr. Olga Obrezanova
- Principal Scientist at Optibrium Ltd.
- Cambridge, United Kingdom

- Low RMSE (non-significantly different to the winner) **and**
- good correspondence between estimated and calculated errors for the Blind set[1]

[1]Errors were estimated using performances of the methods on the Known set and provided confidences

CADASTER Newsletter, July 2011

Outline

CADASTER has joined the EUROECOTOX network

EUROECOTOX
European Network for Alternative Testing Strategies in Ecotoxicology

Within the FP7 Environment Programme, the coordination action EUROECOTOX was recently funded by the European Commission. EUROECOTOX is a European Network established to promote the integration of European activities on the replacement and reduction of animal experiments in ecotoxicology. EUROECOTOX aims to foster the

http://www.qspr-thesaurus.eu

Revision 5844 by midnighter checked in on 2011-08-29 17:05:57. Built from 146.107.60.52 on 2011-08-29 18:01:03

Chrome 13 on Mac - Partially supported

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Welcome to the QSPR-THESAURUS database!

The QSPR-THESAURUS has been developed within the EU FP7 CADASTER project.
It contains physico-chemical data and models for four classes of compounds:

Polybrominated diphenylethers (PBDE)

Polybrominated diphenylethers (PBDE), typically being a class of hydrophobic chemicals that pose a threat to man and the environment.

Perfluoroalkylated substances

Perfluoroalkylated substances and their transformation products, like perfluoroalkylated sulfonamides, alkanoic acids, sulfonates. Fluorinated compounds are typically a class of persistent, relatively hydrophilic compounds that may be toxic for man and environment.

Substituted musks/fragrances

Substituted musks/fragrances, being a heterogenic group of chemicals of varying composition. Examples include substituted benzophenones, polycyclic musks, terpene derivatives. In view of their typical use pattern, the chemicals have a common emission pattern in the environment.

Triazoles/benzotriazoles

Triazoles/benzotriazoles, a class of chemicals that are increasingly used as pesticides and anti-corrosives.

Experimental properties

CADASTER models

Revision 5844 by midnighter checked in on 2011-08-29 17:05:57. Built from 146.107.60.52 on 2011-08-29 18:01:03

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Step 1. Select a model from the list

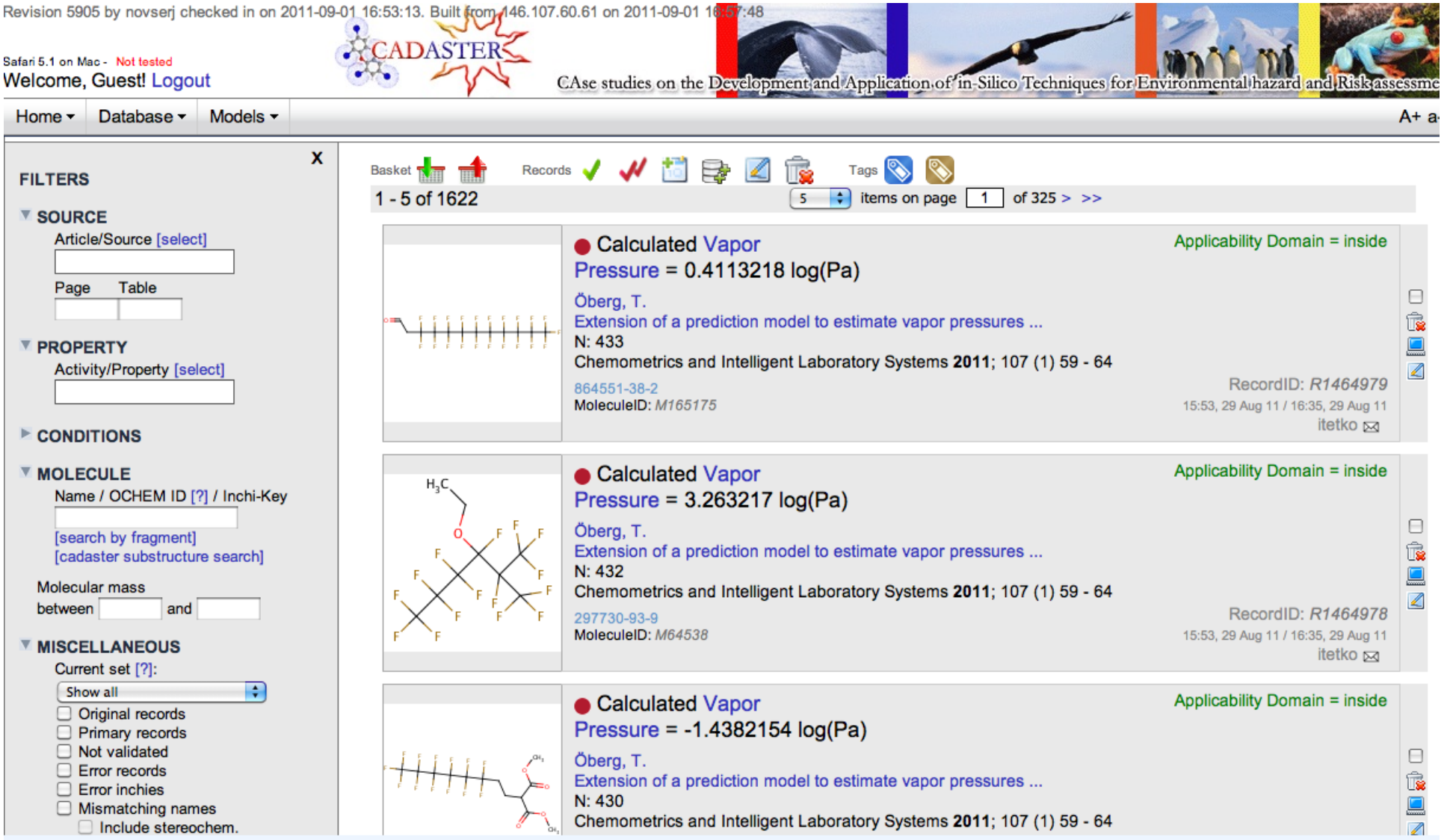
Filter by model name: and property name: or by article id: Models visibility:

Public and private [refresh]

1 - 8 of 8

Compound class	Endpoint	Partner	Reference	Training set	Method	Creation date	
PFC	Aqueous Solubility	UI	Ref.	PFC_LogWS_Training set (20)	MLRA	*2010-11-11*	Model profile
PFC	Vapor Pressure	UI	Ref.	logVP_PFCs (35)	MLRA	*2011-05-26*	Model profile
PFC	Boiling Point	HMGU	Ref.	BarunMPBP.BP-28apr10v1-93 (93) validated by BarunMPBP.BP-PERFORCE-28apr10v1-25 (25)	MLRA	*2010-08-05*	Model profile
PFC	Boiling Point	HMGU	Ref.	PFC BP Training 93 (93) validated by PFC BP Test 25 (25)	MLRA	*2010-08-25*	Model profile
PFC	Boiling Point	HMGU	Ref.	PFC BP Training 93 (93) validated by PFC BP Test 25 (25)	MLRA	*2010-09-06*	Model profile

Predicted properties



MOPAC database

About mopac@home

mopac@home is a research project that uses Internet-connected computers to do research in quantum chemistry. You can participate by downloading and running a free program on your computer.

mopac@home is based at HelmholtzZentrum Muenchen

- Homepage of the CADASTER project
- People involved in this project

Join mopac@home

- Read our rules and policies
- This project uses BOINC. If you're already running BOINC, select Attach to Project. If not, download BOINC.
- When prompted, enter **http://mopac.cadaster.eu/**
- If you're running a command-line or pre-5.0 version of BOINC, create an account first.
- If you have any problems, get help here.

Returning participants

What is the use of mopac@home ?

The CADASTER project is an FP7-funded project by the EU that aims to provide a Decision Support System (DSS) to asses the hazard and risk for chemicals belonging to four compound classes. Therefore QSAR models will be developed and validated, as the basic philosophy behind this project is minimizing animal testing, costs, and time. These models need a solid base, which is primarily founded by the knowledge of reliable structures for chemical compounds. The semiempirical quantum chemistry program MOPAC can, aside from several other important chemical qualities, provide such structures.

Why should you join mopac@home ???

- **Environment protection**
  The basic task of the CADASTER project is to protect the environment. Every single computed molecule can decisively contribute to improve the quality of models that asses the risk of a chemical compound to your ecosystem.

- **Animal protection**
  The usual technique for assesment of hazard and risk, is animal experiments. Contrary to that, our scientific work aims to avoid these experiments. The data collected by **mopac@home** should enable QSAR-models

User of the day

Stefan brandmaier
I am a PhD student at the Helmholtz-Zentrum in Munich and one of the guys that helped to realized this project.

News

Several fixes
September 27, 2010
Problems with creating profiles and group joining should be fixed now. Sorry for the delay, but this was caused by a cold that affected both our system admin and me.

Problems with web configuration
August 27, 2010
Our system admin just returned from vacation so on monday we will face the problems with the site configuration. Within the first days of the next week, both the joining of groups as the profile edditing should work. Nice weekend to all of you ... ;)

Forum is open

MOPAC statistics

- Volunteers computing all around world
- > 1,200,000 optimized conformations*
- > 200,000 molecules

- Web services to search optimized molecules
  - Starting from a given conformation
  - Preserving stereochemistry
  - Ignoring stereochemistry

Collaboration with OpenTox

AD assessment

- [x] Calculate leverage
- [ ] Calculate AMBIT: Tanimoto
- [ ] Calculate AMBIT: Missing fragments
- [x] Calculate AMBIT: Leverage
- [x] Calculate AMBIT: Euclidian distance
- [ ] Calculate AMBIT: City block distance
- [ ] Calculate AMBIT: PCA ranges

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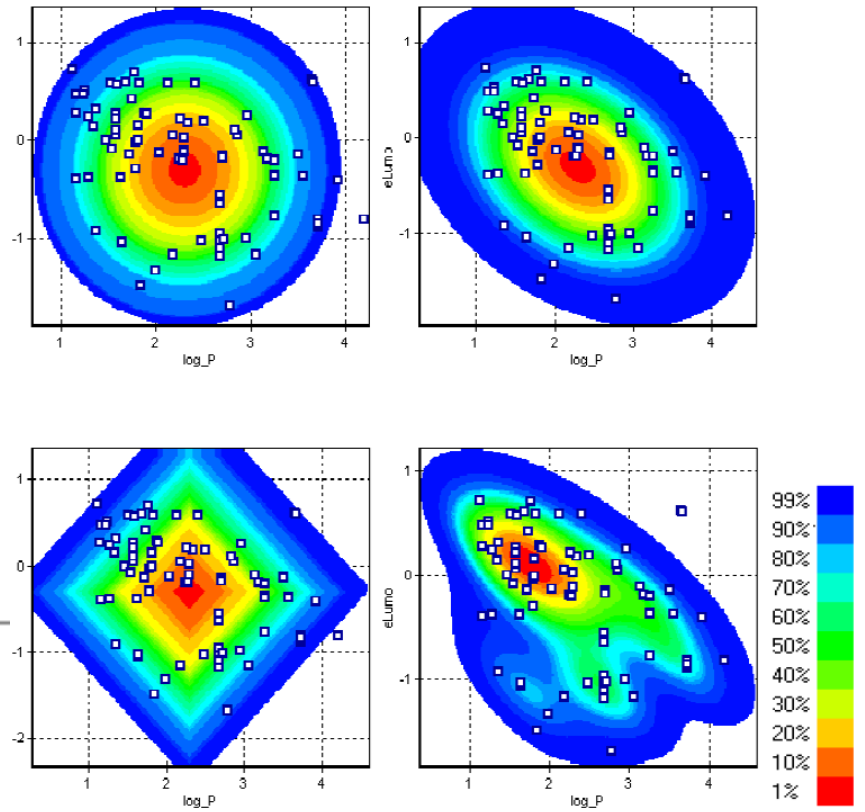


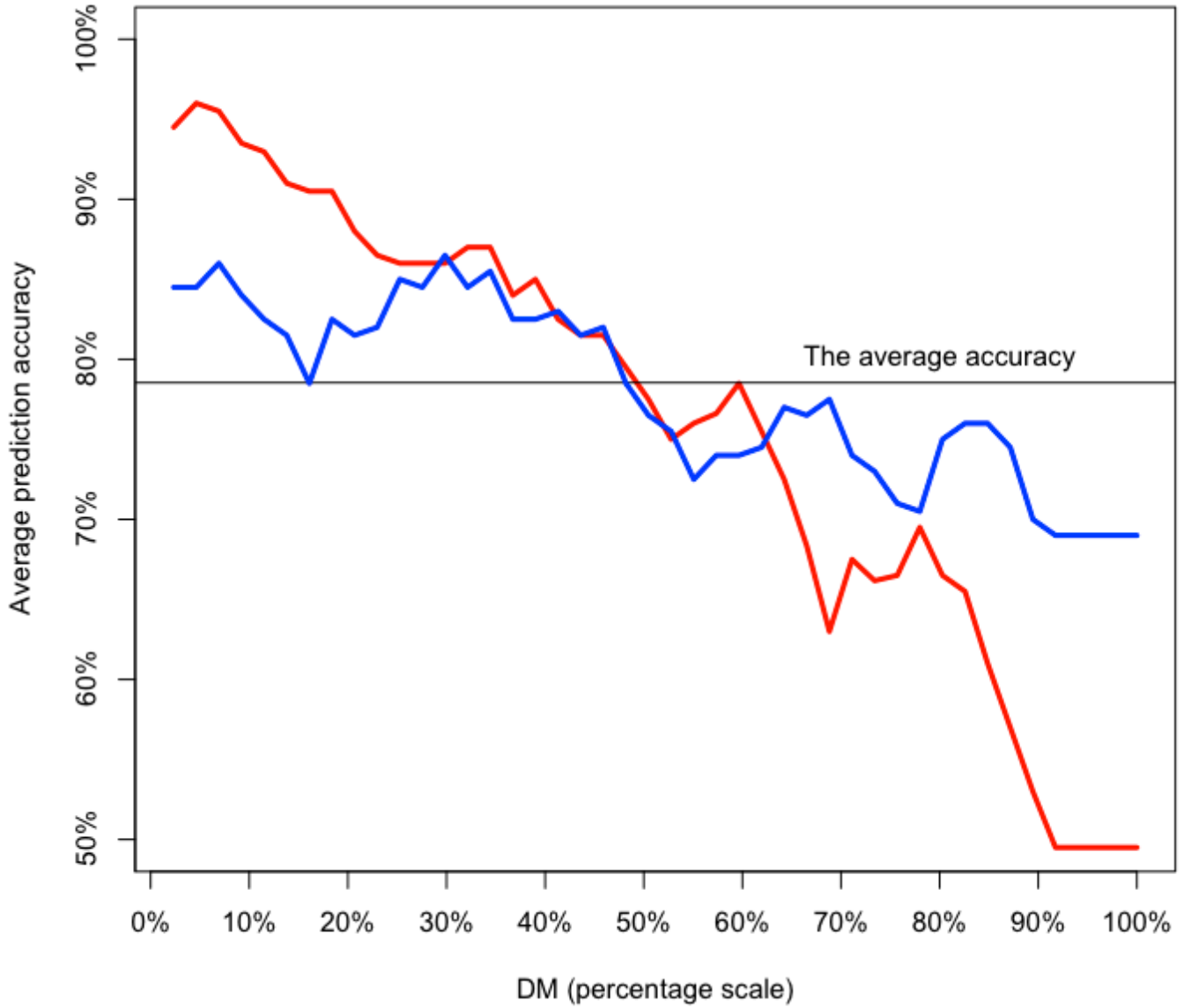
Jaworska et al, *ATLA*, 2005, *33*, 445-459.

Applicability domain of models

- PhD thesis by Iurii Sushko (TUM, March 1st, 2011, magna summa cum laude)
- Comparison of different distances to models
- Measures of quality of predictions for quantitative and qualitative models
- Identification of predictions having experimental accuracy

Collaborative efforts with WP3 and WP4

Discrimination power of different distances to models



Experimental design

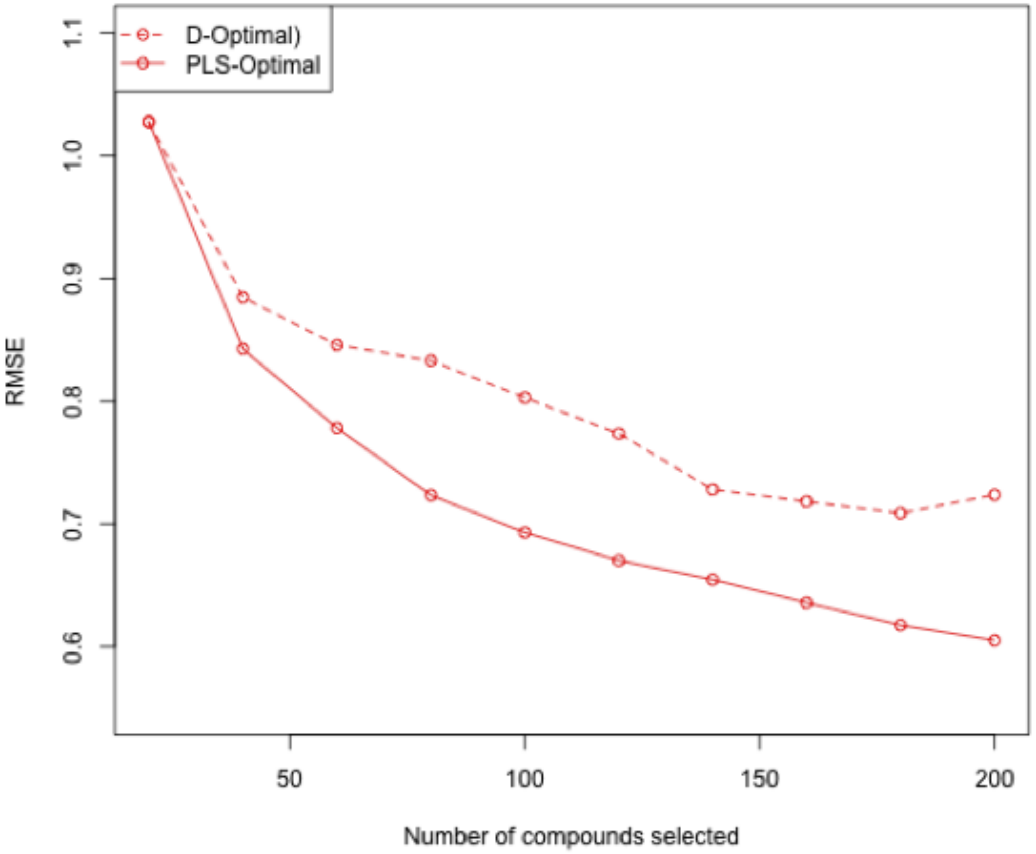
D optimal design

PLS-optimal design

→

Optimal set of molecules to build model

IGC 50



CADASTER: EU-China collaboration

EU-China Environment Research: Looking back and moving forward together

2nd July 2011

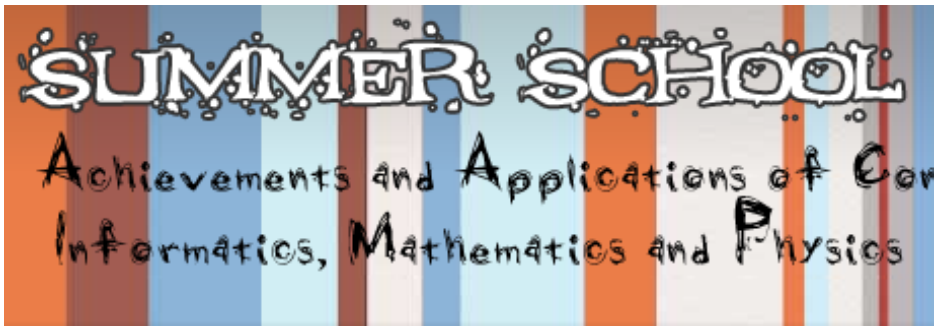
Guohong Hotel, Muxidi No. 11, Xicheng District, Beijing

Large-scale collaborative projects involving partners from multiple countries and regions are needed to tackle the big environment issues of the future. Opportunities for strategic EU-China research addressing sustainability and the environment are increasing, supported by the focus on sustainable growth and environment protection promoted by Europe's 2020 strategy and China's 12th Five Year Plan.

In this innovative meeting, invited speakers from large and medium-scale collaborative EU and China projects will present the best of existing collaborative research in the environment sector. Information on ongoing and upcoming funding opportunities from both the EU and China will be distributed.

Session 2 – FP6 & 7: Topical Break-out sessions		
	Breakout 1	Breakout 2
10:40	DeSURVEY (FP7) **Juan Puidefabregas**	CADASTER & MC ITN ECO (FP7) **Igor Tetko**
11:00	SENSOR (FP6) **Lin Zhen**	LIVEDIVERSE (FP7) **Geoffrey Gooch**
11:20	SURE (FP7) **Nico Heerink**	TRANSPHORM (FP7) **Menno Keuken**
11:40	EAB **Eugenia Sanchez Cruz & Juan Puidefabregas**	RenErGo (FP7) **Bettina Bleumling**
12:00	CNRS & Sino-French collaborations **Patrick Nedellec & Mu Yujin**	

CADASTER: mentoring



Course coordinator — Dr. Igor V. Tetko, Group leader, Institute of Bioinformatics and Systems Biology, Helmholtz Zentrum Muenchen.

Language of the course — English.

The course will introduce the chemoinformatics and will highlights requirements to this discipline in the light of new EU legislation concerning the registration, evaluation, authorization and restriction of chemicals (REACH). It will start with a basic description of the chemoinfomatics and its role in drug discovery and environmental protection. An overview of modern challenges in the field, unsolved and actively addressed problems will be discussed. Several examples of practical application of chemoinformatics in drug discovery and environment will be given by the leading scientists from EU and the Ukraine. The course will be completed by practical training to the web-based tools to develop quantitative structure-activity(property) relationship (QSAR/QSPR) models.

Other course tutors:

Prof. Willie Peijnenburg, The Netherlands, RIVM, coordinator of CADASTER project (to be confirmed).

Prof. Victor Kuzmin, vice director of A.V.Bogatsky Physico-Chemical Institute of the National Academy of Sciences of Ukraine.

Dr. Vasyl Kovalishyn, senior scientist, Institute of Bioorganic & Petrochemistry, Kyiv, Ukraine.

Mr. Iurii Sushko and Mr. Sergii Novotarskyi, Institute of Bioinformatics and Systems Biology, Helmholtz Zentrum Muenchen.

Supported with Germany-Ukraine bilateral grant UKR 008/006, FP7 project CADASTER

ECO MC ITN

MARIE CURIE ACTIONS

eco
environmental chemoinformatics
marie curie initial training network

- 11 PhD positions (36 months)
- 37 short-term fellowships
- Six summer and winter schools
- Internship within partners and associated partners

Next school: 19-30 September, Leiden, the Netherlands

First ECO school at UFS Schneefernerhaus, Zugspitze

http://www.eco-itn.eu

CADASTER Workshop 2012*

*Preliminary planned in Autumn, Munich 2012

Thank you for your attention.