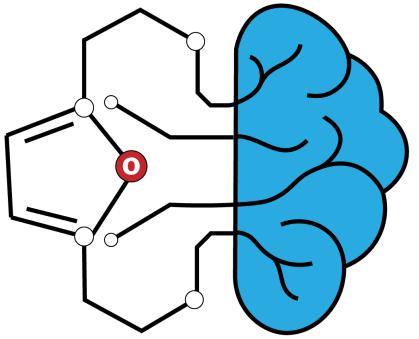


MSCA actions, AIDD, AiChemist and HMGU

Igor V. Tetko

Helmholtz Munich and BIGCHEM GmbH

Joint School of AIDD and AiChemist projects

March 4, 2024, Berlin

HELMHOLTZ MUNICH

Marie Skłodowska-Curie Actions 2021-2027

Developing talents, advancing research

Under Pillar I of Horizon Europe, the MSCA are the European Union's reference programme for doctoral education and postdoctoral training. They support researchers from all over the world, at all stages of their careers, with a focus on their training, skills and career development.

Under Horizon 2020 (2014-2020), the MSCA:

Funded **1080 doctoral programmes**, of which 156 industrial doctoral programmes and 76 joint doctorates

Involved **4 700 companies**, of which **2 200 SMEs**

Involved **37% of researchers** from non-EU countries and around **1300 organisations** from non-EU and non-associated countries

Since 1996

budget
14 billion €

researchers
140 000
(39 000 PhDs)

Horizon Europe (2021-2027)

budget
6.6 billion €

researchers
65 000
(25 000 PhDs)

Under Horizon Europe, the MSCA will:

Strengthen organisations
The MSCA support excellent doctoral and postdoctoral programmes and collaborative projects worldwide, promoting structuring impact on organisations

Foster research and innovation beyond academia
The MSCA boost ties between academia and other non-academic organisations with various incentives, increasing fellows' exposure to other sectors

Build international links
The MSCA are key in attracting talent to Europe, building international, strategic partnerships, and promoting global research mobility and science cooperation

The MSCA have 5 main actions

Postdoctoral Fellowships

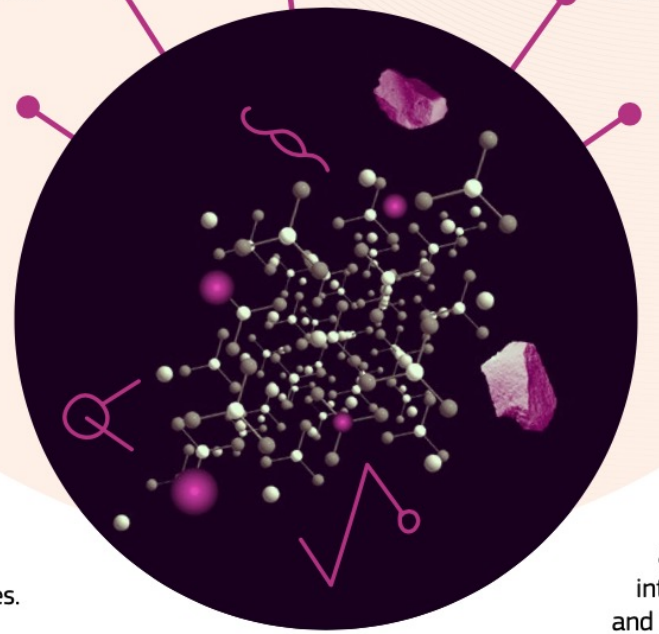
support researchers' careers and foster excellence in research and innovation. Researchers holding a PhD can carry out their research activities, acquire new skills and develop their careers abroad, whilst developing competences in non-academic sectors and working within interdisciplinary teams.

Doctoral Networks

implement doctoral programmes (including joint doctorates and industrial doctorates) **by international partnerships** of organisations from different sectors. They train highly-skilled doctoral candidates, stimulate their creativity, enhance their innovation capacities and boost their employability in the long-term.

Staff Exchanges

encourage short-term international and inter-sectoral exchanges of research and innovation staff through sustainable, collaborative projects in Europe and beyond. By doing so, they enhance knowledge and skills transfer and increase organisations' research and innovation capacities.



MSCA and Citizens

brings research and researchers closer to children, families and the public at large through the European Researchers' Night - the annual research communication and promotion event taking place at the end of September across EU Member States and Horizon Europe Associated Countries.

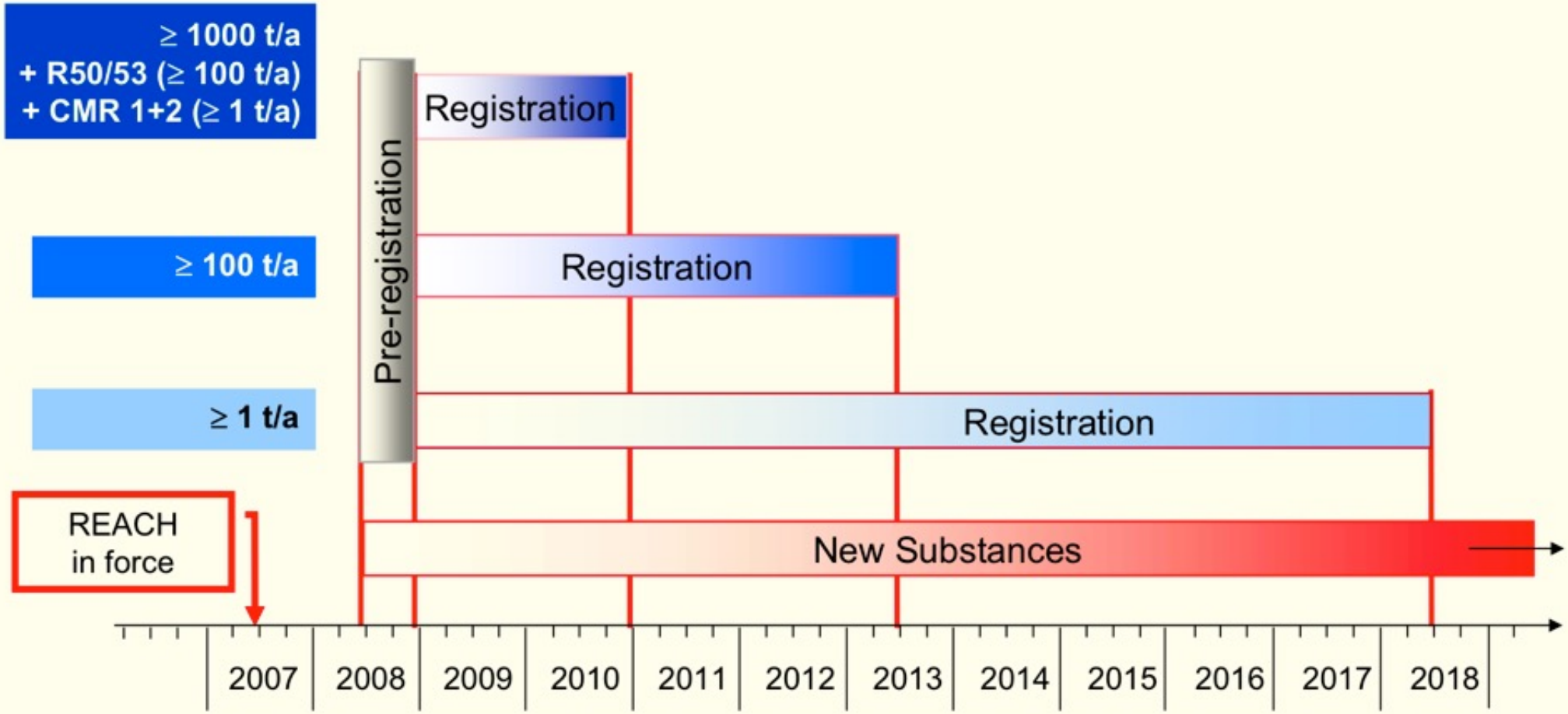
COFUND

co-finances regional, national and international doctoral and postdoctoral programmes for researchers' training and career development. The COFUND action spreads MSCA's best practices by setting high standards and excellent working conditions, and boosts training and international, interdisciplinary and inter-sectoral mobility.

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

ECO http://ecoitn.eu

Environmental ChemOinformatics

ECO | NEWS | REACH | FELLOWS | SCHOOLS | PUBLICATIONS | CONTACT

SITE STRUCTURE

- ECO
  - Description
    - General information
    - Synergism
    - Methodology
    - Dissemination
    - Abbreviations
  - Training
  - Partners
  - Projects involved
- News
  - Archive
- REACH
- Fellows
- Schools
  - Final Conference 2013
  - Winter School 2013
  - Summer School 2012
  - Winter School 2012
  - Autumn School 2011
  - Winter School 2011
  - Autumn School 2010
- Publications
- Contact

News

ECO News and Events

31 PhDs were awarded to the former ECO fellows. See the impact of ECO ITN publications at Google Scholar.

Saturday, 7 March 2020

10 doctoral (PhD) positions in Big Data Analysis in Chemistry, Marie Skodowska-Curie ITN BIGCHEM (http://bigchem.eu)

BIGCHEM (BIG data in CHEMistry) is a Marie Skodowska-Curie Innovative Training Network (ITN) for Early Stage Researchers (ESR) funded by the European Commission under the H2020 Programme. The BIGCHEM ITN will provide a comprehensive and cross-disciplinary structured curriculum for doctoral students in large chemical data analysis using machine-learning, computational chemistry and chemoinformatics methods. The innovative research program will be implemented with the target users, large pharma companies and SMEs, which generate and analyse large chemical data.

Tuesday, 12 February 2016

ECO publication received 2016 SLAS ReadersChoice Awards

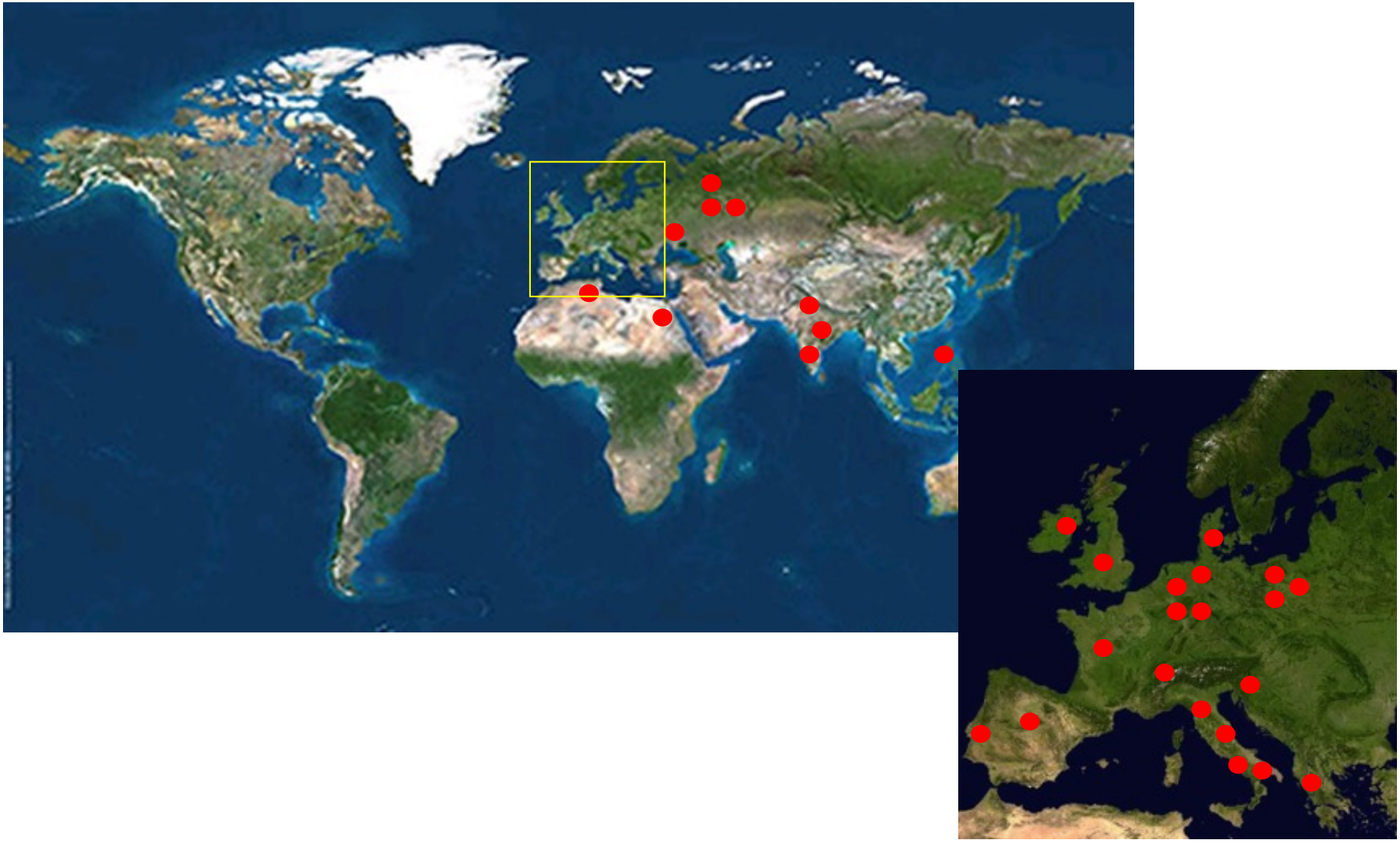
On January 26 2016, SLAS announced that article of Schorpp, K. et al Identification of Small-Molecule Frequent Hitters from AlphaScreen High-Throughput Screens *J. Biomol. Screen. 2014, 19 715-726* received 2016 JBS Readers Choice Award. ECO fellow Mrs. Elena Salmina contributed to the chemoinformatics analysis of this study during her short-term fellowship in HMGU, group of Dr. Tetko.

Tuesday, 26 January 2016

19th successful PhD in ECO network

On December 9 2015, Dr. Alessandra Pirovano successfully defended her PhD thesis at the Radboud University. Dr. Prirovano was ECO fellow at the same University. The topic of her thesis is "Quantifying biotransformation of xenobiotics in mammals" under supervisor of Prof. dr. ir. A.J. Hendriks.

Origin of the fellows



The final School of the ECO project (September 2013)

ECO ITN publications

FOLLOW

Environmental ChemOinformatic - FP7 Marie Curie Innovative Training Network
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REACH chemoinformatics Ecotoxicology Nanotoxicology QSAR

TITLE	CITED BY	YEAR
Online chemical modeling environment (OCHEM): web platform for data storage, model development and publishing of chemical information I Sushko, S Novotarskyi, R Körner, AK Pandey, M Rupp, W Teetz, ... Journal of computer-aided molecular design 25, 533-554	583	2011
Comparison of different approaches to define the applicability domain of QSAR models F Sahigara, K Mansouri, D Ballabio, A Mauri, V Consonni, R Todeschini Molecules 17 (5), 4791-4810	463	2012
Relative importance of microplastics as a pathway for the transfer of hydrophobic organic chemicals to marine life A Bakir, IA O'Connor, SJ Rowland, AJ Hendriks, RC Thompson Environmental pollution 219, 56-65	440	2016
Internalization and cytotoxicity of graphene oxide and carboxyl graphene nanoplatelets in the human hepatocellular carcinoma cell line Hep G2 T Lammel, P Boisseaux, ML Fernández-Cruz, JM Navas Particle and fibre toxicology 10, 1-21	410	2013
Quantitative structure–activity relationship models for ready biodegradability of chemicals K Mansouri, T Ringsted, D Ballabio, R Todeschini, V Consonni Journal of chemical information and modeling 53 (4), 867-878	257	2013
ToxAlerts: a web server of structural alerts for toxic chemicals and compounds with potential adverse reactions I Sushko, E Salmina, VA Potemkin, G Poda, IV Tetko Journal of chemical information and modeling 52 (8), 2310-2316	241	2012
Degree of deacetylation of chitosan by infrared spectroscopy and partial least squares IKD Dimzon, TP Knepper International journal of biological macromolecules 72, 939-945	150	2015

Cited by

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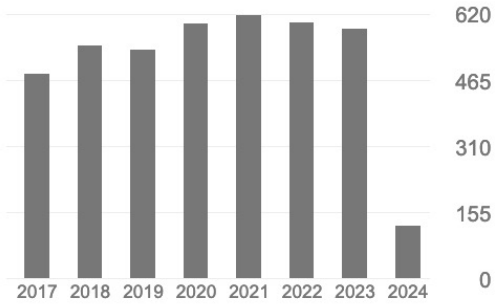
	All	Since 2019
Citations	5101	3068
h-index	35	27
i10-index	58	51



Co-authors

VIEW ALL

- Igor V. Tetko — BIGCHEM GmbH & Helmholtz M…
- Roberto Todeschini — University of Milano-Bicocca - Fu…
- Peijnenburg Willie — RIVM - Center for Safety of Subs…
- A. Jan Hendriks — Professor of Environmental Scie…
- Faizan Sahigara — in silico modelling expert
- Tobias Lammel — Researcher at University of Goth…
- Kamel Mansouri [orcid: 0000-0002-642…

ECO ITN publications

FOLLOW

Environmental ChemOinformatic - FP7 Marie Curie Innovative Training Network
Verified email at ecoitn.eu

REACH chemoinformatics Ecotoxicology Nanotoxicology QSAR

TITLE	CITED BY	YEAR
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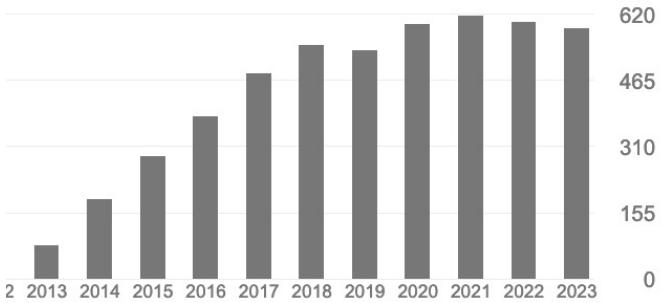

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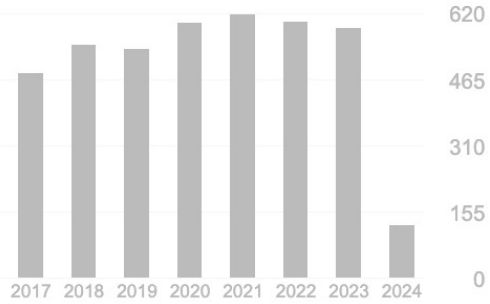

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- A. Jan Hendriks — Professor of Environmental Scie…
- Faizan Sahigara — in silico modelling expert
- Tobias Lammel — Researcher at University of Goth…
- … orcid: 0000-0002-642…

Screenshot

Faizan Sahigara · 1st

Business Development & Brand Manager | QSAR Modeling Expert

Paris, Île-de-France, France · **Contact info**

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Joachim Vogt, **Dr. Ahmed Sayed, MBA**, and 149 other mutual connections

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Message More

Accelerated Early staGe drug dIScovery

AEGIS

Accelerated Early staGe drug dIScovery

EC HORIZON 2020 Marie Skłodowska-Curie
Innovative Training Network (ITN)

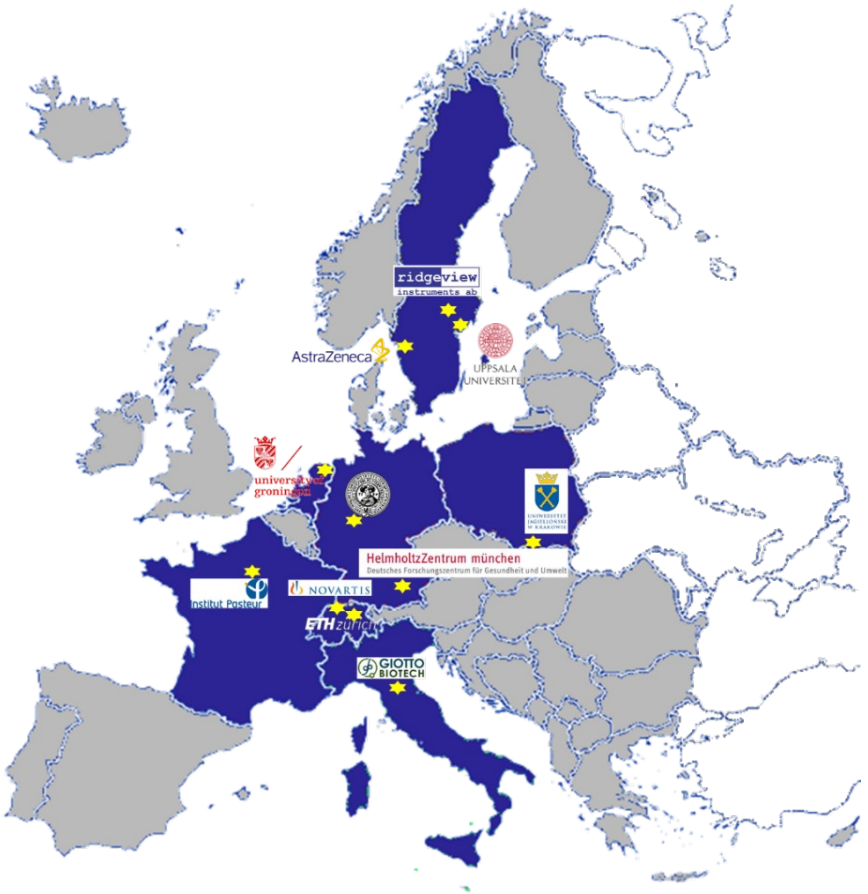
Coordination:
Michael Sattler, Helmholtz Zentrum München

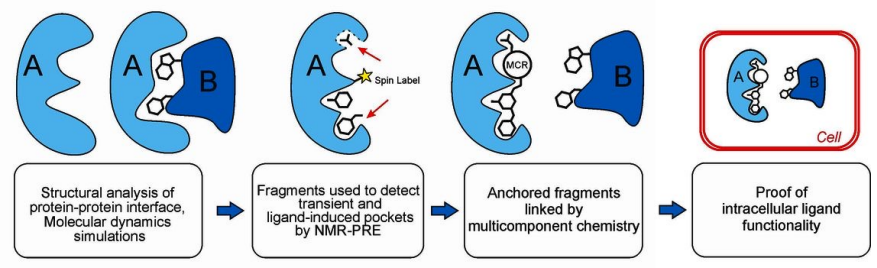
NOVARTIS

AstraZeneca

ridgeview instruments ab

GIOTTO BIOTECH





BigChem http://bigchem.eu

big data in chemistry + informatics = chemoinformatics

The **increasing volume of biomedical data** in chemistry and life sciences requires development of **new methods and approaches for their analysis**.

The BIGCHEM project will provide **innovative education in large chemical data analysis**. The innovative research program will be implemented with the target users, **large pharma companies and SMEs**, which generate and analyze large chemical data as well as will promote technology transfer from academy to industrial applications.

Marie Skłodowska-Curie Innovative Training Network
European Industrial Doctorate

BIGCHEM fellows: three years after the project end

Two fellows who joined BICGHEM later

Dr. Raquel Rodríguez-Pérez, University of Bonn/Boehringer Ingelheim - PhD by University of Bonn - now **Principal Scientist at Novartis,** Basel, Switzerland

Dr. Arkadii Lin, University of Strasbourg/Boehringer Ingelheim - PhD by University of Strasbourg -now **Team Leader in Chemoinformatics at Insilico Medicine**, Abu Dhabi

Dr. Dipan Ghosh, Helmholtz Zentrum München/LDC - PhD by Technical University of München - now **Scientist at Lead Discovery Center GmbH,** Dortmund, Germany

Laurianne David, University of Bonn/AstraZeneca - now **Computational Chemist at Evotec**, Toulouse, France

Dr. Josep Arús-Pous, University of Bern/AstraZeneca - PhD by University of Berm - now **Senior Machine Learning Engineer at Roche,** Basel, Switzerland

Dr. Xuejin Zhang, ETH Zürich/Boehringer Ingelheim - PhD by ETH Hönggerberg -now **ML/AI Scientist at VantAI, USA**

Thomas Blaschke, AstraZeneca/University of Bonn (finishing PhD, **working on a start-up in the UK**)

Dr. Amol Thakkar, University of Bern/AstraZeneca - PhD by University of Berm - now **Research Scientist at IBM Research,** Zurich,

Michael Withnall, Helmholtz Zentrum München/AstraZeneca - now **Head of Computational Chemistry at Apheris AI,** Berlin

Oliver Laufkötter, AstraZeneca/University of Bonn (finishing PhD)

Benedict Mutimba,* Boehringer Ingelheim - now **Technical Project Manager & Scrum Master at Klick Health,** Toronto, Canada

Eric March Vila,* University of Modena and Reggio Emilia, now - **Research Associate at Universitat Pompeu Fabra,** Barcelona

BIGCHEM publications

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Horizon2020 Marie Skłodowska-Curie Innovative Training Network European Industrial Doctorate

Verified email at bigchem.eu

big data chemoinformatics cheminformatics

TITLE	CITED BY	YEAR
The rise of deep learning in drug discovery H Chen, O Engkvist, Y Wang, M Olivecrona, T Blaschke Drug discovery today 23 (6), 1241-1250	1525	2018
Molecular de-novo design through deep reinforcement learning M Olivecrona, T Blaschke, O Engkvist, H Chen Journal of cheminformatics 9 (1), 1-14	1000	2017
Automating drug discovery G Schneider Nature reviews drug discovery 17 (2), 97-113	621	2018
QSAR without borders EN Muratov, J Bajorath, RP Sheridan, IV Tetko, D Filimonov, V Poroikov, ... Chemical Society Reviews 49 (11), 3525-3564	564	2020
Application of Generative Autoencoder in *De Novo* Molecular Design T Blaschke, M Olivecrona, O Engkvist, J Bajorath, H Chen Molecular informatics 37 (1-2), 1700123	408	2018
Molecular representations in AI-driven drug discovery: a review and practical guide L David, A Thakkar, R Mercado, O Engkvist Journal of Cheminformatics 12 (1), 1-22	328	2020
Interpretation of machine learning models using shapley values: application to compound potency and multi-target activity predictions R Rodríguez-Pérez, J Bajorath Journal of computer-aided molecular design 34, 1013-1026	295	2020
A de novo molecular generation method using latent vector based generative adversarial network O Prykhodko, SV Johansson, PC Kotsias, J Arús-Pous, EJ Bjerrum, ...	278	2019

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	All	Since 2019
Citations	8692	8317
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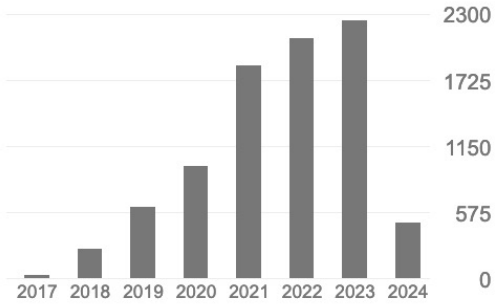
i10-index	56	55



Co-authors

VIEW ALL

- Ola Engkvist, AstraZeneca R&D Gothenburg O…
- Hongming Chen, Bioland Laboratory
- Jürgen Bajorath, Professor of Life Science Inform…
- Jean-Louis Reymond, University of Bern
- Thomas Blaschke, Phd student, AstraZeneca/Unive…
- Igor V. Tetko, BIGCHEM GmbH & Helmholtz M…
- Evinova (AstraZeneca)

Screenshot

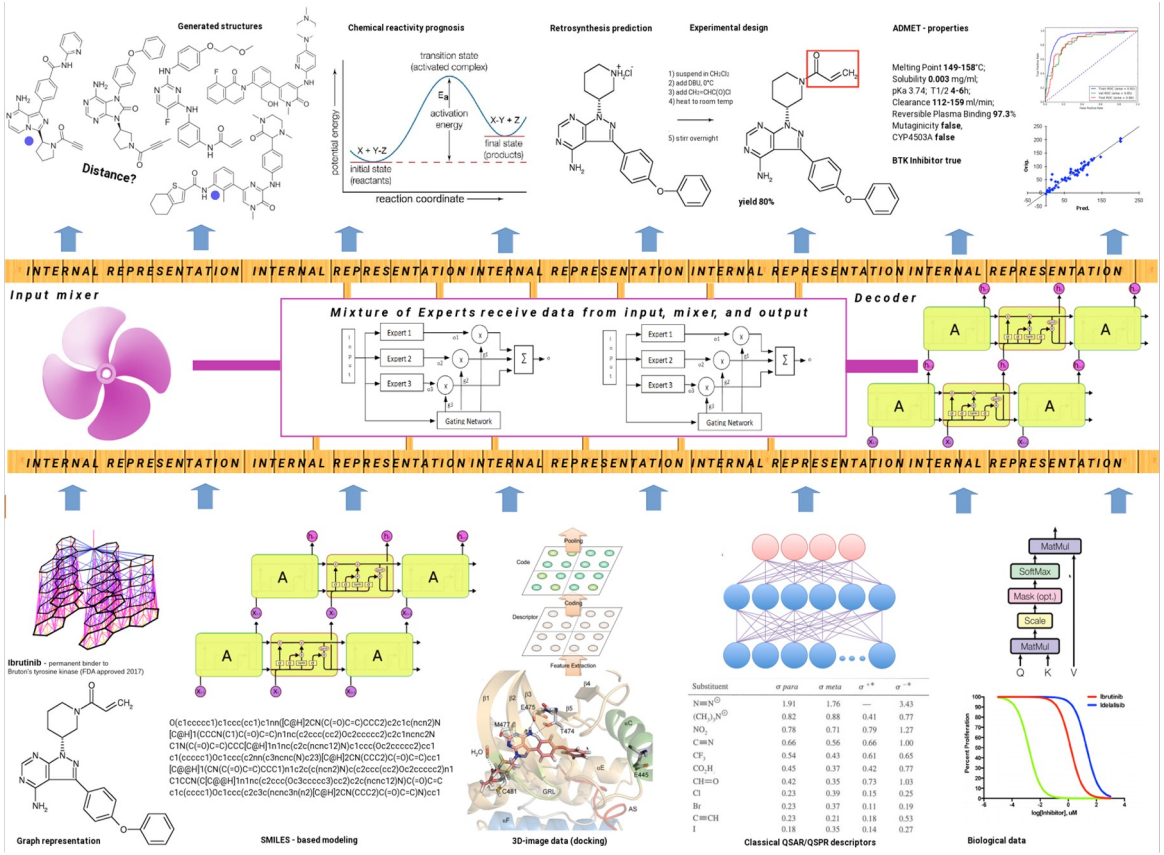
AIDD ITN https://ai-dd.eu

Advanced machine Learning for Innovative drug discovery

Marie Skłodowska-Curie Actions

HELMHOLTZ MUNICH

16 PhDs
17 beneficiaries
13 partners
5 companies
17 countries
3.93 M€



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Bayer
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Pfizer

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JKU
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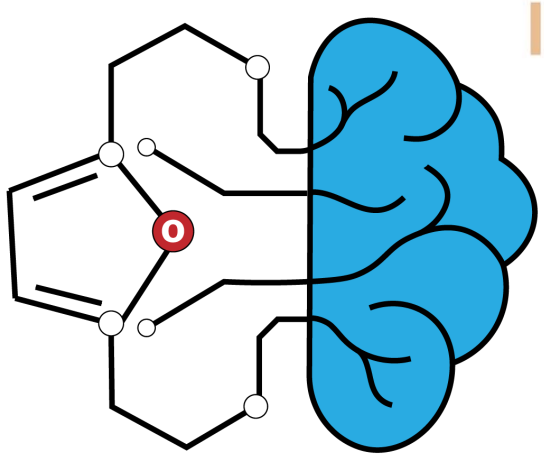
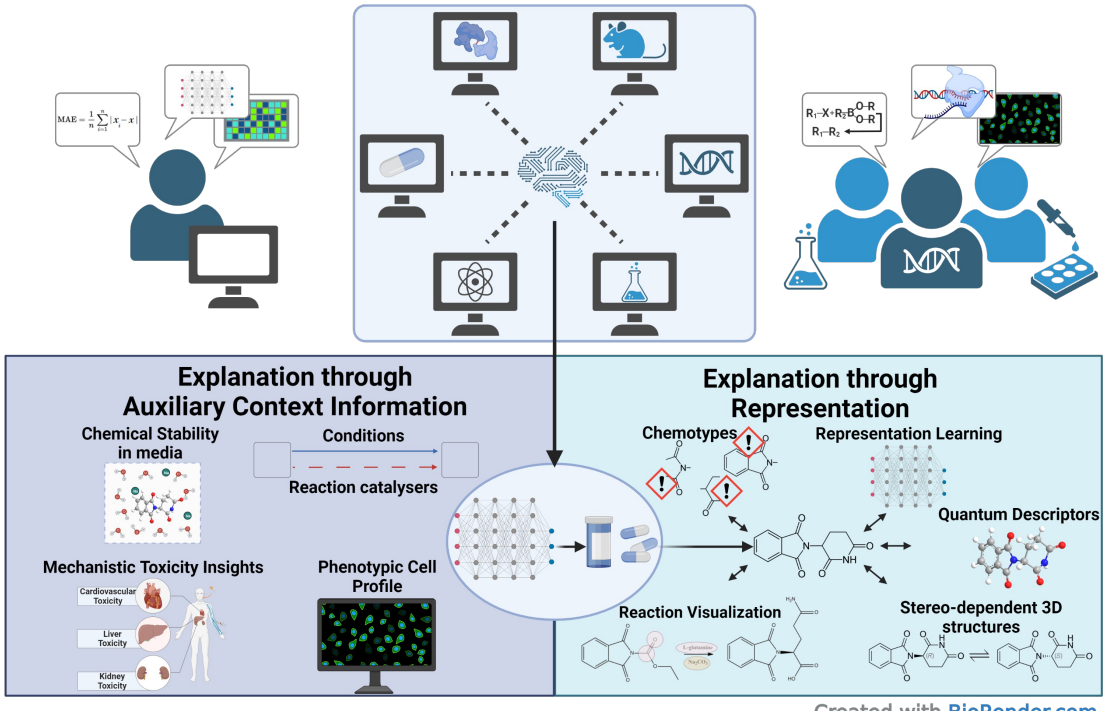
technische universität dortmund
JG|U
Aalto University
UNIVERSITÄT LUXEMBURG
Scuola universitaria professionale della Svizzera italiana
SUPSI
Freie Universität Berlin
universität wien

Explainable AI for molecules - https://aichemist.eu






HELMHOLTZ
MUNICH
German Research Center for Environmental Health

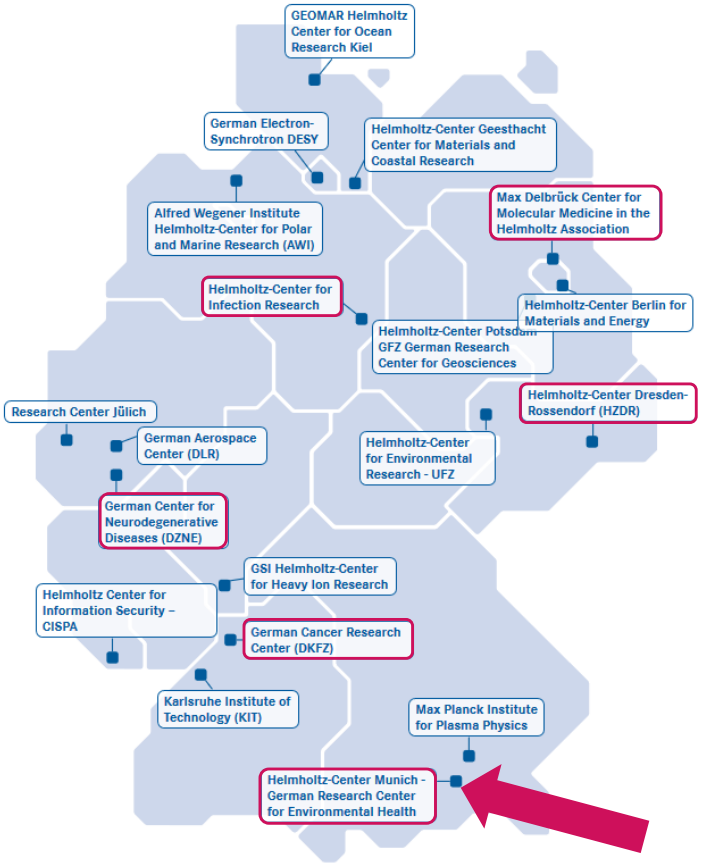
Helmholtz Association – Facts and Figures

Germany´s largest research organization

- 19 research centers
- Budget: 5 Billion €, more than 42.000 staff

6 Research Fields

6 centers represent the Research Field Health.



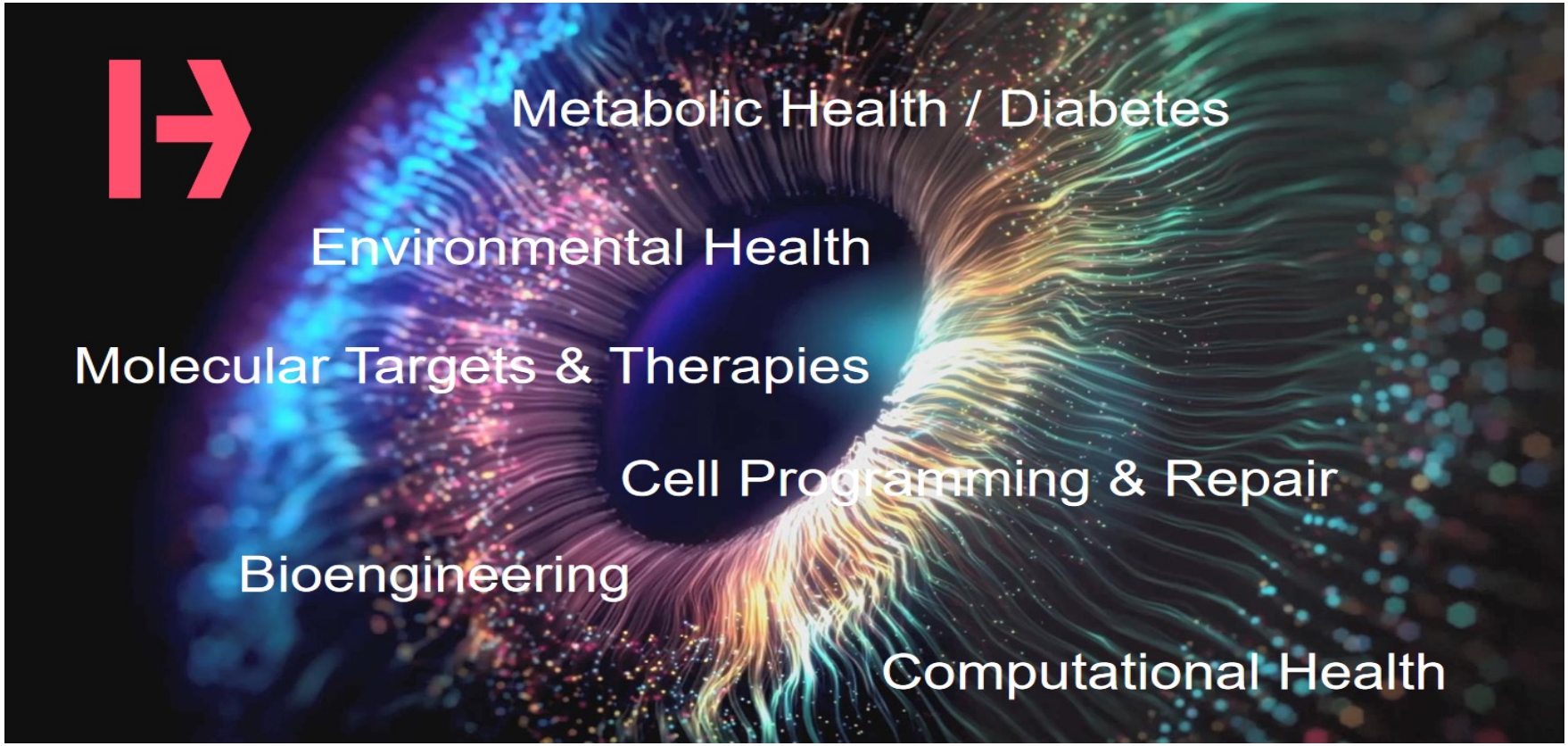
- Our Mission

Discovering personalized solutions for **environmentally triggered diseases** such as diabetes, obesity, allergies, and lung diseases

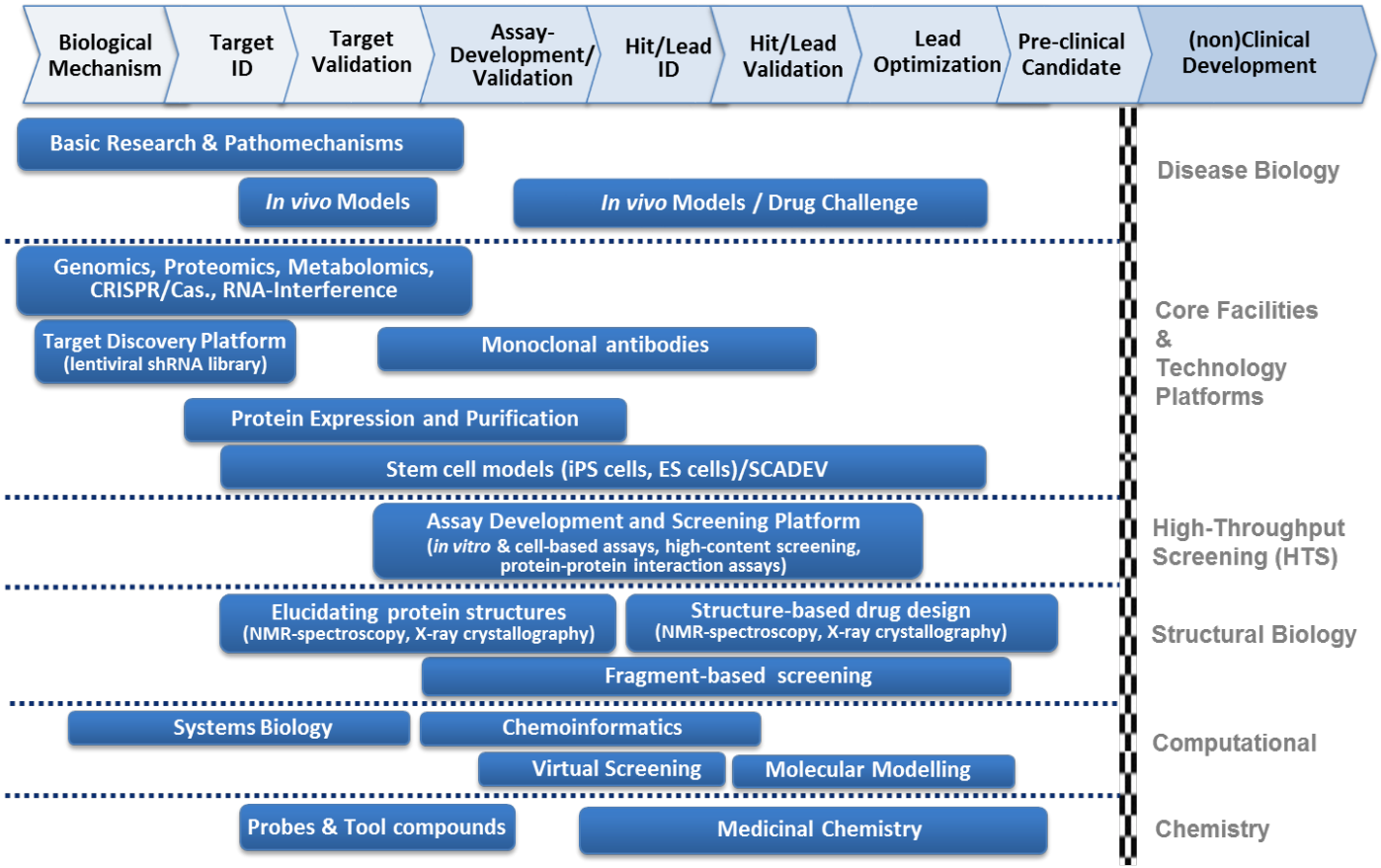
2.475	85	1.604	650
Employees	Nations	Publications in 2021	PhD students

27	48
Spin-Offs	ERC Grants

- Outstanding Research in 6 Departments



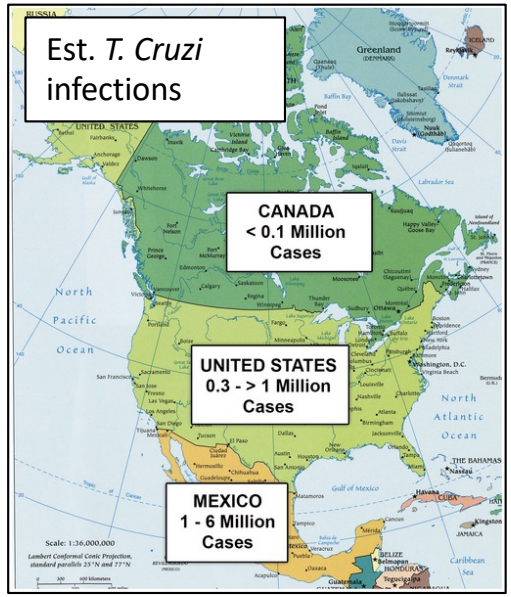
- Cutting-Edge Scientific Infrastructure



Target: Trypanosomatids caused by Kinetoplastida

Human Diseases

Disease	Parasite	Epidemilogy	Region
African sleeping sickness	*Trypanosoma brucei*	7216 Confirmed cases (2012) 20 000 estimated total 70 million in endangered area	Equatorial Africa. „Tse-tse zone“
Chagas disease	*Trypanosoma Cruzi*	41 000 New cases (2010) 10 000 Deaths	**USA, Canada** Latin America, Spain,
Leischmaniasis	*Leishmania Donovani*	1.5-2 million cases yearly, 52 000 deaths 350 million in endangered area	88 (sub)tropical countries, mainly India but also Southern America and **Texas**

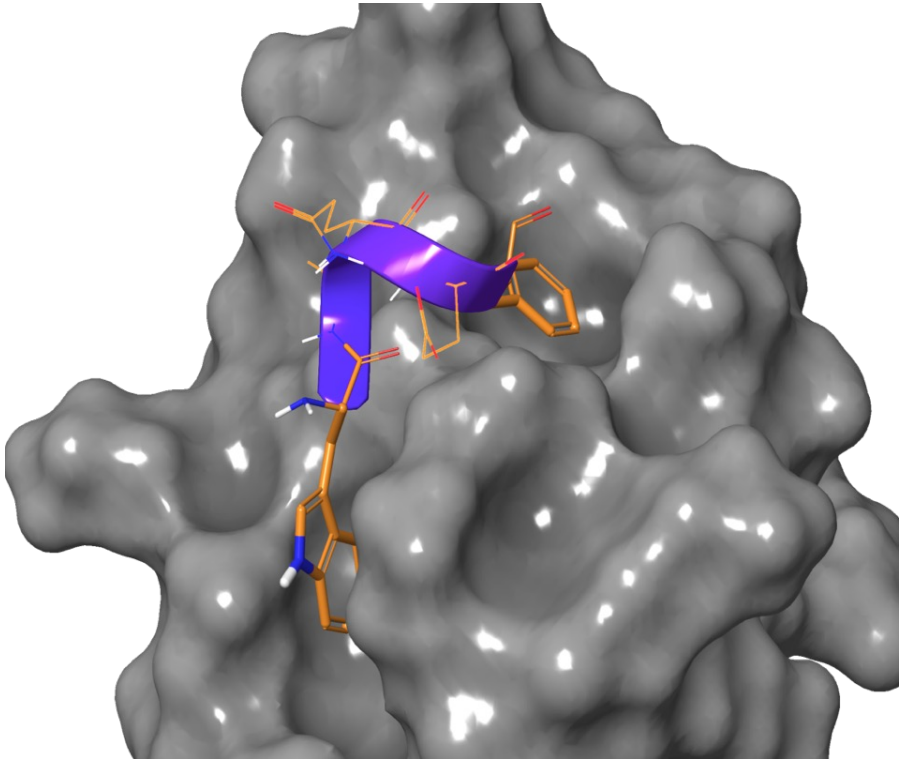


Animal Diseases

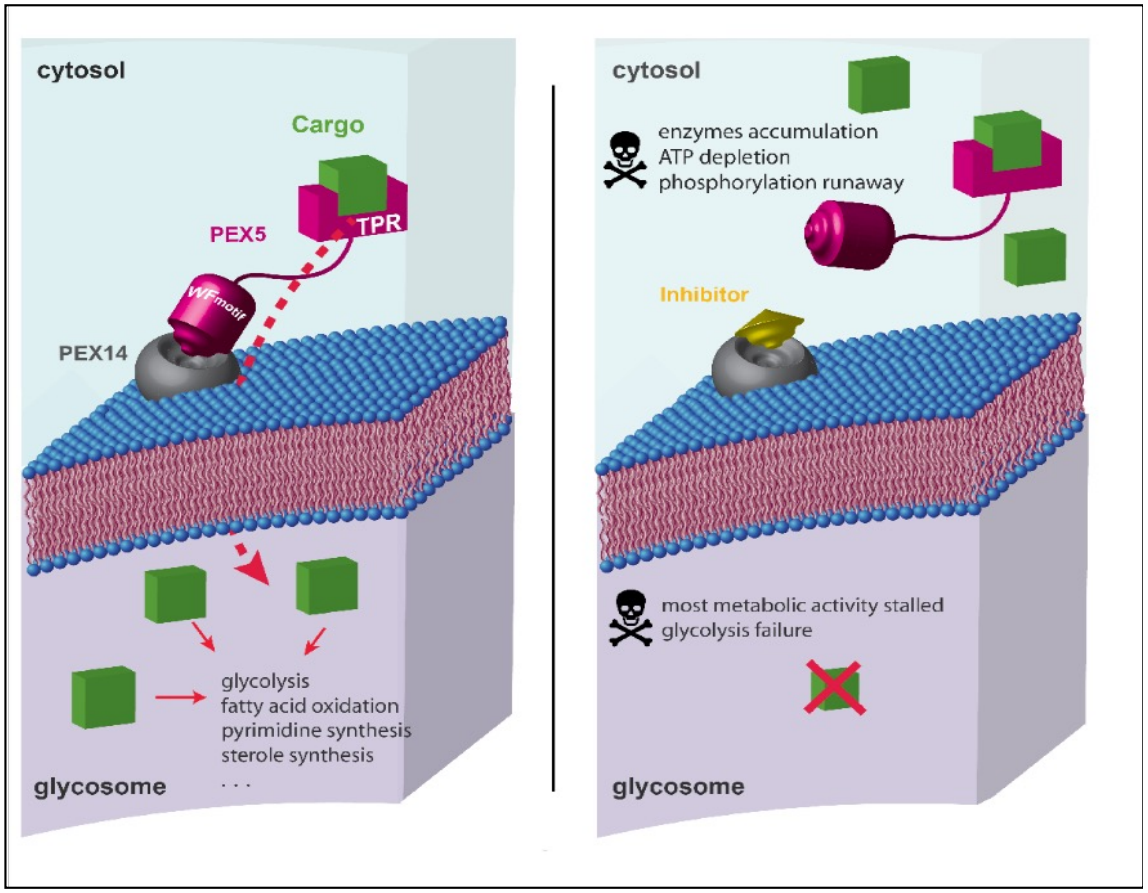
Disease	Parasite	Animals	Region
Nagana	*T. Congolese* *T. Vivax*	Cattle, sheep, pigs, horses, camels, monkeys	37 African countries
Dourine (Covering sickness)	*T. Equiperdum*	Horses, donkeys, mules **-untreatable-**	Africa, Asiatic Russia, Middle East **Europe (2011 Outbreak in Italy)**
Surra	*T. Evansi* *T. Suis*	Horses, donkeys, mules, cattle, camels,	South America, Africa, Middle East, Philippines
Sheep Ked	*T. Melophagium*	Sheep (benign)	**Northern UK**, Croatia (86%), Turkey (8%)
	T. Irwini	Koalas	Australia

Source: WHO Fact sheet N°259 FAO- PAAT
Hotez. PJ. Et al PLoS Negl Trop Dis. 7(10): e2300.

Hypothesized Target



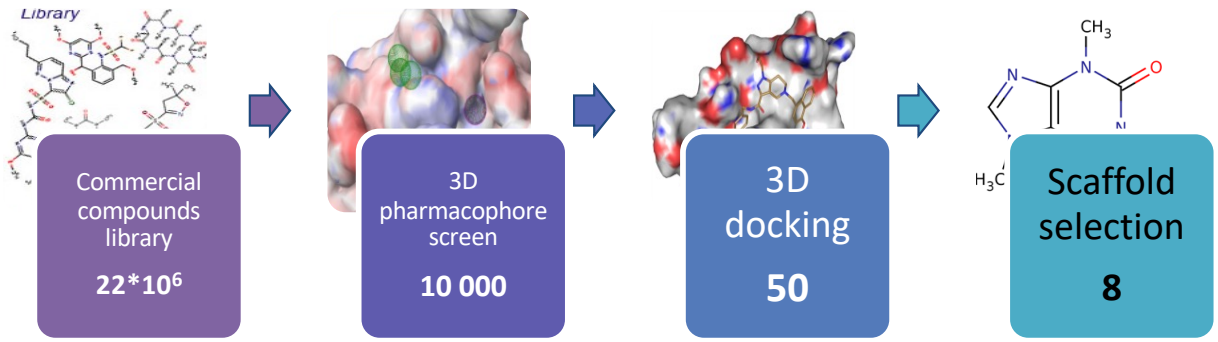
PPI interface

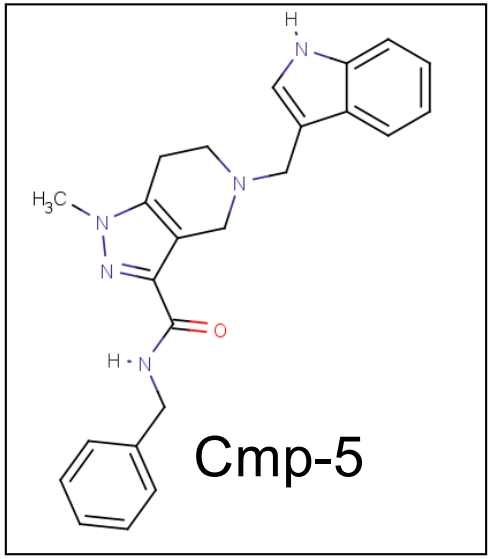


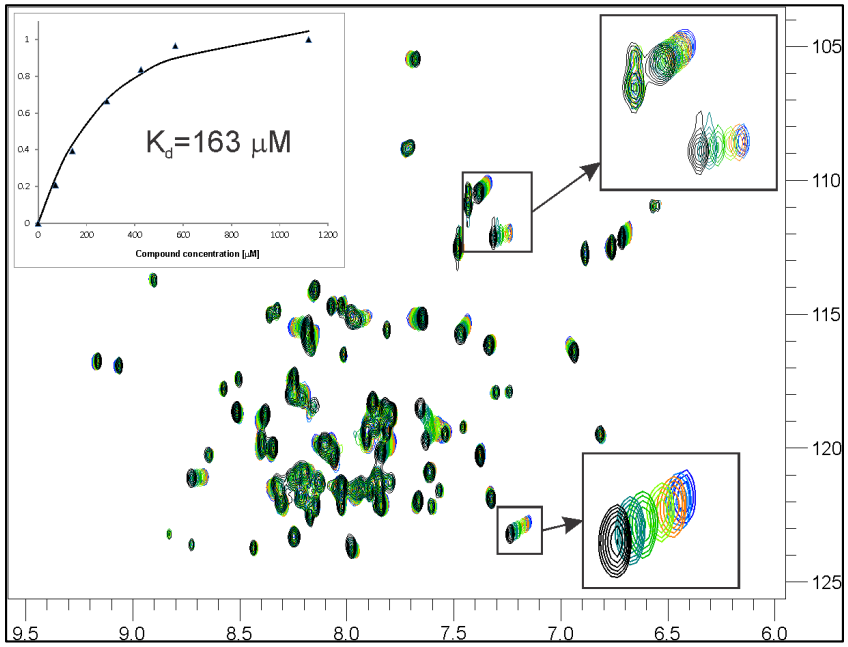
Neufeld, C. … Sattler, M. (2009) EMBO J. 28: 745-754

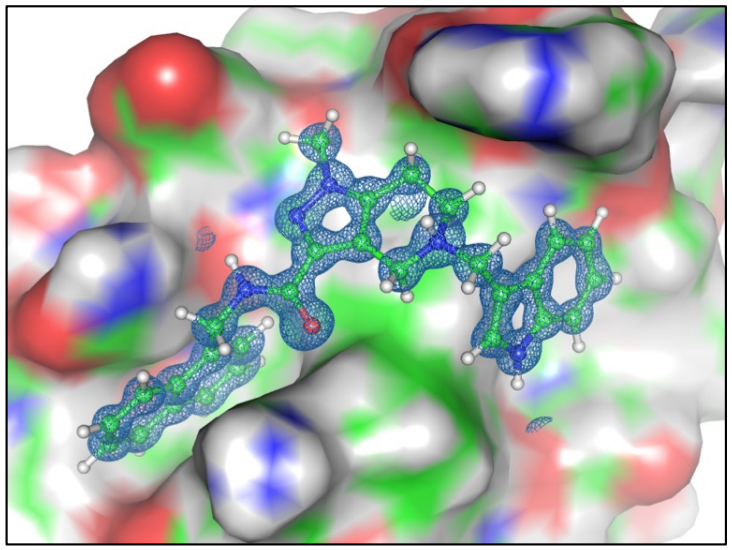
Peroxins Pex14/Pex5 are responsible for transport of glycosomal enzymes from cytoplasm to glycosomes for glucose metabolism

Hit identification



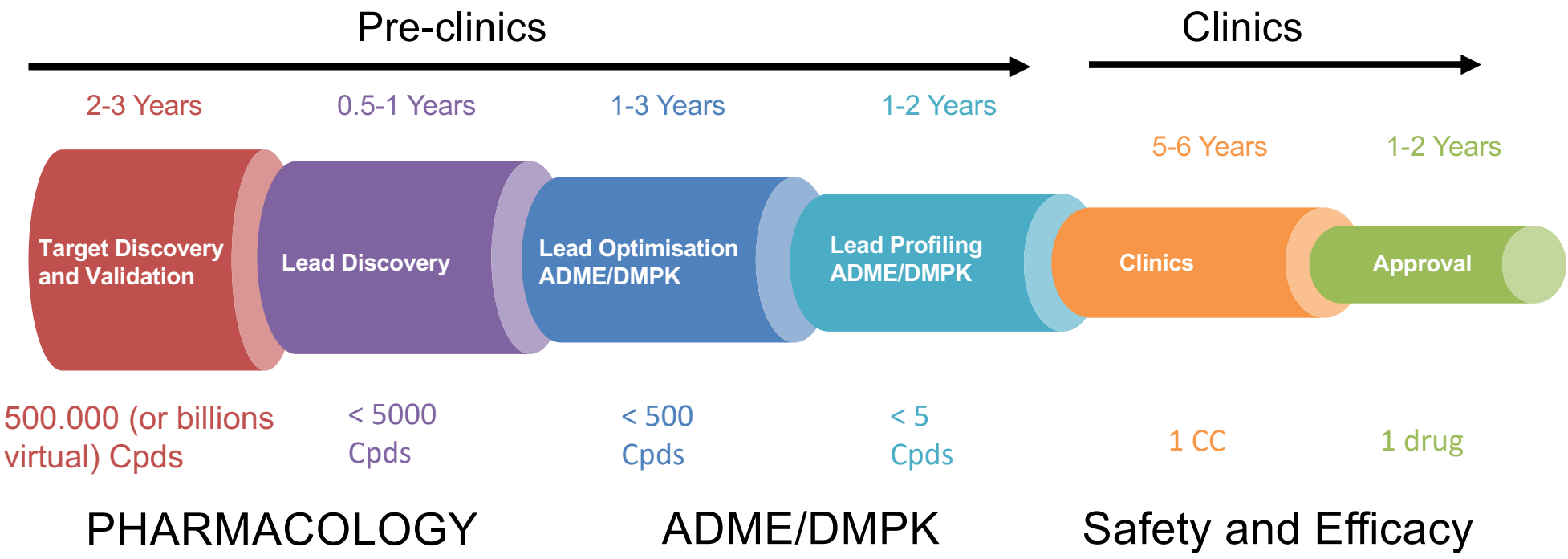






Dawidowski, M., … Popowicz, G. M. Science 2017, 355, 1416-1420.

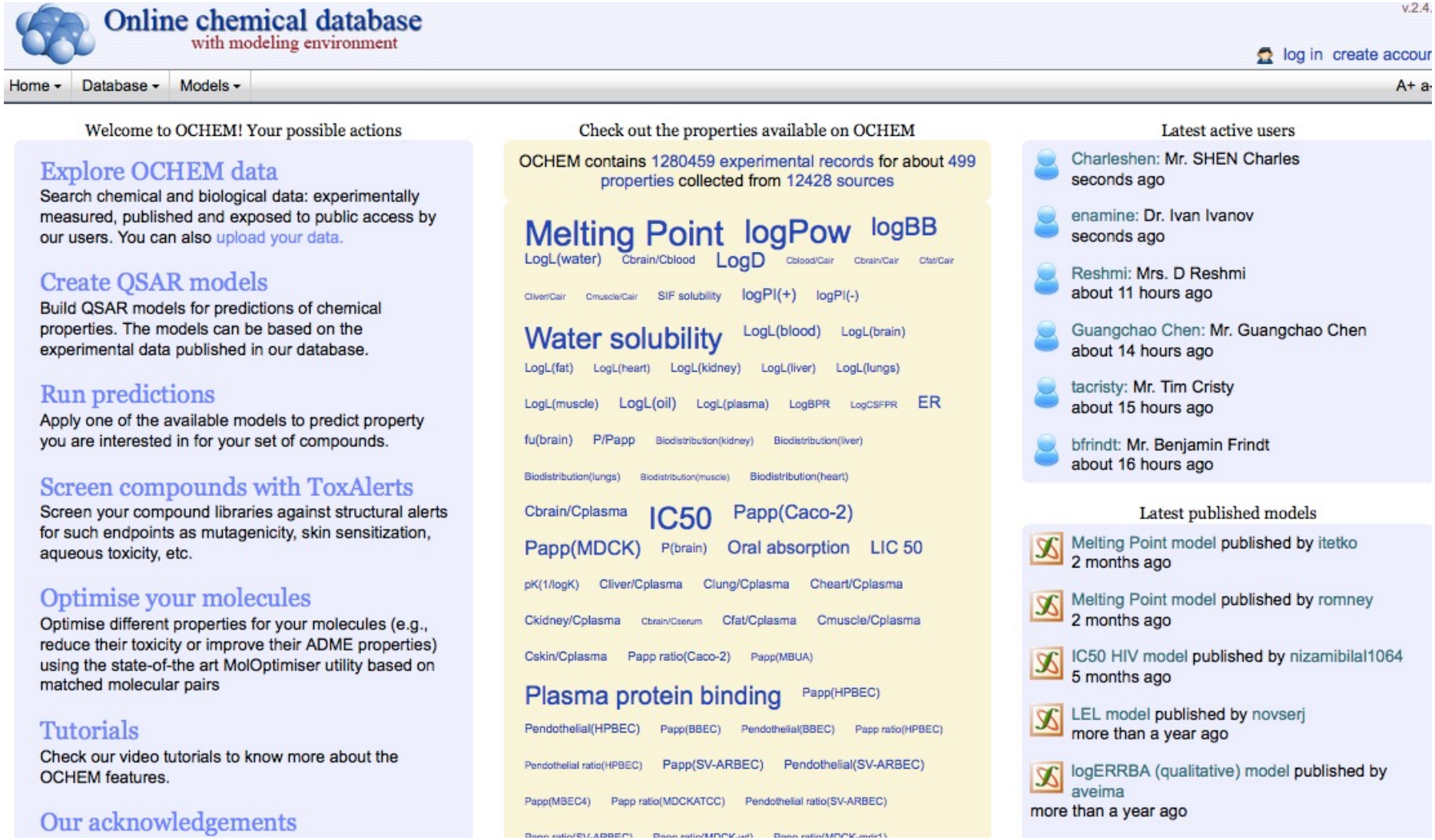
Traditional Process of Drug Discovery



- Profiling and screening in the virtual space helps to identify the most promising candidates

Slide courtesy of Dr. C. Höfer, Merck

Data storage and model development: http://ochem.eu



openOCHEM https://github.com/openochem

Overview | Repositories 3 | Projects | Packages | Stars

openochem / README.md

Open OCHEM -- AI models for drug discovery and environmental chemistry

The Open OCHEM is open source version of the On-line Chemical database and Modelling Environment Platform (http://ochem.eu)

It is a user-contributed repository of referenced experimental data, computational tools and models of ADMET properties of chemical compounds. The OCHEM algorithms can reliably identify compounds predicted with experimental accuracy: there is no need to test them in a lab. The OCHEM can be used for timely and low-cost identification of scaffolds with lower risks of failure due to the unfavorable physico-chemical and/or biological properties. The free open source of OCHEM is a reference system for academic users thus accumulating data and knowledge produced in academia. The developed OCHEM workflow allows an unbiased comparison of different existing and new machine learning algorithms which can be easily integrated in OCHEM by its users.

OCHEM software can be used to develop QSPR and QSAR models for various biological and physico-chemical projects. It can work with millions of molecules and can be configured to use hundreds of CPUs or GPUs. Open OCHEM allows you to install the fully functional version of the software and analyse your data privately. The closed source version is also available from BIGCHEM GmBH and provides several additional optimized software packages which were contributed by the company or its partners.

The open OCHEM currently supports tens methods and descriptors packages, which were developed and contributed by different providers and are distributed under the open source or respective license agreements (most of them are free of charge for academic, educational, recreational or evaluation purposes - check each respective license agreement).

See installation instructions how to install and run open the OCHEM.

We wish you a happy computing!

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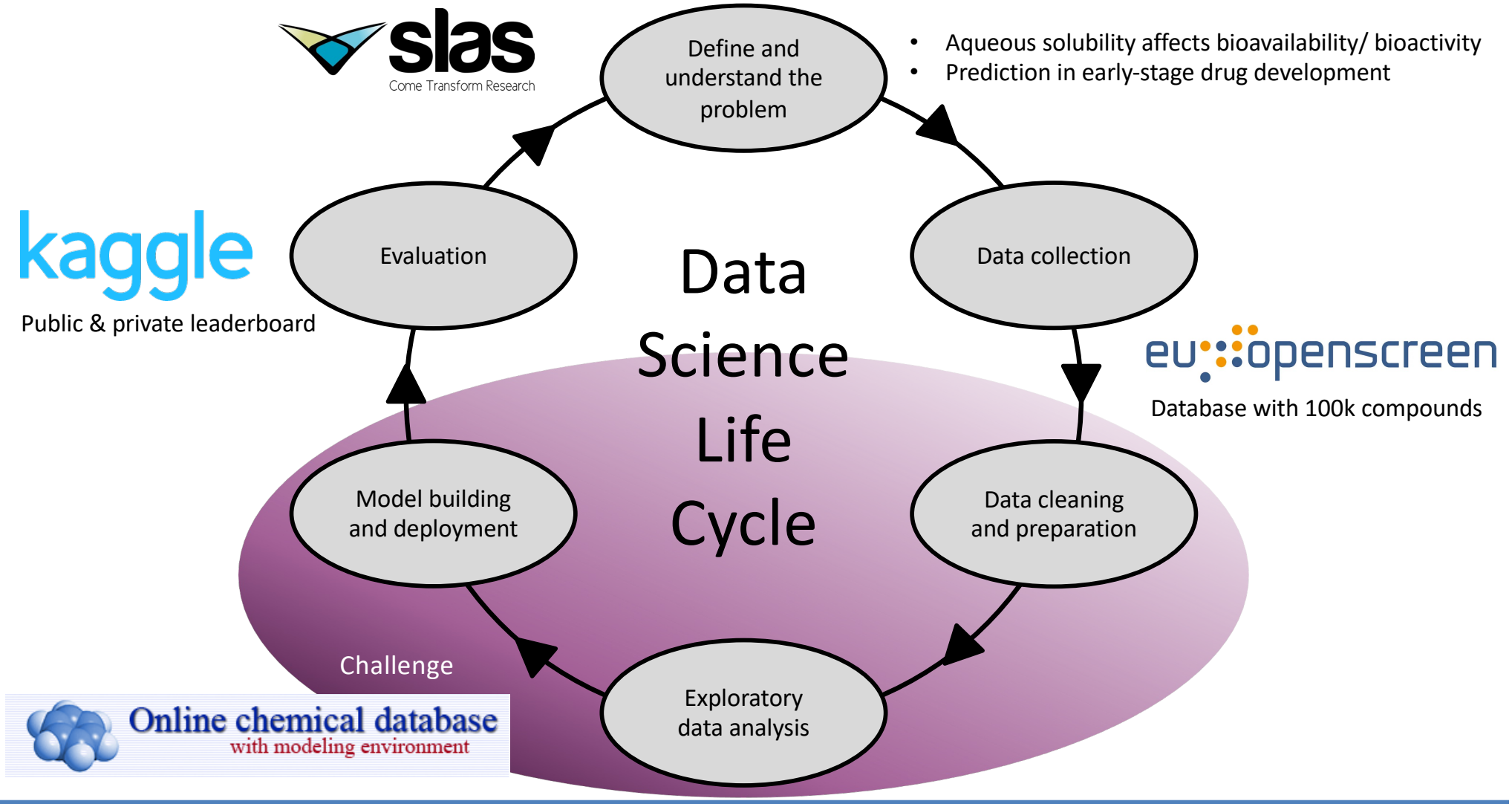

A. Hunklinger et al, *SLAS Discovery*, 2024.

National Center for Advancing Translational Sciences

Tox21 Data Challenge 2014

Login

Open call ends: November 14, 2014

About the Data

The Challenge

The 2014 Tox21 data challenge is designed to help scientists understand the potential of the chemicals and compounds being tested through the Toxicology in the 21st Century initiative to disrupt biological pathways in ways that may result in toxic effects.

The goal of the challenge is to "crowdsource"

All challenge winners will receive the opportunity to submit a paper for publication in a special thematic issue of *Frontiers in Environmental Science* and recognition on the NCATS website and via social media.

www.epa.gov/ncct/challenges.html

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Key Links

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EPA Exposure Research
Research Projects
Chemical Databases
ToxCast Stakeholder Events
EPA Chemical Safety Research
Research Publications
Scientific Reviews
Communities of Practice
ToxCast Data Challenges
Staff Profiles
CompTox Partners
Jobs and Opportunities

ToxCast Chemical Data Challenges and Release

EPA's high-throughput screening data on 1,800 chemicals is accessible through the interactive Chemical Safety for Sustainability Dashboards (iCSS dashboard). The iCSS dashboard provides user-friendly and customizable access to toxicity data from ToxCast and Tox21 high-throughput chemical screening technologies.

Using the TopCoder and InnoCentive crowd-sourcing platform, EPA invited the science and technology community to work with the data and provide solutions for how the new toxicity data can be used to predict potential health effects. The ToxCast data challenges focused on using this data and other publicly available data to predict the lowest effect level from traditional toxicity studies using laboratory animals. Challenge winners received awards for solving this challenge.

Key Links

- Lowest Effect Level Challenge Results (PDF, 497KB, 18pp)
- Chemical Safety for Sustainability Dashboards
- Complete ToxCast Phase II Data & Files
- TopCoder Challenge
- InnoCentive Challenge
- Stakeholder Workshops

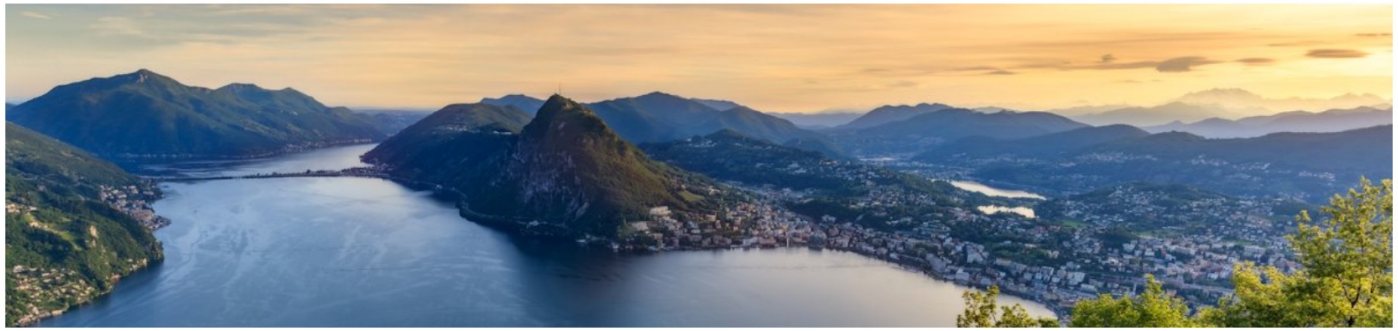
Novotarskyi, S. et al. *Chem. Res. Toxicol*. 2016, 29, 768-75.

https://icann2024.org

ICANN24

33rd International Conference on Artificial Neural Networks

MENU



Welcome to ICANN 2024

The 33rd International Conference on Artificial Neural Networks.
A conference of the European Neural Network

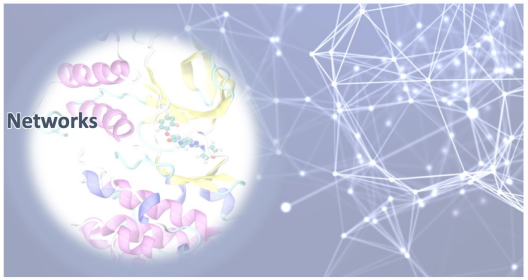
Submission deadline March 15 (April 15*)

Workshop on

AI in Drug Discovery at the

33rd International Conference on Artificial Neural Networks

ICANN24



The Workshop on AI in Drug Discovery, to be held within the esteemed 33rd International Conference on Artificial Neural Networks (ICANN 2024), invites cutting-edge contributions in the rapidly evolving field of AI-driven drug discovery. We are seeking submissions encompassing various facets such as generative models, explainable AI, model distillation, uncertainty quantification, reaction informatics and synthetic route prediction, quantum machine learning for reactivity, methodologies for mining very large compound data sets, federated learning, analysis of HTS data and identification of frequent hitters and other topics related to the use of ML in chemistry. This workshop aims to bring together machine learning experts, computational chemists and chemoinformaticians working on the development and application of ML in chemistry, environmental health and (eco)toxicology.

WORKSHOP TOPICS

We look forward to receiving contributions from all researchers active in the field, whether they are developing novel methodologies or expanding the scope of established methodologies. A non-exhaustive list of topics includes:

- Big Data and Advanced Machine Learning in Chemistry
- Use of Deep Learning to Predict Molecular Properties
- Modeling and Predication of Chemical Reaction Data
- eXplainable AI (XAI) in Chemistry
- Chemoinformatics
- Generative Models

SUBMISSION INSTRUCTIONS

Contributions (full/short papers or extended abstracts) should be submitted through the regular ICANN submission system at https://icann2024.org. Select track "AI in Drug Discovery Workshop". Accepted papers will appear in the proceedings of the ICANN 2024. The authors of accepted articles/abstracts will be invited to submit new or updated papers to a special issue of a journal before end of September 2024 with a discount (negotiations ongoing).

IMPORTANT DATES

- Deadline for full, short papers and extended abstracts via submission system: 15th of March
- Deadline for extended abstract submission by e-mail to aidd@icann2024.org: 15th of April
- Notification of acceptance: 15th of May
- Conference dates: 17 – 20 September 2024

PROGRAM COMMITTEE

Ola Engkvist, Matteo Aldeghi, Hugo Ceulemans, Samuel Kaski, Frank Noé, Yves Moreau, Günter Klambauer, Sepp Hochreiter, Jürgen Schmidhuber, Michael Wand, Paul Czodrowski, Mike Preuss, Alexandre Tkatchenko, Johannes Kirchmaier, Gianni de Fabritiis, Artem Cherkasov, Fabian Theis, Marc Bianciotto, Chihae Yang, Jan Halborg Jensen, Alexandre Varnek, Alessandra Roncaglioni, Francesca Grisoni, Rodolphe Vuilleumier, Philippe Schwaller, Hyun Kil Shin

ORGANIZERS

Dr. Igor Tetko
Group Leader Chemoinformatics and Chemical Biology
Institute of Structural Biology, Helmholtz Zentrum Munich
Neuherberg, Germany
Contact: aidd@icann2024.org

Dr. Djork-Arné Clevert
VP Machine Learning Research
Pfizer
Berlin, Germany
Contact: Djork-Arne.Clevert@pfizer.com

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Peter Hartog
Fabian Krüger
Paula Torren-Peraire
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Katya Ahmad
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