

Leibniz
Wirkstoffe und
Biotechnologie

Bioactives Cloud



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Leibniz Bioactives Cloud



<http://www.leibniz-wirkstoffe.de>

- The big picture
- Concepts and accomplishments
- Plans and tasks for the (near) future

The big picture

- Leibniz Association
 - >80 independent institutions
 - Goals: scientific excellence, competitiveness
- Leibniz research alliances (LRA):
 - funding instrument
 - competitiveness through **cooperation**
- LRA Bioactive Compounds and Biotechnology:
 - Leibniz Conference on Bioactive Compounds
 - Seed money
 - Software platform “**Leibniz Bioactives Cloud**”

Semantic web technology

- Supplementation of additional facts
- Ontologies are fact databases
- Community provides ontologies for
 - organisms
 - extracts
 - assays
 - compounds
 - reactions
 - etc.

Class:	Oomycota
Order:	Peronosporales
Family:	Pythiaceae
Genus:	<i>Phytophthora</i>

BIOACTIVE FUNGAL METABOLITES

Infections with *Phytophthora infestans*, the causal agent of potato and tomato late blight disease, are difficult to control and can lead to considerable agricultural losses. Thus, the development of new effective agents against the pathogen is of great interest. In previous work, (*E*)-4-oxohexadec-2-enoic acid (**compound I**) was isolated from *Hygrophorus eburneus*, which exhibited fungicidal activity against *Cladosporium cucumerinum*. In our on-

⇒ **Search: Oomycota AND fatty acid**

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Existing software projects:

- Web based
- Advanced technologies
- Distributed infrastructure
- Chemistry aware



BioSolr 

 ckan

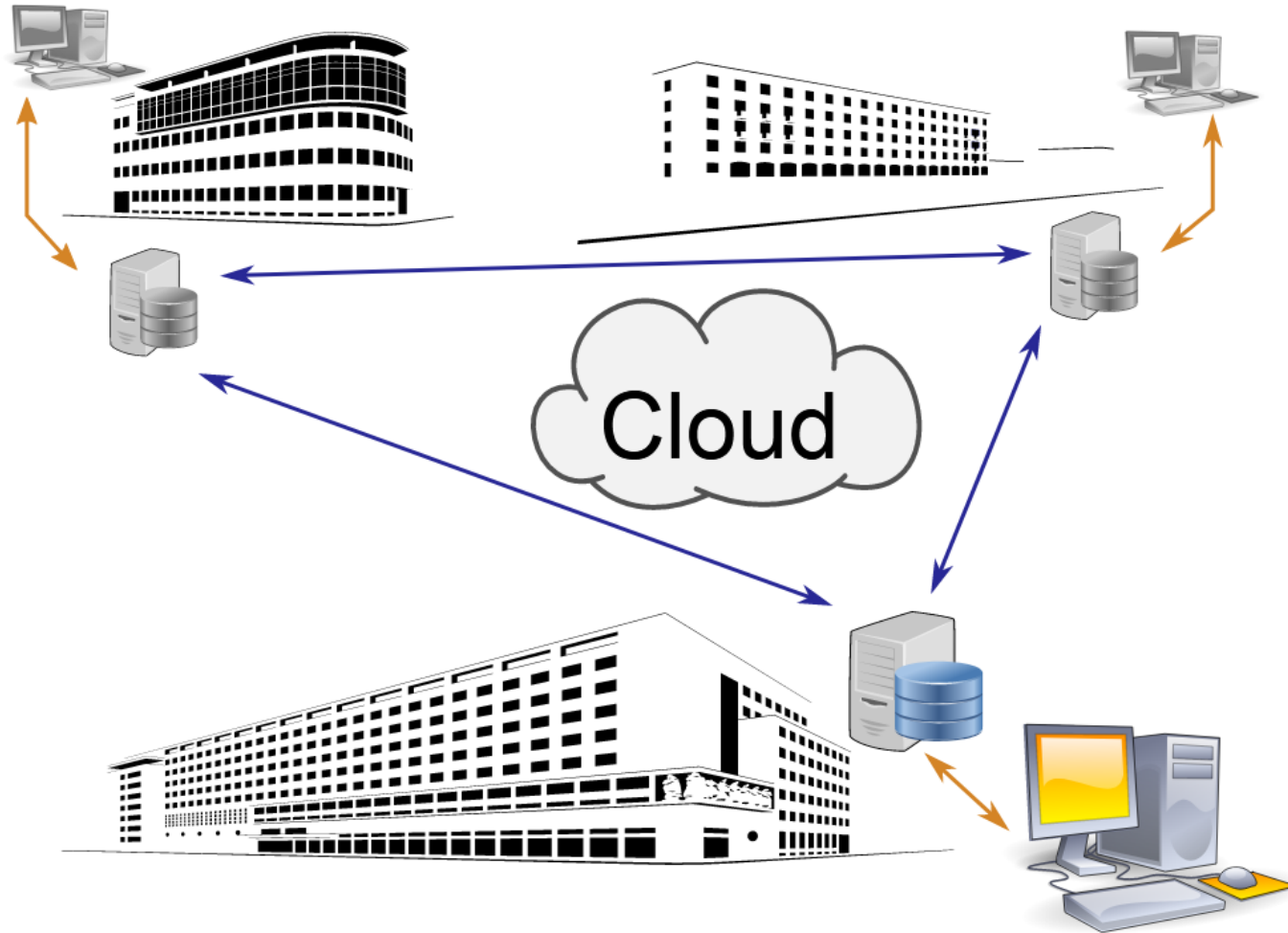
 LAILAPS
THE PLANT SCIENCE SEARCH ENGINE

 ZB MED Search Portal
for Life Sciences
LIVIVO

 RADAR
eu:openscreen

 BASE
Bielefeld Academic Search Engine

Architecture



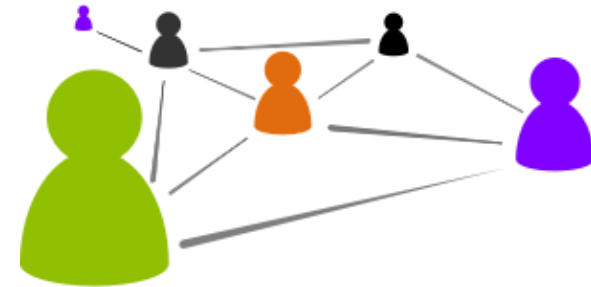
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“Smart data warehouse”

- Exchange of text documents (grey literature, ...)
- Advanced technologies: semantic annotation / ontologies, chemistry awareness, mining and analysis of research data

“Social networking” for scientists

- Personal profiles highlighting expertise
- Establishing contacts



“Market place”

- For scientific know how, services, data or samples



inhibitor AND parp



Dateien zum Upload auswählen ...

Show entries

Dokument	Quelle	Relevanz
 PPHeym_Dissertation.pdf	Public collection @ICA Halle (ICA Halle)	90
 jahresbericht_09100_Layout_1.pdf	Public collection @IPB Halle (IPB Halle)	48
 2013_sr_119_fuer_web.pdf	Public collection @IPB Halle (IPB Halle)	57

Showing 1 to 3 of 3 entries

Previous

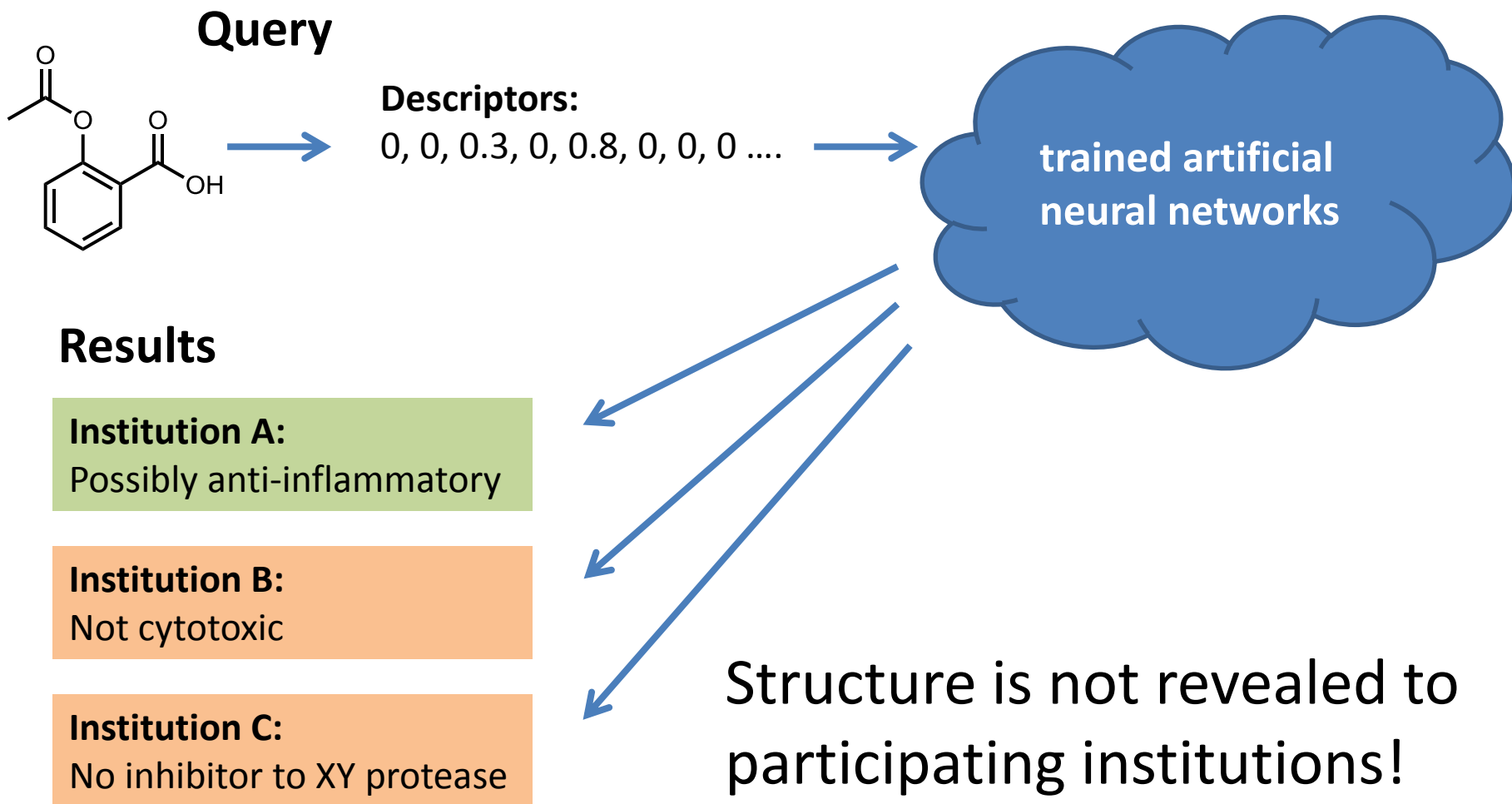
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Next

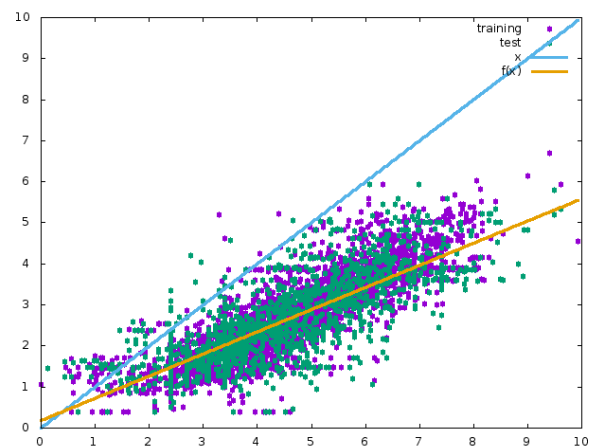
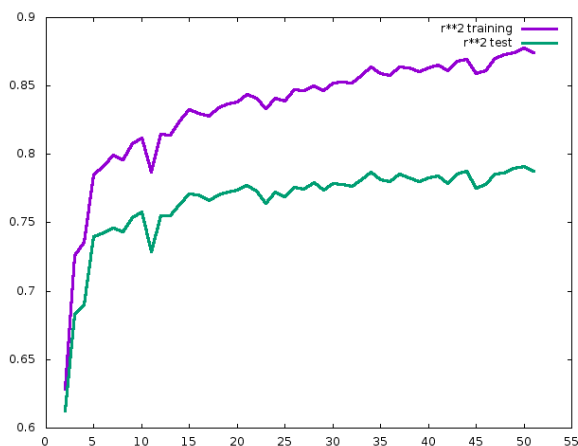
Accomplishments

- Distributed network of nodes
- Document handling
(upload, indexing, searching & download)
- Basic authorization
- Automated installation procedure
- Extensive project documentation
(see: <http://www.leibniz-wirkstoffe.de>)

Distributed SAR



Distributed SAR



- Superior performance ($r^2 > 0.75$)
- Integration into the web portal will be accomplished within the next few months
- SAR could assist in matching compound owners with assay providers

Your Support Needed



Rollout to
additional institutions

Documents & data to
feed into the cloud



“Test drivers”

