

BRENDA



Date: 23.10.2019 (09.00-17.00)
24.10.2019 (09.00-13.00)

Location:
TU Braunschweig, BRICS
Rebenring 56, Room 44

Learning goals:

- Introduction to the **BRENDA** enzyme database and exploiting the potential of enzyme structures in **ProteinsPlus**
- Learning and understanding the scope and organization of the databases
- Learning and working with the tools of the database

Introduction to BRENDA:

- History, scope and contents
- Data sources and updates
- Application areas

BRENDA web interface:

- Query engine – data access
 - Text-based queries, numerical queries
 - Genome explorer, EC explorer, Taxonomy tree explorer, Ontologies
 - Ligand query via chemical structure or substructure – molecule editor
 - Pathway based queries
 - Complex combination queries

Result pages:

- Enzyme summary page and Ligand summary page
- Word maps
- Pathway maps
- Enzyme/disease relation
- Expected taxonomic range
- Protein 3D structure – amino acid sites
- Enzyme functional parameters – statistical analysis
- Text-mining results

Registration Deadline

15.10.2019

Computer-based BRENDA access:

- SOAP
- SBML output

Introduction to ProteinsPlus:

- Experimental protein structures
- Protein-ligand interactions
- Basics and challenges of molecular modelling

ProteinsPlus server:

- Application area and computational methods behind ProteinsPlus
- Workflow and the interactive visualization concept
- Download options

ProteinsPlus applications:

- Structure preparation and quality assessment
- Protein-ligand binding site and druggability prediction
- Analysis of interactions in protein structures
 - Protein-ligand interactions, metal coordination and 2D visualization
- Protein conformation analysis
- Protein-protein interface classification

Prerequisites:

- Basic knowledge in biochemistry, molecular biology and microbiology
- We recommend that you bring your own laptop

Contact, information and registration:

The training is free of charge. The participants have to cover their traveling and hotel expenses. A list of hotels will be supplied.

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