

Steinbeck Research Group

Cheminformatics and Computational Metabolomics

Institute for Inorganic and Analytical Chemistry (IAAC)

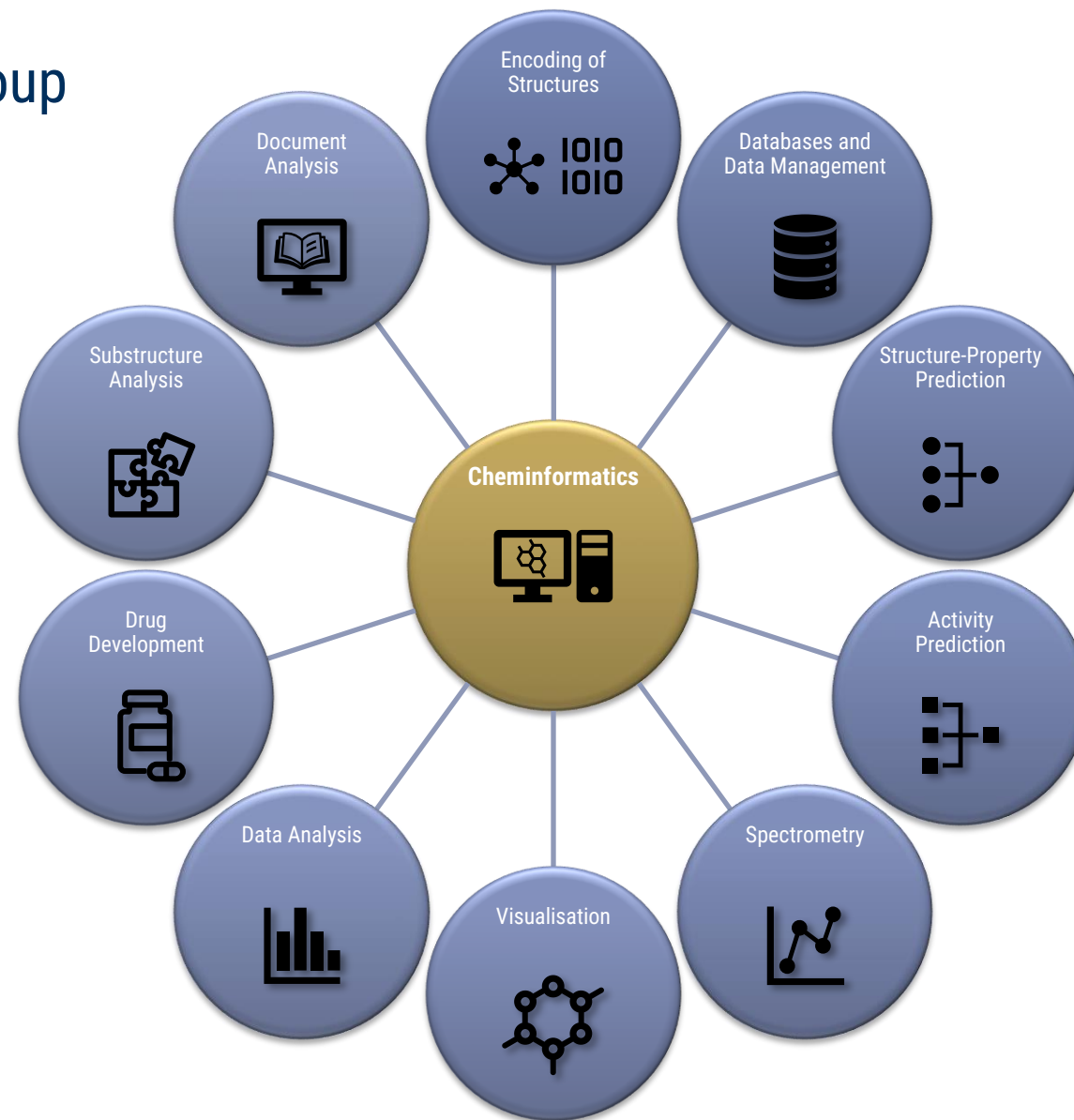


We are part of:



Steinbeck Research Group

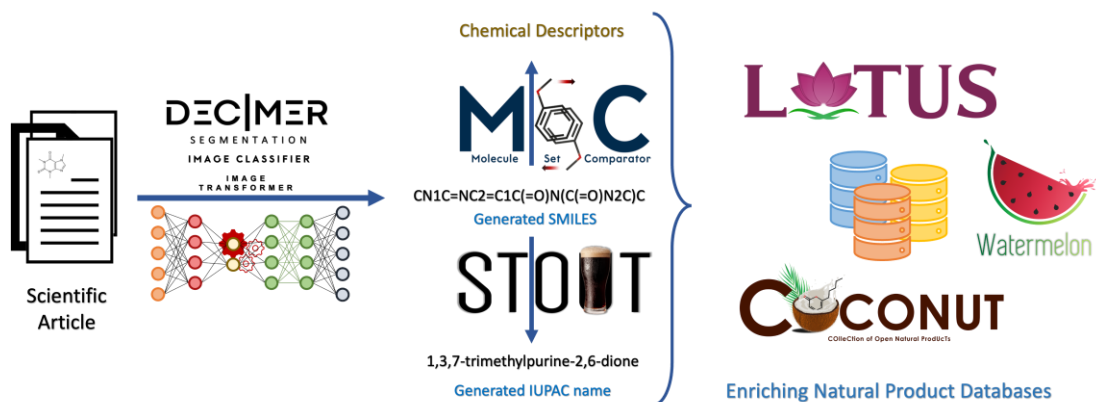
- Cheminformatics



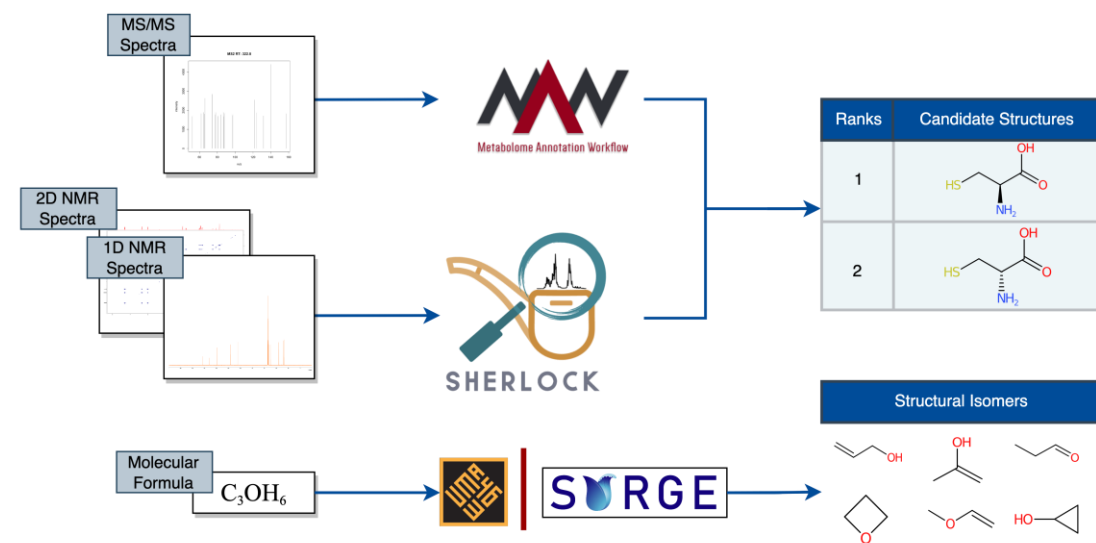
Steinbeck Research Group

- Our Research

Chemical Information Extraction & Natural Product Databases



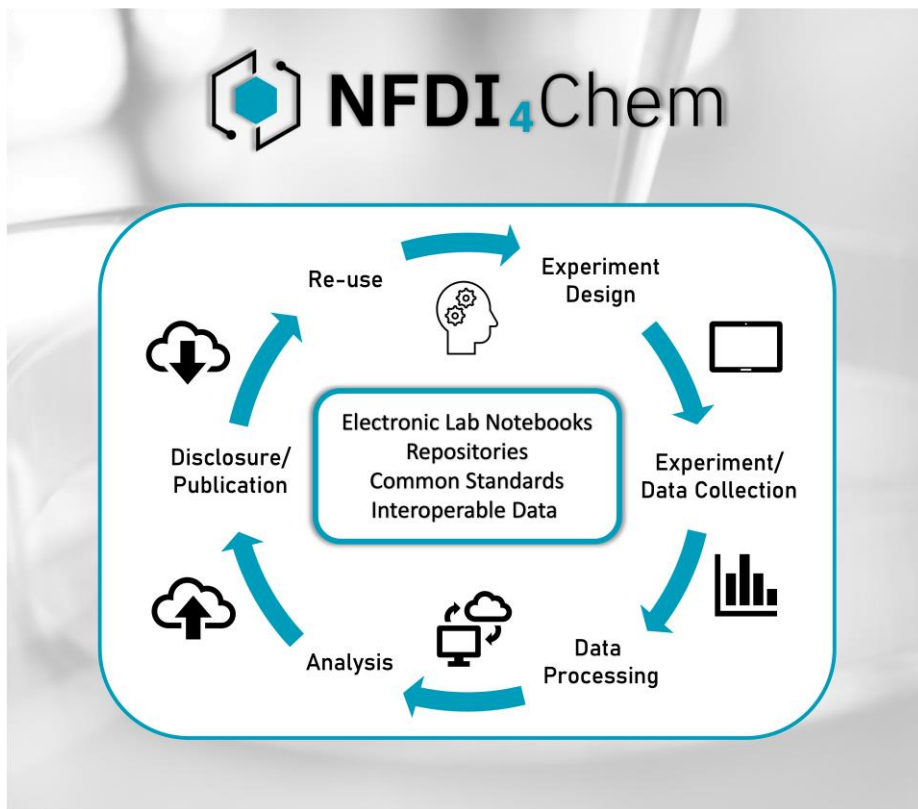
Computational Metabolomics & Structure Elucidation



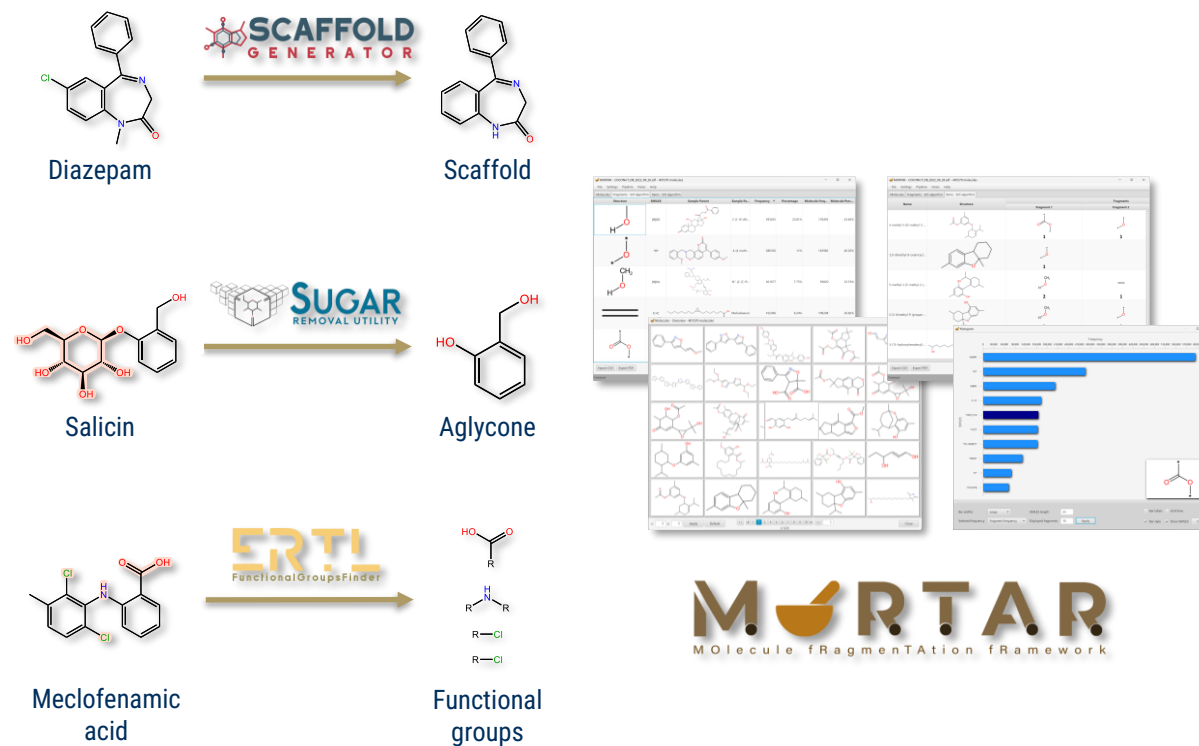
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- Our Research

National Research Data Infrastructure for Chemistry



Structural Cheminformatics and Substructure Analysis



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- Some Notes

- Contains 0.0 % lab work
- Con: you have to learn programming (well)
- Pro: you will learn how to do that with us (mainly Python and Java, some R; preexisting skills welcome)
- International team and field (good English skills required!)
- We do completely *open* science
- Our research-related lectures in the chemistry master's programme (recommended to visit beforehand):
 - Analytical Chemistry I Metabolomics MC2.1.1 (summer semester)
 - Analytical Chemistry II Cheminformatics MC3.1.1 (winter semester)
- Career prospects (extra vague!):
 - Cheminformatics, e.g. in pharma companies
 - Machine learning and data scientist
 - Software development
 - Academia

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- Contact

- Dr Jonas Schaub (jonas.schaub@uni-jena.de)

- Prof. Dr Steinbeck personally



- More information: <https://cheminf.uni-jena.de>

Cheminformatics and Computational Metabolomics
Friedrich-Schiller-University, Jena, Germany

RESEARCH TEACHING INFRASTRUCTURE WEB-SERVICES MEMBERS PUBLICATIONS NEWS JOBS

Cheminformatics and Computational Metabolomics

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Computational Metabolomics and Natural Products Research

Algorithms

Chemical Information

NEWS

DECIMER.ai: an open platform for automated optical chemical structure identification, segmentation and recognition in scientific publications

MAW: the reproducible Metabolome Annotation Workflow for untargeted tandem mass spectrometry

Notes on molecular fragmentation and parameter settings for a dissipative particle dynamics study of a C₁₀E₄/water mixture with lamellar bilayer formation

Open data and algorithms for open science in AI-driven molecular informatics

Sherlock—A Free and Open-Source System for the Computer-Assisted Structure Elucidation of Organic Compounds from NMR Data