Details

Chemotion repository (Chemotion)

The chemotion repository is an initiative of the Prof. Stefan Bräse group at the Karlsruhe Institute of Technology (KIT) (Institute of Organic Chemistry and Institute of Toxicology and Genetics). The chemotion database is a collection of synthetic compounds, their analytics and details that have been provided by single researchers. All information that is available can be provided and shared with others via very easy upload protocols for structures, analytics or descriptive resources. Other researchers and universities are invited to join and to use the repository. All compounds and datasets can be published and are automatically citable via DOI® and available on PubChem. Examples for available datasets are: descriptions and primary data of 1H NMR data, 13C NMR data, mass-, IR-, Raman-, UV-spectra and data, HPLC and GCMS results, crystal structures, TLC information und pictures, identifiers.

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To website

Host Institution

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Scientific Domain

Primary Subjects:
- Chemistry

Secondary Subjects:
- Biology
- Materials Science and Engineering

Category

Research data repositories

Scientific Services

The Chemotion Repository offers the opportunity to save scientific data electronically and to share them with others if the researcher is willing to do so. It is possible to structure own work and to invite others to discuss about the results that have been gained. The repository offers a very fast and easy process of sharing of information and it supports the collaboration in interdisciplinary projects. The project is a collection of analytical data that allows the comparison of results with researchers that had these results before and offers this service without the need of commercial databases. The use of IT-solutions that are available as Open Source contributes to an independent and comprehensive backup process with storage function and allows the use of up to date research data. With the support of Chemotion, the researcher is able to ask for the basic data of the desired compound without the use of further programs (as important chemistry IT-solutions have been implemented into Chemotion). Additionally useful information is automatically available (e.g. listing in PubChem). Via Chemotion, the researcher gets a citable DOI in an very fast and automatic manner, independent of the institution he belongs to and independent of the kind of chemistry reserach data he wants to get citable.

Scientific Equipment

Keywords

- management of research data
- chromatography data
- analytics
- Descriptions
- Primary Data
- IT Infrastructure to store research data
- IT Infrastructure as Open Source
- Integrated databases
- DOI management/DOI name generation

Networks

InchiTrust
http://www.inchi-trust.org/

PubChem
https://pubchem.ncbi.nlm.nih.gov/

DataCite
https://www.datacite.org/

Users per annum

Internal Users:
External Users in total: siehe oben
External Users:
External Users in the EU:
External Users outside of EU:

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