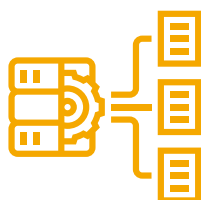# ioChem-BD

Empowering chemical and materials research through innovative data management solutions

DISRUPTIVE TECHNOLOGY

ioChem-BD provides web services for creating enriched chemical databases from data obtained in **quantum mechanics and molecular simulations.** The software integrates advanced textparsing technologies, data visualisation, and cheminformatics tools. With a flexible architecture and modular design, users can customise and extend the functionality of the software to suit their specific research needs. It also offers unique tools for releasing FAIR OpenData datasets.

PROBLEM SOLVING

R&D departments in computational materials design face challenges managing vast data volumes. Traditional storage methods hinder accessibility, collaboration, and reproducibility. The lack of centralised repositories limits sharing findings and deriving new data-driven research. Funding agencies requires researchers to adopt OpenData good practices.

ioChem-BD offers a comprehensive **solution to the data management challenges:** it enables to reduce storage needs and organises data in a structured manner, facilitating easy retrieval, collaboration, and reproducibility. This solution holds a proved 10 years' experience and broad acceptance among companies (already with customers) and the academic community.

ADVANTAGES

- Material science, small molecules, catalysis, biomolecules.
- Open-source.
- Data tools.
- Visual tools integrated in the platform.
- Data saving and data sharing.
- Specific file formats.

USES CASES

Companies

- Dataset management for training AI and ML models.
- Single private database for unifying data formats and saving storage space.
- Internal usage for scientific software development.
- Proprietary repository for publishing companies, for storing data associated with scientific manuscripts.

Academia

- Storage and publication of main research results and datasets for academia (>450 users worldwide)

SECTORS

Chemistry, energy, pharma, publishers, academia

KEYWORDS

Software, open data, open science, research, chemical data, storage

AVAILABILITY
Open use

Store

Visualise

Share

Analyse

Search

ICIQ

Knowledge and Technology Transfer