

CHEMeDATA projects



CHEMeDATA-Schema

CHEMeDATA objects are schema-based JSON objects collecting key data and metadata from common chemistry files

CHEMeDATA manifest files are collections of CHEMeDATA objects. They describe the content of archive files

CHEMeDATA-Finder



CHEMeDATA manifest files make chemistry data easily **Findable** and **Accessible** with standard search engines

CHEMeDATA-Viewer

CHEMeDATA objects such as NMR spectra, 3D structures, etc. can be visualized, from the browser where they have been found with CHEMeDATA-Viewers



CHEMeDATA-Converter

CHEMeDATA objects of files with proprietary format could be converted in a *preferred* format before exploitation or visualization making them more **Interoperable** and **Reusable**

CHEMeDATA-Archeology

CHEMeDATA-Archeology aims at generating CHEMeDATA objects from pre-digital era publications, thesis, hard copies of spectra, etc.

CHEMeDATA-Release

CHEMeDATA-Release aims at facilitating the publication of private collections of chemistry data. Whether they are personal, institutional, or industrial, collections of chemistry data may require processing, filtering, anonymization, before they can be published

CHEMeDATA-Evolution

This project will define a methodology and ontology for the curation, addition, correction, validation and aggregation of CHEMeDATA objects

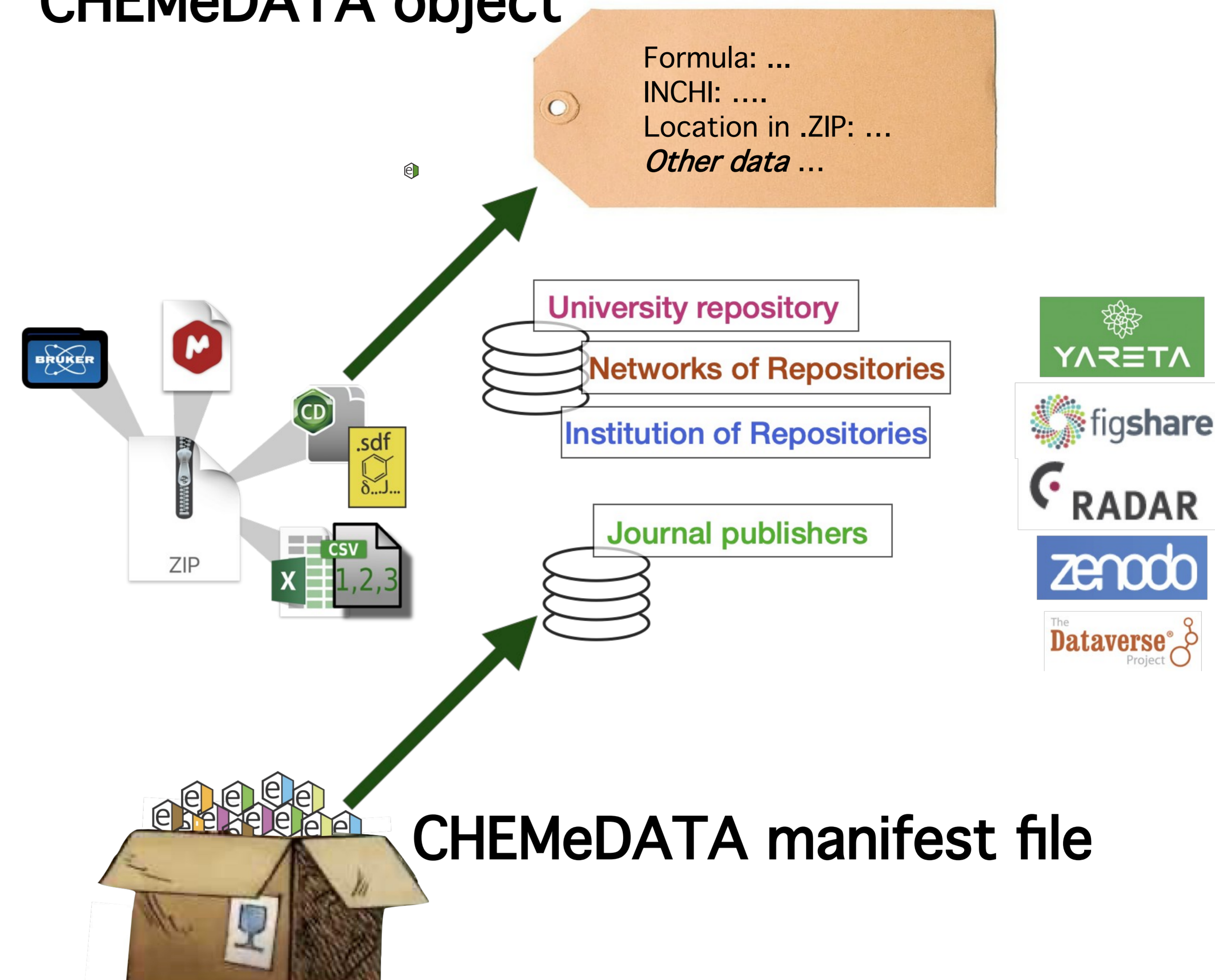
Relation to NMRReDATA

CHEMeDATA ambitions to be to chemistry what NMRReDATA was to the NMR assignment of small molecules

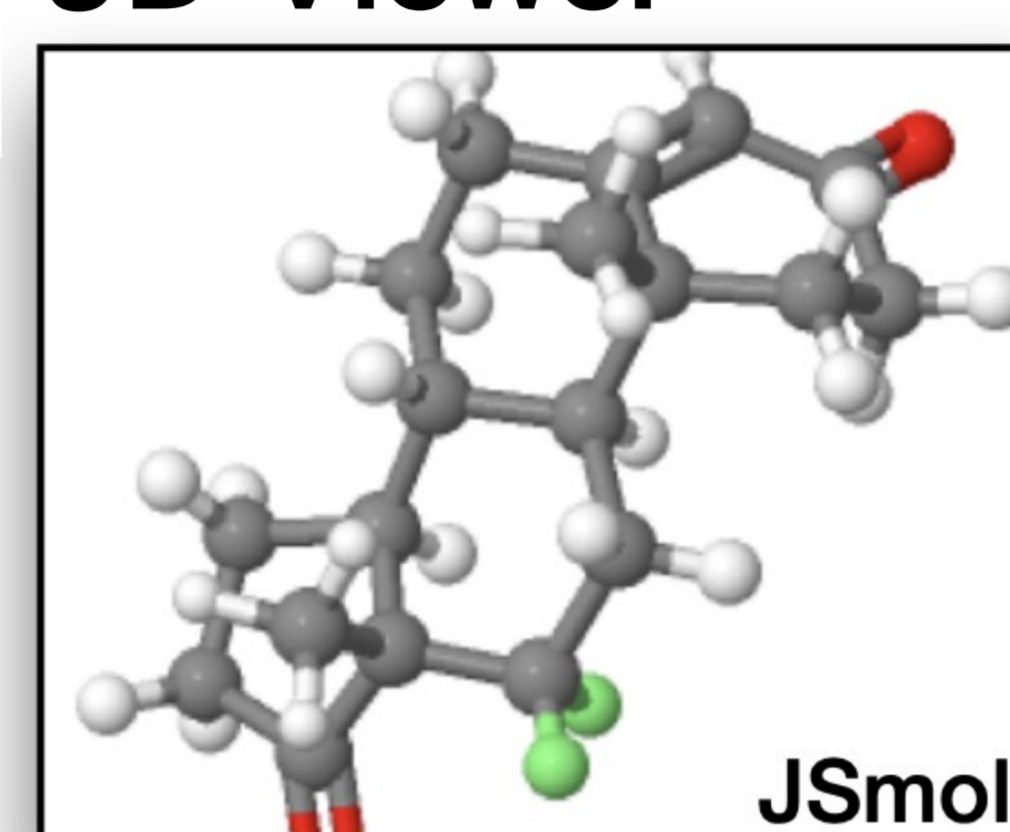
License

CHEMeDATA is currently a completely non-profit initiative. Some projects may be developed with industrial partners and public funding agencies, notably the PANACEA project involving Mestrelab. But anything called CHEMeDATA must remain an "open" initiative with MIT licensing and the generated data free and open. Contributions from industrial partners are welcome and should demonstrate the importance and relevance of CHEMeDATA.

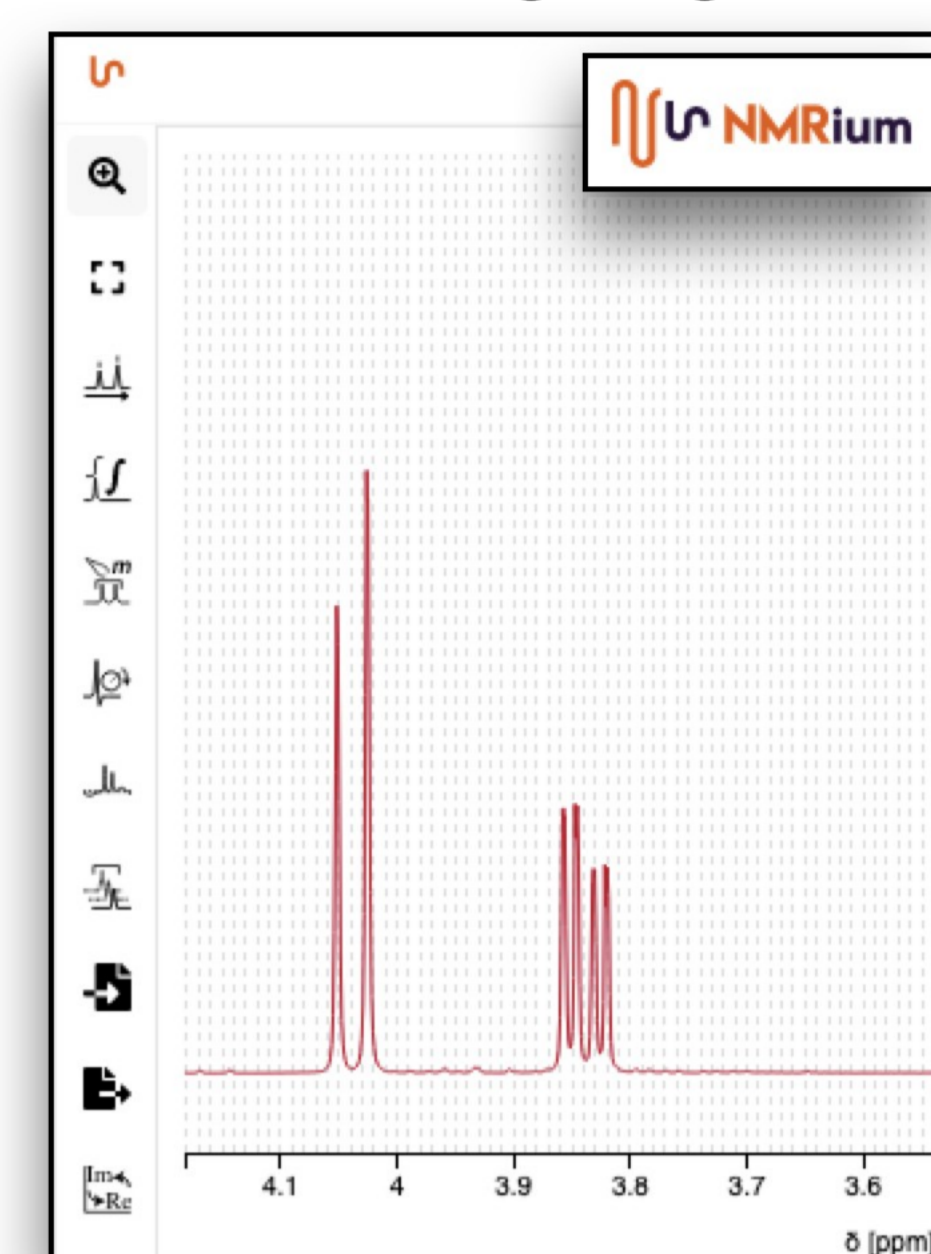
CHEMeDATA object



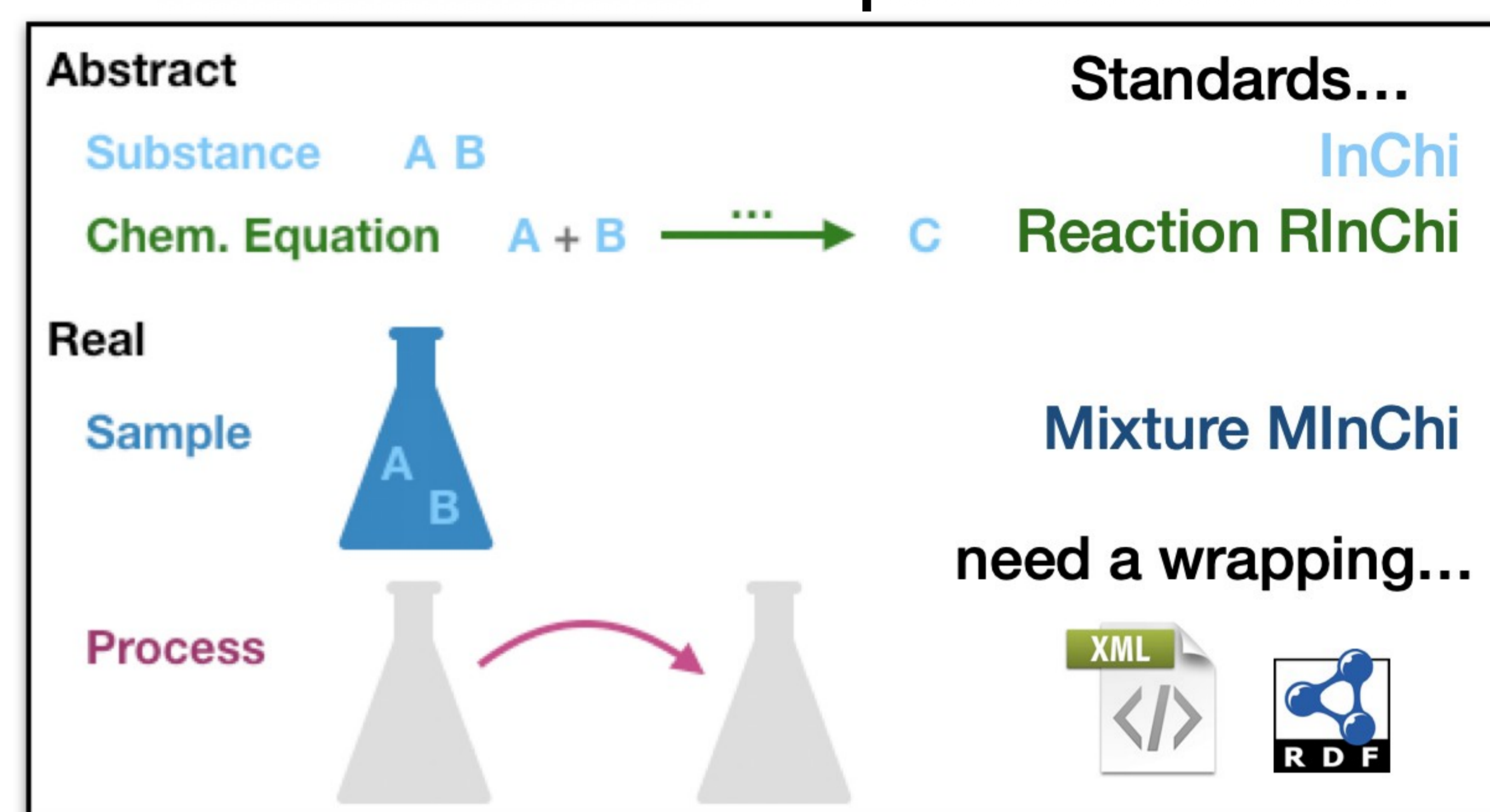
3D Viewer



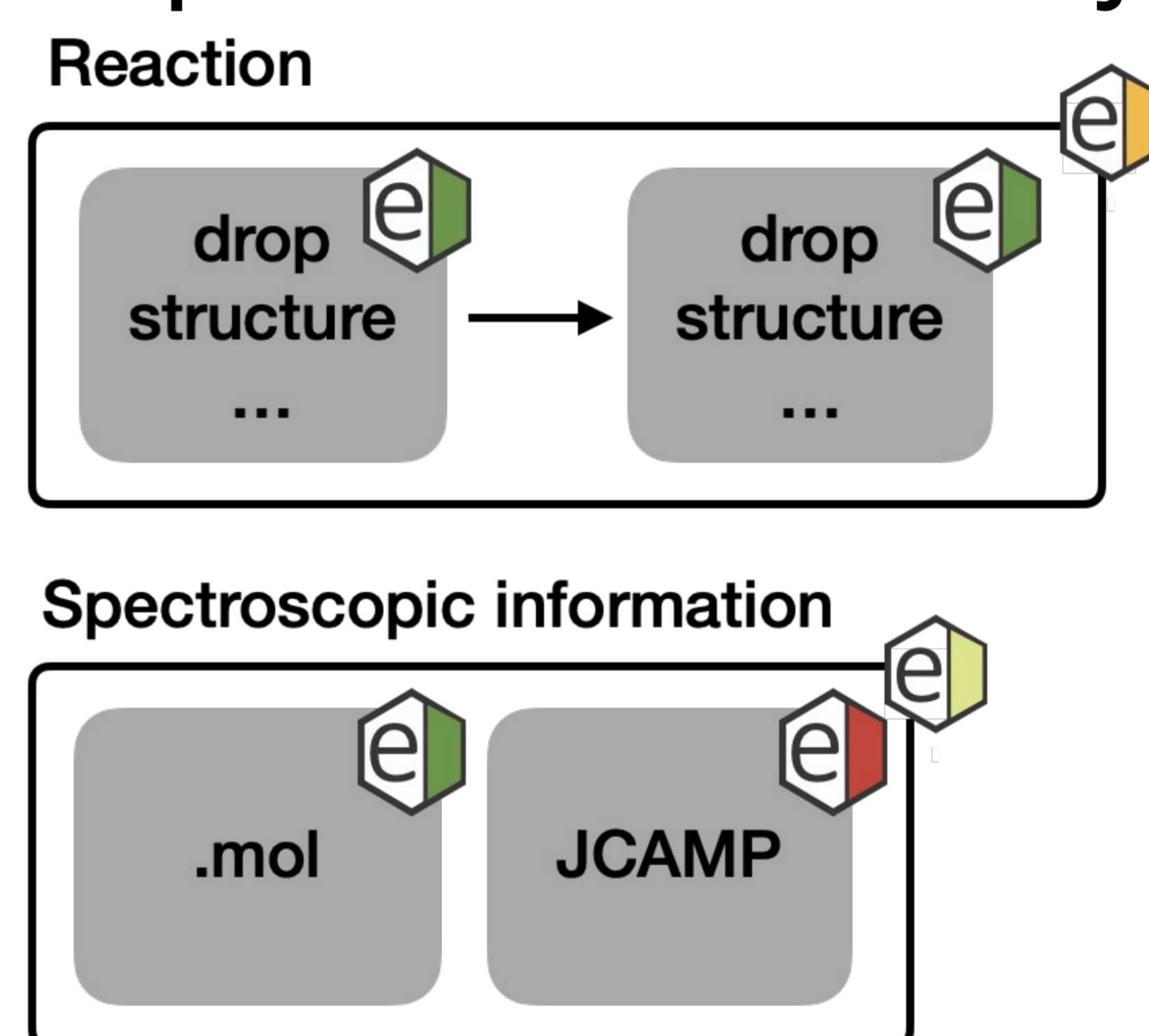
NMR Viewer



Some of the basic concepts of CHEMeDATA



Example of CHEMeDATA objects

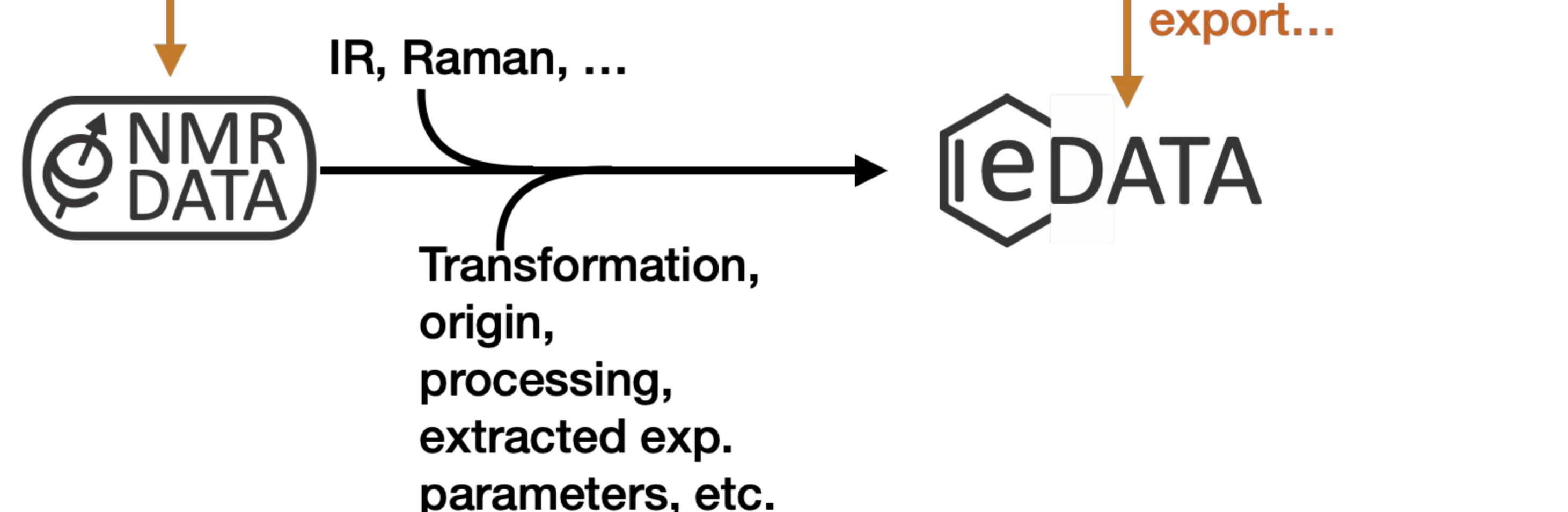
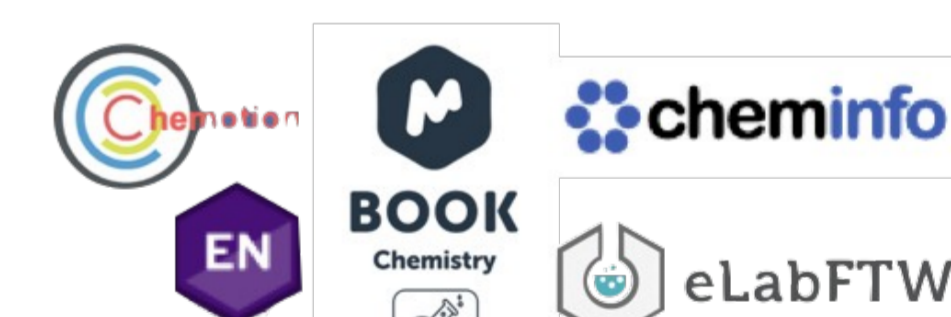


- Type of "objects" accepted / mandatory
- Types of set of objects accepted / mandatory

CASE software



Electronic notebook



More details:



<https://chemedata.github.io/projects/allProjectsPresentedSmash>