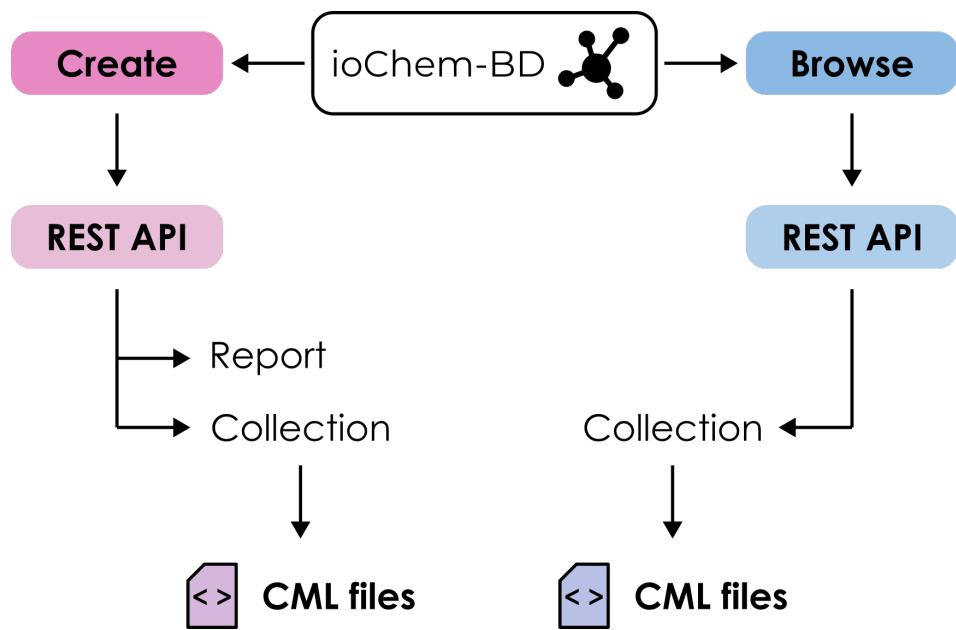




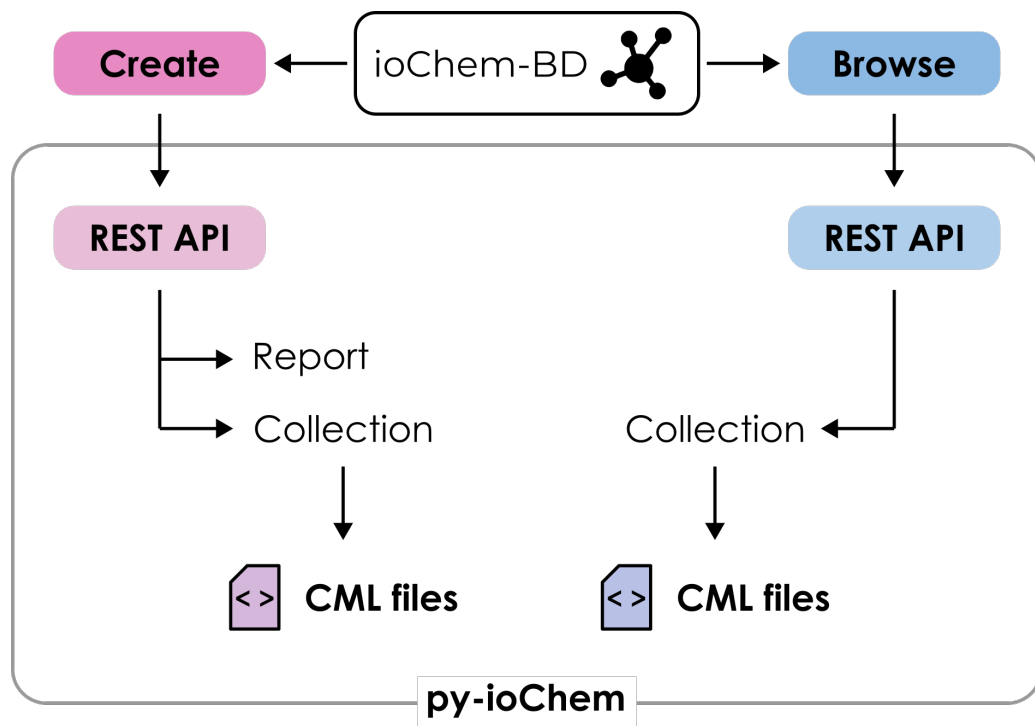
Connecting Python and ioChem-BD

Diego Garay-Ruiz (dgaray@iciq.es)

14 May 2024, RDM Seminars



Independent APIs for Browse and Create
Create allows to define reports including additional information



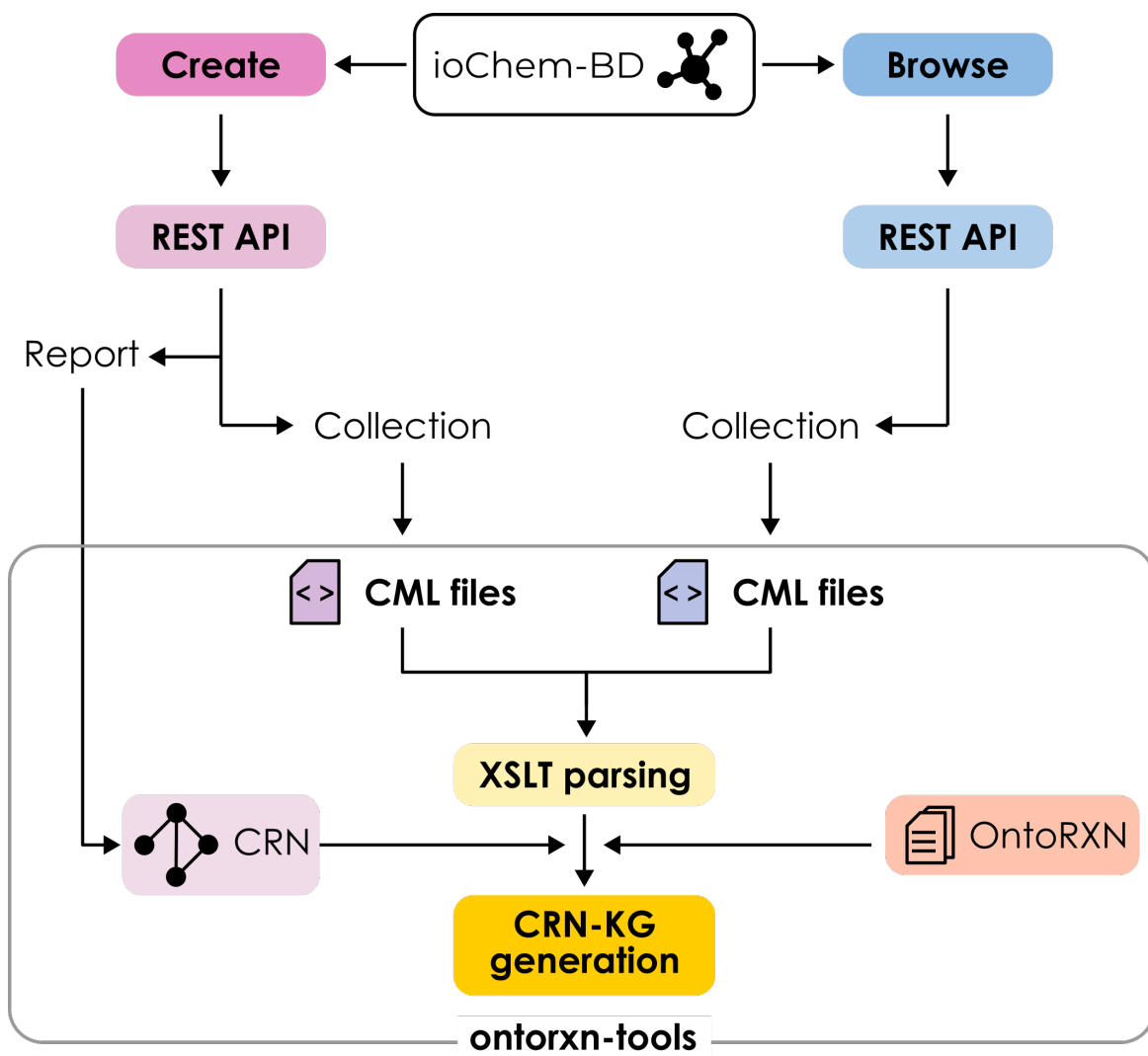
py-ioChem:

Python package to simplify user interaction with the API

- Manage HTML requests
- Filter and download files
- Extract fields from CML

Available on GitLab:

gitlab.com/dgarayr/ontorxn_tools/py_iochem



ontorxn-tools^[1]:

Python package to apply semantic organization scheme to reaction networks from ioChem-BD: building CRN-KGs

[1] D. Garay-Ruiz, C. Bo, *J. Cheminf.*, **2022**, 29

Available on GitLab:

gitlab.com/dgarayr/ontorxn_tools