Using SEEK in computational modelling – API & outlook

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COMBINE2019, FAIRDOM user meeting
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Physiologically based pharmacokinetics models

**Models**
- Ordinary differential equations (ODE)

**Datasets**
- Time course data of test substance and products (plasma & urine)
- Pharmacokinetic parameters (clearance, half-lifes)
PK-DB – pharmacokinetics data

- Standardized pharmacokinetics data
- Meta-information for stratification & individualization (characteristica & genetic variants)
- Tables and figures
**Rest API Basics**

- **HTTP GET**:
  - `/allUsers`
  
- **HTTP POST**:
  - `/newUser`

**Rest API**

- Receives HTTP requests from Clients and does whatever request needs. i.e create users

**Response**: When the Rest API has what it needs, it sends back a response to the clients. This would typically be in JSON or XML format.

**Database**

- Our Rest API queries the database for what it needs.
SEEK API

- REST API for interaction with SEEK
  - https://seek.lisym.org/studies/30
  - https://github.com/matthiaskoenig/ipython_for_SEEK-API

- Allows to automate repetitive tasks (upload many resources)
- Integration in modeling workflows
SEEK API

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- Challenges
  - Complicated to get ids (which are necessary to query end points).
    Necessary to look at all the assets (manually :/)
  - Some work to build the correct JSON (templates?)
Nightmare of digitized datasets

- Digitize experimental data from publications
  - publication (PDF) → images (PNG) → Spreadsheets (XLSX) → CSV → modeling pipeline
- Need for annotation format for spreadsheet/csv
  - Ontologies
- How to store metadata? How to provide this for instance for SEEK to search.

![Table Example](image.png)
The Future: Metadata for Datasets

CSV + annotations?

- Data packages https://frictionlessdata.io/