ETH zürich

Institute of Molecular Systems Biology

Linked Open Data: Hands-on

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Practice time

Based on the previous presentation and on some examples, we will try to write down queries for our research question.

Surface sensing triggers a broad-spectrum antimicrobial response in *Pseudomonas aeruginosa*

https://doi.org/10.1111/1462-2920.15139

- What are the compounds found in *Pseudomonas aeruginosa*?
  Define them by their canonical SMILES, isomeric SMILES, InChI, InChIKey.
- What are the compounds found in *Pseudomonas* or children taxa?
- What are the spectra corresponding to compounds found in *P. aeruginosa*?
- Which compounds corresponding to a mass of 324.0602 ± 10ppm are found in which organism(s)?
- What are the compounds that are subclasses of Rhamnolipids?
- … of classes Rhamnolipids are subclasses of?
- … that are similar to siderophores or iron chelating agents?
- … that are similar to compounds treating gram positive bacterial infections?
- … known to have a relationship to things linked to subclasses of cell-cell signalling?

Further resources

These are not meant to be used today, but rather to serve as examples for the future.

- Very interesting endpoints:
  - Wikipathways: https://sparql.wikipathways.org/
  - IDMS: https://idsm.elixir-czech.cz/sparql
- Tutorials/examples:
  - https://www.wikidata.org/wiki/Wikidata:SPARQL_tutorial
  - https://www.wikidata.org/wiki/Wikidata:WikiProject_Chemistry_Natural_products#Queries
  - https://adafede.github.io/sparql/