



Status of LC-UV Data Model

November 2018

Agenda

- Scope
- Workflow
- Submission
- Patterns
- What can you do with it?
- Future work



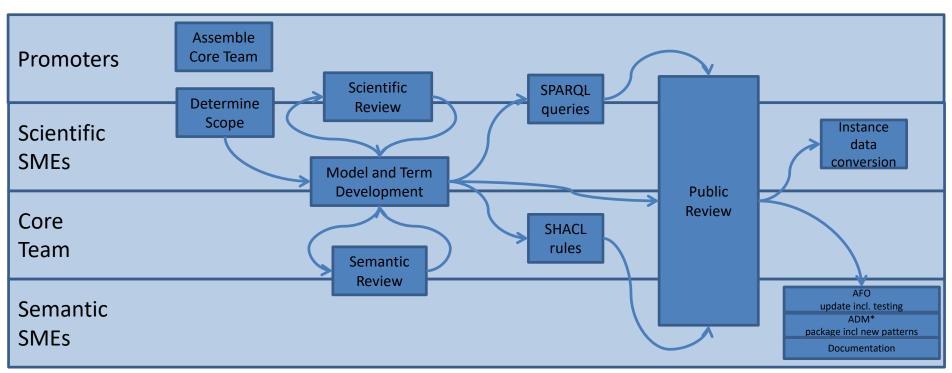
Initial Release Use-Cases

- As an analytical chemist I need to be able to retrieve my HPLC-UV analytical method parameters from a standardized file format.
 - Confirm the correct method parameters were used in obtaining the data
 - Data Mining to be able to predict/prioritize effective conditions for method development
- As an analytical chemist I need to retrieve standard HPLC-UV results and instrument descriptions.
 - Automated Result Reporting
 - Data Mining for Lot Trend analysis, control chart analysis of instrument / method performance.



Full Graph Development Workflow

Initiation Development Cycle Finalize Review Release





What's in a submission?

Required:

- Class model diagrams (CMAP)
 - Visual documentation of the proposed models, including all entities, relationships, and cardinalities
- New term definitions (Excel)
 - Listing of the new semantic terms required to by this model, for addition to AFO
- Example test data (native and TTL)
 - Example dataset in a native format and a TTL version of the same dataset conforming to the proposed model
- SPARQL queries (RQ)
 - Example SPARQL queries i.e. how to ask questions of the proposed model.

Optional:

- Automated SHACL rules (SHACL/TTL)
 - SHACL implementation of the proposed model, to automatically verify that data matches the model
- Pattern model diagrams (CMAP)
 - Visual documentation of any new patterns defined by the model that should be reused in development of other models

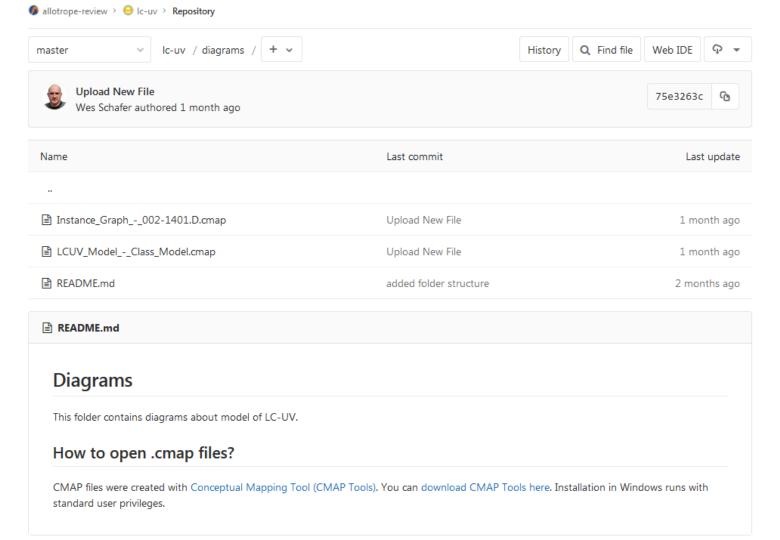


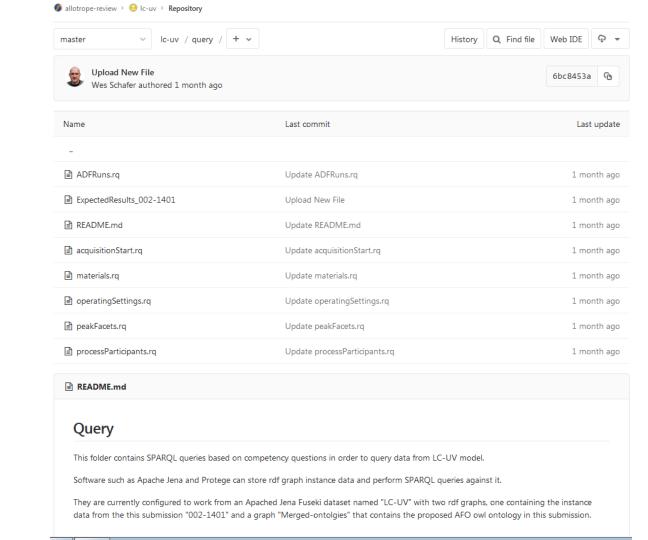
GitLab

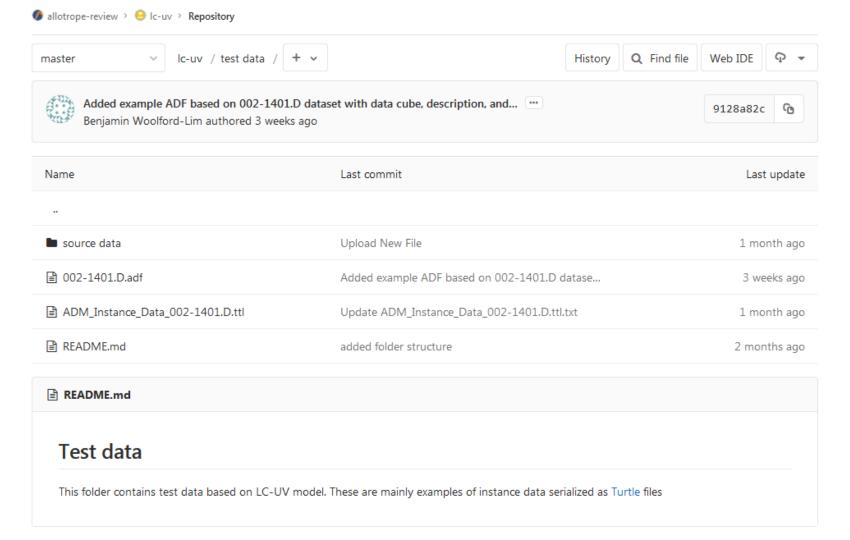
- Everything hosted on GitLab repository
- Link is https://gitlab.com/allotrope-review/lc-uv
- Please raise any issues or comments on the issue tracker there

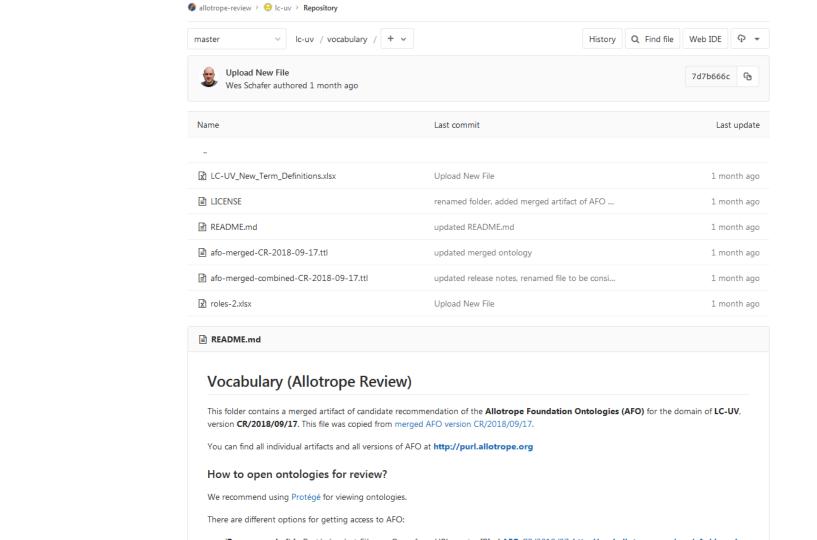


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miscellaneous	renamed folder	1 month ago
p attern	updated release notes, renamed file to be consistent, added pa	1 month ago
q uery	Upload New File	1 month ago
test data	Added example ADF based on 002-1401.D dataset with data c	3 weeks ago
■ validation	Upload New File	1 month ago
vocabulary	Upload New File	1 month ago
:gitignore	initial commit	2 months ago
README.md	Update README.md	1 month ago



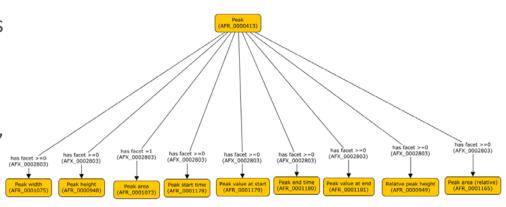






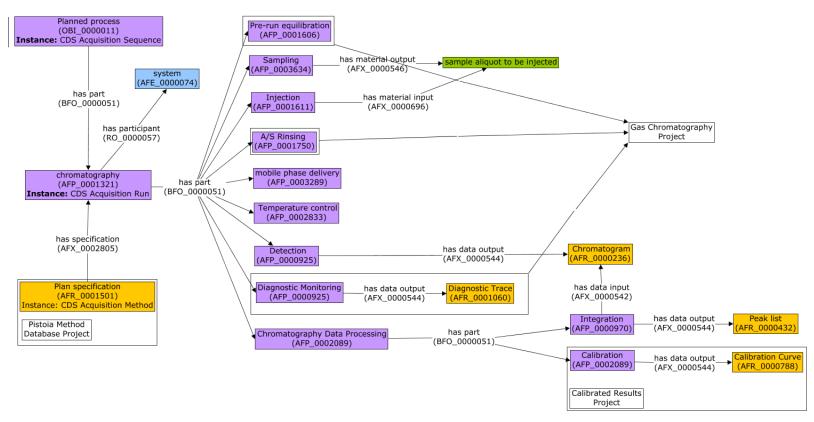
Patterns

- Part of the process of modelling involves identifying reusable patterns
- These patterns should be small subgraphs that have a consistent shape throughout
- Patterns may be specific to a domain, e.g. the pattern for an LC-UV system, or apply across domains, e.g. the pattern for a piece of equipment
- Development of patterns and their use ensures consistency across different datasets and domains





Chromatography ADM





What can we do with it?

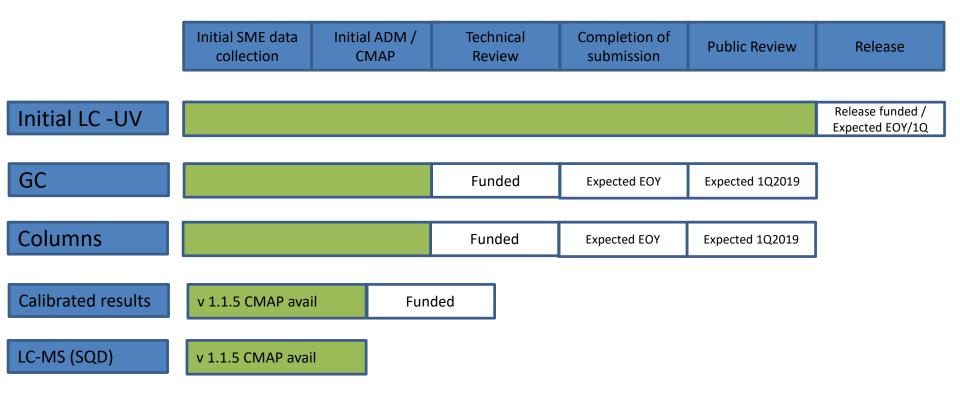
Answer key questions about your experiments through SPARQL queries

- Who?
 - Who submitted the sample?
- What?
 - What sample was submitted?
- Where?
 - Where was the experiment performed?
- When?
 - When was the sample processed?
- How?
 - How was the experiment performed?
- Why?
 - What was the purpose of the experiment?





On-Going Efforts



Non-chromatography full graph models: DSC (in-progress), XRPD, TGA (planned)



Next steps

- Try it!
 - APN members can integrate this model into their products and give feedback for improvement
 - Allotrope can provide targeted support and maintenance for APN members building LC-UV converters using ADM
- Test consistency of model across implementations
 - Once multiple converters are available to generate LC-UV ADFs, the consistency in ADM application will be assessed and adjustments made if warranted
- Extend the data model suite
 - Include additional domains needed to support workflows (materials, specifications, analytical procedures, etc)

