The Chemical Analysis Metadata Platform (ChAMP): Thoughts and Ideas on the Semantic Identification of Analytical Metrics

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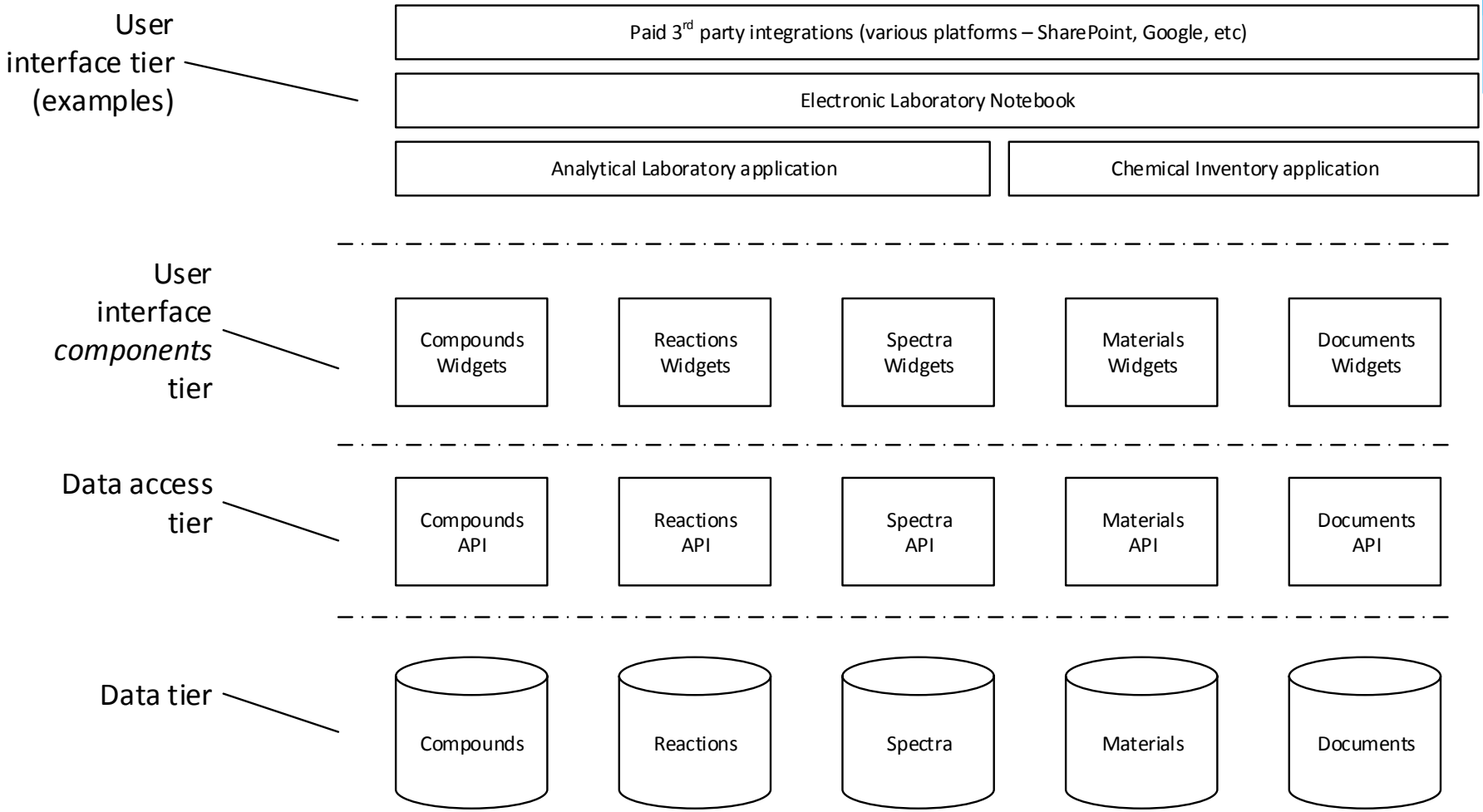
Initial Idea

* Develop a set of data standards for representation/ annotation of chemical analysis information
* Are there important characteristics (metadata) about analysis methodologies that, if captured, would add value to a resource?
* Must be easy to implement
* Must be useful across multiple disciplines

RSC Data Repository



Motivation

* Access to knowledge in existing literature
* Annotation of research in future publications
* Annotation of unpublished/self published (but potentially useful) work
* Annotation of data captured in ELN's
* Data ingest into the RSC's Data Repository

* Complements/enhances existing activities

* The haystack is so big – we need to make it easy to make the needle show up

Why a Platform?

* Develop it to be as broadly applicable as possible
* Chemical analysis is a not tangible like a spectrum
* Users have domain specific needs
* Users has a favorite/required format to store information
  * SQL Relational Database
  * Excel Spreadsheet
  * XML, YAML
  * JSON or JSON-LD
* ChAMP should define the types of metadata and general organization of the information, not the format it is stored in (this is like MIAME [1])

[1] http://www.mged.org/Workgroups/MIAME/miame.html

First Thoughts

* Covers metadata for a chemical analysis methodology not raw analytical instrument data

* Two main sections?
  * Fundamental method development
  * Method application

* How big should the platform scope be?
* What information is most important?
* How do we get community involvement/buy-in?

Pieces of the Puzzle

* Ontology of chemical analysis terms
* Taxonomy of chemical analysis metadata
* Controlled vocabularies for specific metadata items
* Definitions of required metadata (in context)
* Naming and design rules

Existing Resources

* Ontologies
  * Chemical Methods Ontology (CMO) [2]
  * SemanticScience CHEMINF Ontology [3]
  * ChEBI [4]
  * “Ontology on Property” by René Dybkær [5]
  * Ontobee (ontology search) [6]

[2] http://ontology.iupac.org/
[3] http://www.rsc.org/ontologies/CMO/
[4] https://code.google.com/p/semanticscience/
[5] http://www.ebi.ac.uk/chebi/
[6] http://www.ontobee.org/

Existing Resources

* Controlled Vocabularies/Taxonomies
  * MESH [6]
  * LCSH [7]
  * CAS Subject Headings [8]
  * IUPAC Orange Book [9]
  * IUPAC Gold Book [10]
  * … do they address how to organize the metadata?

[6] http://www.ncbi.nlm.nih.gov/mesh
[7] http://id.loc.gov/authorities/subjects.html
[8] http://cas.org
[9] http://iupac.org/publications/analytical_compendium
[10] http://goldbook.iupac.org/

Existing Resources

* Other
  * JCAMP-DX [11]
  * Analytical Information Markup Language (AnIML) [12]
  * Units Markup Language (UnitsML) [13]
  * NASA Quantities, Units, Dimensions and Data Types [14]
  * Electronic Laboratory Notebook Manifest (elnItemManifest) [15]

[11] JCAMP-DX – http://www.jcamp-dx.org/
[12] AnIML – http://animl.sourceforge.net/
[13] UnitsML – http://unitsml.nist.gov/
[14] QUDT– http://qudt.org/
[15] elnItemManifest –http://www.jcheminf.com/content/5/1/52

What are the Most Important Metadata?

* Depends on who you talk to…
* Platform should describe (as completely as possible) the types of metadata important in analysis…
* … but leave the description of what's important to the users
* Standards for different industries, with different requirements, could be developed based on the platform

Minimum Information About a Chemical Analysis?

* MIAChA (my-ache-a?)

* Can the community agree on a minimum set of metadata items needed to annotate an analysis?

* Must be for a more specific area of analysis
  * MIASA – Spectrochemical Analysis
  * MIACA – Chromatographic Analysis
  * MIAEA – Electrochemical Analysis
  * MIATA – Thermal Analysis

Different Perspectives on a Chemical Analysis

* Users and publishers have different needs/wants when they view/present information
* Defining perspectives(views) would extract out of a record only what a certain type of chemist would expect to see
* Could be defined broadly or narrowly
* This could include aggregation and/or calculation of new metrics derived from the basic metadata

Example: Metadata Categories in XML

```
<?xml version="1.0" encoding="UTF-8"?>
<chemicalAnalysis id="http://example.com/analysis_007">
  <description>
    <title/><focus/><citation/><doi/><analysisType/><applicationArea/>...
  </description>
  <analytes>
    <analyte id="http://www.chemspider.com/…" type="sci:CHEMINF_000000">
      <inchikey/><name/>...
    </analyte>
  </analytes>
  <matrices>
    <matrix id="http://champ.org/ont/champ:m0000001" type="champ:MAT_000001">
      <name/><state/><form/>...
    </matrix>
  </matrices>
  <instruments>
    <instrument id="http://champ.org/ont/champ:i0000001" type="champ:INS_000001">
      <name/><description/><settings/>...
    </instrument>
  </instruments>
  <validation>
    <srmAnalysis/><recoveryStudy/><methodComparison/><interferences/>...
  </validation>
  <samplePrep>
    <collection/><stabilization/><storage/><workup/>...
  </samplePrep>
</chemicalAnalysis>
```

Example: Metadata Categories in JSON-LD

```
{
  "@context":"http://champ.org/chemicalanalysis.jsonld",
  “@id”: “http://example.com/analysis_007”,
  “description”: { “title”: …, “focus”: …, “citation”: …, “doi”: …
                   “analysisType”: …, “applicationArea”: … }
  "analytes": [{"@id”: …, "@type”: …, "inchikey”: …, "name": … },… ],
  "matrices": [{"@id”: …, "@type": …, "name": …, “state”: …, “form”: … }, … ]
  "instruments": [{"@id": …, "@type": …, "name": …, "description”: …,
                  "settings": … }, … ],
  "metrics": { "detection limit”: …, “linear dynamic range”: … },
  “validation”: { "reference material": …, “recovery study”: …,
                  “method comparison”: …, “interferences”: … },
  “samplePrep”: { “collection”: …, “stabilization”: …, “storage”: …,
                  “workup”: … }
}
```

Immediate Plans

* Get the word out
* Put up a website to provide focal point for project
* Get on social media and promote, encourage participation
* Survey the community
* Do an analysis of existing literature for metadata
* Using resources develop an initial alpha (first pass) version of the platform
* Provide mechanism for crowdsourced feedback
* Publish examples of the use in different scenarios

Longer Term Plan

* Version 1 of platform
* Controlled vocabularies
* Example documents
* Example applications

Conclusion

* This approach to metadata identification will provide value to existing resources
* It will enhance basic searching
* It will allow semantic searching
* It will provide efficient annotation of large amounts of curated data that is not from traditional publishing

Conclusion

* It also fits well with the mission of the Research Data Alliance (RDA) [16]
  * **RDA Vision**: Researchers and innovators openly sharing data across technologies, disciplines, and countries to address the grand challenges of society.
  * **RDA Mission**: The Research Data Alliance (RDA) builds the social and technical bridges that enable open sharing of data.

[16] http://rd-alliance.org

Questions?

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