This presentation: 10.5281/zenodo.3258123

Standardization efforts around deposition of isotopic tracer data

ELIXIR Implementation Study on Standardizing fluxomics workflows

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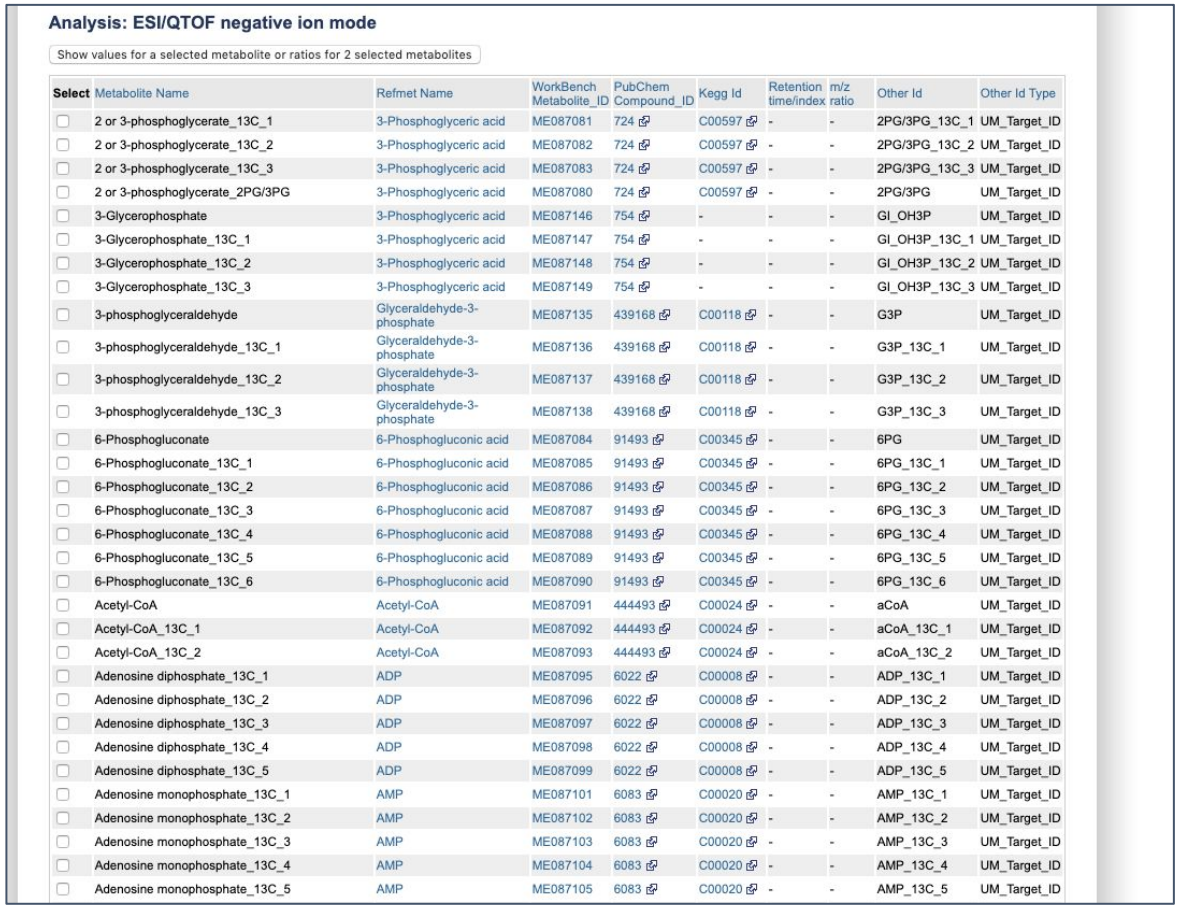
Outline

- Bringing awareness to existing resources
  - Request for extending IUPAC InChi specification to support isotopologue reporting
    - (Hunter Moseley)
  - A controlled Terminology: MSIO
  - A syntax for describing experimental setup: ISA
    - Used by EMBL-EBI Metabolights Repository
  - Fluxomics use case require specific handling
    - Dedicated ISA-Configurations reflecting annotation needs formulated by the community
    - Dedicated Data Matrix Formats:
      - Option 1: derived from MAF file for compatibility with ISAcreator plugin
        - Validation
        - Layout: wide table + fixed height (i.e. fixed number of molecular dimensions)
      - Option 2: Exploratory JSON Tabular Data packages
        - Layout: long table + fixed width (i.e. fixed number of measurement dimensions)

SIRM & flux studies != Metabolite profiling studies

- A lot in common for acquisition techniques (MS,NMR)
- BUT
  - labeling experiments require specific descriptors
  - analytical tools differ
  - Reporting results require specific descriptors



Analysis: ESI/QTOF negative ion mode

Show values for a selected metabolite or ratios for 2 selected metabolites

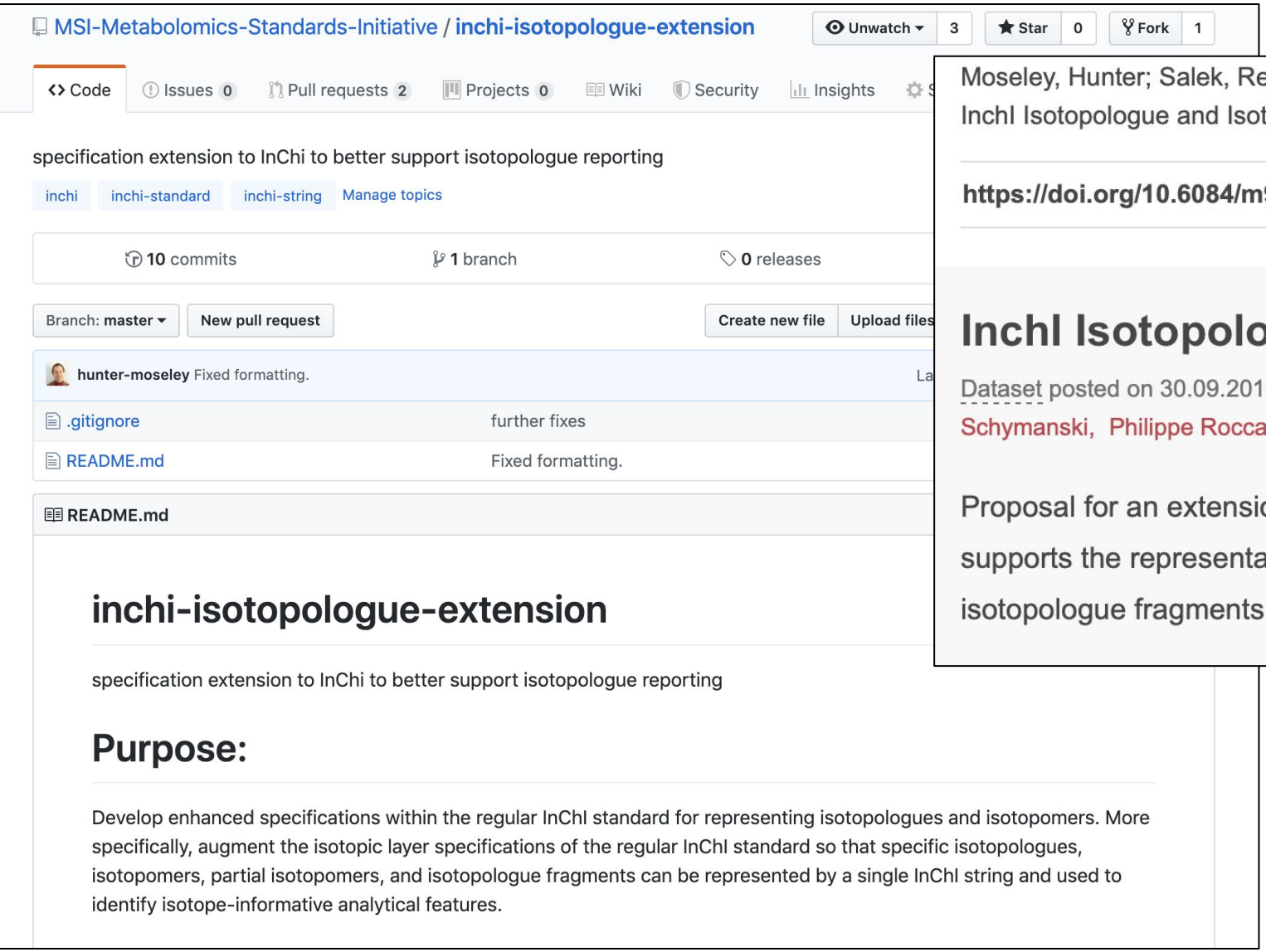
Select	Metabolite Name	Refmet Name	WorkBench Metabolite_ID	PubChem Compound_ID	Kegg Id	Retention time/index	m/z ratio	Other Id	Other Id Type
☐	2 or 3-phosphoglycerate_13C_1	3-Phosphoglyceric acid	ME087081	724	C00597	-	-	2PG/3PG_13C_1	UM_Target_ID
☐	2 or 3-phosphoglycerate_13C_2	3-Phosphoglyceric acid	ME087082	724	C00597	-	-	2PG/3PG_13C_2	UM_Target_ID
☐	2 or 3-phosphoglycerate_13C_3	3-Phosphoglyceric acid	ME087083	724	C00597	-	-	2PG/3PG_13C_3	UM_Target_ID
☐	2 or 3-phosphoglycerate_2PG/3PG	3-Phosphoglyceric acid	ME087080	724	C00597	-	-	2PG/3PG	UM_Target_ID
☐	3-Glycerophosphate	3-Phosphoglyceric acid	ME087146	754	-	-	-	GI_OH3P	UM_Target_ID
☐	3-Glycerophosphate_13C_1	3-Phosphoglyceric acid	ME087147	754	-	-	-	GI_OH3P_13C_1	UM_Target_ID
☐	3-Glycerophosphate_13C_2	3-Phosphoglyceric acid	ME087148	754	-	-	-	GI_OH3P_13C_2	UM_Target_ID
☐	3-Glycerophosphate_13C_3	3-Phosphoglyceric acid	ME087149	754	-	-	-	GI_OH3P_13C_3	UM_Target_ID
☐	3-phosphoglyceraldehyde	Glyceraldehyde-3-phosphate	ME087135	439168	C00118	-	-	G3P	UM_Target_ID
☐	3-phosphoglyceraldehyde_13C_1	Glyceraldehyde-3-phosphate	ME087136	439168	C00118	-	-	G3P_13C_1	UM_Target_ID
☐	3-phosphoglyceraldehyde_13C_2	Glyceraldehyde-3-phosphate	ME087137	439168	C00118	-	-	G3P_13C_2	UM_Target_ID
☐	3-phosphoglyceraldehyde_13C_3	Glyceraldehyde-3-phosphate	ME087138	439168	C00118	-	-	G3P_13C_3	UM_Target_ID
☐	6-Phosphogluconate	6-Phosphogluconic acid	ME087084	91493	C00345	-	-	6PG	UM_Target_ID
☐	6-Phosphogluconate_13C_1	6-Phosphogluconic acid	ME087085	91493	C00345	-	-	6PG_13C_1	UM_Target_ID
☐	6-Phosphogluconate_13C_2	6-Phosphogluconic acid	ME087086	91493	C00345	-	-	6PG_13C_2	UM_Target_ID
☐	6-Phosphogluconate_13C_3	6-Phosphogluconic acid	ME087087	91493	C00345	-	-	6PG_13C_3	UM_Target_ID
☐	6-Phosphogluconate_13C_4	6-Phosphogluconic acid	ME087088	91493	C00345	-	-	6PG_13C_4	UM_Target_ID
☐	6-Phosphogluconate_13C_5	6-Phosphogluconic acid	ME087089	91493	C00345	-	-	6PG_13C_5	UM_Target_ID
☐	6-Phosphogluconate_13C_6	6-Phosphogluconic acid	ME087090	91493	C00345	-	-	6PG_13C_6	UM_Target_ID
☐	Acetyl-CoA	Acetyl-CoA	ME087091	444493	C00024	-	-	aCoA	UM_Target_ID
☐	Acetyl-CoA_13C_1	Acetyl-CoA	ME087092	444493	C00024	-	-	aCoA_13C_1	UM_Target_ID
☐	Acetyl-CoA_13C_2	Acetyl-CoA	ME087093	444493	C00024	-	-	aCoA_13C_2	UM_Target_ID
☐	Adenosine diphosphate_13C_1	ADP	ME087095	6022	C00008	-	-	ADP_13C_1	UM_Target_ID
☐	Adenosine diphosphate_13C_2	ADP	ME087096	6022	C00008	-	-	ADP_13C_2	UM_Target_ID
☐	Adenosine diphosphate_13C_3	ADP	ME087097	6022	C00008	-	-	ADP_13C_3	UM_Target_ID
☐	Adenosine diphosphate_13C_4	ADP	ME087098	6022	C00008	-	-	ADP_13C_4	UM_Target_ID
☐	Adenosine diphosphate_13C_5	ADP	ME087099	6022	C00008	-	-	ADP_13C_5	UM_Target_ID
☐	Adenosine monophosphate_13C_1	AMP	ME087101	6083	C00020	-	-	AMP_13C_1	UM_Target_ID
☐	Adenosine monophosphate_13C_2	AMP	ME087102	6083	C00020	-	-	AMP_13C_2	UM_Target_ID
☐	Adenosine monophosphate_13C_3	AMP	ME087103	6083	C00020	-	-	AMP_13C_3	UM_Target_ID
☐	Adenosine monophosphate_13C_4	AMP	ME087104	6083	C00020	-	-	AMP_13C_4	UM_Target_ID
☐	Adenosine monophosphate_13C_5	AMP	ME087105	6083	C00020	-	-	AMP_13C_5	UM_Target_ID

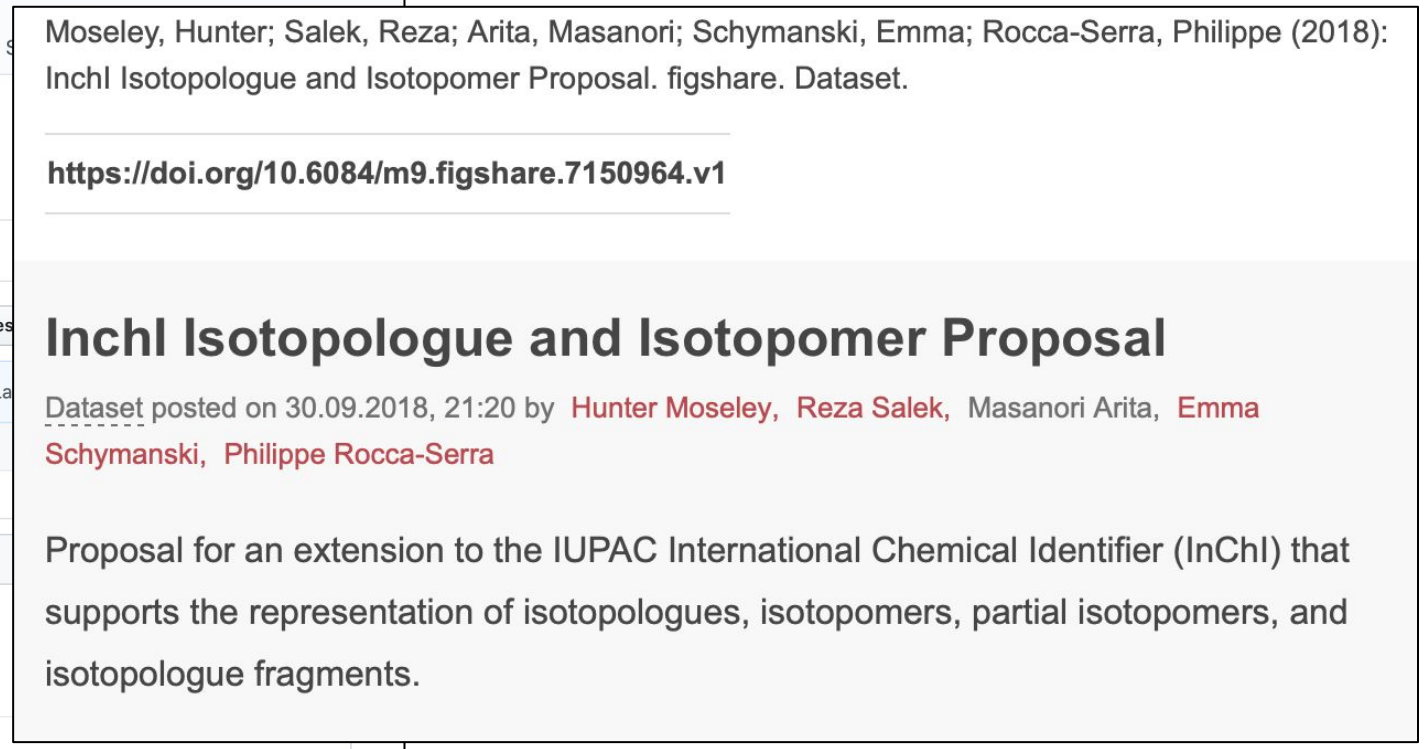
Issue 1: Molecular Identity

- **InchI Isotopologue and Isotopomer Proposal**

https://github.com/MSI-Metabolomics-Standards-Initiative/inchi-isotopologue-extension

Molecular Identification: Extension to Inchi Proposal





- https://doi.org/10.6084/m9.figshare.7150964.v1

Isotopically-Resolved Isotopologue Specification:

In the following proposed specifications, isotopologue designations are indicated by parentheses with the *element* identified first, while isotopomer designations lack parentheses with the *atom position* identified first: e.g. /a(C2+1) for isotopologue and /i7+1 for isotopomer. The lack of parentheses for isotopomers ensures backwards compatibility with previous InChI specifications. See individual specifications below for details.

Isotopically-Resolved Isotopologue Specification:
Rationale: to enable the use of InChI to specify an isotopologue or isotopologue fragment.
Simple Definition: /a(Ee#<+|->#[,#]...)
Complete Definition:
/a(<element><isotope_count><isotope_designation>[,<atom_number>])
<element> - one or two letter Element code (Ee).
<isotope_count> - number of atoms with the designated isotope (#).
<isotope_designation> - isotope designation indicated by a sign (+ or -) and number indicating the unit mass difference from the rounded average atomic mass of the element. For example, the average atomic mass of Sn (118.710) is rounded to 119. We specify two ^{118}Sn atoms as "/a(Sn2-1)".
<atom_number> - specific atom(s) that may have the specified isotope. If empty, then all atoms of the given element may have the specified isotope (# in [,#]). If multiple atoms need to be specified, these are comma separated.
Regular Expression Definition: [/]a[(][A-Z][a-z]?\d+[+-]\d+([,]\d+)*[)]

Examples:
1. $^{13}C_2$ isotopologue of alpha-D-glucopyranose:
InChI=1/C6H12O6/c7-1-2-3(8)4(9)5(10)6(11)12-2/h2-11H,1H2/t2-,3-,4+,5-,6+/m1/s1/a(C2+1)
2. $^{13}C_2{}^2H_3$ isotopologue of alpha-D-glucopyranose:
InChI=1/C6H12O6/c7-1-2-3(8)4(9)5(10)6(11)12-2/h2-11H,1H2/t2-,3-,4+,5-,6+/m1/s1/a(C2+1),(H3+1)
3. $^{17}O_2{}^{18}O_1$ isotopologue of alpha-D-glucopyranose:
InChI=1/C6H12O6/c7-1-2-3(8)4(9)5(10)6(11)12-2/h2-11H,1H2/t2-,3-,4+,5-,6+/m1/s1/a(O2+1),(O1+2)

Augmented Range Specification:

Augmented Range Specification:

Rationale: to enable a more concise string representation of isotopomer and isotopologues. Note in the isotopologue definition, the first sign and following number indicates the isotope, whereas in the isotopomer definition the last sign and following number indicates the isotope.

Simple Isotopologue Definition: /a(Ee#<+|->#[,#-#|,#]...)

Complete Isotopologue Definition:

/a(<element><isotope_count><isotope_designation>[,<start_atom_number>-<end_atom_number>])

Simple Isotopomer Definition: /i#-#<+|->#

The augmented isotopomer range specification is limited to a single atom_range and isotope_designation, due to parsing ambiguities that would arise if mixed atom_range and single atom designations were allowed.

Complete Isotopomer Definition:

/i<start_atom_number>-<end_atom_number><isotope_designation>

Examples:

1. $^{13}C_2$ limited to atoms 4,5,6 isotopologue fragment of alpha-D-glucopyranose:
   InChI=1/C6H12O6/c7-1-2-3(8)4(9)5(10)6(11)12-2/h2-11H,1H2/t2-,3-,4+,5-,6+/m1/s1/a(C2+1,4-6)
2. $^{13}C_6$ isotopomer of alpha-D-glucopyranose:
   InChI=1/C6H12O6/c7-1-2-3(8)4(9)5(10)6(11)12-2/h2-11H,1H2/t2-,3-,4+,5-,6+/m1/s1/i1-6+1

Nominal-Mass Isotopologue Specification:

Nominal-Mass Isotopologue Specification:

Rationale: to enable an InChI representation for mass spectral features that are not isotope-resolved.

Simple Nominal-Mass Isotopologue Definition: /a(#n[,#]...)

Complete Nominal-Mass Isotopologue Definition:

/a(<neutron_count>n[,<atom_number>])

<neutron_count> - number of neutrons of extra mass.

Notice the reversal of neutron_count relative to the "n" representing neutron. This is done so that no ambiguity will exist with the isotopically-resolved isotopologue specification, where the element is indicated first and the isotope_count second.

Examples:

1. M+3 isotopologue of alpha-D-glucopyranose:

   InChI=1/C6H12O6/c7-1-2-3(8)4(9)5(10)6(11)12-2/h2-11H,1H2/t2-,3-,4+,5-,6+/m1/s1/a(3n)

   The lack of a specified list of atoms indicates the whole molecule.

2. M+4 isotopologue limited to carbon atoms of alpha-D-glucopyranose:

   InChI=1/C6H12O6/c7-1-2-3(8)4(9)5(10)6(11)12-2/h2-11H,1H2/t2-,3-,4+,5-,6+/m1/s1/a(4n,1,2,3,4,5,6)

   With augmented range specifications:

   InChI=1/C6H12O6/c7-1-2-3(8)4(9)5(10)6(11)12-2/h2-11H,1H2/t2-,3-,4+,5-,6+/m1/s1/i(4n,1-6)

   This situation could arise from use of tandem mass spectrometry features that localize the extra mass to certain elements.

Partial Isotopomer Specification:

Partial Isotopomer Specification:

Rationale: to enable an InChI representation of a partial isotopomer, which is directly useful for describing most individual nuclear magnetic resonance spectroscopy spectral features.

Simple Definition: same as the full isotopomer specification but with the unknown isotope specifications removed (Example 2). The designation of the isotope for all atoms of a given element will represent a full isotopomer (Example 1).

Examples:

1. ^{13}C at 4th carbon for full isotopomer (with respect to carbon) of alpha-D-glucopyranose:

   InChI=1/C6H12O6/c7-1-2-3(8)4(9)5(10)6(11)12-2/h2-11H,1H2/t2-,3-,4+,5-,6+/m1/s1/i1+0,2+0,3+0,4+1,5+0,6+0

   With augmented range specification:

   InChI=1/C6H12O6/c7-1-2-3(8)4(9)5(10)6(11)12-2/h2-11H,1H2/t2-,3-,4+,5-,6+/m1/s1/i1-3+0,4+1,5-6+0

2. ^{13}C at 4th carbon for partial isotopomer of alpha-D-glucopyranose:

   InChI=1/C6H12O6/c7-1-2-3(8)4(9)5(10)6(11)12-2/h2-11H,1H2/t2-,3-,4+,5-,6+/m1/s1/i4+1

   Only the atom with the known isotopic composition is indicated.

Cross-Constitutional Isomer Isotopologue Specification:

Cross-Constitutional Isomer Isotopologue Specification:

Rationale: to enable a nonstandard InChI representation of isotopologues that span multiple constitutional isomers, i.e. either a fully or partially isotopically-resolved molecular formula. This specification is directly useful for describing individual features in mass spectrometry when the specific constitutional isomer is unknown.

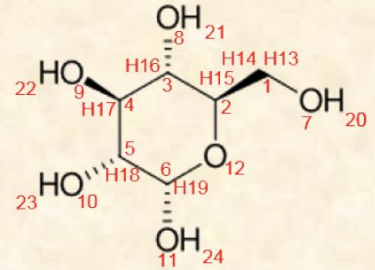
Simple Definition: 1/Ee#[Ee#].../a(Ee#<+|->#) OR 1/Ee#[Ee#].../a(#n)

Examples:

1. $^{13}C_2$ isotopologue of molecules with molecular formula $C_6H_{12}O_6$:
   InChI=1/C6H12O6//a(C2+1)
2. $^{13}C_1{}^{18}O_1$ isotopologue of molecules with molecular formula $C_6H_{12}O_6$:
   InChI=1/C6H12O6//a(C2+1),(O1+2)
3. M+3 isotopologue of molecules with molecular formula $C_6H_{12}O_6$:
   InChI=1/C6H12O6//a(3n)

   This last example enables a major use-case in mass spectrometry spectral feature assignment.

The Proposal



alpha-D-glucopyranose

- **Full isotopomer with respect to carbon for alpha-D-glucopyranose with ^{13}C at the 4th carbon:**
  - InChI=1/C6H12O6/c7-1-2-3(8)4(9)5(10)6(11)12-2/h2-11H,1H2/t2-,3-,4+,5-,6+/m1/s1/i1+0,2+0,3+0,4+1,5+0,6+0
- **Partial isotopomer of alpha-D-glucopyranose with ^{13}C at the 1st and 2nd carbons:**
  - InChI=1S/C6H12O6/c7-1-2-3(8)4(9)5(10)6(11)12-2/h2-11H,1H2/t2-,3-,4+,5-,6+/m1/s1/i1+1,2+1
- **$^{13}C_2{}^{2}H_3$ isotopologue of alpha-D-glucopyranose:**
  - InChI=1/C6H12O6/c7-1-2-3(8)4(9)5(10)6(11)12-2/h2-11H,1H2/t2-,3-,4+,5-,6+/m1/s1/a(C2+1)
- **$^{13}C_2$ limited to atoms 4,5,6 isotopologue fragment of alpha-D-glucopyranose:**
  - InChI=1/C6H12O6/c7-1-2-3(8)4(9)5(10)6(11)12-2/h2-11H,1H2/t2-,3-,4+,5-,6+/m1/s1/a(C2+1,4,5,6)

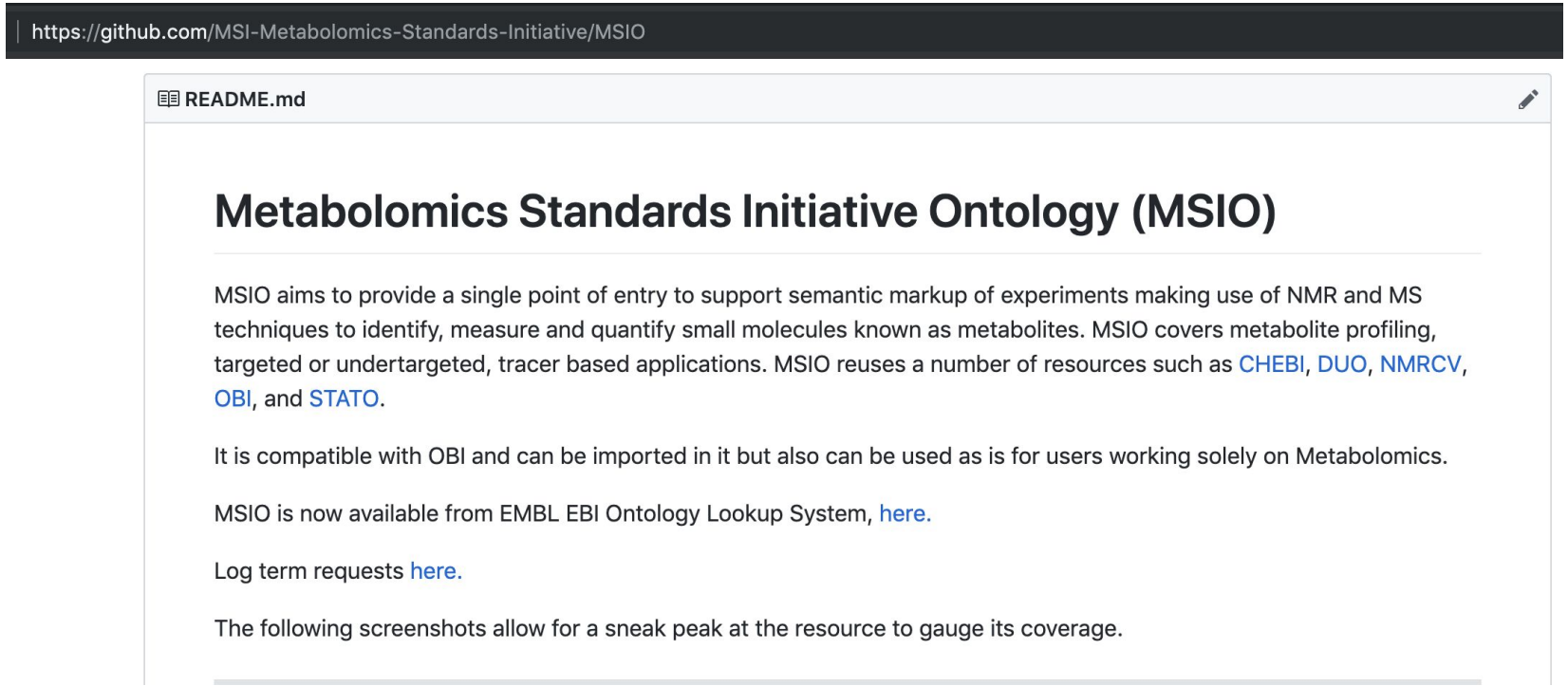
- Credit: Hunter Moseley, University of Kentucky

Issue 2: **describing and depositing Stable Isotope Resolved Metabolomic Studies to Metabolights @EMBL-EBI**

- **ISA the syntax**
- **MSIO the terminology**

Quick Overview of MSIO:

- https://github.com/MSI-Metabolomics-Standards-Initiative/MSIO



Application ontology: Built by reusing ontology modules extracted from exisiting resources

Enriched and augmented by the term additions collected during the COSMOS and PhenoMenal Work

Quick Overview of MSIO:

- OBI
- CHEBI
- STATO
- PSI-MS
- NMR-CV
- DUO

MSIO v1.0.1

Edit

proccaserra released this on 5 Oct 2018 · 2 commits to master since this release

MSIO v1.0.1:

minor service release from MSIO v1.0 to address ontology metadata for serving by EMBL-EBI Ontology Lookup Service

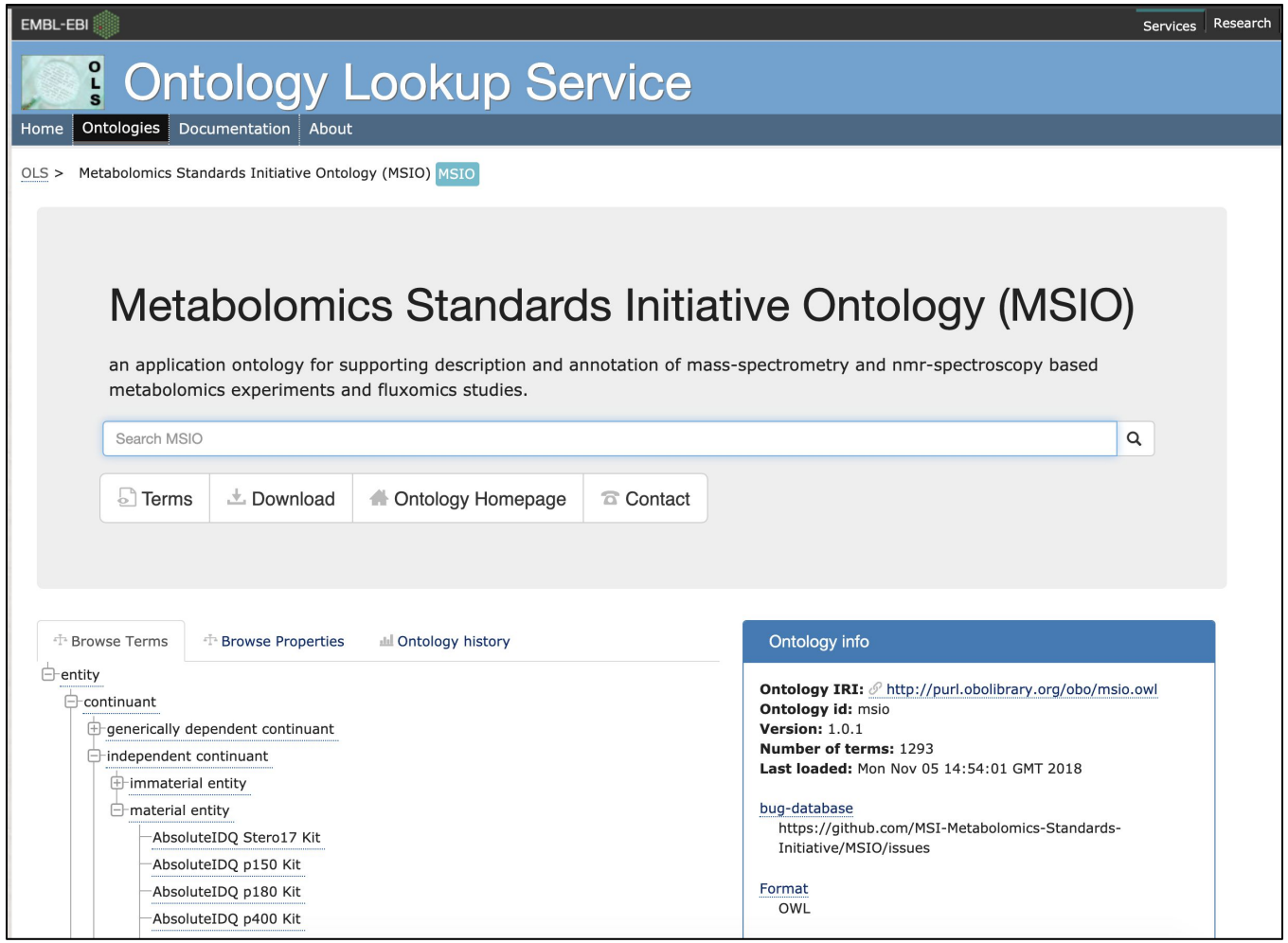
*support for Stable Isotope Resolved Metabolomics
*support for MS and NMR based metabolomics studies
*support for QA/QC reporting (both description of elements and type of quality controls)
*support for derivatisation processes and reagents (import of chemical compounds from CHEBI)
*support for description of data matrices (MzTab-M, MAF or Metabolomics specific JSON data packages)
*support for data use and consent information reporting (import of terms from DUO)

*compatible with the Ontology of BioMedical Investigations OBI
*compatible and optional import of STATO, the ontology for statistics

Acknowledgments:

*produced with support from H2020 PhenoMeNal (H2020-EU.1.4.1.3, 654241)

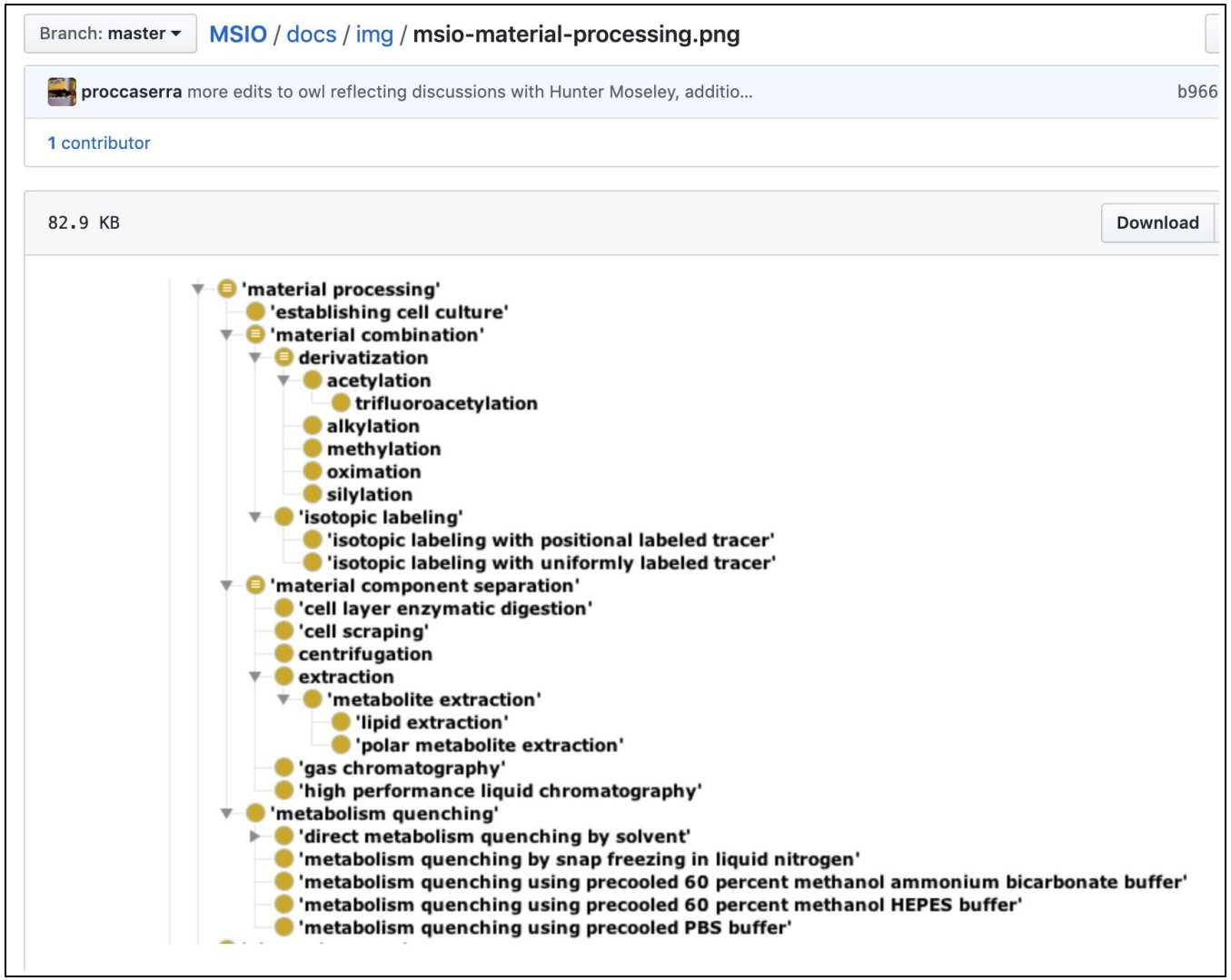
In production, available from EMBL-EBI OLS



- What is posted is a reasoned and merged version of the ontology
- It is updated with every release automatically

MSIO has 3 main branches

- Process branch:
  - covering actions such as:
    - Material processing



MSIO has 3 main branches

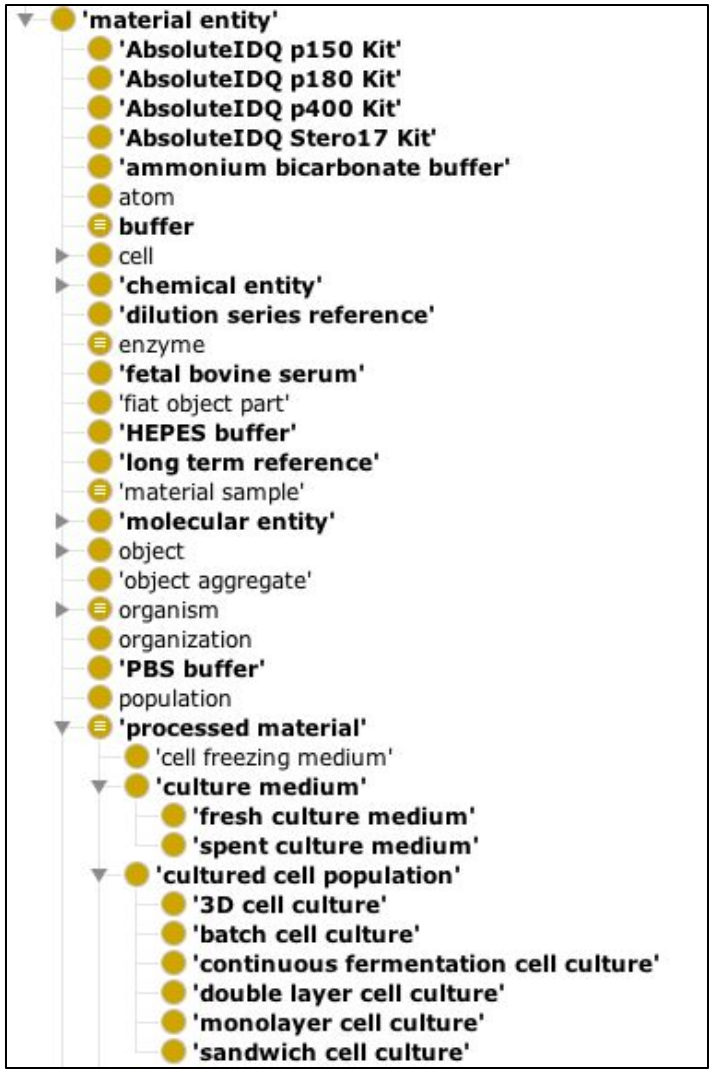
- Process branch:
  - covering actions such as:
    - Assay/ Data Acquisition

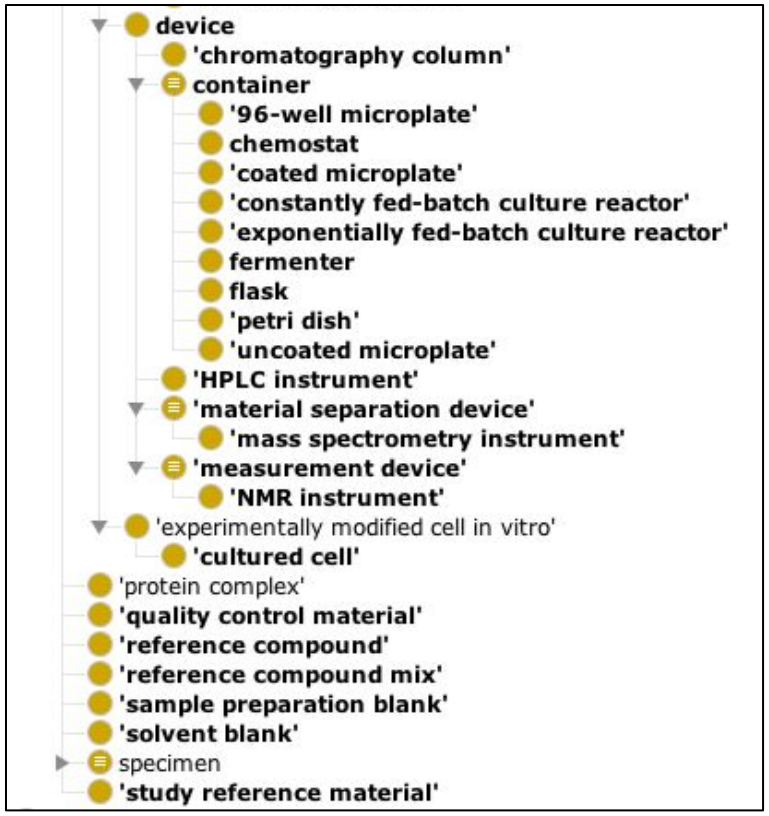
MSIO has 3 main branches

- Process branch:
  - covering actions such as:
    - Data Transformation

MSIO has 3 main branches

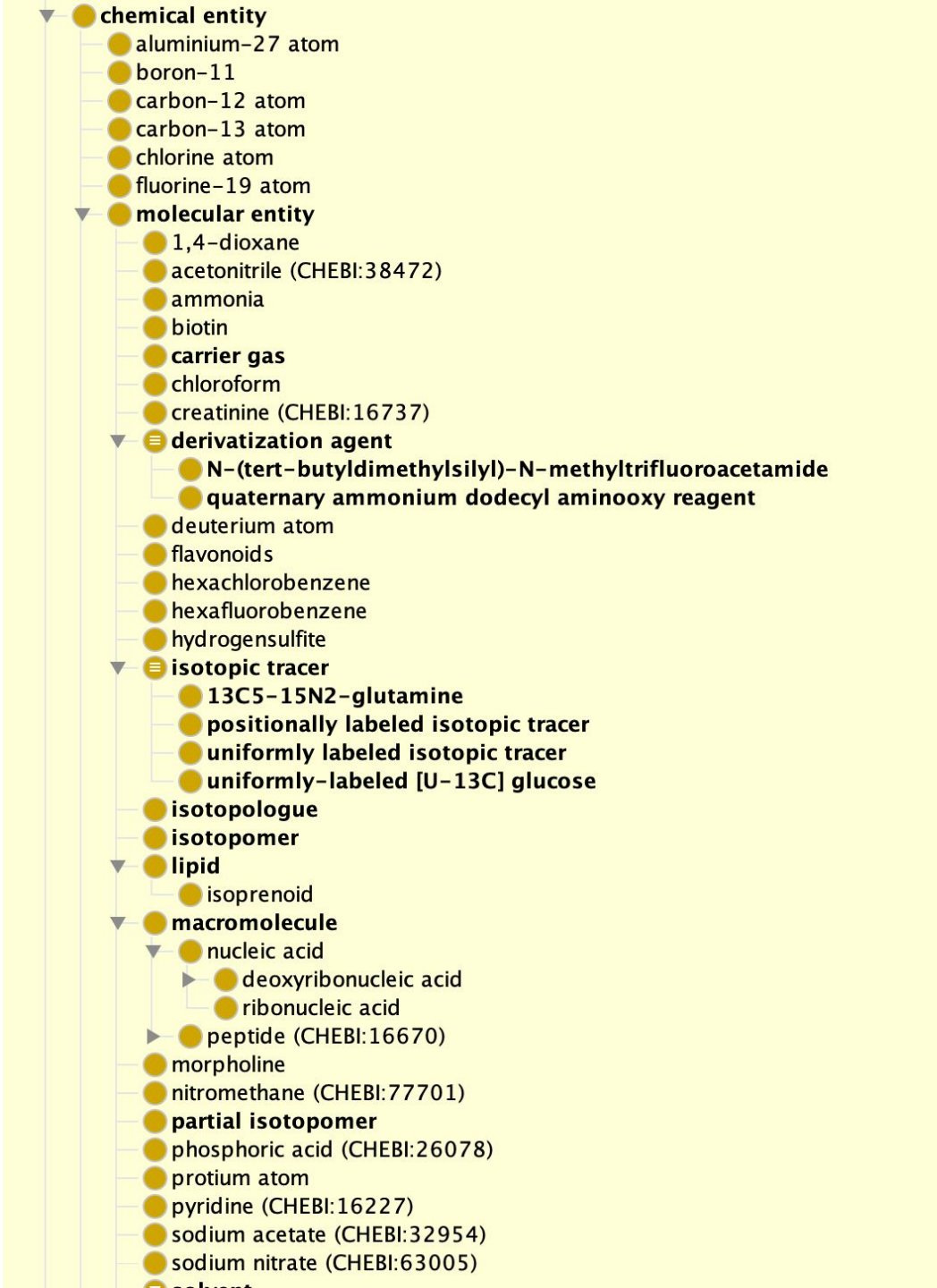
- Process branch:
  - covering actions such as:
    - Material Entity
    - MSIO includes Terms supporting reporting Quality Control Elements





MSIO has 3 main branches

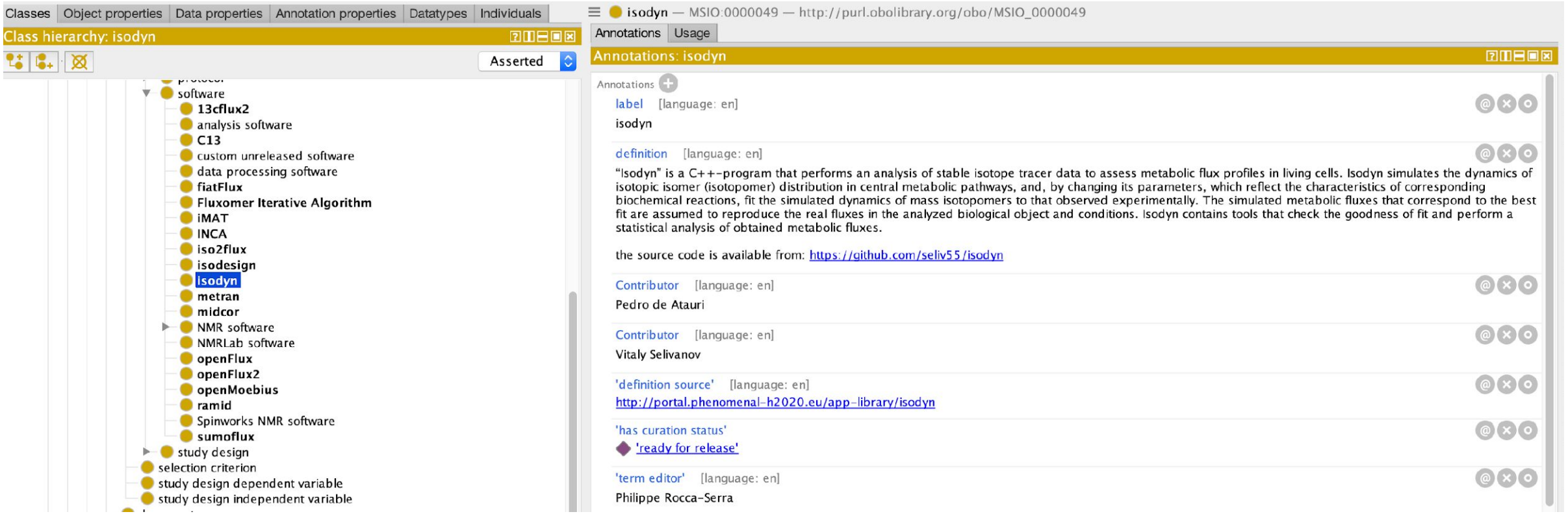
- Process branch:
  - covering actions such as:
    - Molecular Entity
      - Mostly imports from CHEBI



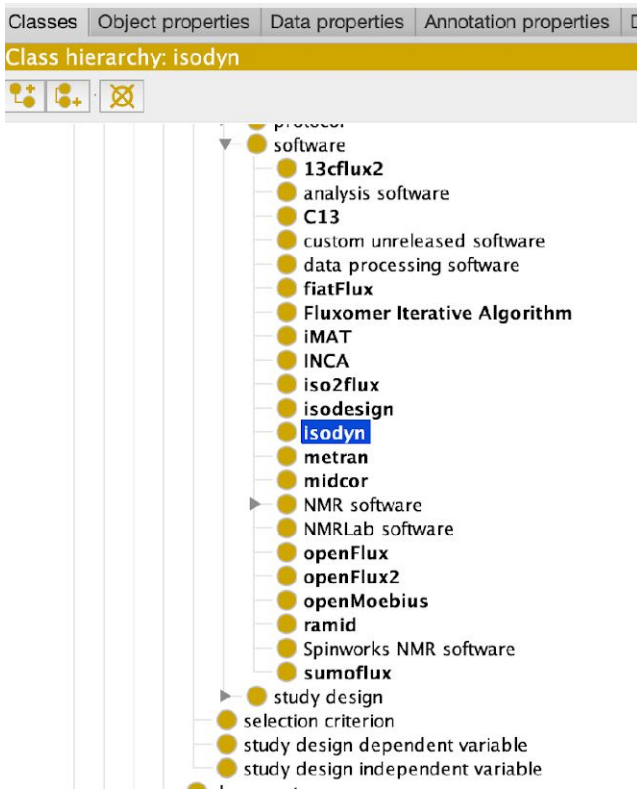
MSIO has 3 main branches

- Information Entity
  - covering actions such as:
    - Measurement types/datum

MSIO support for Fluxomics specific software



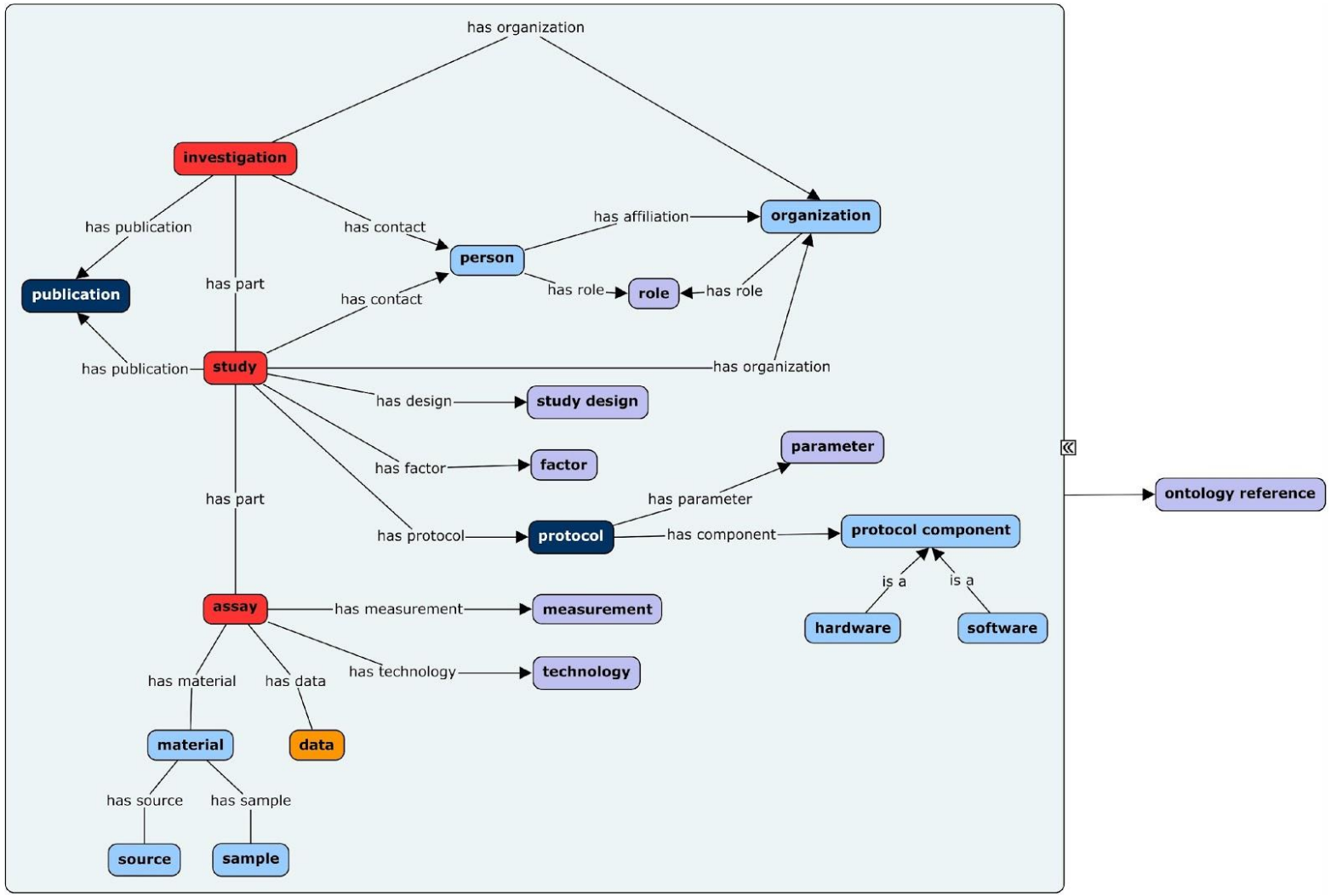
MSIO support for Fluxomics specific software



- Need more ?
  - **No problem, there a template for that!**
  - Take advantage of OBO Foundry Robot tools for submitting, requesting new terms (http://robot.obolibrary.org/)
  - As simple as filling a spreadsheet
  - At minima, provide
    - A name of the software class
    - A definition including a reference to a code repository and/or a DOI / Pubmed ID to a publication (as shown in the example)
  - Log issues / term requests at MSIO github issue tracker
  - https://github.com/MSI-Metabolomics-Standards-Initiative/MSIO/issues

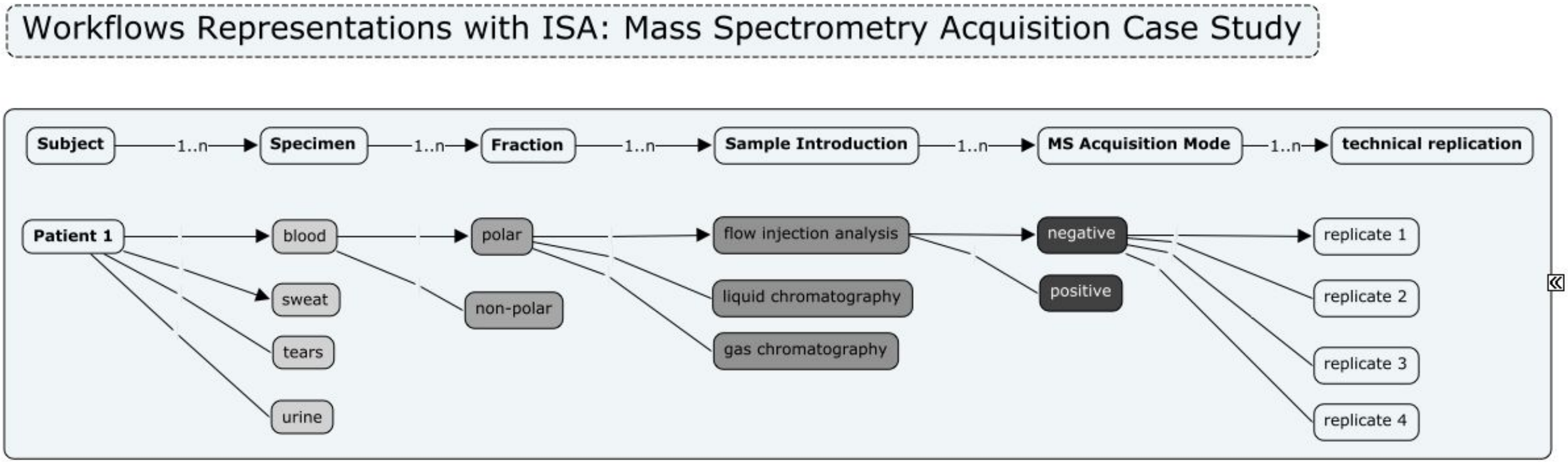
ISA Syntax – EMBL-EBI Metabolights Format

- Information Entity
  - covering actions such as:
    - Measurement types/datum



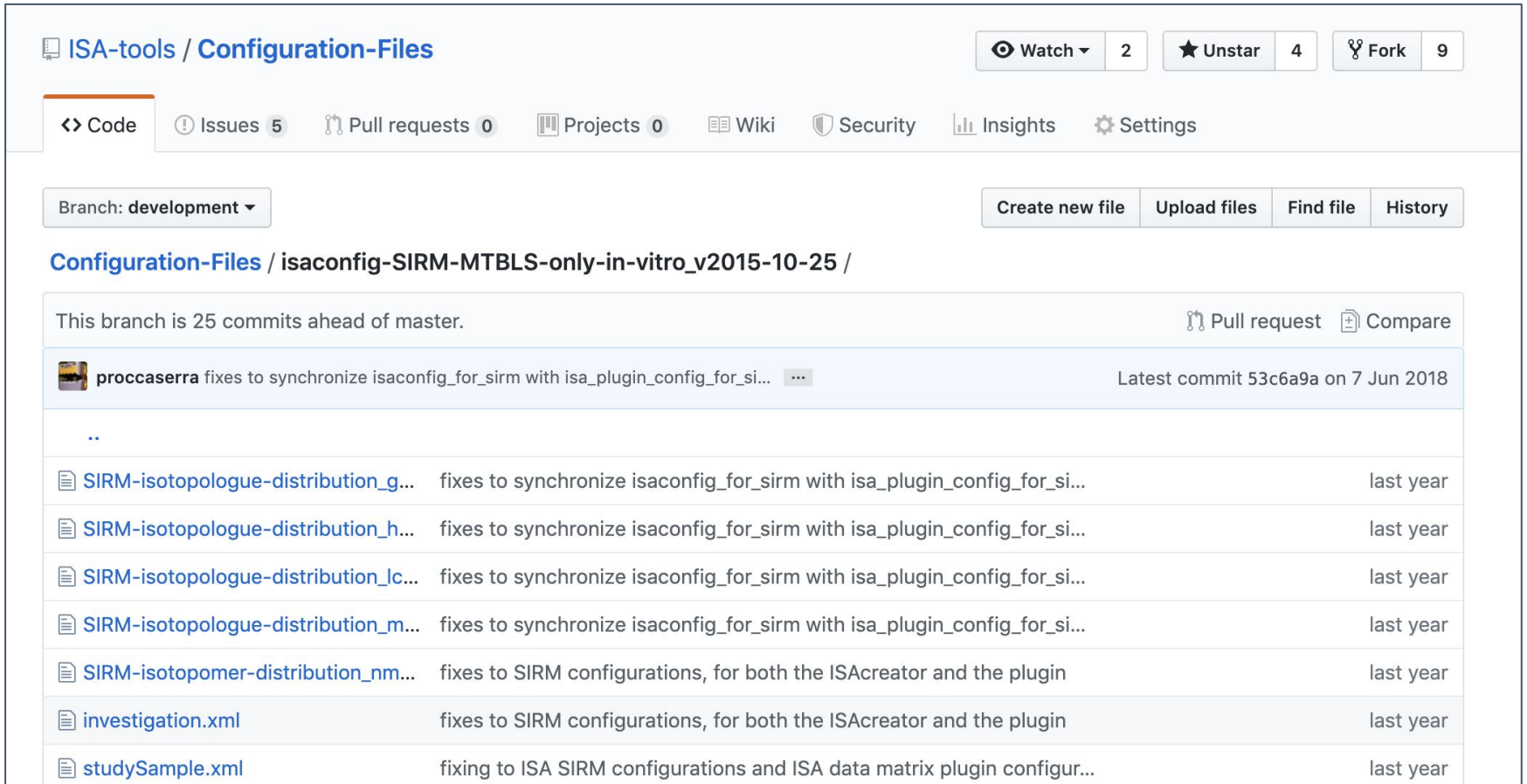
ISA Syntax – EMBL-EBI Metabolights Format

- Serialization as Tabular text file or JSON document
- JSON-LD context files are available (OBO foundry + Schema.org (not as rich))



ISA Syntax – EMBL-EBI Metabolights Format

- Fluxomics Specific Annotation Requirements via a set of ISA configurations



ISA Syntax – EMBL-EBI Metabolights Format

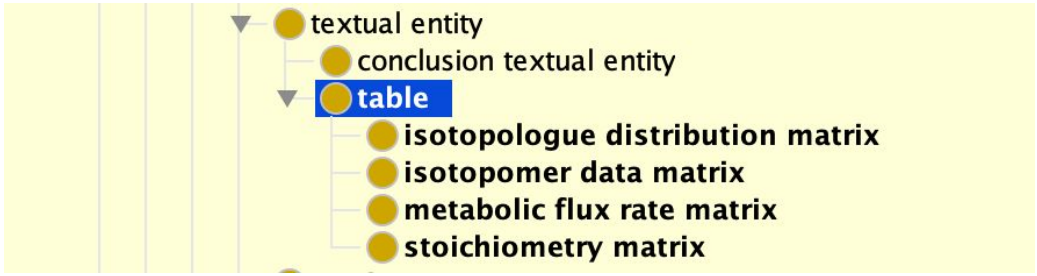
- Several studies from Marta Cascante's team have been submitted
- https://www.ebi.ac.uk/metabolights/MTBLS247
- https://www.ebi.ac.uk/metabolights/MTBLS412

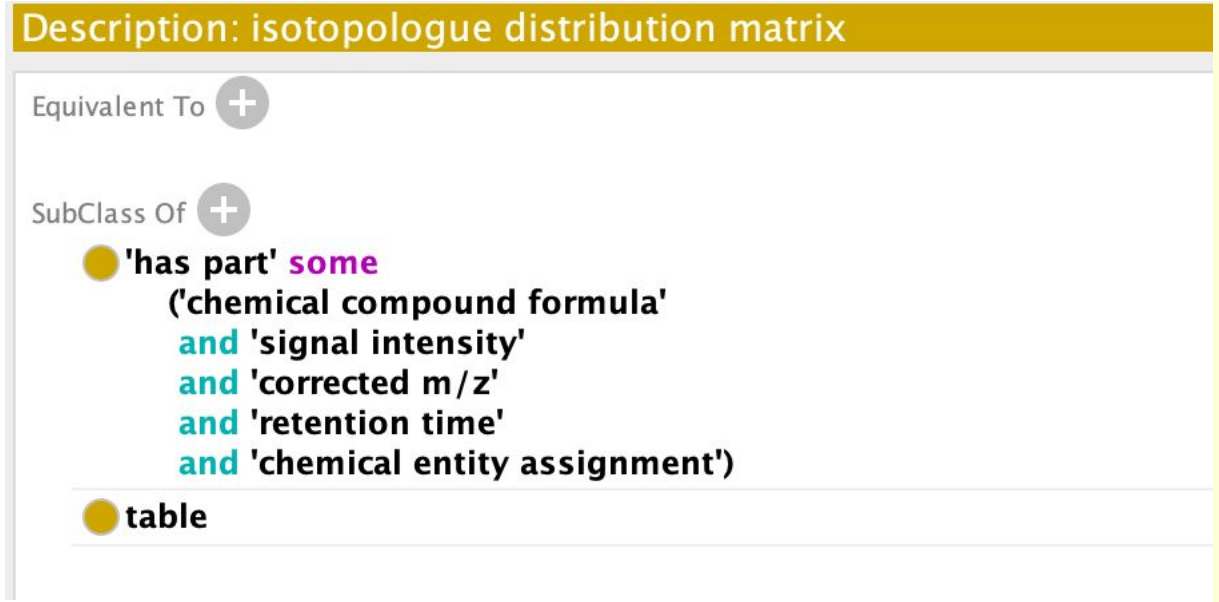
- ISA converter can retrieve Metabolomics Workbench Data and convert to ISA syntax (pb = absence of raw data files from the US repository)
- ISA python code to convert US DCC JSON to ISA format
  - Caveat: free text only, not semantic markup, could be done post-hoc by NER.

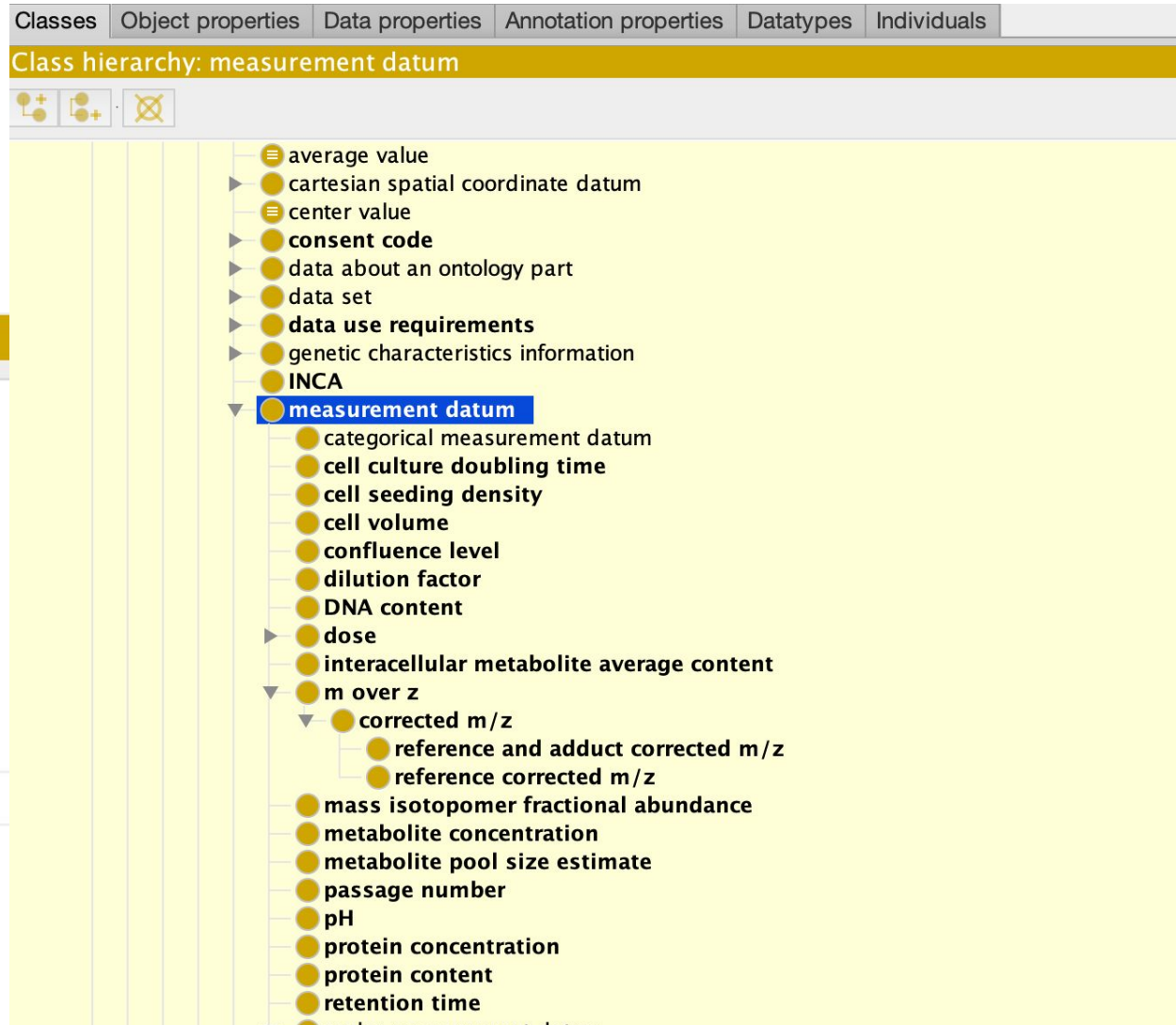
Issue 3: Data Matrix Results

- **Again, both syntax and semantics to be agreed upon**
- Dedicated Data Matrix Formats:
  - Option 1: derived from MAF file for compatibility with ISAcreator plugin
    - Validation
    - Layout: wide table + fixed height (i.e. fixed number of molecular dimensions)
  - Option 2: Exploratory JSON Tabular Data packages
    - Layout: long table + fixed width (i.e. fixed number of measurement dimensions)

Modeling Data Matrices







Provisioning for FAIR data matrices – MS

implementation as a ISA Table for ISACreator Plugin:

https://github.com/ISA-tools/Configuration-Files/blob/development/datamatrix-plugin-configuration/configuration_SIRM_ms.xml

```
<!-- OPTIONAL REPORTING OF TRACER MOLECULE INFORMATION -->
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<field header="post_collision_mass_to_charge" data-type="String" is-file-field="false" is-multiple-value="false" is-required="false" is-hidden="false"> [5 lines]
<field header="selected_ion_mass_to_charge" data-type="String" is-file-field="false" is-multiple-value="false" is-required="false" is-hidden="false"> [5 lines]
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```

Provisioning for FAIR data matrices - NMR

implementation as a ISA Table for ISACreator Plugin:
https://github.com/ISA-tools/Configuration-Files/blob/development/datamatrix-plugin-configuration/configuration_SIRM_nmr.xml

```
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<field header="smiles" data-type="String" is-file-field="false" is-multiple-value="false" is-required="false"  is-hidden="false"> [5 lines]
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```
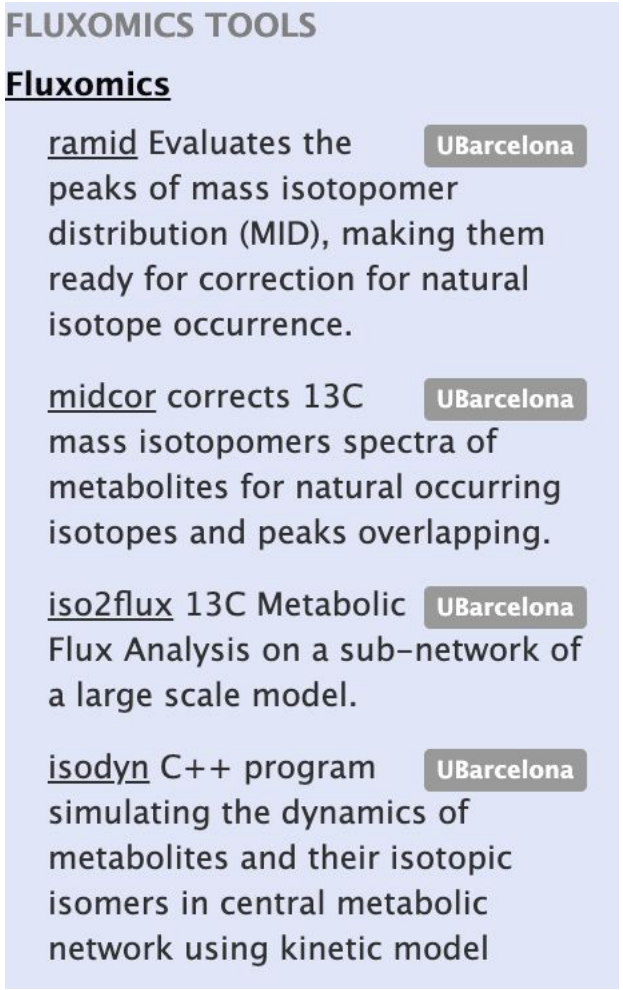
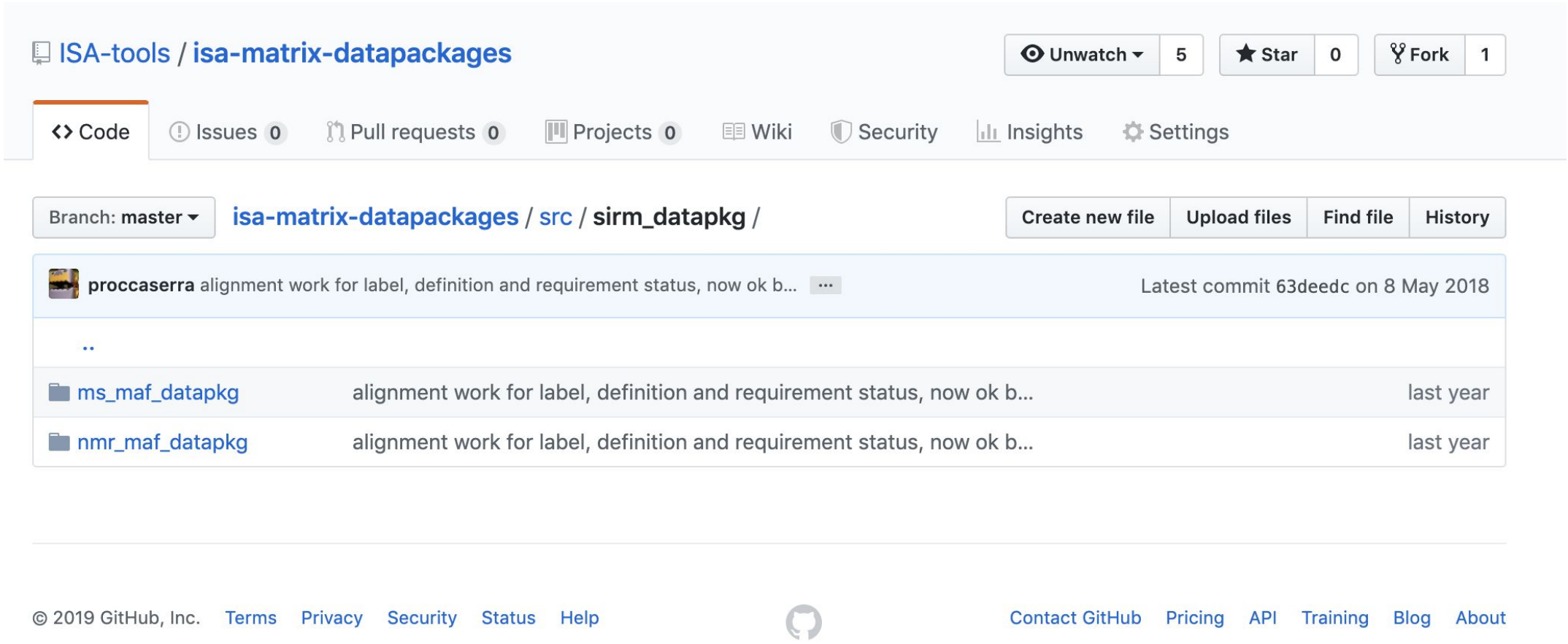

Provisioning for FAIR data matrices – Analysis Tools

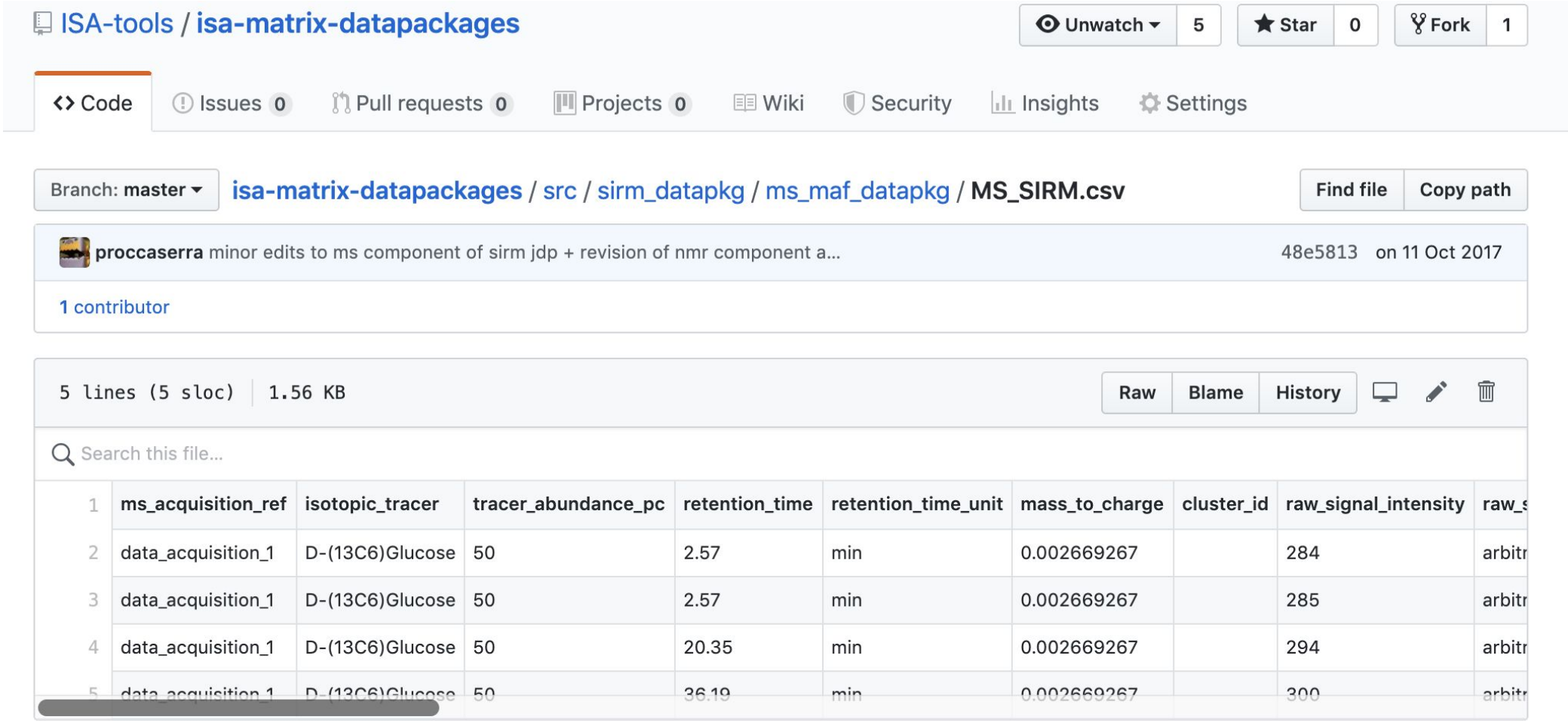
- Output of Ramid, Midcor and iso2flux implement the current recommendations
  - (credits to Vitaly Selivanov, Pedro de Atauri, Marta Cascante, Silvia Marin, University of Barcelona)



- Option 2: Exploratory JSON Tabular Data package



- Option 2: Exploratory JSON Tabular Data package



ISA-tools / isa-matrix-datapackages

Unwatch 5 | Star 0 | Fork 1

Code | Issues 0 | Pull requests 0 | Projects 0 | Wiki | Security | Insights | Settings

Branch: master — isa-matrix-datapackages / src / sirm_datapkg / ms_maf_datapkg / MS_SIRM.csv — Find file | Copy path

proccaserra minor edits to ms component of sirm jdp + revision of nmr component a... 48e5813 on 11 Oct 2017

1 contributor

5 lines (5 sloc) | 1.56 KB — Raw | Blame | History

Search this file...

	ms_acquisition_ref	isotopic_tracer	tracer_abundance_pc	retention_time	retention_time_unit	mass_to_charge	cluster_id	raw_signal_intensity	raw_s
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3	data_acquisition_1	D-(13C6)Glucose	50	2.57	min	0.002669267		285	arbitr
4	data_acquisition_1	D-(13C6)Glucose	50	20.35	min	0.002669267		294	arbitr
5	data_acquisition_1	D-(13C6)Glucose	50	36.19	min	0.002669267		300	arbitr

- Option 2: Exploratory JSON Tabular Data package


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    "email": "proccaserra@gmail.com",
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Future Work

- More testing
  - BYOD and creation ISA formatted documents for deposition to Metolights
  - Hackathon with tool developers to implement regularized outputs and self standing data matrices
  - Vocabulary development
    - submit terms where a need arises
    - make some resources used by MSIO more robust with resolvable uri (e.g. NMR cv)

Acknowledgements

- FP7 COSMOS: grant agreement number: EC312941
- H2020 PhenoMeNal: grant agreement number: 654241

All thanks go to:
Marta Cascante, Vitaly Selivanov, Pedro de Atauri, Kenneth Haug, Reza Salek, Claire o'Donovan, Chris Steinbeck, Hunter Moseley, Teresa Fan, Andrew Lane

Questions