Deliverable 9.4

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Abstract

This report provides an update on existing software tools, workflows and analytical pipelines supported in PhenoMeNal, covering the new developments since the *D9.1 Report on existing software tools, workflows and analytical pipelines initially supported in the PhenoMeNal grid*.

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1 Executive Summary

This report provides an update on existing software tools, workflows and analytical pipelines supported in PhenoMeNal, covering the new developments since the *D9.1 Report on existing software tools, workflows and analytical pipelines initially supported in the PhenoMeNal grid*.

The project has now updated the tool list for ISA support, extended NMR coverage, ported new tools from the Workflow4Metabolomics project, updated the fluxomics tools and workflow, and is supporting OpenMS on the PhenoMeNal e-Infrastructure. Along with these new tools we now support new Formats, i.e. the ISA-Tab and nmrML data standards are now Galaxy recognized data types.

2 Contribution towards the project objectives

The deliverable has contributed towards the following project objectives:

- 9.1 Specify and integrate software pipelines and tools utilised in the PhenoMeNal e-Infrastructure into VMIs, adhering to data standards developed in WP8 and supporting the interoperability and federation middleware developed in WP5. We will develop new applications only to complete 'missing links' in pipelines. We will use public repositories and continuous integration to always provide development snapshots of the infrastructure VMIs.
- 9.2 Develop methods to scale-up software pipelines for high-throughput analysis, supporting distributed execution on e.g. local clusters, private clouds, federated clouds, or GRIDs.
- 9.3 Add quality control and quality assurance to pipelines to ensure high quality and reliable data, keep an audit trail of intermediate steps and results.
- 9.4 Develop methods to present and summarize the results of the pipelines in biomedical and disease contexts.

3 Detailed report on the deliverable

3.1 Background

This is an update of D9.1 Report on existing software tools, workflows and analytical pipelines initially supported in the PhenoMeNal grid[1].

[1] http://phenomenal-h2020.eu/home/wp-content/uploads/2016/09/D9.1.pdf

Strategy for the collection of tools, workflows and analytical pipelines supported in the PhenoMeNal infrastructure

We have continued to extend the collection of tools, workflows and analytical pipelines already started with D9.1. We first concentrated on tools and workflows that are useable in medical phenotyping. This initial tool and workflow selection strategy was governed by a questionnaire and UX meeting (described in earlier deliverables). As a second selection criteria we now integrated additional robust and well-known open source tools that already have a large user base. We also added new tools that were recently developed and which will improve our workflows (e.g. rDolphin and nmrProcFlow). After that, we continued to update the list, driven by new observations we made during our own use of the workflows, and feedback from users during the user training. At the same time, we also deprecated several tools which were considered less relevant due to different reasons, including lack of upstream support and no workflows using the tool. Already packaged tools remain available in the container registry.

3.2 ISA support

The PhenoMeNal consortium has made the support of the ISA data model and -format one of the goals of the tool development.

New Galaxy datatypes: ISA-Tab and ISA-JSON

Three new Galaxy datatypes (nmrML, ISA-Tab and ISA-JSON) have been developed by CRS4, UOXF and CEA in order to handle the ISA format natively inside Galaxy. We have developed an ISA data type and implemented support in the Galaxy workflow system. Several tools were upgraded in order to take advantage of the new Galaxy datatypes ISA-Tab and ISA-JSON developed by the PhenoMeNal team.

Mtbls-dwnld, which initially was a downloader of ISA studies from MetaboLights and a converter to W4M (Workflow4Metabolomics) format into Galaxy, has been split in two:

1. The **mtbls-dwnld** tool itself now deals only with the downloading of MetaboLights studies, and outputs an ISA-Tab dataset.
2. A new tool, **isa2w4m**, has now been developed that converts an ISA-Tab dataset into the W4M format (3 tabular datasets for variables, samples and data matrix) and the conversion code has been translated to Python and integrated inside the ISA-API Python library developed by UOXF.

Other tools using an ISA archive for input are now being upgraded in order to use this new datatype. This will allow better modularity of the tools, leaving downloading and conversion to specialised tools, and facilitate the connection of tools inside workflows (i.e.: tools input and output will be adapted to the new ISA-Tab datatype).

ISAcreate-tool, which is built on the ISA API and the galaxy tool definition, now supports the creation of ISA documents and follows implementation guidelines reported in D8.4.2. This allows both prospective and retrospective study reporting and ensure regularization of metadata input in the PhenoMeNal workflows.

3.3 Extended NMR coverage

An NMR data processing pipeline has already been part of the PhenoMeNal installation in 2017. To continue the development of this pipeline, a workshop on NMR[2] was held from 23th to 25th January 2018 at EMBL-EBI, with participants from both PhenoMeNal and external developers of NMR tools. The workshop opened with discussions related to improving the current NMR pre-processing Galaxy workflow, considering consolidating existing tools and integrating new, more powerful, tools. It was agreed that in the long term the pipeline must become more flexible, to allow for a more comprehensive coverage of common NMR data analysis workflows, with as little dependence to external tools as possible. As a result, initial steps towards enabling user interactivity, for those tools that require interactive user adjustments via a web GUI, can now run in Galaxy and their output are automatically integrated into the Galaxy history. Action points for the release Cerebellin were also discussed. During the workshop the participants added several new tools to PhenoMeNal:

tameNMR, **rDolphin** and **stocsy**. The **dimpsy** tool was also added, but note that in the time of writing, is still in early development. The **rnmr1d** and related tools depend on the **speaq-library,** containers were created depending on the **speaq-container** and with microservices in mind. Containers and testing was completed for these new tools. Documentation for the tools and how they are used in the PhenoMeNal infrastructure is already well under way. Participants also began to write functions that interconnect the new tools with each other, e.g. **rDolphin2metabomatching**.

During the workshop, participants initiated the implementations with the goal to make the existing tools more interoperable. A new tool **nmrml2batman** was created that allows **BATMAN** to load nmrML data files directly. Further, steps were taken to connect the existing rnmr1d (nmrProcFlow) data output to other tools such as tameNMR and metabomatching.

At the workshop, participants also added a new **nmrML datatype** to Galaxy and this was suggested for general inclusion to the global Galaxy community.

At the workshop, a working prototype of the **nmrProcFlow Galaxy Interactive Environment (IE)** was implemented. NMR data pre-processing is very specific to the use-case, i.e. requires feedback loops and parameter adjustment iterations. Hence such tools tend to require a more complex user interface (GUI) and integration as a standard Galaxy tool could result in a lessen user experience. E.g. the web based nmrProcFlow allows the user to interactively set and test pre-processing parameters in a user-friendly, web based, GUI interface. This interactive interface can now be embedded directly into Galaxy. Source files are injected into the interactive environment. The generated macro (output) file containing the pre-processing settings is part of the Galaxy history and can now be directly used by the existing NMR-workflow. Previously this file had to be created and downloaded externally form the Galaxy environment, which introduced a 'media break' in the Galaxy workflow. We internally documented the steps involved. As this requires changes in Galaxy, a pull request will be made to the Galaxy community once the functionality is ready.

[2] https://docs.google.com/document/d/1HD6o1pS7nJAfP_uCdYTwmE4Gr5LrccYujil6vakqXvY/

During the reporting period, **metabomatching** was partially rewritten to more properly interface with Galaxy, which allowed access to all parameters in the most recent implementation of the metabomatching container. The method paper was published in PLoS Comp Bio in December [https://doi.org/10.1371/journal.pcbi.1005839]. Companion tools, including **STOCSY** and the iterative signature algorithm, that feed into the metabomatching-container have been written, but performance issues encountered in porting existing Matlab code into an open source language will need to be solved before deployment into PheNoMenal and larger workflows.

3.4 Port of Workflow4Metabolomics (CEA/INRA) tools

The Workflow4Metabolomics infrastructure is operated by the french MetaboHUB infrastructure and bioinformatics platforms (IFB: Institut Français de Bioinformatique) is an open, public and centrally managed Galaxy instance for metabolomics. The institutions CEA and INRA are part of both Workflow4Metabolomics and PhenoMeNal.

Several tools which are extensively used in the Workflow4Metabolomics platform were ported into PhenoMeNal to harmonise tools and workflows across Galaxy installations. Together they now allow to build comprehensive statistical workflows which take as input preprocessed MS and NMR data and perform data exploration, prediction modeling and biomarker selection. In addition, by using the updated MetaboLights downloader, such workflows can be directly applied to the data sets from the MetaboLights[3] repository (as demonstrated by the MTBLS404[4] data set example).

Univariate: a module that performs univariate analysis. The methods implemented are: two sample tests (t-test and Wilcoxon rank test), analysis of variance and Kruskal-Wallis rank test, and correlation tests (by using either the Pearson or the Spearman correlation)

Multivariate: a module that performs multivariate analysis (PCA, PLS and OPLS).

Biosigner: a module that implements a new feature selection algorithm to assess the relevance of the variables for the prediction performances of the classifier.

Several tools have been selected and ported more recently: they are listed below.

Lcmsmatching (new): performs LC/MS matching on an input list of MZ/RT values, using either a provided in-house single file database or a connection to the Peakforest database.

Batch correction (new): corrects the offset differences between batches, using QC samples.

Generic filtering (new): removes all samples and/or variables corresponding to specific values regarding designated factors or numerical variables.

Quality metrics (new): provides quality metrics of the samples and variables, and visualization of the data matrix.

[3] https://www.ebi.ac.uk/metabolights/
[4] https://www.ebi.ac.uk/metabolights/MTBLS404

Transformation (new): performs a transformation of the data matrix intensity values to stabilize variance.

Normalisation (new): performs a normalisation, where an operation is applied to each (preprocessed) individual spectrum of the data.

The development of the above-mentioned mtbls-dwnld and isa2w4m modules, as well as the porting of these five new normalization tools is a major achievement for the *interoperability* between the reference resources for data reposition (MetaboLights) and analysis workflows (PhenoMeNal and Workflow4Metabolomics). As a real use case with a human cohort study, a workflow starting with the MTBLS404 dataset from MetaboLights and performing a comprehensive statistical analysis (W4M00001; Guitton et al., 2017) was successfully built and run on PhenoMeNal (Peters et al., *in preparation*).

3.5 Updated fluxomics tools and workflow

The tools for fluxomics support stable isotope tracing data analysis aimed in evaluation of metabolic fluxes (biochemical reactions) catalysed within selected intracellular metabolic pathways of interest. The last release includes a new tool (**cdf2mid**) that supports the first step of this workflow: extraction of mass spectra (mass isotopomer distribution, MID) from mass spectrometer written CDF files. Its functionality is similar to that of the implemented before tool RaMID. The difference is that cdt2mid is designed to the analysis of new experiments, yet not presented in MetaboLights. Cdf2mid presents the evaluated spectra in the format compatible with MetaboLights, so that the provided data can be aggregated into this database. In addition to CDF files, containing time course of mass spectra of metabolites of interest, it uses a brief description of experimental conditions, provided by owners of the data.

3.6 Supporting OpenMS on the PhenoMeNal e-Infrastructure

As already mentioned in D9.1, OpenMS is one of the prominent Open Source Platforms for the analysis of computational mass spectrometry data. It is mainly used in Proteomics, but increasingly also in Metabolomics. OpenMS consists of C++ libraries, many command line tools, and graphical interfaces. This platform is now fully supported by the PhenoMeNal analysis environment. During the PhenoMeNal project, the OpenMS team has released several updates to the OpenMS software suite, in particular OpenMS 2.1 (2016), OpenMS 2.1 (2017), OpenMS 2.3 (2018). We have upgraded the OpenMS tools in the current development branch to OpenMS-2.3.

The Caramba team[5] at Uppsala hospital is using metabolomics to perform pre-clinical and clinical research, targeting endogenous and exogenous molecules, with the overall goal to improve human health care and disease prevention, using state-of-the-art as well as novel mass spectrometry and bioinformatics-based methods for use in routine clinical applications. The tools previously used individually, and during the project runtime were now integrated into PhenoMeNal, as also described below in Demonstrator 2.

[5] http://www.caramba.clinic/

We also identified several functionality gaps where new tools had to be developed over the course of PhenoMeNal to improve the interoperability between the R-based MS data processing using xcms and CAMERA, and the OpenMS framework. Specifically, these included:

1. **featureXMLToCAMERA**: converts featureXML files to CAMERA
2. **featureXMLToXcms**: converts featureXML files to xcmsSet
3. **ConsensusXMLToXcms**: converts consensusXML files to xcmsSet

Together with these tools we were able to drastically improve the coverage of our MS data processing workflows, as shown in the following Demonstrators.

3.7 Demonstrators

The presented use cases in D9.1 were used to develop demonstrators that cover the analysis of MS, NMR and fluxomics related data sets to illustrate the usage and applicability of given Phenomenal workflows and software tools for those scenarios. The four demonstrators are described in more detail in the manuscript "*Interoperable and scalable metabolomics data analysis with microservices*" (Emami Khoonsari et. al.), a collaborative effort of the consortium. A preprint of the manuscript is available from bioRxiv[6]; the demonstrators being covered in detail in the supplemental information. In summary, Demonstrator 1 shows how Luigi[7] and Jupyter[8] support use cases with interactive scripting and scaleable scientific computing. Demonstrators 2 (MS), 3 (NMR) and 4 (Fluxomics) show workflows for different application domains and illustrate how PhenoMeNal can simplify the implementation of complex workflows through the Galaxy[9] workflow engine.

Demonstrator 1: Scalability of microservices in a cloud environment in the analysis of a human renal proximal tubule cells dataset

The objective of this analysis was to demonstrate the scalability of an existing workflow on a large dataset (MetaboLights ID: MTBLS233[10]). The experiment includes 528 mass spectrometry samples from whole cell lysates of human renal proximal tubule cells that were pre-processed through a five-step workflow (consisting of peak picking, feature finding, linking, file filtering and exporting) using the OpenMS software. This preprocessing workflow was reimplemented using Docker containers and run using the Luigi workflow engine. Scalability of concurrent running tools (on 40 Luigi workers, each worker receives tasks from the scheduler and executes them) was measured using weak scaling efficiency (WSE), where the workload assigned to each worker stays constant and additional workers are used to solve a larger total problem. The WSE was computed to reach 88% with an execution time of approximately four hours, compared with the ideal case of 100% where linear scaling is achieved if the run time stays constant while the workload is increased. In addition, the final result of the workflow was identical to that presented by the original MTBLS233 study (Ranninger et al.) in negative ionization mode. However, in the

[6] https://www.biorxiv.org/content/early/2017/11/24/213603
[7] https://github.com/spotify/luigi
[8] http://jupyter.org/
[9] https://galaxyproject.org/
[10] http://www.ebi.ac.uk/metabolights/MTBLS233

positive ionization mode, one m/z feature was found in a different group (m/z range 400-1000) than it was originally reported by Ranninger et al. (m/z range 200-400). More detailed results regarding the scaling efficiency and feature quantification are shown in tables S2 and S3 of Emami Khoonsari et. al.[5]

Demonstrator 2: Start-to-end LC-MS-analysis workflow on Multiple Sclerosis data using tools from Bioconductor and OpenMS

The objective of this analysis was to demonstrate interoperability as well as to present a real-world scenario in which patients' data are processed using a microservices-based platform. We used a dataset consisting of 37 clinical cerebrospinal fluid (CSF) samples including thirteen relapsing-remitting multiple sclerosis (RRMS) patients and 14 secondary progressive multiple sclerosis (SPMS) patients as well as ten non-multiple sclerosis controls. Twenty-six quality controls (19 blank and 7 dilution series samples) were also added to the experiment. In addition, 8 pooled CSF samples containing MS/MS data were included in the experiment for improving identification (MetaboLights ID: MTBLS558[11]). The samples were processed and analysed on the Galaxy platform applying the Liquid Chromatography-MS (LC-MS) workflow illustrated in Figure 1 (below), running in a PhenoMeNal VRE behind the Uppsala University Hospital firewall to be compliant with local ELSI (Ethical, Legal and Social Implications) regulations.

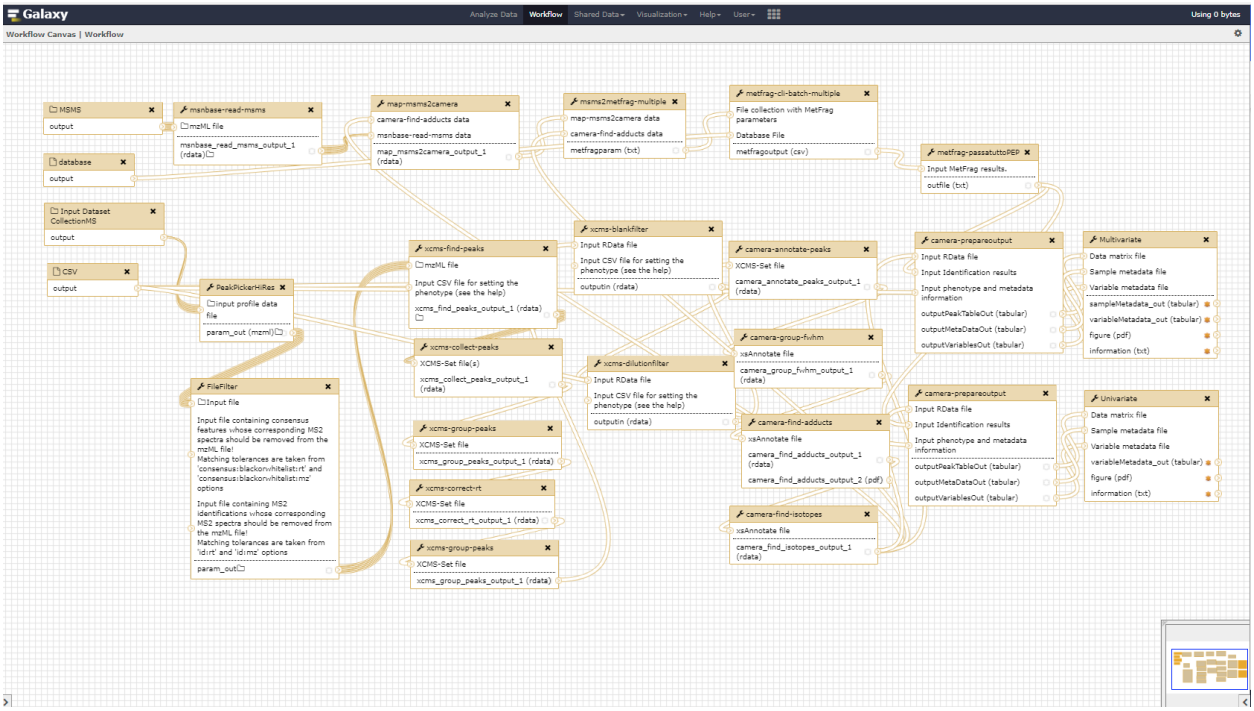

Figure 1: Overview of the full data mass spectrometry preprocessing and data analysis workflow in Galaxy used for demonstrator 2.

The result of multivariate analysis showed a clear difference in the metabolic constitution between the three disease groups of RRMS, SPMS and non-multiple sclerosis controls. In

[11] http://www.ebi.ac.uk/metabolights/MTBLS558

addition, the univariate analysis resulted in a total of three metabolites being significantly altered ($p<0.05$) between multiple sclerosis subtypes and control samples, namely alanyltryptophan and indoleacetic acid with higher and linoleoyl ethanolamide with lower abundance in both RRMS and SPMS compared to controls.

Demonstrator 3: 1D NMR-analysis workflow on human type 2 diabetes mellitus data

This NMR-based metabolomics study was originally performed by Salek et al. on urine of type 2 diabetes mellitus (T2DM) patients and controls (MetaboLights ID: MTBLS1[12]). In total, 132 samples (48 T2DM and 84 controls) were processed using the workflow performing MetaboLights import, nmrML conversion, signal preprocessing and the Orthogonal Projections to Latent Structures Discriminant Analysis (OPLS-DA) on extracted study related experiment factors. A total of 726 metabolites were quantified and used to perform the OPLS-DA which resulted in a clear separation between T2DM and controls, reproducing previous findings. The results are shown in Figure 5 of Emami Khoonsari et. al.[5]

Demonstrator 4: Start-to-end fluxomics workflow on HUVEC cells under hypoxia

The purpose of this demonstrator was to show the integrated use of separately developed tools covering subsequent steps of the study of metabolic fluxes based on 13C stable isotope-resolved metabolomics (SIRM). Here we implemented the analysis of flux distributions in HUVEC cells under hypoxia (MetaboLights ID: MTBLS412[13]), from raw mass spectra contained in netCDF files, using the workflow illustrated in Figure 2 using the Ramid, Midcor, Iso2Flux and Escher-fluxomics software tools integrated in the Galaxy platform. The result was a detailed description of the magnitudes of the fluxes through the reactions accounting for glycolysis and pentose phosphate pathway.

[12] http://www.ebi.ac.uk/metabolights/MTBLS1
[13] http://www.ebi.ac.uk/metabolights/MTBLS412

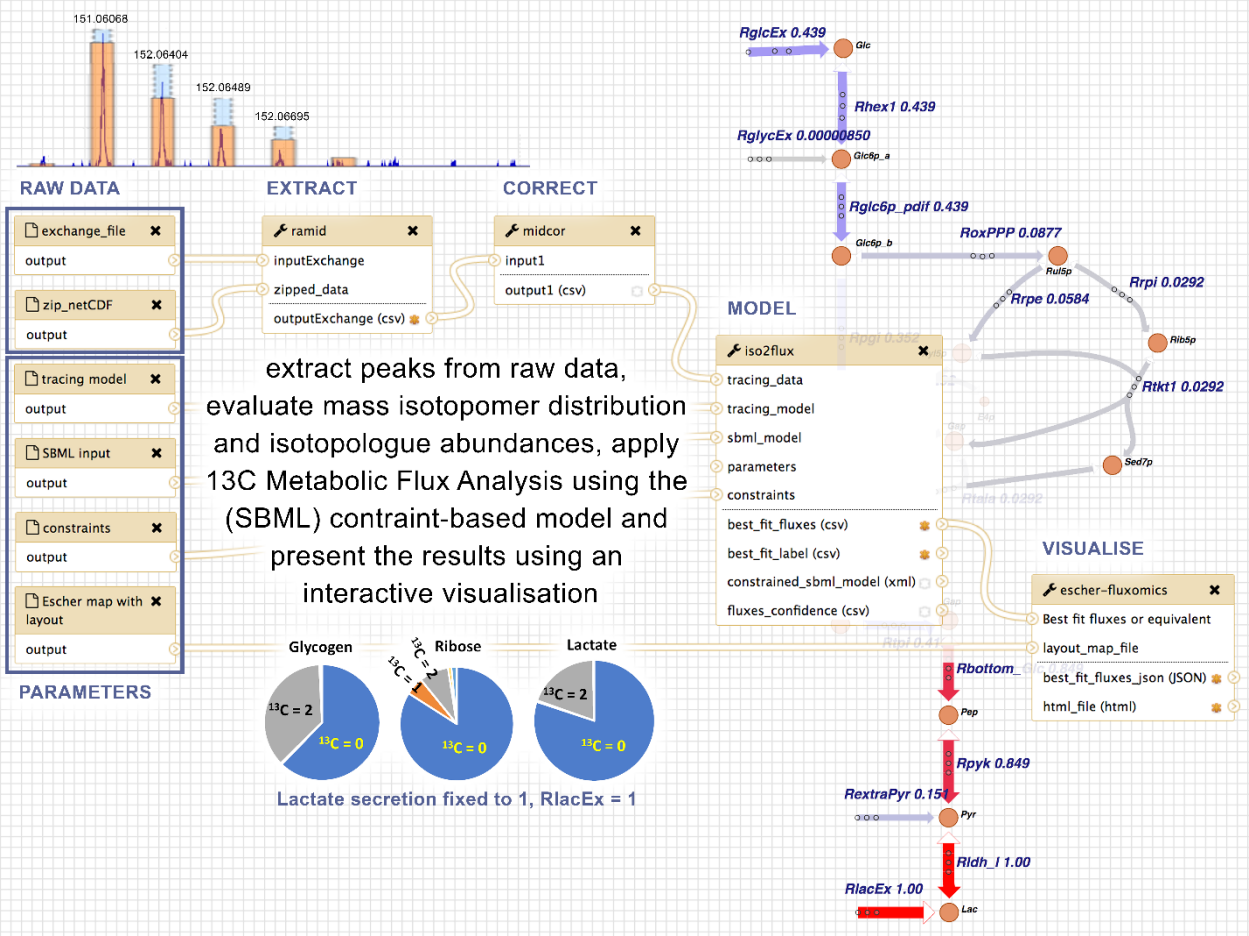

Figure 2: Overview of the fluxomics workflow in Galaxy used for demonstrator 4.

4 Conclusion

Recent activities have largely cantered around increasing robustness and coverage of representative biomedical Phenomics workflows in PhenoMeNal. These efforts were also guided by recent real-life test scenarios during tutorial workshops with target users from the clinical domain. Aside emerging new tools and more complete workflows now covering biomedical analysis pipelines from data generation (or download) over data processing, statistics and result depositions in appropriate data repositories, we have introduced lower level IT set-up changes to the infrastructure that increased performance stability in cloud setups. To support the processing tools with comprehensive data exchange, communication channels and storage formats, we have made Galaxy aware of data standards for raw (e.g. nmrML) and metadata (e.g. ISA Tab) formats. In the remaining

5 Delivery and Schedule

The delivery is delayed: No

6 Annex: List of phenomenalized tools

Table: List of tools in PhenoMeNal. Listed are also their status in the Continuous Integration and for the upcoming release and availability in the PhenoMeNal portal.

Tool	Case worker	Topic Tags	Status of Container Cerebellin (2018.02)Release	Container Git Repository
batch_correction	Nils Paulhe, Pierrick Roger	Normalization	Ready	
BATMAN	Jianliang Gao / Pablo Moreno	NMR	Ready	https://github.com/phnmnl/docker-batman
Biosigner	Pierrick Roger	Statistics	Ready	https://github.com/phnmnl/container-biosigner.git
bruker2batman	Jianliang Gao		Ready	
CAMERA	Christoph Ruttkies	MS	Ready	https://github.com/phnmnl/container-camera.git
cdf2mid	Vitaly Selivanov	MS; Fluxomics	Ready	https://github.com/phnmnl/container-cdf2mid
escher-fluxomics	Pablo Moreno	Visualization	Ready	https://github.com/phnmnl/container-escher-fluxomics
galaxy-k8s-runtime	Pablo Moreno	Runtime	Ready	https://github.com/phnmnl/container-galaxy-k8s-runtime.git
isa2w4m	Phillipe Rocca-Serra		Ready	
isajson-validator	David Johnson	Converter	Ready	https://github.com/phnmnl/container-isajson-validator.git
isatab-validator	David Johnson	Converter	Ready	https://github.com/phnmnl/container-isatab-validator.git
isatab2json	David Johnson	Converter	Ready	https://github.com/phnmnl/container-isatab2json.git
iso2flux	Pablo Moreno, Pedro Atauri	MS; Fluxomics	Ready	https://github.com/phnmnl/docker-iso2flux
isodyn	Pablo Moreno, Vitaly Selivanov	MS; Fluxomics	Ready	https://github.com/phnmnl/docker-isodyn
json2isatab	David Johnson	Converter	Ready	https://github.com/phnmnl/container-json2isatab.git
jupyter	Marco Capuccini, Pablo Moreno	Runtime	Ready	
lcmsmatching	Pierrick Roger	MS	Ready	https://github.com/phnmnl/container-lcmsmatching.git
Luigi	Marco Capuccini, Pablo Moreno	Runtime	Ready	

metabolab	Michelle Thompson	NMR	Ready	
MetaboliteIDConverter	Benjamin Merlet	Converter	Ready	https://github.com/phnmnl/container-MetaboliteIDConverter.git
metabomatching	Rico Rueedi	NMR	Ready	https://github.com/phnmnl/container-metabomatching.git
metfrag-cli	Christoph Ruttkies	MS	Ready	https://github.com/phnmnl/container-metfrag-cli
metfrag-cli-batch	Christoph Ruttkies	MS	Ready	https://github.com/phnmnl/container-metfrag-cli-batch
metfrag-vis	Christoph Ruttkies	MS	Ready	https://github.com/phnmnl/container-metfrag-vis.git
midcor	Pablo Moreno, Vitaly Selivanov	MS; Fluxomics	Ready	https://github.com/phnmnl/docker-midcor
ms-vfetc	Michael van Vliet	MS	Ready	https://github.com/phnmnl/container-ms-vfetc
msnbase	Kristian Peters, Payam Emami	MS	Ready	
mtbl-labs-uploader	Pablo Moreno	Transfer	Ready	https://github.com/phnmnl/container-mtbl-labs-uploader.git
mtblisa	David Johnson, Pablo Moreno	Converter	Ready	https://github.com/phnmnl/container-mtblisa.git
mtbls-dwnld	Pierrick Roger	Transfer	Ready	https://github.com/phnmnl/container-mtbls-dwnld
mtbls-factors-viz	Pablo Moreno	Visualization	Ready	
Multivariate	Pierrick Roger	Statistics	Ready	https://github.com/phnmnl/container-multivariate
mw2isa	Phillipe Rocca-Serra	Converter	Ready	https://github.com/phnmnl/container-mw2isa
mzML2isa	Pablo Moreno, Thomas Lawson	Converter	Ready	https://github.com/phnmnl/container-mzml2isa.git
nmrML2BATMAN	Jianliang Gao	NMR	Ready	https://github.com/phnmnl/container-nmrML2BATMAN
nmrML2isa	Pablo Moreno, Thomas Lawson	Converter	Ready	
nmrmlconv	Kristian Peters	NMR	Ready	https://github.com/phnmnl/docker-nmrmlconv
normalization	Nils Paulhe, Pierrick Roger	Normalization	Ready	
openms	Christoph Ruttkies	MS	Ready	https://github.com/phnmnl/container-openms.git
papy	Jianliang Gao	Statistics	Ready	
passatutto			Ready	

pathwayEnrichment	Etiennee Camenem		Ready	
phenomenal-portal	Sijin He	Portal	Ready	
qualitymetrics	Nils Paulhe, Pierrick Roger	Quality Control	Ready	
ramid	Pablo Moreno, Vitaly Selivanov	MS; Fluxomics	Ready	https://github.com/phnmnl/container-ramid
rbase	Kristian Peters, Pablo Moreno	Statistics	Ready	https://github.com/phnmnl/container-rbase
rnmr1d	Kristian Peters	NMR	Ready	https://github.com/phnmnl/container-rnmr1d
scp-aspera	Pablo Moreno	Transfer	Ready	https://github.com/phnmnl/container-scp-aspera.git
speaq	Kristian Peters	NMR	Ready	https://github.com/phnmnl/container-speaq
tool-generic_filter	Nils Paulhe, Pierrick Roger	Filtering	Ready	
transformation	Pierrick Roger	STAT	Ready	https://github.com/phnmnl/container-transformation
Univariate	Pierrick Roger	STAT	Ready	https://github.com/phnmnl/container-univariate
xcms	Kristian Peters	MS	Ready	https://github.com/phnmnl/container-xcms
xcms-1.x	Kristian Peters	MS	Ready	https://github.com/phnmnl/container-xcms-1.x