

USMI Galaxy Demonstrator(UGD): a collection of tools to integrate microorganisms information



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Background

As a result of several heterogeneous repositories, which collect information on microorganisms, some web platforms gather microorganisms information and provide services to mBRCs in limited way. The USMI Galaxy Demonstrator(UGD), presented at Bioinformatics Italian Society (BITS) meeting in June 2015, support both researchers and mBRC staffs to perform bioinformatics pipelines in an automatic way, importing available microbial catalogues, enriching them with enzyme data, ribosomal RNA sequences and taxon IDs according to MIRRI' aims.

Scope

In this new version of UGD, we want to extend the integrative capabilities providing tools that are able to avoid manual, potentially long, searches on the web and to identify and select microorganisms of interest using metabolite, ligand, enzyme and protein names via new tools: *From alignment of proteins to microbial strain* and *Compound and enzyme*.

USMI Galaxy Demonstrator (UGD)

The USMI Galaxy Demonstrator is publicly available on-line at <http://bioinformatics.hsanmartino.it:8080>, Galaxy version 15.07. The developed tools are available in two sections, **Get microbial data** (box 1) and **Retrieval external information** (box 2), under the general label 'BASIC TOOLS FOR MIRRI'. The new tool **From alignment of proteins to microbial strain** integrates alignment of proteins with strain number, taxon ID, link to CABRI and related DBs by using data provided by blastp. **Compound and enzyme** retrieves strain number, link to CABRI, Compound/ligand accession number, EC number, name and synonyms by using a biological term. Galaxy allows to set up workflows to rerun, store and share both specific analyses and data. As shown in fig. 1, tools may be set in various ways in order to define own pipelines. Indeed, implementing basic tools as modular elements allows to make up several pipelines.

CABRI, Common access to biological resource and information, Network Services (<http://cabri.org>) offer access to 28 catalogues from European Biological Resources Centers (BRCs), since 2000.

MIRRI, Microbial Resource Research Infrastructure, is a pan-European distributed research infrastructure in its preparatory phase which aims to connect all European **mBRCs**, microBiological Resource Centres, with the aim of providing improved and extended services to the research and industry communities. **MIRRI** wants to reach the integration of information on microorganisms with further data that can be found and retrieved from a wide range of biological databases like NCBI, EMBL, BRENDA and UNIPROT.

Results

The most recently developed UGD tools, fig. 2, are able to identify which microorganisms that are related to a molecule or a protein of interest to the end user by integrating information both from mBRCs catalogues and from external data sources.

Running workflow "Taxonomy and INSDC"

Associate taxonIDs and 16s rRNA accession number to species name

Expand All Collapse

Step 1: Taxonomy (version 1.0.2)
1st step (part 1): Retrieves all taxonomy from NCBI and makes it available in text form

Step 2: Microbial INSDC rRNA (version 1.0.0)
1st step (part 2): Retrieves all accession numbers related to catalogue' acronym

Catalogue' Acronym

Type of output
Text

Step 3: TaxonID (version 1.0.1)
2nd step: retrieves the Taxon ID from NCBI

Select MCL file
22: Get Catalogues (BCCM_LMG)

Select taxonomy file
Output dataset 'out' from step 1

Step 4: INSDC rRNA (version 1.0.1)
3rd step: retrieves all small subunit (SSU) rRNA related to strains in a catalogue

Send results to a new history

Run workflow

Figure 1 An UGD workflow

Taxonomy retrieves all taxonomy information
Microbial INSDC rRNA retrieves information by using a Catalogue acronym
Upload file is a Galaxy' generic tool
Get Catalogues is a 'data_source' tool to import catalogues from external-web storage

box 1

TaxonID retrieves taxonomy ID for all strains
ECNumber gathers information when enzyme names are collected in Catalogue
Protein FASTA retrieves protein sequences by using protein accession number
INSDC rRNA retrieves rRNA accession number related to Strains in Catalogue
PMID and DOI retrieves Pubmed IDs and Digital Object Identifiers (DOIs) of given bibliographic references
FASTA from INSDC retrieves rRNA sequences by using accession number
Uniprot retrieves protein accession number by using all strains

box 2

Galaxy

1	2	3	4	5	6
ProteinAccession	ProteinDefinition	Identity	TaxonID	Taxon	Strain
WP_045394981.1	glutamate synthase [Enterobacter aerogenes]	100.00	548	Enterobacter aerogenes	n/a
WP_047067233.1	glutamate synthase [Enterobacter aerogenes]	99.93	548	Enterobacter aerogenes	n/a
WP_045377996.1	glutamate synthase [Enterobacter aerogenes]	99.93	548	Enterobacter aerogenes	n/a
WP_015369486.1	glutamate synthase [Enterobacter aerogenes]	99.79	548	Enterobacter aerogenes	n/a
WP_047047532.1	glutamate synthase [Enterobacter aerogenes]	99.93	548	Enterobacter aerogenes	n/a
WP_047061743.1	glutamate synthase [Enterobacter aerogenes]	99.72	548	Enterobacter aerogenes	n/a
WP_047038716.1	glutamate synthase [Enterobacter aerogenes]	99.86	548	Enterobacter aerogenes	n/a
WP_047080089.1	glutamate synthase [Enterobacter aerogenes]	99.72	548	Enterobacter aerogenes	n/a
WP_045359696.1	glutamate synthase [Enterobacter aerogenes]	99.72	548	Enterobacter aerogenes	n/a
WP_047062770.1	glutamate synthase [Enterobacter aerogenes]	99.72	548	Enterobacter aerogenes	n/a
WP_015703611.1	glutamate synthase subunit alpha [Enterobacter aerogenes]	99.79	548	Enterobacter aerogenes	n/a
WP_047466516.1	glutamate synthase [Enterobacter aerogenes]	99.72	548	Enterobacter aerogenes	n/a
KGB04685.1	Enterobacter aerogenes glutamate synthase [NADPH] large chain	99.72	548	Enterobacter aerogenes	EAX

Galaxy

UGD - List of strains
 EZF78209.1 - Trichophyton soudanense CBS 452.61
 TaxonID: 1215331
 Strain: CBS 452.61
 Catalogue(s): CBS_FIL
 Link: [http://cabri.org/CABRI/srs-bin/wgetz?-newId=-e-\[CBS_FIL:%27CBS%20452.61%27\]](http://cabri.org/CABRI/srs-bin/wgetz?-newId=-e-[CBS_FIL:%27CBS%20452.61%27])

EGD93143.1 - Trichophyton tonsurans CBS 112818
 TaxonID: 647933
 Strain: CBS 112818
 Catalogue(s): CBS_FIL
 Link: [http://cabri.org/CABRI/srs-bin/wgetz?-newId=-e-\[CBS_FIL:%27CBS%20112818%27\]](http://cabri.org/CABRI/srs-bin/wgetz?-newId=-e-[CBS_FIL:%27CBS%20112818%27])

Figure 2 The new tools provide a tabular format output (a) and an HTML format (b). Data are retrieved from BRENDA, kegg, NCBI, ENA and CABRI.

References

- The MIRRI Project: www.mirri.org
- The Galaxy project: <http://galaxyproject.org>
- Colobraro DP and Romano P. A Galaxy approach to integrate microbial data: the USMI Galaxy demonstrator. Proceedings of BITS 2015, 3-5 June, Milano. Guffanti A et al. (eds) (in press)

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