



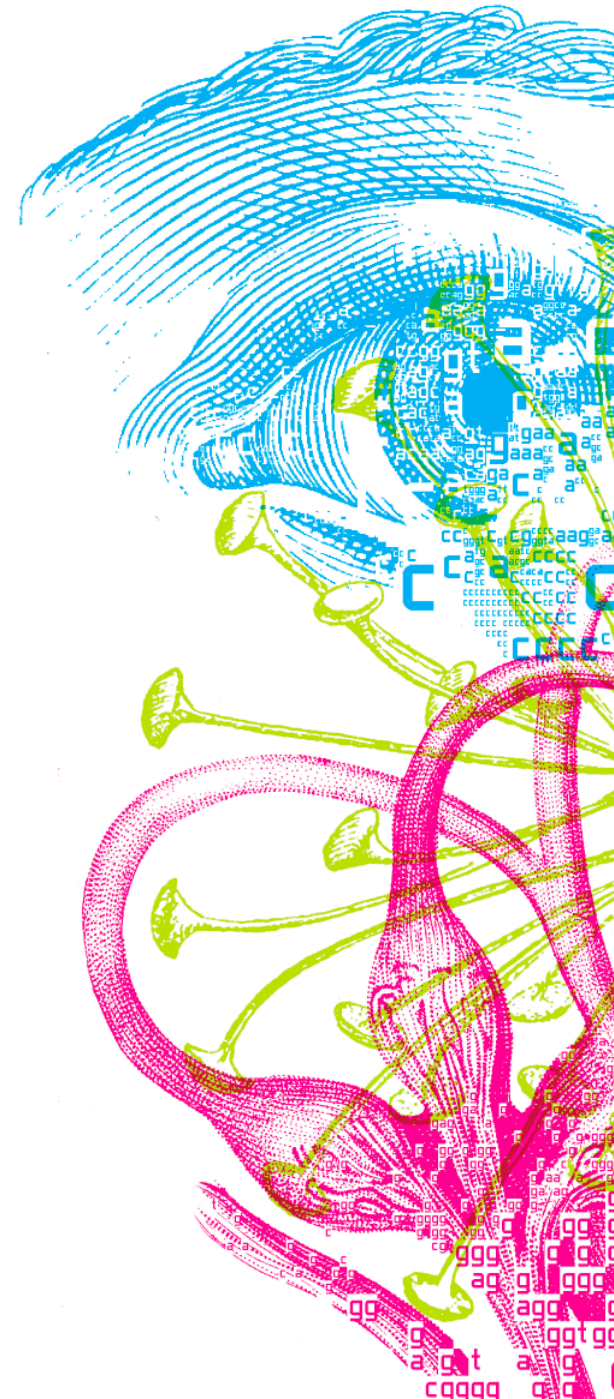
Netherlands
Bioinformatics
Centre

Workflows Accessibility in Bioinformatics

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Workflows / Pipelines

- Large data sets
 - e.g. NGS
- Data analysis
 - multiple steps
 - automation
 - flexibility
 - reusability
- User groups
 - biologists
 - bioinformaticians

Simple Task

- List all enzymes catalyzing reactions involving a given compound
- Services on the Internet provide this functionality
 - e.g. KEGG services
 - <http://www.genome.jp/kegg/>
- Scripts
- Galaxy
- Taverna
- Taverna-Galaxy
- Taverna-Web

Script/Program (1)

```
#!/usr/bin/env ruby

require 'soap/wsdlDriver'

wsdl = "http://soap.genome.jp/KEGG.wsdl"
kegg_service = SOAP::WSDLDriverFactory.new(wsdl).create_rpc_driver

enzyme_classifications = []

begin
  reactions = kegg_service.get_reactions_by_compound(ARGV[0])
rescue => err
  puts err.message
end

reactions.each do |reaction|
  begin
    enzyme_classifications << kegg_service.get_enzymes_by_reaction(reaction)
  rescue => err
    puts err.message
  end
end

enzyme_classifications.uniq.each { |ec| puts ec }
```

Script/Program (2)

```
$ ./simpleGetEnzymesFromCompoundWkf.rb C15973  
  
ec:2.3.1.12  
ec:2.3.1.61  
ec:2.3.1.61  
ec:2.3.1.168  
ec:2.3.1.168  
ec:2.3.1.168  
ec:1.8.1.4  
  
$
```

Script/Program (2)

```
$ ./simpleGetEnzymesFromCompoundWkf.rb C15973
```

```
ec:2.3.1.12
```

```
ec:2.3.1.61
```

```
ec:2.3.1.61
```

```
ec:2.3.1.168
```

```
ec:2.3.1.168
```

```
ec:2.3.1.168
```

```
ec:1.8.1.4
```

```
$
```

Who does what?



Workflows Accessibility in Bioinformatics



Multiple Scripts

superscript
is needed

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enzyme_classifications = []

begin
  reactions = kegg_service.get_reactions_by_compound(ARGV[0])
rescue => err
  puts err.message
end

reactions.each do |reaction|
  begin
    enzyme_classifications <<
    kegg_service.get_enzymes_by_reaction(reaction)
  rescue => err
    puts err.message
  end
end

enzyme_classifications.uniq.each { |ec| puts ec }
```

```
#!/usr/bin/env ruby

require 'soap/wsdlDriver'

wsdl = "http://soap.genome.jp/KEGG.wsdl"
kegg_service = SOAP::WSDLDriverFactory.new(wsdl).create_rpc_driver

genes = []

enzymes.each do |ec|
  begin
    enzyme_classifications << kegg_service.get_genes_by_enzymes(ec)
  rescue => err
    puts err.message
  end
end

genes.uniq.each { |gene| puts gene }
```

Multiple Scripts

superscript
is needed

```
#!/usr/bin/env ruby

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wsdl = "http://soap.genome.jp/KEGG.wsdl"
kegg_service = SOAP::WSDLDriverFactory.new(wsdl).create_rpc_driver

enzyme_classifications = []

begin
  reactions = kegg_service.get_reactions_by_compound(ARGV[0])
rescue => err
  puts err.message
end

reactions.each do |reaction|
  begin
    enzyme_classifications <<
    kegg_service.get_enzymes_by_reaction(reaction)
  rescue => err
    puts err.message
  end
end

enzyme_classifications.uniq.each { |ec| puts ec }
```

```
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wsdl = "http://soap.genome.jp/KEGG.wsdl"
kegg_service = SOAP::WSDLDriverFactory.new(wsdl).create_rpc_driver

genes = []

enzymes.each do |ec|
  begin
    enzyme_classifications << kegg_service.get_genes_by_enzymes(ec)
  rescue => err
    puts err.message
  end
end

genes.uniq.each { |gene| puts gene }
```

e.g. GAPSS pipeline

Multiple Scripts - Issues

- Difficult to manage
 - many scripts/programs
 - many arguments per script/program
 - many directories/files (scripts' I/Os)
- Difficult to reuse
 - due to low-level description
 - inconsistent program arguments

In Galaxy Web Portal (1)

The screenshot displays the Galaxy Web Portal interface in a Mozilla Firefox browser window. The browser's address bar shows the URL `http://localhost:8080/`. The Galaxy header includes navigation links: **Analyze Data**, **Workflow**, **Shared Data**, **Help**, and **User**.

Tools Panel (Left): A sidebar containing various tool categories. The 'Get enzyme classifications of a compound' tool is highlighted with a red dashed box and a red arrow pointing to it.

Main Tool Interface:

- Get enzyme classifications of a compound**
- Select source for compound_id:** A dropdown menu set to 'Type manually'.
- Enter compound_id:** A text input field containing 'C15973'.
- Would you also like the raw results as a zip file:** A dropdown menu set to 'No'.
- Execute** button.
- What it does:** A description stating: 'Given a compound we want to know all the reactions that it participates in so that we get all the enzymes that drive those reactions. It uses KEGG services.'
- Inputs:** A list item: **compound_id** The compound id (from KEGG). Examples include:
 - C15973
- Outputs:** A list item: **enzymeClassificationList** Enzyme classifications Examples include:
 - ec:2.3.1.168

History Panel (Right): A sidebar showing a message: 'Your history is empty. Click 'Get Data' on the left pane to start'.

In Galaxy Web Portal (1)

Galaxy - Mozilla Firefox

File Edit View History Bookmarks Tools Help

Galaxy

Analyze Data Workflow Shared Data Help User

Tools Options

manipulation

NGS: Mapping

NGS: Indel Analysis

NGS: RNA Analysis

NGS: SAM Tools

NGS: Peak Calling

NGS: Simulation

SNP/WGA: Data; Filters

SNP/WGA: QC; LD; Plots

SNP/WGA: Statistical Models

Human Genome Variation

VCF Tools

Taverna Workflows

EBI InterProScan for Taverna 2

Workflow1

Workflow2

BioAID ProteinDiscovery

Get enzyme classifications of a compound

Get enzyme classifications of a compound

Select source for compound_id:

Type manually

Enter compound_id:

C15973

Would you also like the raw results as a zip file:

No

Execute

What it does

Given a compound we want to know all the reactions that it participates in so that we get all the enzymes that drive those reactions. It uses KEGG services.

Inputs

- compound_id The compound id (from KEGG). Examples include:
 - C15973

Outputs

- enzymeClassificationList Enzyme classifications Examples include:
 - ec:2.3.1.168

History Options

Your history is empty. Click 'Get Data' on the left pane to start

In Galaxy Web Portal (1)

Galaxy - Mozilla Firefox

File Edit View History Bookmarks Tools Help

http://localhost:8080/

Galaxy

Analyze Data Workflow Shared Data Help User

Tools manipulation Options

NGS: Mapping

NGS: Indel Analysis

NGS: RNA Analysis

NGS: SAM Tools

NGS: Peak Calling

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Human Genome Variation

VCF Tools

Taverna Workflows

EBI InterProScan for Taverna 2

Workflow1

Workflow2

BioAID ProteinDiscovery

Get enzyme classifications of a compound

Get enzyme classifications of a compound

Select source for compound_id:

Type manually

Enter compound_id:

C15973

Would you also like the raw results as a zip file:

No

Execute

What it does

Given a compound we want to know all the reactions that it participates in so that we get all the enzymes that drive those reactions. It uses KEGG services.

Inputs

- compound_id The compound id (from KEGG). Examples include:
 - C15973

Outputs

- enzymeClassificationList Enzyme classifications Examples include:
 - ec:2.3.1.168

History Options

Your history is empty. Click 'Get Data' on the left pane to start

In Galaxy Web Portal (2)

Galaxy - Mozilla Firefox

File Edit View History Bookmarks Tools Help

MBIC BioAs... Spark Workflow: ... BullionVaul... Διαδικτυακ... Problem lo... Rich UI Wid... Outlook W... Firefox 4: e... Screencast... Galaxy-Tav... eGalaxy - el... Galaxy start_tcp_... myExperim...

http://localhost:8080/

Galaxy Analyze Data Workflow Shared Data Help User

Tools Options

manipulation

NGS: Mapping

NGS: Indel Analysis

NGS: RNA Analysis

NGS: SAM Tools

NGS: Peak Calling

NGS: Simulation

SNP/WGA: Data; Filters

SNP/WGA: QC; LD; Plots

SNP/WGA: Statistical Models

Human Genome Variation

VCF Tools

Taverna Workflows

- EBI InterProScan for Taverna 2
- Workflow1
- Workflow2
- BioAID ProteinDiscovery
- Get enzyme classifications of a compound

ec:2.3.1.12
ec:2.3.1.61
ec:2.3.1.61
ec:2.3.1.168
ec:2.3.1.168
ec:2.3.1.168
ec:1.8.1.4

History Options

4: enzymeClassificationList

In Galaxy Web Portal (3)

The screenshot displays the Galaxy Web Portal interface in a Mozilla Firefox browser window. The browser's address bar shows the URL: `http://localhost:8080/workflow/editor?id=f2db41e1fa331b3e`. The Galaxy header includes navigation links: **Analyze Data**, **Workflow** (selected), **Shared Data**, **Help**, and **User**.

Tools Panel (Left): A sidebar with a search bar and a list of tool categories: **Get Data**, **Send Data**, **ENCODE Tools**, **Lift-Over**, **Text Manipulation**, **Filter and Sort**, **Join, Subtract and Group**, **Convert Formats**, **Extract Features**, **Fetch Sequences**, **Fetch Alignments**, **Get Genomic Scores**, **Operate on Genomic Intervals**, **Statistics**, **Wavelet Analysis**, **Graph/Display Data**, **Regional Variation**, **Multiple regression**, **Multivariate Analysis**, **Evolution**, and **Motif Tools**.

Workflow Canvas (Center): Titled "Get enzyme classification of a compound", it shows a workflow with two steps: "Get enzyme classifications of a compound" and "Add column". The first step has inputs "enzymeClassificationList (tabular)" and "result_zip (zip)". A yellow arrow connects the output of the first step to the input of the second step. The second step has inputs "to Dataset" and "out_file1".

Details Panel (Right): Contains configuration options for the selected tool: "Get enzyme classifications of a compound". It includes a "Select source for compound_id:" dropdown set to "Type manually", an "Enter compound_id:" text field with the value "C15973", and a "Would you also like the raw results as a zip file?" dropdown set to "No". Below this is the "Edit Step Actions" section with a "Rename Dataset" dropdown set to "enzymeClassificationList" and a "Create" button. A note states: "Add actions to this step; actions are applied when this workflow step completes." The "Edit Step Attributes" section is also visible.

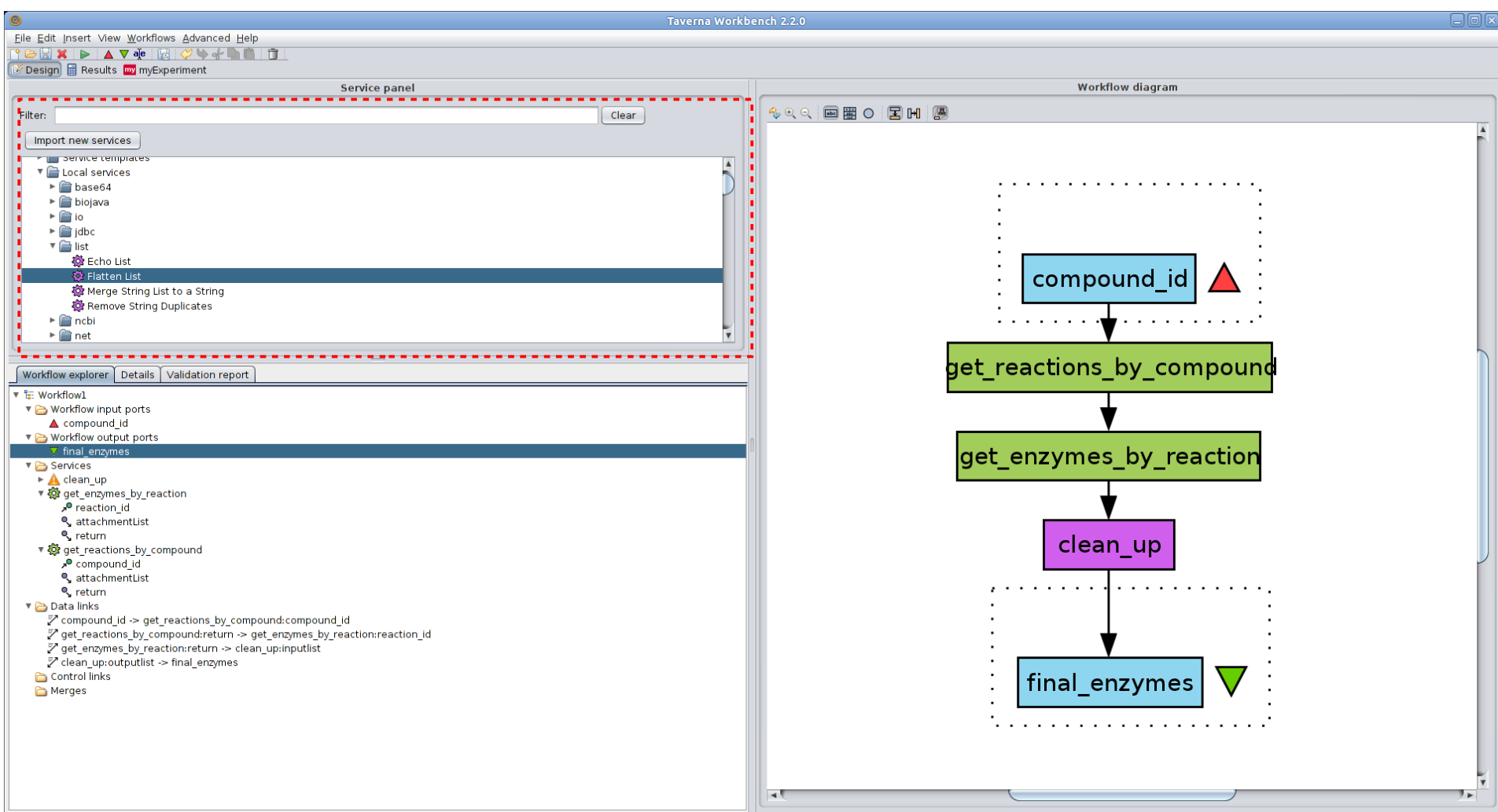
In Galaxy Web Portal (3)

The screenshot displays the Galaxy Web Portal interface in a Mozilla Firefox browser window. The address bar shows the URL: `http://localhost:8080/workflow/editor?id=f2db41e1fa331b3e`. The top navigation bar includes links for **Analyze Data**, **Workflow** (selected), **Shared Data**, **Help**, and **User**.

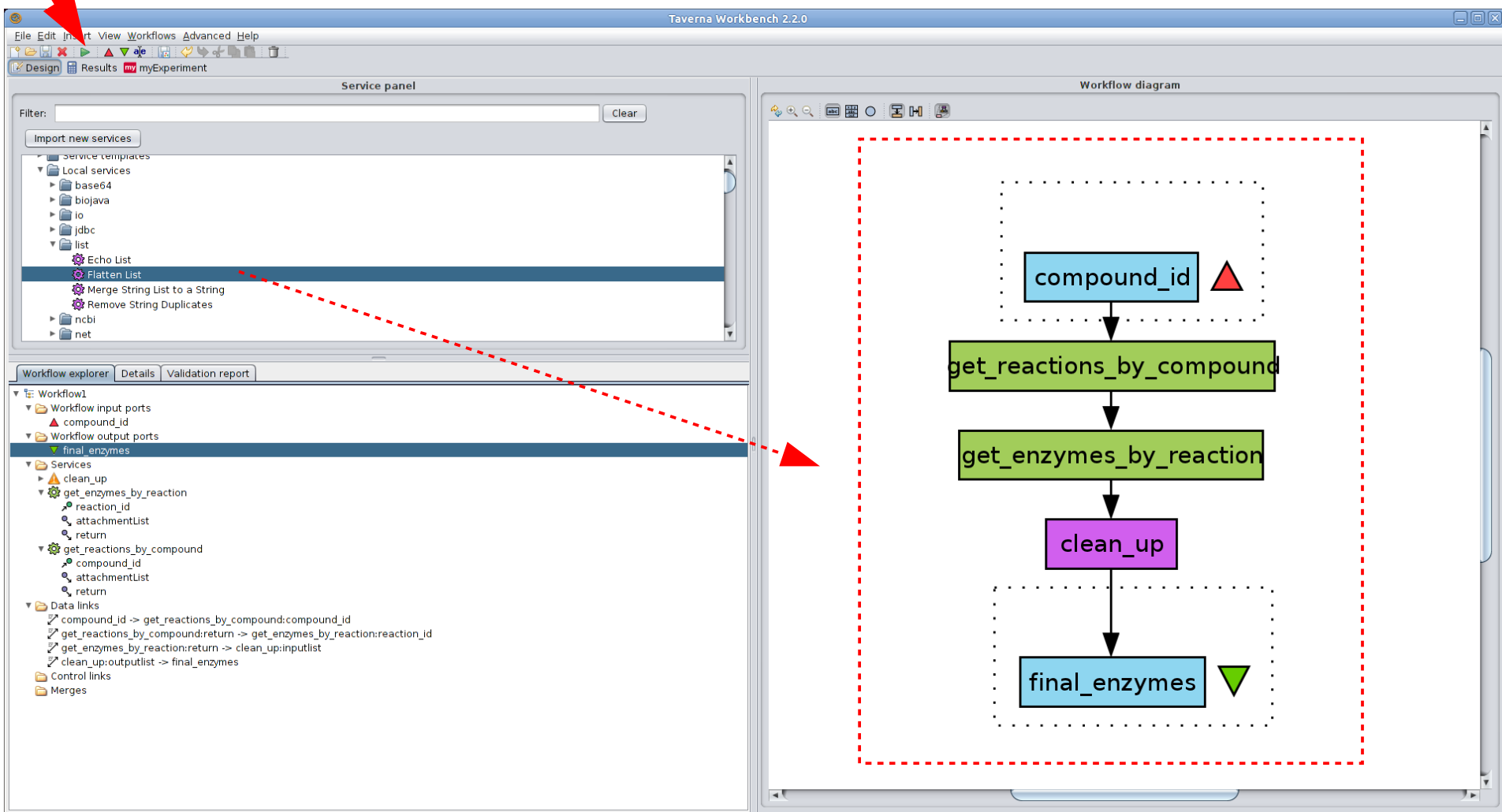
The main interface is divided into three panels:

- Tools Panel (Left):** A sidebar with a search bar and a list of tool categories including **Get Data**, **Send Data**, **ENCODE Tools**, **Lift-Over**, **Text Manipulation**, **Filter and Sort**, **Join, Subtract and Group**, **Convert Formats**, **Extract Features**, **Fetch Sequences**, **Fetch Alignments**, **Get Genomic Scores**, **Operate on Genomic Intervals**, **Statistics**, **Wavelet Analysis**, **Graph/Display Data**, **Regional Variation**, **Multiple regression**, **Multivariate Analysis**, **Evolution**, and **Motif Tools**.
- Workflow Canvas (Center):** Titled "Get enzyme classification of a compound", it shows a workflow with two steps:
 - Get enzyme classifications of a compound:** Inputs are `enzymeClassificationList (tabular)` and `result_zip (zip)`.
 - Add column:** Input is `to Dataset`, output is `out_file1`.A yellow box highlights the first step, and a line connects it to the second step.
- Details Panel (Right):** Contains configuration options for the selected tool:
 - Tool:** Get enzyme classifications of a compound
 - Select source for compound_id:** Type manually
 - Enter compound_id:** C15973
 - Would you also like the raw results as a zip file:** No
 - Edit Step Actions:** Includes a "Rename Dataset" dropdown set to `enzymeClassificationList` and a **Create** button.
 - Edit Step Attributes:** Includes an **Annotation / Notes** field.

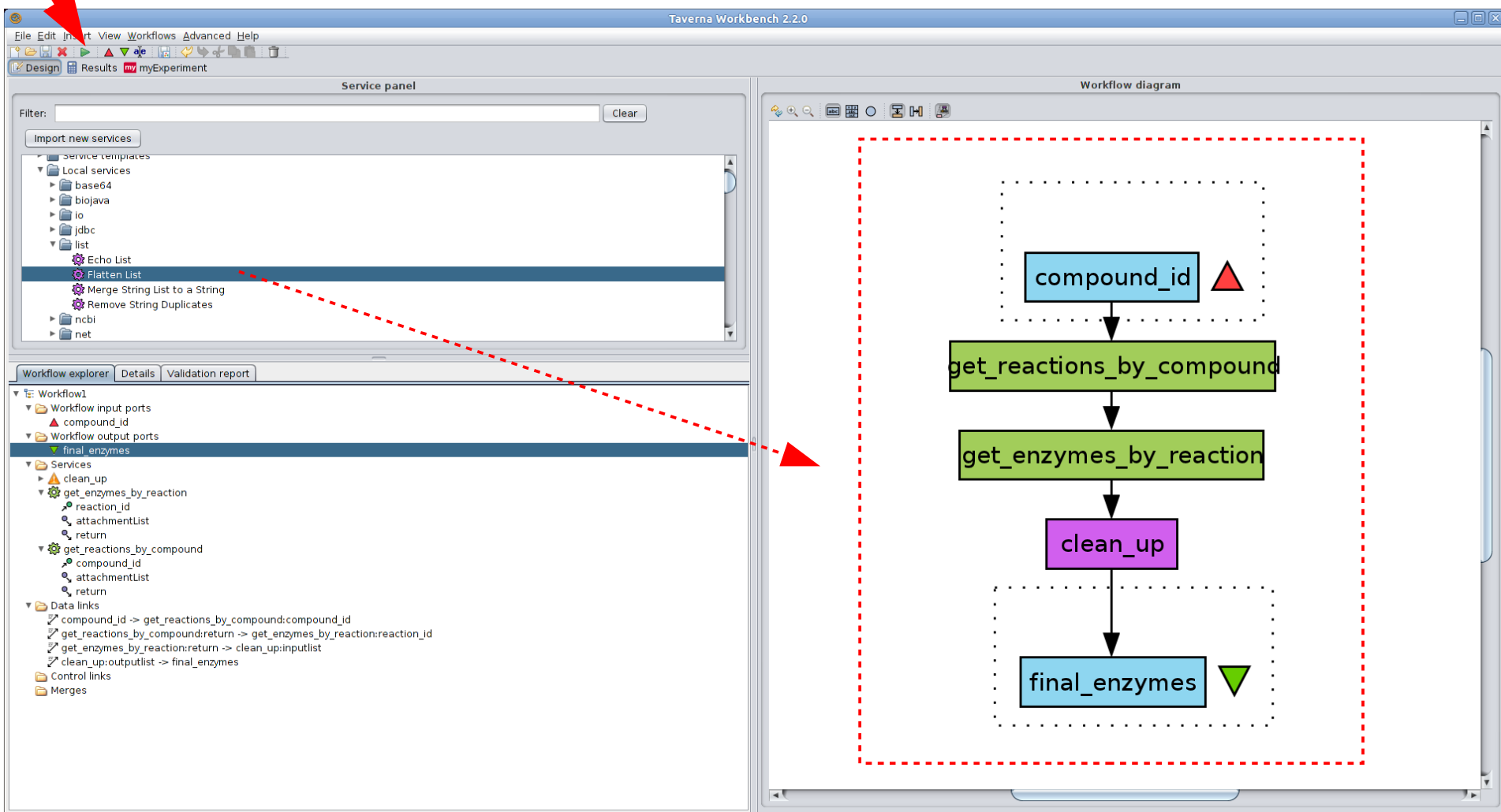
In Taverna Workbench (1)



In Taverna Workbench (2)



In Taverna Workbench (2)



In Taverna Workbench (3)

The screenshot displays the Taverna Workbench 2.2.0 interface. The top menu bar includes File, Edit, Insert, View, Workflows, and Advanced Help. Below the menu is a toolbar with icons for Design, Results, and myExperiment. The main workspace shows a workflow diagram with the following steps: `compound_id` (blue box with a red triangle), `get_reactions_by_compound` (grey box), `get_enzymes_by_reaction` (green box, highlighted with a red dashed border), `clean_up` (orange box), and `final_enzymes` (blue box with a green triangle). The left sidebar lists workflow runs with timestamps, and the bottom section shows workflow results for `compound_id` and `final_enzymes`.

Taverna Workbench 2.2.0

File Edit Insert View Workflows Advanced Help

Design Results myExperiment

Workflow runs Remove

Click on a run to see its values
Click on a service in the diagram
to see intermediate values (if available)

Workflow1 2011-10-06 12:28:51
Workflow1 2011-10-06 12:27:08
Workflow1 2011-10-06 12:25:11
Workflow1 2011-10-06 12:23:12
Workflow1 2011-10-06 12:21:35
Workflow1 2011-10-06 12:19:31
Workflow1 2011-10-06 12:12:56
Workflow1 2011-10-06 12:10:12
Workflow1 2011-10-06 12:09:12
Workflow1 2011-10-06 12:02:27
Workflow1 2011-10-06 11:58:22
Workflow1 2011-10-06 11:55:04
Workflow1 2011-10-06 11:50:15
Workflow1 2011-10-06 11:49:11
Workflow1 2011-10-06 11:46:08
Workflow1 2011-10-06 11:38:57

Graph Progress report

compound_id
get_reactions_by_compound
get_enzymes_by_reaction
clean_up
final_enzymes

Running Pause Cancel

Refresh intermediate values Show workflow results

Save all values

Workflow results

compound_id final_enzymes

Click in tree to view values

Value type Refresh

Save value

In Taverna Workbench (4)

The screenshot displays the Taverna Workbench 2.2.0 interface. The top menu bar includes File, Edit, Insert, View, Workflows, and Advanced Help. Below the menu is a toolbar with icons for Design, Results, and myExperiment. The main workspace shows a workflow diagram with the following steps: `compound_id` (input), `get_reactions_by_compound`, `get_enzymes_by_reaction`, `clean_up`, and `final_enzymes` (output). The workflow is enclosed in a dashed box. The left sidebar lists workflow runs with timestamps, and the bottom panel shows the results for the `final_enzymes` output, displaying a list of EC numbers: `ec:2.3.1.12`, `ec:2.3.1.61`, `ec:2.3.1.61`, `ec:2.3.1.168`, `ec:2.3.1.168`, `ec:2.3.1.168`, and `ec:1.8.1.4`.

Taverna Workbench 2.2.0

File Edit Insert View Workflows Advanced Help

Design Results myExperiment

Workflow runs Remove

Click on a run to see its values
Click on a service in the diagram
to see intermediate values (if available)

Workflow1 2011-10-06 12:27:08
Workflow1 2011-10-06 12:25:11
Workflow1 2011-10-06 12:23:12
Workflow1 2011-10-06 12:21:35
Workflow1 2011-10-06 12:19:31
Workflow1 2011-10-06 12:12:56
Workflow1 2011-10-06 12:10:12
Workflow1 2011-10-06 12:09:12
Workflow1 2011-10-06 12:02:27
Workflow1 2011-10-06 11:58:22
Workflow1 2011-10-06 11:55:04
Workflow1 2011-10-06 11:50:15
Workflow1 2011-10-06 11:49:11
Workflow1 2011-10-06 11:46:08
Workflow1 2011-10-06 11:38:57

Graph Progress report

compound_id
get_reactions_by_compound
get_enzymes_by_reaction
clean_up
final_enzymes

Refresh intermediate values Show workflow results

Finished Pause Cancel

Workflow results

compound_id final_enzymes

Click in tree to view values

Value type Text Refresh

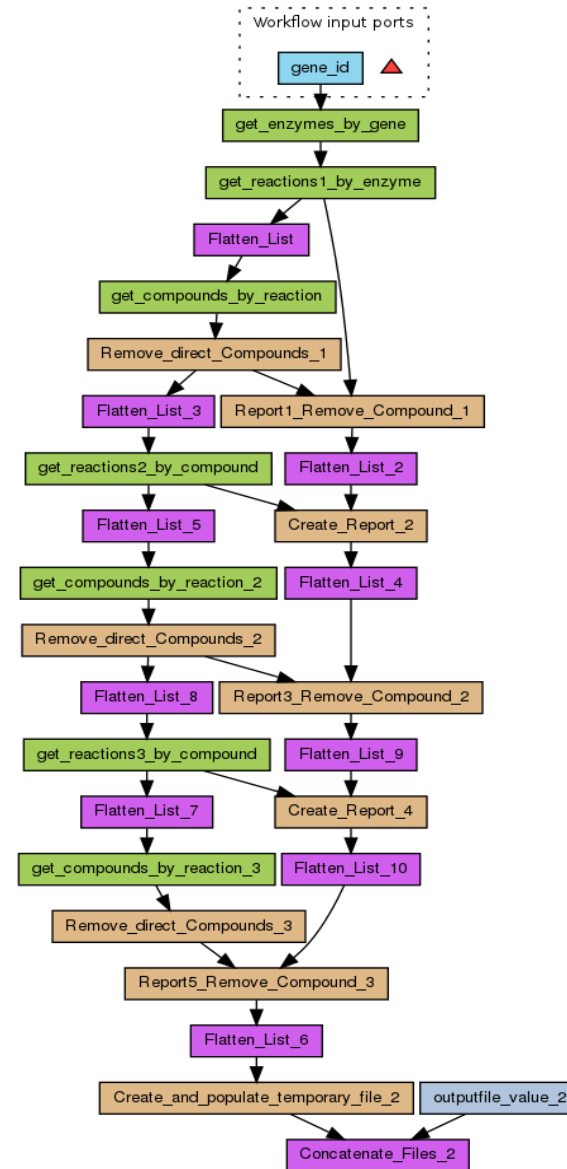
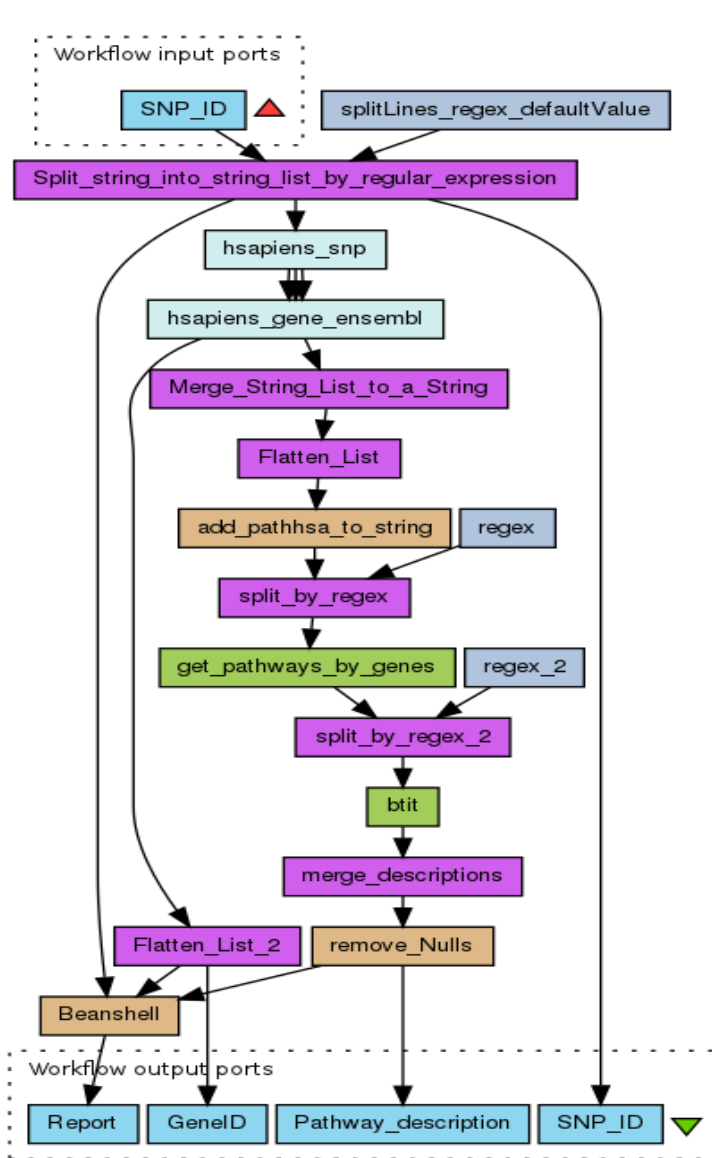
Value 1

ec:2.3.1.12
ec:2.3.1.61
ec:2.3.1.61
ec:2.3.1.168
ec:2.3.1.168
ec:2.3.1.168
ec:1.8.1.4

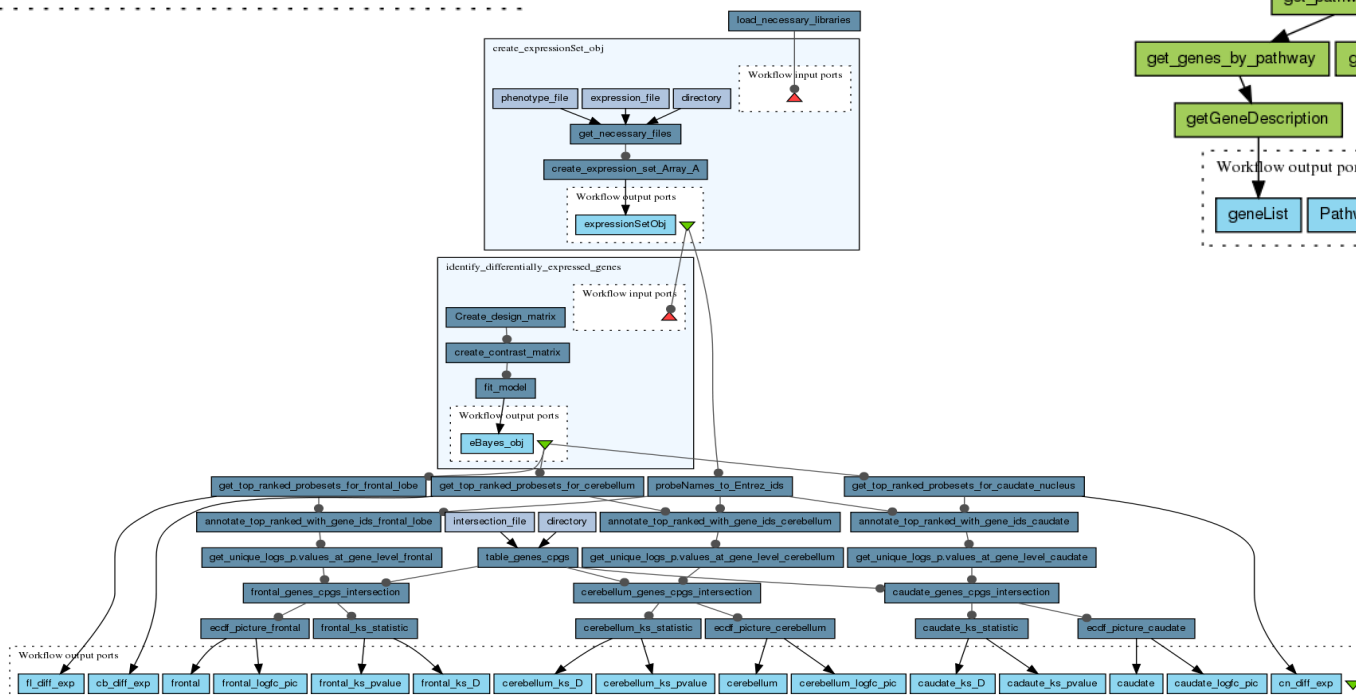
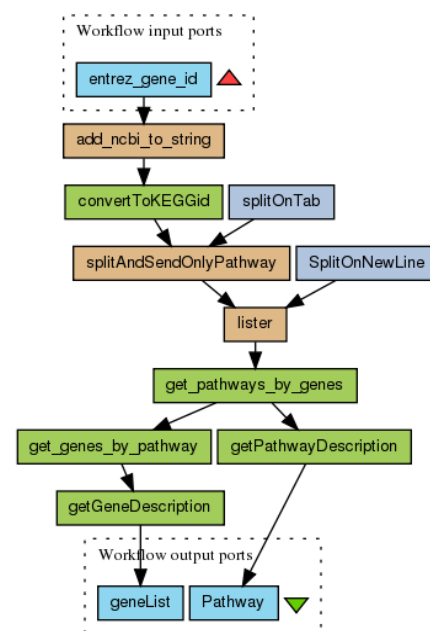
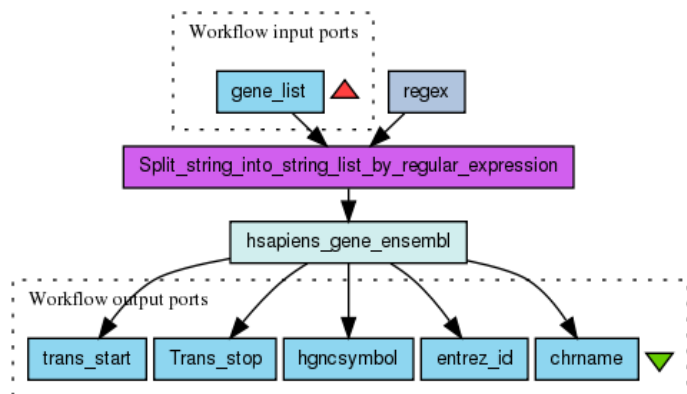
Save all values

Save value

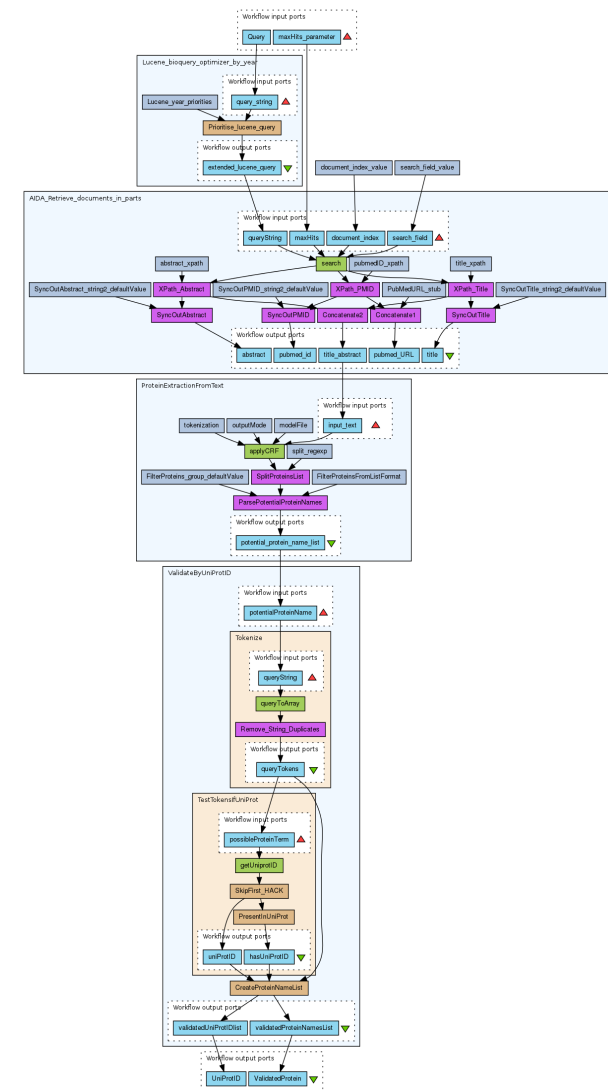
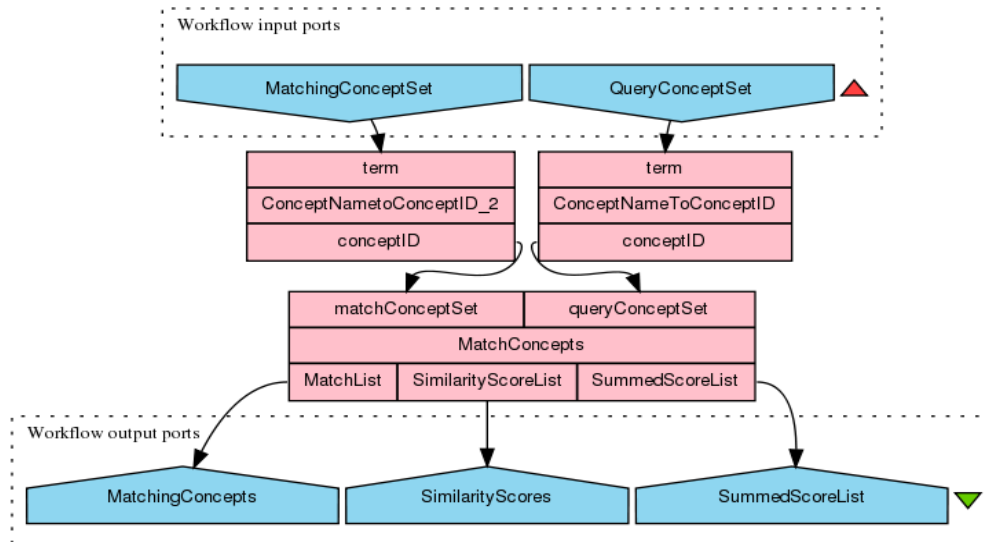
Harish's Workflows (GWAS: Metabolic Syndrome)



Eleni's Workflows (Huntington's Disease)



Marco's workflows (Semantic Text Mining)



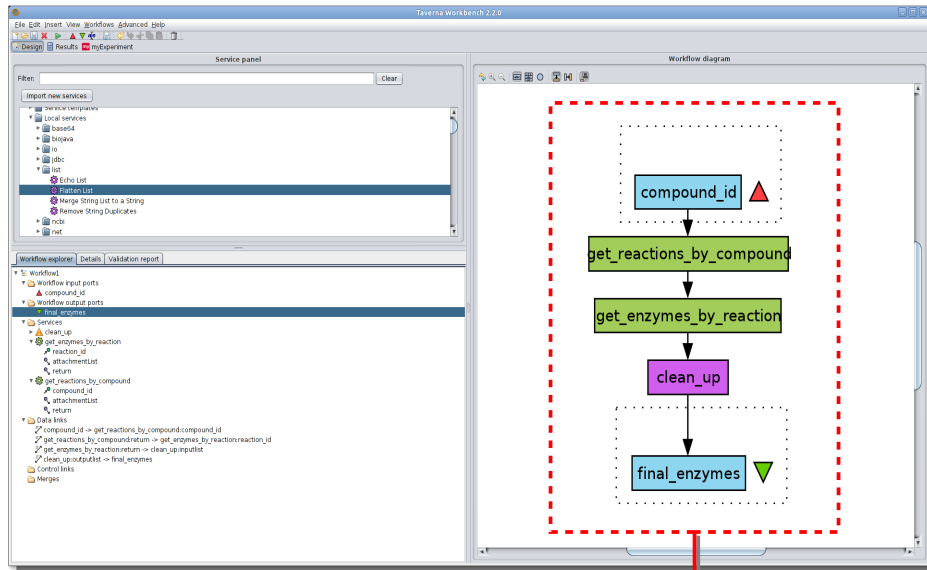
Taverna and Galaxy workflows

- The systems have a different focus
 - Some overlapping functionality but different strengths
 - Different fan clubs!

Galaxy	Taverna
straightforward workflows	very expressive workflows
exposing existing scripts	exposing existing web services
typically local tools	typically remote tools

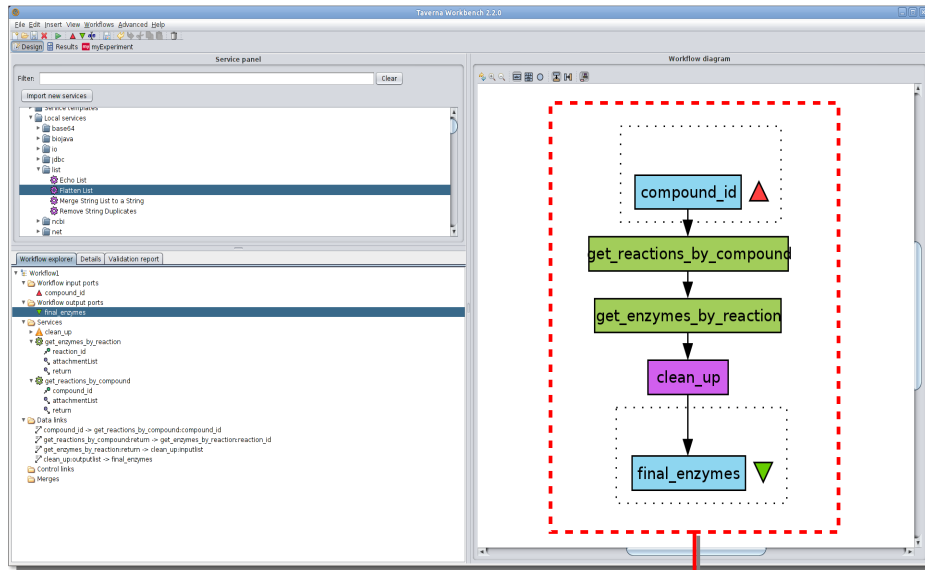
- Do we have to make a choice?
- Does that limit our potential users?
- How to make them more interoperable?

Taverna Workflows in Galaxy (1)



The screenshot shows the Galaxy web interface. The 'Tools' panel on the left lists various tools, with 'Taverna Workflows' highlighted. The main panel displays the 'Get enzyme classifications of a compound' tool. The tool has a 'Select source for compound_id:' dropdown set to 'Type manually', an 'Enter compound_id:' text box containing 'C15973', and a 'Would you also like the raw results as a zip file?' checkbox set to 'No'. The 'Execute' button is visible. The 'Outputs' section shows the output as 'enzymeClassificationList' with an example value 'ec:2.3.1.168'. The 'History' panel on the right shows a message: 'Your history is empty. Click "Get Data" on the left pane to start.'

Taverna Workflows in Galaxy (1)



Galaxy

Tools manipulation

- NGS: Mapping
- NGS: Indel Analysis
- NGS: RNA Analysis
- NGS: SAM Tools
- NGS: Peak Calling
- NGS: Simulation
- SNP/WGA: Data; Filters
- SNP/WGA: QC; LD; Plots
- SNP/WGA: Statistical Models
- Human Genome Variation
- VCF Tools
- Taverna Workflows**
 - EBI_InterProScan for Taverna 2
 - Workflow1
 - Workflow2
 - BioAID_ProteinDiscovery
 - Get enzyme classifications of a compound**

Get enzyme classifications of a compound

Select source for compound_id:

Type manually

Enter compound_id:

C15973

Would you also like the raw results as a zip file:

No

Execute

What it does

Given a compound we want to know all the reactions that it participates in so that we get all the enzymes that drive those reactions. It uses KEGG services.

Inputs

- compound_id The compound id (from KEGG). Examples include:
 - C15973

Outputs

- enzymeClassificationList Enzyme classifications Examples include:
 - ec:2.3.1.168

History

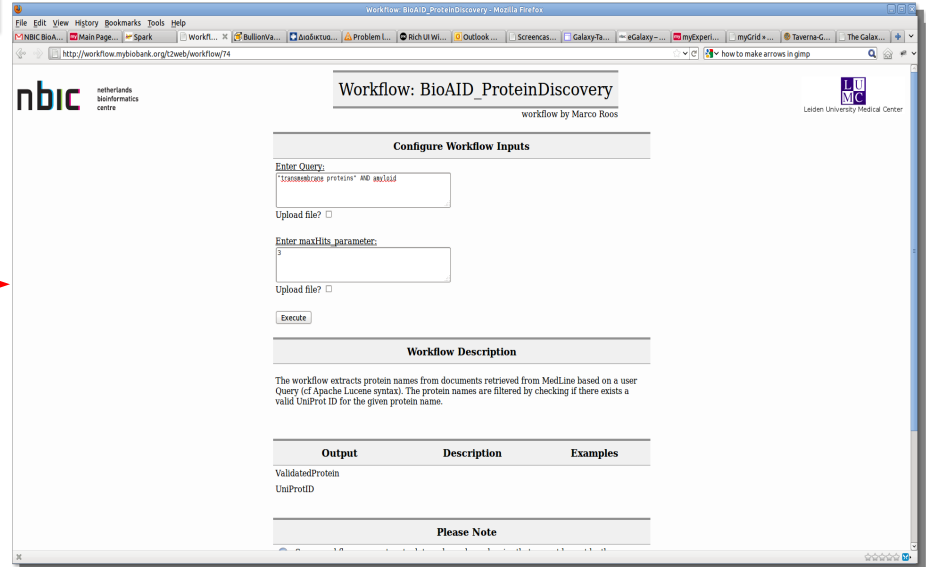
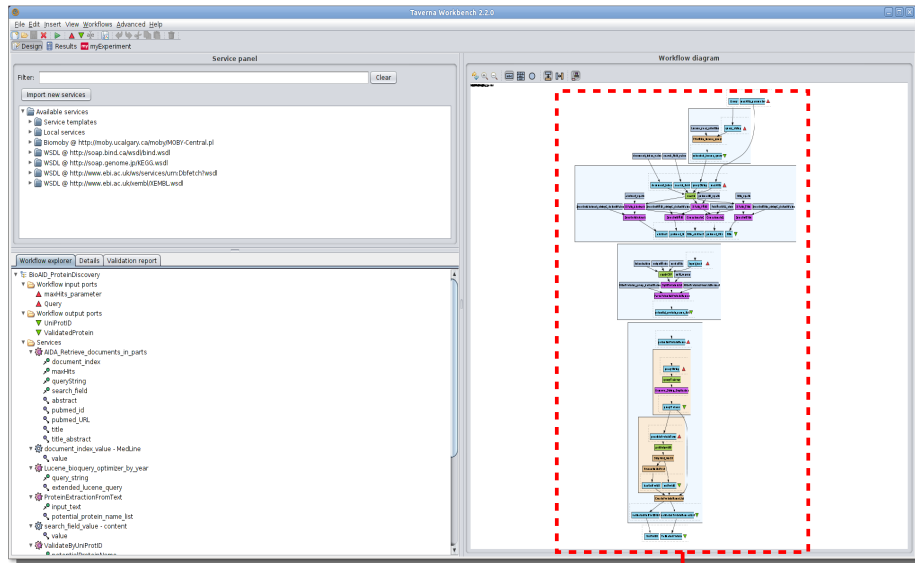
Your history is empty. Click 'Get Data' on the left pane to start

Who does what?

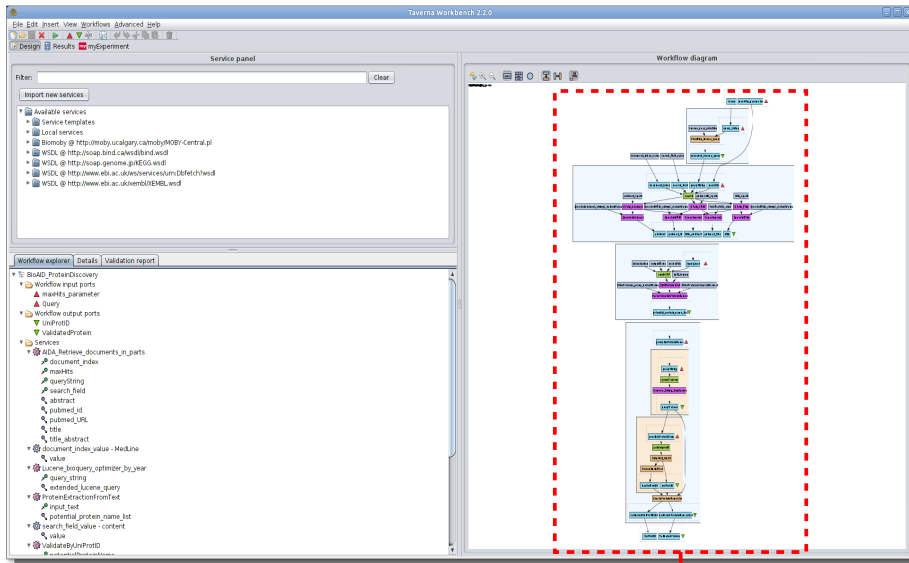
Taverna Workflows in Galaxy (2)

The screenshot displays the Galaxy web interface in a Mozilla Firefox browser window. The address bar shows the URL `http://localhost:8080/`. The interface includes a top navigation bar with links for **Analyze Data**, **Workflow**, **Shared Data**, **Help**, and **User**. On the left, a sidebar lists various tool categories under the heading **Tools**, including **manipulation**, **NGS: Mapping**, **NGS: Indel Analysis**, **NGS: RNA Analysis**, **NGS: SAM Tools**, **NGS: Peak Calling**, **NGS: Simulation**, **SNP/WGA: Data; Filters**, **SNP/WGA: QC; LD; Plots**, **SNP/WGA: Statistical Models**, **Human Genome Variation**, **VCF Tools**, and **Taverna Workflows**. The **Taverna Workflows** section is expanded, showing a list of workflows: **EBI InterProScan for Taverna 2**, **Workflow1**, **Workflow2**, **BioAID ProteinDiscovery**, and **Get enzyme classifications of a compound**. The main workspace area displays a list of workflow steps: `ec:2.3.1.12`, `ec:2.3.1.61`, `ec:2.3.1.61`, `ec:2.3.1.168`, `ec:2.3.1.168`, `ec:2.3.1.168`, and `ec:1.8.1.4`. On the right, a **History** panel shows a list of workflow instances. The instance **4: final_enzymes** is highlighted with a red dashed border, indicating it is the current selection. The **History** panel also includes an **Options** dropdown menu.

Taverna Workflows on a Web Browser (1)



Taverna Workflows on a Web Browser (1)



The screenshot shows the Taverna web interface for the 'Workflow: BioAID_ProteinDiscovery' workflow. The interface includes a 'Configure Workflow Inputs' section with fields for 'Enter Query' and 'Enter maxHits parameter'. Below this is the 'Workflow Description' section, which provides a brief overview of the workflow's purpose. At the bottom, there is a table with columns for 'Output', 'Description', and 'Examples'.

Output	Description	Examples
ValidatedProtein		
UniProtID		

Who does what?



Workflows Accessibility in Bioinformatics

Taverna Workflows on a Web Browser (2)

The screenshot shows a Mozilla Firefox browser window with the address bar displaying <http://workflow.mybiobank.org/t2web/workflow/74>. The page title is "Workflow: BioAID_ProteinDiscovery" by Marco Roos. The left sidebar features the nbic logo and the text "netherlands bioinformatics centre". The top right corner shows the Leiden University Medical Center logo.

The main content area is divided into sections:

- Configure Workflow Inputs**: Contains two input fields. The first, labeled "Enter Query:", contains the text `"transmembrane proteins" AND amyloid`. The second, labeled "Enter maxHits parameter:", contains the value `3`. Both fields have an "Upload file?" checkbox. Below these is an "Execute" button, which is highlighted by a red arrow.
- Workflow Description**: Contains a paragraph: "The workflow extracts protein names from documents retrieved from MedLine based on a user Query (cf Apache Lucene syntax). The protein names are filtered by checking if there exists a valid UniProt ID for the given protein name."
- Output**: A table with three columns: "Output", "Description", and "Examples". The "Output" column lists "ValidatedProtein" and "UniProtID".
- Please Note**: A section at the bottom of the page.

Taverna Workflows on a Web Browser (3)

The screenshot shows a Mozilla Firefox browser window with the address bar displaying <http://workflow.mybiobank.org/t2web/enact>. The page title is "Workflow: BioAID_ProteinDiscovery" and it is credited to "workflow by Marco Roos". The page features the nbic logo (Netherlands Bioinformatics Centre) and the Leiden University Medical Center logo. On the left side, there are two tabs: "ValidatedProtein" and "UniProtID", with the latter highlighted by a red dashed box. The main content area displays a list of protein accession numbers: P70386, Q02527, Q09327, Q10470, Q14CK5, Q61C49, Q9UH32, P70386, Q02527, Q09327, Q10470, Q14CK5, Q61C49, Q9UH32, P70386, Q02527, Q09327, Q10470, Q14CK5, Q61C49, Q9UH32, P70386, Q02527, Q09327, Q10470, Q14CK5, Q61C49, Q9UH32, A8K7C2, O73815, P02571, P02579, P12714, P14104, P53478, P60010, P63259, P63260, P63261, and P60010. A status bar at the bottom indicates "Transferring data from workflow.mybiobank.org...".

Summary

- Workflow example using several approaches
- Taverna workflows can be accessed in Galaxy
 - Bioinformatician *creates/finds* appropriate workflow
 - He uses Taverna-Galaxy to create new tool and installs it
 - ... biologist will see the new tool in the Galaxy server
 - The taverna workflow can now take part in a Galaxy workflow
- Taverna workflows can be accessed via the web
 - Bioinformatician *creates/finds* appropriate workflow
 - ... sends the URL to biologist

- More information

- <http://galaxy.psu.edu/>
- <http://www.taverna.org.uk/>
- <https://trac.nbic.nl/elabfactory/wiki/eGalaxy>

- Questions?

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