Portals and workflows:
Taverna Workbench

Paolo Romano
National Cancer Research Institute, Genova
(paolo.romano@istge.it)

Summary

- Information and data integration in biology
- Web Services and workflow management
- Taverna Workbench
- A workflow enactment portal

Information in biology: well known facts

- Biomedical research produces an increasing quantity of new data and new data types
  - EMBL size: ver 82 7,3% more vs ver 81 (3 months), 112,9% vs ver 74 (24 months)
- Emerging domains, like mutation and variation analysy, polymorphisms, metabolism, as well as new technologies, e.g., microarrays, will contribute with even huger amounts of data
- Analysis softwares must interoperate with databases
  - Databases as input for softwares
  - Results as new data to record and analyze

Heterogeneicity of databanks

- A few dbs are managed in an almost homogenous way (e.g., sequences at EBI, NCBI, DDBJ)
- Secondary databases are of high quality (good and extended annotation, quality control)
- Many databases are highly specialized, e.g. by gene, organism, disease, mutation, etc…
- Many databanks are created by small groups or by single researchers
- Databanks are distributed:
  - Different DBMS, data structures, query methods
  - Different information, semantics

Goals of the integration

In this context, data integration and work automation are needed to:

- Carry out analysis and/or searches involving more databases and softwares automatically
- Perform analysis involving large data sets effectively

- Achieve a better and wider view of all available information
- Carry out a real data mining

Data integration longevity

- Integration needs stability
  - Standardization……
  - Good domain knowledge
  - Well defined data
  - Well defined goals
- Integration fears:
  - Heterogeneicity of data and systems
  - Uncertain domain knowledge
  - Fast evolution of data
  - Highly specialized data
  - Lacking of predefined, clear goals
  - Originality, experimentalism (“*let me see if this works”*)

Integration of biological information

In biology:

- A pre-analysis and reorganization of the data is very difficult, because data and related knowledge change very quickly
- Complexity of information makes it difficult to design data models which can be valid for different domains and over time
- Goals and needs of researchers evolve very quickly according to new theories and discoveries

Integration must therefore be carried out by using flexible systems that are easy to adapt and to extend

Integration methods

From syntactical to semantical links:

- Explicit (reciprocal) links (xrefs)
- Implicit links (e.g., names)
- Common contents (vocabularies)
- Shared data models and schemas
- Common Semantics (ontologies)

Web Services in brief

- XML based network services
- Implement standard transport protocols (SOAP, HTTP)
- Standards also available for retrieval and identification (UDDI), description (WSDL) and composition (WSFL)
- Allow software applications to access data “intelligently”: identification of contents, interpretation of semantics information
- Metadata needed
- Web Services already implemented by many Institutes and service centers

Workflow management

"**A computerized facilitation or automation of a business process, in whole or part**". (Workflow Management Coalition)

Main goal is:

- the implementation of data analysis processes in standardized environments

Main advantages relate to:

- **effectiveness**: being an automatic procedure, it frees bio-scientists from repetitive interactions with the web and it supports good practice,
- **reproducibility**: analysis can be replicated over time,
- **reusability**: intermediate results can be reused,
- **traceability**: the workflow is carried out in a transparent analysis environment where data provenance can be checked and/or controlled.

Workflow management software

Workflow management software for bioinformatics applications:

- Biopipe, an add-on to bioperl
- GPipe, an extension of the Pise interface
- Taverna (EBI), a component of the myGrid platform
- Wildfire (Bioinformatics Institute, Singapore)
- Pipeline Pilot (SciTegic)
- BioWBI, Bioinformatic Workflow Builder Interface, from IBM

They all require knowledge of the systems and skills and time for development of the workflows.

Workflow management: Taverna

Taverna Workbench

- builds complex analysis workflows
- is able to access both remote and local processors
- defines alternative processors
- runs workflows
- visualizes the results

It includes a an ontology for bioinformatics data

Requirements: java, Windows or Linux
Open source: http://taverna.sourceforge.net/
Current version: 1.3.1 (stable, next version 2.0)

Taverna: GUI

Graphical user interface (GUI) including:

- Advanced Model Explorer (AME)
- Workflow diagram
- Available services
- Run workflow
- Enactor invocation

Options: default services, workflow editor, debug
Extra features: FETA search engine

Taverna: available processors (services)

WSDL services
- Web Service Description Language (WSDL) file: adds WSDL based service nodes

Soaplab servers
- Soaplab server: adds a list of soaplab provided services

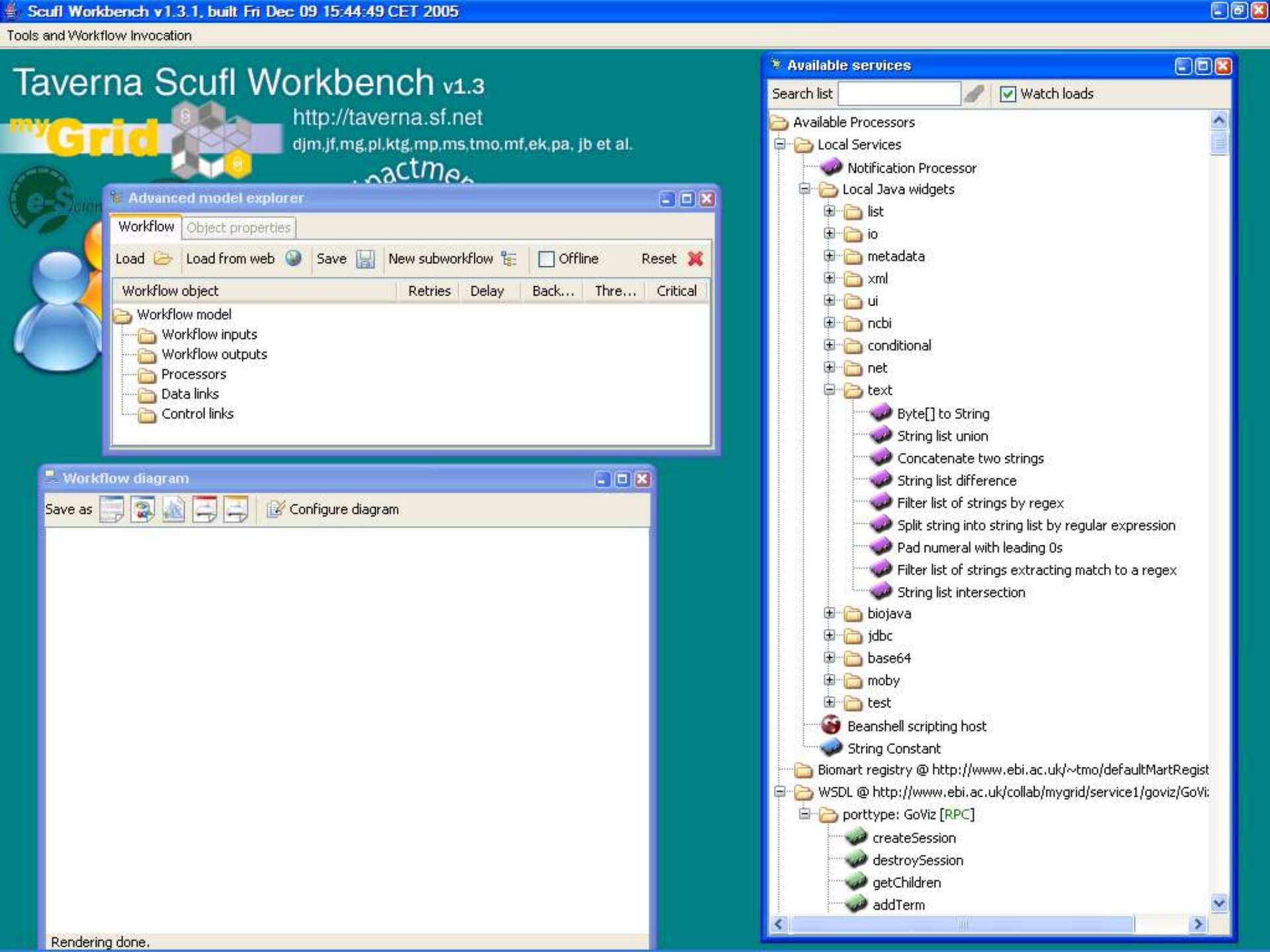
BioMOBY registries
- Moby Central repository: determines hosts and their services

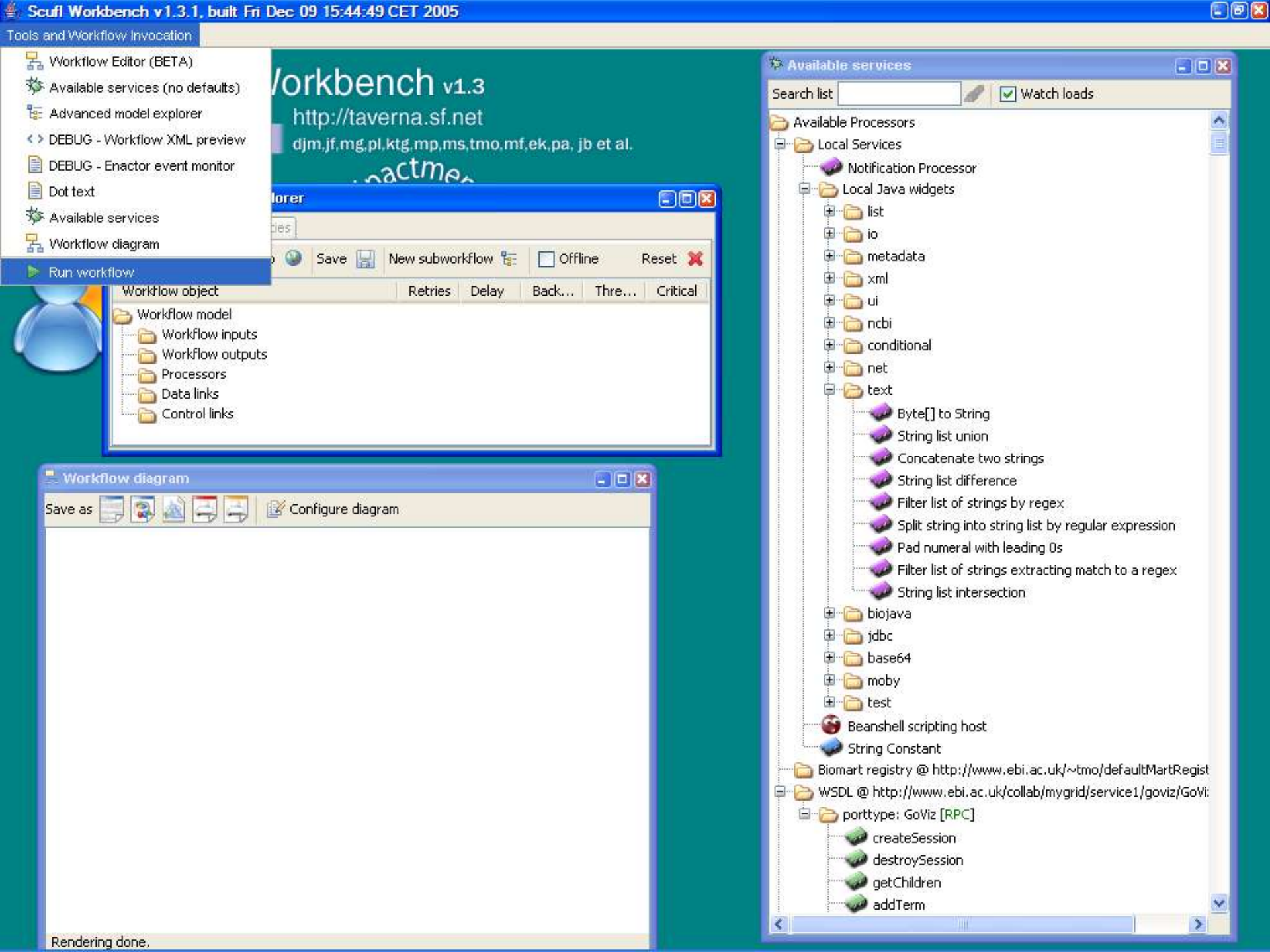
Workflows
- XScufl definition file: either adds the workflow as a sub-workflow or imports processors

Biomart databases
- Biomart data warehouse: allows for searching all available data sets

Local processors
- Simple list/string processors, r/w, extra special remote links, constant values, beanshell scripts

Other processors
- Styx, Talisman, Seqhound, API Consumer


Scufl Workbench v1.3.1, built Fri Dec 09 15:44:49 CET 2005
Tools and Workflow Invocation
Taverna Scufl Workbench v1.3
myGrid
http://taverna.sf.net
djm,jf,mg,pl,ktg,mp,ms,tmo,mf,ek,pa, jb et al.
Advanced model explorer
Workflow
Object properties
Load
Load from web
Save
New subworkflow
Offline
Reset
Workflow object
Retries
Delay
Back...
Thre...
Critical
Workflow model
Workflow inputs
Workflow outputs
Processors
Data links
Control links
Workflow diagram
Save as
Configure diagram
Rendering done.
Available services
Search list
Watch loads
Available Processors
Local Services
Notification Processor
Local Java widgets
list
io
metadata
xml
ui
ncbi
conditional
net
text
Byte[] to String
String list union
Concatenate two strings
String list difference
Filter list of strings by regex
Split string into string list by regular expression
Pad numeral with leading 0s
Filter list of strings extracting match to a regex
String list intersection
biojava
jdbc
base64
moby
test
Beanshell scripting host
String Constant
Biomart registry @ http://www.ebi.ac.uk/~tmo/defaultMartRegist
WSDL @ http://www.ebi.ac.uk/collab/mygrid/service1/goviz/GoVi
porttype: GoViz [RPC]
createSession
destroySession
getChildren
addTerm


Scufl Workbench v1.3.1, built Fri Dec 09 15:44:49 CET 2005
Tools and Workflow Invocation
Workflow Editor (BETA)
Available services (no defaults)
Advanced model explorer
DEBUG - Workflow XML preview
DEBUG - Enactor event monitor
Dot text
Available services
Workflow diagram
Run workflow
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http://taverna.sf.net
djm,jf,mg,pl,ktg,mp,ms,tmo,mf,ek,pa, jb et al.
Save
New subworkflow
Offline
Reset
Workflow object
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String list union
Concatenate two strings
String list difference
Filter list of strings by regex
Split string into string list by regular expression
Pad numeral with leading 0s
Filter list of strings extracting match to a regex
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biojava
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moby
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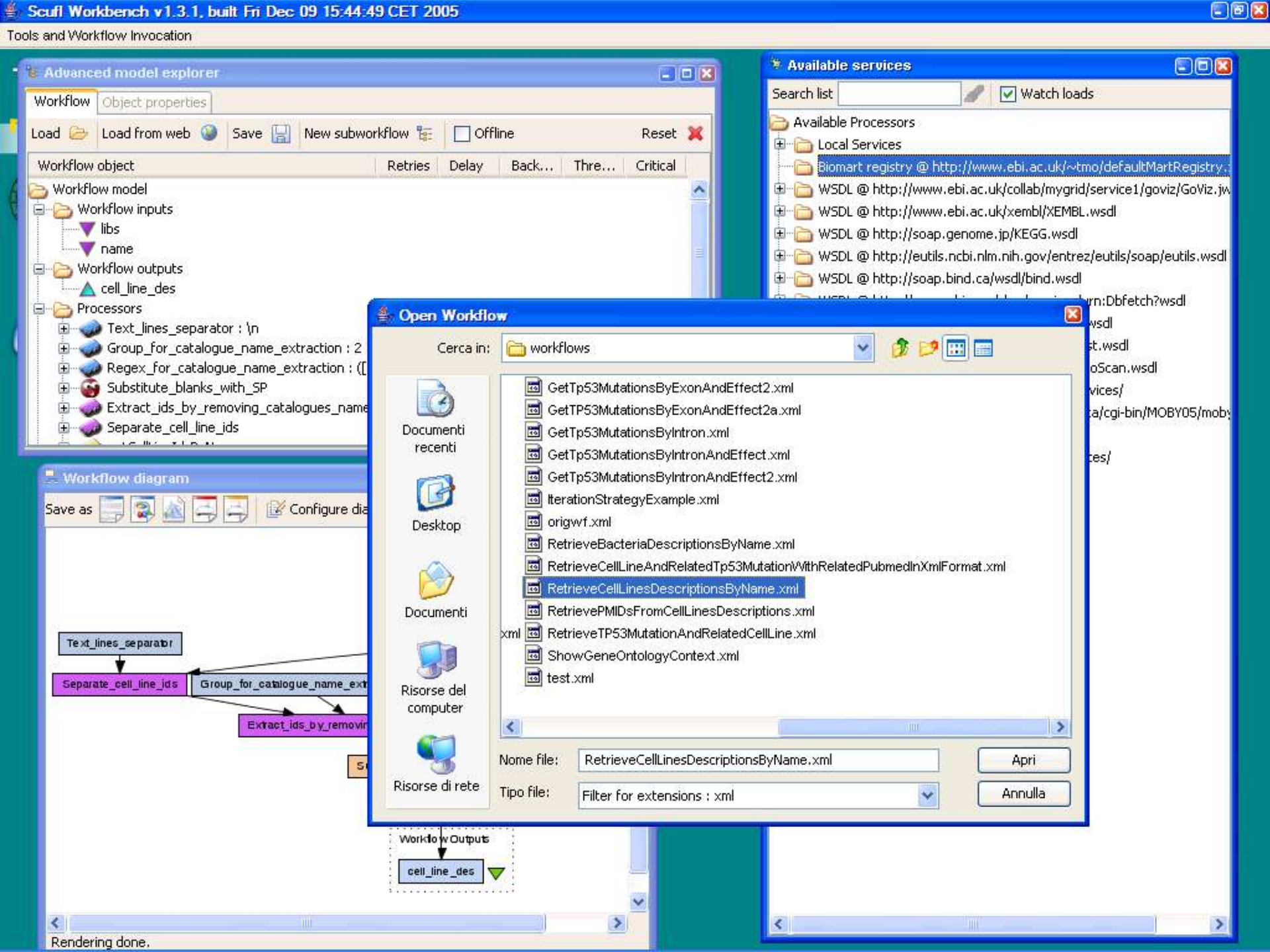
Beanshell scripting host
String Constant
Biomart registry @ http://www.ebi.ac.uk/~tmo/defaultMartRegist
WSDL @ http://www.ebi.ac.uk/collab/mygrid/service1/goviz/GoVi
porttype: GoViz [RPC]
createSession
destroySession
getChildren
addTerm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Tools and Workflow Invocation
Advanced model explorer
Workflow
Object properties
Load
Load from web
Save
New subworkflow
Offline
Reset
Workflow object
Retries
Delay
Back...
Thre...
Critical
Workflow model
Workflow inputs
libs
name
Workflow outputs
cell_line_des
Processors
Text_lines_separator : \n
Group_for_catalogue_name_extraction : 2
Regex_for_catalogue_name_extraction : ([
Substitute_blanks_with_SP
Extract_ids_by_removing_catalogues_name
Separate_cell_line_ids
Available services
Search list
Watch loads
Available Processors
Local Services
Biomart registry @ http://www.ebi.ac.uk/~tmo/defaultMartRegistry
WSDL @ http://www.ebi.ac.uk/collab/mygrid/service1/goviz/GoViz.jw
WSDL @ http://www.ebi.ac.uk/xembl/XEMBL.wsdl
WSDL @ http://soap.genome.jp/KEGG.wsdl
WSDL @ http://eutils.ncbi.nlm.nih.gov/entrez/eutils/soap/eutils.wsdl
WSDL @ http://soap.bind.ca/wsdl/bind.wsdl
Open Workflow
Cerca in:
workflows
Documenti recenti
Desktop
Documenti
Risorse del computer
Risorse di rete
GetTp53MutationsByExonAndEffect2.xml
GetTP53MutationsByExonAndEffect2a.xml
GetTp53MutationsByIntron.xml
GetTp53MutationsByIntronAndEffect.xml
GetTp53MutationsByIntronAndEffect2.xml
IterationStrategyExample.xml
origwf.xml
RetrieveBacteriaDescriptionsByName.xml
RetrieveCellLineAndRelatedTp53MutationWithRelatedPubmedInXmlFormat.xml
RetrieveCellLinesDescriptionsByName.xml
RetrievePMIDsFromCellLinesDescriptions.xml
RetrieveTP53MutationAndRelatedCellLine.xml
ShowGeneOntologyContext.xml
test.xml
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RetrieveCellLinesDescriptionsByName.xml
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Filter for extensions : xml
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Workflow diagram
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Workflow Outputs
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Rendering done.

Scufl Workbench v1.3.1, built Fri Dec 09 15:44:49 CET 2005

Tools and Workflow Invocation

Advanced model explorer

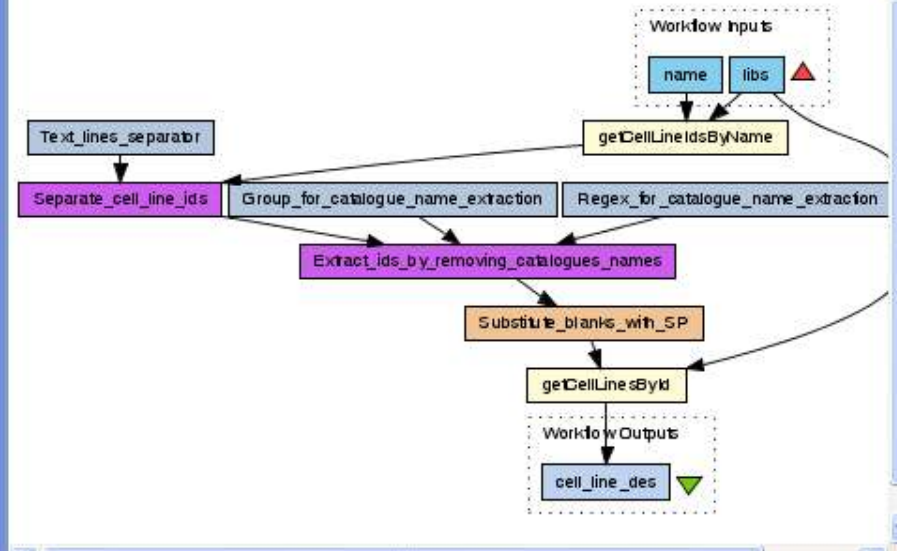
Workflow | Object properties

Load | Load from web | Save | New subworkflow | Offline | Reset

Workflow object	Retries	Delay	Back...	Thre...	Critical
Workflow model					
Workflow inputs					
libs					
name					
Workflow outputs					
cell_line_des					
Processors					
Text_lines_separator : \n	0	0	1	1	
Group_for_catalogue_name_extraction : 2	0	0	1	1	
Regex_for_catalogue_name_extraction : ([A-	0	0	1	1	
Substitute_blanks_with_SP	0	0	1	1	
Extract_ids_by_removing_catalogues_names	0	0	1	1	
Separate_cell_line_ids	0	0	1	1	

Workflow diagram

Save as | Configure diagram

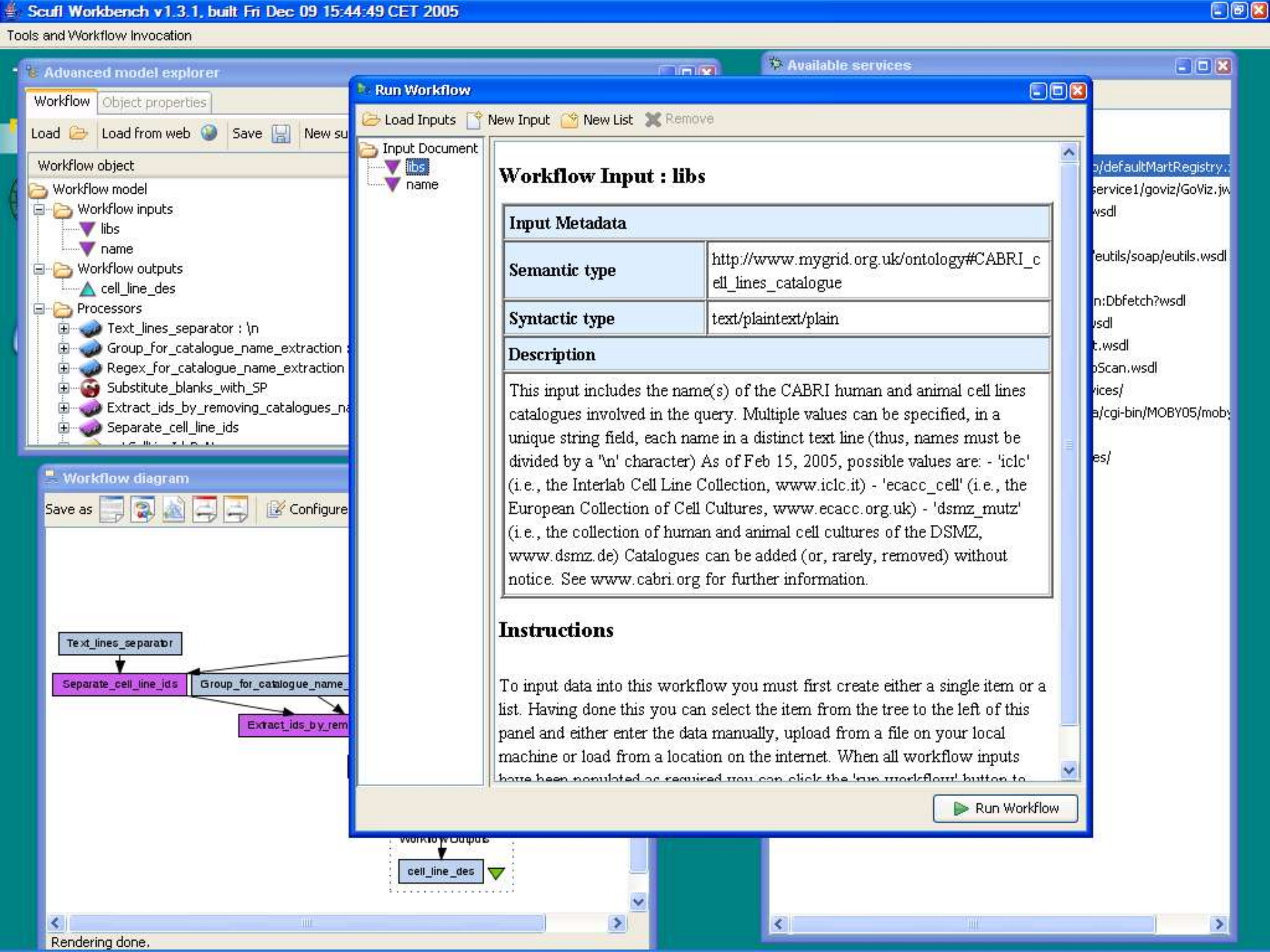


Rendering done.

Available services

Search list | Watch loads

- Available Processors
  - Local Services
  - Biomart registry @ http://www.ebi.ac.uk/~tmo/defaultMartRegistry.
  - WSDL @ http://www.ebi.ac.uk/collab/mygrid/service1/goviz/GoViz.jw
  - WSDL @ http://www.ebi.ac.uk/xembl/XEMBL.wsdl
  - WSDL @ http://soap.genome.jp/KEGG.wsdl
  - WSDL @ http://eutils.ncbi.nlm.nih.gov/entrez/eutils/soap/eutils.wsdl
  - WSDL @ http://soap.bind.ca/wsdl/bind.wsdl
  - WSDL @ http://www.ebi.ac.uk/ws/services/urn:Dbfetch?wsdl
  - WSDL @ http://www.ebi.ac.uk/ws/WSFasta.wsdl
  - WSDL @ http://www.ebi.ac.uk/ws/WSWUBlast.wsdl
  - WSDL @ http://www.ebi.ac.uk/ws/WSInterProScan.wsdl
  - Soaplab @ http://www.ebi.ac.uk/soaplab/services/
  - Biomoby @ http://mobycentral.icapture.ubc.ca/cgi-bin/MOBY05/moby
  - SeqHound @ seqhound.blueprint.org
  - Soaplab @ http://www.o2i.it:8080/axis/services/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Tools and Workflow Invocation
Advanced model explorer
Workflow
Object properties
Load
Load from web
Save
Workflow object
Workflow model
Workflow inputs
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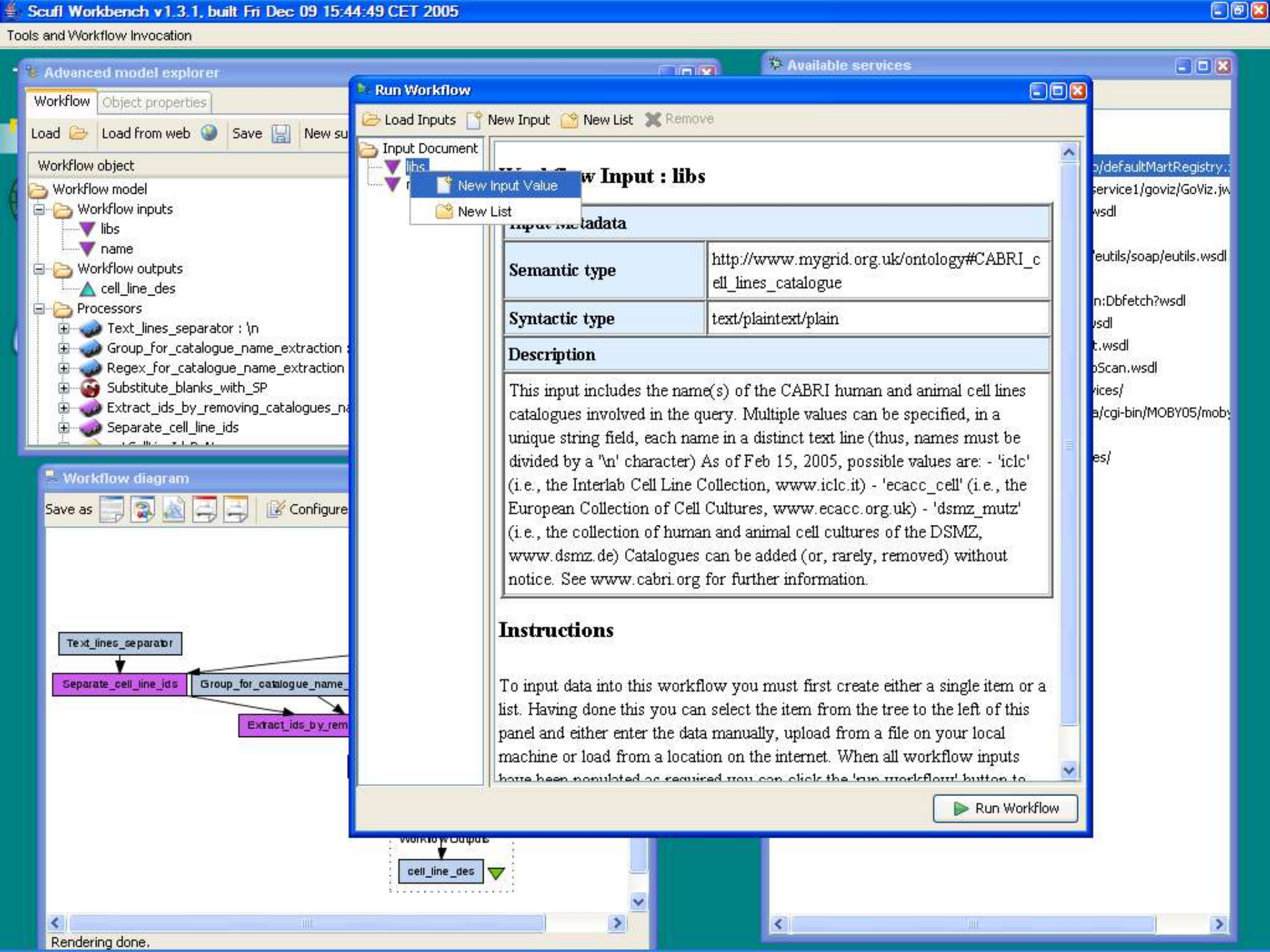
name
Workflow outputs
cell_line_des
Processors
Text_lines_separator : \n
Group_for_catalogue_name_extraction
Regex_for_catalogue_name_extraction
Substitute_blanks_with_SP
Extract_ids_by_removing_catalogues_na
Separate_cell_line_ids
Run Workflow
Load Inputs
New Input
New List
Remove
Input Document
libs
name
Workflow Input : libs
Input Metadata
Semantic type
http://www.mygrid.org.uk/ontology#CABRI_cell_lines_catalogue
Syntactic type
text/plaintext/plain
Description
This input includes the name(s) of the CABRI human and animal cell lines catalogues involved in the query. Multiple values can be specified, in a unique string field, each name in a distinct text line (thus, names must be divided by a '\n' character) As of Feb 15, 2005, possible values are: - 'iclc' (i.e., the Interlab Cell Line Collection, www.iclc.it) - 'ecacc_cell' (i.e., the European Collection of Cell Cultures, www.ecacc.org.uk) - 'dsmz_mutz' (i.e., the collection of human and animal cell cultures of the DSMZ, www.dsmz.de) Catalogues can be added (or, rarely, removed) without notice. See www.cabri.org for further information.
Instructions
To input data into this workflow you must first create either a single item or a list. Having done this you can select the item from the tree to the left of this panel and either enter the data manually, upload from a file on your local machine or load from a location on the internet. When all workflow inputs
Run Workflow
Workflow diagram
Save as
Configure
Text_lines_separator
Separate_cell_line_ids
Group_for_catalogue_name_
Extract_ids_by_rem
cell_line_des
Rendering done.
Available services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Tools and Workflow Invocation
Advanced model explorer
Workflow
Object properties
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Workflow object
Workflow model
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Workflow outputs
cell_line_des
Processors
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Regex_for_catalogue_name_extraction
Substitute_blanks_with_SP
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Separate_cell_line_ids
Workflow diagram
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Configure
Text_lines_separator
Separate_cell_line_ids
Group_for_catalogue_name_
Extract_ids_by_rem
cell_line_des
Rendering done.
Run Workflow
Load Inputs
New Input
New List
Remove
Input Document
libs
New Input Value
New List
w Input : libs
adata
Semantic type
http://www.mygrid.org.uk/ontology#CABRI_cell_lines_catalogue
Syntactic type
text/plaintext/plain
Description
This input includes the name(s) of the CABRI human and animal cell lines catalogues involved in the query. Multiple values can be specified, in a unique string field, each name in a distinct text line (thus, names must be divided by a '\n' character) As of Feb 15, 2005, possible values are: - 'iclc' (i.e., the Interlab Cell Line Collection, www.iclc.it) - 'ecacc_cell' (i.e., the European Collection of Cell Cultures, www.ecacc.org.uk) - 'dsmz_mutz' (i.e., the collection of human and animal cell cultures of the DSMZ, www.dsmz.de) Catalogues can be added (or, rarely, removed) without notice. See www.cabri.org for further information.
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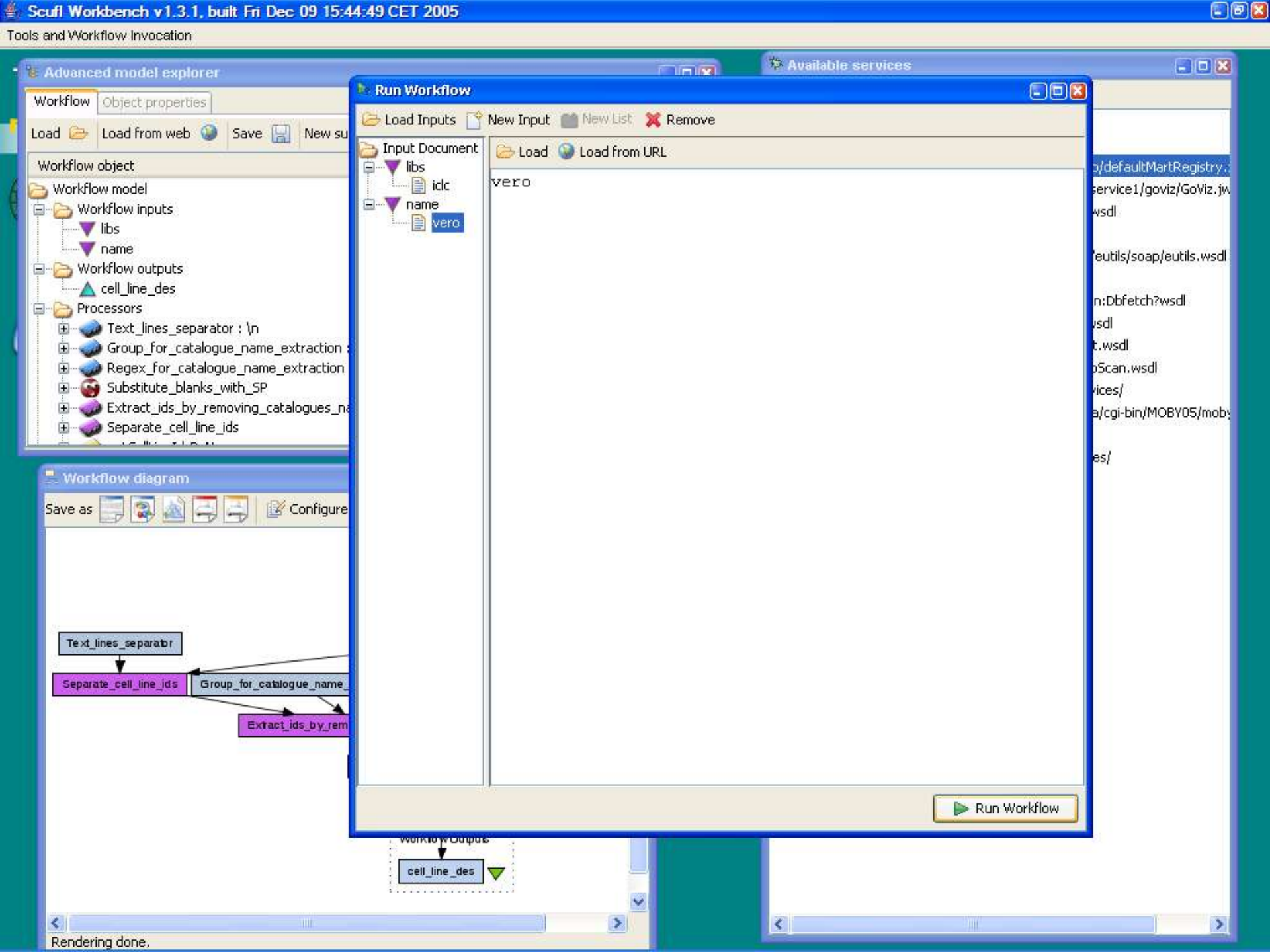
Run Workflow
Available services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Tools and Workflow Invocation
Advanced model explorer
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Workflow outputs
cell_line_des
Processors
Text_lines_separator : \n
Group_for_catalogue_name_extraction
Regex_for_catalogue_name_extraction
Substitute_blanks_with_SP
Extract_ids_by_removing_catalogues_na
Separate_cell_line_ids
Run Workflow
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New List
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Load from URL
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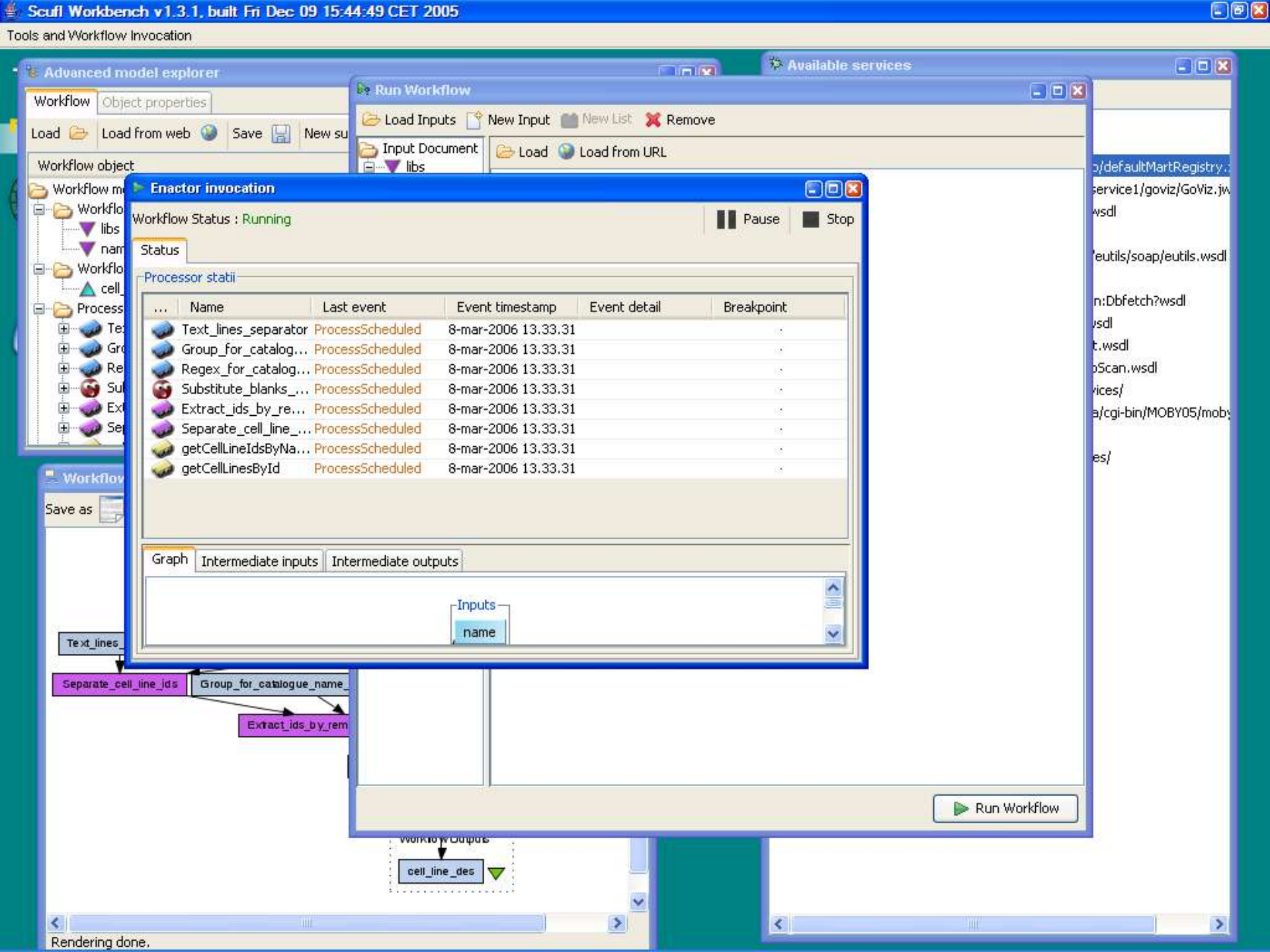
Run Workflow
Available services
Workflow diagram
Save as
Configure
Text_lines_separator
Separate_cell_line_ids
Group_for_catalogue_name_
Extract_ids_by_rem
cell_line_des
Rendering done.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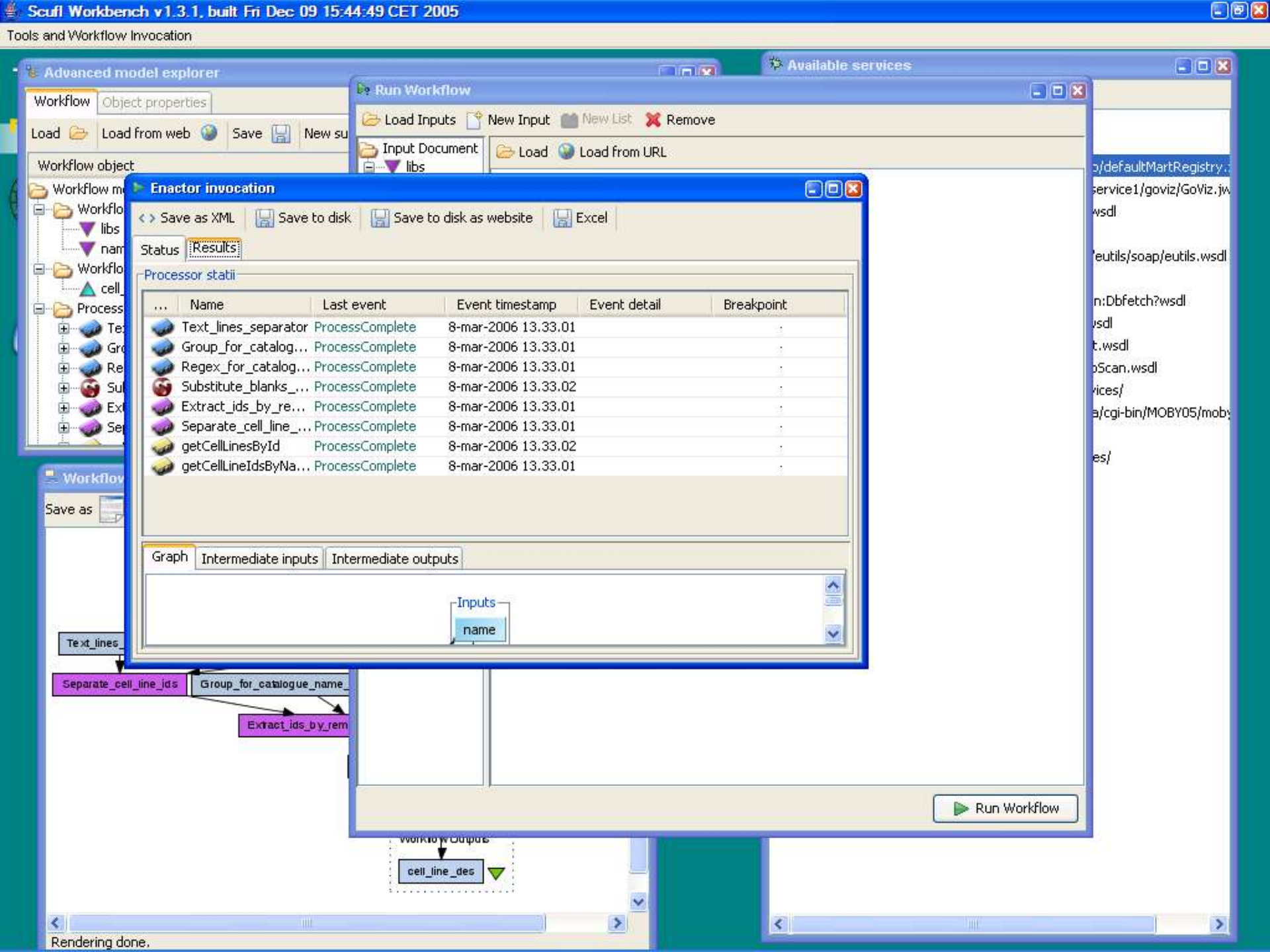
Tools and Workflow Invocation
Advanced model explorer
Workflow
Object properties
Load
Load from web
Save
Workflow object
Run Workflow
Load Inputs
New Input
New List
Remove
Input Document
libs
Load
Load from URL
Available services
Enactor invocation
Workflow Status : Running
Pause
Stop
Status
Processor statii
... Name Last event Event timestamp Event detail Breakpoint
Text_lines_separator ProcessScheduled 8-mar-2006 13.33.31
Group_for_catalog... ProcessScheduled 8-mar-2006 13.33.31
Regex_for_catalog... ProcessScheduled 8-mar-2006 13.33.31
Substitute_blanks_... ProcessScheduled 8-mar-2006 13.33.31
Extract_ids_by_re... ProcessScheduled 8-mar-2006 13.33.31
Separate_cell_line_... ProcessScheduled 8-mar-2006 13.33.31
getCellLineIdsByNa... ProcessScheduled 8-mar-2006 13.33.31
getCellLinesById ProcessScheduled 8-mar-2006 13.33.31
Graph
Intermediate inputs
Intermediate outputs
Inputs
name
Save as
Text_lines_
Separate_cell_line_ids
Group_for_catalogue_name_
Extract_ids_by_rem
cell_line_des
Run Workflow
Rendering done.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New List
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Save as XML
Save to disk
Save to disk as website
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Status
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Processor statii
... Name Last event Event timestamp Event detail Breakpoint
Text_lines_separator ProcessComplete 8-mar-2006 13.33.01
Group_for_catalog... ProcessComplete 8-mar-2006 13.33.01
Regex_for_catalog... ProcessComplete 8-mar-2006 13.33.01
Substitute_blanks_... ProcessComplete 8-mar-2006 13.33.02
Extract_ids_by_re... ProcessComplete 8-mar-2006 13.33.01
Separate_cell_line_... ProcessComplete 8-mar-2006 13.33.01
getCellLinesById ProcessComplete 8-mar-2006 13.33.02
getCellLineIdsByNa... ProcessComplete 8-mar-2006 13.33.01
Graph
Intermediate inputs
Intermediate outputs
Inputs
name
Save as
Text_lines_
Separate_cell_line_ids
Group_for_catalogue_name_
Extract_ids_by_rem
cell_line_des
Run Workflow
Rendering done.

Scufl Workbench v1.3.1, built Fri Dec 09 15:44:49 CET 2005

Tools and Workflow Invocation

Advanced model explor

Workflow | Object properties

Load | Load from web

Workflow object

- Workflow model
  - Workflow inputs
    - libs
    - name
  - Workflow outputs
    - cell_line_des
  - Processors
    - Text_lines_separ
    - Group_for_catalo
    - Regex_for_catal
    - Substitute_blank
    - Extract_ids_by_r
    - Separate_cell_lin

Workflow diagram

Save as

Text_lines_separator

Separate_cell_line_ids

Rendering done.

Enactor invocation

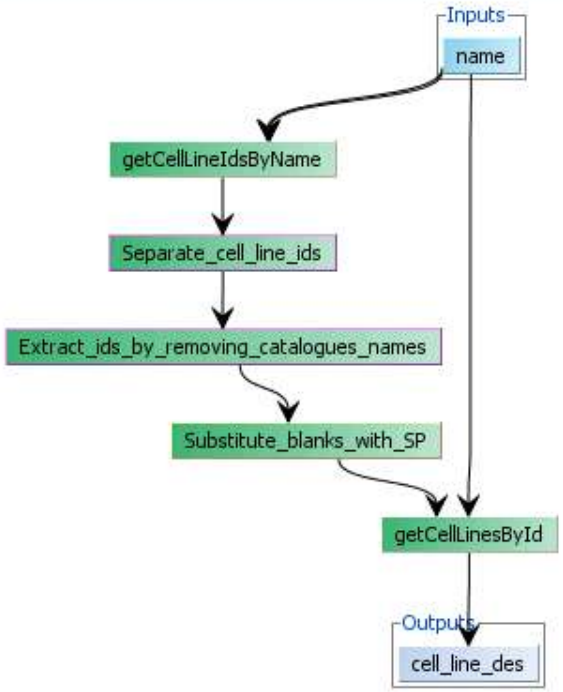
Save as XML | Save to disk | Save to disk as website | Excel

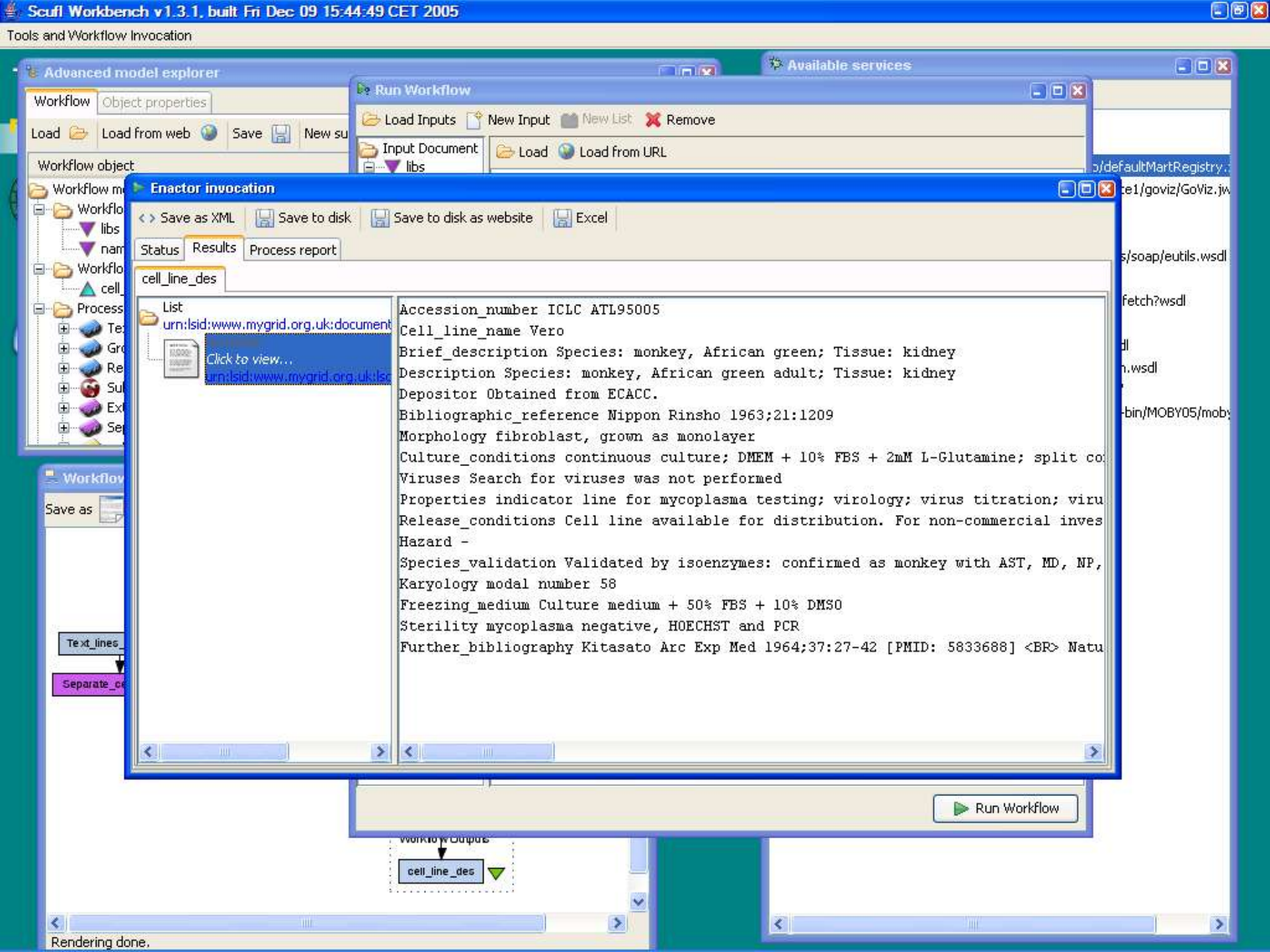
Status | Results | Process report

Processor statii

...	Name	Last event	Event timestamp	Event detail	Breakpoint
	Text_lines_separator	ProcessComplete	8-mar-2006 13.33.31		
	Group_for_catalogue_nam...	ProcessComplete	8-mar-2006 13.33.31		
	Regex_for_catalogue_nam...	ProcessComplete	8-mar-2006 13.33.31		
	Substitute_blanks_with_SP	ProcessComplete	8-mar-2006 13.33.31		
	Extract_ids_by_removing_...	ProcessComplete	8-mar-2006 13.33.31		
	Separate_cell_line_ids	ProcessComplete	8-mar-2006 13.33.31		

Graph | Intermediate inputs | Intermediate outputs

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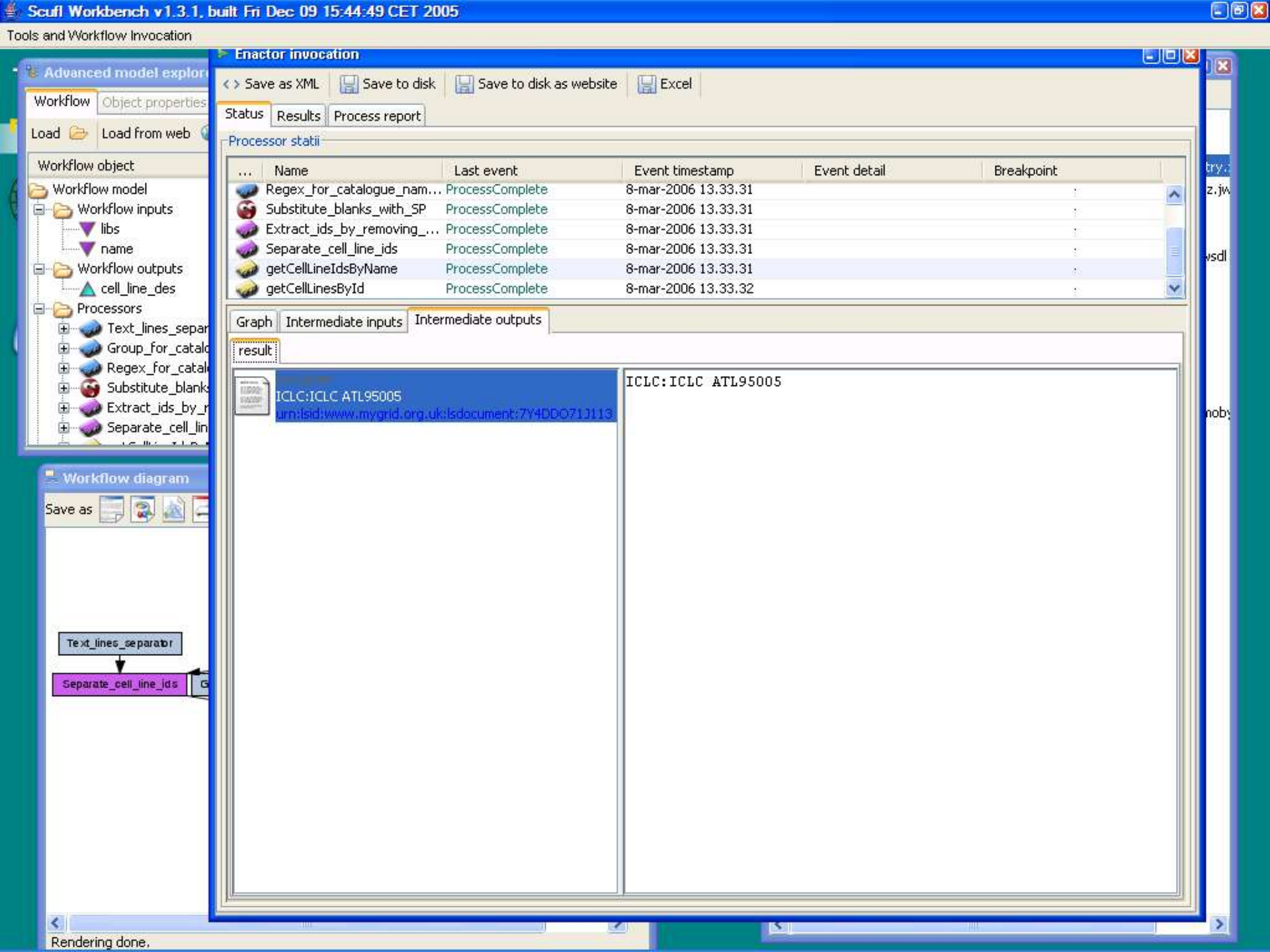
Tools and Workflow Invocation
Advanced model explorer
Workflow
Object properties
Load
Load from web
Save
Workflow object
Run Workflow
Load Inputs
New Input
New List
Remove
Input Document
libs
Load
Load from URL
Available services
Enactor invocation
Save as XML
Save to disk
Save to disk as website
Excel
Status
Results
Process report
cell_line_des
List
urn:lsid:www.mygrid.org.uk:document
Click to view...
Accession_number ICLC ATL95005
Cell_line_name Vero
Brief_description Species: monkey, African green; Tissue: kidney
Description Species: monkey, African green adult; Tissue: kidney
Depositor Obtained from ECACC.
Bibliographic_reference Nippon Rinsho 1963;21:1209
Morphology fibroblast, grown as monolayer
Culture_conditions continuous culture; DMEM + 10% FBS + 2mM L-Glutamine; split co
Viruses Search for viruses was not performed
Properties indicator line for mycoplasma testing; virology; virus titration; viru
Release_conditions Cell line available for distribution. For non-commercial inves
Hazard -
Species_validation Validated by isoenzymes: confirmed as monkey with AST, MD, NP,
Karyology modal number 58
Freezing_medium Culture medium + 50% FBS + 10% DMSO
Sterility mycoplasma negative, HOECHST and PCR
Further_bibliography Kitasato Arc Exp Med 1964;37:27-42 [PMID: 5833688]
 Natu
Save as
Text_lines
Separate_ce
cell_line_des
Run Workflow
Rendering done.


Scufl Workbench v1.3.1, built Fri Dec 09 15:44:49 CET 2005
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Substitute_blanks
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Separate_cell_line_ids
Rendering done.
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Save to disk
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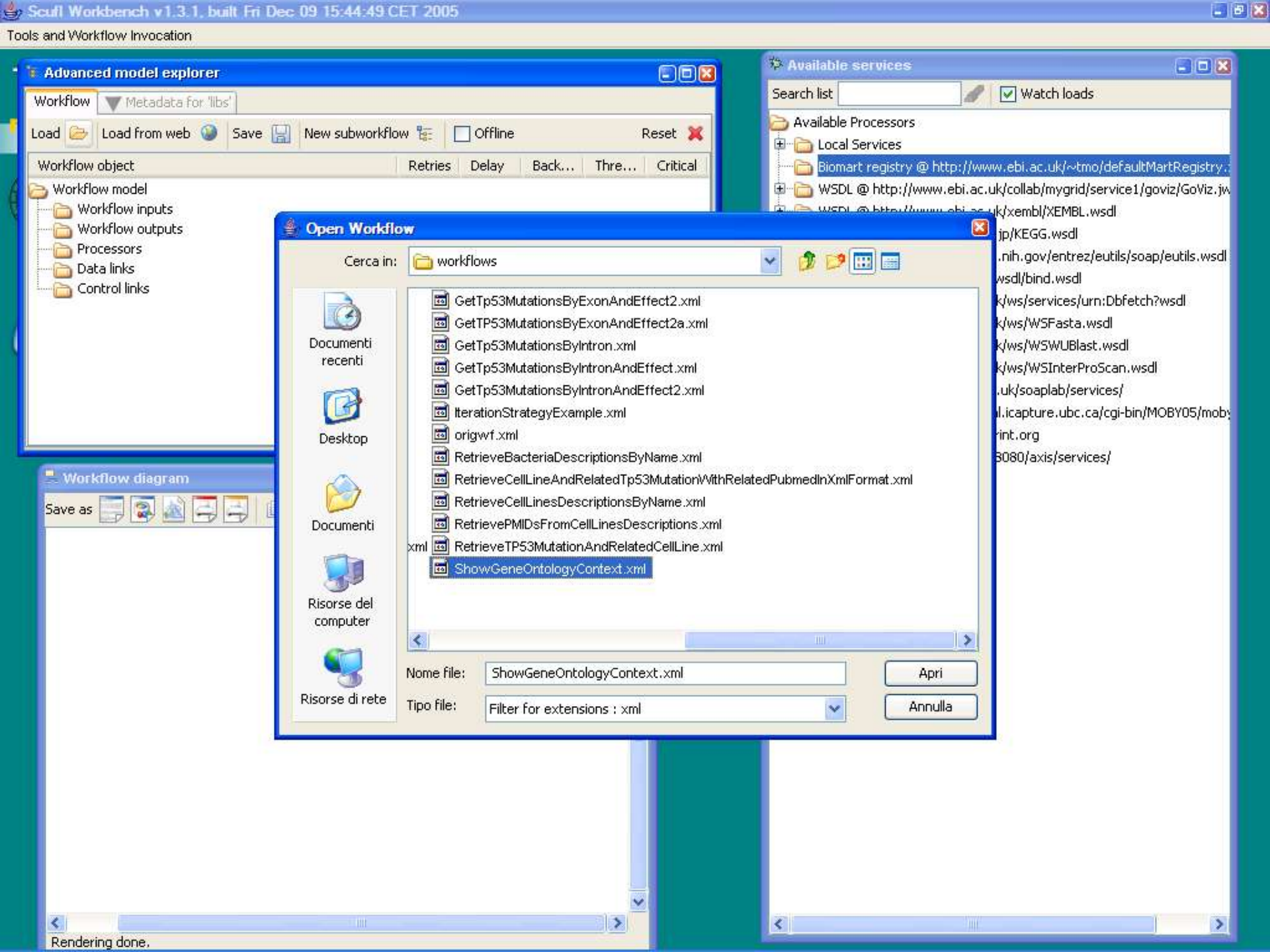
... Name Last event Event timestamp Event detail Breakpoint
Regex_for_catalogue_nam... ProcessComplete 8-mar-2006 13.33.31
Substitute_blanks_with_SP ProcessComplete 8-mar-2006 13.33.31
Extract_ids_by_removing_... ProcessComplete 8-mar-2006 13.33.31
Separate_cell_line_ids ProcessComplete 8-mar-2006 13.33.31
getCellLineIdsByName ProcessComplete 8-mar-2006 13.33.31
getCellLinesById ProcessComplete 8-mar-2006 13.33.32
Graph
Intermediate inputs
Intermediate outputs
result
ICLC:ICLC ATL95005
urn:lsid:www.mygrid.org.uk:lsdocument:7Y4DDO71J113
ICLC:ICLC ATL95005


Scufl Workbench v1.3.1, built Fri Dec 09 15:44:49 CET 2005
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Biomart registry @ http://www.ebi.ac.uk/~tmo/defaultMartRegistry.
WSDL @ http://www.ebi.ac.uk/collab/mygrid/service1/goviz/GoViz.jw
/xembl/XEMBL.wsdl
jp/KEGG.wsdl
.nih.gov/entrez/eutils/soap/eutils.wsdl
wsdl/bind.wsdl
k/ws/services/urn:Dbfetch?wsdl
k/ws/WSFasta.wsdl
k/ws/WSWUBlast.wsdl
k/ws/WSInterProScan.wsdl
.uk/soaplab/services/
l.icapture.ubc.ca/cgi-bin/MOBY05/moby
int.org
8080/axis/services/
Open Workflow
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workflows
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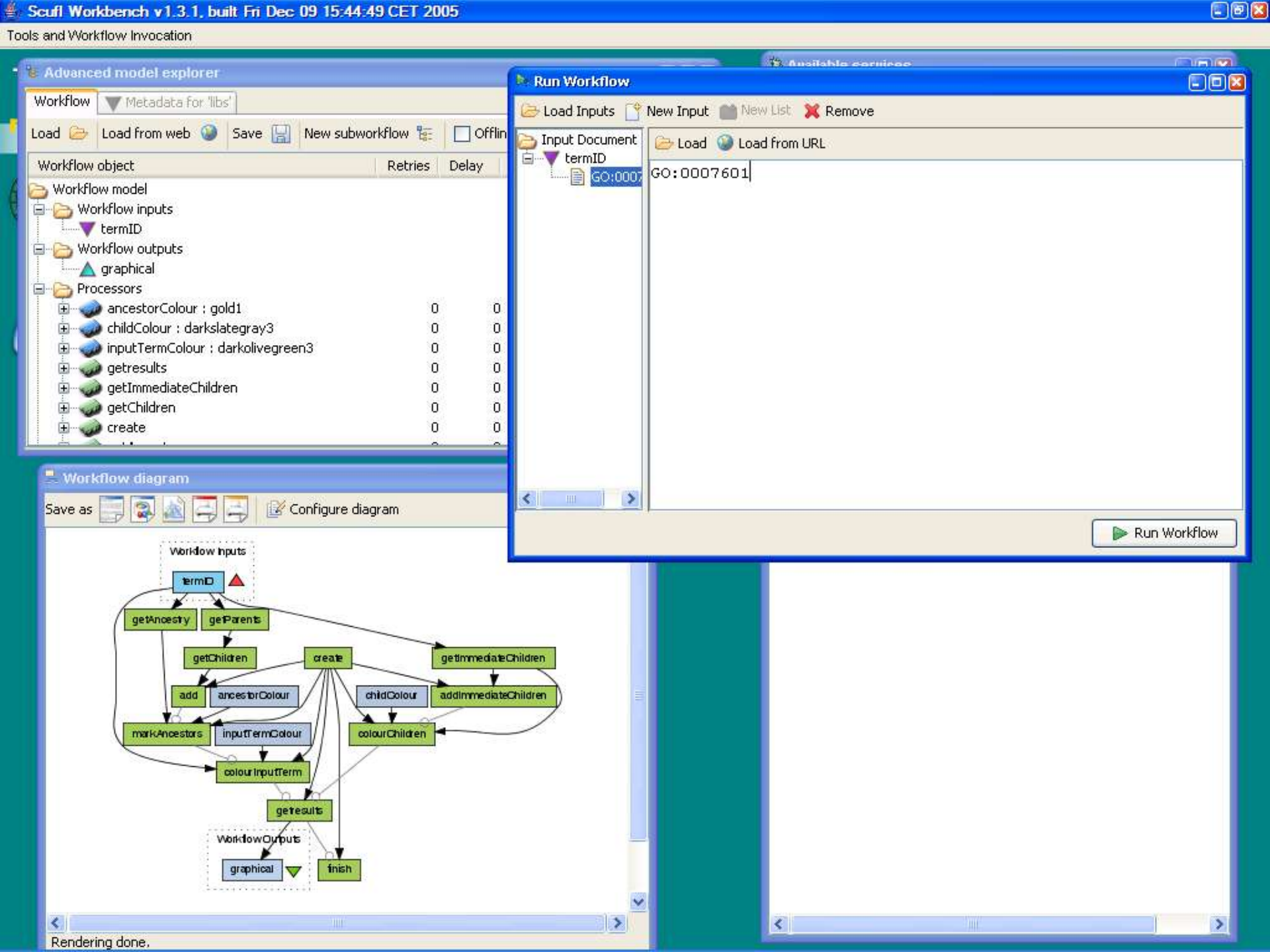
GetTp53MutationsByExonAndEffect2.xml
GetTP53MutationsByExonAndEffect2a.xml
GetTp53MutationsByIntron.xml
GetTp53MutationsByIntronAndEffect.xml
GetTp53MutationsByIntronAndEffect2.xml
IterationStrategyExample.xml
origwf.xml
RetrieveBacteriaDescriptionsByName.xml
RetrieveCellLineAndRelatedTp53MutationWithRelatedPubmedInXmlFormat.xml
RetrieveCellLinesDescriptionsByName.xml
RetrievePMIDsFromCellLinesDescriptions.xml
xml
RetrieveTP53MutationAndRelatedCellLine.xml
ShowGeneOntologyContext.xml
Nome file:
ShowGeneOntologyContext.xml
Tipo file:
Filter for extensions : xml
Apri
Annulla
Workflow diagram
Save as
Rendering done.


Scufl Workbench v1.3.1, built Fri Dec 09 15:44:49 CET 2005
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childColour : darkslategray3
inputTermColour : darkolivegreen3
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getChildren
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Remove
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GO:0007
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GO:0007601
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Rendering done.

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Tools and Workflow Invocation

Enactor invocation

Workflow Status : Running

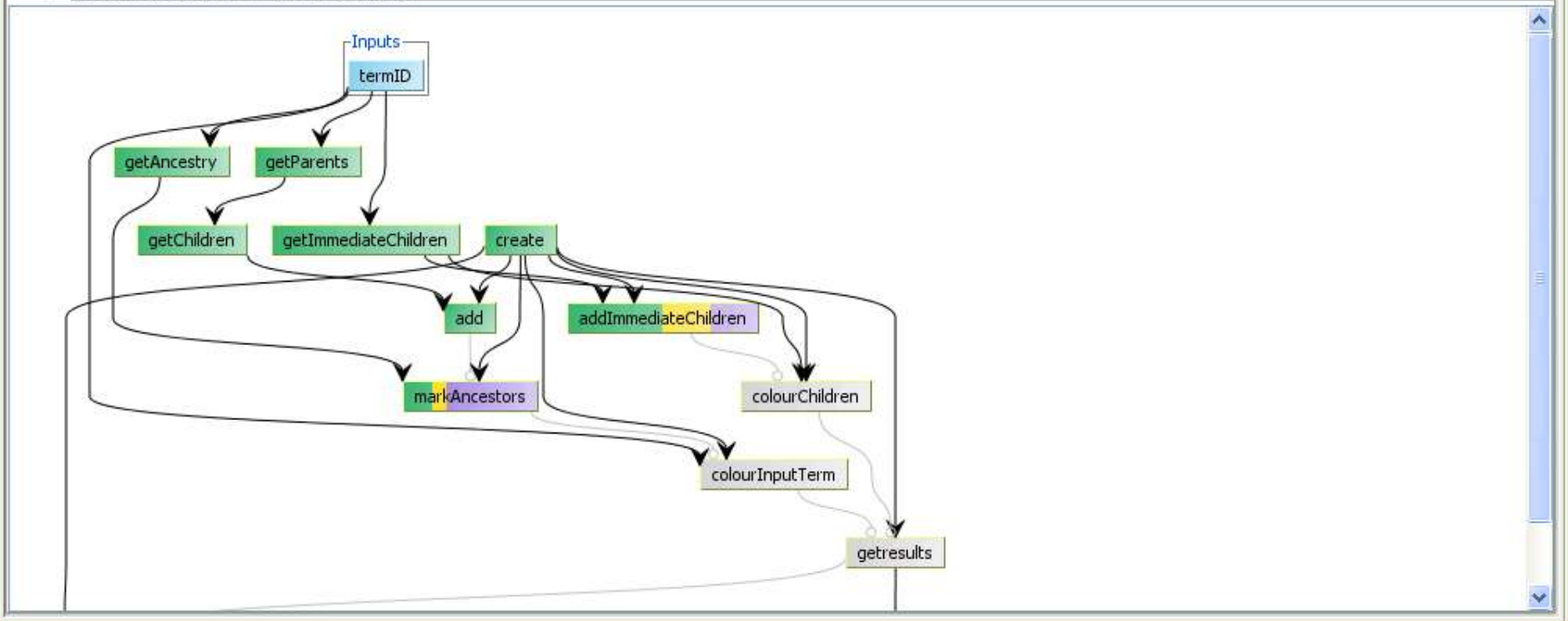
Pause Stop

Status

Processor statii

...	Name	Last event	Event timestamp	Event detail	Breakpoint
	ancestorColour	ProcessComplete	8-mar-2006 14.20.21		
	childColour	ProcessComplete	8-mar-2006 14.20.21		
	inputTermColour	ProcessComplete	8-mar-2006 14.20.21		
	getresults	ProcessScheduled	8-mar-2006 14.20.21		
	getImmediateChildren	ProcessComplete	8-mar-2006 14.20.24		
	getChildren	ProcessComplete	8-mar-2006 14.20.37		
	create	ProcessComplete	8-mar-2006 14.20.24		
	getAncestry	ProcessComplete	8-mar-2006 14.20.24		
	finish	ProcessScheduled	8-mar-2006 14.20.21		
	markAncestors	InvokingWithIteration	8-mar-2006 14.20.38	IterationNumber='3' IterationTotal='9' ActiveWorkers...	
	add	ProcessComplete	8-mar-2006 14.20.38		

Graph | Intermediate inputs | Intermediate outputs



Scufl Workbench v1.3.1, built Fri Dec 09 15:44:49 CET 2005

Tools and Workflow Invocation

Enactor invocation

Save as XML | Save to disk | Save to disk as website | Excel

Status | Results | Process report

graphical

Click to view...

urn:lsid:www.myg /4DDO71J139

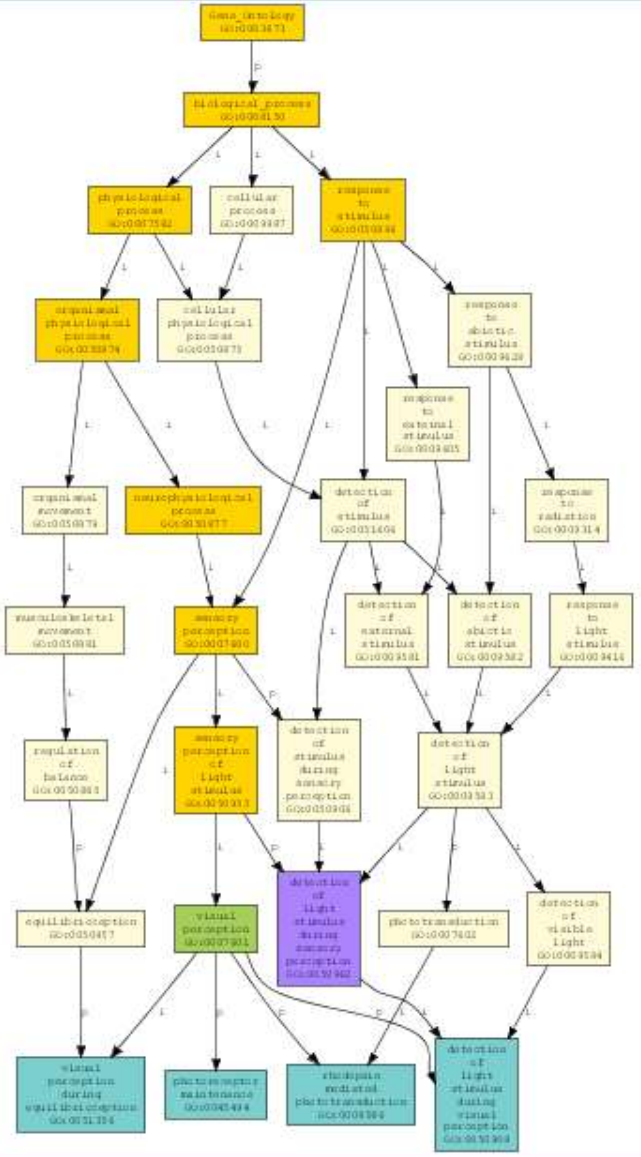
Save to file

Viewers

X-Graphviz

Text

Table



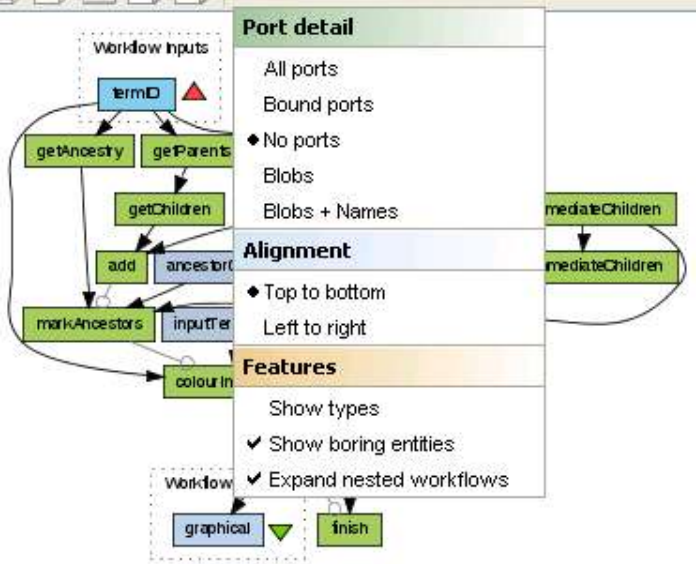
Scufl Workbench v1.3.1, built Fri Dec 09 15:44:49 CET 2005

Tools and Workflow Invocation

Workflow diagram

Save as

Configure diagram



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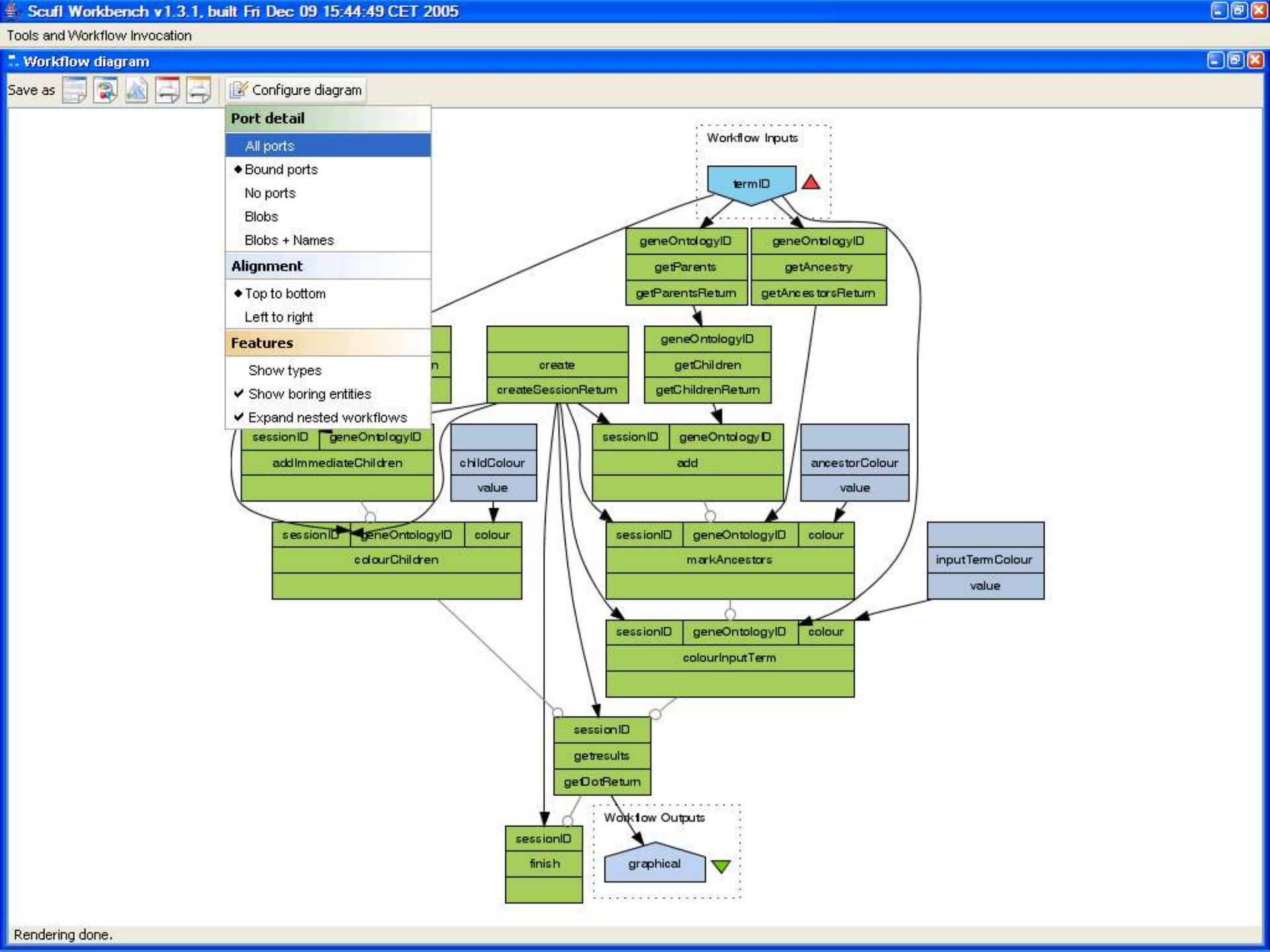
Scufl Workbench v1.3.1, built Fri Dec 09 15:44:49 CET 2005
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Bound ports
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geneOntologyID
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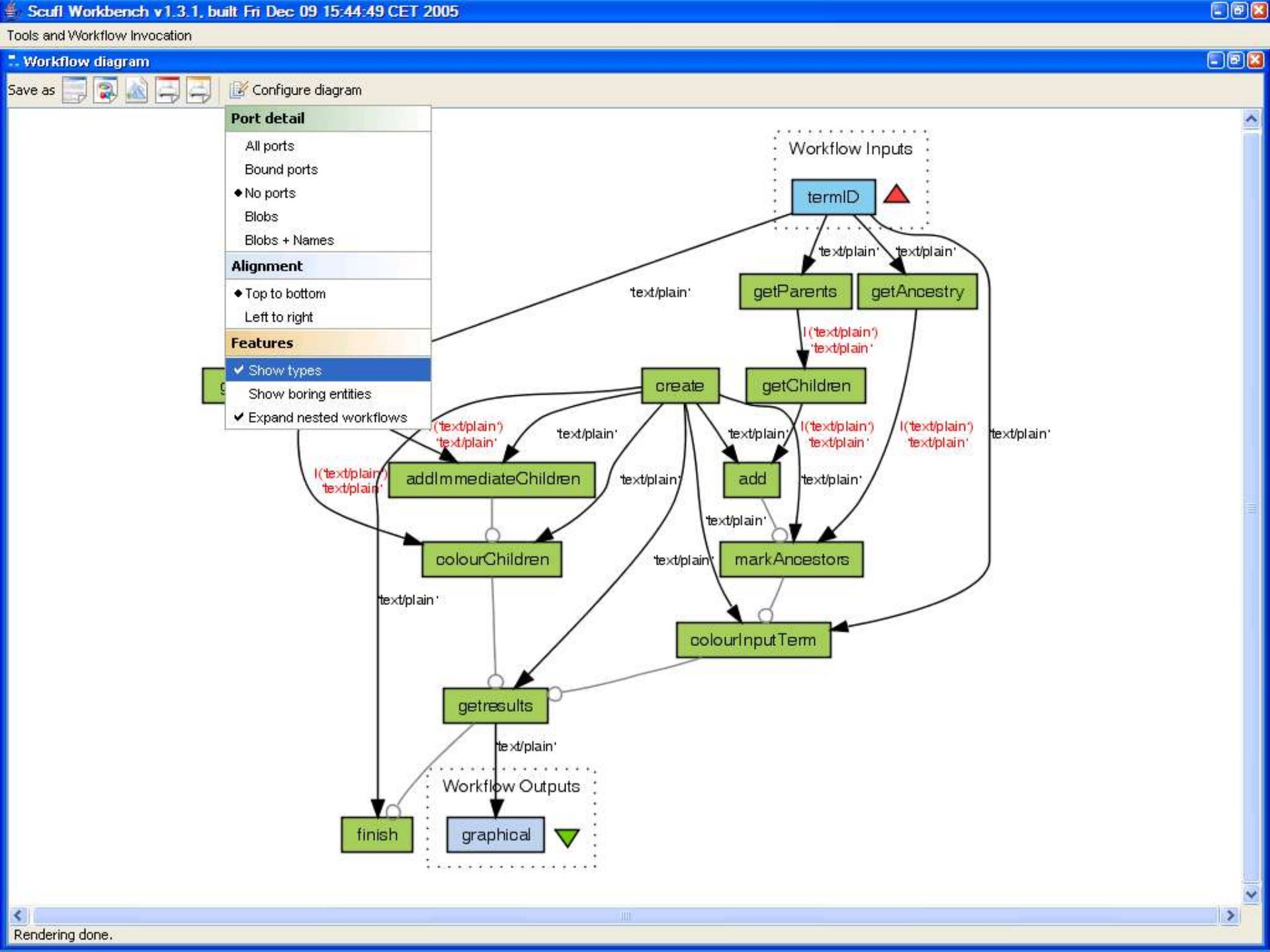
Rendering done.


Scufl Workbench v1.3.1, built Fri Dec 09 15:44:49 CET 2005
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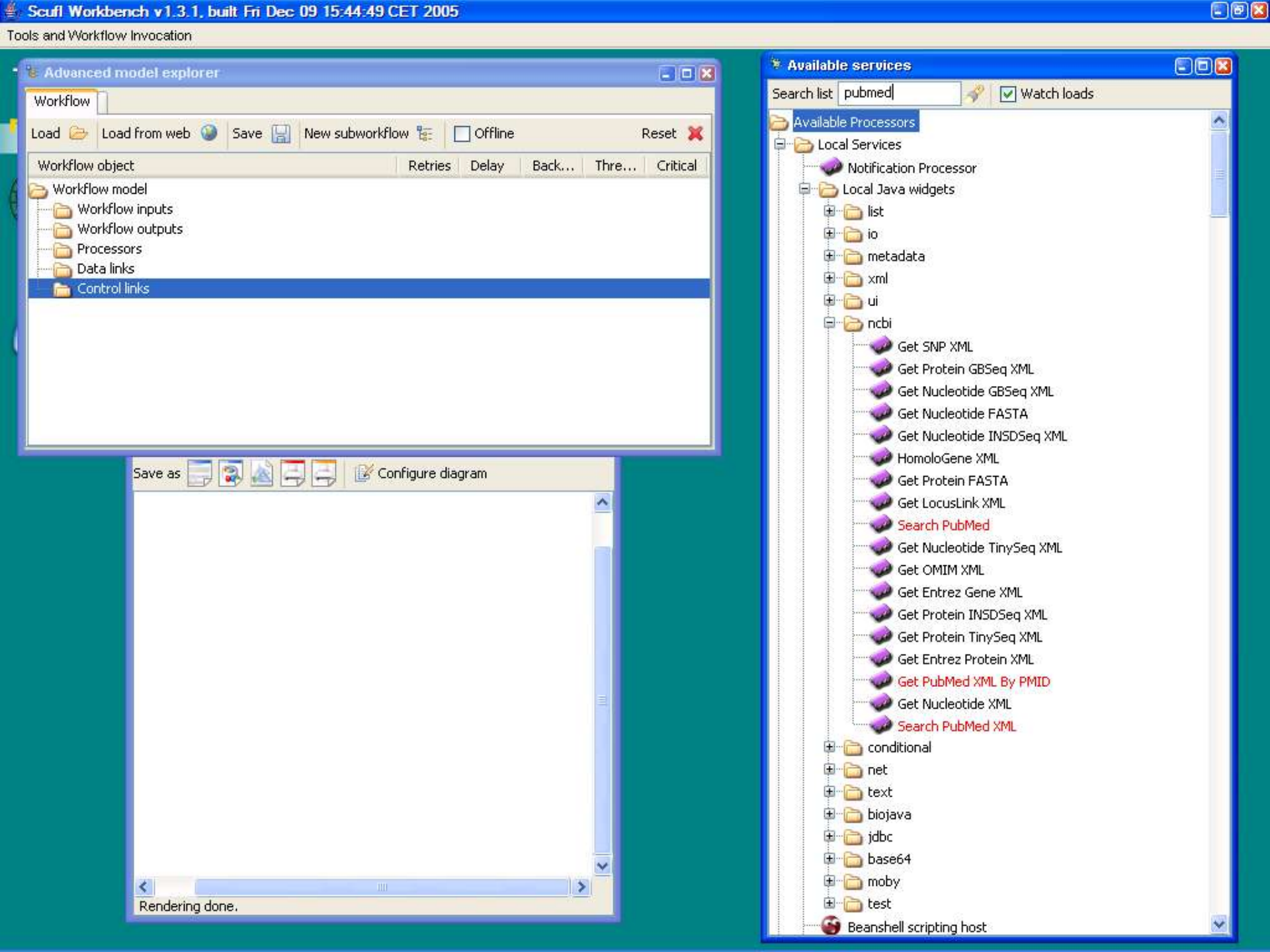
Rendering done.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Get Entrez Gene XML
Get Protein INSDSeq XML
Get Protein TinySeq XML
Get Entrez Protein XML
Get PubMed XML By PMID
Get Nucleotide XML
Search PubMed XML
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net
text
biojava
jdbc
base64
moby
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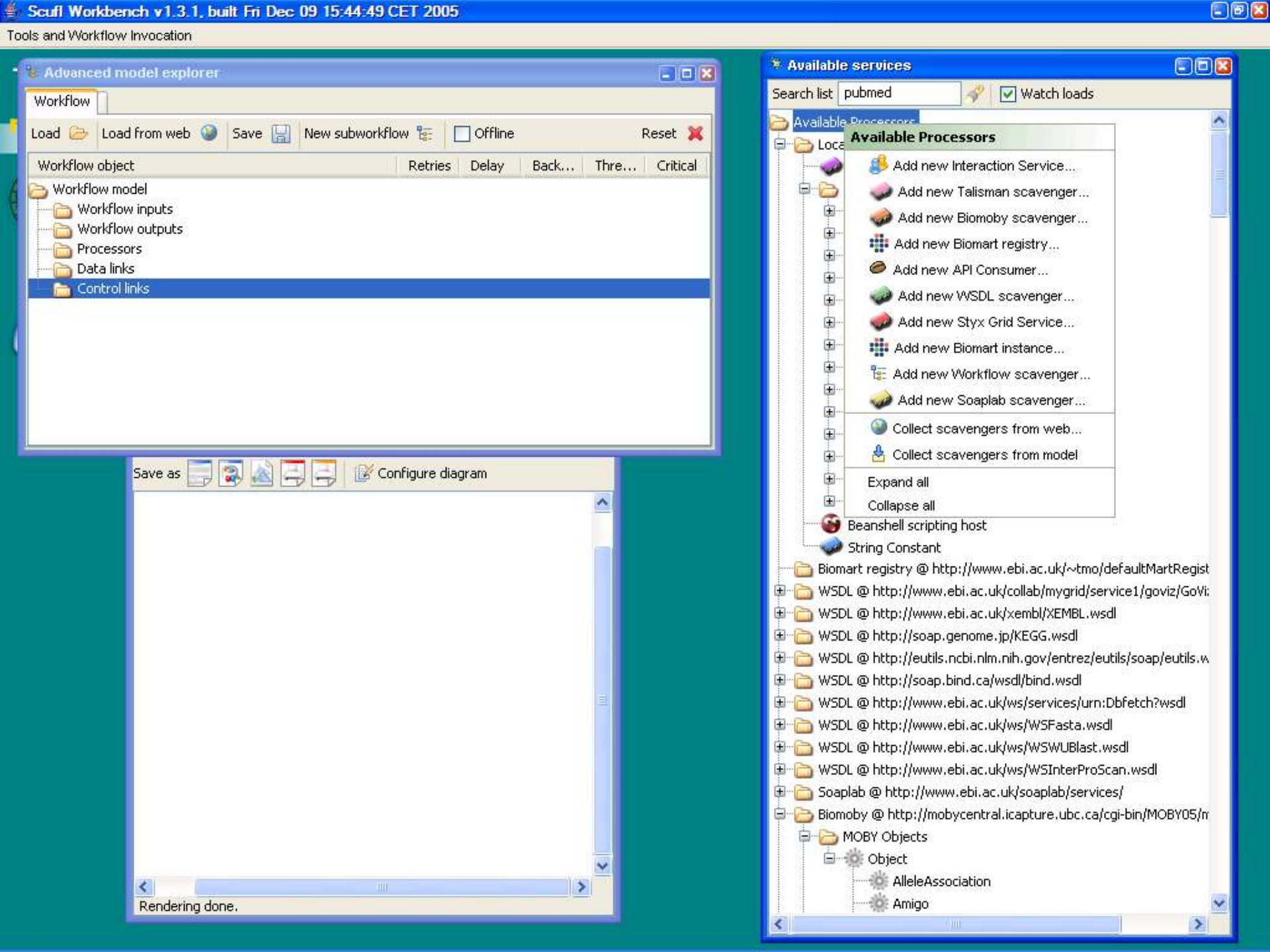
Beanshell scripting host


Scufl Workbench v1.3.1, built Fri Dec 09 15:44:49 CET 2005
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Add new Biomoby scavenger...
Add new Biomart registry...
Add new API Consumer...
Add new WSDL scavenger...
Add new Styx Grid Service...
Add new Biomart instance...
Add new Workflow scavenger...
Add new Soaplab scavenger...
Collect scavengers from web...
Collect scavengers from model
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Collapse all
Beanshell scripting host
String Constant
Biomart registry @ http://www.ebi.ac.uk/~tmo/defaultMartRegist
WSDL @ http://www.ebi.ac.uk/collab/mygrid/service1/goviz/GoVi
WSDL @ http://www.ebi.ac.uk/xembl/XEMBL.wsdl
WSDL @ http://soap.genome.jp/KEGG.wsdl
WSDL @ http://eutils.ncbi.nlm.nih.gov/entrez/eutils/soap/eutils.w
WSDL @ http://soap.bind.ca/wsdl/bind.wsdl
WSDL @ http://www.ebi.ac.uk/ws/services/urn:Dbfetch?wsdl
WSDL @ http://www.ebi.ac.uk/ws/WSFasta.wsdl
WSDL @ http://www.ebi.ac.uk/ws/WSWUBlast.wsdl
WSDL @ http://www.ebi.ac.uk/ws/WSInterProScan.wsdl
Soaplab @ http://www.ebi.ac.uk/soaplab/services/
Biomoby @ http://mobycentral.icapture.ubc.ca/cgi-bin/MOBY05/m
MOBY Objects
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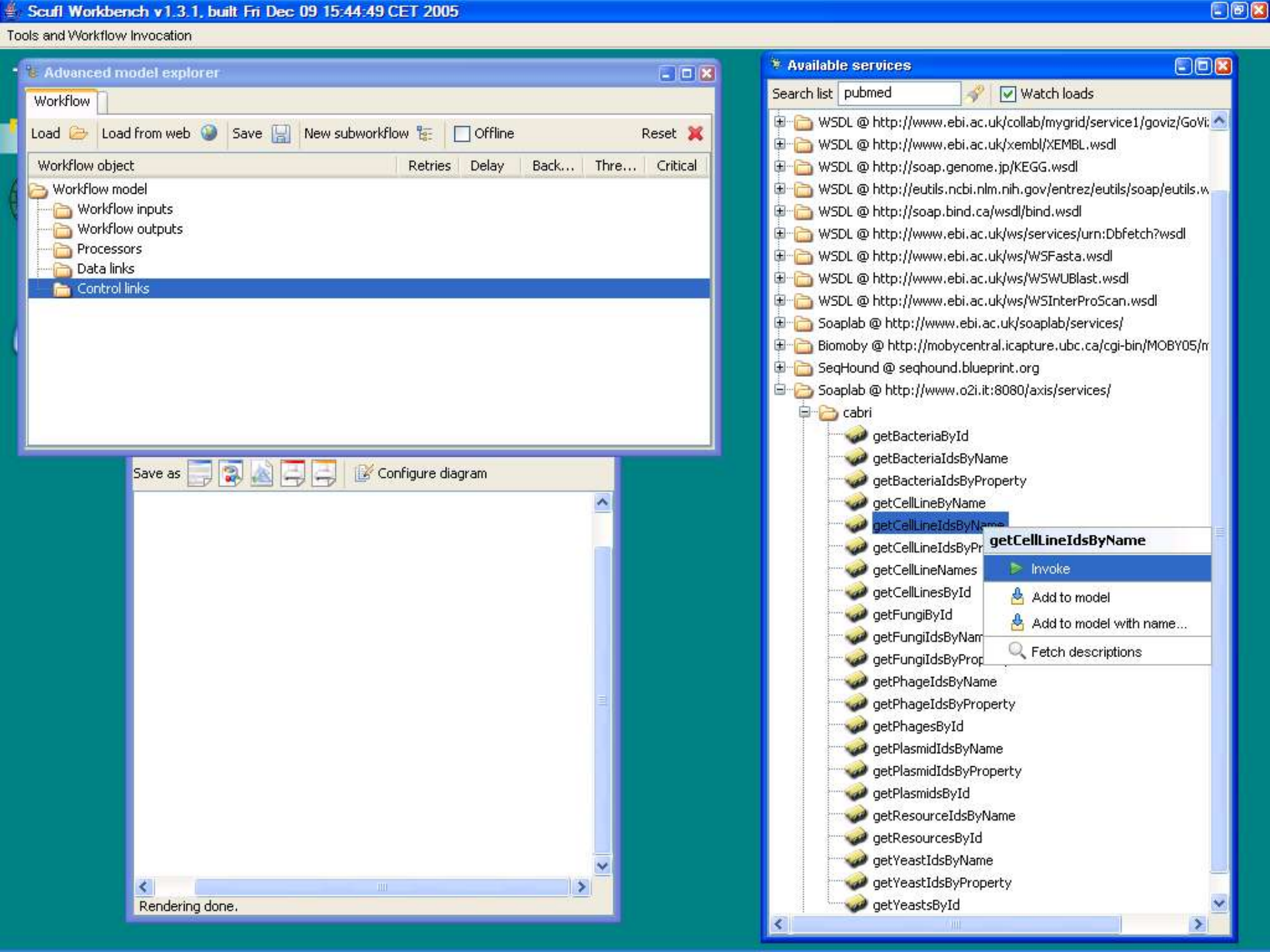
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WSDL @ http://www.ebi.ac.uk/xembl/XEMBL.wsdl
WSDL @ http://soap.genome.jp/KEGG.wsdl
WSDL @ http://eutils.ncbi.nlm.nih.gov/entrez/eutils/soap/eutils.w
WSDL @ http://soap.bind.ca/wsdl/bind.wsdl
WSDL @ http://www.ebi.ac.uk/ws/services/urn:Dbfetch?wsdl
WSDL @ http://www.ebi.ac.uk/ws/WSFasta.wsdl
WSDL @ http://www.ebi.ac.uk/ws/WSWUBlast.wsdl
WSDL @ http://www.ebi.ac.uk/ws/WSInterProScan.wsdl
Soaplab @ http://www.ebi.ac.uk/soaplab/services/
Biomoby @ http://mobycentral.icapture.ubc.ca/cgi-bin/MOBY05/m
SeqHound @ seqhound.blueprint.org
Soaplab @ http://www.o2i.it:8080/axis/services/
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getBacteriaById
getBacteriaIdsByName
getBacteriaIdsByProperty
getCellLineByName
getCellLineIdsByName
getCellLineIdsByPr
getCellLineNames
getCellLinesById
getFungiById
getFungiIdsByNam
getFungiIdsByProp
getPhageIdsByName
getPhageIdsByProperty
getPhagesById
getPlasmidIdsByName
getPlasmidIdsByProperty
getPlasmidsById
getResourceIdsByName
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getYeastIdsByProperty
getYeastsById
getCellLineIdsByName
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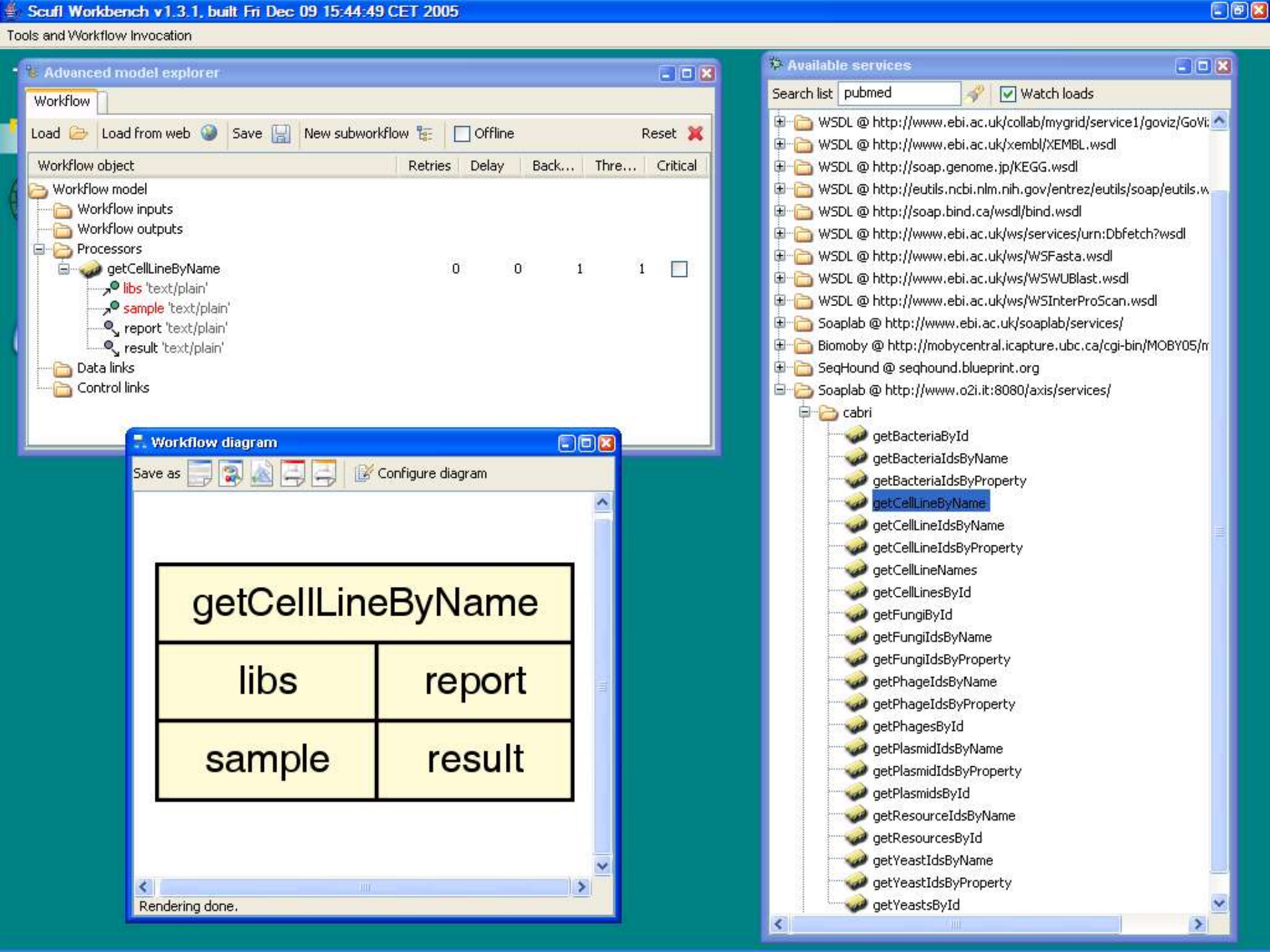
Add to model
Add to model with name...
Fetch descriptions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0
1
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WSDL @ http://soap.genome.jp/KEGG.wsdl
WSDL @ http://eutils.ncbi.nlm.nih.gov/entrez/eutils/soap/eutils.w
WSDL @ http://soap.bind.ca/wsdl/bind.wsdl
WSDL @ http://www.ebi.ac.uk/ws/services/urn:Dbfetch?wsdl
WSDL @ http://www.ebi.ac.uk/ws/WSFasta.wsdl
WSDL @ http://www.ebi.ac.uk/ws/WSWUBlast.wsdl
WSDL @ http://www.ebi.ac.uk/ws/WSInterProScan.wsdl
Soaplab @ http://www.ebi.ac.uk/soaplab/services/
Biomoby @ http://mobycentral.icapture.ubc.ca/cgi-bin/MOBY05/m
SeqHound @ seqhound.blueprint.org
Soaplab @ http://www.o2i.it:8080/axis/services/
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getBacteriaIdsByName
getBacteriaIdsByProperty
getCellLineByName
getCellLineIdsByName
getCellLineIdsByProperty
getCellLineNames
getCellLinesById
getFungiById
getFungiIdsByName
getFungiIdsByProperty
getPhageIdsByName
getPhageIdsByProperty
getPhagesById
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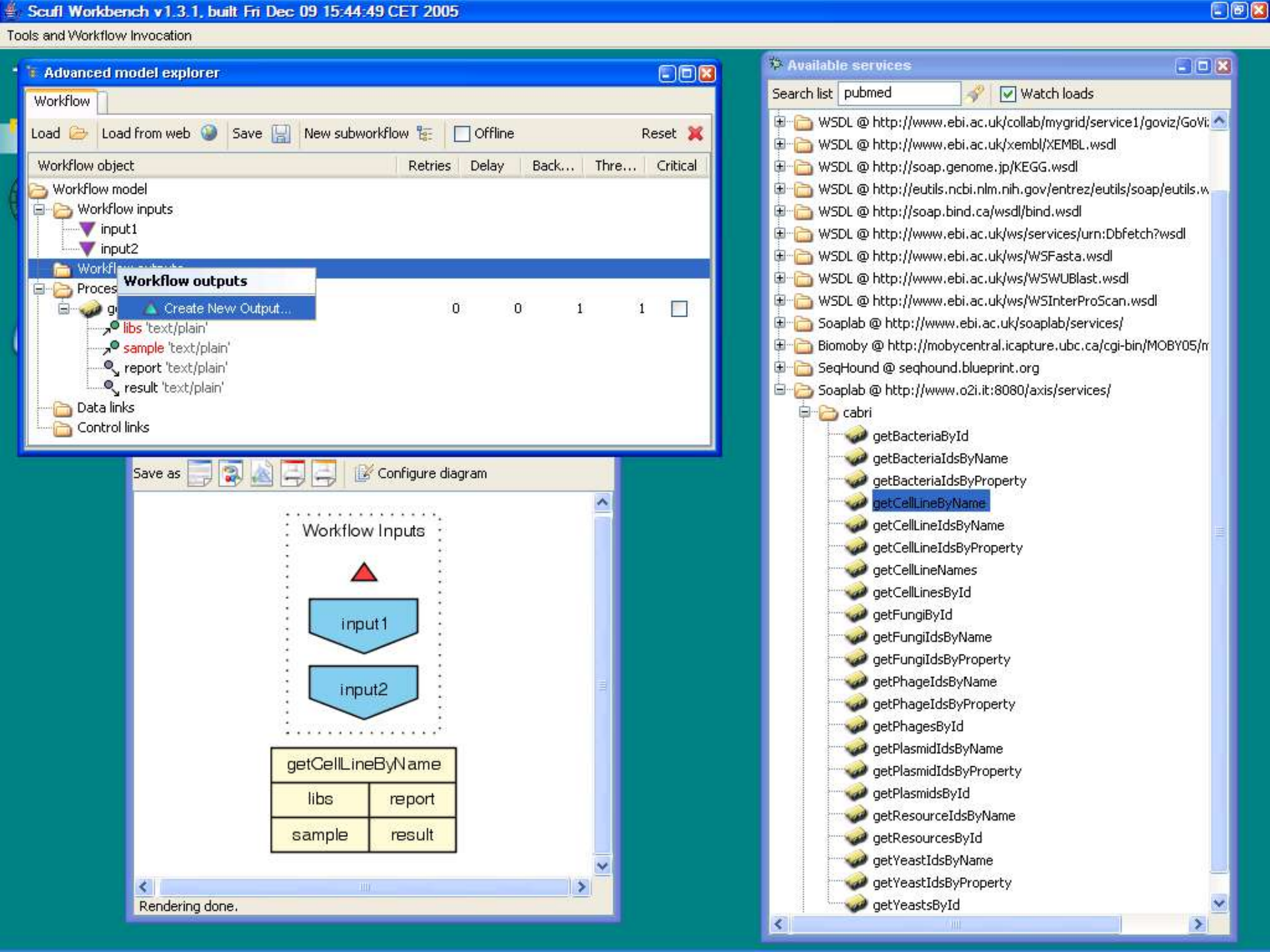
getPlasmidsById
getResourceIdsByName
getResourcesById
getYeastIdsByName
getYeastIdsByProperty
getYeastsById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WSDL @ http://soap.bind.ca/wsdl/bind.wsdl
WSDL @ http://www.ebi.ac.uk/ws/services/urn:Dbfetch?wsdl
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getBacteriaById
getBacteriaIdsByName
getBacteriaIdsByProperty
getCellLineByName
getCellLineIdsByName
getCellLineIdsByProperty
getCellLineNames
getCellLinesById
getFungiById
getFungiIdsByName
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getPhageIdsByProperty
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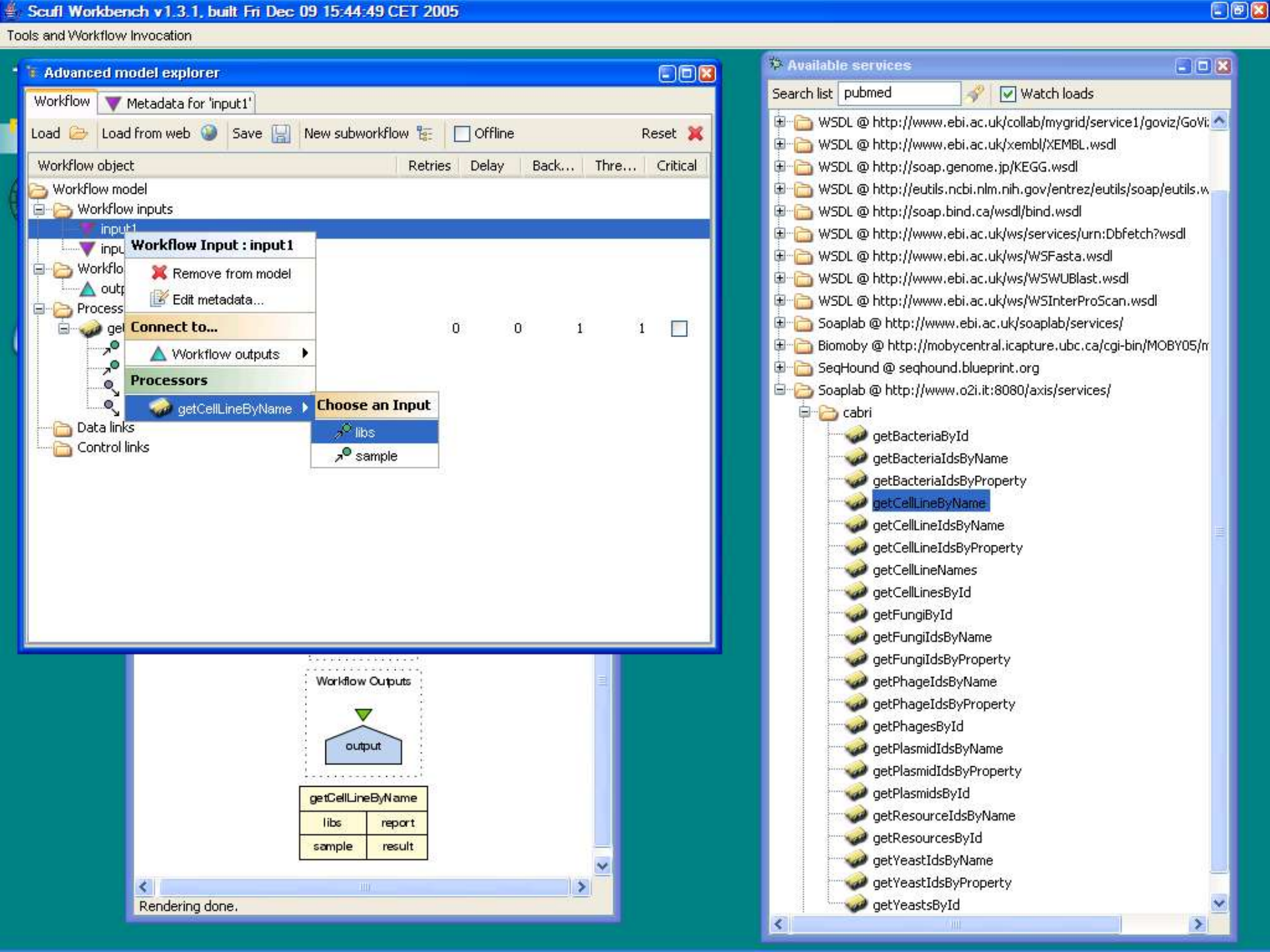
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Tools and Workflow Invocation
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1
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WSDL @ http://www.ebi.ac.uk/ws/WSFasta.wsdl
WSDL @ http://www.ebi.ac.uk/ws/WSWUBlast.wsdl
WSDL @ http://www.ebi.ac.uk/ws/WSInterProScan.wsdl
Soaplab @ http://www.ebi.ac.uk/soaplab/services/
Biomoby @ http://mobycentral.icapture.ubc.ca/cgi-bin/MOBY05/m
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getCellLineNames
getCellLinesById
getFungiById
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getResourceIdsByName
getResourcesById
getYeastIdsByName
getYeastIdsByProperty
getYeastsById

Scufl Workbench v1.3.1, built Fri Dec 09 15:44:49 CET 2005

Tools and Workflow Invocation

Advanced model explorer

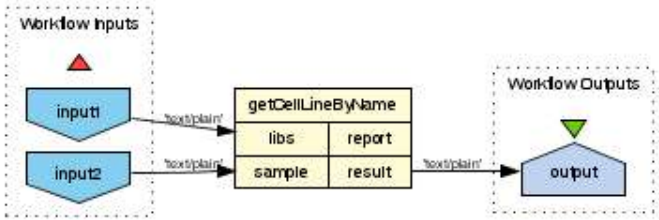
Workflow

Load | Load from web | Save | New subworkflow | Offline | Reset

Workflow object	Retries	Delay	Back...	Thre...	Critical
Workflow model					
Workflow inputs					
input1					
input2					
Workflow outputs					
output					
Processors					
getCellLineByName	0	0	1	1	☐
libs 'text/plain'					
sample 'text/plain'					
report 'text/plain'					
result 'text/plain'					
Data links					
input1-getCellLineByName:libs					
input2-getCellLineByName:sample					
getCellLineByName:result-output					
Control links					

Workflow diagram

Save as | Configure diagram

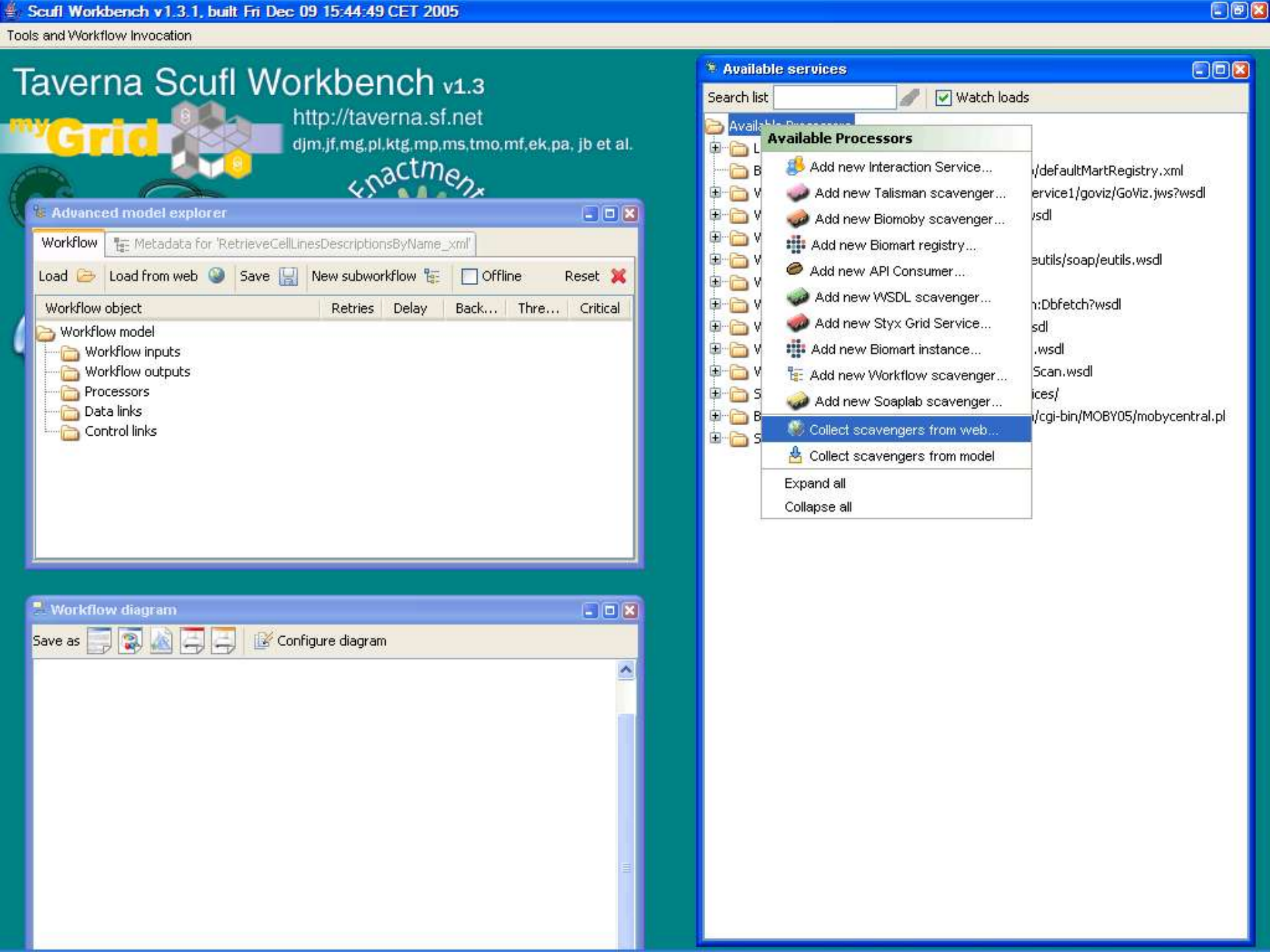


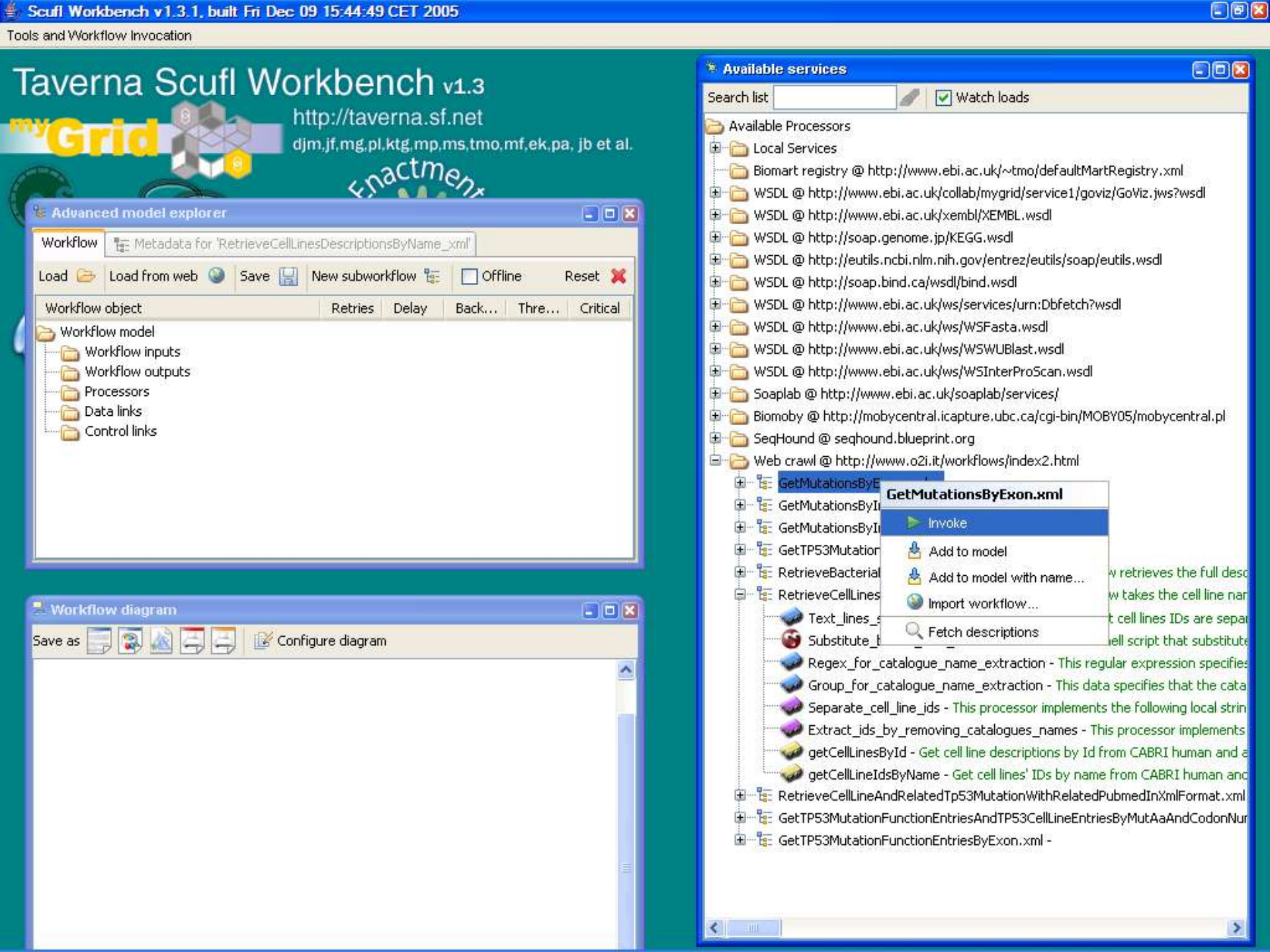
Rendering done.

Available services

Search list: pubmed | Watch loads

- WSDL @ http://www.ebi.ac.uk/collab/mygrid/service1/goviz/GoVi
- WSDL @ http://www.ebi.ac.uk/xembl/XEMBL.wsdl
- WSDL @ http://soap.genome.jp/KEGG.wsdl
- WSDL @ http://eutils.ncbi.nlm.nih.gov/entrez/eutils/soap/eutils.w
- WSDL @ http://soap.bind.ca/wsdl/bind.wsdl
- WSDL @ http://www.ebi.ac.uk/ws/services/urn:Dbfetch?wsdl
- WSDL @ http://www.ebi.ac.uk/ws/WSFasta.wsdl
- WSDL @ http://www.ebi.ac.uk/ws/WSWUBlast.wsdl
- WSDL @ http://www.ebi.ac.uk/ws/WSInterProScan.wsdl
- Soaplab @ http://www.ebi.ac.uk/soaplab/services/
- Biomoby @ http://mobycentral.icapture.ubc.ca/cgi-bin/MOBY05/m
- SeqHound @ seqhound.blueprint.org
- Soaplab @ http://www.o2i.it:8080/axis/services/
  - cabri
    - getBacteriaById
    - getBacteriaIdsByName
    - getBacteriaIdsByProperty
    - getCellLineByName
    - getCellLineIdsByName
    - getCellLineIdsByProperty
    - getCellLineNames
    - getCellLinesById
    - getFungiById
    - getFungiIdsByName
    - getFungiIdsByProperty
    - getPhageIdsByName
    - getPhageIdsByProperty
    - getPhagesById
    - getPlasmidIdsByName
    - getPlasmidIdsByProperty
    - getPlasmidsById
    - getResourceIdsByName
    - getResourcesById
    - getYeastIdsByName
    - getYeastIdsByProperty
    - getYeastsById


Scufl Workbench v1.3.1, built Fri Dec 09 15:44:49 CET 2005
Tools and Workflow Invocation
Taverna Scufl Workbench v1.3
http://taverna.sf.net
djm,jf,mg,pl,ktg,mp,ms,tmo,mf,ek,pa, jb et al.
myGrid
Enactment
Advanced model explorer
Workflow
Metadata for 'RetrieveCellLinesDescriptionsByName_xml'
Load
Load from web
Save
New subworkflow
Offline
Reset
Workflow object
Retries
Delay
Back...
Thre...
Critical
Workflow model
Workflow inputs
Workflow outputs
Processors
Data links
Control links
Workflow diagram
Save as
Configure diagram
Available services
Search list
Watch loads
Available Processors
Add new Interaction Service...
Add new Talisman scavenger...
Add new Biomoby scavenger...
Add new Biomart registry...
Add new API Consumer...
Add new WSDL scavenger...
Add new Styx Grid Service...
Add new Biomart instance...
Add new Workflow scavenger...
Add new Soaplab scavenger...
Collect scavengers from web...
Collect scavengers from model
Expand all
Collapse all
/defaultMartRegistry.xml
ervice1/goviz/GoViz.jws?wsdl
sdl
eutils/soap/eutils.wsdl
:Dbfetch?wsdl
sdl
.wsdl
Scan.wsdl
ices/
/cgi-bin/MOBY05/mobycentral.pl


Scufl Workbench v1.3.1, built Fri Dec 09 15:44:49 CET 2005
Tools and Workflow Invocation
Taverna Scufl Workbench v1.3
http://taverna.sf.net
djm,jf,mg,pl,ktg,mp,ms,tmo,mf,ek,pa, jb et al.
Advanced model explorer
Workflow
Metadata for 'RetrieveCellLinesDescriptionsByName_xml'
Load
Load from web
Save
New subworkflow
Offline
Reset
Workflow object
Retries
Delay
Back...
Thre...
Critical
Workflow model
Workflow inputs
Workflow outputs
Processors
Data links
Control links
Workflow diagram
Save as
Configure diagram
Available services
Search list
Watch loads
Available Processors
Local Services
Biomart registry @ http://www.ebi.ac.uk/~tmo/defaultMartRegistry.xml
WSDL @ http://www.ebi.ac.uk/collab/mygrid/service1/goviz/GoViz.jws?wsdl
WSDL @ http://www.ebi.ac.uk/xembl/XEMBL.wsdl
WSDL @ http://soap.genome.jp/KEGG.wsdl
WSDL @ http://eutils.ncbi.nlm.nih.gov/entrez/eutils/soap/eutils.wsdl
WSDL @ http://soap.bind.ca/wsdl/bind.wsdl
WSDL @ http://www.ebi.ac.uk/ws/services/urn:Dbfetch?wsdl
WSDL @ http://www.ebi.ac.uk/ws/WSFasta.wsdl
WSDL @ http://www.ebi.ac.uk/ws/WSWUBlast.wsdl
WSDL @ http://www.ebi.ac.uk/ws/WSInterProScan.wsdl
Soaplab @ http://www.ebi.ac.uk/soaplab/services/
Biomoby @ http://mobycentral.icapture.ubc.ca/cgi-bin/MOBY05/mobycentral.pl
SeqHound @ seqhound.blueprint.org
Web crawl @ http://www.o2i.it/workflows/index2.html
GetMutationsByExon.xml
Invoke
Add to model
Add to model with name...
Import workflow...
Fetch descriptions
RetrieveCellLines
Regex_for_catalogue_name_extraction - This regular expression specifies
Group_for_catalogue_name_extraction - This data specifies that the cata
Separate_cell_line_ids - This processor implements the following local strin
Extract_ids_by_removing_catalogues_names - This processor implements
getCellLinesById - Get cell line descriptions by Id from CABRI human and a
getCellLineIdsByName - Get cell lines' IDs by name from CABRI human and
RetrieveCellLineAndRelatedTp53MutationWithRelatedPubmedInXmlFormat.xml
GetTP53MutationFunctionEntriesAndTP53CellLineEntriesByMutAaAndCodonNur
GetTP53MutationFunctionEntriesByExon.xml -

Scufl Workbench v1.3.1, built Fri Dec 09 15:44:49 CET 2005

Tools and Workflow Invocation

Advanced model explorer

Workflow | Metadata for 'RetrieveCellL

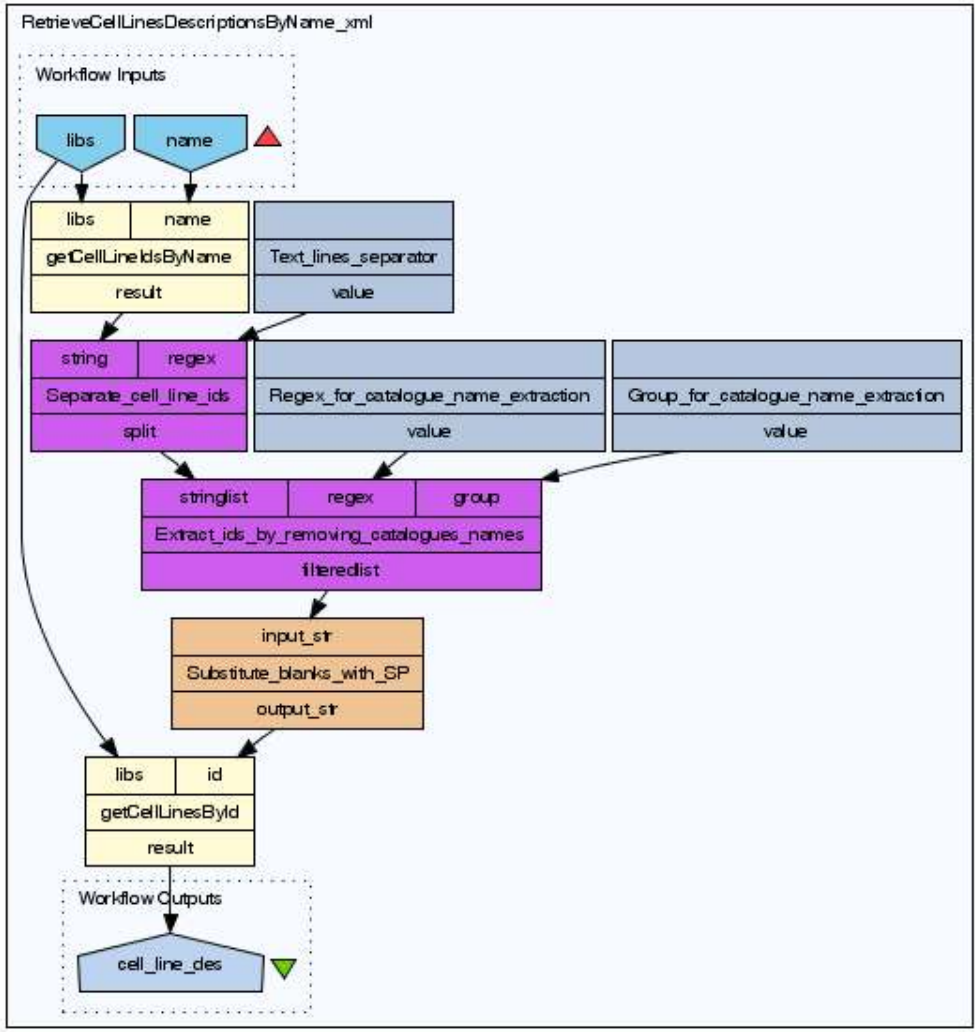
Load | Load from web | Save

Workflow object

- Workflow model
  - Workflow inputs
  - Workflow outputs
  - Processors
    - RetrieveCellLinesDescriptionsBy
      - libs 'text/plain'
      - name 'text/plain'
      - cell_line_des 'text/plain'
  - Data links
  - Control links

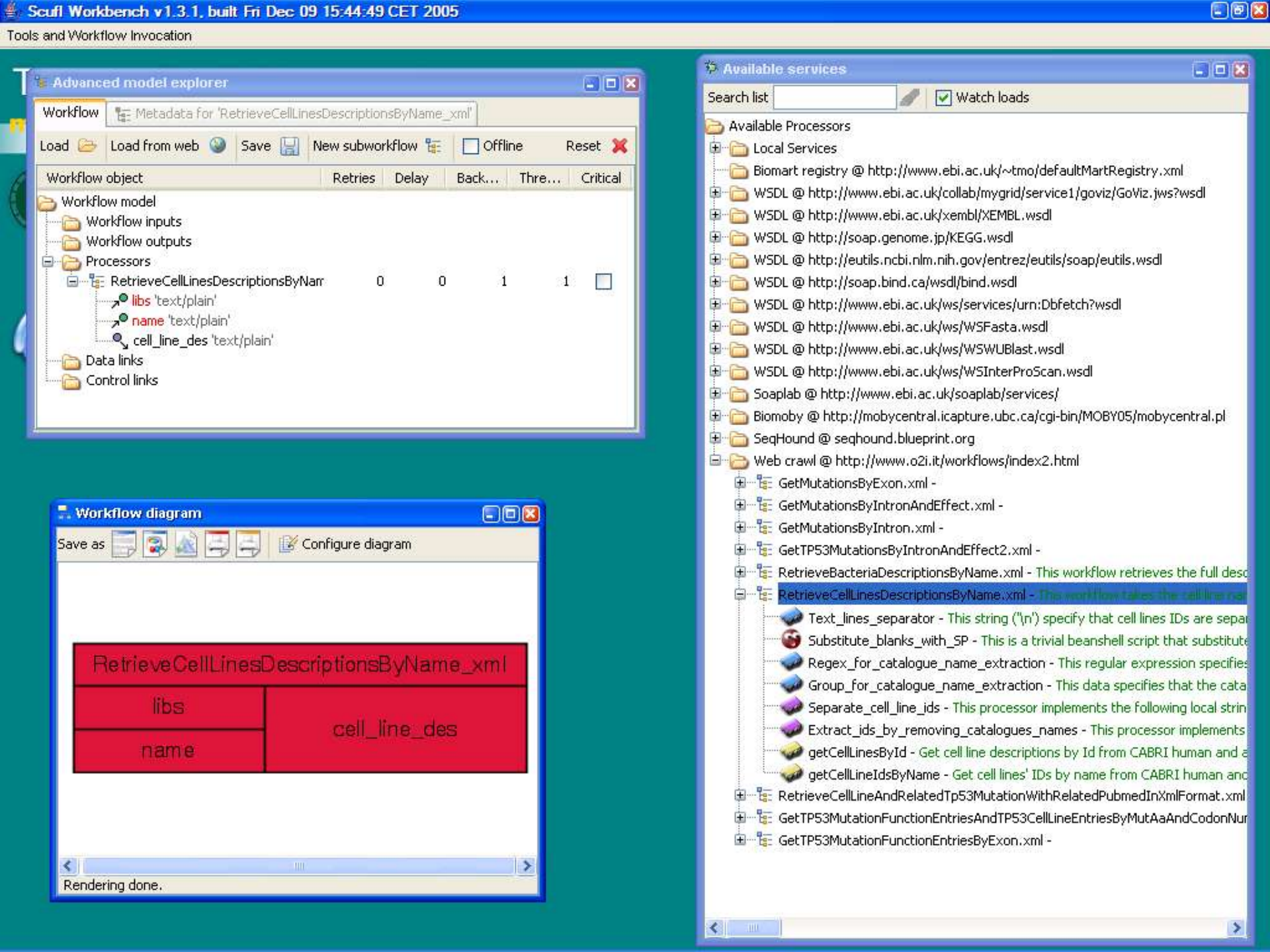
Workflow diagram

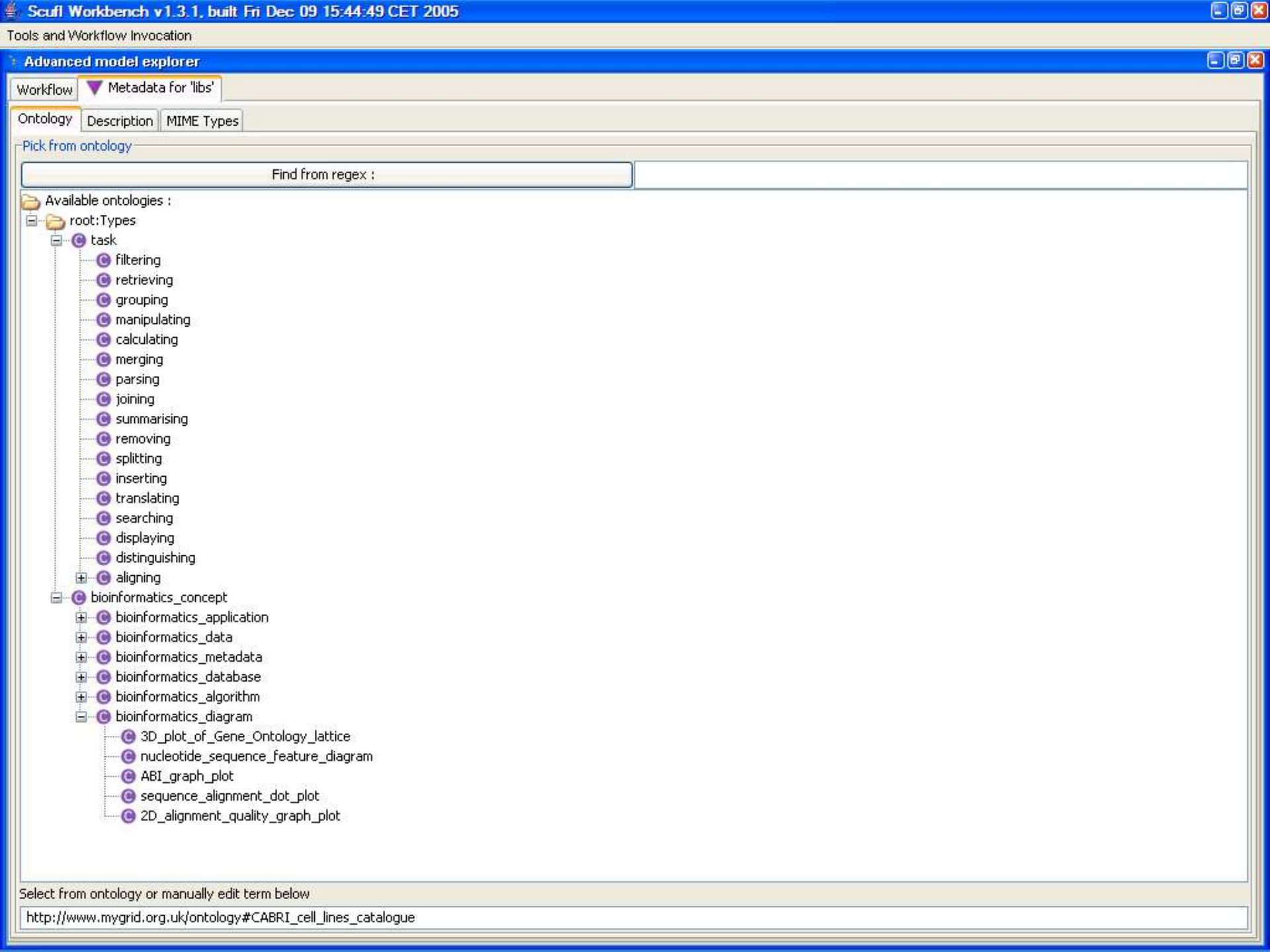
Save as | Configure diagram



Rendering done.

Available services


Scufl Workbench v1.3.1, built Fri Dec 09 15:44:49 CET 2005
Tools and Workflow Invocation
Advanced model explorer
Workflow
Metadata for 'RetrieveCellLinesDescriptionsByName_xml'
Load
Load from web
Save
New subworkflow
Offline
Reset
Workflow object
Retries
Delay
Back...
Thre...
Critical
Workflow model
Workflow inputs
Workflow outputs
Processors
RetrieveCellLinesDescriptionsByNam
0
0
1
1
libs 'text/plain'
name 'text/plain'
cell_line_des 'text/plain'
Data links
Control links
Workflow diagram
Save as
Configure diagram
RetrieveCellLinesDescriptionsByName_xml
libs
name
cell_line_des
Rendering done.
Available services
Search list
Watch loads
Available Processors
Local Services
Biomart registry @ http://www.ebi.ac.uk/~tmo/defaultMartRegistry.xml
WSDL @ http://www.ebi.ac.uk/collab/mygrid/service1/goviz/GoViz.jws?wsdl
WSDL @ http://www.ebi.ac.uk/xembl/XEMBL.wsdl
WSDL @ http://soap.genome.jp/KEGG.wsdl
WSDL @ http://eutils.ncbi.nlm.nih.gov/entrez/eutils/soap/eutils.wsdl
WSDL @ http://soap.bind.ca/wsdl/bind.wsdl
WSDL @ http://www.ebi.ac.uk/ws/services/urn:Dbfetch?wsdl
WSDL @ http://www.ebi.ac.uk/ws/WSFasta.wsdl
WSDL @ http://www.ebi.ac.uk/ws/WSWUBlast.wsdl
WSDL @ http://www.ebi.ac.uk/ws/WSInterProScan.wsdl
Soaplab @ http://www.ebi.ac.uk/soaplab/services/
Biomoby @ http://mobycentral.icapture.ubc.ca/cgi-bin/MOBY05/mobycentral.pl
SeqHound @ seqhound.blueprint.org
Web crawl @ http://www.o2i.it/workflows/index2.html
GetMutationsByExon.xml -
GetMutationsByIntronAndEffect.xml -
GetMutationsByIntron.xml -
GetTP53MutationsByIntronAndEffect2.xml -
RetrieveBacteriaDescriptionsByName.xml - This workflow retrieves the full desc
RetrieveCellLinesDescriptionsByName.xml -
Text_lines_separator - This string ("\n") specify that cell lines IDs are separ
Substitute_blanks_with_SP - This is a trivial beanshell script that substitute
Regex_for_catalogue_name_extraction - This regular expression specifies
Group_for_catalogue_name_extraction - This data specifies that the cata
Separate_cell_line_ids - This processor implements the following local strin
Extract_ids_by_removing_catalogues_names - This processor implements
getCellLinesById - Get cell line descriptions by Id from CABRI human and a
getCellLineIdsByName - Get cell lines' IDs by name from CABRI human and
RetrieveCellLineAndRelatedTp53MutationWithRelatedPubmedInXmlFormat.xml
GetTP53MutationFunctionEntriesAndTP53CellLineEntriesByMutAaAndCodonNur
GetTP53MutationFunctionEntriesByExon.xml -


Scufl Workbench v1.3.1, built Fri Dec 09 15:44:49 CET 2005
Tools and Workflow Invocation
Advanced model explorer
Workflow
Metadata for 'libs'
Ontology
Description
MIME Types
Pick from ontology
Find from regex :
Available ontologies :
root:Types
task
filtering
retrieving
grouping
manipulating
calculating
merging
parsing
joining
summarising
removing
splitting
inserting
translating
searching
displaying
distinguishing
aligning
bioinformatics_concept
bioinformatics_application
bioinformatics_data
bioinformatics_metadata
bioinformatics_database
bioinformatics_algorithm
bioinformatics_diagram
3D_plot_of_Gene_Ontology_lattice
nucleotide_sequence_feature_diagram
ABI_graph_plot
sequence_alignment_dot_plot
2D_alignment_quality_graph_plot
Select from ontology or manually edit term below
http://www.mygrid.org.uk/ontology#CABRI_cell_lines_catalogue

Scufl Workbench v1.3.1, built Fri Dec 09 15:44:49 CET 2005

Tools and Workflow Invocation

Advanced model explorer

Workflow | Remote resource usage

Save HTML description

Workflow information

This report applies to the workflow titled 'Search CABRI human and animal cell lines catalogues by cell line name and retrieve full cell line descriptions' authored by 'Paolo Romano, IST, Genova, Italy (paolo.romano@istge.it)' and with LSID 'urn:lsid:www.mygrid.org.uk:operation:US38XCRXJA0'. The textual description, if any is shown below :

> *This workflow takes the cell line name and the catalogue(s) name(s) as input and retrieve the full cell line description(s) by first retrieving the cell lines' unique IDs associated with the input (done via a call to the getCellLineIdsByName web service) and then using IDs for retrieving the full cell lines descriptions (done via a call to the getCellLinesById's web service).*

Resource usage report

This display shows the various external resources used by the current workflow. It does not show resources such as local operations or string constants which are run within the enactment engine. Services are categorized by resource host and type, and the name of the instance of each service shown to the right.

Resources on **www.o2i.it**, 2 instances.		
Soaplab	Service rooted at */axis/services*	
	App category and name	Processors
	/axis/services/cabri::getCellLineIdsByName	getCellLineIdsByName
	/axis/services/cabri::getCellLinesById	getCellLinesById

Oncology over Internet (O_2I)

We designed a web system that:

- allows for the carrying out of a set of predefined workflows (of oncology interest)
- supports workflows annotation by using a simple ontology for bioinformatics processors (domain, task, i/o)
- implements search of workflows on the basis of their annotation
- supports retrieval of workflows based on users' registration and profiling
- allows storing and retrieval of workflows' executions and related results

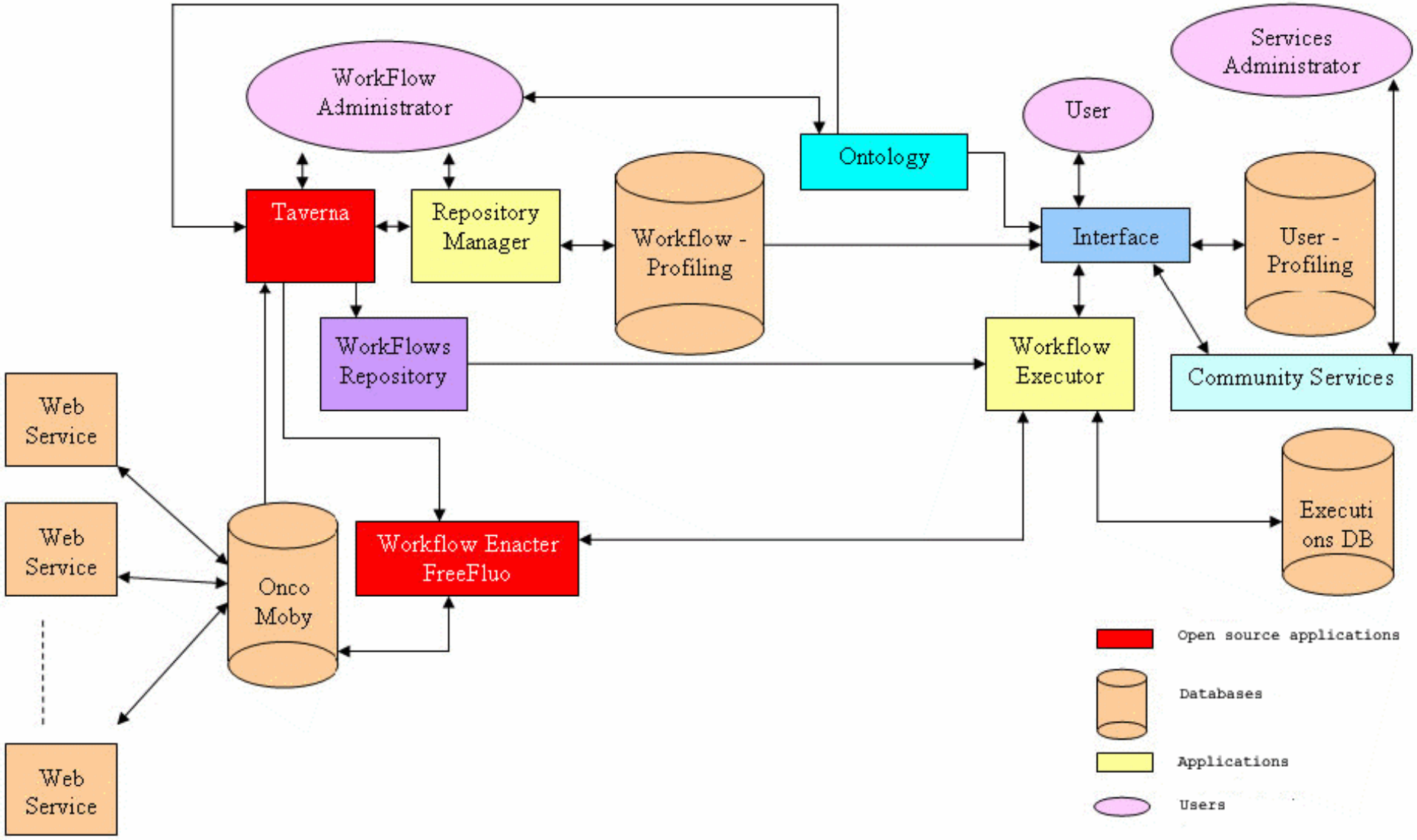
Oncology over Internet (O_2I)

We designed a web system that:

- makes access to and retrieves data from Web Services and registries of Web Services
- stores workflows using the Simple conceptual unified flow language (Scufl) format
- is partially based on open source tools (Taverna WB, FreeFluo and mySQL)

Prototype available on-line: http://www.o2i.it:8080/portal/

O_2I architecture



Predefined workflows

Workflows are:

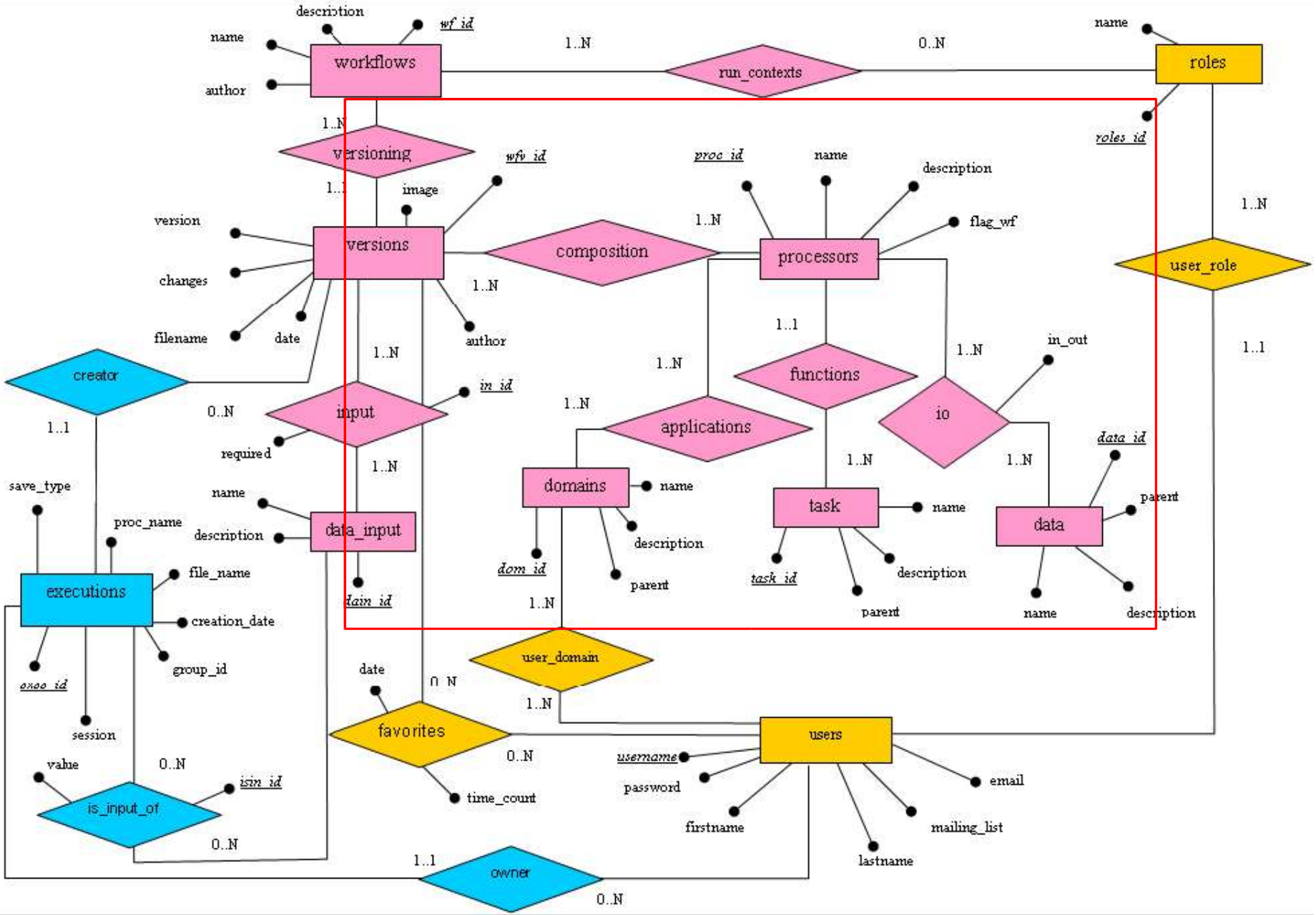
- created by internal staff using Taverna
- stored in Scufl format
- maintained (workflow vs version)
- submitted by:
  - users
  - service providers

Annotation of workflows

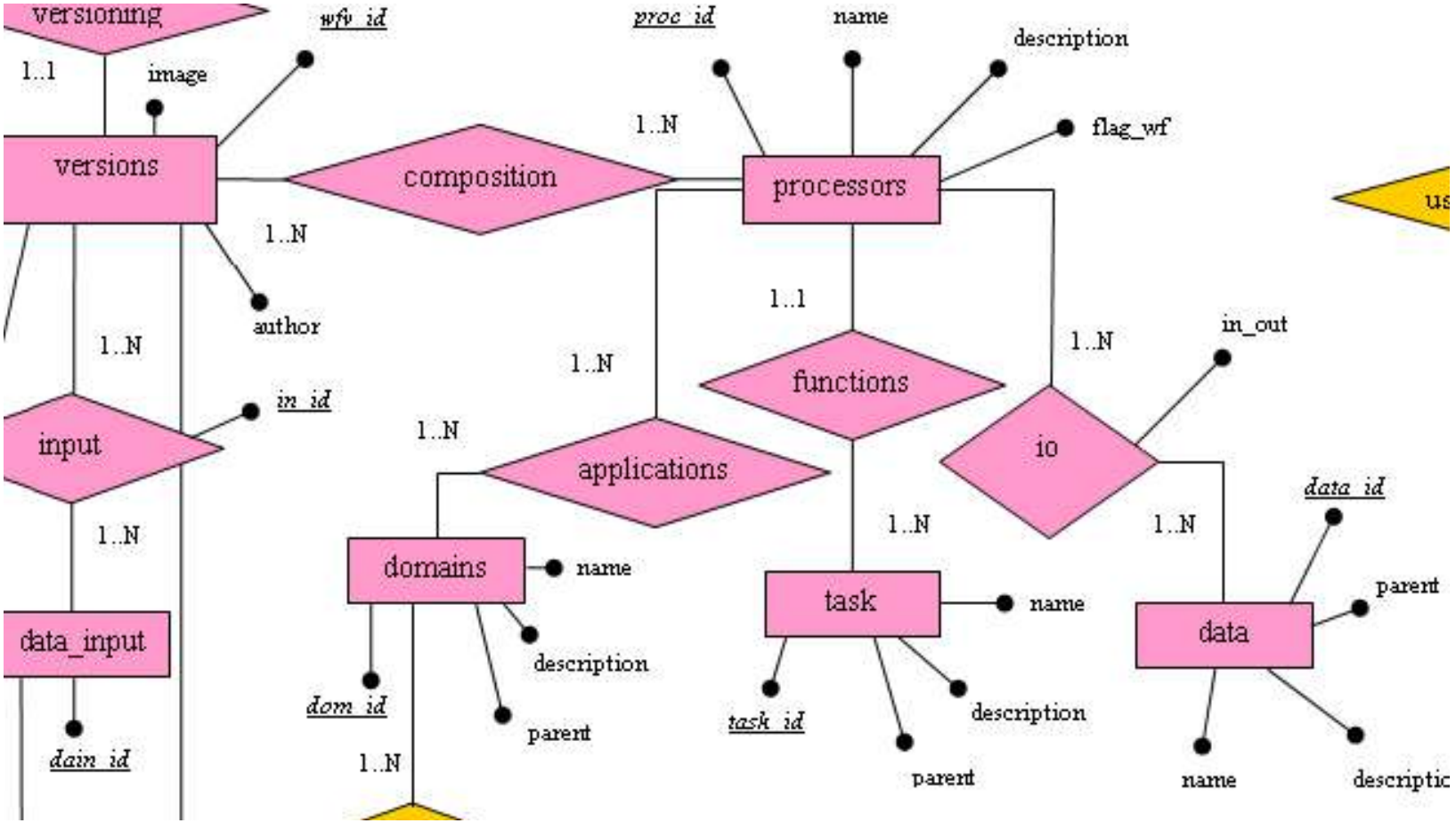
Workflows are annotated on the basis of:

- a simple ontology for bioinformatics processors:
  - application domains
  - task
  - inputs/outputs
- ontology derived from Taverna:
  - new structure
  - some additions (biological resources, images, …)
  - under further development

O_2I ERA schema



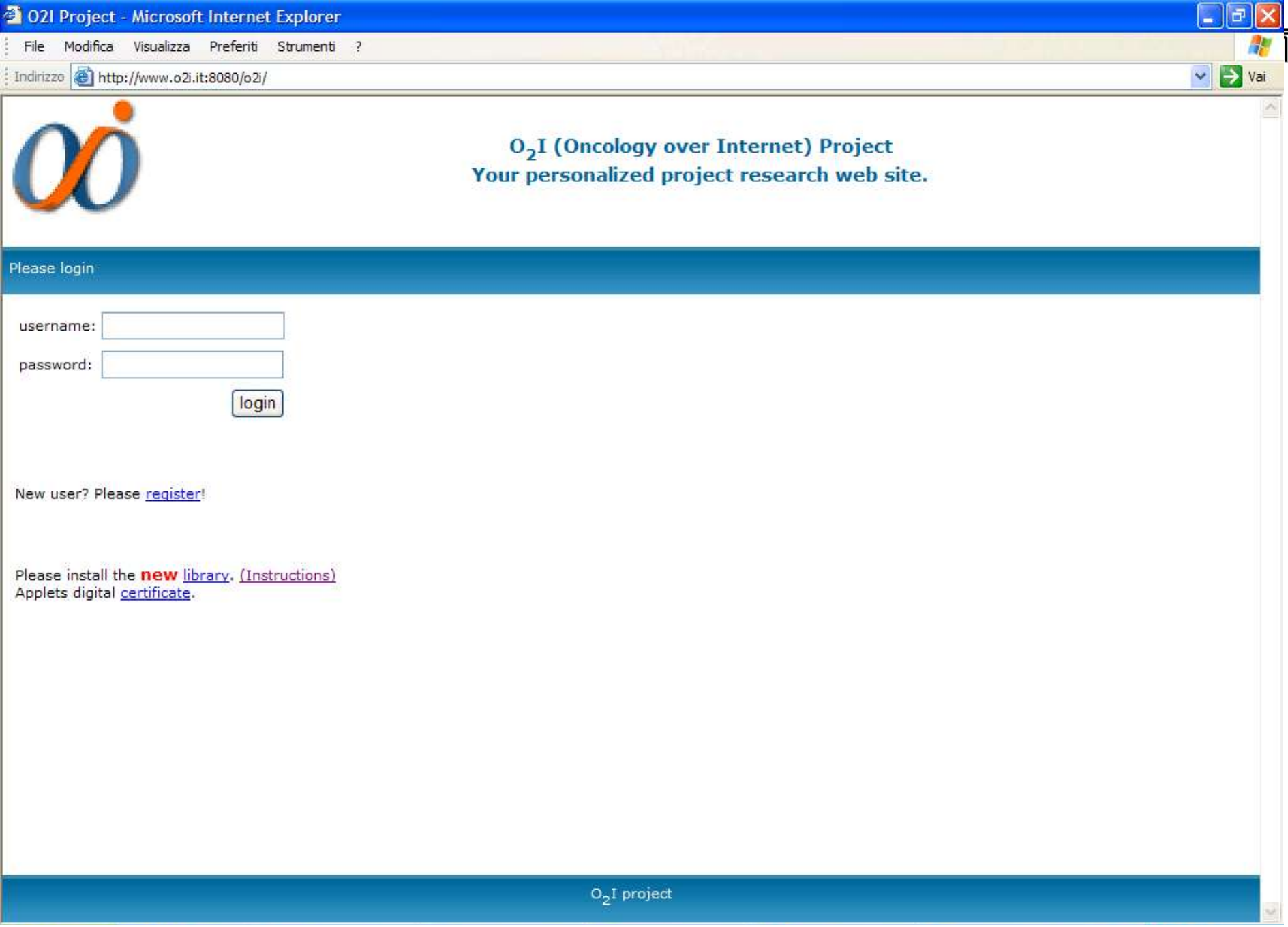
O_2I workflows annotation

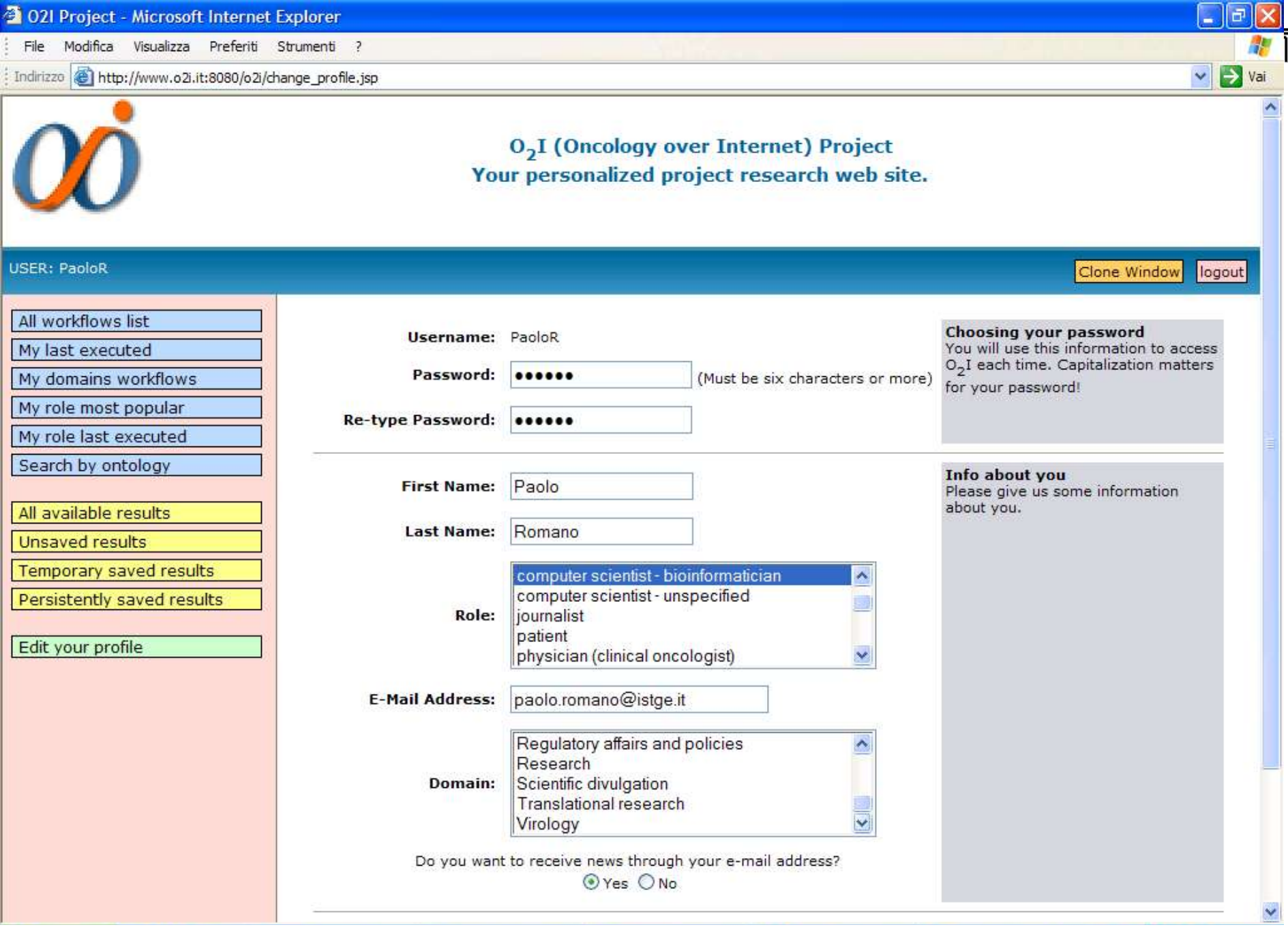


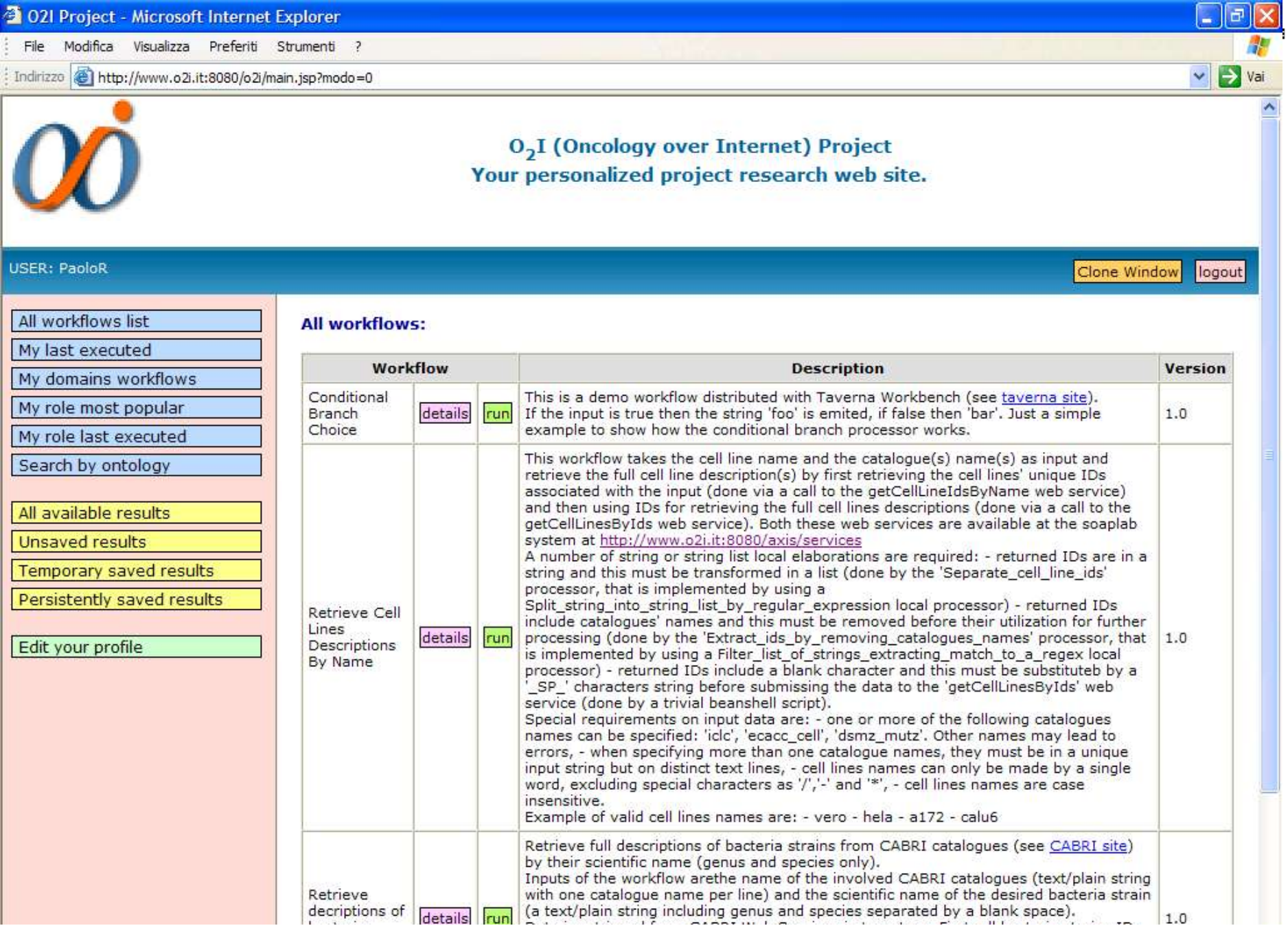
Users' registration and profiling

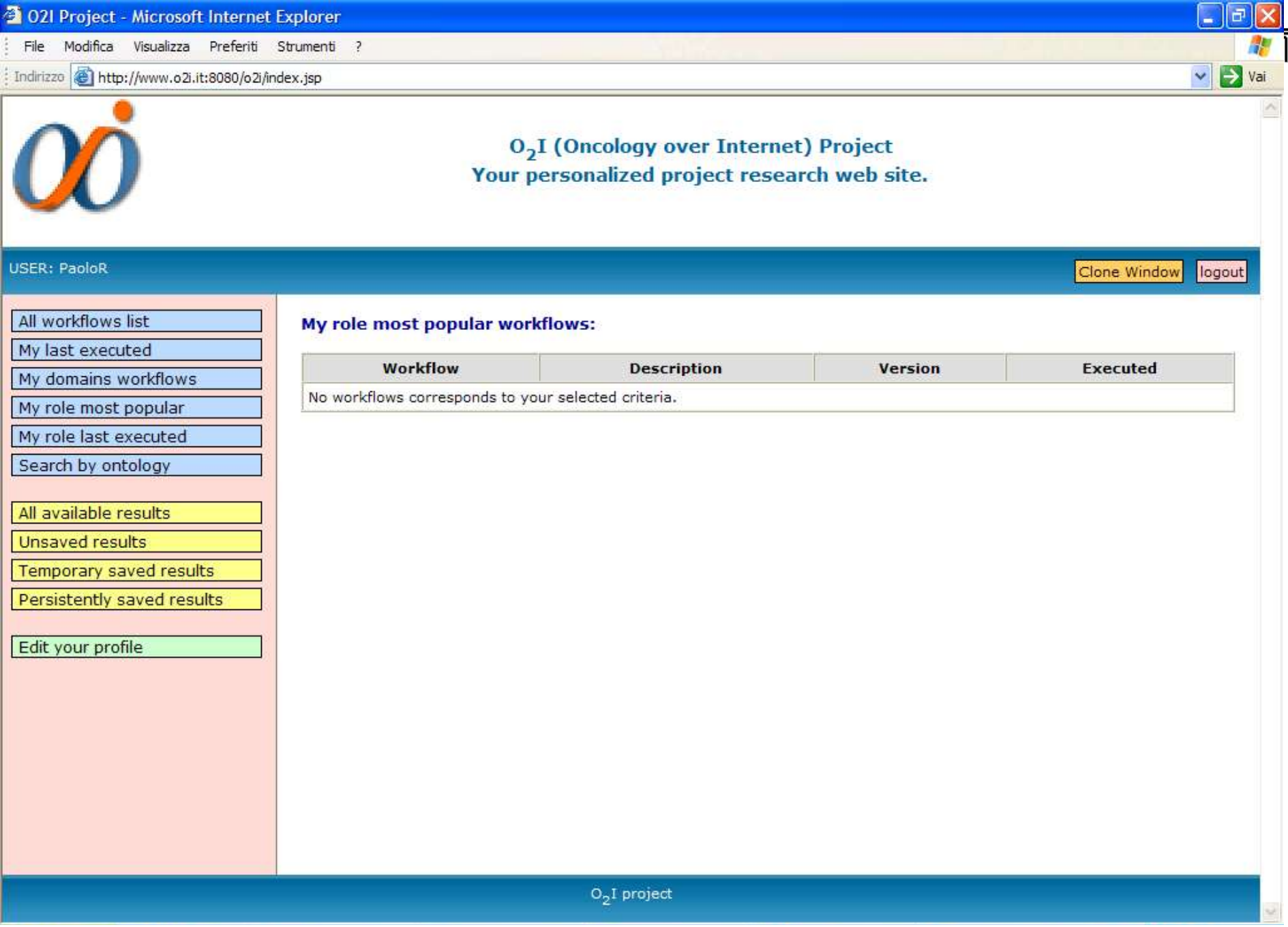
Users are profiled on the basis of:

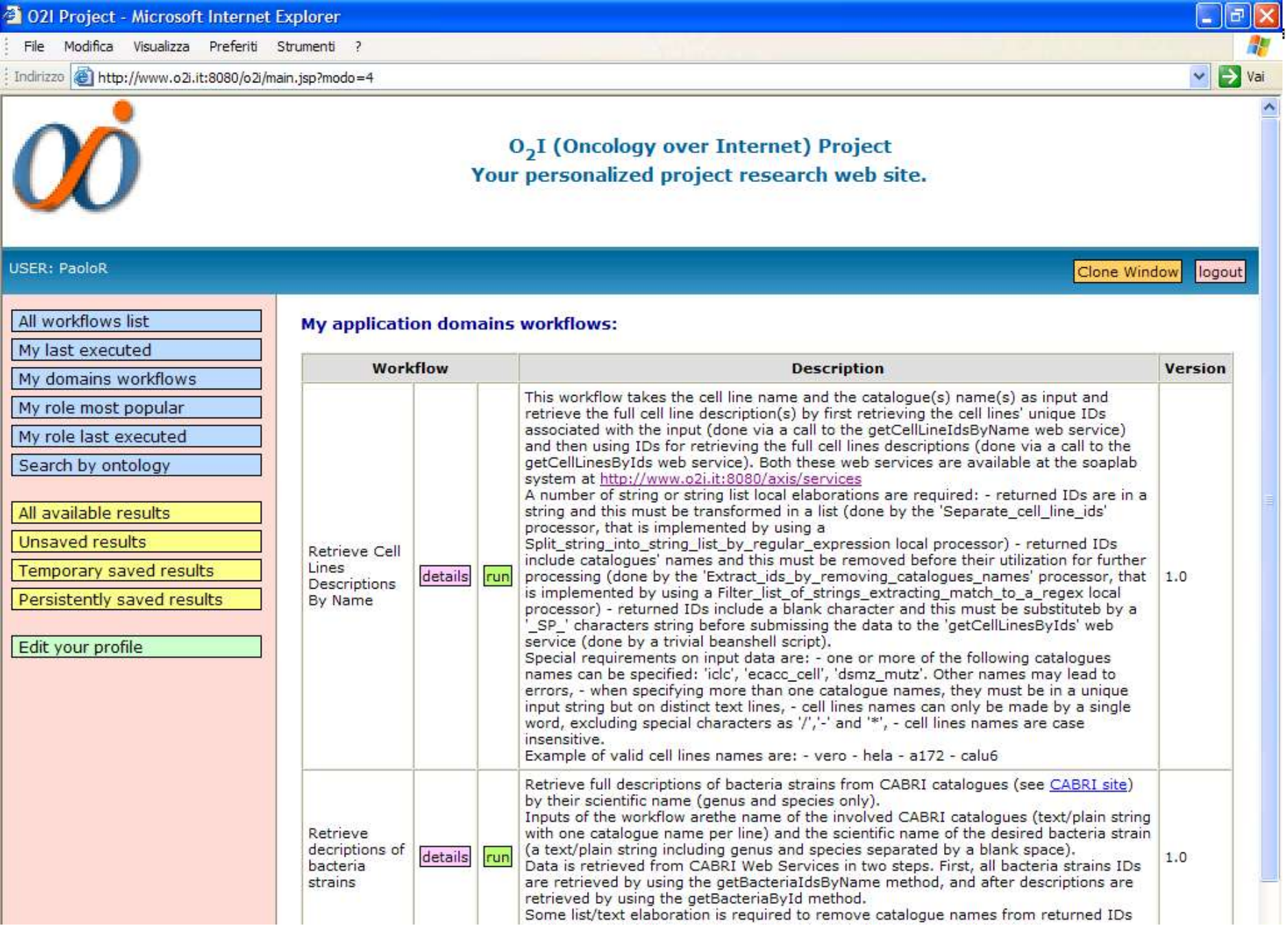
- role in their organization
  - computer scientist / physician / researcher / patient / journalist / …
- domains of interest
- past workflows' executions


O2I Project - Microsoft Internet Explorer
File Modifica Visualizza Preferiti Strumenti ?
Indirizzo http://www.o2i.it:8080/o2i/
Vai
O2I (Oncology over Internet) Project
Your personalized project research web site.
Please login
username:
password:
login
New user? Please register!
Please install the new library. (Instructions)
Applets digital certificate.
O2I project

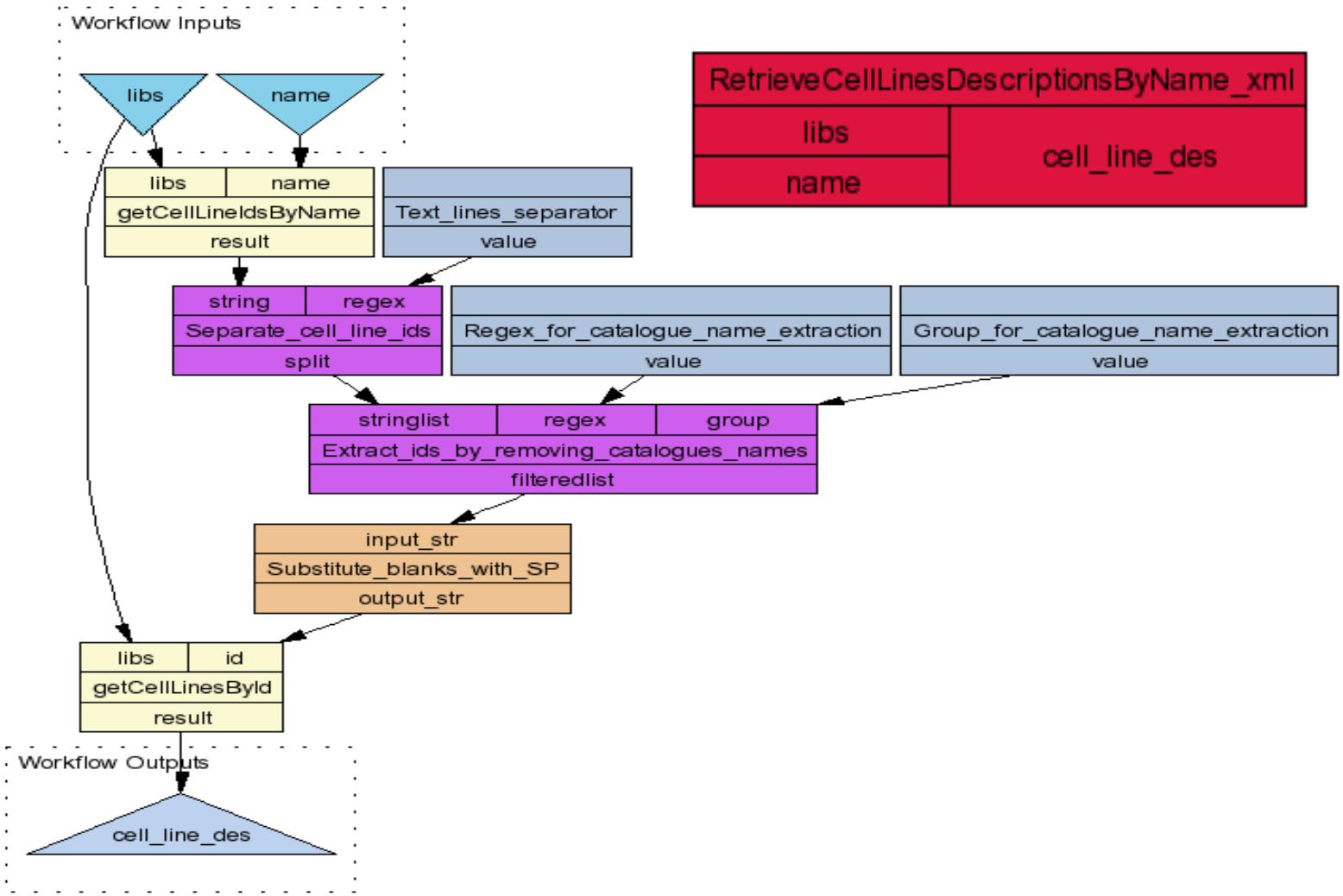

O2I Project - Microsoft Internet Explorer
File Modifica Visualizza Preferiti Strumenti ?
Indirizzo http://www.o2i.it:8080/o2i/change_profile.jsp
Vai
O2I (Oncology over Internet) Project
Your personalized project research web site.
USER: PaoloR
Clone Window
logout
All workflows list
My last executed
My domains workflows
My role most popular
My role last executed
Search by ontology
All available results
Unsaved results
Temporary saved results
Persistently saved results
Edit your profile
Username: PaoloR
Password: ••••••
(Must be six characters or more)
Re-type Password: ••••••
Choosing your password
You will use this information to access O2I each time. Capitalization matters for your password!
First Name: Paolo
Last Name: Romano
Role:
computer scientist - bioinformatician
computer scientist - unspecified
journalist
patient
physician (clinical oncologist)
E-Mail Address: paolo.romano@istge.it
Info about you
Please give us some information about you.
Domain:
Regulatory affairs and policies
Research
Scientific divulgation
Translational research
Virology
Do you want to receive news through your e-mail address?
Yes
No

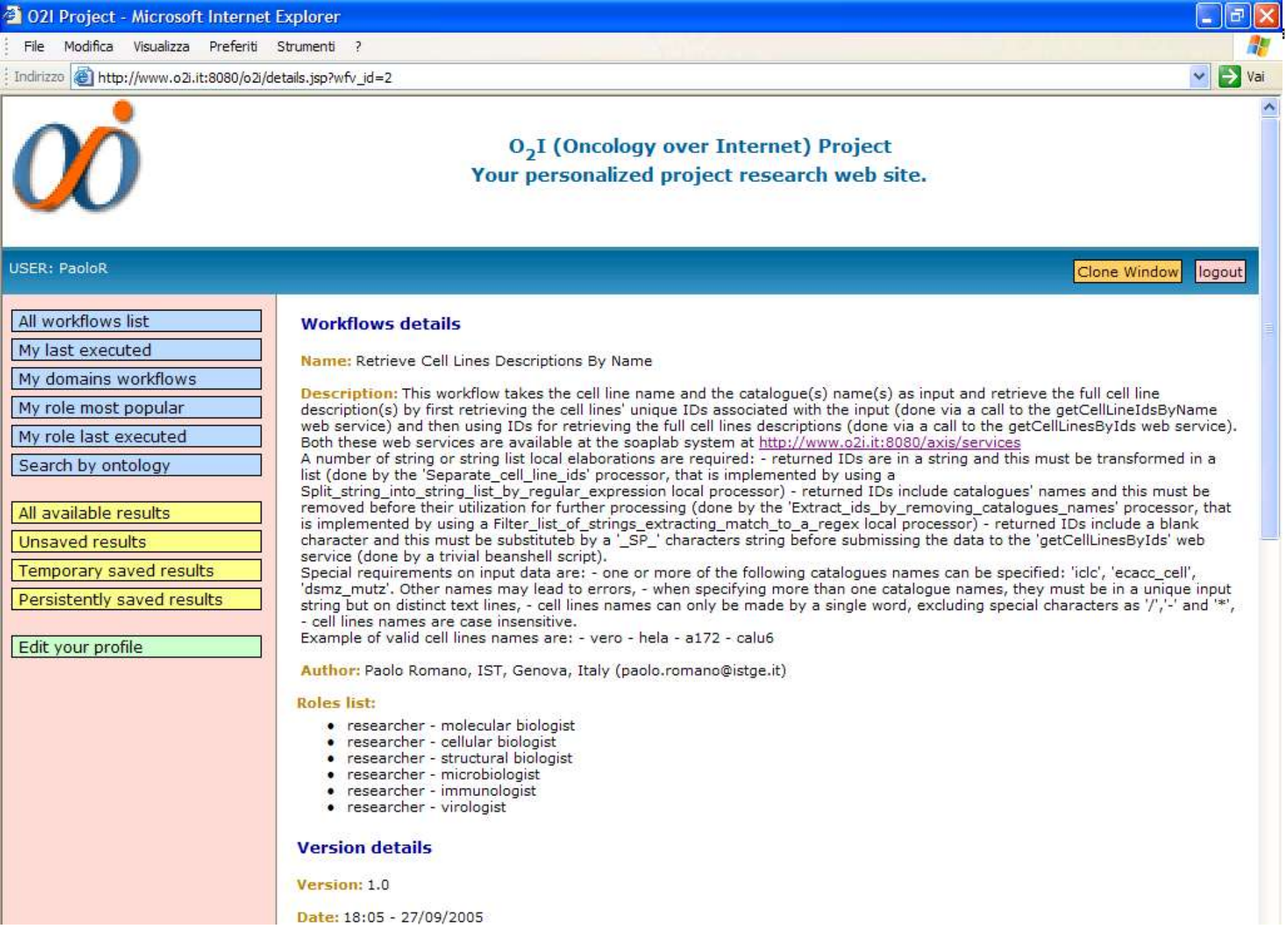

O2I Project - Microsoft Internet Explorer
File Modifica Visualizza Preferiti Strumenti ?
Indirizzo http://www.o2i.it:8080/o2i/main.jsp?modo=0
Vai
O2I (Oncology over Internet) Project
Your personalized project research web site.
USER: PaoloR
Clone Window
logout
All workflows list
My last executed
My domains workflows
My role most popular
My role last executed
Search by ontology
All available results
Unsaved results
Temporary saved results
Persistently saved results
Edit your profile
All workflows:
Workflow
Description
Version
Conditional Branch Choice
details
run
This is a demo workflow distributed with Taverna Workbench (see taverna site). If the input is true then the string 'foo' is emited, if false then 'bar'. Just a simple example to show how the conditional branch processor works.
1.0
Retrieve Cell Lines Descriptions By Name
details
run
This workflow takes the cell line name and the catalogue(s) name(s) as input and retrieve the full cell line description(s) by first retrieving the cell lines' unique IDs associated with the input (done via a call to the getCellLineIdsByName web service) and then using IDs for retrieving the full cell lines descriptions (done via a call to the getCellLinesByIds web service). Both these web services are available at the soaplab system at http://www.o2i.it:8080/axis/services
A number of string or string list local elaborations are required: - returned IDs are in a string and this must be transformed in a list (done by the 'Separate_cell_line_ids' processor, that is implemented by using a Split_string_into_string_list_by_regular_expression local processor) - returned IDs include catalogues' names and this must be removed before their utilization for further processing (done by the 'Extract_ids_by_removing_catalogues_names' processor, that is implemented by using a Filter_list_of_strings_extracting_match_to_a_regex local processor) - returned IDs include a blank character and this must be substituteb by a '_SP_' characters string before submissing the data to the 'getCellLinesByIds' web service (done by a trivial beanshell script).
Special requirements on input data are: - one or more of the following catalogues names can be specified: 'iclc', 'ecacc_cell', 'dsmz_mutz'. Other names may lead to errors, - when specifying more than one catalogue names, they must be in a unique input string but on distinct text lines, - cell lines names can only be made by a single word, excluding special characters as '/','-' and '*', - cell lines names are case insensitive.
Example of valid cell lines names are: - vero - hela - a172 - calu6
1.0
Retrieve decriptions of
details
run
Retrieve full descriptions of bacteria strains from CABRI catalogues (see CABRI site) by their scientific name (genus and species only).
Inputs of the workflow arethe name of the involved CABRI catalogues (text/plain string with one catalogue name per line) and the scientific name of the desired bacteria strain (a text/plain string including genus and species separated by a blank space).
1.0


O2I Project - Microsoft Internet Explorer
File Modifica Visualizza Preferiti Strumenti ?
Indirizzo http://www.o2i.it:8080/o2i/index.jsp
Vai
O2I (Oncology over Internet) Project
Your personalized project research web site.
USER: PaoloR
Clone Window
logout
All workflows list
My last executed
My domains workflows
My role most popular
My role last executed
Search by ontology
All available results
Unsaved results
Temporary saved results
Persistently saved results
Edit your profile
My role most popular workflows:
Workflow
Description
Version
Executed
No workflows corresponds to your selected criteria.
O2I project


O2I Project - Microsoft Internet Explorer
File Modifica Visualizza Preferiti Strumenti ?
Indirizzo http://www.o2i.it:8080/o2i/main.jsp?modo=4
Vai
O2I (Oncology over Internet) Project
Your personalized project research web site.
USER: PaoloR
Clone Window
logout
All workflows list
My last executed
My domains workflows
My role most popular
My role last executed
Search by ontology
All available results
Unsaved results
Temporary saved results
Persistently saved results
Edit your profile
My application domains workflows:
Workflow
Description
Version
Retrieve Cell Lines Descriptions By Name
details
run
This workflow takes the cell line name and the catalogue(s) name(s) as input and retrieve the full cell line description(s) by first retrieving the cell lines' unique IDs associated with the input (done via a call to the getCellLineIdsByName web service) and then using IDs for retrieving the full cell lines descriptions (done via a call to the getCellLinesByIds web service). Both these web services are available at the soaplab system at http://www.o2i.it:8080/axis/services
A number of string or string list local elaborations are required: - returned IDs are in a string and this must be transformed in a list (done by the 'Separate_cell_line_ids' processor, that is implemented by using a Split_string_into_string_list_by_regular_expression local processor) - returned IDs include catalogues' names and this must be removed before their utilization for further processing (done by the 'Extract_ids_by_removing_catalogues_names' processor, that is implemented by using a Filter_list_of_strings_extracting_match_to_a_regex local processor) - returned IDs include a blank character and this must be substituteb by a '_SP_' characters string before submissing the data to the 'getCellLinesByIds' web service (done by a trivial beanshell script).
Special requirements on input data are: - one or more of the following catalogues names can be specified: 'iclc', 'ecacc_cell', 'dsmz_mutz'. Other names may lead to errors, - when specifying more than one catalogue names, they must be in a unique input string but on distinct text lines, - cell lines names can only be made by a single word, excluding special characters as '/','-' and '*', - cell lines names are case insensitive.
Example of valid cell lines names are: - vero - hela - a172 - calu6
1.0
Retrieve decriptions of bacteria strains
details
run
Retrieve full descriptions of bacteria strains from CABRI catalogues (see CABRI site) by their scientific name (genus and species only).
Inputs of the workflow arethe name of the involved CABRI catalogues (text/plain string with one catalogue name per line) and the scientific name of the desired bacteria strain (a text/plain string including genus and species separated by a blank space).
Data is retrieved from CABRI Web Services in two steps. First, all bacteria strains IDs are retrieved by using the getBacteriaIdsByName method, and after descriptions are retrieved by using the getBacteriaById method.
Some list/text elaboration is required to remove catalogue names from returned IDs
1.0

Simple demo workflow

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File Modifica Visualizza Preferiti Strumenti ?
Indirizzo http://www.o2i.it:8080/o2i/details.jsp?wfv_id=2
Vai
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logout
All workflows list
My last executed
My domains workflows
My role most popular
My role last executed
Search by ontology
All available results
Unsaved results
Temporary saved results
Persistently saved results
Edit your profile
Workflows details
Name: Retrieve Cell Lines Descriptions By Name
Description: This workflow takes the cell line name and the catalogue(s) name(s) as input and retrieve the full cell line description(s) by first retrieving the cell lines' unique IDs associated with the input (done via a call to the getCellLineIdsByName web service) and then using IDs for retrieving the full cell lines descriptions (done via a call to the getCellLinesByIds web service). Both these web services are available at the soaplab system at http://www.o2i.it:8080/axis/services
A number of string or string list local elaborations are required: - returned IDs are in a string and this must be transformed in a list (done by the 'Separate_cell_line_ids' processor, that is implemented by using a Split_string_into_string_list_by_regular_expression local processor) - returned IDs include catalogues' names and this must be removed before their utilization for further processing (done by the 'Extract_ids_by_removing_catalogues_names' processor, that is implemented by using a Filter_list_of_strings_extracting_match_to_a_regex local processor) - returned IDs include a blank character and this must be substituteb by a '_SP_' characters string before submissing the data to the 'getCellLinesByIds' web service (done by a trivial beanshell script).
Special requirements on input data are: - one or more of the following catalogues names can be specified: 'iclc', 'ecacc_cell', 'dsmz_mutz'. Other names may lead to errors, - when specifying more than one catalogue names, they must be in a unique input string but on distinct text lines, - cell lines names can only be made by a single word, excluding special characters as '/','-' and '*', - cell lines names are case insensitive.
Example of valid cell lines names are: - vero - hela - a172 - calu6
Author: Paolo Romano, IST, Genova, Italy (paolo.romano@istge.it)
Roles list:
researcher - molecular biologist
researcher - cellular biologist
researcher - structural biologist
researcher - microbiologist
researcher - immunologist
researcher - virologist
Version details
Version: 1.0
Date: 18:05 - 27/09/2005

- researcher - virologist

Version details

Version: 1.0

Date: 18:05 - 27/09/2005

Author: Paolo Romano, IST, Genova, Italy (paolo.romano@istge.it)

Filename: RetrieveCellLinesDescriptionsByName.xml

Changes: Original version

Image: show in a new window

Input list:

- biological resource database (required)
- cell line name (required)

Output list:

- CABRI human and animal cell lines record

Domains list:

- Microbiology
- Cellular Biology

Processors:
Please be advised that is only a list of main components of the workflow. They are not ordered.

Name	Description	Task	Domains	Inputs	Outputs
Get cell lines id by name	Retrieve CABRI cell lines' IDs after a search in CABRI Web Services by cell lines' name	biological resource retrieval	Microbiology Cellular Biology	biological resource database cell line name	biological resource identifier
Get cell lines descriptions by id	Retrieves cell lines' descriptions by CABRI id	biological resource retrieval	Microbiology Cellular Biology	biological resource database biological resource identifier	CABRI human and animal cell lines record

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Indirizzo http://www.o2i.it:8080/o2i/details.jsp?wfv_id=2

- researcher - virologist

Version details

Version: 1.0

Date: 18:05 - 27/09/2005

Author: Paolo Romano, IST, Genova, Ita

Filename: RetrieveCellLinesDescriptionsI

Changes: Original version

Image: show in a new window

Input list:

- biological resource database (requ
- cell line name (required)

Output list:

- CABRI human and animal cell lines

Domains list:

- Microbiology
- Cellular Biology

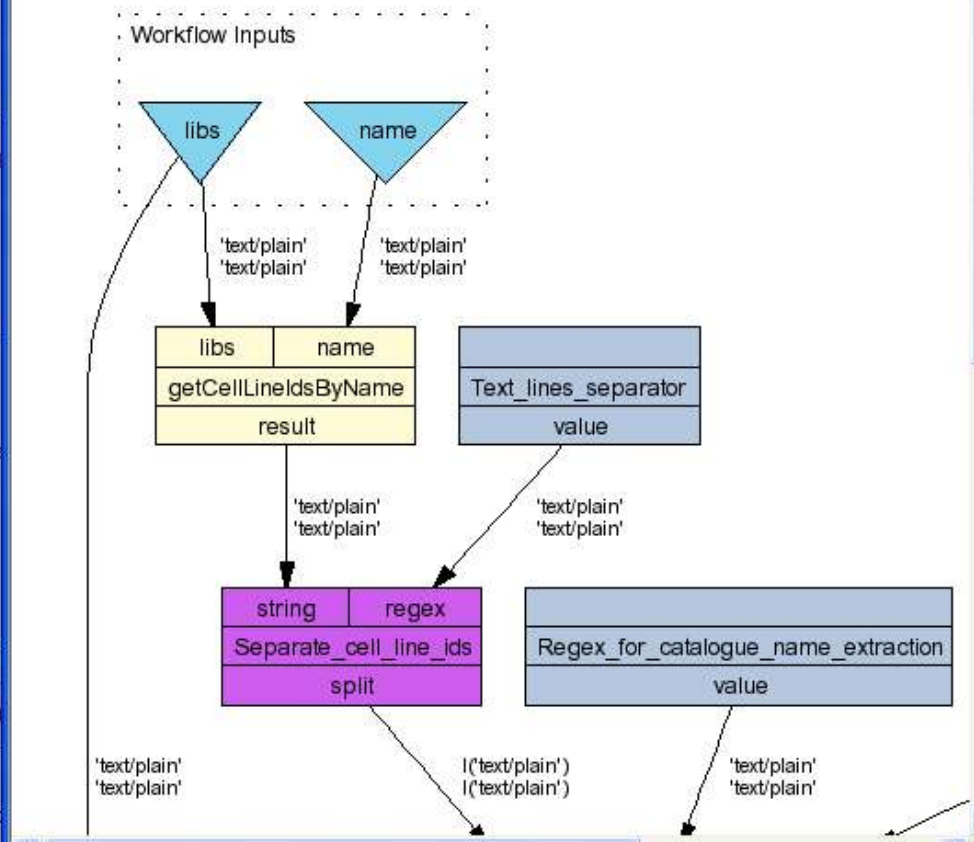
Processors:
Please be advised that is only a list of ma

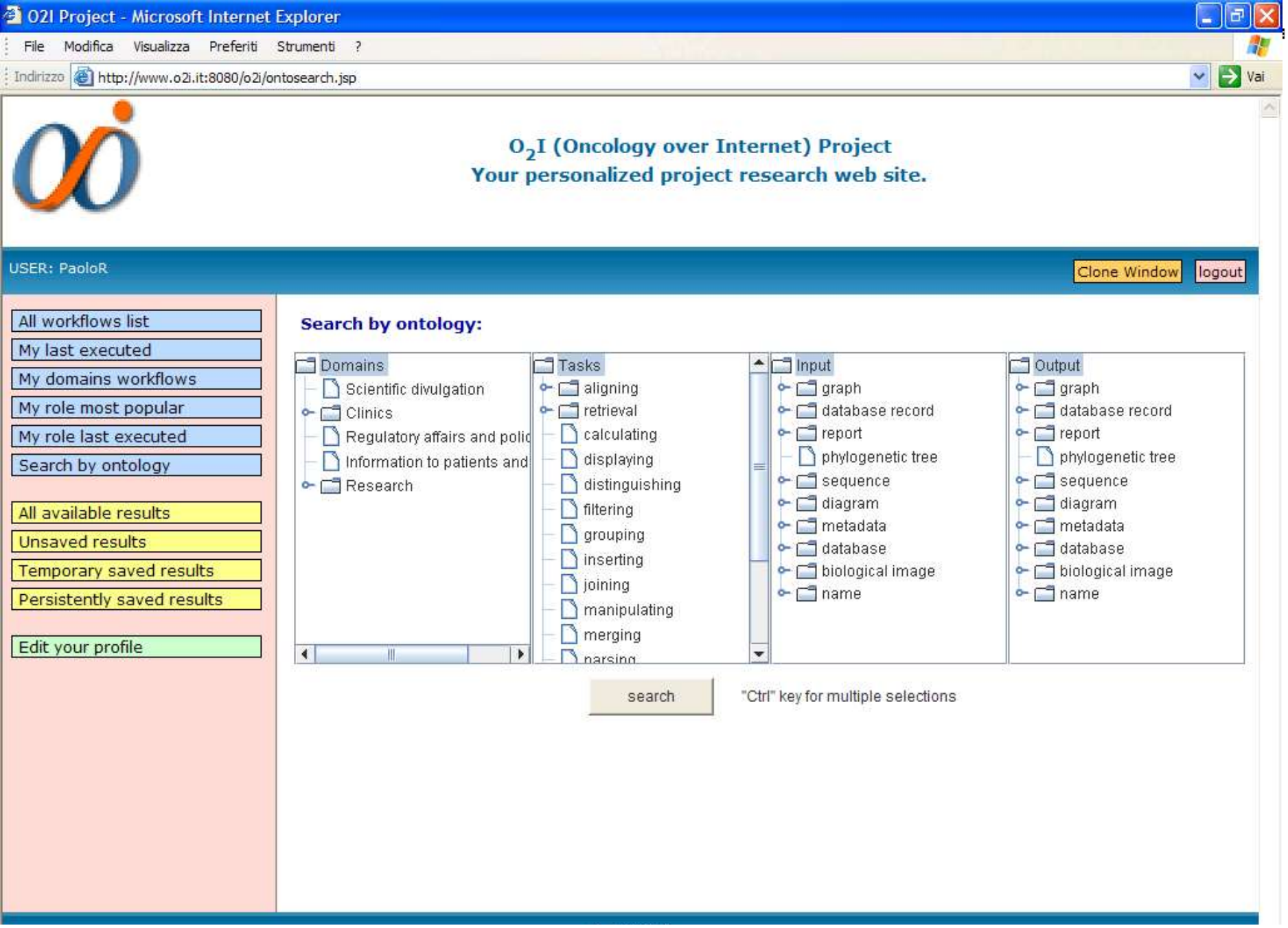
Name	Descript				
Get cell lines id by name	Retrieve CABRI c after a search in Services by cell				
Get cell lines descriptions by id	Retrieves cell lines' descriptions by CABRI id	biological resource retrieval	Microbiology Cellular Biology	biological resource database biological resource identifier	CABRI human and animal cell lines record

http://www.o2i.it:8080/o2i/wf_images/RetrieveCellLinesDescriptions...

File Modifica Visualizza Preferiti Strumenti ?

Indirizzo http://www.o2i.it:8080/o2i/wf_images/RetrieveCellLinesDescriptionsByName.png Vai

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File Modifica Visualizza Preferiti Strumenti ?
Indirizzo http://www.o2i.it:8080/o2i/ontosearch.jsp
Vai
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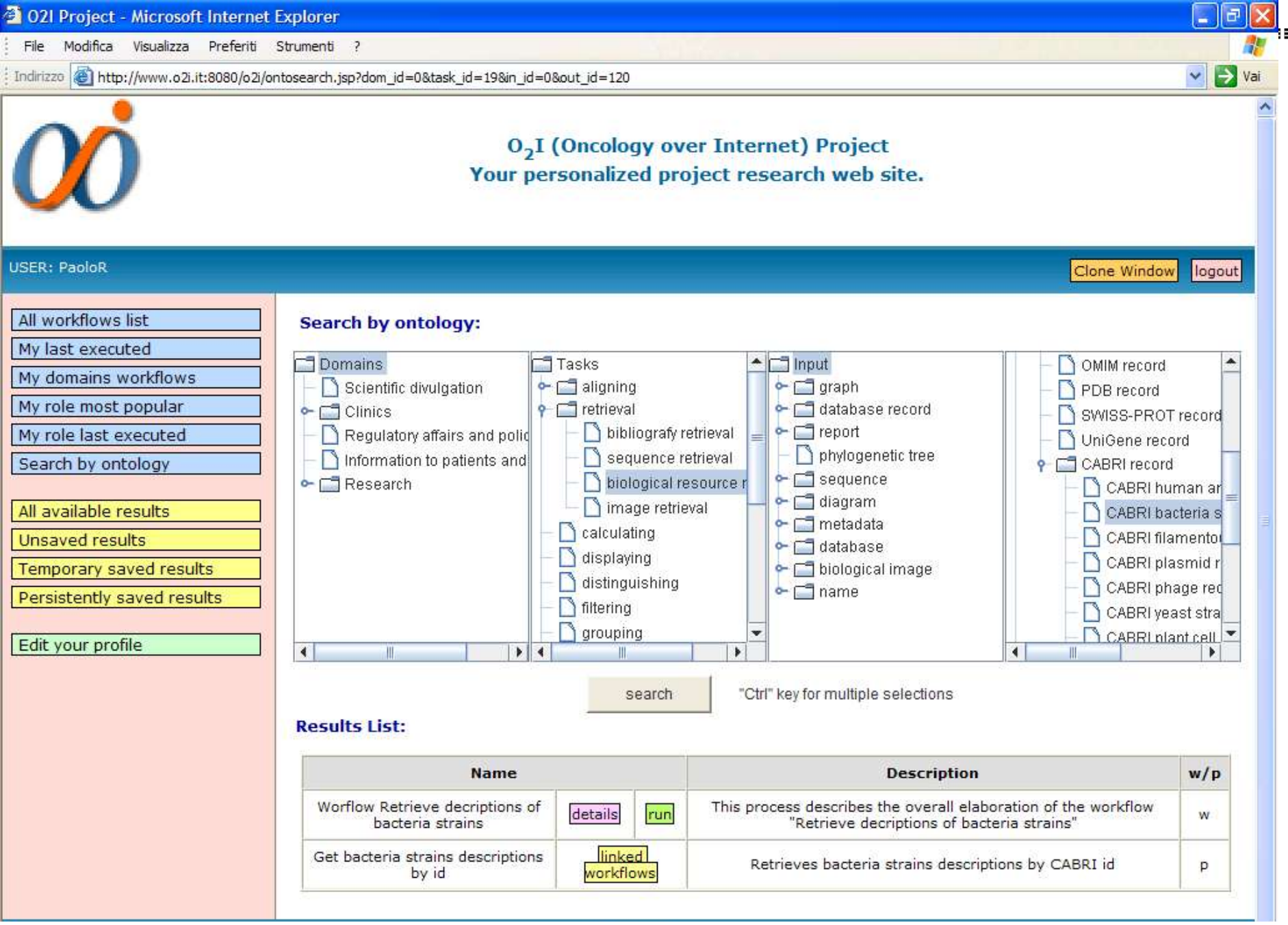
Clone Window
logout
All workflows list
My last executed
My domains workflows
My role most popular
My role last executed
Search by ontology
All available results
Unsaved results
Temporary saved results
Persistently saved results
Edit your profile
Search by ontology:
Domains
Scientific divulgation
Clinics
Regulatory affairs and polic
Information to patients and
Research
Tasks
aligning
retrieval
calculating
displaying
distinguishing
filtering
grouping
inserting
joining
manipulating
merging
parsing
Input
graph
database record
report
phylogenetic tree
sequence
diagram
metadata
database
biological image
name
Output
graph
database record
report
phylogenetic tree
sequence
diagram
metadata
database
biological image
name
search
"Ctrl" key for multiple selections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File Modifica Visualizza Preferiti Strumenti ?
Indirizzo http://www.o2i.it:8080/o2i/ontosearch.jsp?dom_id=0&task_id=19&in_id=0&out_id=120
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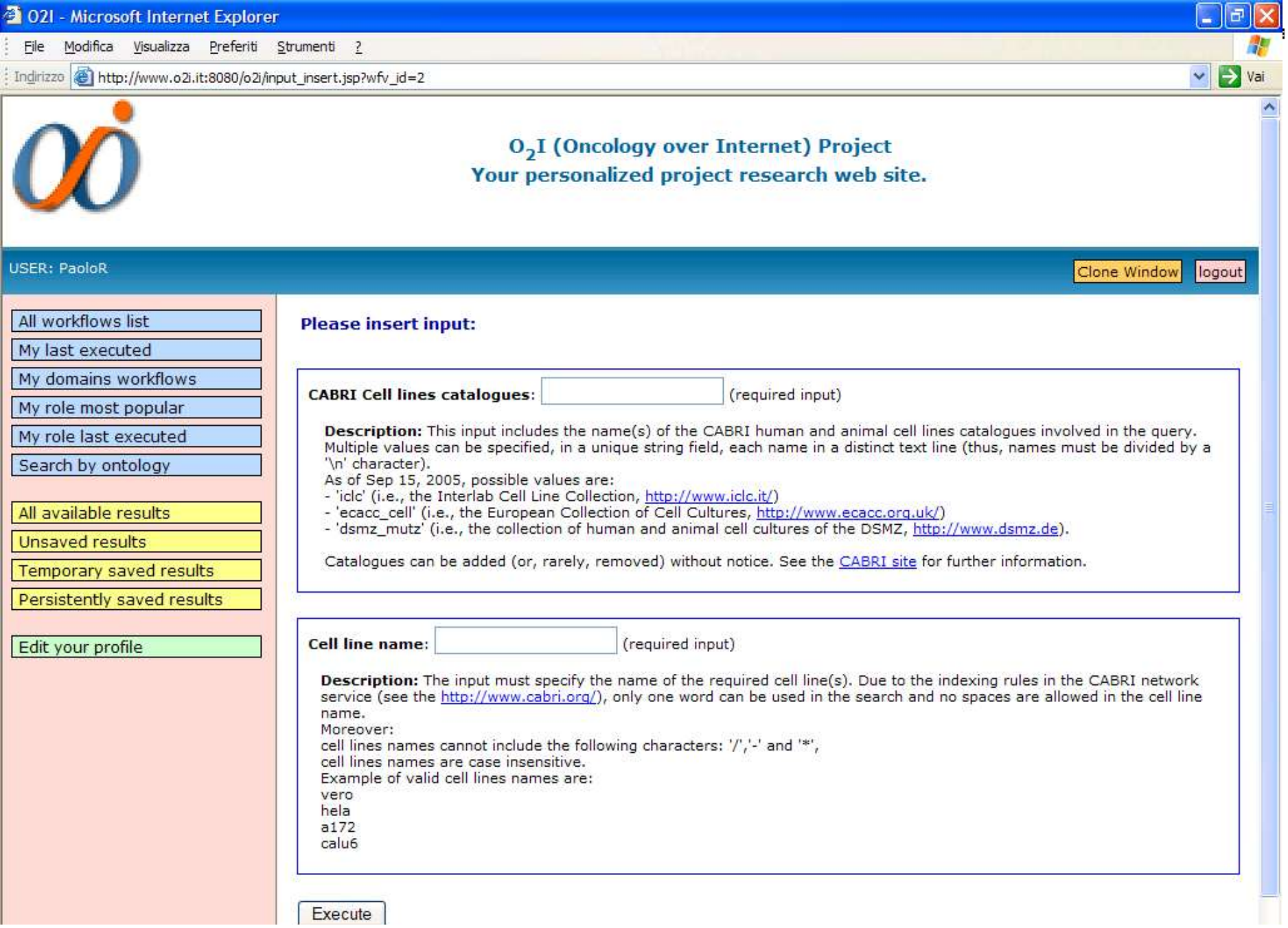
My last executed
My domains workflows
My role most popular
My role last executed
Search by ontology
All available results
Unsaved results
Temporary saved results
Persistently saved results
Edit your profile
Search by ontology:
Domains
Scientific divulgation
Clinics
Regulatory affairs and polic
Information to patients and
Research
Tasks
aligning
retrieval
bibliografy retrieval
sequence retrieval
biological resource r
image retrieval
calculating
displaying
distinguishing
filtering
grouping
Input
graph
database record
report
phylogenetic tree
sequence
diagram
metadata
database
biological image
name
OMIM record
PDB record
SWISS-PROT record
UniGene record
CABRI record
CABRI human ar
CABRI bacteria s
CABRI filamento
CABRI plasmid r
CABRI phage rec
CABRI yeast stra
CABRI plant cell
search
"Ctrl" key for multiple selections
Results List:
Name
Description
w/p
Worflow Retrieve decriptions of bacteria strains
details
run
This process describes the overall elaboration of the workflow "Retrieve decriptions of bacteria strains"
w
Get bacteria strains descriptions by id
linked workflows
Retrieves bacteria strains descriptions by CABRI id
p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File Modifica Visualizza Preferiti Strumenti ?
Indirizzo http://www.o2i.it:8080/o2i/input_insert.jsp?wfv_id=2
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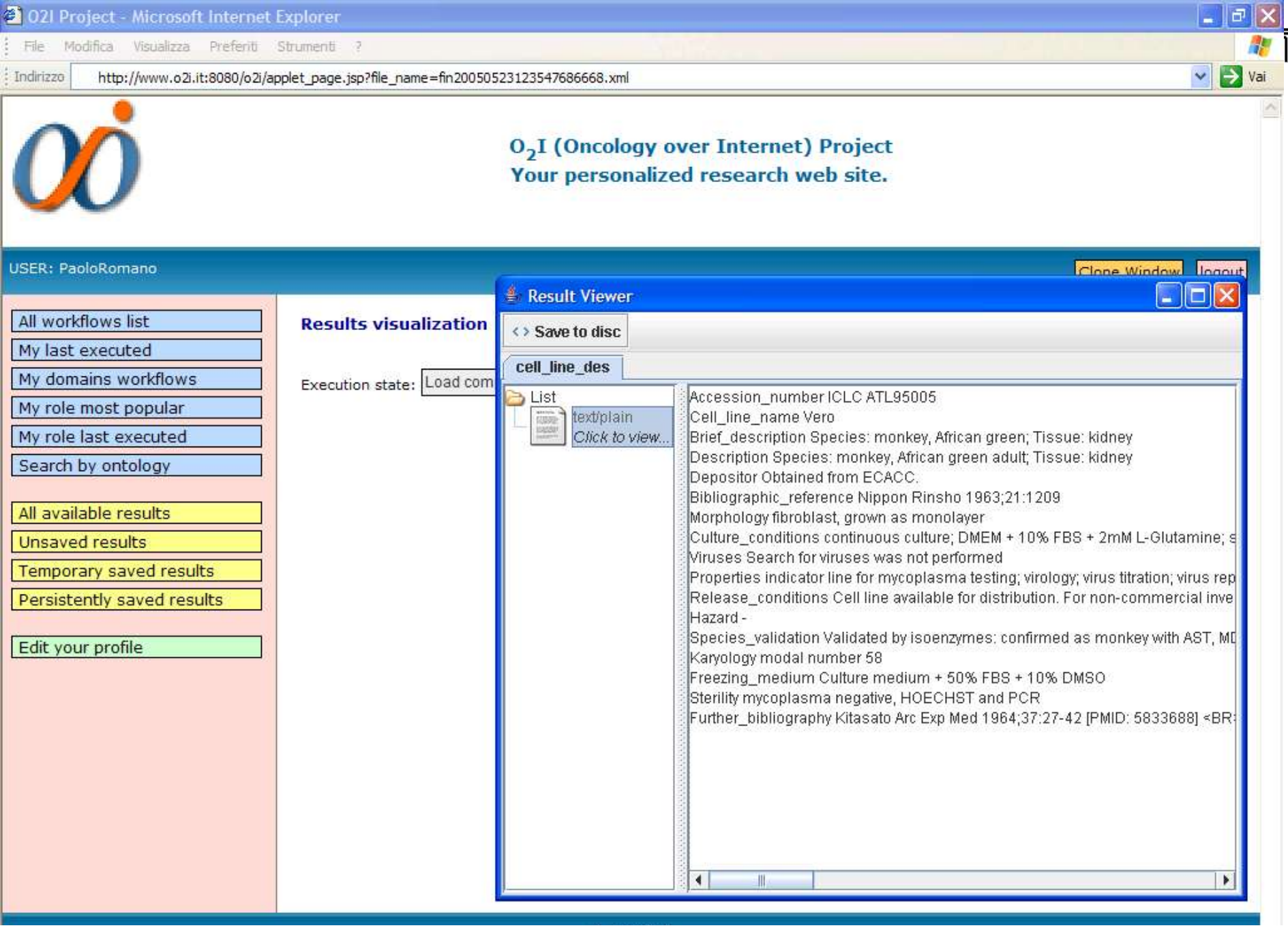
All workflows list
My last executed
My domains workflows
My role most popular
My role last executed
Search by ontology
All available results
Unsaved results
Temporary saved results
Persistently saved results
Edit your profile
Please insert input:
CABRI Cell lines catalogues: (required input)
Description: This input includes the name(s) of the CABRI human and animal cell lines catalogues involved in the query. Multiple values can be specified, in a unique string field, each name in a distinct text line (thus, names must be divided by a '\n' character).
As of Sep 15, 2005, possible values are:
- 'iclc' (i.e., the Interlab Cell Line Collection, http://www.iclc.it/)
- 'ecacc_cell' (i.e., the European Collection of Cell Cultures, http://www.ecacc.org.uk/)
- 'dsmz_mutz' (i.e., the collection of human and animal cell cultures of the DSMZ, http://www.dsmz.de).
Catalogues can be added (or, rarely, removed) without notice. See the CABRI site for further information.
Cell line name: (required input)
Description: The input must specify the name of the required cell line(s). Due to the indexing rules in the CABRI network service (see the http://www.cabri.org/), only one word can be used in the search and no spaces are allowed in the cell line name.
Moreover:
cell lines names cannot include the following characters: '/','-' and '*',
cell lines names are case insensitive.
Example of valid cell lines names are:
vero
hela
a172
calu6
Execute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Indirizzo http://www.o2i.it:8080/o2i/applet_page.jsp?file_name=fin20050523123547686668.xml
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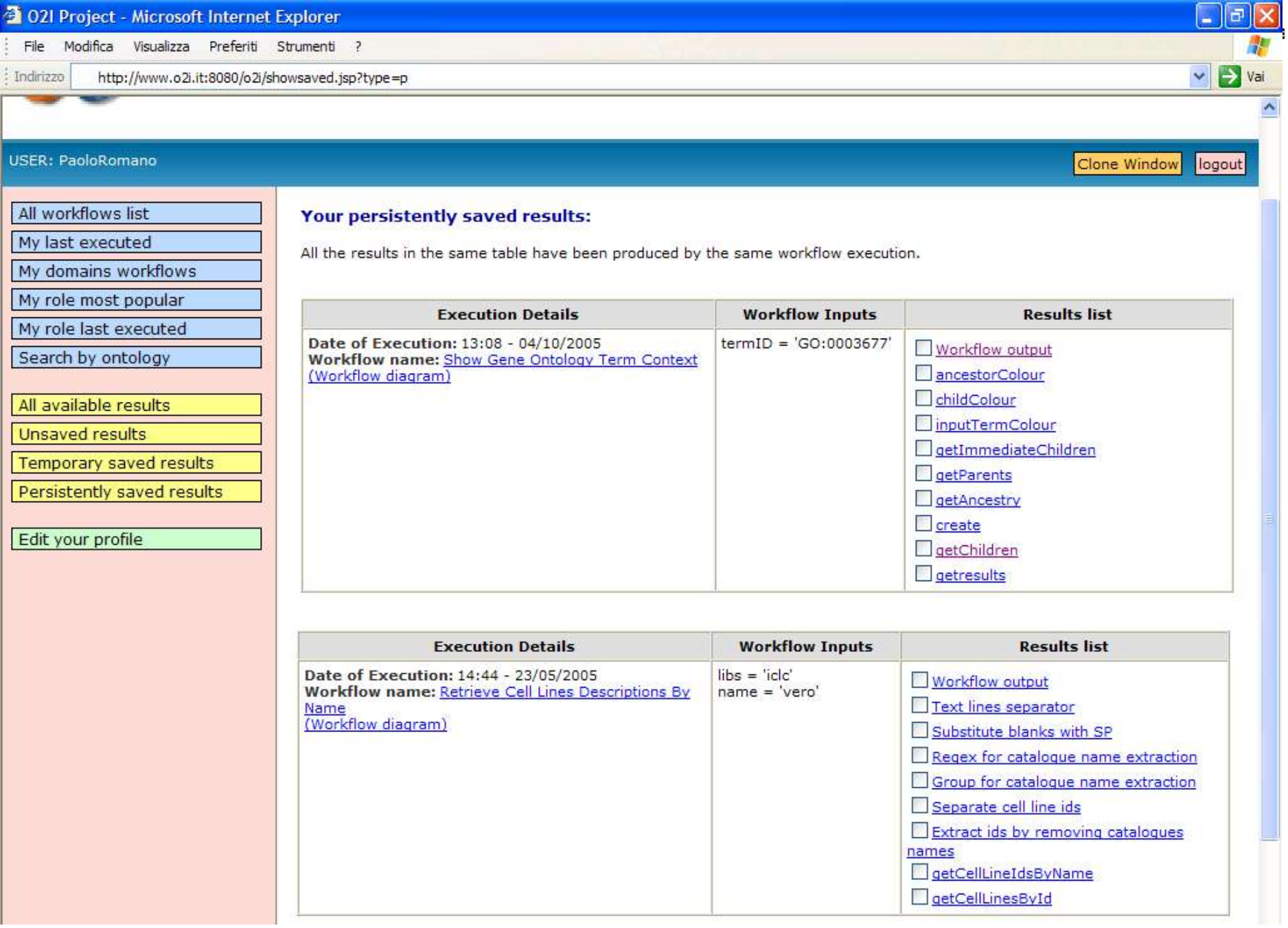
All workflows list
My last executed
My domains workflows
My role most popular
My role last executed
Search by ontology
All available results
Unsaved results
Temporary saved results
Persistently saved results
Edit your profile
Results visualization
Execution state:
Load com
Result Viewer
Save to disc
cell_line_des
List
text/plain
Click to view...
Accession_number ICLC ATL95005
Cell_line_name Vero
Brief_description Species: monkey, African green; Tissue: kidney
Description Species: monkey, African green adult; Tissue: kidney
Depositor Obtained from ECACC.
Bibliographic_reference Nippon Rinsho 1963;21:1209
Morphology fibroblast, grown as monolayer
Culture_conditions continuous culture; DMEM + 10% FBS + 2mM L-Glutamine; s
Viruses Search for viruses was not performed
Properties indicator line for mycoplasma testing; virology; virus titration; virus rep
Release_conditions Cell line available for distribution. For non-commercial inve
Hazard -
Species_validation Validated by isoenzymes: confirmed as monkey with AST, MD
Karyology modal number 58
Freezing_medium Culture medium + 50% FBS + 10% DMSO
Sterility mycoplasma negative, HOECHST and PCR
Further_bibliography Kitasato Arc Exp Med 1964;37:27-42 [PMID: 5833688] <BR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File Modifica Visualizza Preferiti Strumenti ?
Indirizzo http://www.o2i.it:8080/o2i/showsaved.jsp?type=p
Vai
USER: PaoloRomano
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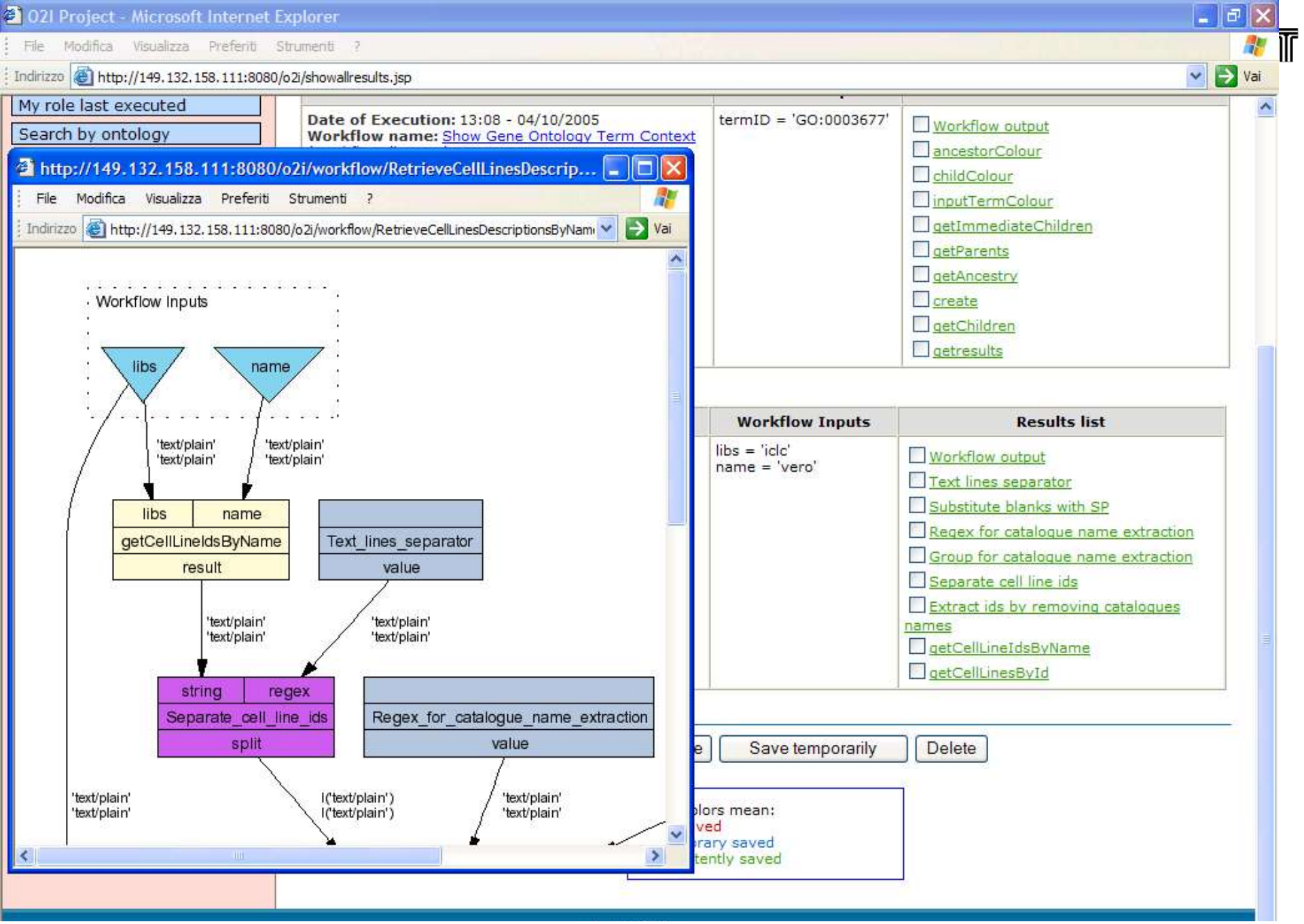
logout
All workflows list
My last executed
My domains workflows
My role most popular
My role last executed
Search by ontology
All available results
Unsaved results
Temporary saved results
Persistently saved results
Edit your profile
Your persistently saved results:
All the results in the same table have been produced by the same workflow execution.
Execution Details
Workflow Inputs
Results list
Date of Execution: 13:08 - 04/10/2005
Workflow name: Show Gene Ontology Term Context
(Workflow diagram)
termID = 'GO:0003677'
Workflow output
ancestorColour
childColour
inputTermColour
getImmediateChildren
getParents
getAncestry
create
getChildren
getresults
Execution Details
Workflow Inputs
Results list
Date of Execution: 14:44 - 23/05/2005
Workflow name: Retrieve Cell Lines Descriptions By Name
(Workflow diagram)
libs = 'iclc'
name = 'vero'
Workflow output
Text lines separator
Substitute blanks with SP
Regex for catalogue name extraction
Group for catalogue name extraction
Separate cell line ids
Extract ids by removing catalogues names
getCellLineIdsByName
getCellLinesById


O2I Project - Microsoft Internet Explorer
File Modifica Visualizza Preferiti Strumenti ?
Indirizzo http://149.132.158.111:8080/o2i/showallresults.jsp
Vai
My role last executed
Search by ontology
Date of Execution: 13:08 - 04/10/2005
Workflow name: Show Gene Ontology Term Context
termID = 'GO:0003677'
Workflow output
ancestorColour
childColour
inputTermColour
getImmediateChildren
getParents
getAncestry
create
getChildren
getresults
http://149.132.158.111:8080/o2i/workflow/RetrieveCellLinesDescrip...
File Modifica Visualizza Preferiti Strumenti ?
Indirizzo http://149.132.158.111:8080/o2i/workflow/RetrieveCellLinesDescriptionsByNam
Vai
Workflow Inputs
libs
name
'text/plain'
'text/plain'
'text/plain'
'text/plain'
libs
name
getCellLineIdsByName
result
Text_lines_separator
value
'text/plain'
'text/plain'
'text/plain'
'text/plain'
string
regex
Separate_cell_line_ids
split
Regex_for_catalogue_name_extraction
value
'text/plain'
'text/plain'
l('text/plain')
l('text/plain')
'text/plain'
'text/plain'
Workflow Inputs
Results list
libs = 'iclc'
name = 'vero'
Workflow output
Text lines separator
Substitute blanks with SP
Regex for catalogue name extraction
Group for catalogue name extraction
Separate cell line ids
Extract ids by removing catalogues names
getCellLineIdsByName
getCellLinesById
Save temporarily
Delete
lors mean:
ved
rary saved
tently saved

Some acknowledgements…

IST, Genoa
Paolo Romano,
Ulrich Pfeffer,
Domenico Marra,
Valentina Mirisola,
M. Assunta Manniello

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Matteo Fattore

ITB, CNR, Milan
Luciano Milanesi

DISCo, University of Milan Bicocca
Guglielmo Bertolini,
Flavio De Paoli,
Giancarlo Mauri

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Silvia Scaglione

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Ezio Bartocci

This work has partially been supported by the Italian Ministry for Education, University and Research (MIUR), projects "Oncology over Internet– O_2I" and "Laboratory for Interdisciplinary Technologies in Bioinformatics - LITBIO"

… and an announcement!

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