Running Galaxy workflows using the Clc Main Workbench

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July 2nd
Ablynx – company overview

Drug discovery and development company based in Ghent, Belgium

A pioneer in next generation biologics - Nanobodies®

Worldwide exclusive rights to commercialise Nanobody products in human healthcare

~25 programmes in the R&D pipeline

Two products achieved clinical proof-of-concepts in RA

6 Nanobody products in the clinic - 3 Phase II & 3 Phase I

Exclusive rights to >500 patent applications and granted patents

Partnerships with Boehringer Ingelheim, Merck Serono, Novartis and Merck & Co

Cash at 31 March 2013 of €82.2M

>250 employees
What?

- Transparently run Galaxy workflows in the Main Workbench of Clc bio
Why?

.Users don’t like change
  - Yet Another Tool to learn

User friendly
  - Stay in comfort zone
  - No copy/paste or (manual) export of data needed
How?

- Extend functionality of Main Workbench with plugin
  - SDK (http://www.clcbio.com/customized-solutions/software-developer-kit/)
  - blend4j (John Chilton)
    - Github (https://github.com/biologghe/blend4j)
How?

Steps executed by plugin

- Fasta Exporter plugin
  - Export to fasta
  - Create history
  - Upload fasta to Galaxy history
  - Launch Galaxy workflow

- Poll
  - Download Result dataset(s)
  - Import dataset

Importer plugin matching Galaxy datatype (set in configuration)

Clc Object parameter (eg. SequenceList)

Clc Object(s)
Configuration of Galaxy plugin

Galaxy data type mapping using importer and exporter plugins
Galaxy workflows in Toolbox
Set input parameters and launch
History is created

 Saved Histories

<table>
<thead>
<tr>
<th>Name</th>
<th>Datasets</th>
<th>Tags</th>
<th>Sharing</th>
<th>Size on Disk</th>
<th>Created</th>
<th>Last Updated</th>
<th>Status</th>
</tr>
</thead>
<tbody>
<tr>
<td>Galaxy Protein Net Charge Calculation Sun May 19 17:19:04 CEST 2013</td>
<td>2</td>
<td>0 Tags</td>
<td></td>
<td>36.7 KB</td>
<td>1 minute ago</td>
<td>1 minute ago</td>
<td>current history</td>
</tr>
<tr>
<td>Unnamed history</td>
<td></td>
<td>0 Tags</td>
<td></td>
<td>0 bytes</td>
<td>9 minutes ago</td>
<td>9 minutes ago</td>
<td>current history</td>
</tr>
</tbody>
</table>

For 0 selected histories: Rename Delete Delete Permanently Undelete

Histories that have been deleted for more than a time period specified by the Galaxy administrator(s) may be permanently deleted.
Result Dataset import and rendering

- As soon as workflow is finished, result is fetched, imported and rendered

- History visible in navigation area as well
Error handling

Galaxy workflow did not finish properly (status 'ERROR'):
Error for 'IEP table of data 1':
----------------------------- WARNING -----------------------------
MSG: Can not calculate net charge, sequence 'linker' is not protein

OK Cancel