Vernalis KNIME nodes

13th February 2014
James Davidson
About Vernalis

Organisation

• Revenue-generating small pharmaceutical company
• Based outside Cambridge, UK
• ~ 60 staff in Research
• In-house and collaborated drug discovery programmes

Areas of expertise

• Fragment methodology
• Structure-based design
• Structural biology
• Biophysical techniques

Using KNIME since 2010

• KNIME Server customers since Dec 2011
Vernalis KNIME nodes

Overview

- First node released in June 2012 (PDB Connector)
- Now extended with further released nodes, and internal nodes
- Became a Community Contribution in July 2013 (and now with ‘trusted’ status!)
Reproduces RCSB’s web interface for querying the PDB (http://www.pdb.org/pdb/search/advSearch.do)

Lots of possible output fields

Currently liaising with RCSB on a new POST accepting service – much faster

<table>
<thead>
<tr>
<th>POST (secs)</th>
<th>GET (secs)</th>
<th>Iteration</th>
</tr>
</thead>
<tbody>
<tr>
<td>7.533</td>
<td>206.666</td>
<td>0</td>
</tr>
<tr>
<td>7.734</td>
<td>314.979</td>
<td>1</td>
</tr>
<tr>
<td>7.053</td>
<td>208.224</td>
<td>2</td>
</tr>
<tr>
<td>7.443</td>
<td>189.497</td>
<td>3</td>
</tr>
<tr>
<td>6.593</td>
<td>461.388</td>
<td>4</td>
</tr>
<tr>
<td>7.393</td>
<td>224.173</td>
<td>5</td>
</tr>
<tr>
<td>8.034</td>
<td>410.88</td>
<td>6</td>
</tr>
<tr>
<td>7.132</td>
<td>175.411</td>
<td>7</td>
</tr>
<tr>
<td>13.663</td>
<td>174.911</td>
<td>8</td>
</tr>
<tr>
<td>7.842</td>
<td>175.539</td>
<td>9</td>
</tr>
</tbody>
</table>

Substructure query returning ~ 5600 hits

Downloader nodes that will download structures in numerous formats (PDB, Structure Factors, mmCIF, PDBx, FASTA)
Vernalis KNIME nodes

Local PDB Tools

- For transferring between PDB cells and PDB files
  *Local or remote files*
  *Text paths or URI cells*

- Extracts structural information from PDB cells
  *eg Resolution, Space Group, etc*
Extracts Sequence (and optionally header info) from FASTA sequence string cells
Vernalis KNIME nodes

Miscellaneous

- Simple interconversion between multi-line string cells and text files
- A ‘partner’ for KNIME’s List Files node
- It generates a column of random numbers...
- Connects to the ZBH’s SMARTSviewer service ([http://www.smartsview.de/](http://www.smartsview.de/))
Vernalis KNIME nodes

SMARTSviewer example
We also have a growing number of internal nodes.

Some of these will be incorporated into the Community Contributions soon.

*eg* Returns reference details as XML cells that can be parsed with XPATH, etc.
Acknowledgements

Vernalis

Steve Roughley
Richard Sherhod
(Dave Morley)

RCSB

For the PDB RESTful web service

University of Hamburg (ZBH)

For the SMARTSviewer web service

KNIME

Bernd et al. for excellent support

The KNIME Community

For so many useful contributions!

If you are staying for next week’s Developer training, please say “Hi” to Steve and Richard and feel free to quiz them more about the nodes!

Contact:
knime@vernalis.com

Forum:
http://tech.knime.org/forum/vernalis

Node Descriptions:
https://tech.knime.org/book/vernalis-nodes-for-knime-trusted-extension

Company website:
www.vernalis.com