MOCKUP – 1

Data Narratives

Data narratives for result: < Scientific workflow >

Data Narrative 1: Resource summary

The highly connected drugs result was generated in the Wings workflow system by execution 1348628778528 (See figure), which originated from the workflow template AbstractGlobalWorkflow2 (See figure). The file size is 1166 bytes and is stored in the Wings servers on the following location http://www.opmw.org/export /page/resource/WorkflowExecutionArtifact/DE58909D2E17DF26F0BF79D75E12C2D6. The DOI for the result file is: https://dx.doi.org/10.6084/m9.figshare.776887.v1

Data Narrative 2: Inputs and parameters used in the workflow to produce the resource

The highly connected drugs result was generated in the Wings workflow system by execution 1348628778528 (See figure), which originated from the workflow template AbstractGlobalWorkflow2 (See figure).

Several input datasets were used in the execution of the workflow, including the configuration file and the drugBindisngSites for for the CompareLigandBindingSitesV2 steps, the structureForComparison and structureForComparison1 for the CompareLigandBindingSitesV2 and ResultSorterV2 components, the tbProteinInfo and model_info datasets for the FormatStepToCompareDissimi ProteinStructures and FormatPDBToCompareProteinStructures abstract steps and the template_po and the drugKeys for the FormatPDBToCompareProteinStructures and countDrugs steps respectively. The parameter p-value was set up to 0,05.

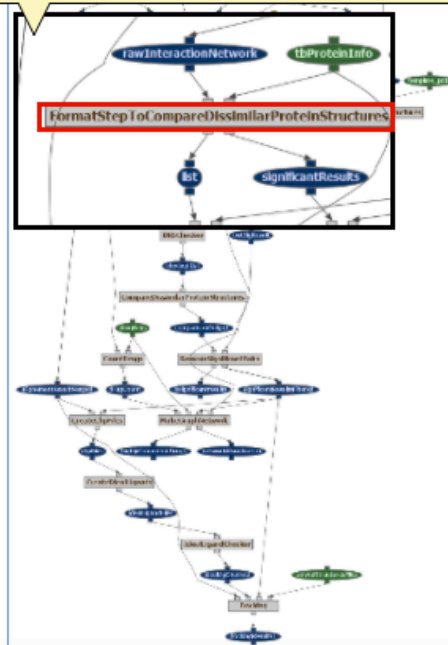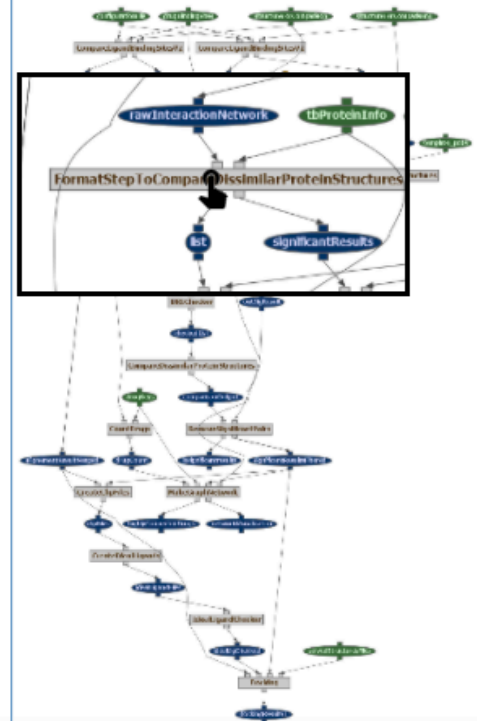### Data Narrative 3: Workflow's main steps.

The highly connected drugs result was generated by an execution of the workflow template AbstractGlobalWorkflow2 (See figure).

AbstractGlobalWorkflow2 performs three main types of analyses on the input data. First, the CompareLigandBindingSitesV2 components is applied, then the CompareDissimilarStructures and finally the Docking component produces the final results.

The highlyConnectedDrugs result is the output of the MakeGraphNetwork component, a visualization step.

Workflow Visualization (Abstract method)

Legend:
- Data Variable
- Parameter Variable
- Data Variable(Input)
- Process

- Linking visualization to the textual description of Data narratives is to be implemented initially.
- On hover over the workflow step in textual summary, corresponding step has to be highlighted on the workflow representation.
- An optional tooltip is provided with color coding representation used for different steps and inputs.

- When a workflow step hover takes place in the flow-chart representation, corresponding text on the summary is highlighted.
- The highlight has to happen for all occurrences of the process/input in every data narratives.