MOCKUP – 2

- On mouse hover in the textual description of a workflow step, the corresponding step in the flow chart, along with its inputs and outputs are highlighted.
- A tooltip appears to facilitate the user in distinguishing the color coding used for different elements of flow chart.

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 templat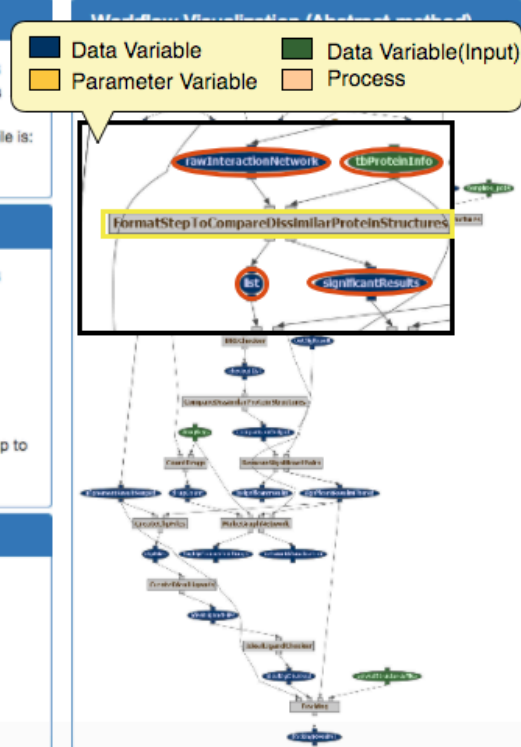e AbstractGlobalWorkflow2 (See figure). The file size is 1166 bytes and is stored in the Wings servers on the following location http://www.opmw.org/export/page/resource/WorkflowExecutionArtifact/DE58909D2E17DF26F0BF79D75E12C2D6. The DOI for the result file is: https://dx.doi.org/10.6084/m9.figshare.776887.v1

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 FormatStepToCompareDissimilarProteinStructures and FormatPDBToCompareProteinStructures abstract steps and the template_pdbs 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.
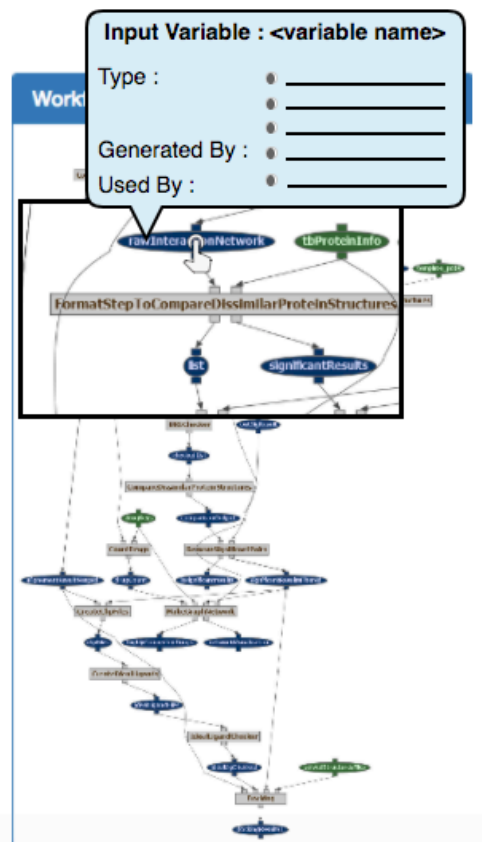
- On mouse hover of any step in the workflow, a tooltip appears with the description of the variable/process
- The description contains the information like whether the hovered element is an Input/Process/Output along with 'Type', 'Generated By', 'Used By' attribute details.