

Supplementary Material: visMOP – A Visual Analytics Approach for Multi-omics Pathways

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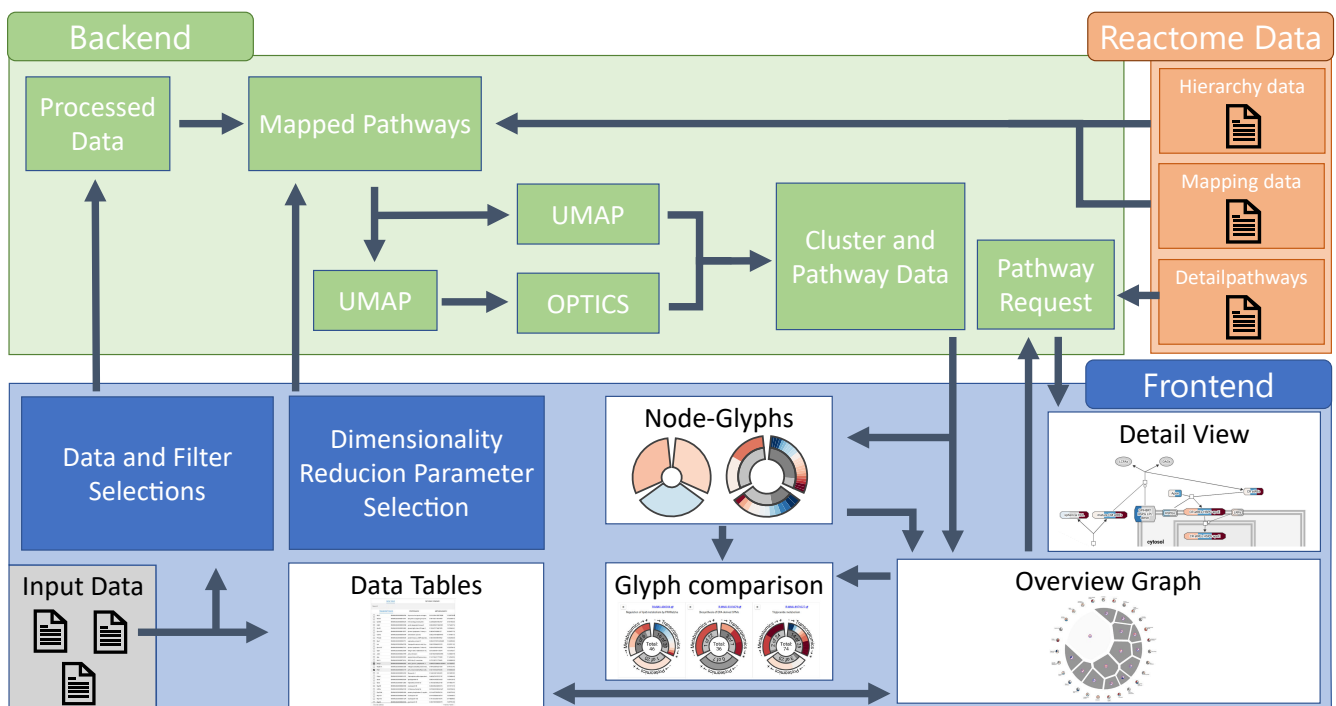


Figure 1: visMOP pipeline overview. Using the interface of the presented prototype, users can input up to three different omics types (transcriptomics, proteomics, metabolomics). These input data is displayed in interactive tables. The user can set up filtering for the data and can choose variables derived from the data to be used in dimensionality reduction. The data is then sent to a backend to be processed for mapping to the Reactome pathways. Using the selected parameters, the pathways are embedded into a lower dimensional space with UMAP. With OPTICS, clusters are detected in this lower dimensional space. Using UMAP a second time, a 2D embedding is generated from the mapped pathway data. Cluster data, including the mapping, the Cluster assignment and cluster positions (as defined by a centroid) are sent to the front end for visualization. The mapping data is then used to generated glyphs for each pathway. These glyphs are then used as nodes in the overview graph. Utilizing the cluster assignment and cluster centroids, a hierarchical treemap is generated. Interaction with the overview graph, coupled with linkage to other visualizations, offers the user an exploratory analysis of the supplied data. The other visualizations include a detail view, in which specific pathways are queried, and the mapped data is visualized in the Reactome pathway layout. Furthermore, multiple pathways can be selected for comparison, here the glyphs become interactive and individual measurements and omics can be investigated.

Table 1: *Selectable features for dimensionality reduction and clustering derived from the input data*

Transcriptomics: Number of values	Absolute number of measured Transcriptomics values mapped to the pathway
Proteomics: Number of values	Absolute number of measured Proteomics values mapped to the pathway
Metabolomics: Number of values	Absolute number of measured Metabolomics values mapped to the pathway
Transcriptomics: % regulated	Percentage of measured Transcriptomics values mapped to the pathway which are considered regulated (over and under user-defined upper-limit/lower-limit)
Proteomics: % regulated	Percentage of measured Proteomics values mapped to the pathway which are considered regulated (over and under user-defined upper-limit/lower-limit)
Metabolomics: % regulated	Percentage of measured Metabolomics values mapped to the pathway which are considered regulated (over and under user-defined upper-limit/lower-limit)
Transcriptomics: % unregulated	Percentage of measured Transcriptomics values mapped to the pathway which are considered unregulated (under and over user-defined upper-limit/lower-limit)
Proteomics: % unregulated	Percentage of measured Proteomics values mapped to the pathway which are considered unregulated (under and over user-defined upper-limit/lower-limit)
Metabolomics: % unregulated	Percentage of measured Metabolomics values mapped to the pathway which are considered unregulated (under and over user-defined upper-limit/lower-limit)
Transcriptomics: % with measured value	Percentage of pathways Transcriptomics values with measured value
Proteomics: % with measured value	Percentage of pathways Proteomics values with measured value
Metabolomics: % with measured value	Percentage of pathways Metabolomics values with measured value
Transcriptomics: Mean expression above limit	mean of transcriptomics measurement level from the values mapped to the pathway above the user defined upper-limit
Proteomics: Mean expression above limit	mean of Proteomics measurement level from the values mapped to the pathway above the user defined upper-limit
Metabolomics: Mean expression above limit	mean of Metabolomics measurement level from the values mapped to the pathway above the user defined upper-limit
Transcriptomics: % values above limit	percentage of Transcriptomics measurements mapped to the pathway above the user defined upper-limit
Proteomics: % values above limit	percentage of Proteomics measurements mapped to the pathway above the user defined upper-limit
Metabolomics: % values above limit	percentage of Metabolomics measurements mapped to the pathway above the user defined upper-limit
Transcriptomics: Mean expression below limit	mean of Transcriptomics measurement level from the values mapped to the pathway below the user defined lower-limit
Proteomics: Mean expression below limit	mean of Proteomics measurement level from the values mapped to the pathway below the user defined lower-limit
Metabolomics: Mean expression below limit	mean of Metabolomics measurement level from the values mapped to the pathway below the user defined lower-limit
Transcriptomics: % values below limit	percentage of Transcriptomics measurements mapped to the pathway below the user defined lower-limit
Proteomics: % values below limit	percentage of Proteomics measurements mapped to the pathway below the user defined lower-limit
Metabolomics: % values below limit	percentage of Metabolomics measurements mapped to the pathway below the user defined lower-limit
Not omic-specific: % values measured over all omics	Percentage of all omics measured and mapped to the pathway combined in relation to all omics entries in the pathway.