Hierarchical Clustering and PCA Plots in Skyline Daily

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Nicholas Shulman
“Cluster” button on the Document Grid

- When you push that button, Skyline will choose a set of numeric columns to perform hierarchical clustering on.
- The clustering works best if some numeric columns have been pivoted by replicate.
What is hierarchical clustering?

- Finds which points are closest to each other, and then finds which points or groups of points are closest to each other.
- In this case, A&E are close to each other, and B&D are close to each other. After that, C is closer to B&D than it is to A&E.
What hierarchical clustering looks like in the Document Grid

• Rows get reordered so that the dendrogram can be drawn without the lines crossing
• Values in “Text” column get colored arbitrarily
• Values in “X” column get colored based on how far they are from zero
Group Comparisons

• The Group Comparison grid in Skyline-Daily now has an additional report available “Clustered”.

• Also, pushing the colorful cluster button automatically switches the report from “default” to “Clustered.”
Clustered Group Comparison Report

• The “Clustered” comparison report displays the replicate abundances in separate columns.

• Hierarchical clustering is performed on the replicate columns, as well as the peptide or protein rows.
Displaying the heat map graph

- There is a dropdown menu item from the cluster button which brings up a heat map graph.