Subject: Re: Assign cluster name based on cluster size Posted by nbehrnd on Sat, 09 Apr 2022 18:29:25 GMT

View Forum Message <> Reply to Message

The following doesn't offer the automatic sort (and perhaps eventual cumulative distribution) you look for.

Yet because each cluster's molecule is labeled by the integer of the cluster, one may use it and request DataWarrior to plot a histogram (bin size 1, starting by 1 along the abscissa, number of molecules per bin along the ordinate) to identify the most populated bin/to check if the distribution of bins perhaps is bi/polymodal. For smaller numbers of bins, it might be helpful to add the number of molecules (view options for statistical graphs) to the drawing.

Norwid

File Attachments

1) example.png, downloaded 153 times