Subject: row lists
Posted by pc419714@ohio.edu on Thu, 25 Apr 2019 18:09:09 GMT
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Say I had a list of ligands that were ranked according to their binding energy from a docking program. The output from the docking program had ligand numbers that corresponded with the .sdf file I exported from DataWarrior after converting to conformers. Would it be possible to take this list of row numbers and use the row list function to view these ligands in order of ranked binding energy? I'm not sure if row lists can be used this way in Data Warrior. I have not tried it yet.

Subject: Re: row lists
Posted by thomas on Thu, 25 Apr 2019 19:47:21 GMT
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I just checked: If you generate conformers from an open DataWarrior window into a new SD-file, then this file contains a column 'ID' containing the original file's row number. If your docking program's output file contains these IDs as well as binding energies in TAB-delimited or CSV format, then you may merge that file into the original DataWarrior file. Because that one does not contain the IDs, you need to generate them first with 'Data -> Add row numbers' starting from 1. Then you can merge using 'Row number' and 'ID', which adds the binding energies as a new column to your original file.

Alternatively, you could create a list from those IDs, if DataWarrior would allow you to select numeric column as key column. Unfortunately, this is not possible till today, which I have now fixed in the source code. Nevertheless, creating a list would also require to create a new column with row numbers. To me merging ernergies into the original file seems to be the better solution anyway.

Thomas