Subject: export jpg/png file from SDF file with datawarrior from command line
Posted by dongkeke on Tue, 09 Jul 2019 06:13:28 GMT
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I often have to find the rules from images from 2D or 3D view in SDF files, it is troublesome to open each SDF file and save images as PNG file. It would be nice to have Datawarrior operate from the command line to export all images form each SDF file in Linux.

Subject: Re: export jpg/png file from SDF file with datawarrior from command line
Posted by thomas on Tue, 09 Jul 2019 11:57:17 GMT
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I suggest that you create a macro file that opens your sd-file with a predefined name, creates and saves the image from the view and then closes the datawarrior application. You may then run this macro from the command line with:
/opt/datawarrior/datawarrior testmacro.dwam

This would launch DataWarrior, open the ds-file, save the view, and exit DataWarrior.

Thomas

Subject: Re: export jpg/png file from SDF file with datawarrior from command line
Posted by nbehrnd on Tue, 09 Jul 2019 14:13:07 GMT
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If your aim is to generate a visual survey about the constitution of the molecules deposit in your .sdf, and assuming each .sdf contains only one model, I would first concatenate the .sdf into one "container" with openbabel. Put them into one folder in common, enter this depot via the CLI, and launch

obabel *.sdf -O container.sdf -d

To optional parameter "-d" will cause openbabel to strip-off all hydrogens except the ones bound to either a hetero atom or on a terminal C. This simplifies the visual output quite a bit.

Request then openbabel to access this poly-model container.sdf a twice, to create a vignette about each molecule, put into a box of an array of all. You choose either a bitmapped .png, or a vectorized .svg as output. The minimal instruction indicates input file type and file name, and name of the output to be written (name including the file extension), e.g.

obabel -isdf container.sdf -O array.svg

There are optional paramers to adjust the formatting (e.g., number of columns, number of rows; a grid, an integer counter next to the structure's original file name about the entry of the

model in the .sdf accessed).

Openabel's Dreiding-like colouring of heteroatoms may be good for a display on screen. This however may be a potential pitfall if the structures are big (consequently, represented at low scale) and print on paper. This is especially true for explict H bound to heteroatoms, Si, F, Cl, S, Se; to lesser extent for O and N. You may request openbabel to use black ink only by "-xu" (without quotation marks). Advantageously, the resolution independent crisp .svg may be postprocessed further (cairosvg, inkscape, etc).

A recent example is https://github.com/nbehrnd/saturated_Murcko_scaffold

File Attachments

1) example.png, downloaded 1301 times

