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 531 times