Subject: Re: ChemAxon plugin
Posted by thomas on Fri, 04 Mar 2022 18:49:48 GMT

Hi Christophe,

if there are files with the same name in the same folder hierarchy, then this is most likely, because the originally separated ChemAxon jar files contained the same external dependencies, which are redundant, if merged. You should be able to just overwrite these files that they are contained just once. Indeed the merged file would be huge, but it should work.

When I did this 15 years ago, I removed all files, which were not needed for the pKa calculation, which reduced the file size by more than a factor of 1000. After trying various other methods for this, I turned to a brute force method: Running a bash script, which was removing one file after another. After every file removal I calculated pKa with the remaining files and checked, if the procedure still worked. If not, then the files was added again and the script continued with removing the next file. Finally, I had to add a few removed files, when I discovered that different structure classes required different Java classes for the pKa calculation, which were invoked with ClassForName.