Subject: Re: ChemAxon plugin
Posted by thomas on Thu, 10 Feb 2022 09:08:03 GMT

Hello Christophe,

you can search this forum for 'capka' and find some posts. I did it myself about 15 years ago and suspect that the same procedure should work also with the current ChemAxon pKa plugin, but since I don't have the current plugin, I cannot confirm this. Basically, you have to unpack all jar files into one directory and then repack everything from that directory into a new 'capka.jar' file. You also have to put the license file where the license code can find it.

If you want, you can contact me offline to work together on creating a reproducible procedure, e.g. a bash script doing the entire conversion, which we could publish afterwards on this forum for others to re-use.

Thomas