Subject: Re: ChemAxon calculated properties
Posted by chemist on Tue, 17 Jan 2017 09:45:31 GMT
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Thanks for creating really great software!

I have been struggling with Chemaxon calculated properties. I also have this free academic lisence but enabling these chemaxon properties seems quite difficult.

What I have tried:

1. Go to chemaxon directory
2. Searh .jar
3. copy all of them to new folder
4. extract all .jars by ticking [x]"Extract archives to subfolders"
5. zip all to capka.zip
6. rename -> capka.jar
7. move to datawarrior.exe location

I have also lisence file in correct location.

I just started to think if in the academic version there is some limitation to batch calculation of pKa values.

I have lisence for following products:
Marvin Applets
Marvin Beans
Instant JChem
JChem Base
Standardizer
Screen
Reactor
JKlustor
Metabolizer
Markush Search
Protonation Plugin Group
Partitioning Plugin Group
Isomers Plugin Group
Markush Enumeration Plugin
Structure to Name Plugin
Name to Structure
JChem for Excel
Structure Search
IUPAC naming plugin
Web Services Server
Structure Checker
Predictor Plugin
MCES

3D Screen
Molecular Descriptors
Instant JChem VIZ
ECFP/FCFP
Document to Structure
NMR Predictor
JChem for Office
Markush Editor
Solubility Plugin
Structural Calculations