Subject: Re: ChemAxon calculated properties
Posted by MussaQ on Thu, 04 Dec 2014 16:46:39 GMT
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Quote:if you have a license to the necessary subset of the ChemAxon software,
you may put all ChemAxon files needed for pKa calculation into a new .jar file

I have an academic license for chemaxon (for the entire Marvin and JChem suites) through my institute, I was wondering if you knew the location of these files required for the LogD calculations? I have had no luck on Mac or windows in trying to locate them.

Much appreciated.