Subject: Integration with KNIME or Python Posted by cfang on Thu, 04 Nov 2021 19:33:19 GMT

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Hi all,

DataWarrior is a great chemistry frontend GUI with a lot of embedded cheminformatics toolkits. But I wonder if it is possible to develop customized tools and publish to the DataWarrior such as utilizing KNIME connection or Python/RDKit etc.

I read an old poster in 2016 that pointed out the integration of KNIME to DataWarrior was on the way. Is there any updates on that? Generally, at current stage, is it possible to do some customization with DataWarrior?

Thanks! Cheng