Subject: python usage
Posted by sukrit2024 on Fri, 04 Oct 2024 22:48:28 GMT
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I am new to data warrior. Can I use the functionality of data warrior from python? I want to use a jupyter notebook and use data warrior.

Subject: Re: python usage
Posted by thomas on Sat, 26 Oct 2024 19:44:40 GMT
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wrapping openchemlib, the chemistry engine behind DataWarrior, to be used with python should be possible, but somebody would have to do that.

Subject: Re: python usage
Posted by Etnolekt on Sat, 02 Aug 2025 10:15:00 GMT
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Hi, I wrote dwar2pd: a wrapper for openchemlib.js that allows you to load .dwar files directly into a Pandas DataFrame and decode idcodes to SMILES. Feel free to give it a try!