Subject: Re: Generate conformers - write to file does nothing Posted by Paul on Thu, 09 Jul 2020 00:46:33 GMT View Forum Message <> Reply to Message

Thanks - I have been able to use the various force fields with success, but only when generating a single conformer as new columns in the DWAR document.

Regardless of the force field, or choosing not to minimize, the output from generate conformers

Paul

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