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Subject: Re: Generate conformers - write to file does nothing

Posted by [nbehrnd](#) on Wed, 08 Jul 2020 22:58:47 GMT

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Hello Paul,

the generation of conformers may, but need not to, include the application of a force field. DW includes MMFF94s, MMFF94s+, and Indorsia; if used (which might be your default) some of the conformers may coalesce. The fourth option next to minimize energy is «don't minimize»; then retaining better the results of the parameters «Algorithm» and «Initial torsions» in display and file written.

Norwid

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