
Subject: Re: Docking score and Datawarrior
Posted by [nbehrnd](#) on Thu, 29 Dec 2022 09:46:08 GMT
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Dear Jon,

> Also what forcefields are used in the minimisation?

In chapter Chemistry 3D, section minimize energy, the documentation shipped with DW lists MMFF94s+, MMFF94s, and Idorsia forcefields.

Because Joel Wahl is mentioned as contributor to MMFF94s+ for «A peer-reviewed publication is in process.», maybe «Accuracy evaluation and addition of improved dihedral parameters for the MMFF94s» by 2019 is the corresponding literature reference[1] to address problems in MMFF94s. DW as distributed here possibly is not on the white list for Idorsia's forcefield.

Norwid

[1] <https://jcheminf.biomedcentral.com/articles/10.1186/s13321-019-0371-6> It is an open access publication; by today, there are 15 citations of this work the journal identified.
