
Subject: Re: Rendering structures from SMILES
Posted by [jwfeng](#) on Mon, 01 May 2017 05:25:07 GMT
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Hi Thomas,

Thanks for the different options. I will convert my SD file into a tab separated file where the first column stores SMILES string of the SD structure. The remaining columns will store SD fields.

I like to store SMILES strings in SD tag where those SMILES could be substructures, near neighbors, or molecular match pairs.

JW
