Subject: Rendering structures from SMILES
Posted by jwfeng on Wed, 05 Apr 2017 17:28:01 GMT

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Hi,

My SD file contains SD tag with SMILES strings as values. Is there a way to render them as structures in DW? Attached is a simple example of what I want to do. The Structure column display what's in the MOL block, the r-group smiles column should render the SMILES string as a structure instead of displaying it as text.

Thanks,

JW

File Attachments
1) Screen Shot 2017-04-05 at 10.26.34 AM.png, downloaded 721 times