Subject: exporting R groups of compounds
Posted by jkulpiii on Wed, 06 Mar 2019 15:00:03 GMT
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When I exported as a SDF file, the R groups or fragment data was lost. When I exported as txt file I did get these columns: Scaffold [idcode] R1 [idcode] R2 [idcode]

What file type is the idcode? I do not recognize it. I would like to convert it to smiles.

Thanks for the help