Subject: Re: Merge File Issues

Posted by nbehrnd on Wed, 17 Apr 2024 10:31:02 GMT

View Forum Message <> Reply to Message

Hello Angus,

can you afford to drop `&` and `or`, the extended stereochemistry of .sdf files (V3000) and subsequently work with the elder syntax of version 2000 instead? The .dwam macro file attached below will export the DW structure array, and exports the subsequent columns as a tag trailing each entry. The file format can be re-read by DW, and hence be serve to merge with an other file, too.

Norwid

File Attachments

1) export_sdf_v2000.dwam, downloaded 340 times