
Subject: Re: V3000 export issue
Posted by [thomas](#) on Mon, 06 Feb 2017 09:17:53 GMT
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Hi Bruno,

my ctfile formats document from 2005 does not seem to specify whether the collection block is part of the CTAB block or should start after the 'END CTAB' tag. However, the example molfile in the 'MDL's Enhanced Stereochemical Representation' document is conform with DataWarrior's way of producing molfiles. An up-to-date version of this document is online available:

<http://accelrys.com/products/pdf/enhanced-stereochemical-representation.pdf>

I also checked what ChemDraw Pro 15 is doing: Their molfiles have the collection block before 'END CTAB' as DataWarrior has.

I am currently waiting for a download link to the newest ctfile document from biovia be sent to me. I assume that this is where you found the specification.

For now it seems that I am in good company, if I keep it as it is. Please let me know, if you come across any software that expects the format differently.

Thomas
