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Subject: Re: Duplicate Molecules

Posted by [thomas](#) on Mon, 02 Mar 2020 17:46:47 GMT

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This would mean that two different canonical SMILES are considered the same structure by DataWarrior. I cannot perceive of a reason for that. If you delete all unique rows from your file, then you retain all these cases. If you can send me some of them, I may have a more detailed explanation.

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