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Subject: Remove duplicate molecules

Posted by [sbembenek18](#) on Sat, 05 Oct 2019 01:08:24 GMT

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is it possible to remove duplicate molecules from a data set and just leave a single occurrence?

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Subject: Re: Remove duplicate molecules

Posted by [nbehrnd](#) on Sun, 06 Oct 2019 21:31:46 GMT

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Assuming you put the structures in one column, duplicates may be removed by selecting the column of interest, followed by choosing Data -> Merge Equivalent Rows.

Norwid

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Subject: Re: Remove duplicate molecules

Posted by [sbembenek18](#) on Fri, 11 Oct 2019 16:42:46 GMT

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thanks!

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