
Subject: Remove duplicate molecules

Posted by [sbembeneck18](#) on Sat, 05 Oct 2019 01:08:24 GMT

[View Forum Message](#) <> [Reply to Message](#)

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

Subject: Re: Remove duplicate molecules

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

[View Forum Message](#) <> [Reply to Message](#)

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

Subject: Re: Remove duplicate molecules

Posted by [sbembeneck18](#) on Fri, 11 Oct 2019 16:42:46 GMT

[View Forum Message](#) <> [Reply to Message](#)

thanks!
