Subject: Drawing Multi-step reaction schemes.
Posted by jeetu270 on Wed, 27 Jan 2016 09:52:24 GMT
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Is there an option for drawing, importing, exporting Multi-step reaction schemes in DataWarrior?

We can only draw and save/share a single step reaction using the Combinatorial library generating option in DW currently.

Thanks
Jitender

Subject: Re: Drawing Multi-step reaction schemes.
Posted by thomas on Thu, 28 Jan 2016 19:57:05 GMT
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No, but usually that is not necessary, because usually you can write any multi-step reaction as single step reaction with multiple reactants. For the purpose of an enumeration it doesn't matter, whether you use a formal one-step-reaction.

Does this answer your question? Or what is your purpose for multi-step reactions?

Kind regards, Thomas

Subject: Re: Drawing Multi-step reaction schemes.
Posted by jeetu270 on Fri, 29 Jan 2016 02:39:32 GMT
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Dear Thomas,
Actually we usually share synthetic schemes (that are generally multi-step reactions) among our colleagues. So I was wondering if we can use DataWarrior's editor for this purpose also. But could not find any option.
It was not for library enumeration use.

Thanks
Jitender