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Subject: Re: PCA

Posted by [thomas](#) on Sun, 08 Jul 2018 16:33:15 GMT

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I am not sure, whether I understand your question correctly. If you intend to make a PCA from multidimensional data and then plot the 2 or 3 most significant dimensions, then you need to do these steps:

- Data-> Calculate Principal Components...
- select the columns that contain your input data (or a descriptor column of chemical structures)
- click OK

Does this answer your question?

Thomas

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