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Subject: Re: Flexophore

Posted by [thomas](#) on Wed, 17 Apr 2019 18:05:58 GMT

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no you cannot, because the flexophore is not a vector. It is a much more complex descriptor: a complete graph of all interaction points, where nodes consist of force field atom types and edges are the distance histogram over a set of representative conformers. A PCA needs many numerical dimensions as input.

Thomas

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