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Title: Molecular Tailoring Approach ap- plied to ab-initio classical dynamics of small proteins

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Abstract: In case of a large molecular chain, calculations become expensive and take time. As resources are limited (i.e CPU, Memory, processor etc.) in such a

computationally expensive situation, this work deals with an approach called molecular tailoring. In which a large molecule chain gets fragmented and calculation is done on each frag- ments. That leads to approximate result with a reasonable error. Calculation on each fragment can be done easily on many parallel

system at a time in a manner to reduce the computing cost.

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