CABS-flex standalone application for fast simulations of flexibility of globular proteins

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The conformational flexibility of protein structures is crucial for their functions. Simulations of protein flexibility remain computationally costly or intractable for most of protein systems using classical modeling tools. Here we present a new standalone version of our method – CABS-flex[1,2] method, so far available as a web server[1]. The method combines a highly efficient, coarse-grained approach with all-atom modeling methods. The CABS-flex predictions reflect the flexibility of an investigated protein and provide a picture complementary to the results obtained from molecular dynamics simulations[3] as well as NMR conformational ensembles[2]. The CABS-flex method was also successfully used for efficient simulations of protein flexibility in predictions of protein-peptide complexes[4,5] and protein aggregation properties[6]. The standalone CABS-flex application allows for customization of the simulation parameters, handling large-sized systems and provides a flexible framework for result analysis. The standalone CABS-flex version is freely available at http://biocomp.chem.uw.edu.pl/CABSflexApp/ and server version at: http://biocomp.chem.uw.edu.pl/CABSflex/.

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