Using Normal Mode Analysis on protein structural models. How far can we go on our predictions?

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Abstract

Normal Mode Analysis is a fast and inexpensive approach that is largely used to gain insight into functional protein motions, and more recently to create conformations for further computational studies. However, when the protein structure is unknown, the use of computational models is necessary. Here, we analyze the capacity of normal mode analysis in internal coordinate space to predict protein motion, its intrinsic flexibility and atomic displacements, using protein models instead of native structures, and the possibility to use it for model refinement. Our results show that normal mode analysis is quite insensitive to modelling errors, but that calculations are strictly reliable only for very accurate models. Our study also suggests that internal normal mode analysis is a more suitable tool for the improvement of structural models, and for integrating them with experimental data or in other computational techniques, such as protein docking or more refined molecular dynamics simulations.

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