Best practices for biomolecular simulation setup : v0.0.1

Rommie E. Amaro[1*], John D. Chodera[2*], David L. Mobley[3*], Antonia Mey[4*], Julien Michel[4*]

***For correspondence:**
email1@example.com (REA);
john.chodera@choderalab.org (JDC); dmobley@mobleylab.org (DLM); email1@example.com (AM); email1@example.com (JM)

[1]Institution 1; [2]Institution 2; [3]Departments of Pharmaceutical Sciences and Chemistry, University of California, Irvine; [4]Institution 4

Abstract Please provide an abstract of no more than 250 words. Your abstract should explain the main contributions of your article, and should not contain any material that is not included in the main text.

Goals

Produce a brief checklist of most critical and most overlooked items that practitioners can follow and potentially reviewers can use. Highlight issues where further study (or references we don?t know about yet) are needed to clarify what should be done; solicit input from the community on how best to handle issues. Guideline on how to report the checklist addressed items in a publication: Note that typical methods sections should provide the information in this checklist. (How to write a methods section by John Chodera: http://klogw.org/2016/07/28/how-to-write-a-methods-section/).

We are not trying to enforce; we are trying to inform.

Scope

Relatively simple biomolecular simulations of soluble proteins that may include small molecule ligands: May not be able to include nucleic acid recommendations initially because of lack of expertise; Toni can potentially cover lipids, but it may be best to have a separate membrane protein doc that follows this. Eventually to include cofactors as part of the consideration

Does NOT include: Generation of parameters, such as for nonstandard nonstandard residues (as opposed to standard nonstandard residues where literature and/or library parameters may already be available), or for complicated lipids or cofactors? AND these will be coupled to force field choice to some extent. Simulation protocol such as minimization, cutoffs, etc.

Checklist

Step 0: Know what you want to simulate

Protein

Ligands

Counterions/water

Other things to think about that didn't make the checklist

Detailed explanation of checklist items

Acknowledgments