# A method for redesigning molecular mechanics force field parameterization by use of a Bayesian statistical framework

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This document describes a collected set of best practices for computing various physical properties from molecular simulations of liquid mixtures.

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# Todo list

## I. Outline

### A. Objectives

- Molecular dynamics simulation is becoming more integral to many scientific studies
  - Observing physical phenomena at a molecular scale (phase changes, ligand docking, etc.
  - Drug discovery and deisgn of new molecules
- The necessity for transferable and accurate force fields is therefore imperative
  - Transferability encourages use and provides convenience for scientists with wide arrays of research interests
  - Inaccurate force fields have been shown to grossly misrepresent even somewhat simple molecular systems (gaff2 lol, check for some other cites)
- A possible solution to the given problem can be by recasting the force field parameterization issue as a bayesian inference problem
- The objective of this paper is introduce a framework for using disparate experimental data in order to parameterize molecular mechanics force fields
- In this paper I will describe the process of collecting and organizing large amounts of high quality thermochemical data and preliminary use of the Multistate Bennett Acceptance Ratio (MBAR) as a means to improve sampling speed during the parameterization process.