

MCCE Documentation

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What is MCCE?

- [Multi-Conformation Continuum Electrostatics - MCCE](#)
- [MCCE Mechanism](#)

MCCE Success Stories

- [Proton Loading Sites in Complex I](#)
- [MCCE Hydrogen Bond Characterization](#)
- [Photosystem II Analysis](#)

Quick Start

- [Install MCCE](#)
- [A simple MCCE example of pH titration](#)

Tutorials

- Calculate pKas of Lysozyme - a 4-step process
- Calculate Em of heme in Cytochrome
- Compute hydrogen bond network
- Sampling more rotamers at "hot" spots
- Gromacs Quick Start
 - Gromacs Server
 - Example 1: Lysozyme
 - Example 2: Biphasic Systems
- Microstate Tools Tutorial
 - What is a microstate?
 - Tautomeric Charge Microstates
- Run MCCE on Multiple PDBs at Once

Knowledgebase

- MCCE Commands

- MCCE Program Run and Debug
 - MCCE Data Analysis
 - MCCE Tools
 - MCCE How Tos
 - How to make a new topology file?
 - How to add rotamer making rules to parameter file?
 - Other HOW-TOs
 - How to install WSL (Windows Subsystem Linux)
 - How to contribute code to MCCE
 - Microstate Analysis Library
 - Microstate Analysis Library Reference
 - Interpret MCCE Results
 - How does changing MCCE's parameters change accuracy?
 - How to break down the energy of a residue ionization?
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