

MCCE Documentation

MCCE Documentation

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](#)
- [Microstate Tools Tutorial](#)
- [Run MCCE on Multiple PDBs at Once](#)

Knowledgebase

- [MCCE Commands](#)
- [MCCE How Tos](#)
- [Other HOW-TOs](#)
- [Microstate Analysis Library](#)
- [Interprete MCCE Results](#)

Revision #8

Created 2 June 2025 17:18:58 by Junjun Mao

Updated 3 June 2025 16:57:59 by Junjun Mao