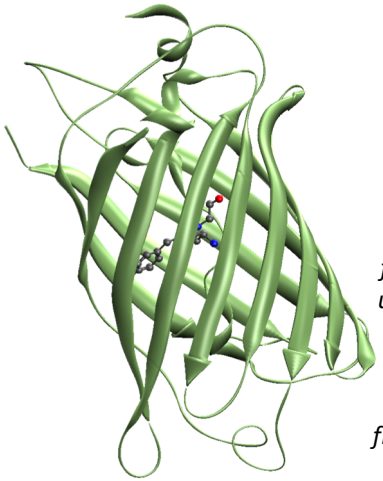
Q-Chem Presents: A New Module for Biomolecular Simulation



The AMOEBA force field can be used for accurate pKa prediction, like in a recent study on the GFP fluorophore (left).

Hybrid Parallel Performance

M-Chem is OpenMP and MPI parallel, allowing for optimal performance on modern HPC hardware.

A One-Stop-Shop For Computational Chemistry

Q-Chem 7.0 includes modules for molecular, material, and biomolecular modeling with no additional licensing.

Learning & Teaching Resources

Free teaching resources, including lab assignments, video tutorials, webinars, workshops, and guest lectures.
https://www.q-chem.com/learn/

Q-Chem Talk Forum

Talk with users, get help, and review an archive of questions and answers.
https://talk.q-chem.com/

Q-Chem Manual

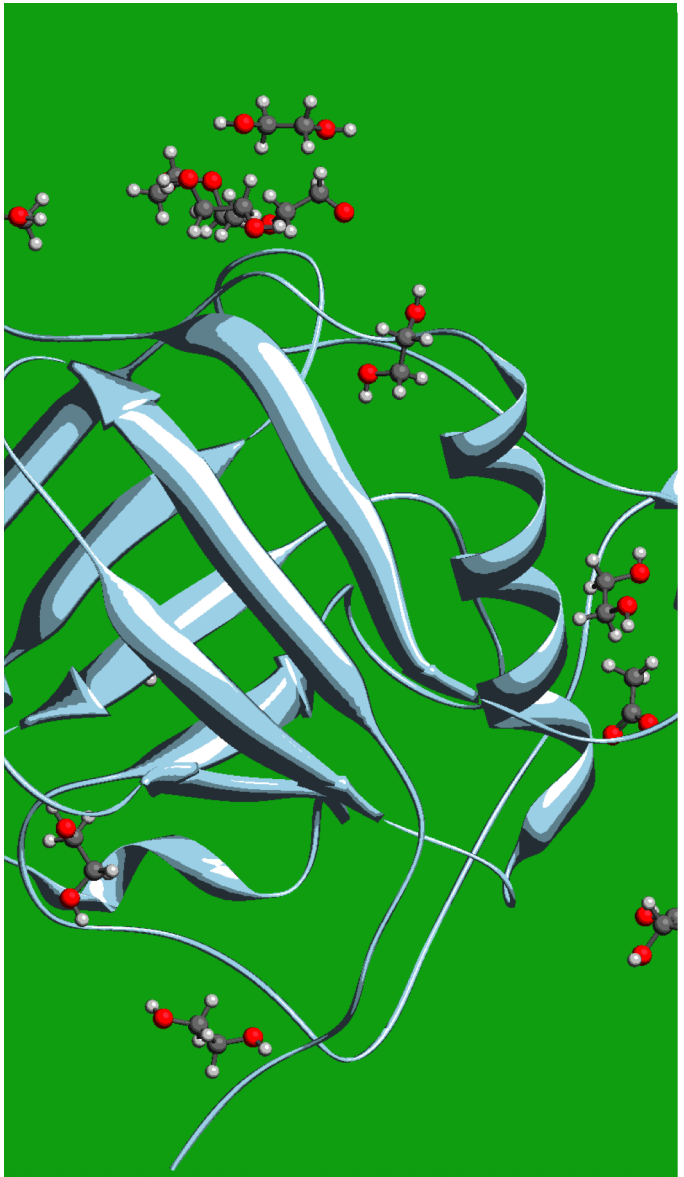
Learn more about features and the underlying theory.
https://manual.q-chem.com/

Contact Us

info@q-chem.com
support@q-chem.com

https://www.q-chem.com

Q-CHEM™
A QUANTUM LEAP INTO THE FUTURE OF CHEMISTRY



M-CHEM
Biomolecular Modeling

Part of the Q-CHEM Suite

Extending Q-Chem To Biomolecular Simulations

M-Chem is a new, state-of-the-art package for modeling large biomolecular systems.

Highlights include: Fast parallel performance; AMOEBA polarizable force field; Python interfacing; ReaxFF; and QForce.

M-Chem Features

AMOEBA Force Field

The AMOEBA force field incorporates polarization effects to provide improved accuracy over traditional non-polarizable force fields.

Python Interfacing

M-Chem includes Python-based interfacing for input processing and system solvation.

ReaxFF

ReaxFF is a reactive force field that enables accurate simulations of bond breaking and formation, making it useful for modeling reactions and materials.

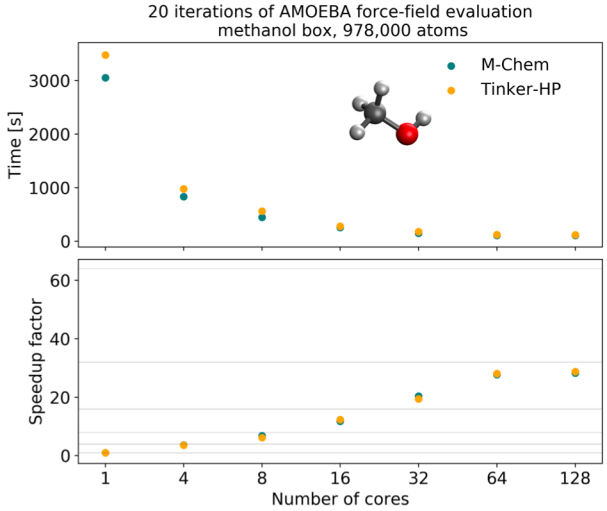
QForce

An automated, open-source toolkit for augmenting transferable force fields with data from QM calculations. The resulting force fields provide improved accuracy at no additional cost.

Read the M-Chem paper!

Try M-Chem

Request a month-long free trial today at https://q-chem.com/try/



Parallel performance benchmarks of M-Chem's AMOEBA for a system of 978,000 atoms.

Fast Parallel Performance

Hybrid MPI/OpenMP Capabilities

- Molecular dyanamics with the AMOEBA force field
- Nose-Hoover thermostat and barostat

Open-MP Capabilities

- Molecular dynamics with AMOEBA and MBUCB force fields
- Single-point calculations with AMOEBA, e.g. for Monte-Carlo simulations
- *In vacuo* molecular dynamics simulations with AMOEBA
- Evaluation of induced electrostatic AMOEBA term with conjugate gradient and extended Lagrangian schemes (iEL/SCF and iEL/0-SCF)