

# OpenPathSampling



<http://openpathsampling.org>

Development at: <http://github.org/openpathsampling/>  
Part of the Omnia consortium: <http://omnia.md>

A Python library for path sampling simulations

- ✓ **Easy to use:** Beginners can quickly learn to use it
- ✓ **Easy to extend:** Advanced users can use it to develop new methods
- ✓ **Independent of dynamics engine:** Useful in many fields and to the broadest audience

```
import openpathsampling as paths
in_file = paths.AnalysisStorage("input_file.nc")
init_traj = in_file.trajectories[0]
engine = in_file.engines[0]
dist = in_file.cvs['my_distance']
stateA = paths.CVRangeVolume(dist, 0.0, 1.0)
stateB = paths.CVRangeVolume(dist, 3.0, float('inf'))
ensemble = paths.TPSEnsemble(stateA, stateB)
shooting_mover = paths.OneWayShootingMover(ensemble)
init_samp = paths.Sample(
    replica=0,
    trajectory=ensemble.split(init_traj)[0],
    ensemble=ensemble)
out_file = paths.Storage("output.nc", "w", init_traj[0])
tps_calc = paths.PathSampling(
    storage=out_file,
    engine=engine,
    move_scheme=paths.LockedMoveScheme(shooting_mover),
    globalstate=paths.SampleSet([init_samp]))
tps_calc.run(1000)
```

DWHS, Prinz, Noé, Bolhuis, Chodera. In prep.

# Take Home Messages

- Path sampling is a powerful tool for gaining insight into biomolecular systems
- Path sampling gives insight into the oncogenic nature of K-Ras mutant Q61L by showing that a channel for opening closes off, keeping the protein active
- Path sampling can be used to study drug binding/unbinding
- New software (OpenPathSampling) and methods are making path sampling more accessible