

HDX

J-coupling

Chemical
Shift

NOE

BICePs v2.0

Preparation

Ensemble

PosteriorSampler

Convergence

Analysis

```
# Prepare data for each conformational state
prep = biceps.Restraint.Preparation(int(nstates), str(top_file))
# Experimental & forward model data
prep.prepare_noe(str(exp_data), str(model_data), str(indices))
prep.prepare_J(str(exp_data), str(model_data), str(indices))
```

```
# Construct an ensemble of conformational states
ensemble = biceps.Ensemble(float(lam), list(energies))
# Apply data restraints
ensemble.initialize_restraints(list(input_data), list(options))
```

```
# Sample the posterior with MCMC (Metropolis-Hastings criterion)
sampler = biceps.PosteriorSampler(object(ensemble))
sampler.sample(int(nsteps), int(burn))
```

```
# Use tools to check MCMC trajectory convergence
C = biceps.Convergence(traj)
C.get_autocorrelation_curves(str(method), int(maxtau))
```

```
# Predict conformational state populations & compute BICePs score
A = biceps.Analysis(list(trajs), int(nstates))
# Plot the posterior distribution & re-weighted populations
A.plot()
```