

```
1 features = FeatureSelector([
2     ('diheds', DihedralFeaturizer(types=['phi', 'psi']),
3     ('contacts', ContactFeaturizer(scheme='ca')))]
4 pipeline = Pipeline([
5     ('featurizer', features),
6     ('tica', tICA(n_components=2)),
7     ('cluster', MiniBatchKMeans(n_clusters=250)),
8     ('msm', MarkovStateModel(n_timescales=3))]
9 ss = ShuffleSplit(28, n_iter=50, test_size=0.5)
10 cv = GridSearchCV(pipeline, cv=ss, param_grid={
11     'featurizer__which_feat': ['contacts', 'diheds'],
12     'tica__lag_time': [1, 4, 16, 64]})
13 cv.fit(trajs)
```