

# CA\_distance\_run1

April 20, 2016

```
In [1]: import mdtraj as md
import os
import numpy as np
import sys
import matplotlib.pyplot as plt
%matplotlib inline
import time
import seaborn as sns
import pandas as pd

In [2]: def _dist_atom_selection(topology, atom1, atom2, verbose, unpythonize):
    """
    Function takes a topology file and residue selection and verifies if
    the latter is possible. It also returns the C-alpha atom selection
    Input:
        topology:
            mdtraj.Topology or string
            Either mdtraj.Topology object or path to trajectory
            to be loaded
        residue_selection:
            string or list with integers
            String will be interpreted with the Mdtraj atom
            selection language. The list will be treated as
            atom number
        selection (by default True):
            boolean
            if true the function will try to return the residue/
            atom selection
    Output:
        atom_subset
            numpy.array
            array with all the atom numbers corresponding to selection
        md_topology
            mdtraj.core.topology.Topology object of protein
    """
    ## First have to load all the inputs if they are defined by a path
    if isinstance(topology, str):
        if os.path.exists(topology):
            try:
                md_topology = md.load_topology(topology)
            except:
                sys.exit('Make sure you have provided a valid path to topology file!')
        else:
            if verbose > 0:
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        print 'The following topology file was successfully loaded: \n %s \n' %(md_t
        elif isinstance(topology, md.core.topology.Topology):
            md_topology = topology
            if verbose > 0:
                print 'The following topology file was successfully loaded: \n %s \n' %(md_topo
        else:
            sys.exit('Invalid input! Must be a valid path to topology file or mdtraj.Topology objec

## check chosen atoms
if isinstance(atom1, str):
    try:
        atom_subset1 = md_topology.select(atom1)
    except:
        sys.exit('Invalid atom selection!')
    else:
        if verbose > 0:
            print 'Atom1 number: %s' %(atom_subset1[0] + 1)

elif isinstance(atom1, int):
    atom1 = atom1 - 1
    try:
        atom_subset1 = []
        if atom1 < md_topology.n_atoms:
            atom_subset1.append(atom1)
    except:
        sys.exit('Atom selection invalid for given topology!')
    else:
        if verbose > 0:
            print 'Atom1 number: %s' %(atom_subset1[0] + 1)

else:
    sys.exit('Invalid atom selection, you need to provide a string or an integer')

if isinstance(atom2, str):
    try:
        atom_subset2 = md_topology.select(atom2)
    except:
        sys.exit('Invalid atom selection!')
    else:
        if verbose > 0:
            print 'Atom2 number: %s' %(atom_subset2[0] + 1)

elif isinstance(atom2, int):
    atom2 = atom2 - 1
    try:
        atom_subset2 = []
        if atom2 < md_topology.n_atoms:
            atom_subset2.append(atom2)
    except:
        sys.exit('Invalid atom selection!')
    else:
        if verbose > 0:

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        print 'Atom2 number: %s' %(atom_subset2[0] + 1)

    else:
        sys.exit('Invalid atom selection, you need to provide a string or an integer')

pair = np.append(atom_subset1, atom_subset2).reshape(1,2)

# should work until 1109
if unpythonize:
    # rename residues (still testing)
    final_resid_name = []
    for i in md_topology.subset(pair).atoms:
        residues = str(i)
        # position to substitute
        pos = []
        num = []
        for i in range(len(residues)):
            # skip first three letters
            if i<6 and residues[i].isdigit():
                pos.append(i)
                num.append(int(residues[i]))
        if len(pos) == 1:
            if num[-1] < 9:
                num[-1] += 1
            else:
                num[-1] = 10
        if len(pos) == 2:
            if num[-1] < 9:
                num[-1] += 1
            else:
                num[-1] = 0
                num[0] += 1
        if len(pos) == 3:
            if num[-1] < 9:
                num[-1] += 1
            else:
                num[1] += 1
                num[-1] = 0
        z = 0
        residues = list(residues)
        for j in pos:
            residues[j] = str(num[z])
            z+=1
        final_resid_name.append("".join(residues))
    final_resid = " - ".join(final_resid_name)

if verbose > 0:
    print 'Calculating distance between following atoms: %s \n' %(final_resid)

return md_topology, pair, final_resid

```

In [3]: def \_dist\_atom\_load(md\_topology, trajectory, pair, verbose, chunk):

```

# first create a list with all the paths that are needed
try:
    trajectory_path = os.listdir(trajectory)
except:
    sys.exit('Make sure you have provided a string for a valid path to a trajectory file!')
else:
    if verbose > 0:
        print 'Loading trajectories from the following files: '
        for trajectory_i in trajectory_path:
            print trajectory_i

all_distances = []
sim_time = []

#try:
for file_i in trajectory_path:
    for chunk_i in md.iterload(trajectory + file_i, chunk, top=md_topology):

        sim_time.append(chunk_i.time)

        if verbose > 1:
            print 'Successfully loaded trajectory: \n %s' %(chunk_i)

        all_distances.append(md.compute_distances(chunk_i, pair))


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all_distances_np = np.concatenate(all_distances) * 10
#except:
#    sys.exit('Make sure you provided a valid path to a folder with trajectory files!')
#else:
#    print '\nSuccessfully calculated atom distances in %s frames!' %(all_distances_np.shape[0])

sim_time = np.concatenate(sim_time) / 1000

return all_distances_np.reshape(all_distances_np.shape[0]), sim_time

```

```

In [4]: def main(topology, trajectory, atom1, atom2, verbose = 1, chunk = 100, unpythonize = True, plot_dist = False):
    """
    Function to calculate distance between two atoms and plot pdf
    """

    if verbose > 0:
        # timer for the whole function
        start = time.time()

        # now load topology and verify selection by calling _dist_atom_selection()
        md_topology, pair, final_residues = _dist_atom_selection(topology, atom1, atom2, verbose, unpythonize)

        # load trajectories and calculate distances
        distance, sim_time = _dist_atom_load(md_topology, trajectory, pair, verbose, chunk)

    if plot_dist:
        # plots:

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# distance as a function of time:
plt.figure(figsize=(12,12))
plt.plot(sim_time, distance, c='k', label = 'Distance')
plt.plot(sim_time, pd.rolling_mean(pd.DataFrame(distance), 50), c='red', label = '50 fr')
plt.legend(loc='best', prop={'size':12})
plt.title('Distance between %s' % final_residues, size = 24)
plt.xlabel('Time (ns)', size = 14)
plt.ylabel('Distance (${\AA}$)', size = 14)
plt.show()

# distance density plot
plt.figure(figsize = (12,12))
ax = sns.distplot(distance, hist=False, rug=False)
ax.set_xlabel('Distance (${\AA}$)', size = 16)
ax.set_ylabel('Density', size = 16)
ax.set_title('Distance between %s' % final_residues, size = 24)
plt.show()

total_trajectory_time = sim_time[-1] - sim_time[0] + 0.02

if verbose > 0:
    print 'Total execution time: %.2f seconds \n' %(time.time() - start)
    print 'Total simulation time of all frames: %s nanoseconds' %(total_trajectory_time)

return distance, final_residues, total_trajectory_time

```

```

In [5]: traj_list = ['/Users/gil_f.hoben/Troponin_md_processed/MD1/run1/Trajectories/',
                 '/Users/gil_f.hoben/Troponin_md_processed/MD2/run1/Trajectories/',
                 '/Users/gil_f.hoben/Troponin_md_processed/MD3/run1/Trajectories/',
                 '/Users/gil_f.hoben/Troponin_md_processed/MD4/run1/Trajectories/',
                 '/Users/gil_f.hoben/Troponin_md_processed/MD5/run1/Trajectories',]
top_list = ['/Users/gil_f.hoben/Troponin_md_processed/MD1/run1/tropomin_egcg_MD1_nowater.prmtop',
            '/Users/gil_f.hoben/Troponin_md_processed/MD2/run1/tropomin_egcg_MD2_nowater.prmtop',
            '/Users/gil_f.hoben/Troponin_md_processed/MD3/run1/tropomin_egcg_MD3_nowater.prmtop',
            '/Users/gil_f.hoben/Troponin_md_processed/MD4/run1/tropomin_egcg_MD4_nowater.prmtop',
            '/Users/gil_f.hoben/Troponin_md_processed/MD5/run1/tropomin_egcg_MD5_nowater.prmtop']
complex_names= ['MD1', 'MD2', 'MD3', 'MD4', 'MD5']
atom1_list = ['name OD1 and resid 64', 'name OD2 and resid 64', 'name OE1 and resid 65',
              'name OE2 and resid 65', 'name OD1 and resid 66',
              'name OD2 and resid 66', 'name OG and resid 68', 'name OG1 and resid 70',
              'name OD1 and resid 72', 'name OD2 and resid 72', 'name OD1 and resid 74',
              'name OD2 and resid 74', 'name OE1 and resid 75', 'name OE2 and resid 75']

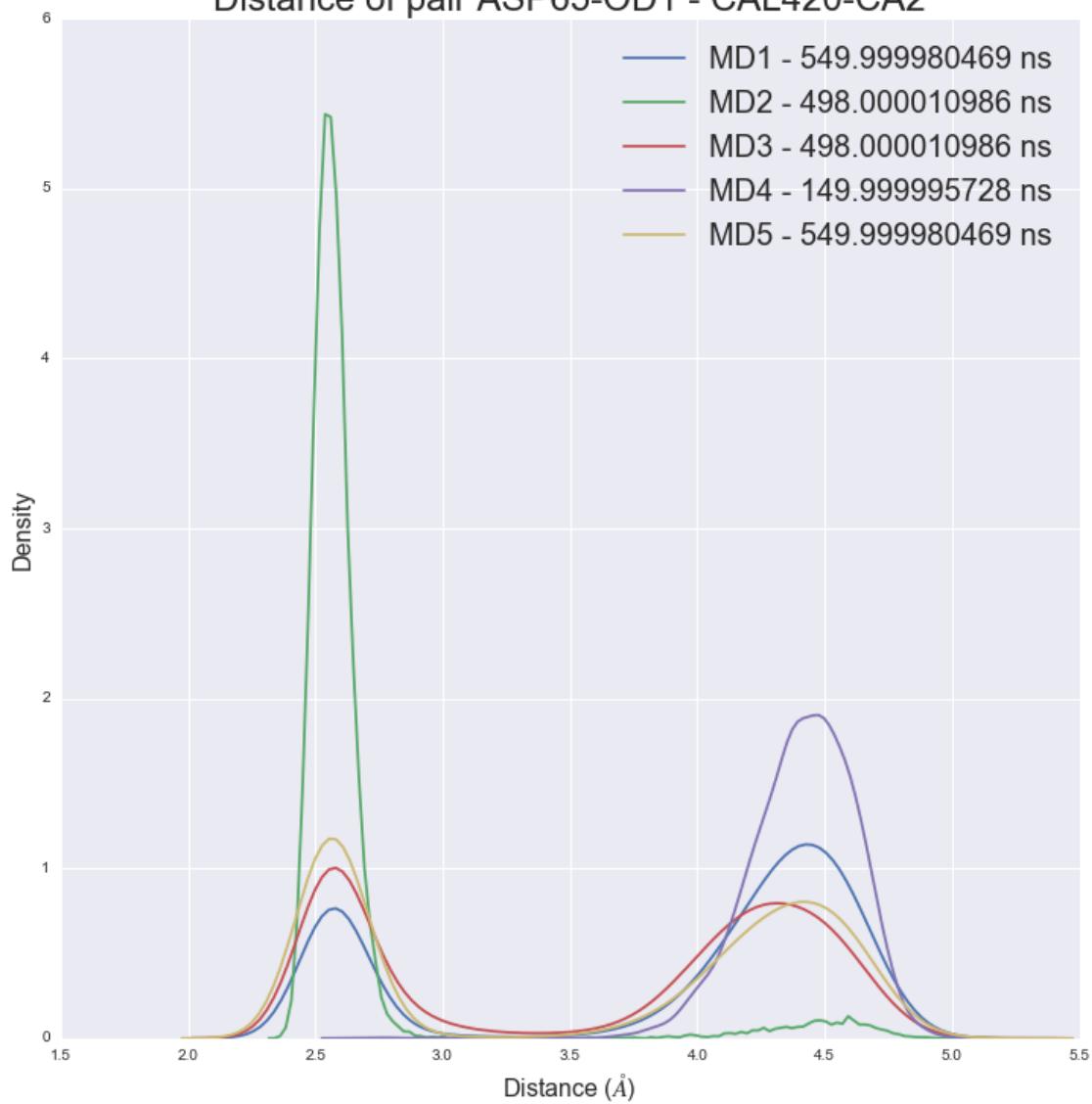

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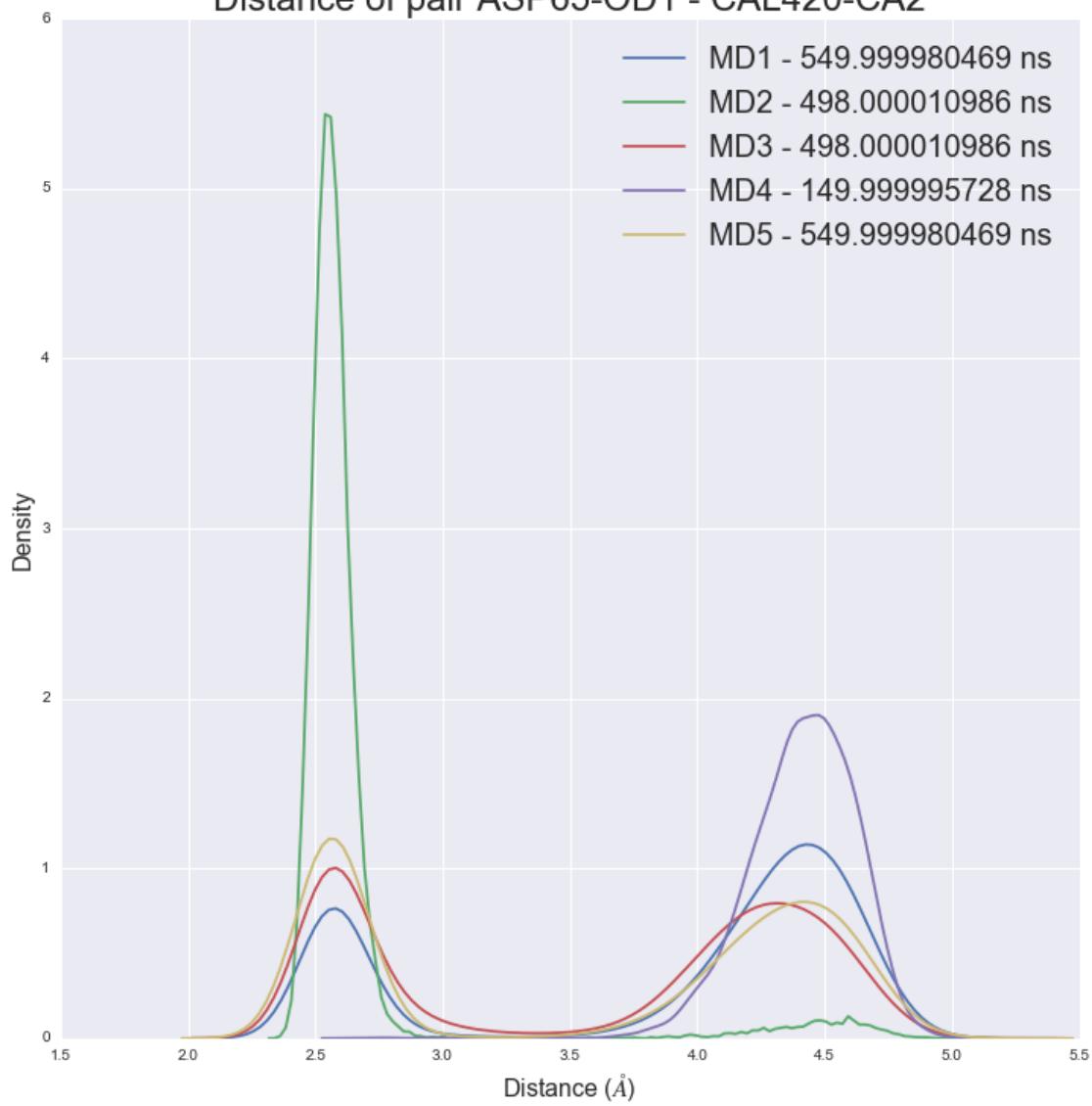
In [16]: atom2 = 'resid 419'
for atom1 in atom1_list:
    plt.figure(figsize = (12,12))
    for traj_i, top_i, name in zip(traj_list, top_list, complex_names):
        distance, pair, time = main(top_i, traj_i, atom1, atom2, verbose = 0, plot_dist = False)
        ax = sns.distplot(distance, hist=False, label= '%s - %s ns' %(name, time))
        ax.set_xlabel('Distance (${\AA}$)', size = 16)
        ax.set_ylabel('Density', size = 16)
        ax.set_title('Distance of pair %s' %(pair) , size = 24)
        ax.legend(loc = 'best', prop={'size':20})
    plt.show()

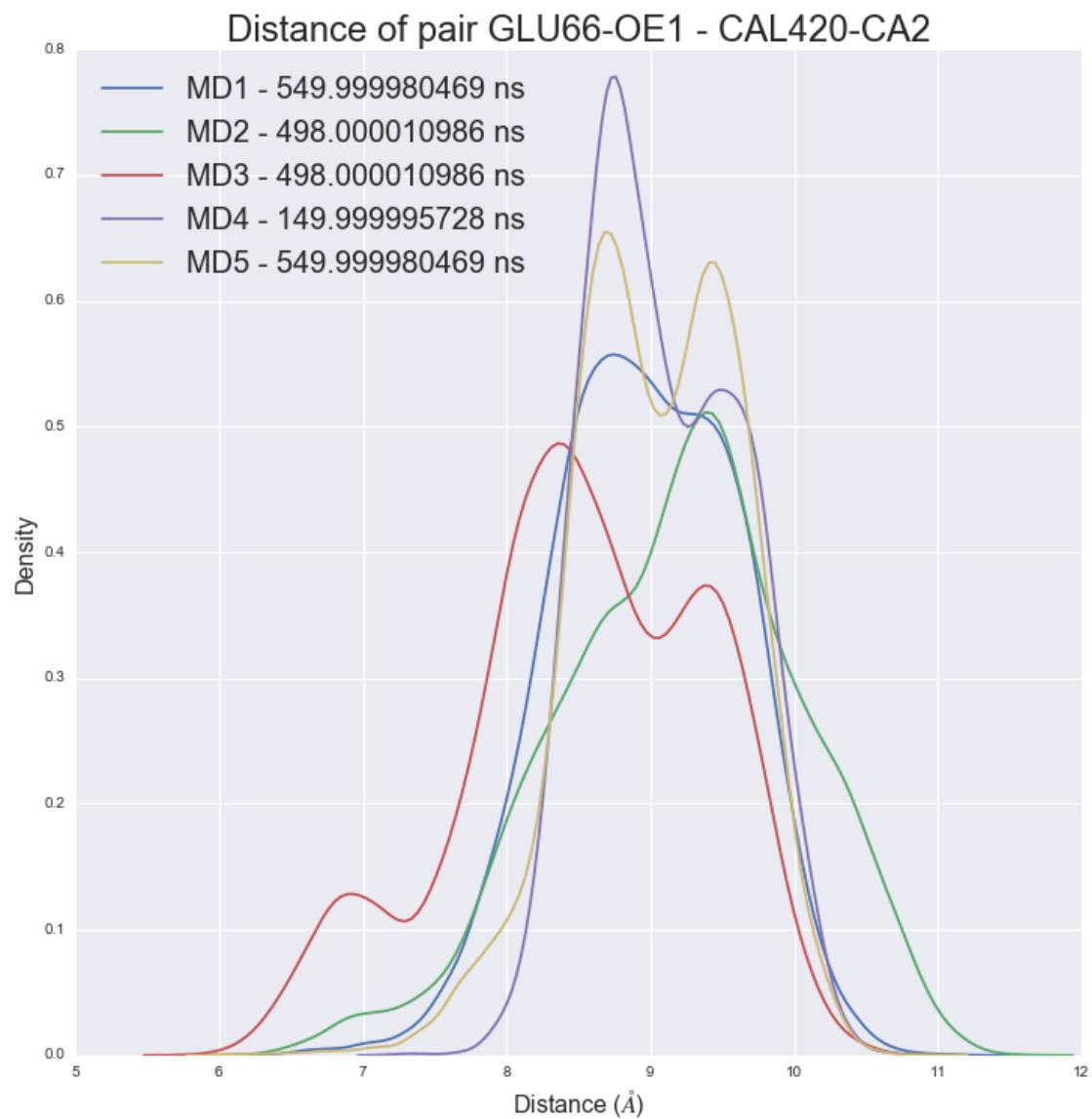
```

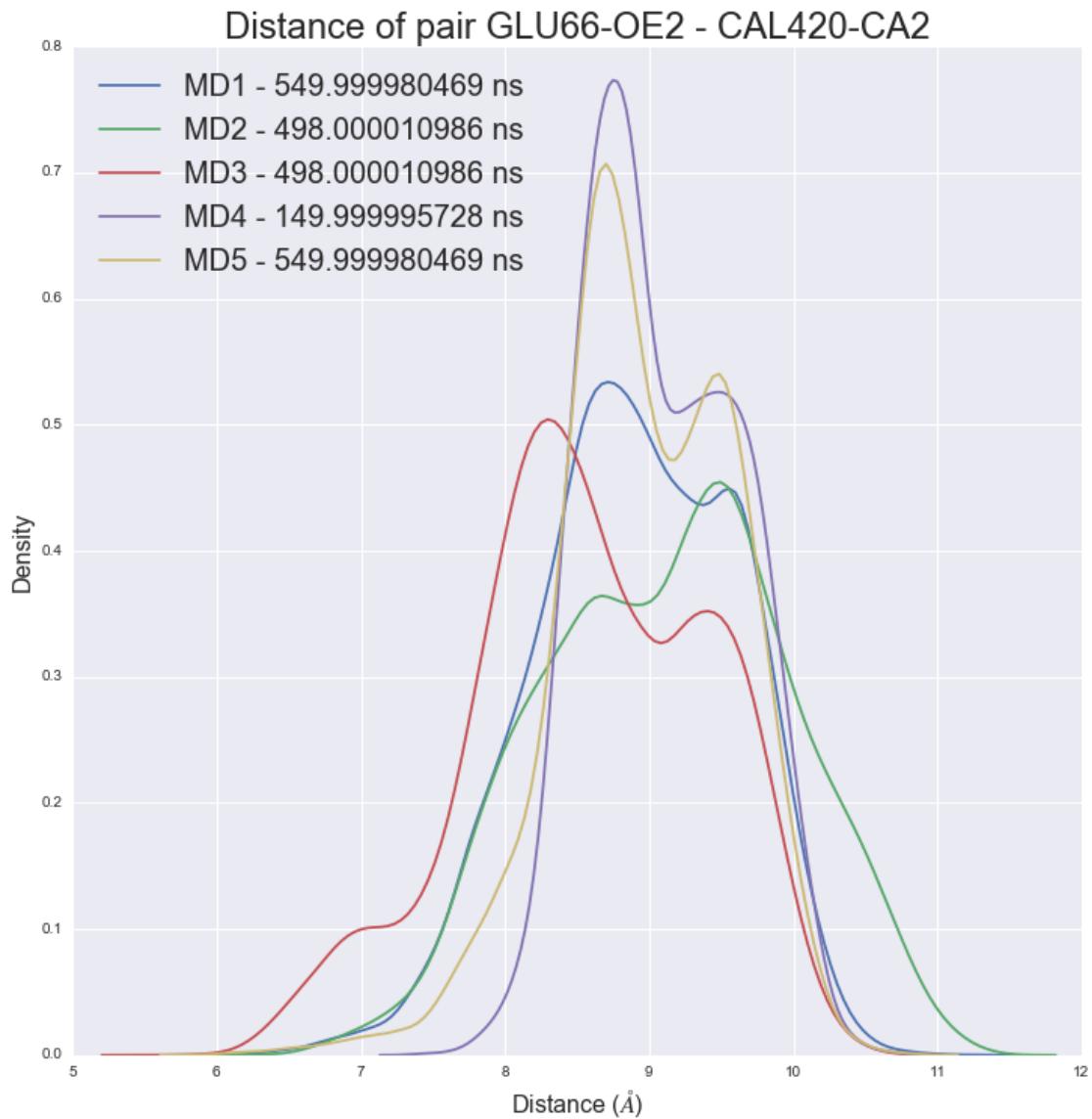
### Distance of pair ASP65-OD1 - CAL420-CA2



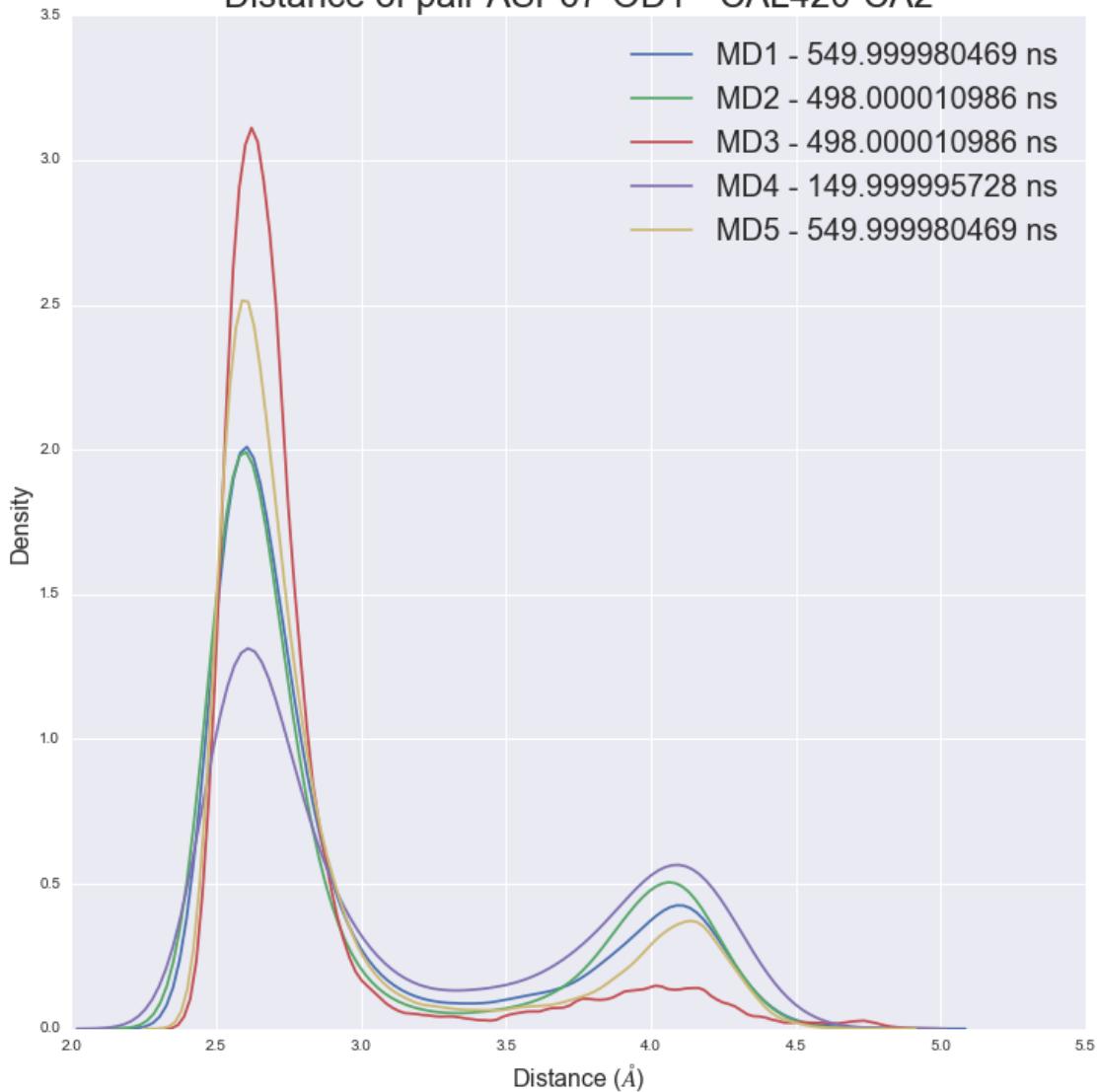
### Distance of pair ASP65-OD1 - CAL420-CA2



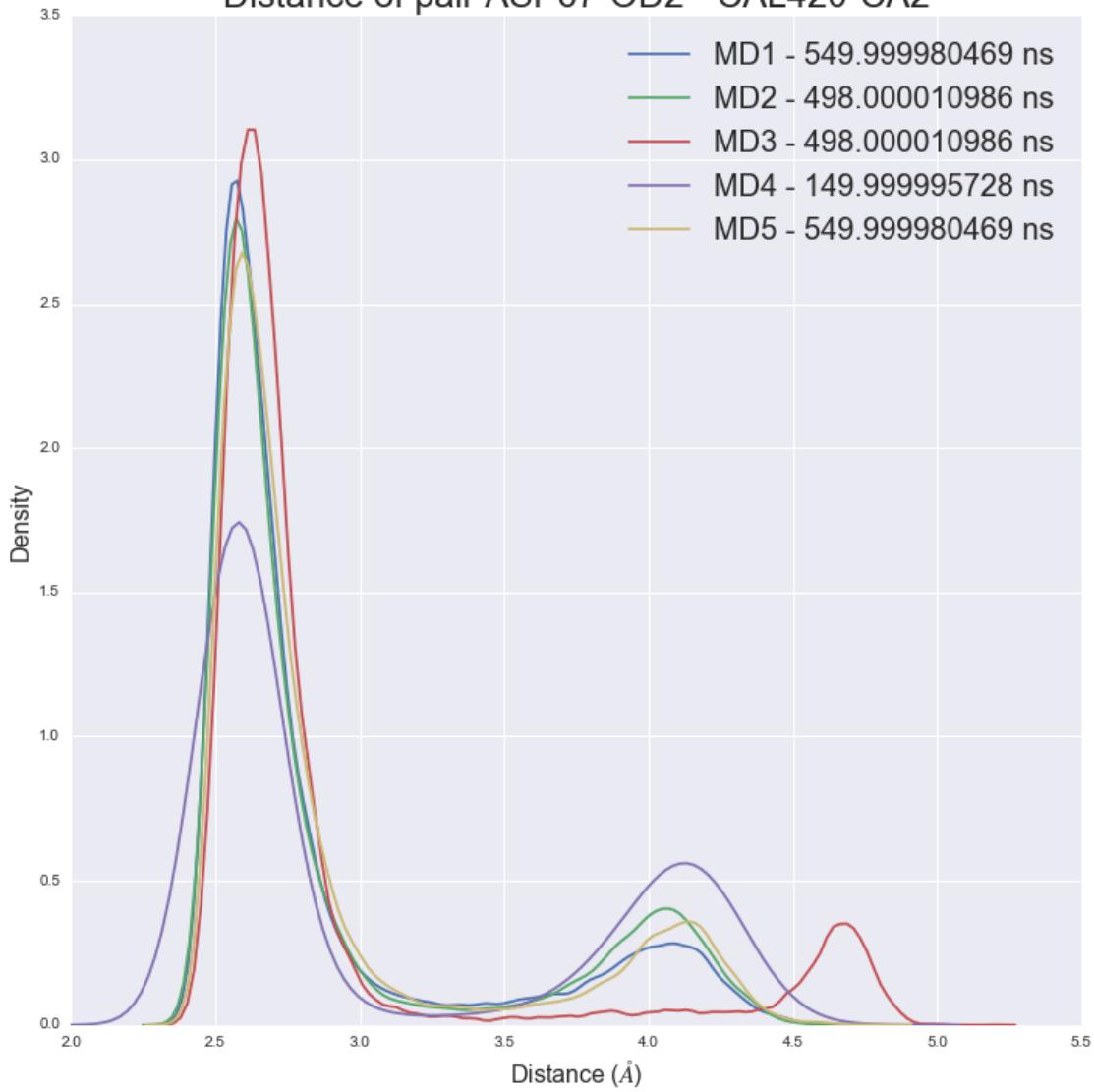


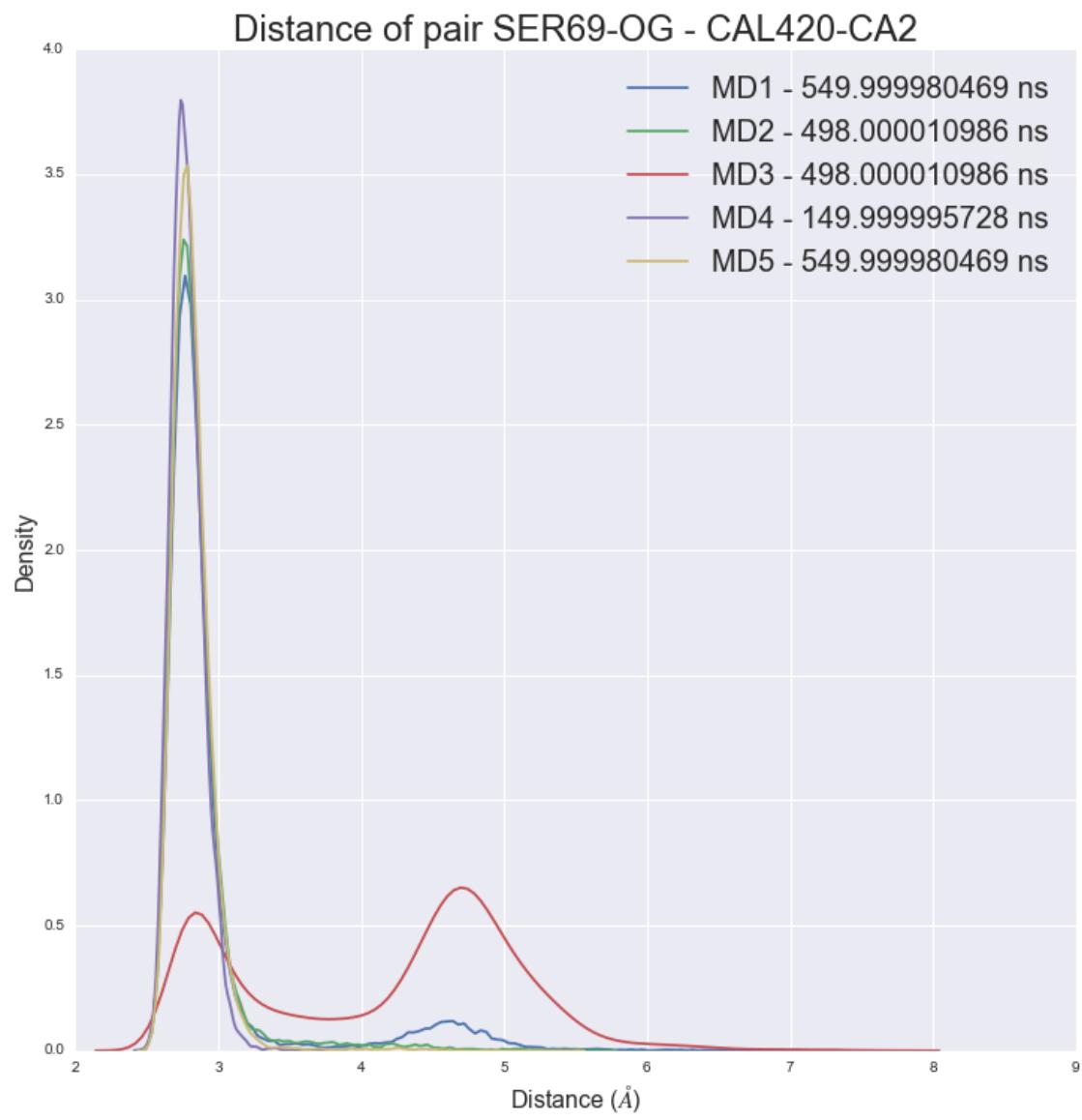


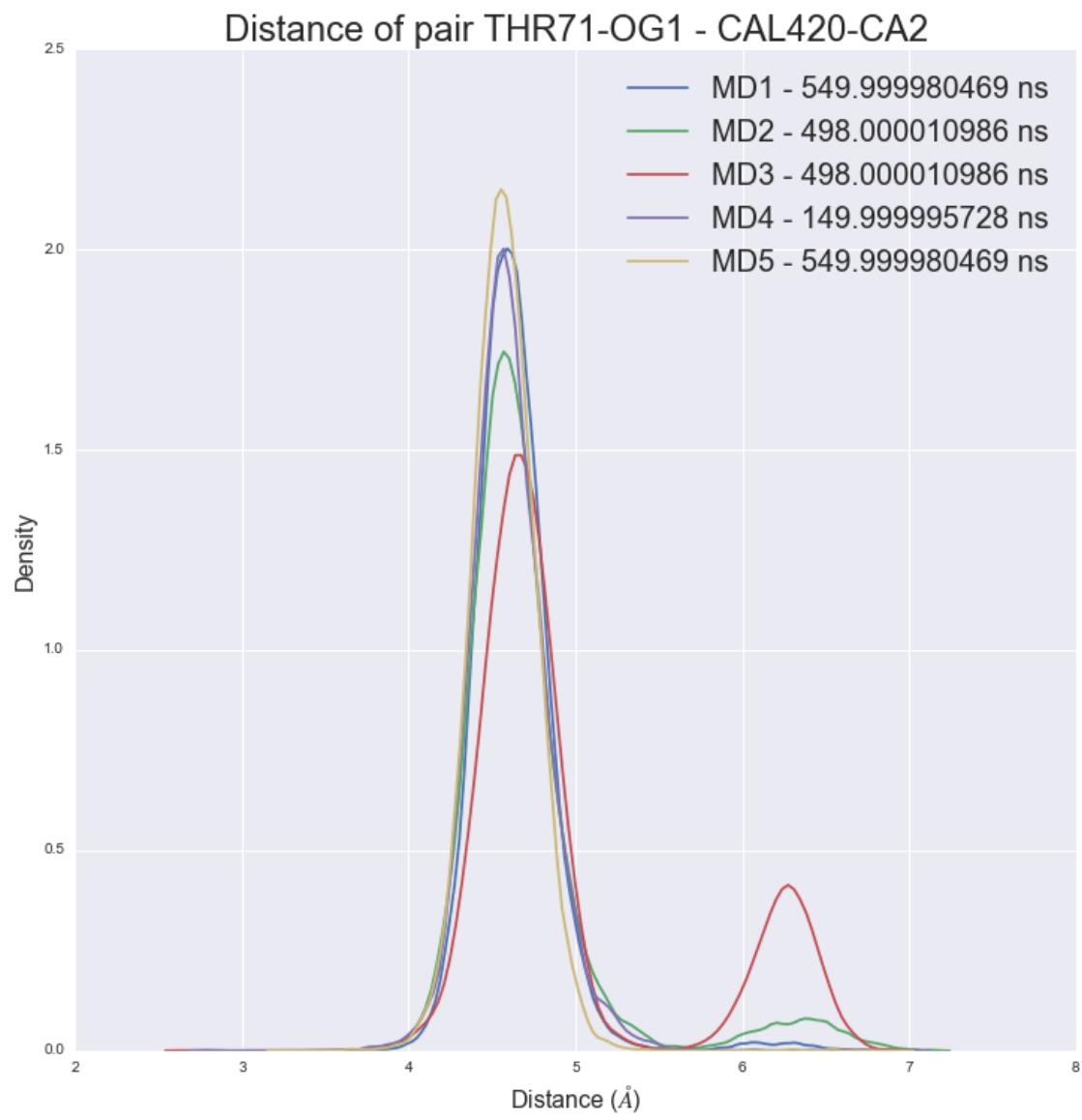
### Distance of pair ASP67-OD1 - CAL420-CA2

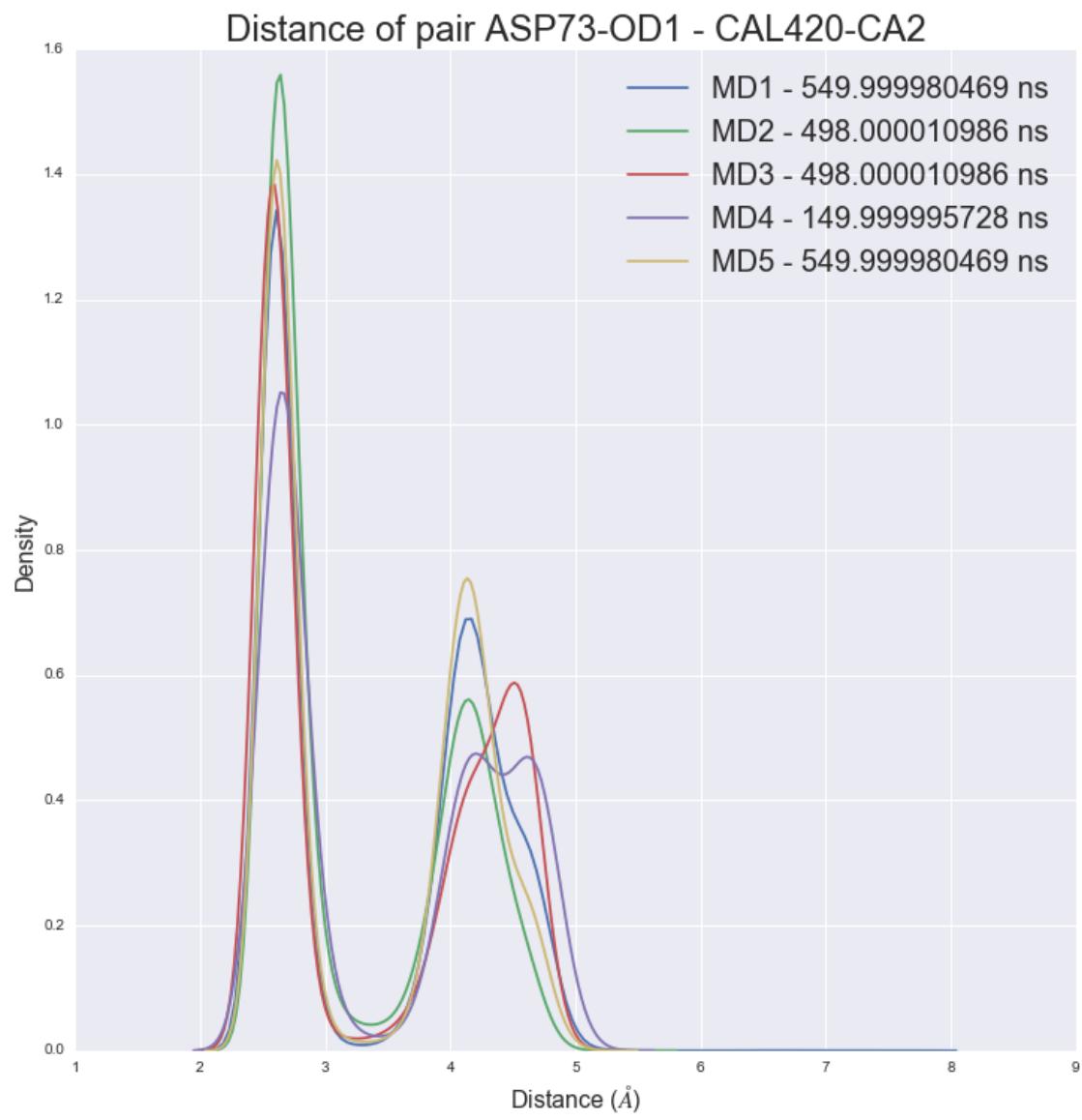


### Distance of pair ASP67-OD2 - CAL420-CA2

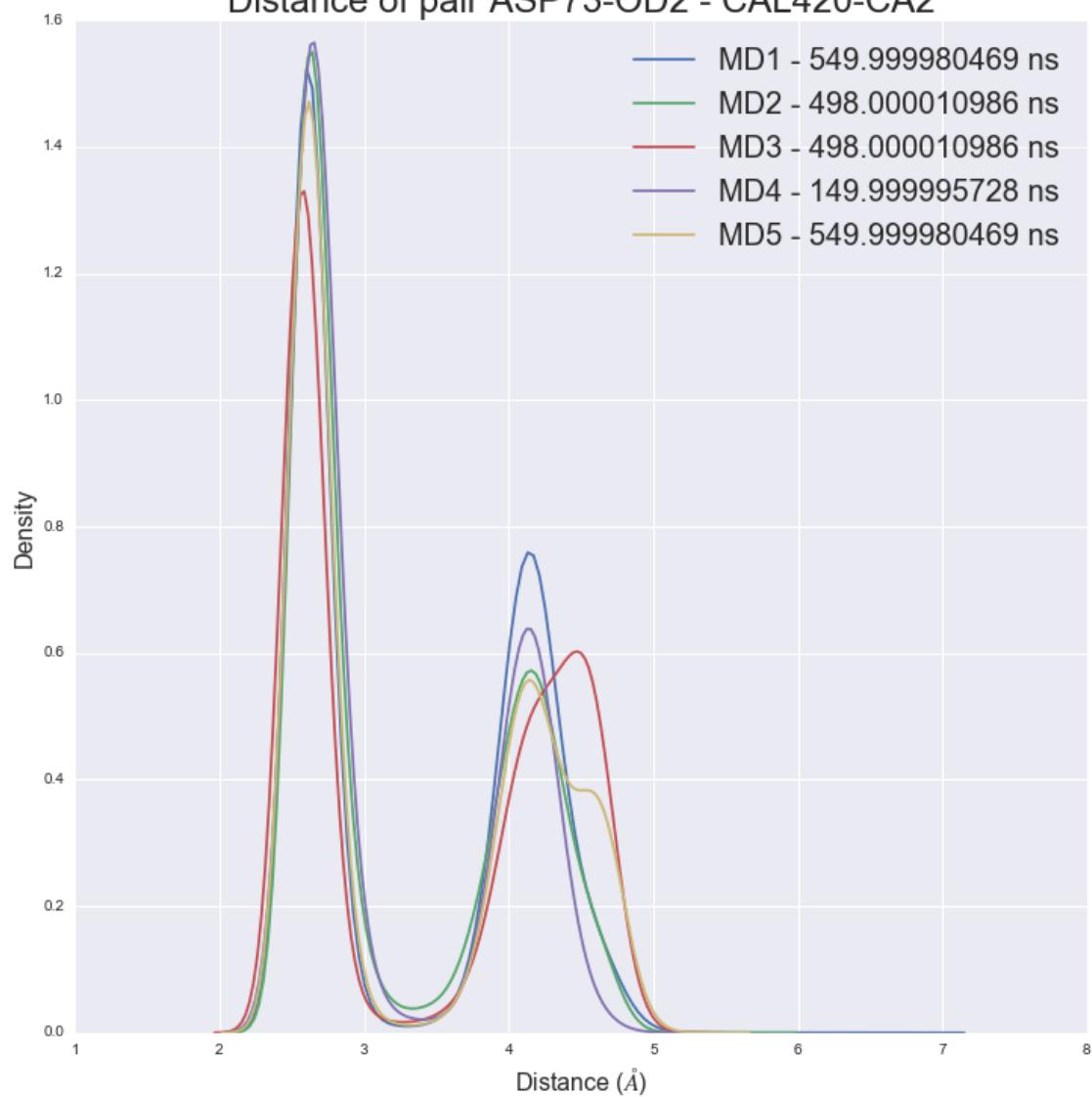


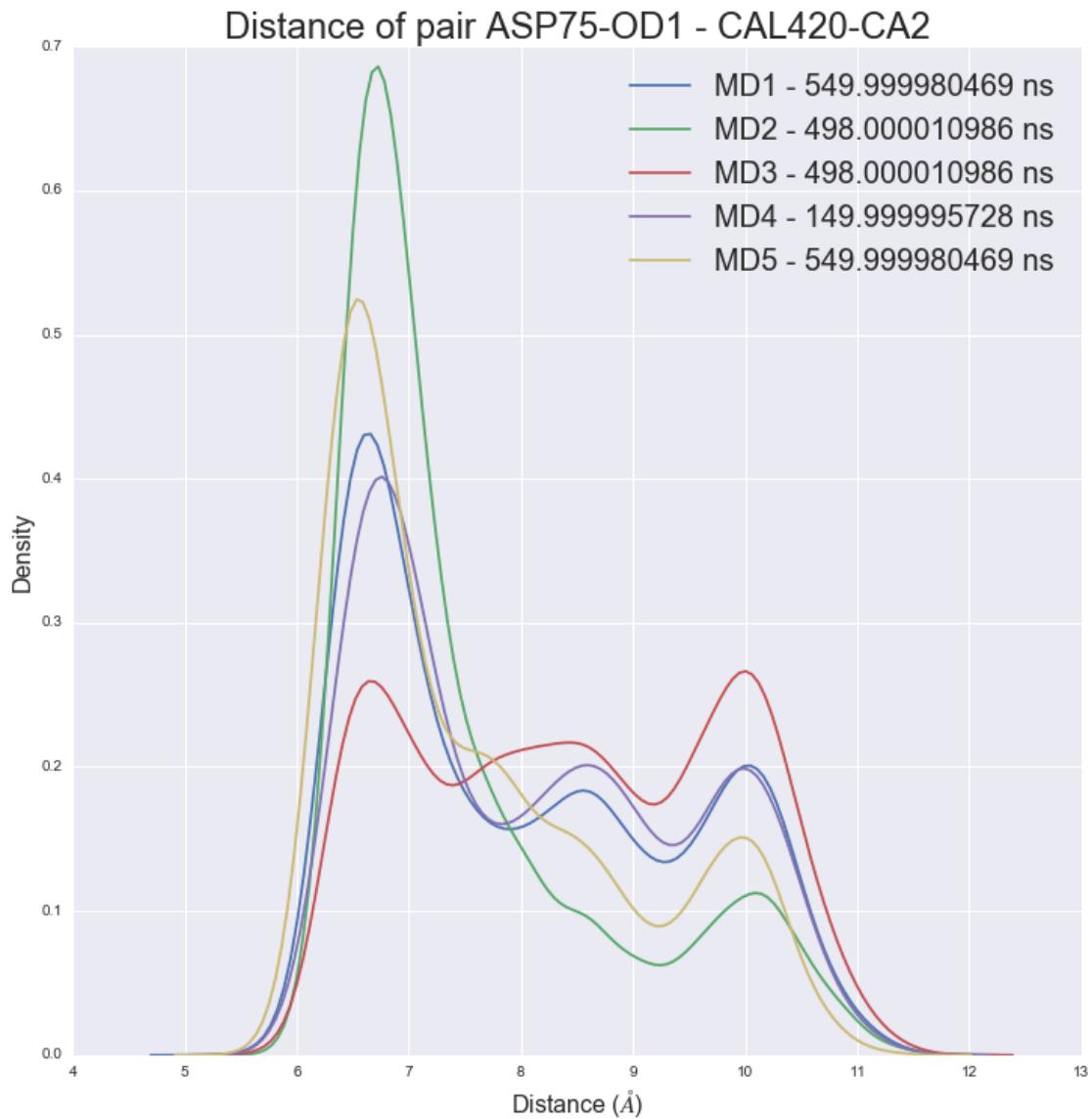


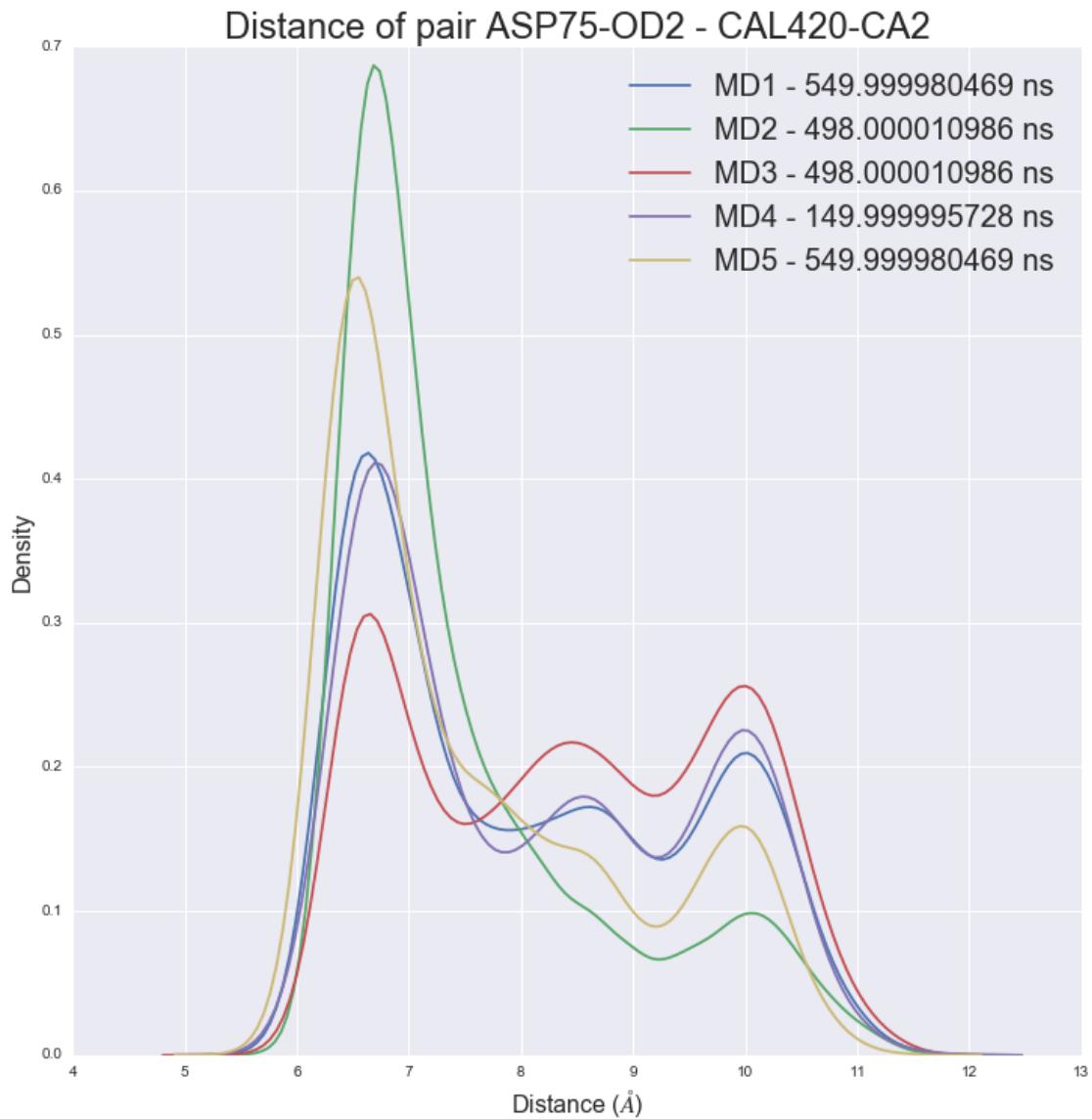


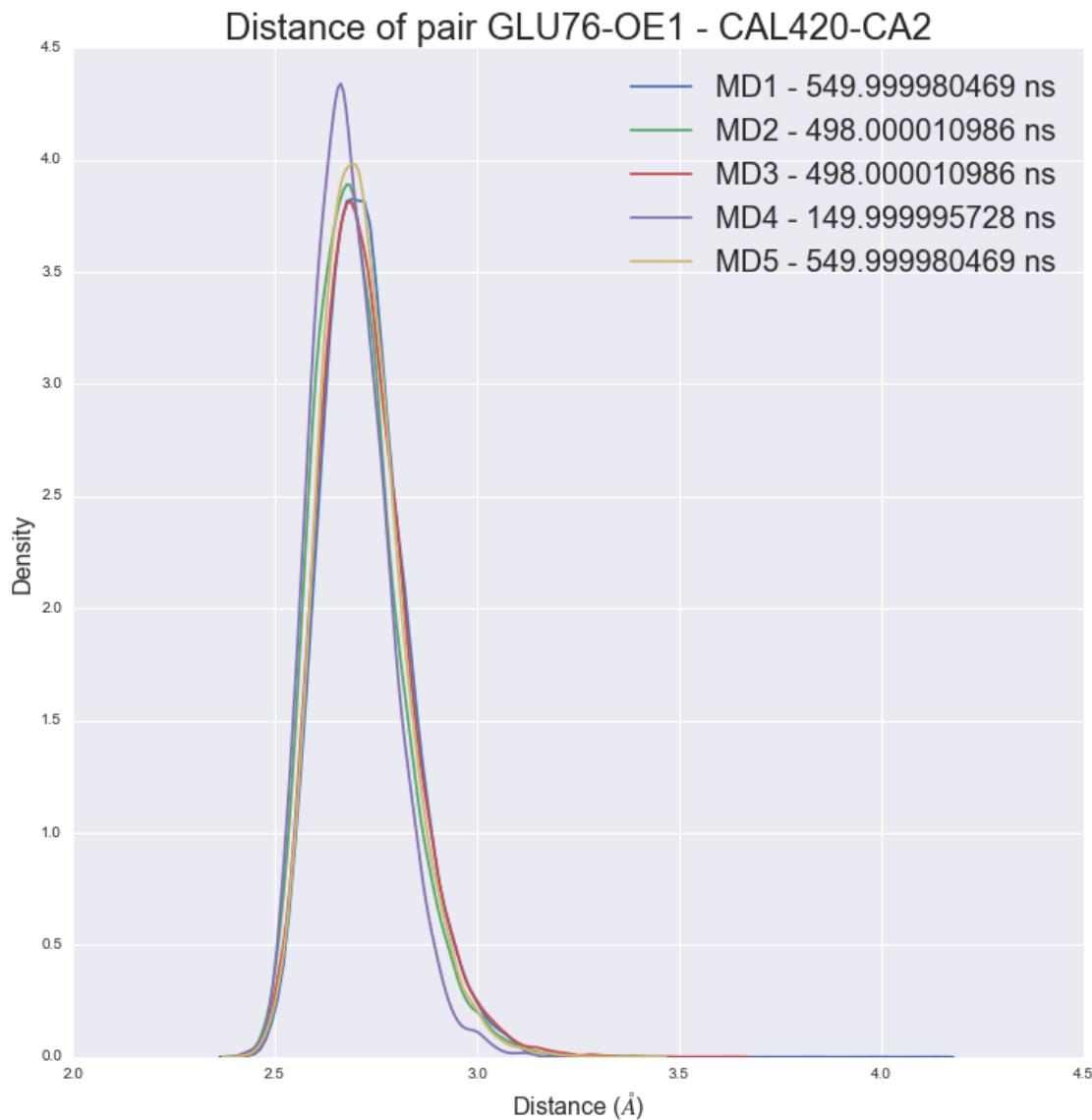


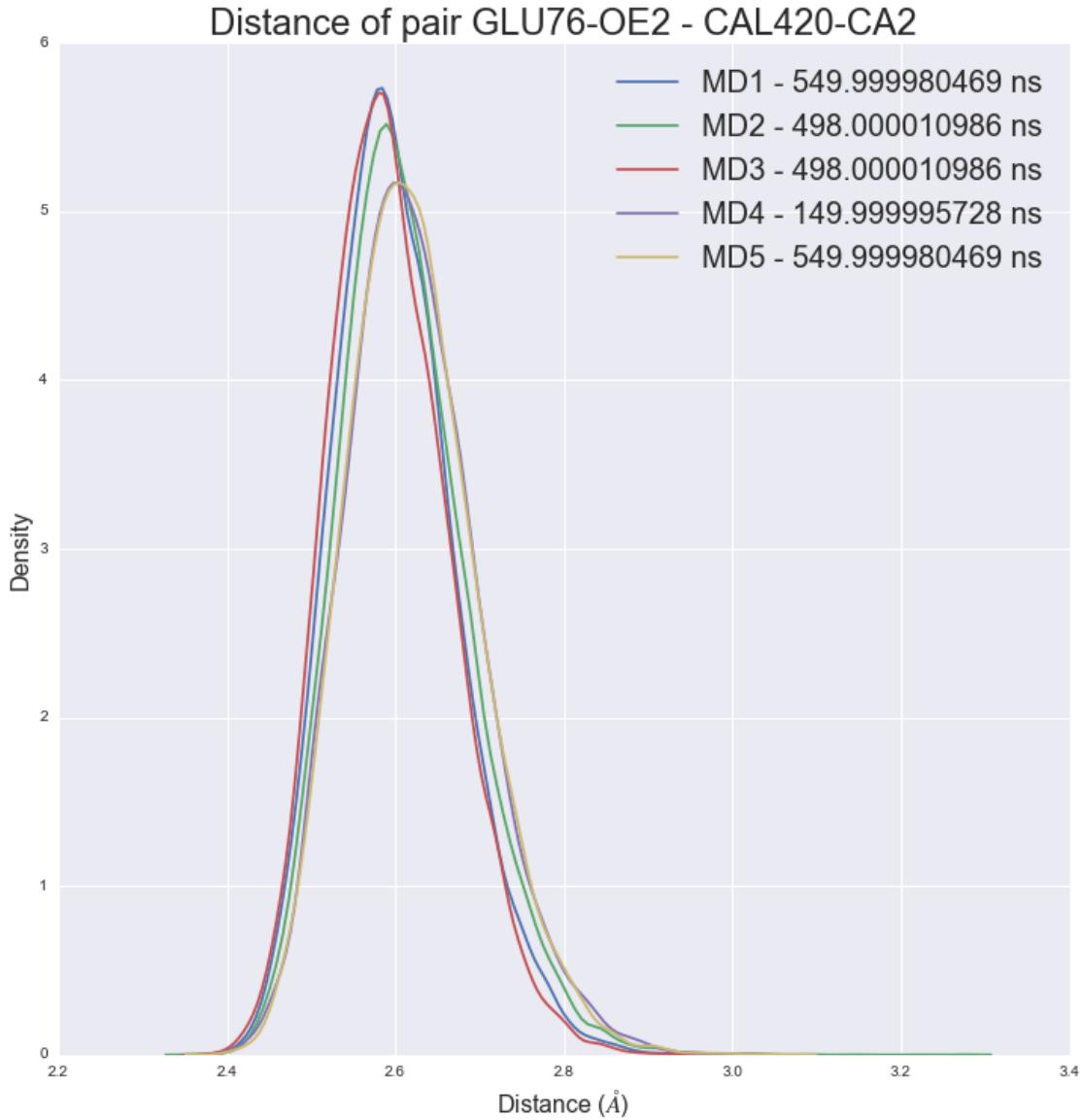
### Distance of pair ASP73-OD2 - CAL420-CA2











## 0.1 MD1

```
In [6]: topology_MD1 = '/Users/gil_f.hoben/Troponin_md_processed/MD1/run1/troponin_egcg_MD1_nowater.prmtop'
trajectory_MD1 = '/Users/gil_f.hoben/Troponin_md_processed/MD1/run1/Trajectories/'
atom1_list = ['name OD1 and resid 64', 'name OD1 and resid 64', 'name OE1 and resid 65',
              'name OE2 and resid 65', 'name OD1 and resid 66',
              'name OD2 and resid 66', 'name OG and resid 68', 'name OG1 and resid 70',
              'name OD1 and resid 72', 'name OD2 and resid 72', 'name OD1 and resid 74',
              'name OD2 and resid 74', 'name OE1 and resid 75', 'name OE2 and resid 75']
atom2 = 'resid 419'

In [7]: for atom1 in atom1_list:
    main(topology_MD1, trajectory_MD1, atom1, atom2, verbose = 1)
```

The following topology file was successfully loaded:  
<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

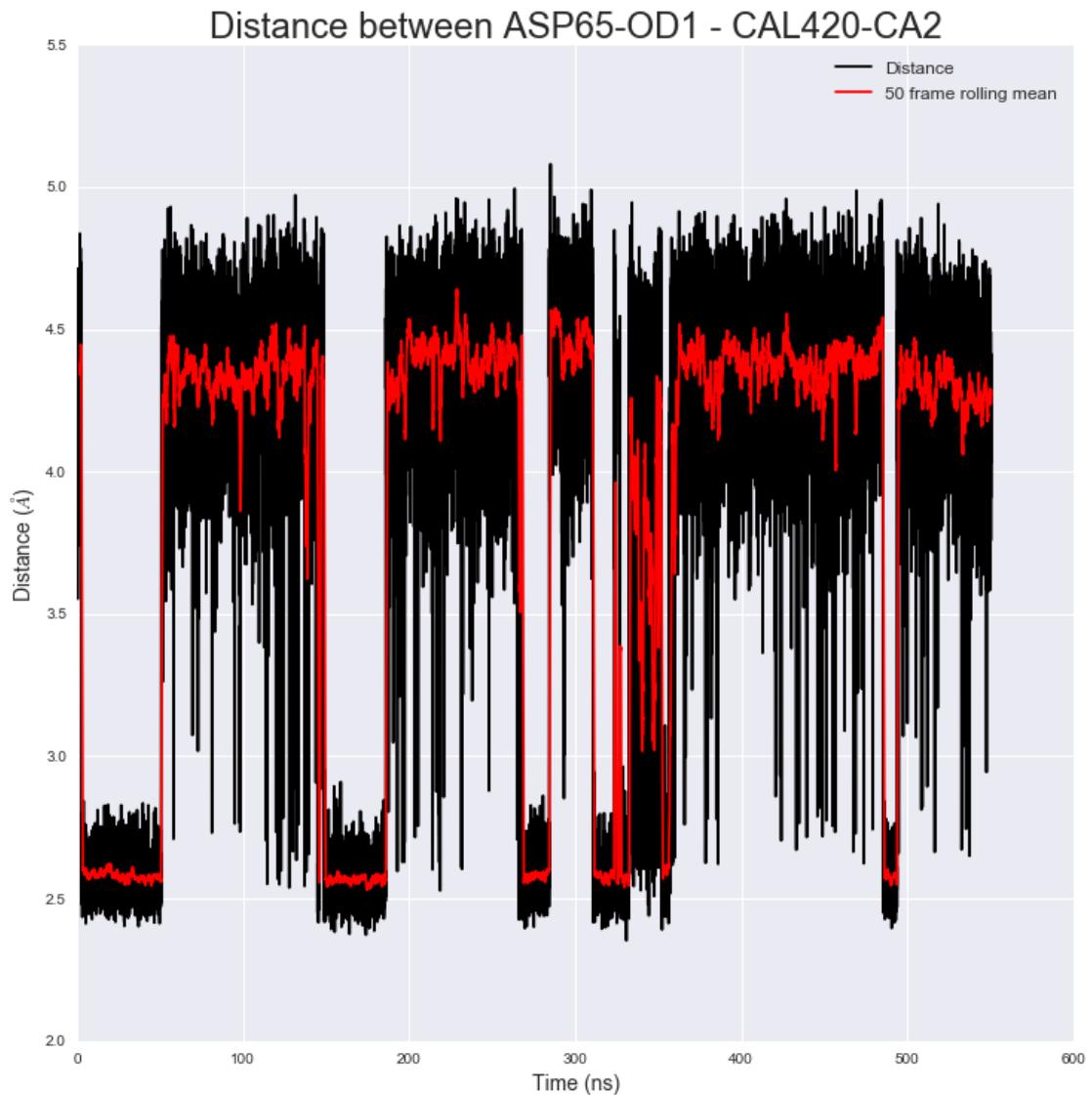
Atom1 number: 1005

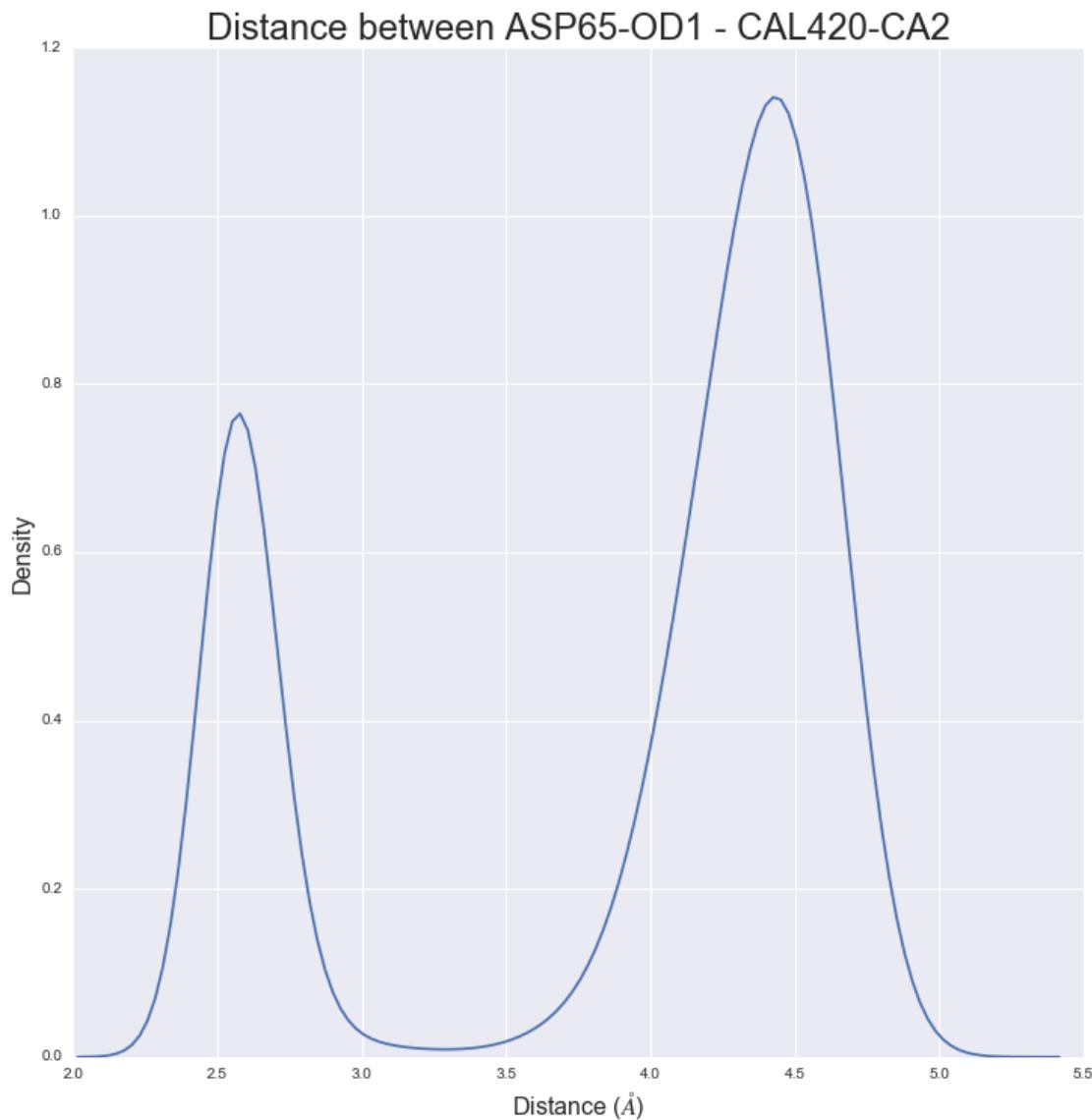
Atom2 number: 6810

Calculating distance between following atoms: ASP65-OD1 - CAL420-CA2

Loading trajectories from the following files:

05\_Prod\_troponin\_egcg\_MD1\_000-050\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_050-100\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_100-150\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_150-200\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_200-250\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_250-300\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_300-350\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_350-400\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_400-450\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_450-500\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_500-550\_run1\_nowater.nc





Total execution time: 7.72 seconds

Total simulation time of all frames: 549.999980469 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1005

Atom2 number: 6810

Calculating distance between following atoms: ASP65-OD1 - CAL420-CA2

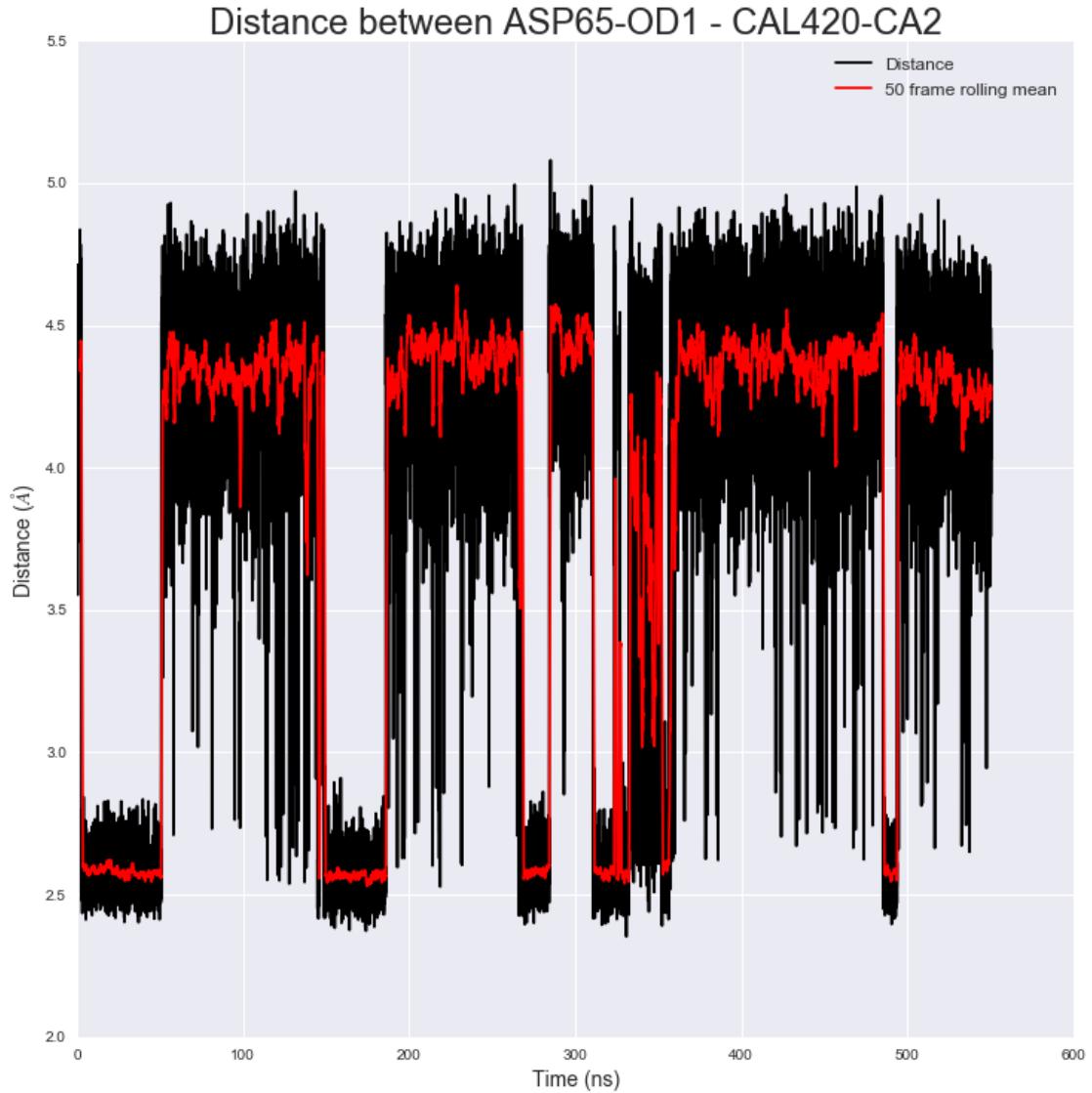
Loading trajectories from the following files:

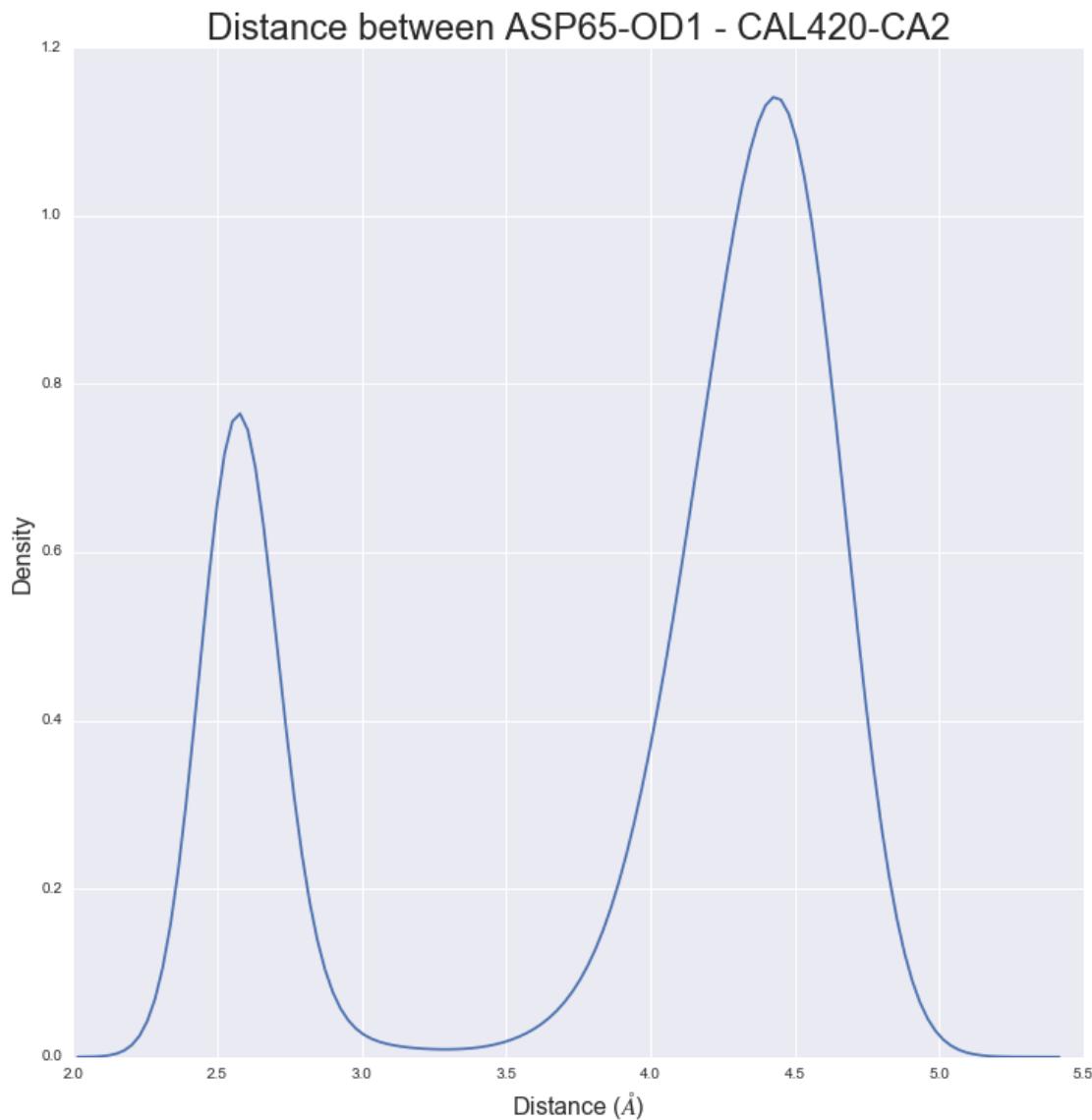
05\_Prod\_troponin\_egcg\_MD1\_000-050\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD1\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD1\_100-150\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD1\_150-200\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_200-250\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_250-300\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_300-350\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_350-400\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_400-450\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_450-500\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_500-550\_run1\_nowater.nc





Total execution time: 5.25 seconds

Total simulation time of all frames: 549.999980469 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1020

Atom2 number: 6810

Calculating distance between following atoms: GLU66-OE1 - CAL420-CA2

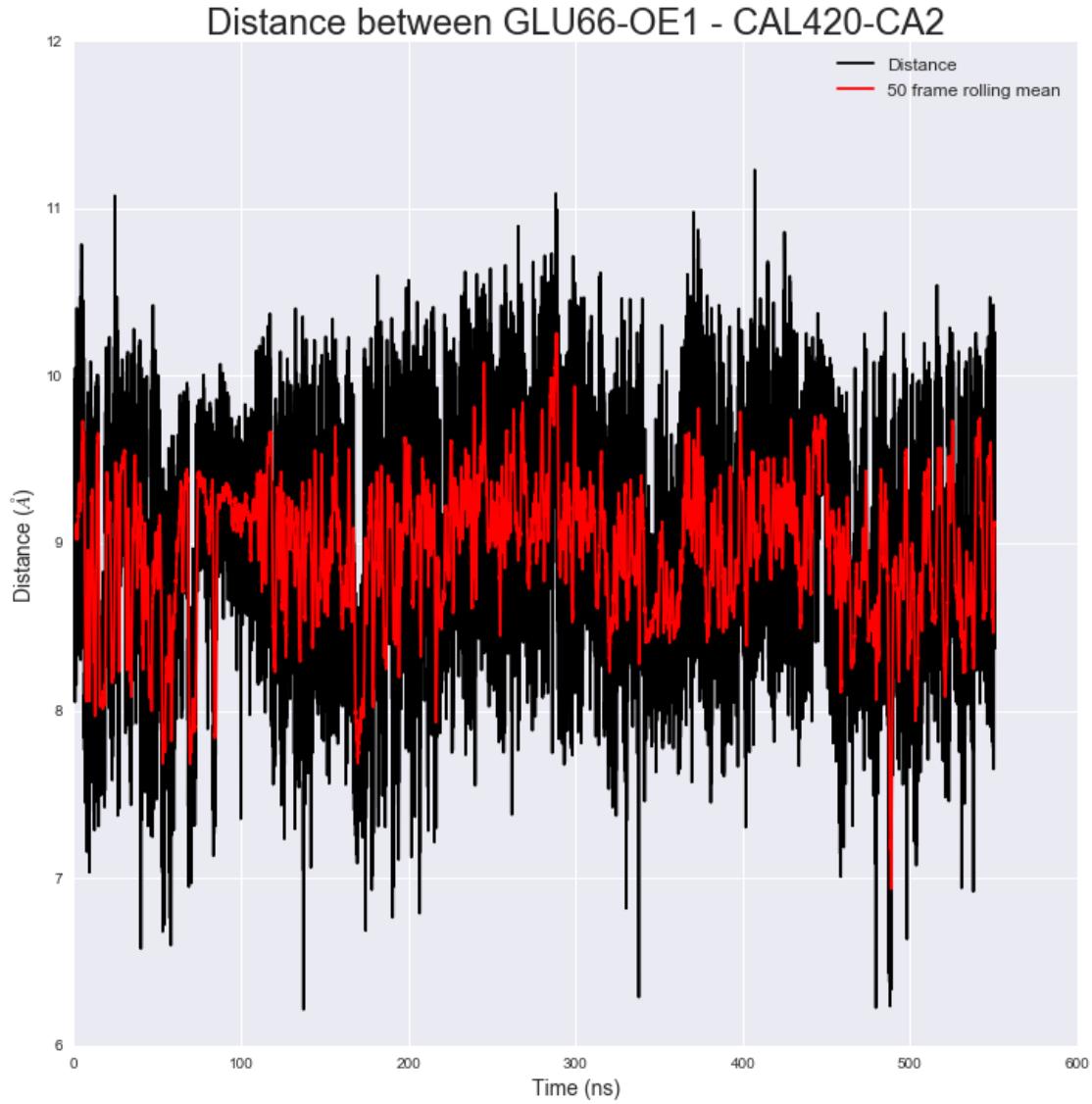
Loading trajectories from the following files:

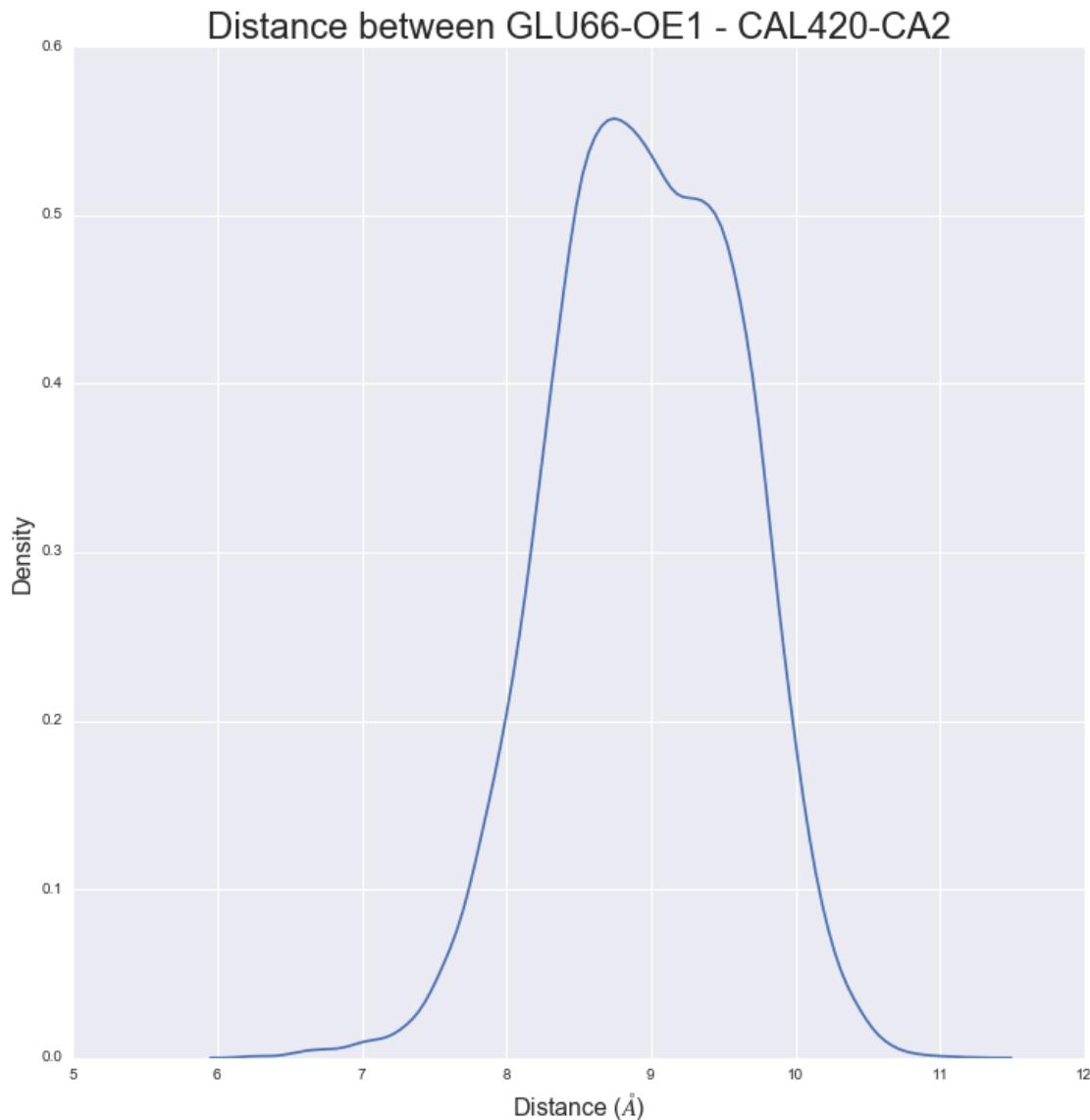
05\_Prod\_troponin\_egcg\_MD1\_000-050\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD1\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD1\_100-150\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD1\_150-200\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_200-250\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_250-300\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_300-350\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_350-400\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_400-450\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_450-500\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_500-550\_run1\_nowater.nc





Total execution time: 4.83 seconds

Total simulation time of all frames: 549.999980469 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1021

Atom2 number: 6810

Calculating distance between following atoms: GLU66-OE2 - CAL420-CA2

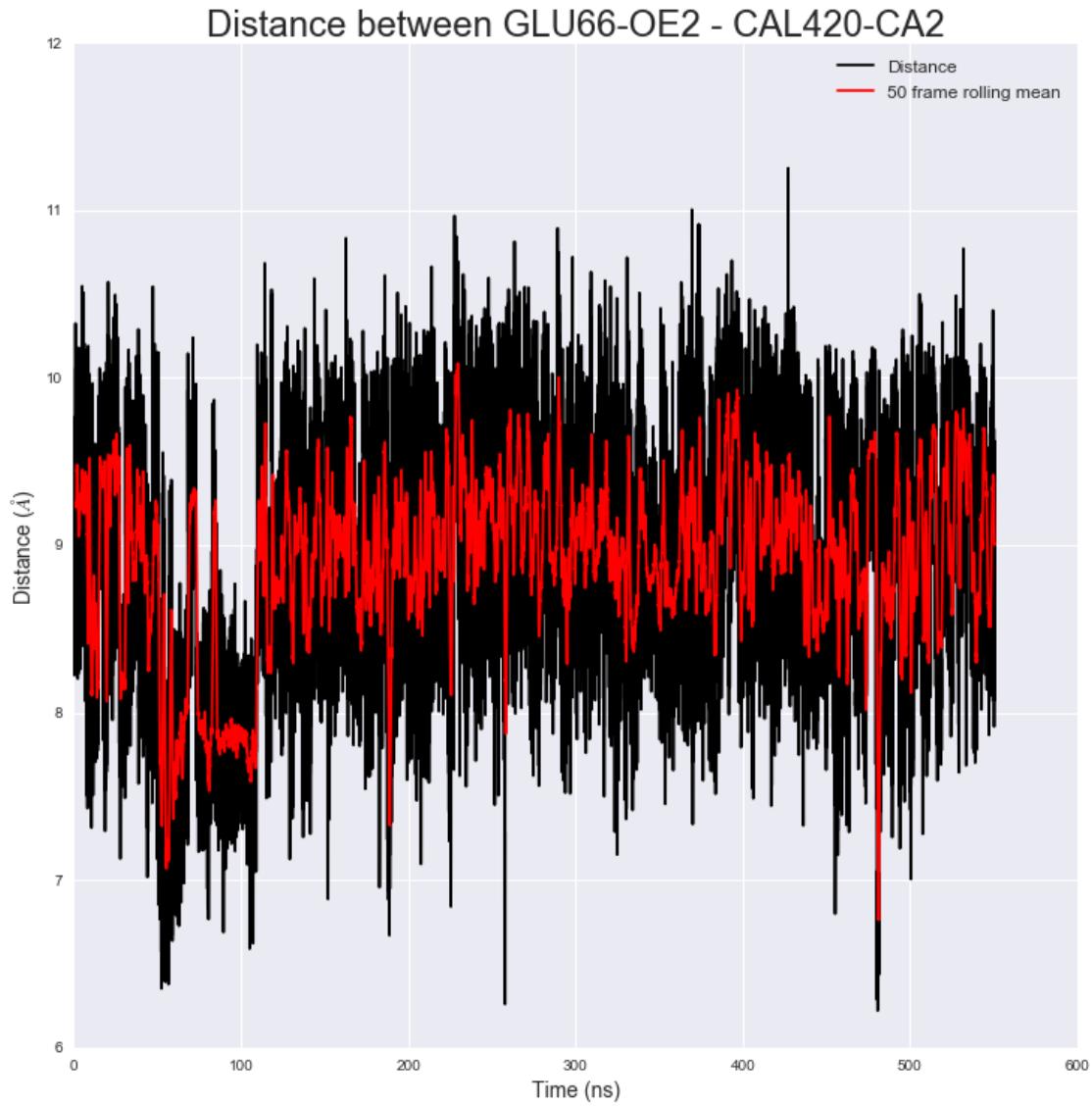
Loading trajectories from the following files:

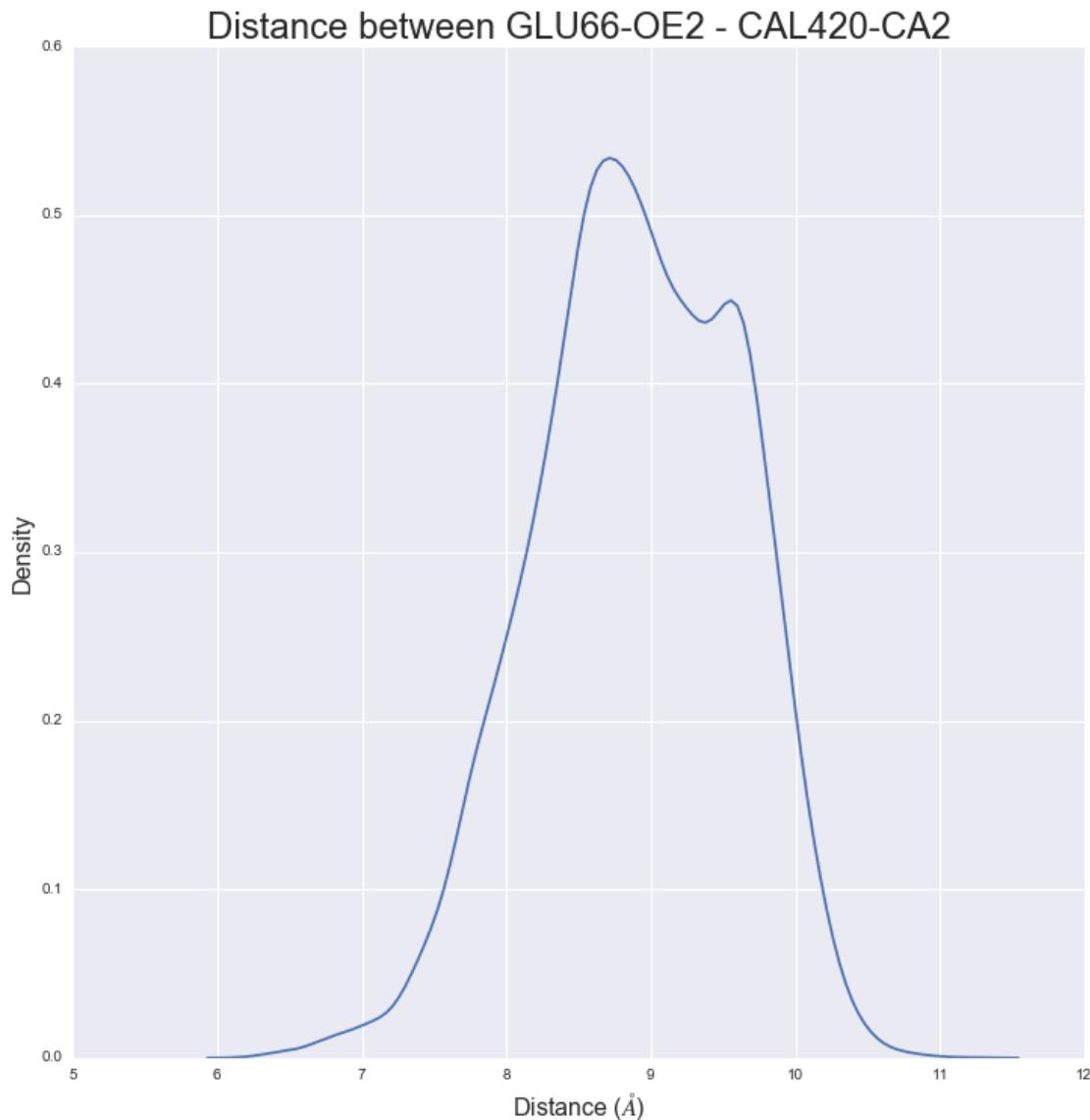
05\_Prod\_troponin\_egcg\_MD1\_000-050\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD1\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD1\_100-150\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD1\_150-200\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_200-250\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_250-300\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_300-350\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_350-400\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_400-450\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_450-500\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_500-550\_run1\_nowater.nc





Total execution time: 4.72 seconds

Total simulation time of all frames: 549.999980469 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1032

Atom2 number: 6810

Calculating distance between following atoms: ASP67-OD1 - CAL420-CA2

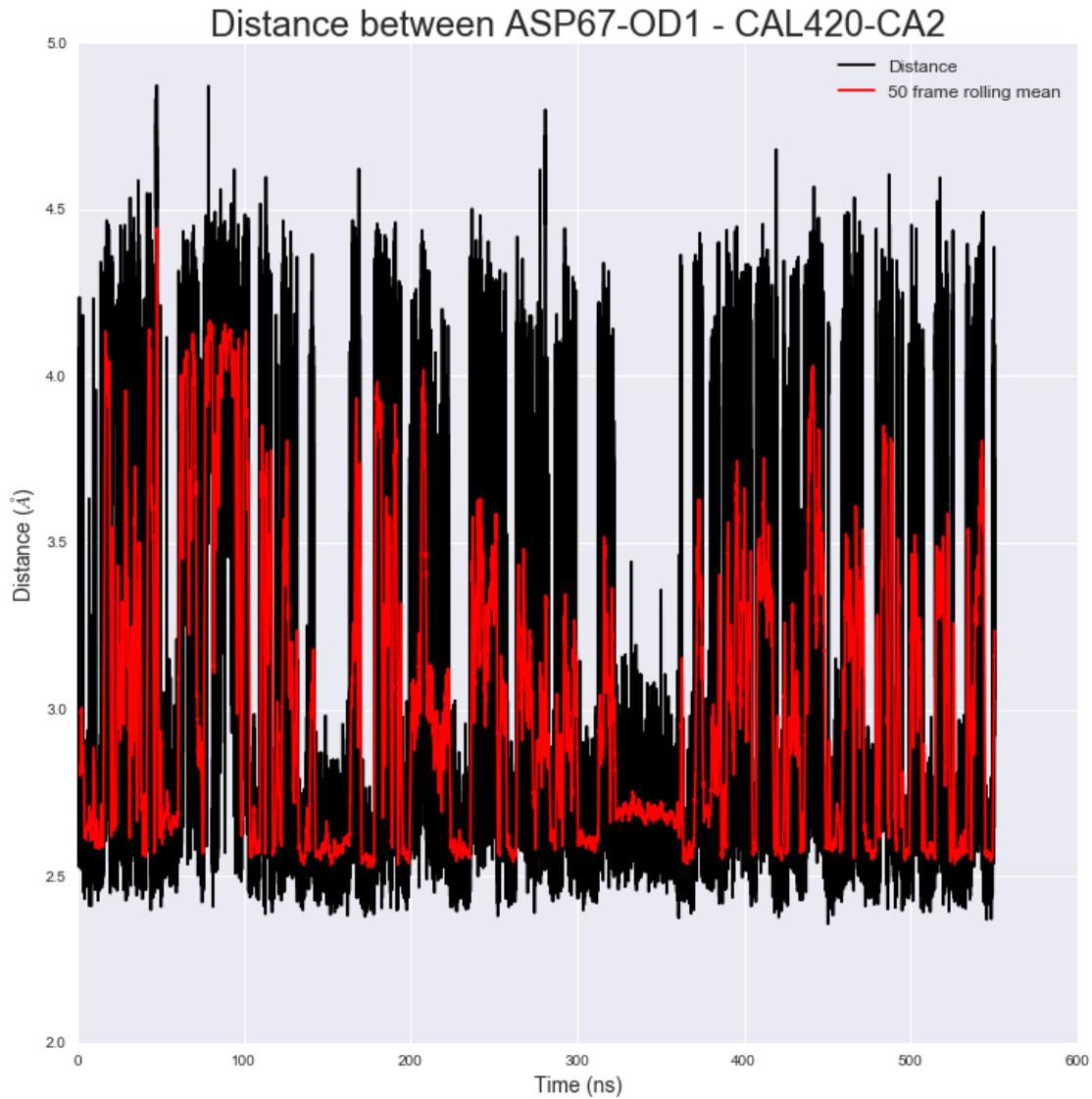
Loading trajectories from the following files:

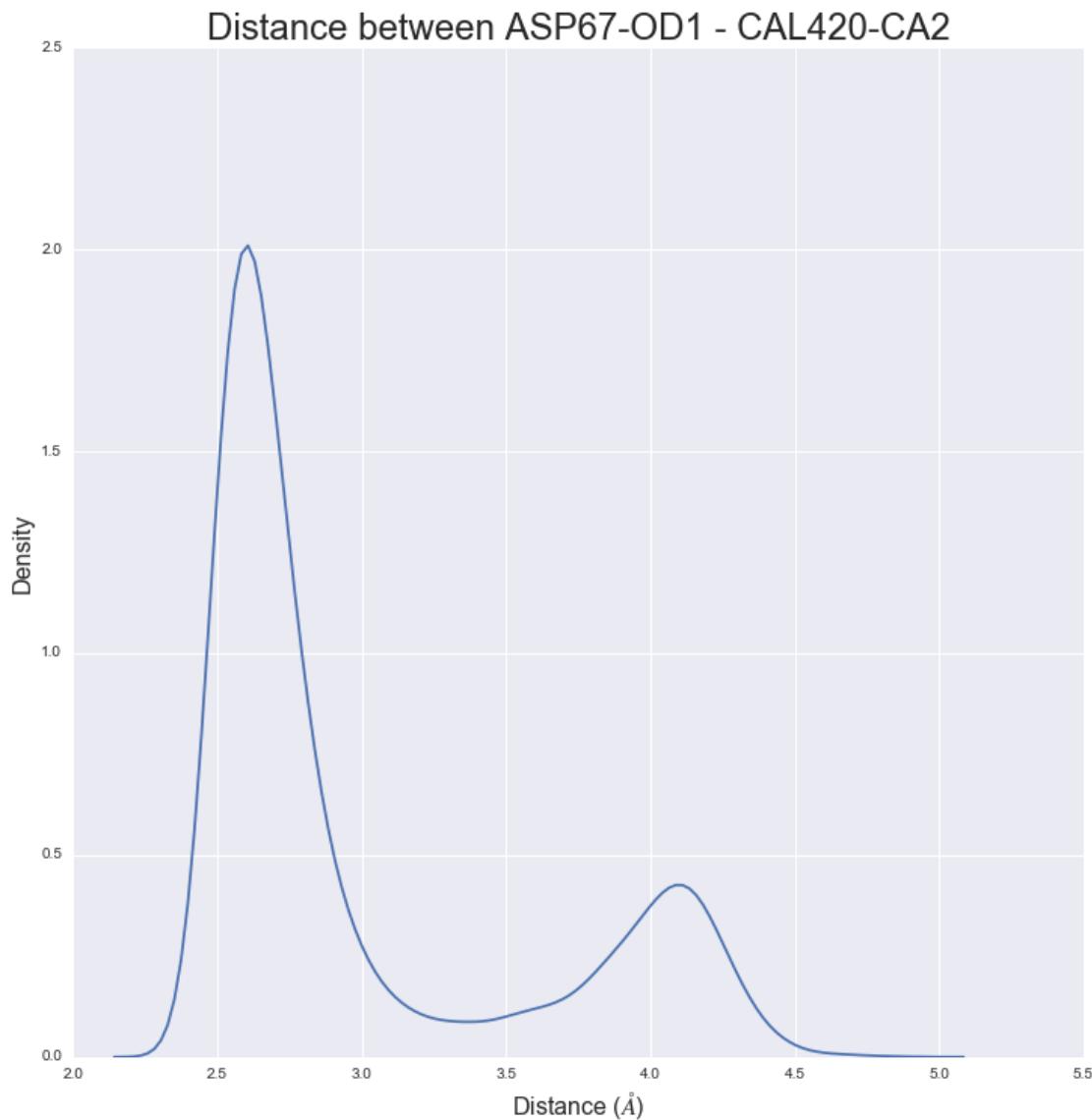
05\_Prod\_troponin\_egcg\_MD1\_000-050\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD1\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD1\_100-150\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD1\_150-200\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_200-250\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_250-300\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_300-350\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_350-400\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_400-450\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_450-500\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_500-550\_run1\_nowater.nc





Total execution time: 4.57 seconds

Total simulation time of all frames: 549.999980469 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1033

Atom2 number: 6810

Calculating distance between following atoms: ASP67-OD2 - CAL420-CA2

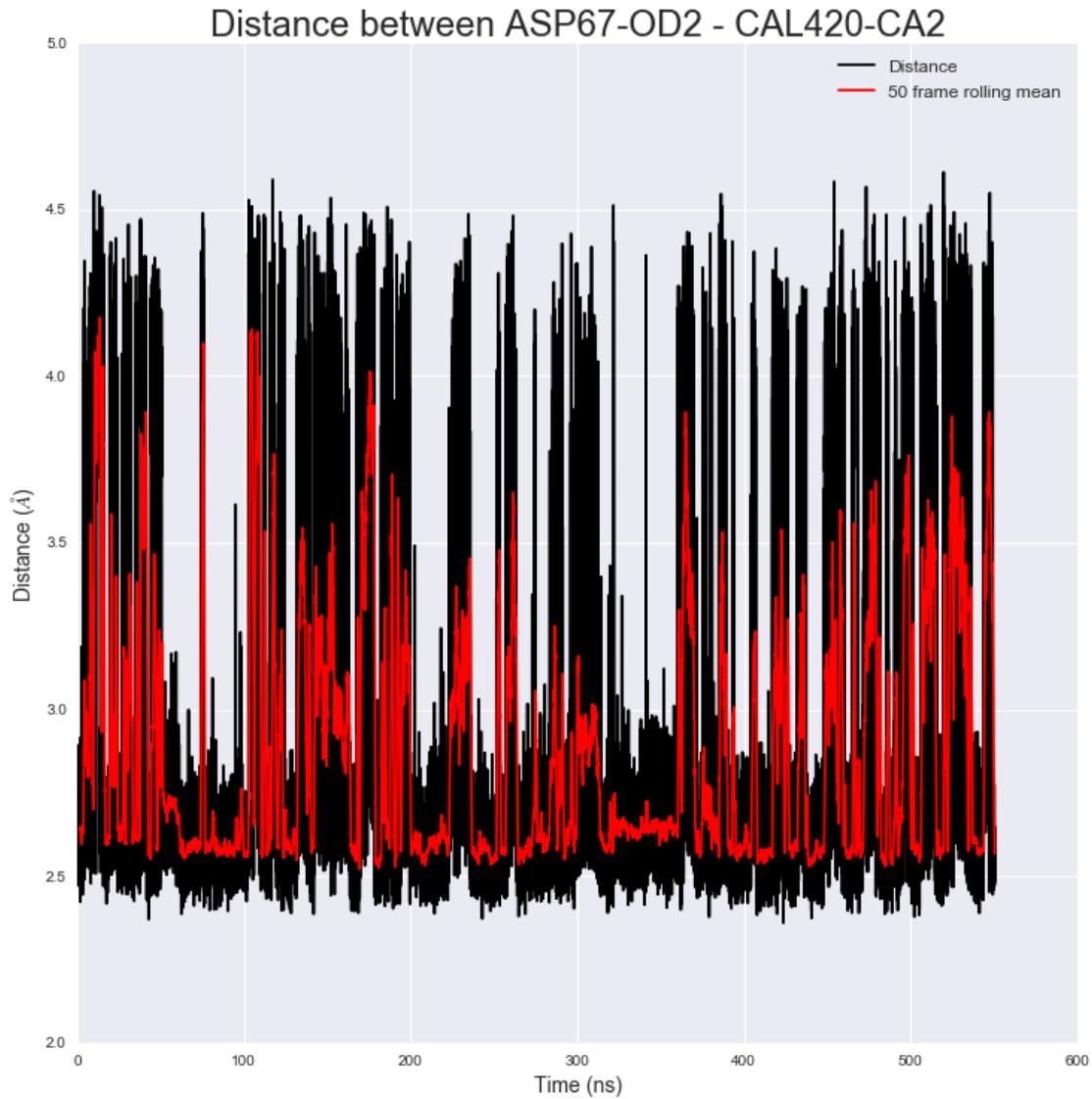
Loading trajectories from the following files:

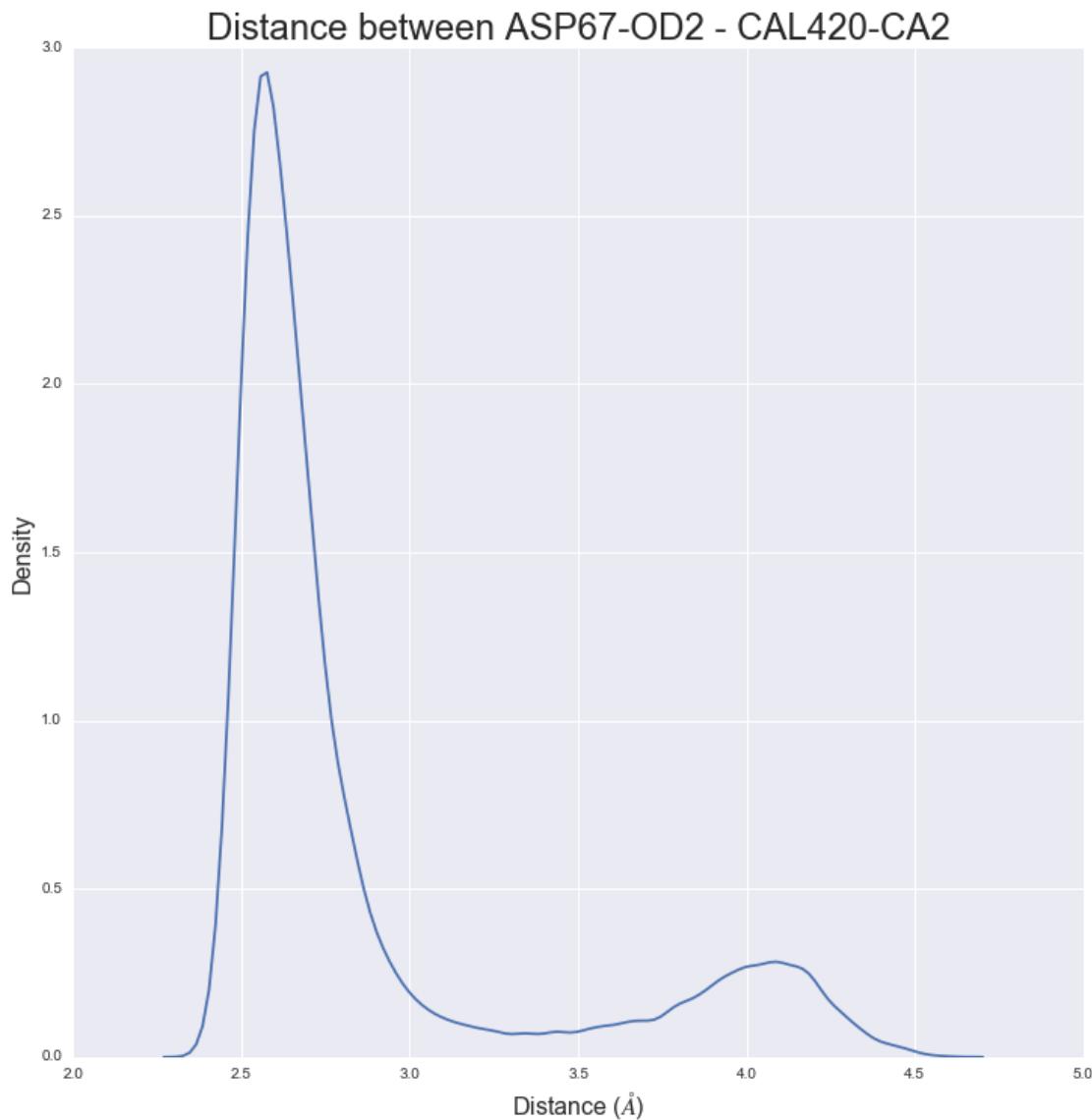
05\_Prod\_troponin\_egcg\_MD1\_000-050\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD1\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD1\_100-150\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD1\_150-200\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_200-250\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_250-300\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_300-350\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_350-400\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_400-450\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_450-500\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_500-550\_run1\_nowater.nc





Total execution time: 4.56 seconds

Total simulation time of all frames: 549.999980469 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1050

Atom2 number: 6810

Calculating distance between following atoms: SER69-OG - CAL420-CA2

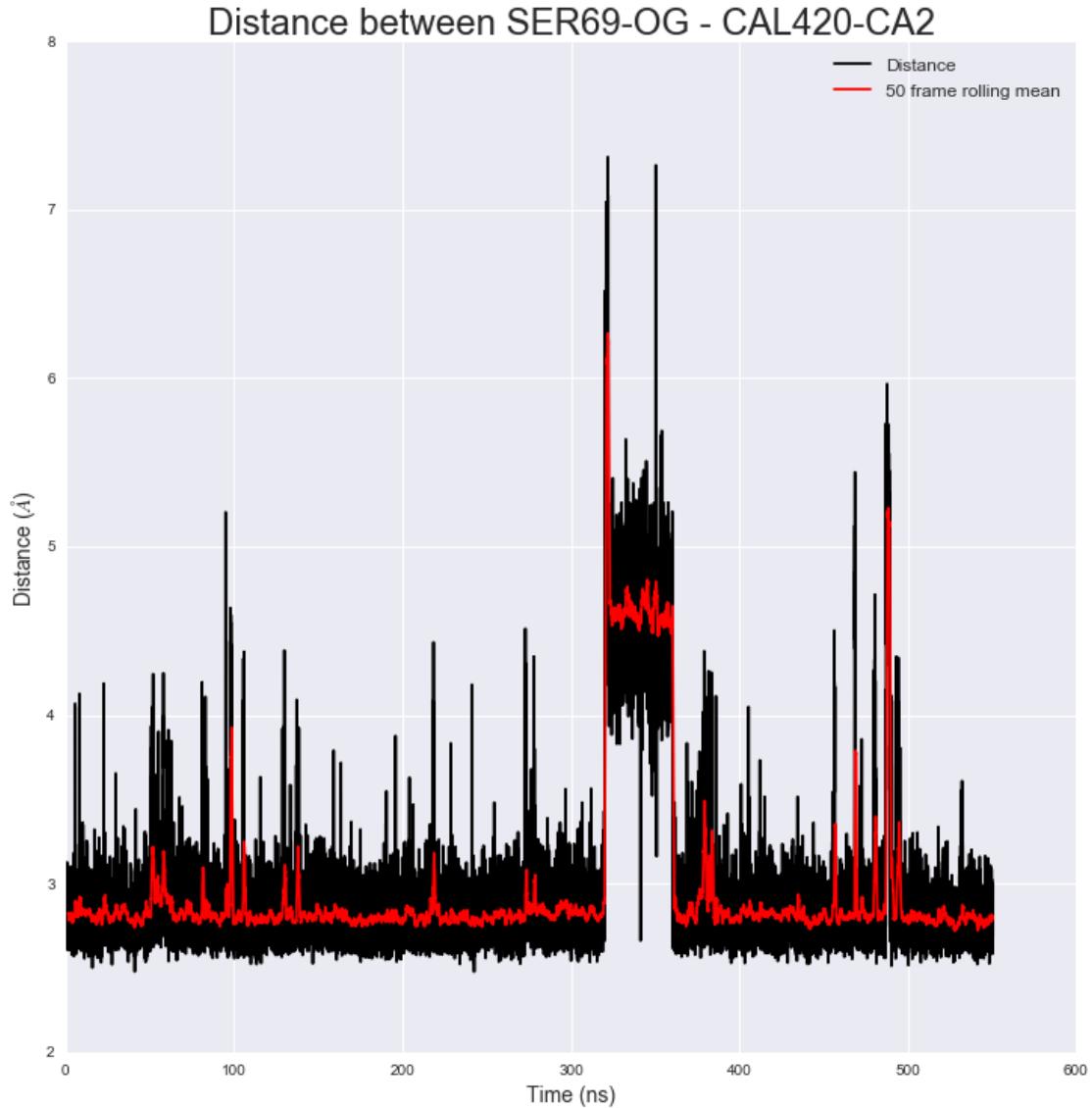
Loading trajectories from the following files:

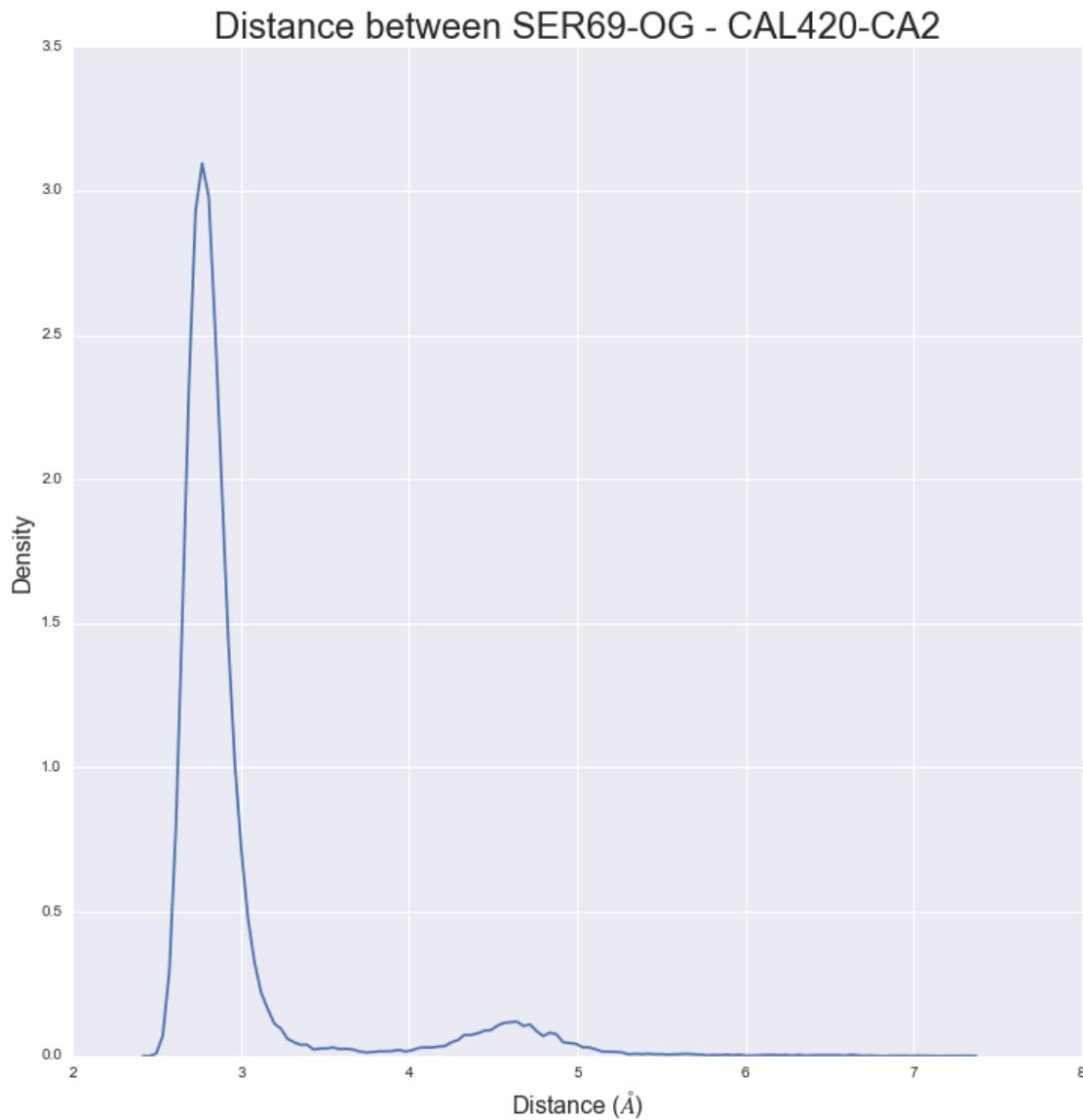
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05\_Prod\_troponin\_egcg\_MD1\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD1\_100-150\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD1\_150-200\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_200-250\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_250-300\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_300-350\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_350-400\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_400-450\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_450-500\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_500-550\_run1\_nowater.nc





Total execution time: 4.28 seconds

Total simulation time of all frames: 549.999980469 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1071

Atom2 number: 6810

Calculating distance between following atoms: THR71-OG1 - CAL420-CA2

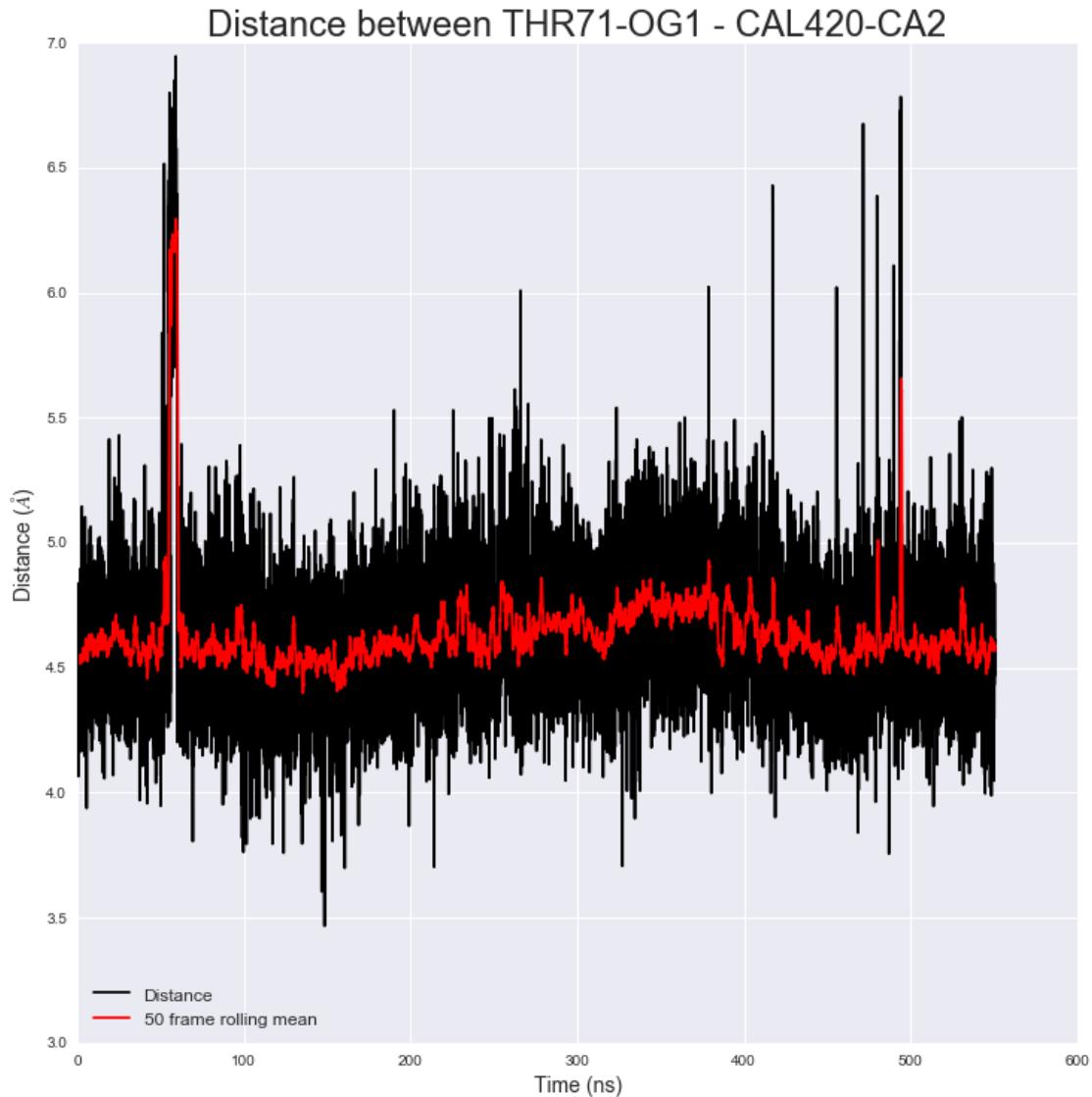
Loading trajectories from the following files:

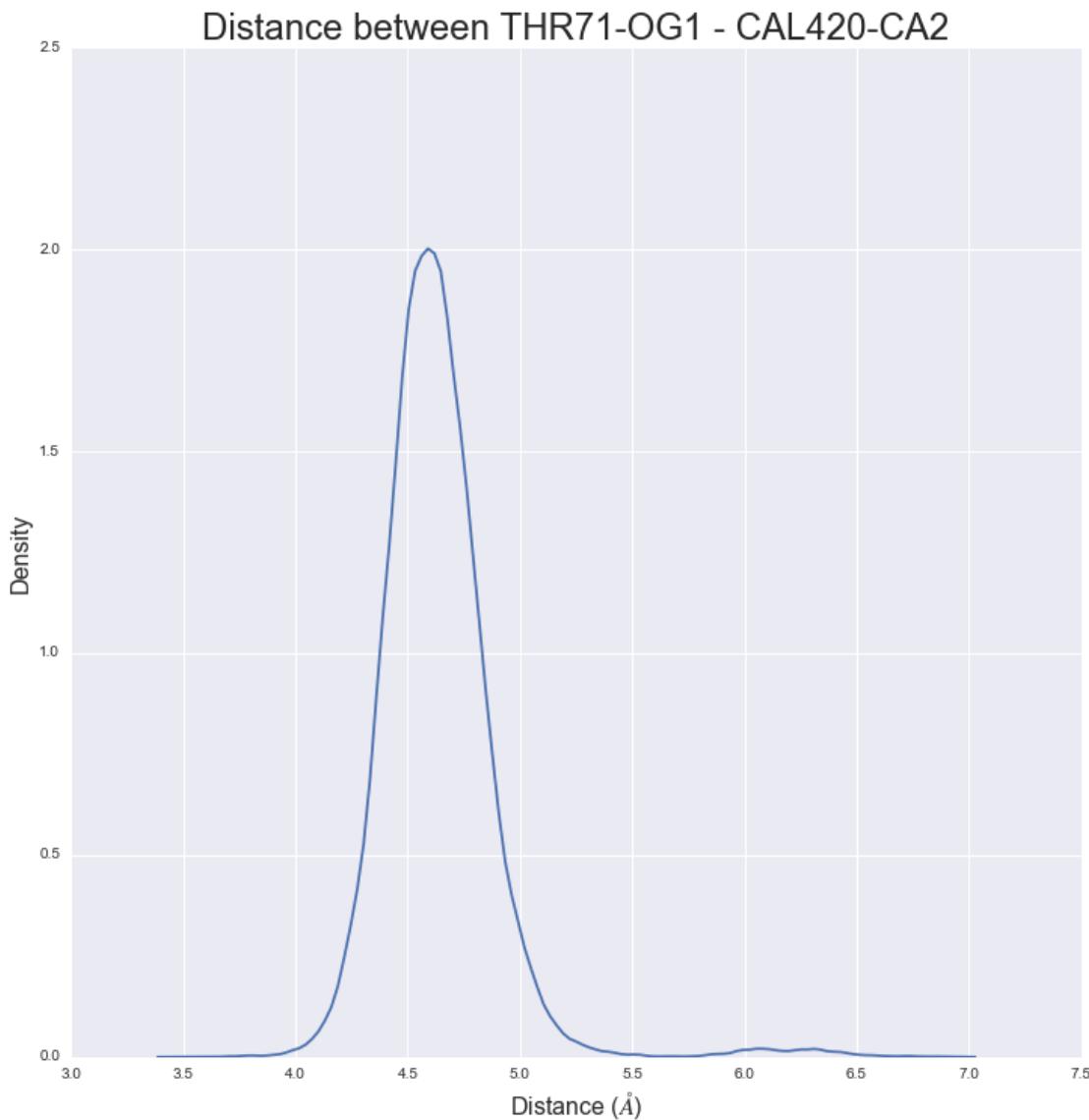
05\_Prod\_troponin\_egcg\_MD1\_000-050\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD1\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD1\_100-150\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD1\_150-200\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_200-250\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_250-300\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_300-350\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_350-400\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_400-450\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_450-500\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_500-550\_run1\_nowater.nc





Total execution time: 4.46 seconds

Total simulation time of all frames: 549.999980469 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1099

Atom2 number: 6810

Calculating distance between following atoms: ASP73-OD1 - CAL420-CA2

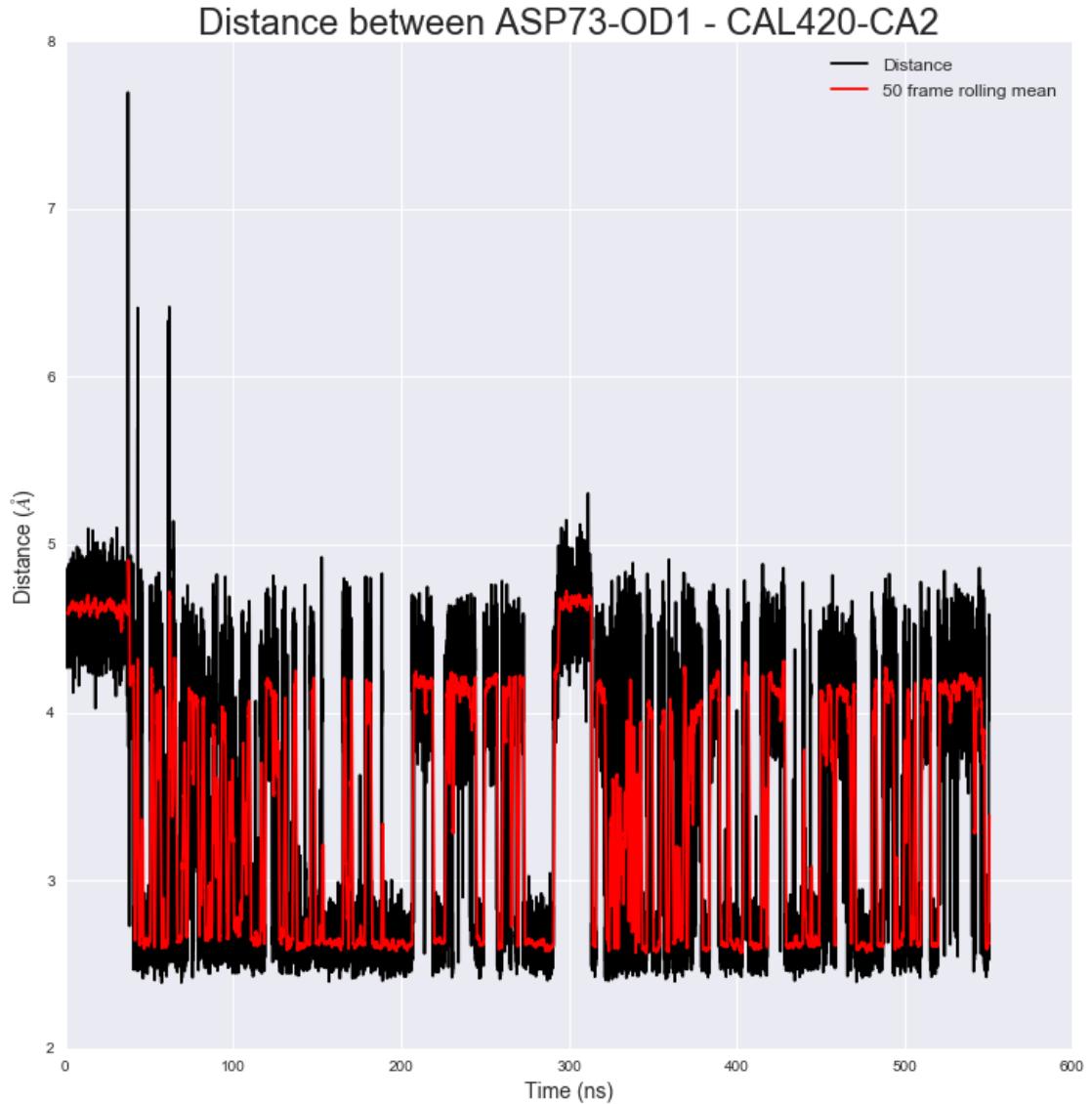
Loading trajectories from the following files:

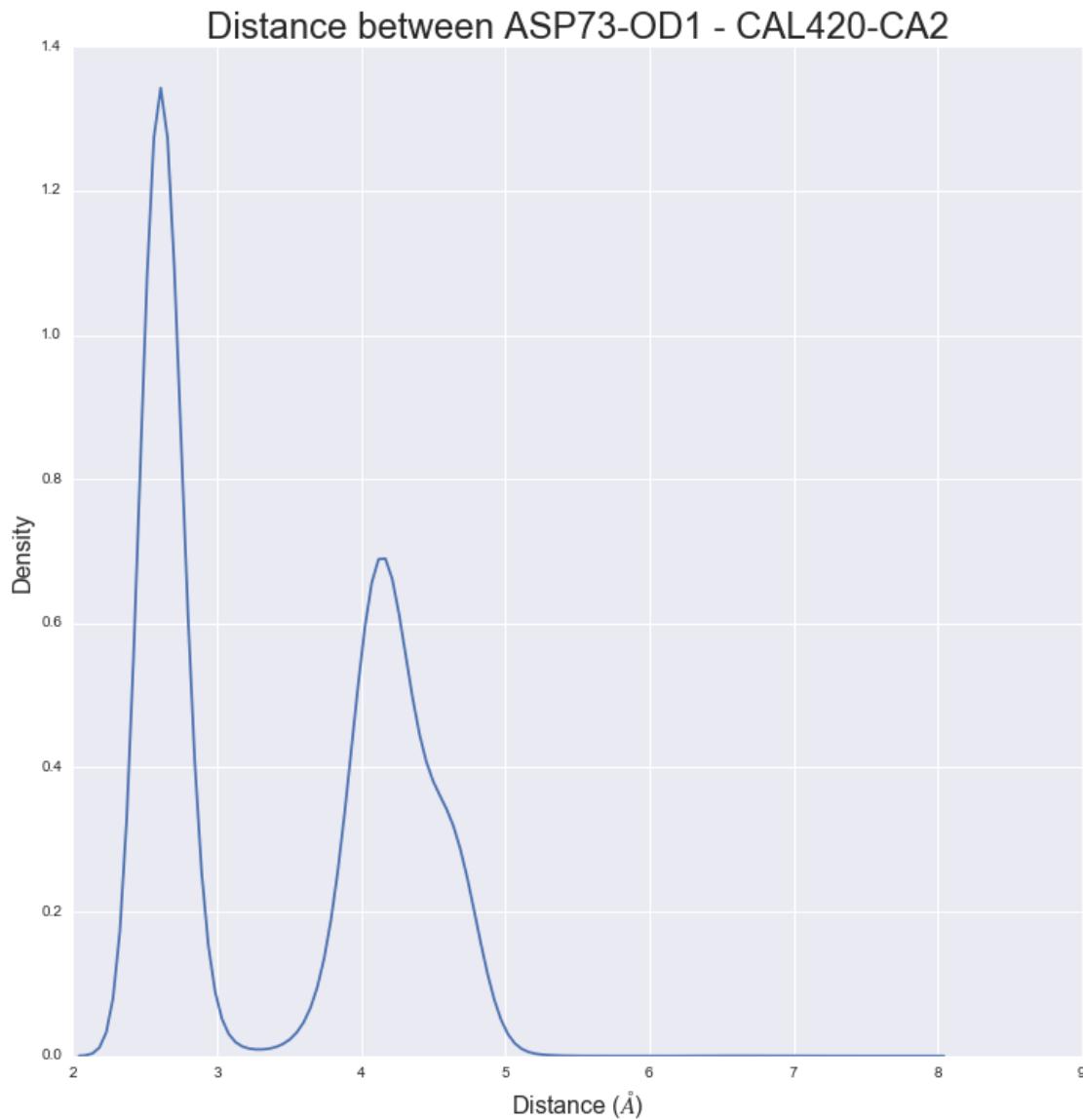
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05\_Prod\_troponin\_egcg\_MD1\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD1\_100-150\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD1\_150-200\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_200-250\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_250-300\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_300-350\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_350-400\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_400-450\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_450-500\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_500-550\_run1\_nowater.nc





Total execution time: 4.43 seconds

Total simulation time of all frames: 549.999980469 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1100

Atom2 number: 6810

Calculating distance between following atoms: ASP73-OD2 - CAL420-CA2

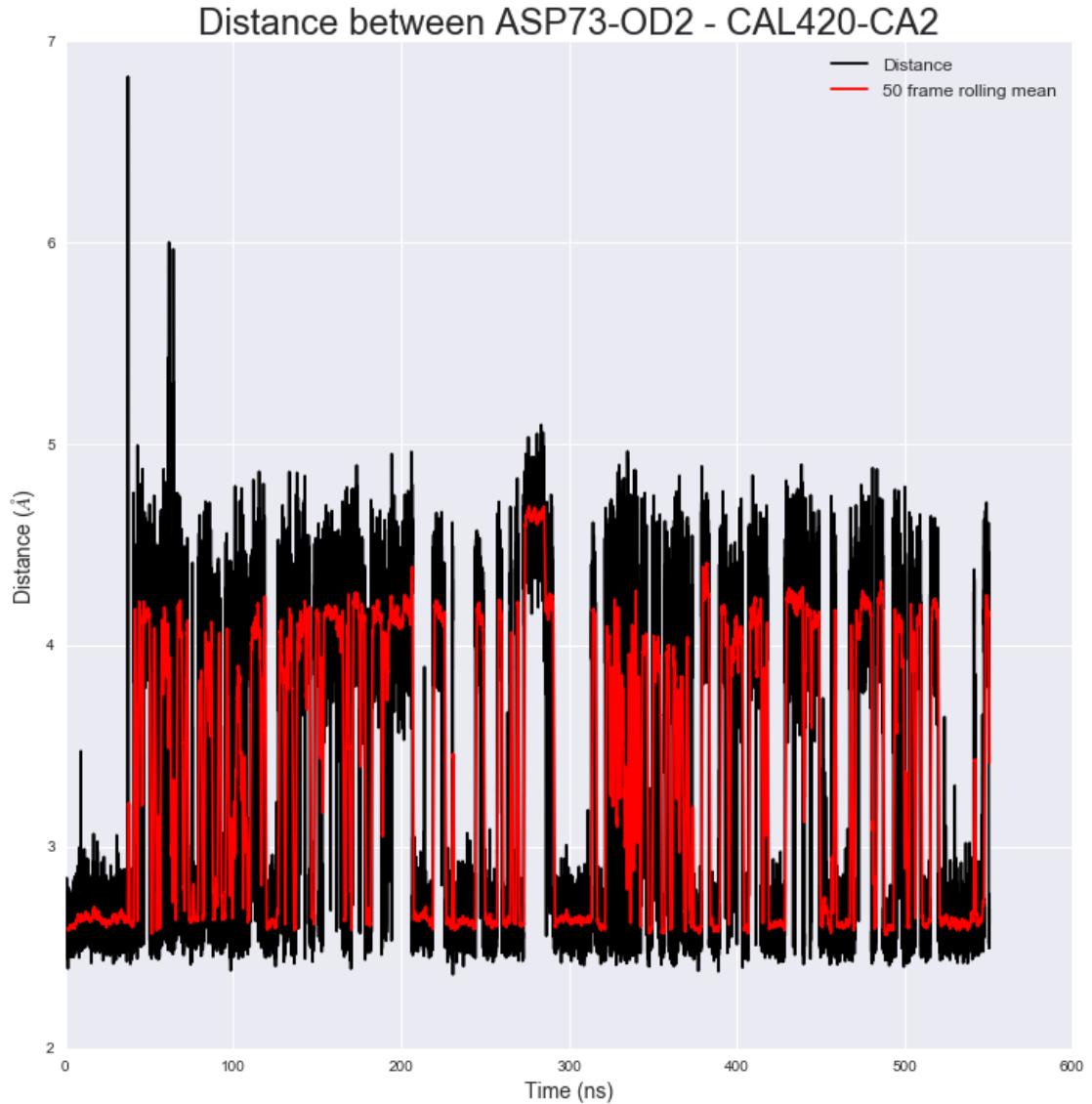
Loading trajectories from the following files:

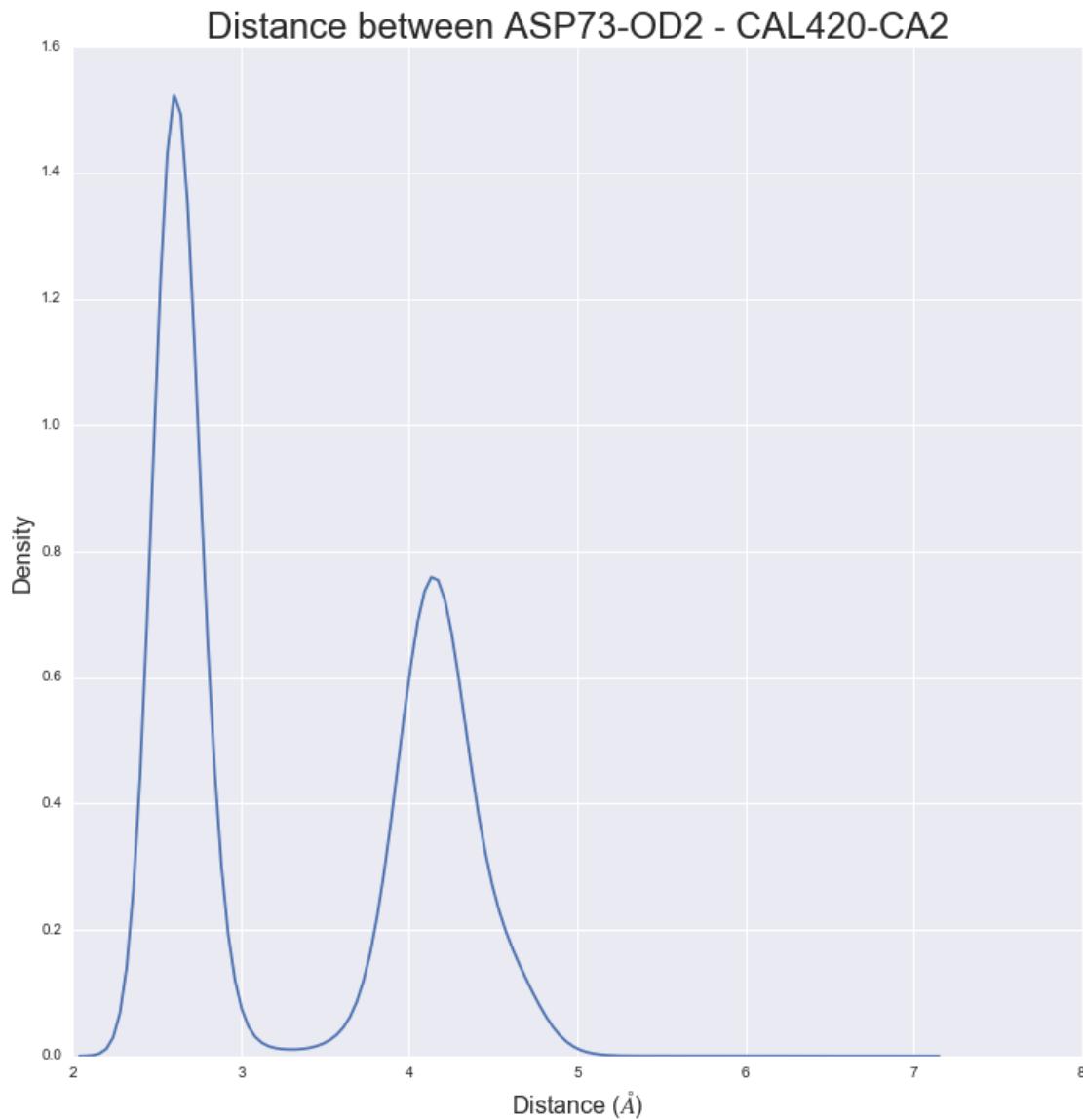
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05\_Prod\_troponin\_egcg\_MD1\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD1\_100-150\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD1\_150-200\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_200-250\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_250-300\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_300-350\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_350-400\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_400-450\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_450-500\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_500-550\_run1\_nowater.nc





Total execution time: 4.25 seconds

Total simulation time of all frames: 549.999980469 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1131

Atom2 number: 6810

Calculating distance between following atoms: ASP75-OD1 - CAL420-CA2

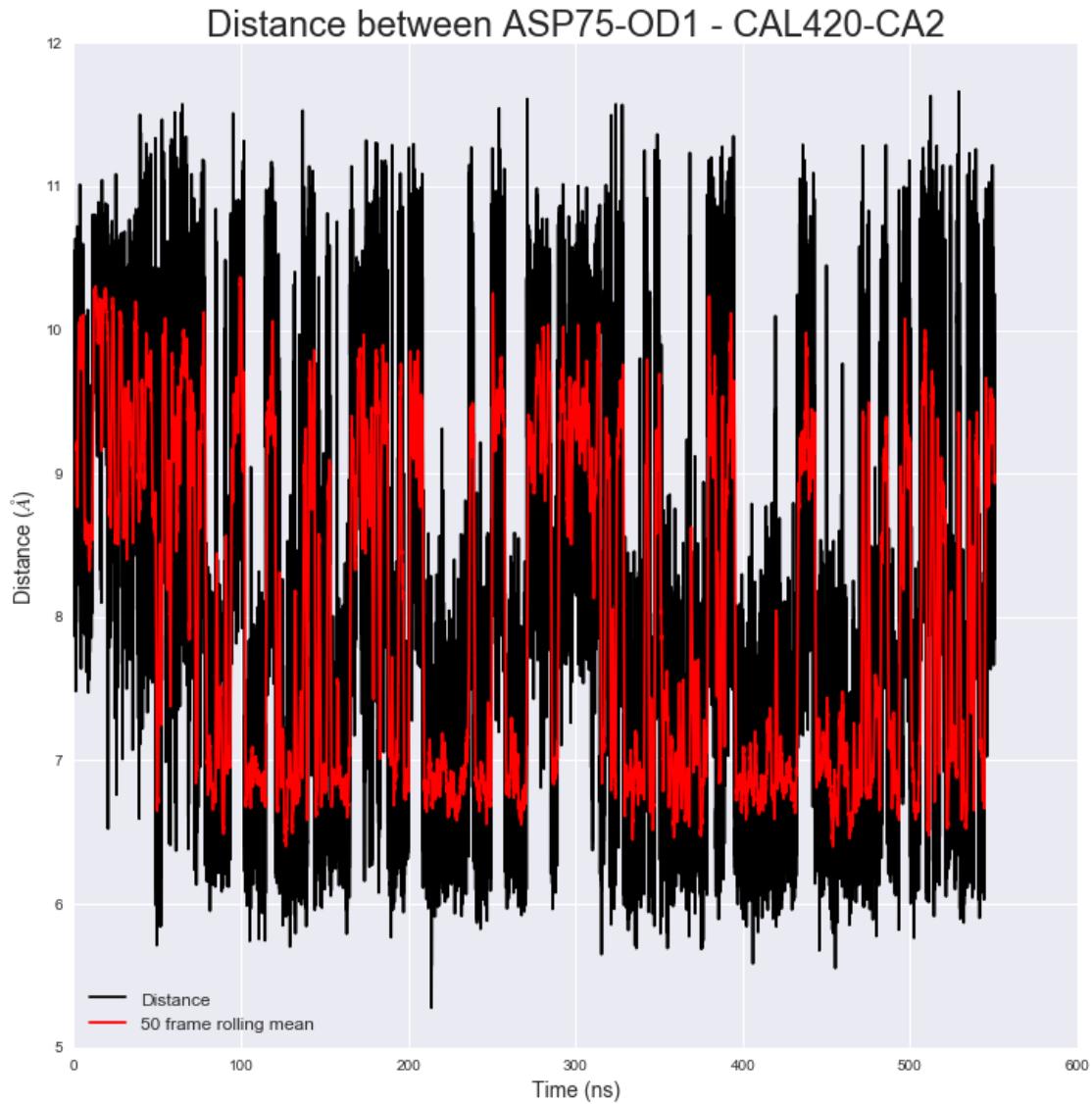
Loading trajectories from the following files:

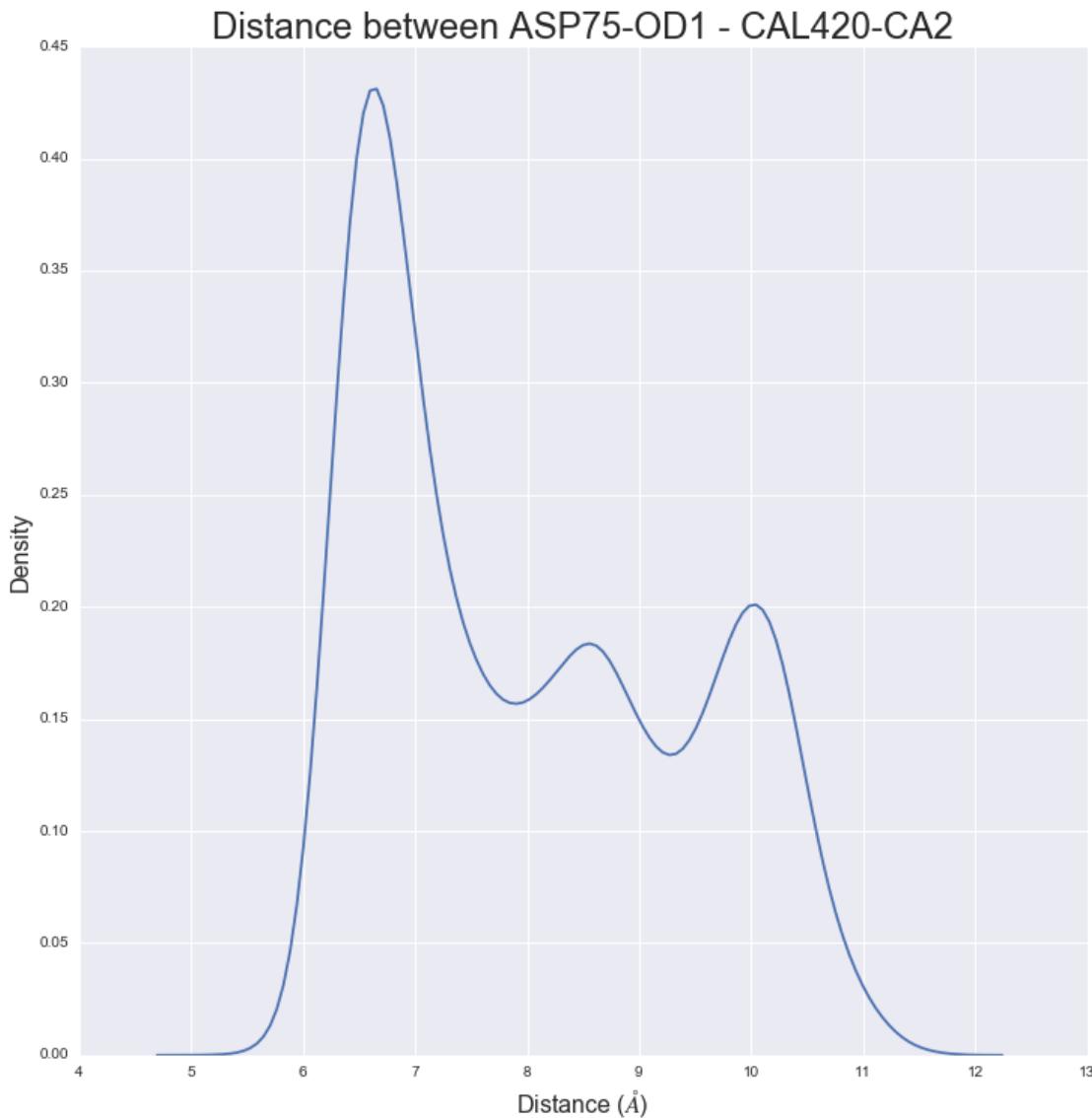
05\_Prod\_troponin\_egcg\_MD1\_000-050\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD1\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD1\_100-150\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD1\_150-200\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_200-250\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_250-300\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_300-350\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_350-400\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_400-450\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_450-500\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_500-550\_run1\_nowater.nc





Total execution time: 4.49 seconds

Total simulation time of all frames: 549.999980469 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1132

Atom2 number: 6810

Calculating distance between following atoms: ASP75-OD2 - CAL420-CA2

Loading trajectories from the following files:

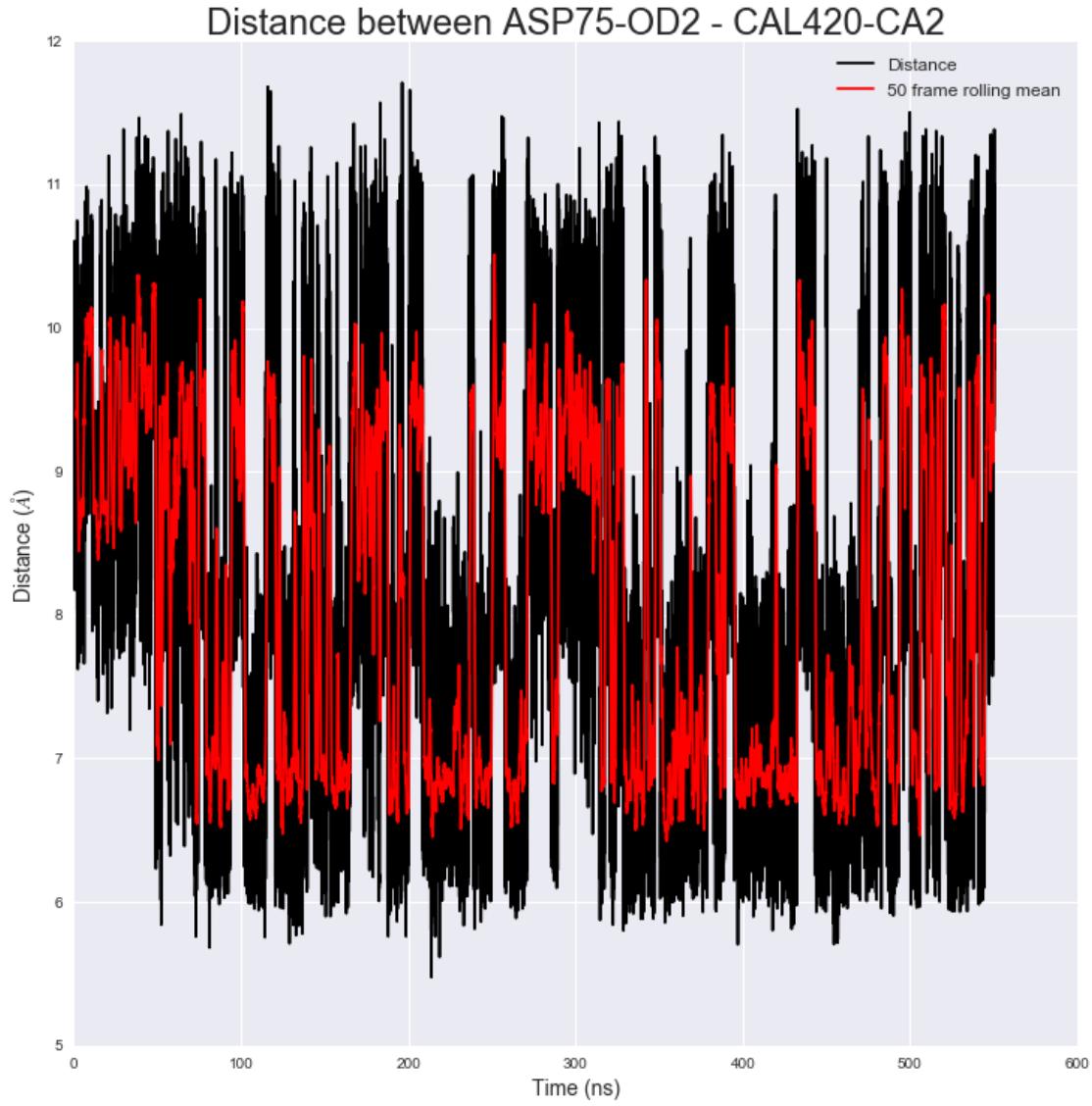
05\_Prod\_troponin\_egcg\_MD1\_000-050\_run1\_nowater.nc

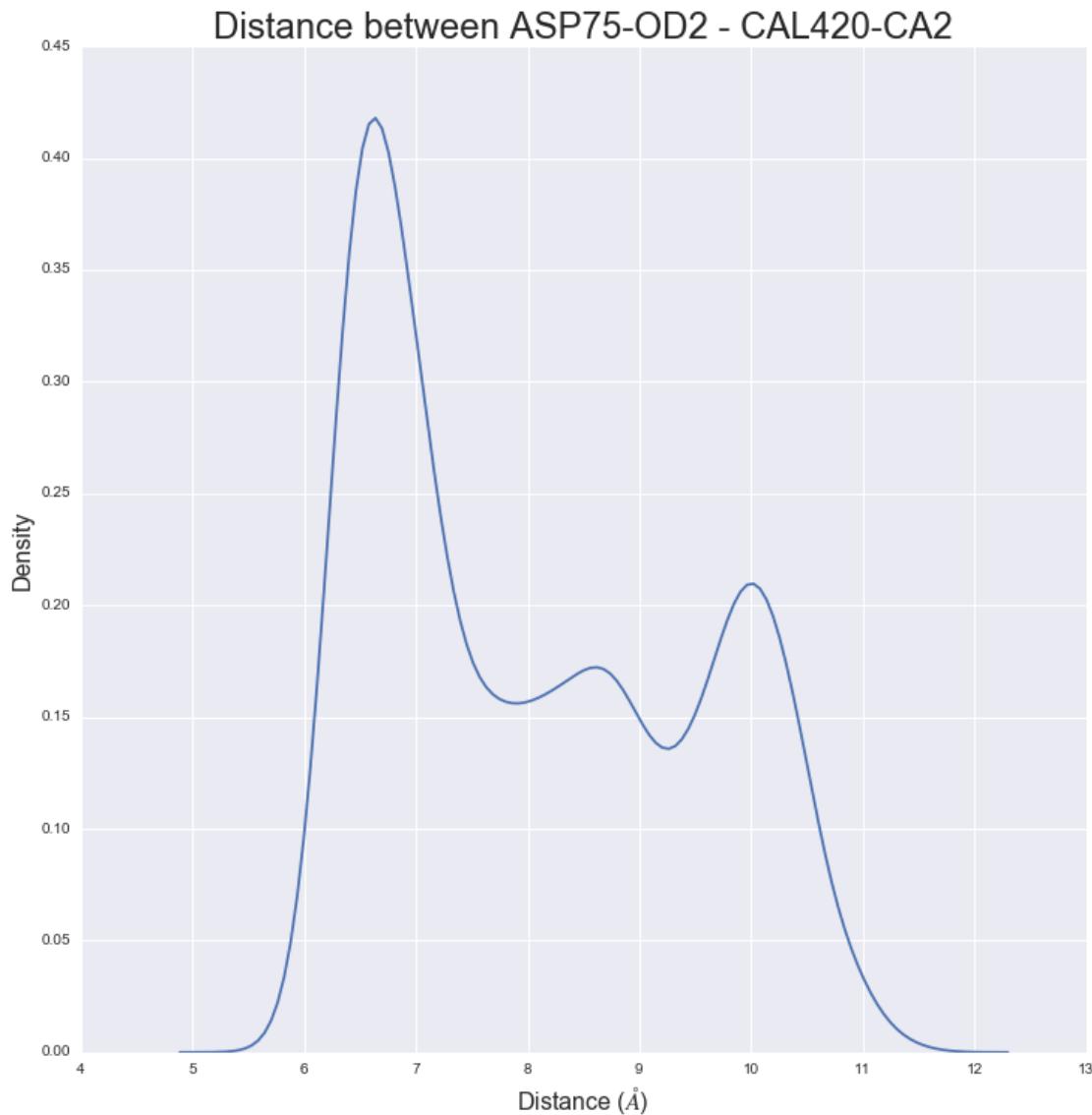
05\_Prod\_troponin\_egcg\_MD1\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD1\_100-150\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD1\_150-200\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD1\_200-250\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_250-300\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_300-350\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_350-400\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_400-450\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_450-500\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_500-550\_run1\_nowater.nc





Total execution time: 4.39 seconds

Total simulation time of all frames: 549.999980469 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1146

Atom2 number: 6810

Calculating distance between following atoms: GLU76-OE1 - CAL420-CA2

Loading trajectories from the following files:

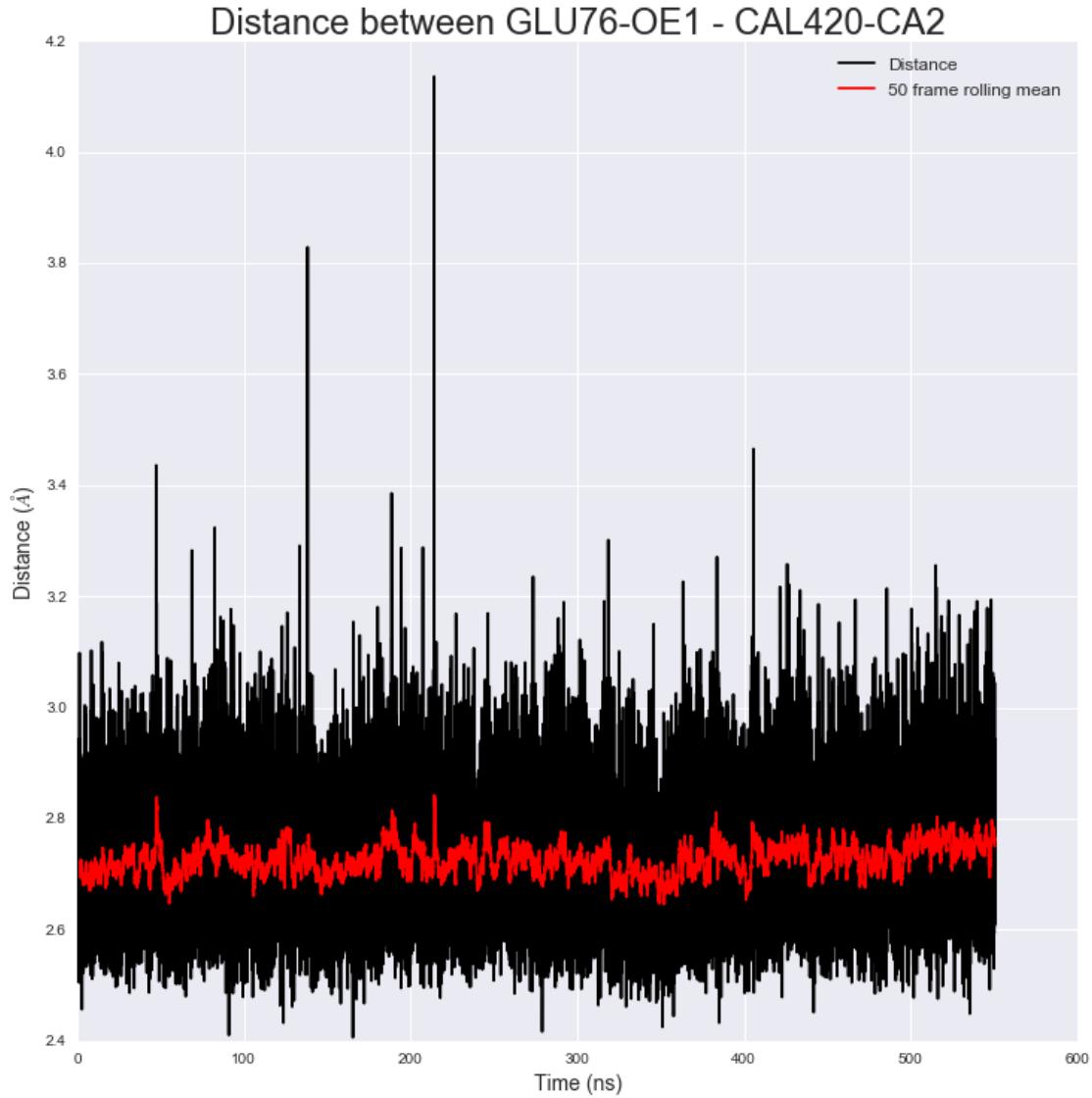
05\_Prod\_troponin\_egcg\_MD1\_000-050\_run1\_nowater.nc

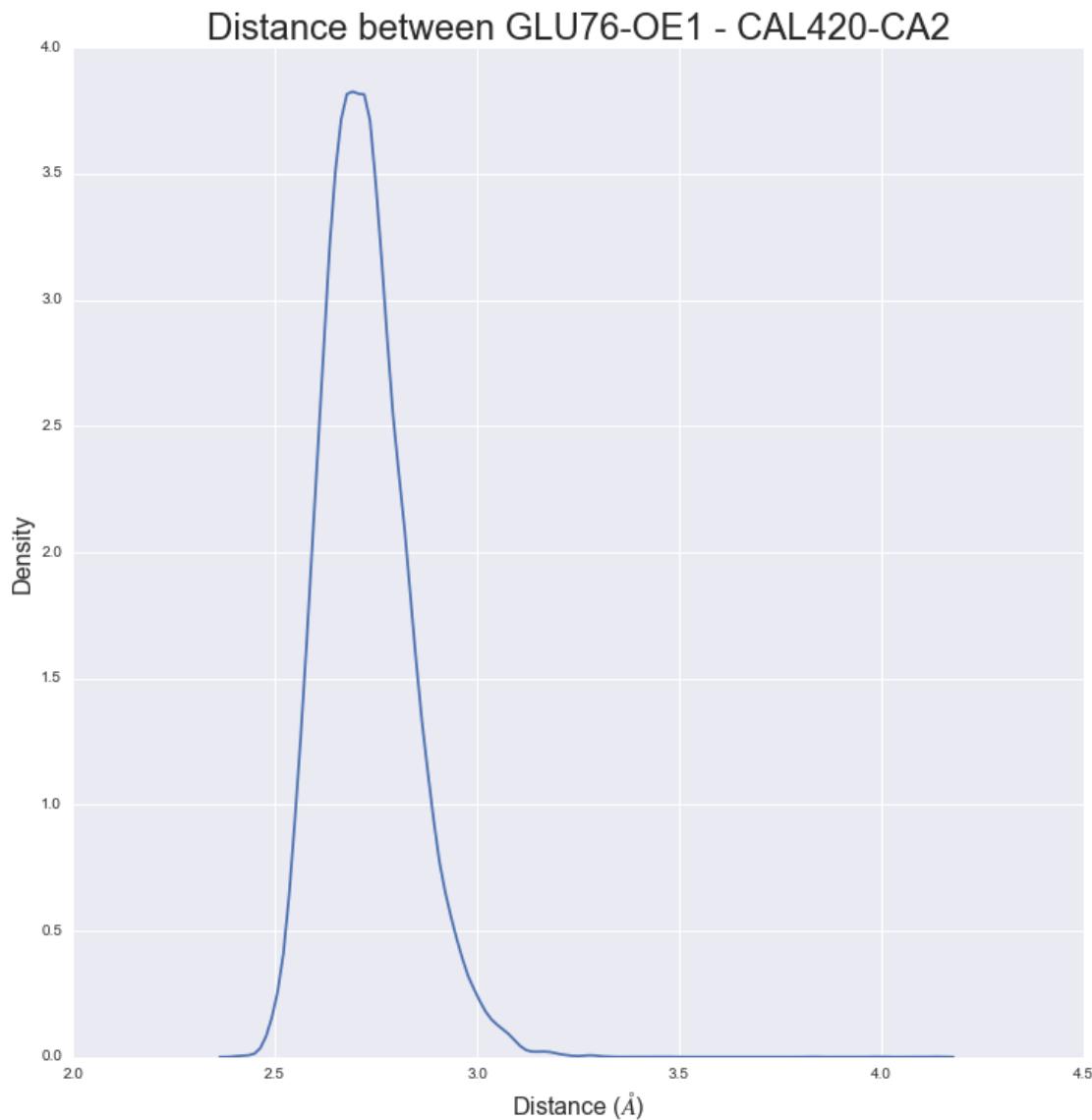
05\_Prod\_troponin\_egcg\_MD1\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD1\_100-150\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD1\_150-200\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD1\_200-250\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_250-300\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_300-350\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_350-400\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_400-450\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_450-500\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_500-550\_run1\_nowater.nc





Total execution time: 4.51 seconds

Total simulation time of all frames: 549.999980469 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1147

Atom2 number: 6810

Calculating distance between following atoms: GLU76-OE2 - CAL420-CA2

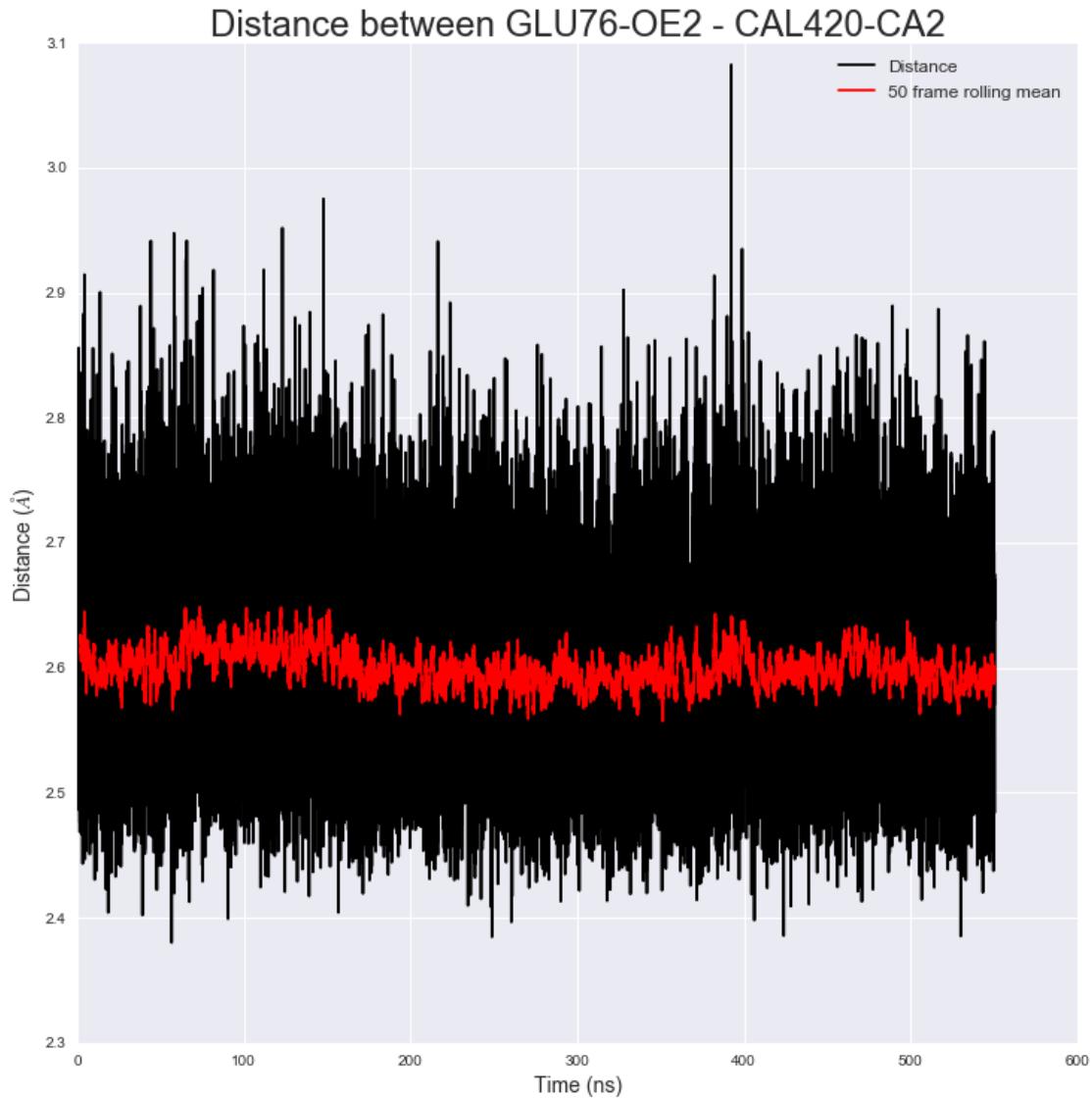
Loading trajectories from the following files:

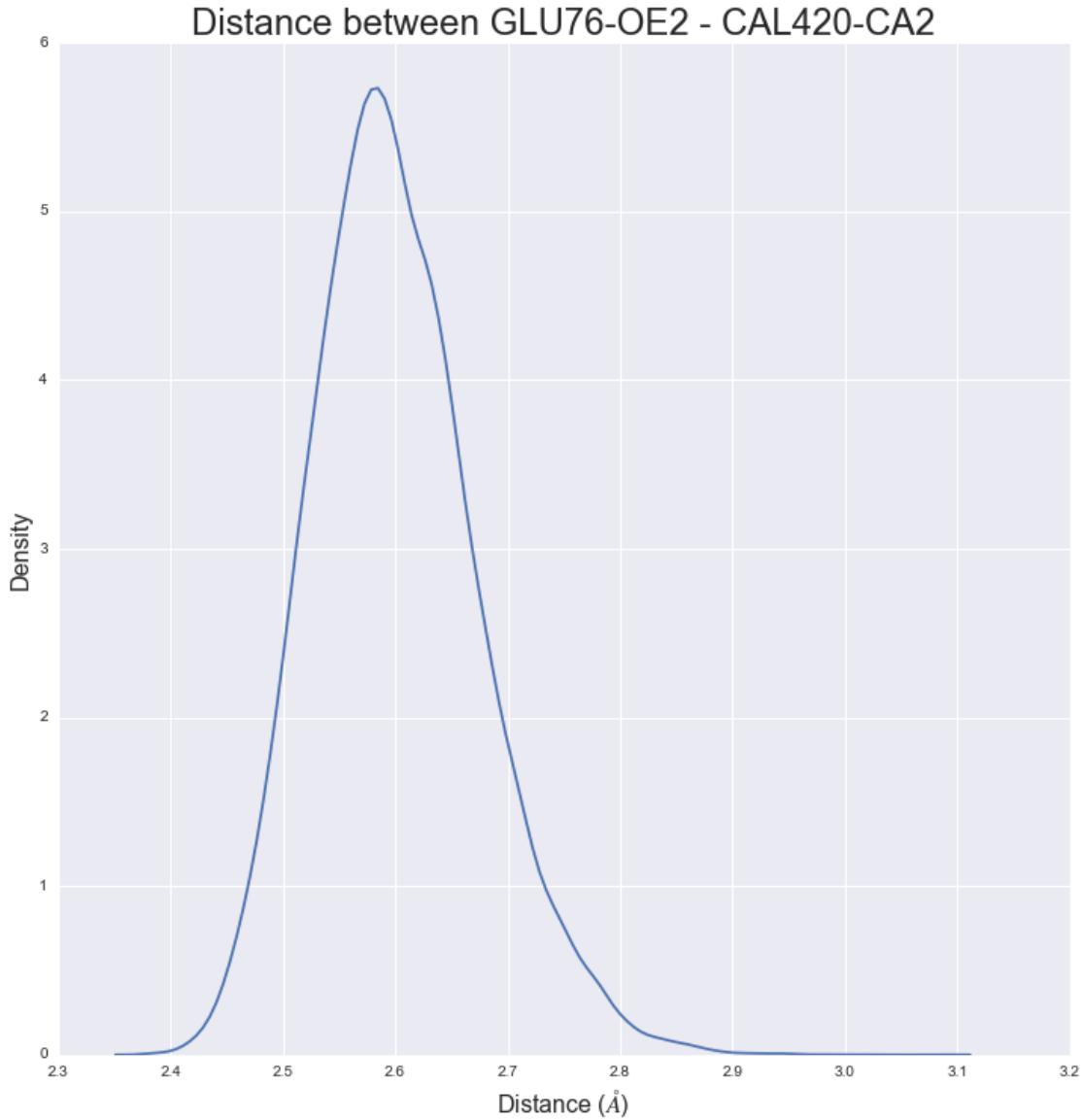
05\_Prod\_troponin\_egcg\_MD1\_000-050\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD1\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD1\_100-150\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD1\_150-200\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_200-250\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_250-300\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_300-350\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_350-400\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_400-450\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_450-500\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD1\_500-550\_run1\_nowater.nc





Total execution time: 4.89 seconds

Total simulation time of all frames: 549.999980469 nanoseconds

## 0.2 MD2

```
In [8]: topology_MD2 = '/Users/gil_f.hoben/Troponin_md_processed/MD2/run1/troponin_egcg_MD2_nowater.prm'
trajectory_MD2 = '/Users/gil_f.hoben/Troponin_md_processed/MD2/run1/Trajectories/'
atom1_list = ['name OD1 and resid 64', 'name OD1 and resid 64', 'name OE1 and resid 65',
              'name OE2 and resid 65', 'name OD1 and resid 66',
              'name OD2 and resid 66', 'name OG and resid 68', 'name OG1 and resid 70',
              'name OD1 and resid 72', 'name OD2 and resid 72', 'name OD1 and resid 74',
              'name OD2 and resid 74', 'name OE1 and resid 75', 'name OE2 and resid 75']
atom2 = 'resid 419'
```

```
In [9]: for atom1 in atom1_list:  
    main(topology_MD2, trajectory_MD2, atom1, atom2, verbose = 1)
```

The following topology file was successfully loaded:  
<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1005

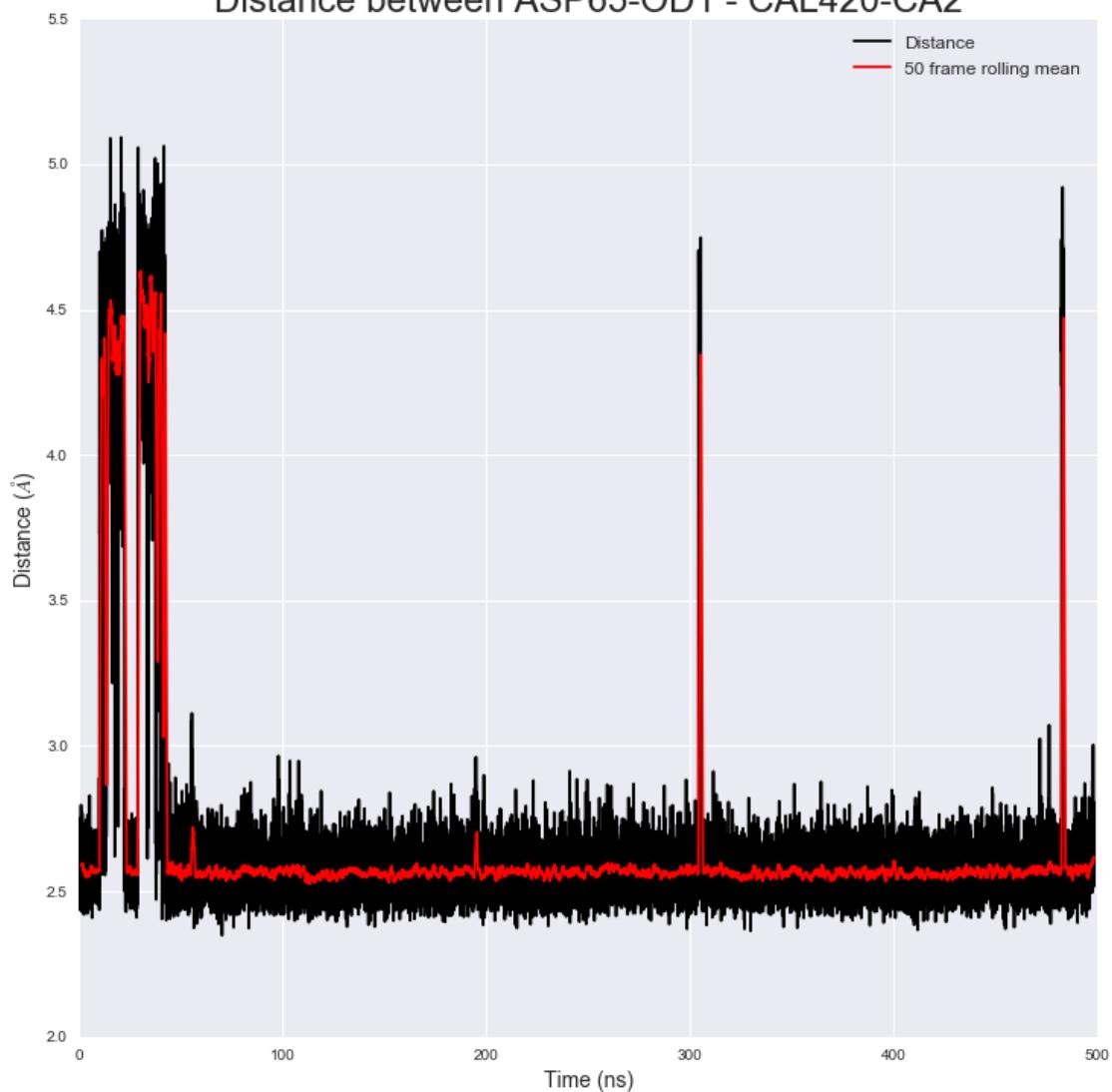
Atom2 number: 6810

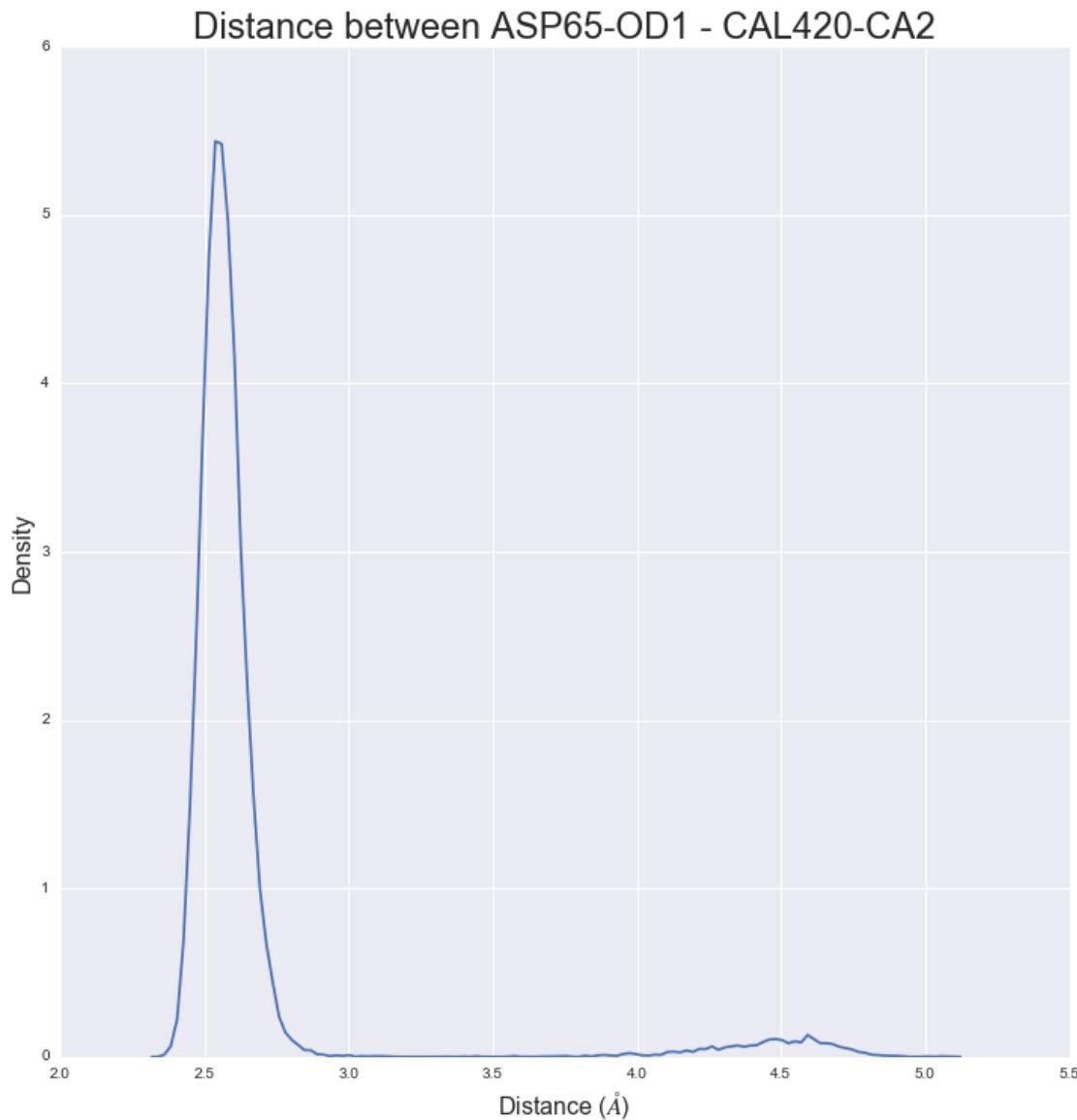
Calculating distance between following atoms: ASP65-OD1 - CAL420-CA2

Loading trajectories from the following files:

05\_Prod\_troponin\_egcg\_MD2\_000-050\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_050-100\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_100-150\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_150-200\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_200-250\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_250-300\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_300-350\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_350-400\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_400-450\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_450-500\_run1\_nowater.nc

### Distance between ASP65-OD1 - CAL420-CA2





Total execution time: 7.60 seconds

Total simulation time of all frames: 498.000010986 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1005

Atom2 number: 6810

Calculating distance between following atoms: ASP65-OD1 - CAL420-CA2

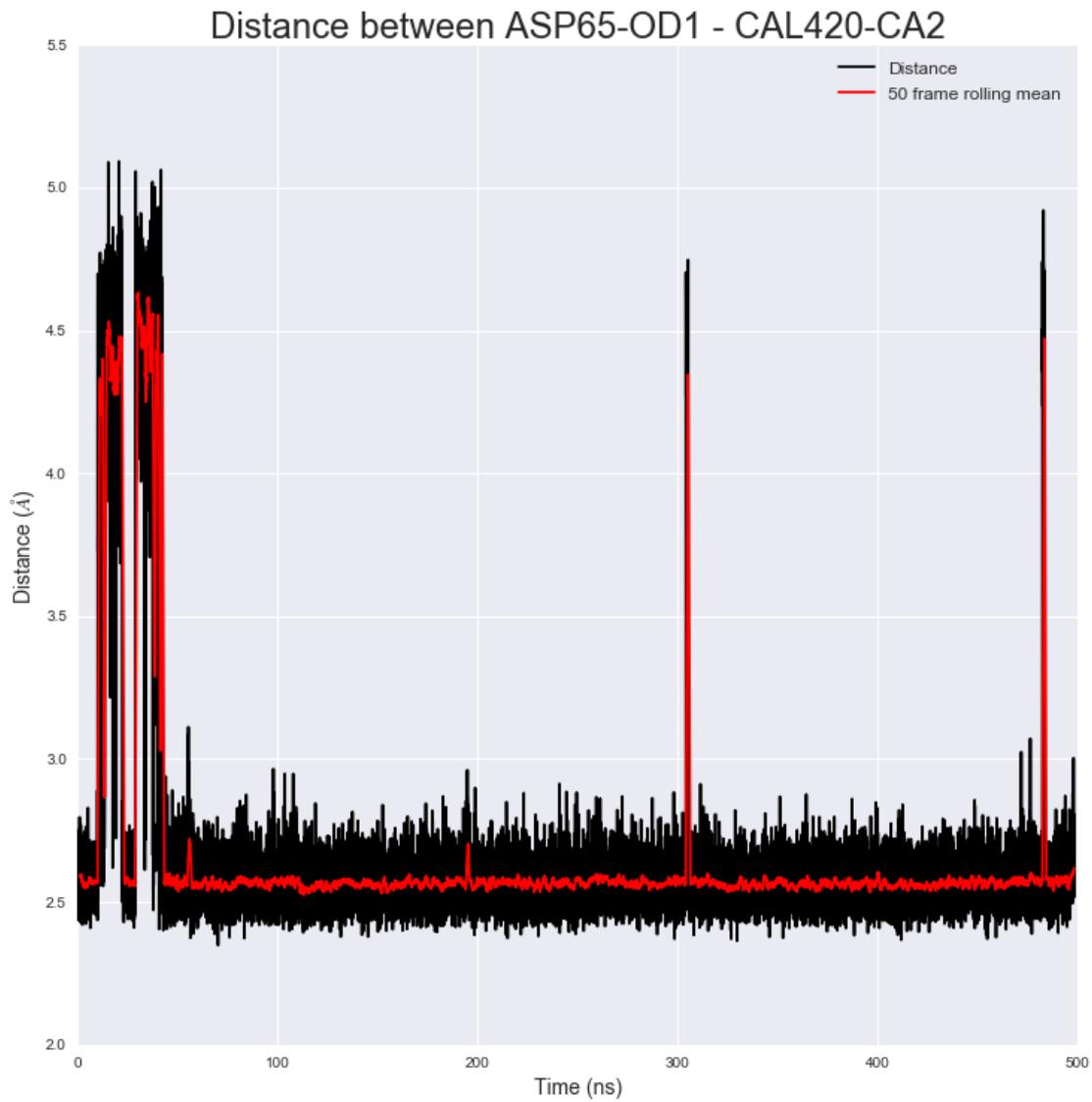
Loading trajectories from the following files:

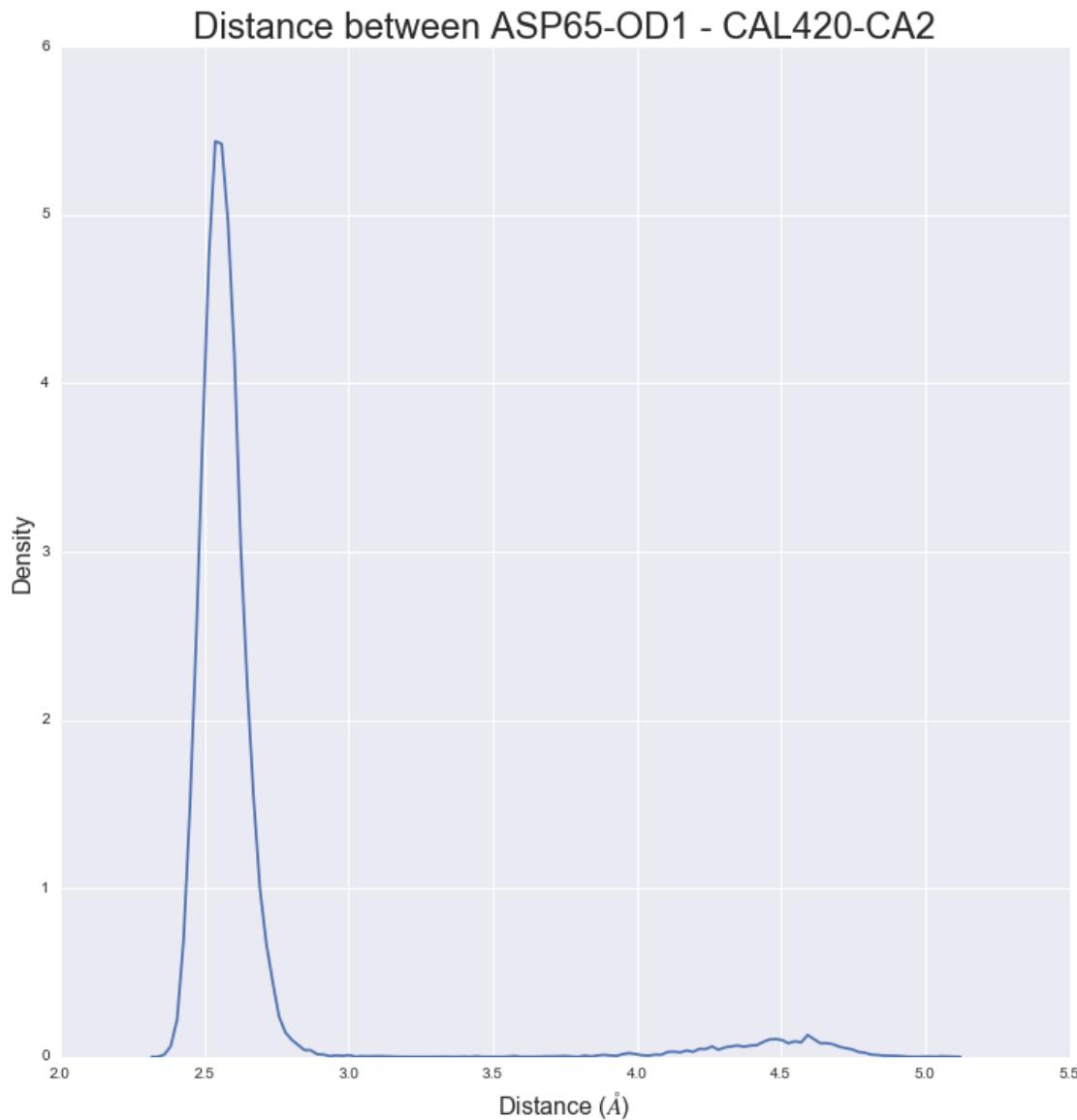
05\_Prod\_troponin\_egcg\_MD2\_000-050\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD2\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD2\_100-150\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD2\_150-200\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_200-250\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_250-300\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_300-350\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_350-400\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_400-450\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_450-500\_run1\_nowater.nc





Total execution time: 4.27 seconds

Total simulation time of all frames: 498.000010986 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1020

Atom2 number: 6810

Calculating distance between following atoms: GLU66-OE1 - CAL420-CA2

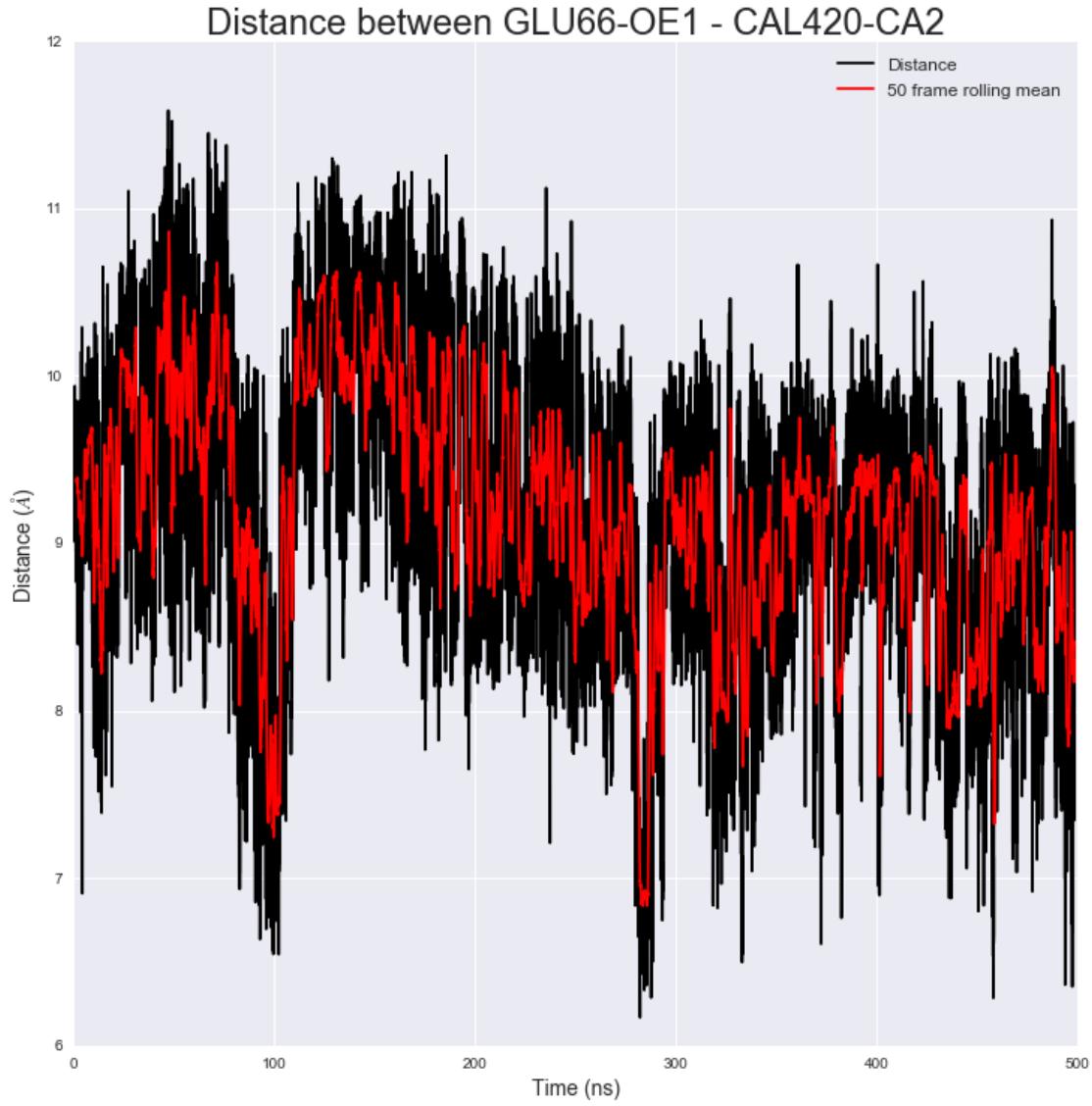
Loading trajectories from the following files:

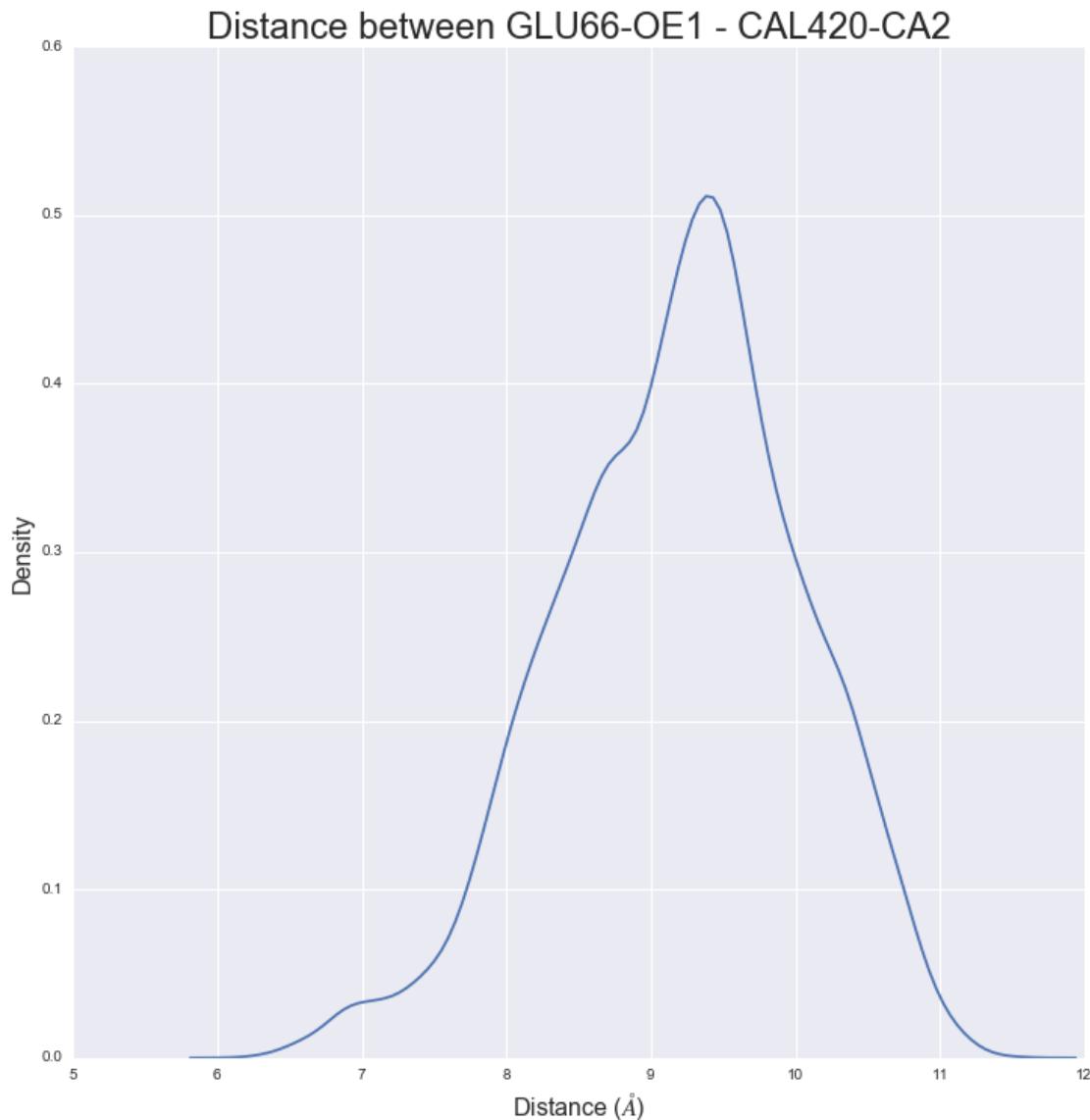
05\_Prod\_troponin\_egcg\_MD2\_000-050\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD2\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD2\_100-150\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD2\_150-200\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_200-250\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_250-300\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_300-350\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_350-400\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_400-450\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_450-500\_run1\_nowater.nc





Total execution time: 4.27 seconds

Total simulation time of all frames: 498.000010986 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1021

Atom2 number: 6810

Calculating distance between following atoms: GLU66-OE2 - CAL420-CA2

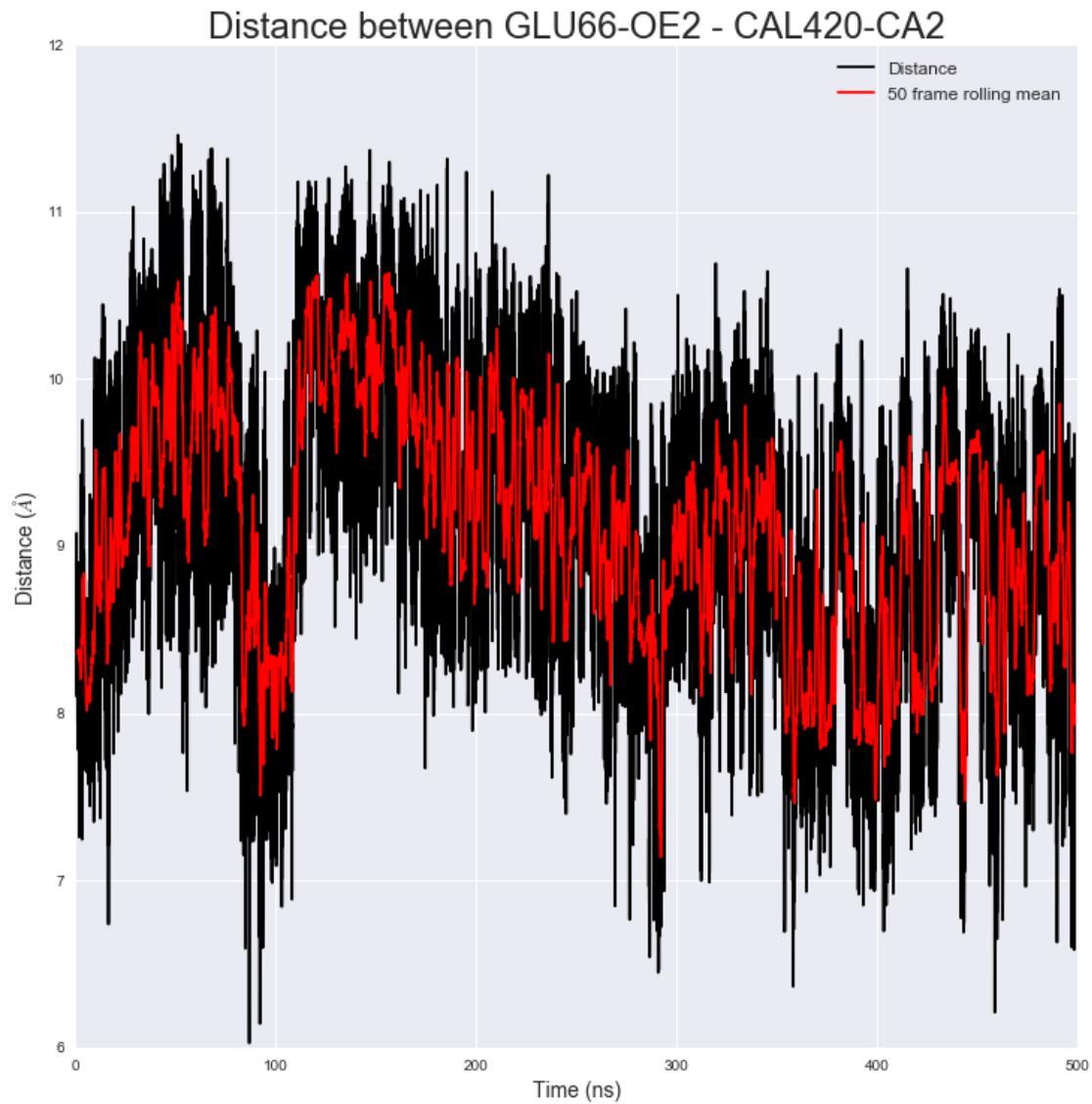
Loading trajectories from the following files:

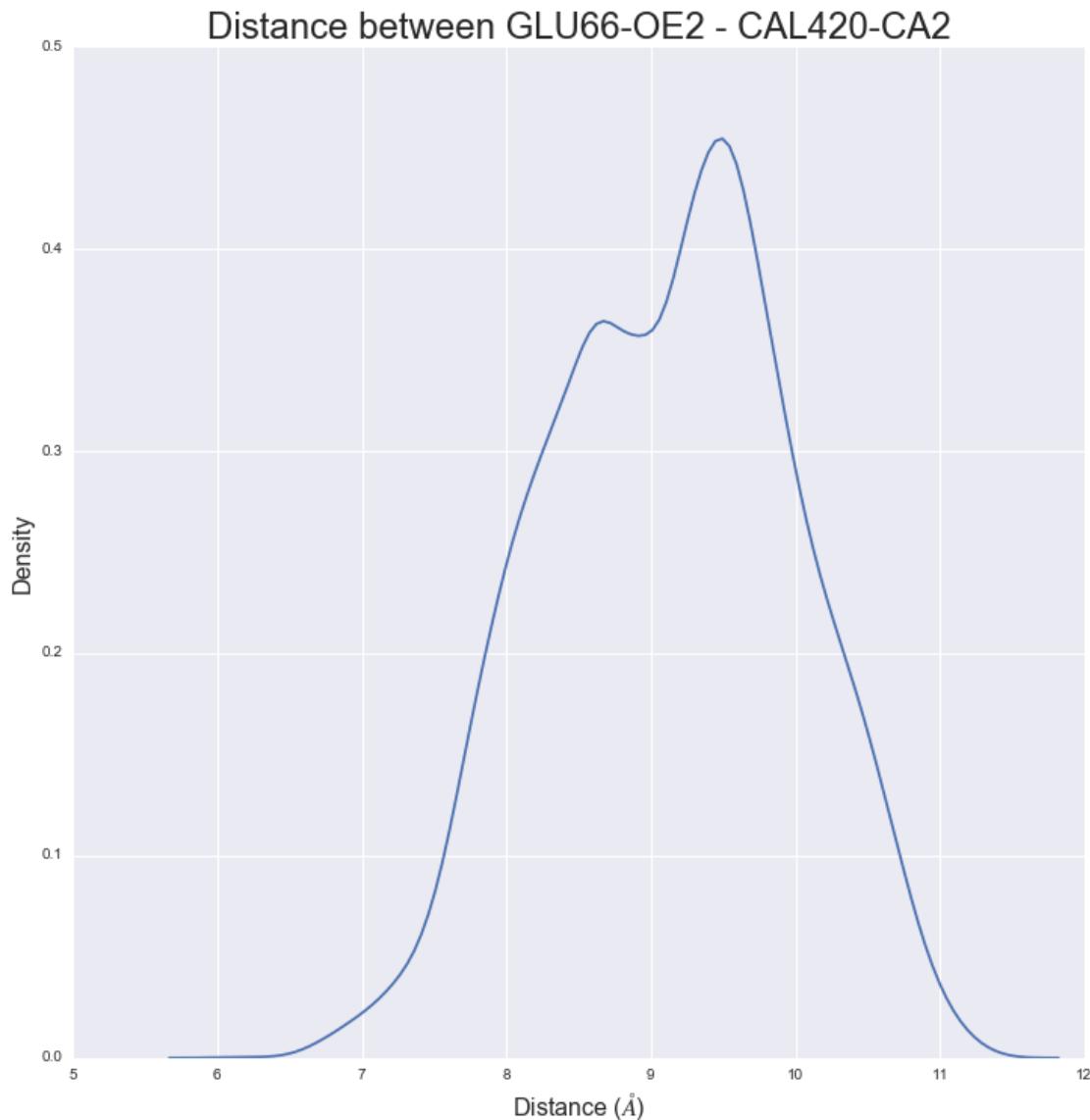
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05\_Prod\_troponin\_egcg\_MD2\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD2\_100-150\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD2\_150-200\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_200-250\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_250-300\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_300-350\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_350-400\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_400-450\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_450-500\_run1\_nowater.nc





Total execution time: 4.27 seconds

Total simulation time of all frames: 498.000010986 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1032

Atom2 number: 6810

Calculating distance between following atoms: ASP67-OD1 - CAL420-CA2

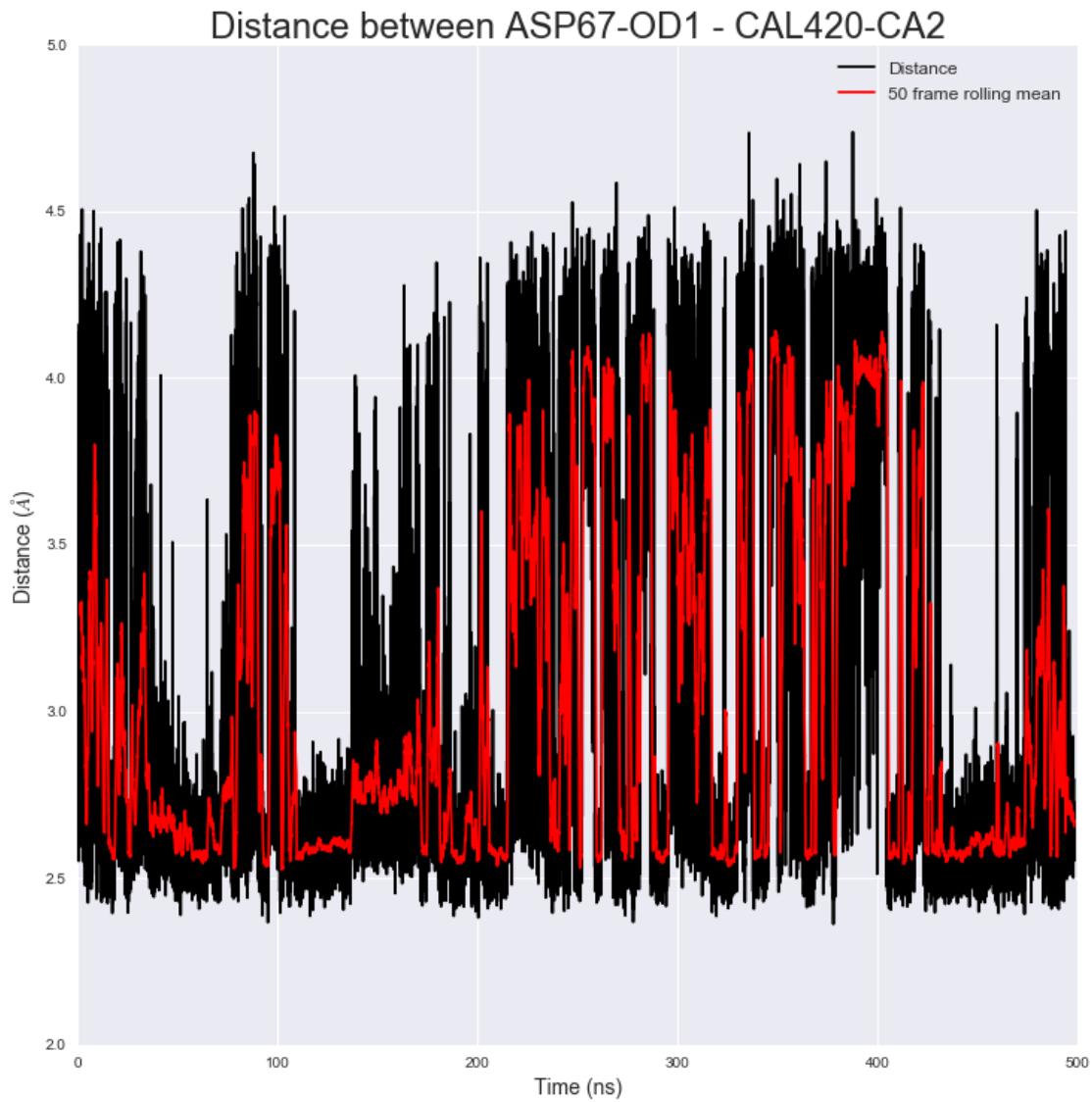
Loading trajectories from the following files:

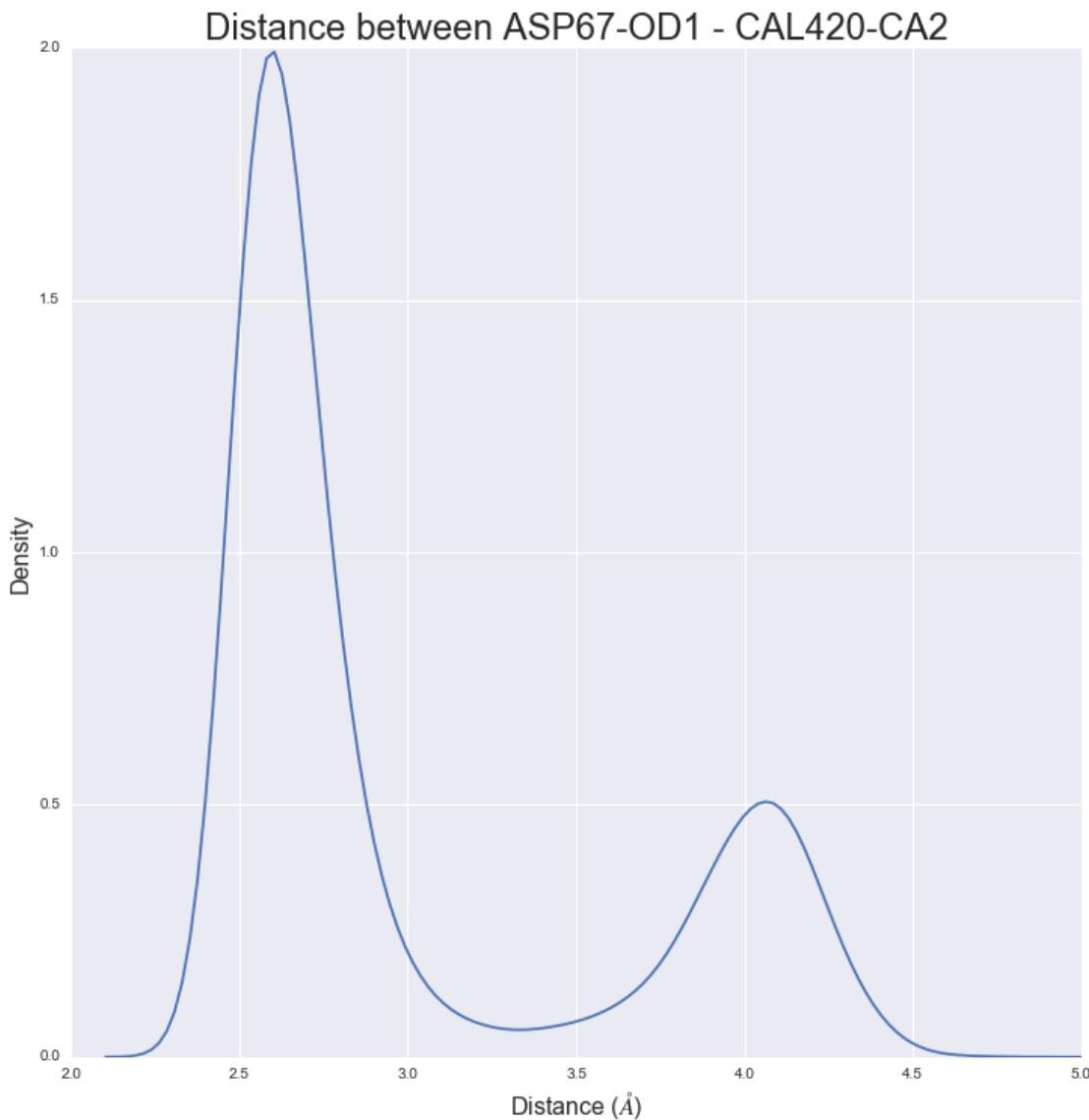
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05\_Prod\_troponin\_egcg\_MD2\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD2\_100-150\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD2\_150-200\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_200-250\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_250-300\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_300-350\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_350-400\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_400-450\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_450-500\_run1\_nowater.nc





Total execution time: 4.45 seconds

Total simulation time of all frames: 498.000010986 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1033

Atom2 number: 6810

Calculating distance between following atoms: ASP67-OD2 - CAL420-CA2

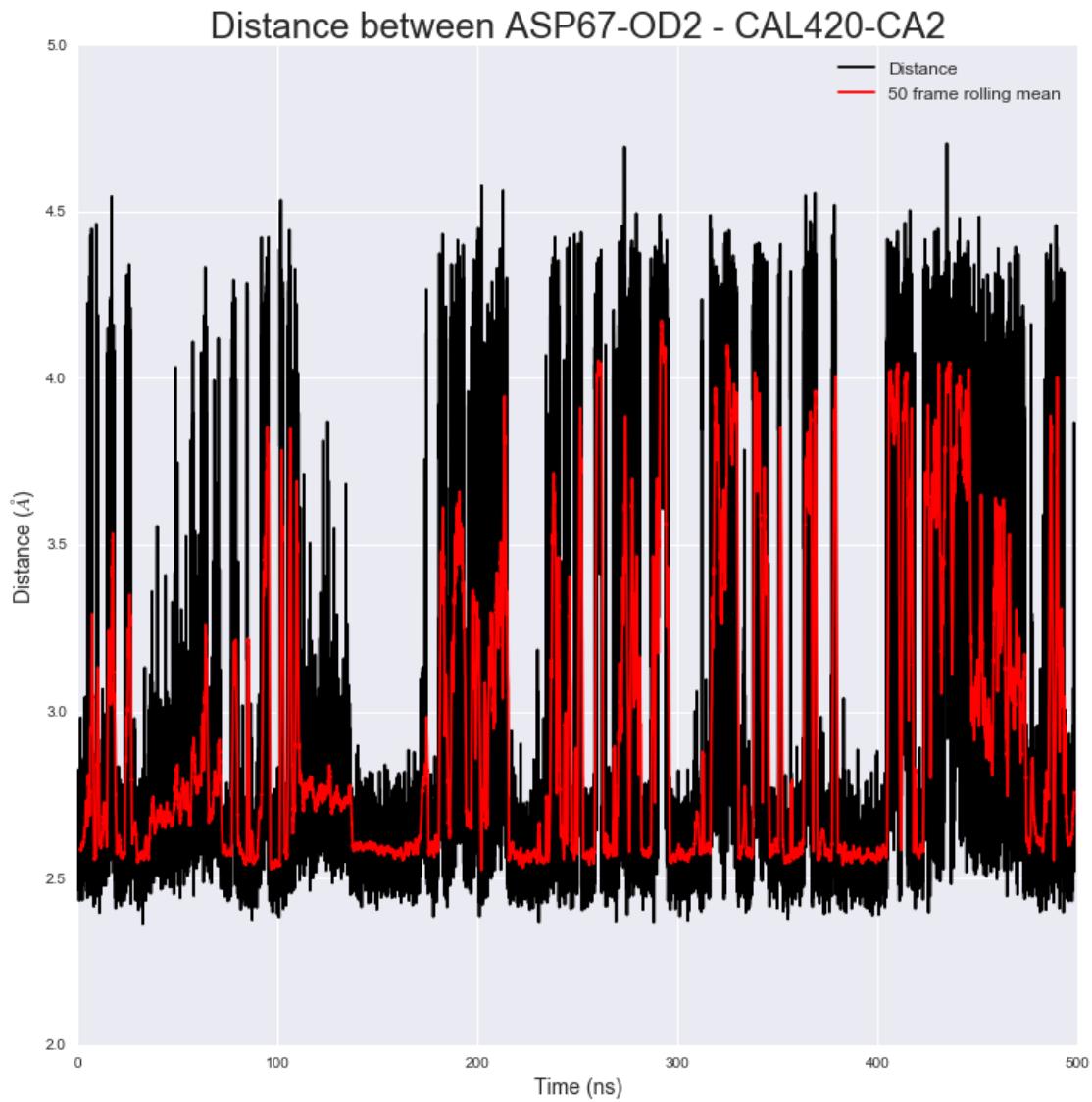
Loading trajectories from the following files:

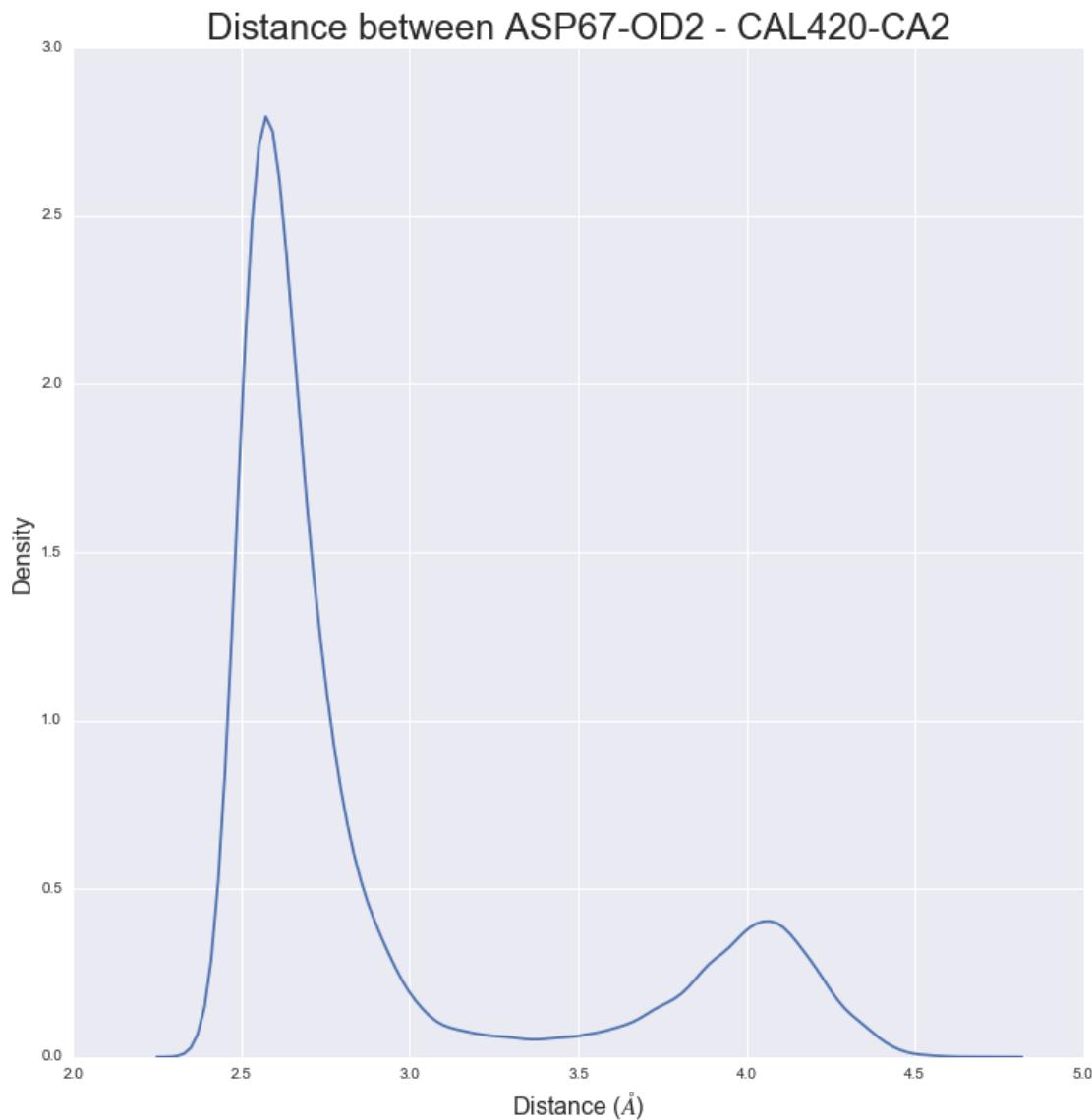
05\_Prod\_troponin\_egcg\_MD2\_000-050\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD2\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD2\_100-150\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD2\_150-200\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_200-250\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_250-300\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_300-350\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_350-400\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_400-450\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_450-500\_run1\_nowater.nc





Total execution time: 4.53 seconds

Total simulation time of all frames: 498.000010986 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1050

Atom2 number: 6810

Calculating distance between following atoms: SER69-OG - CAL420-CA2

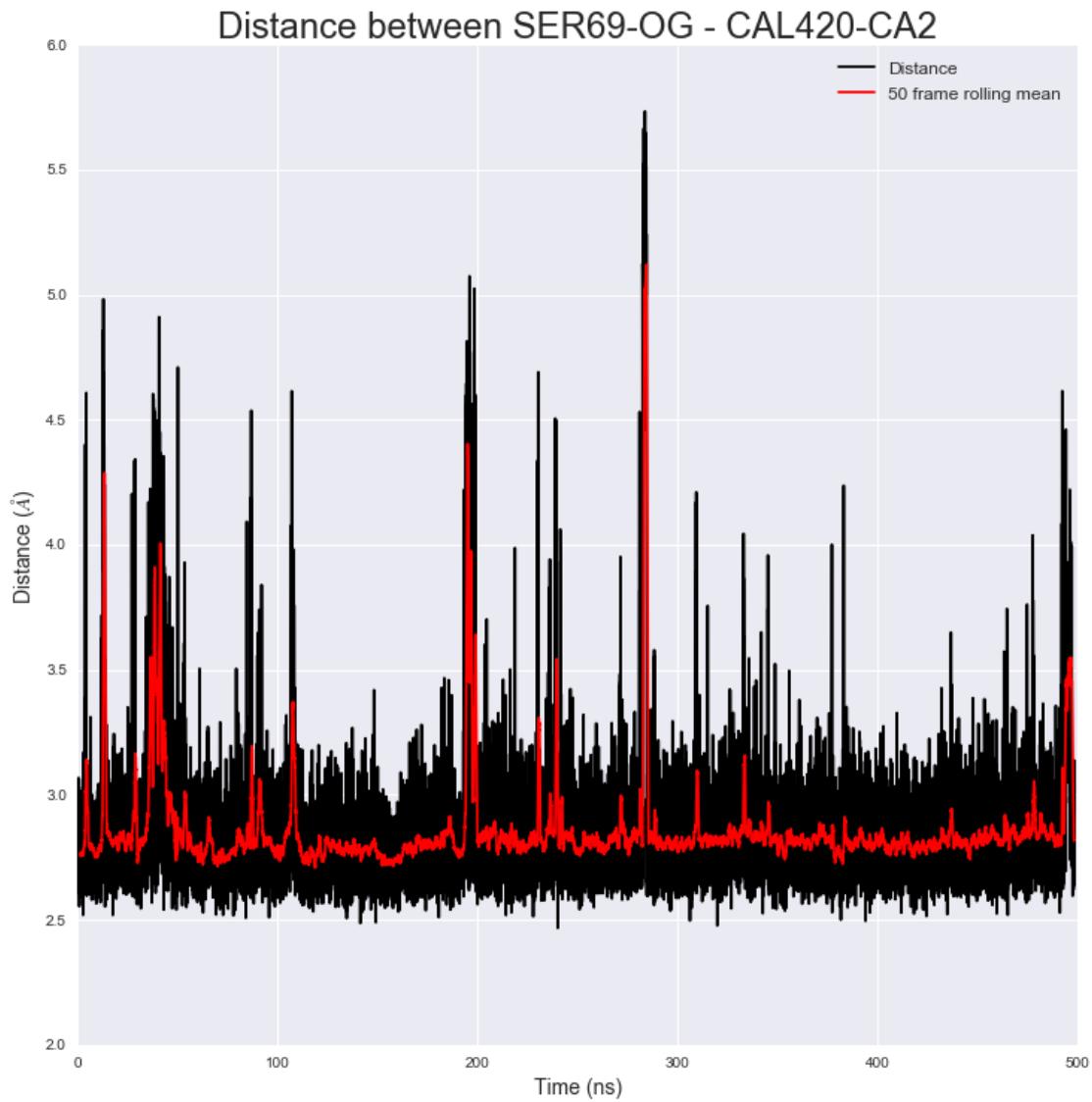
Loading trajectories from the following files:

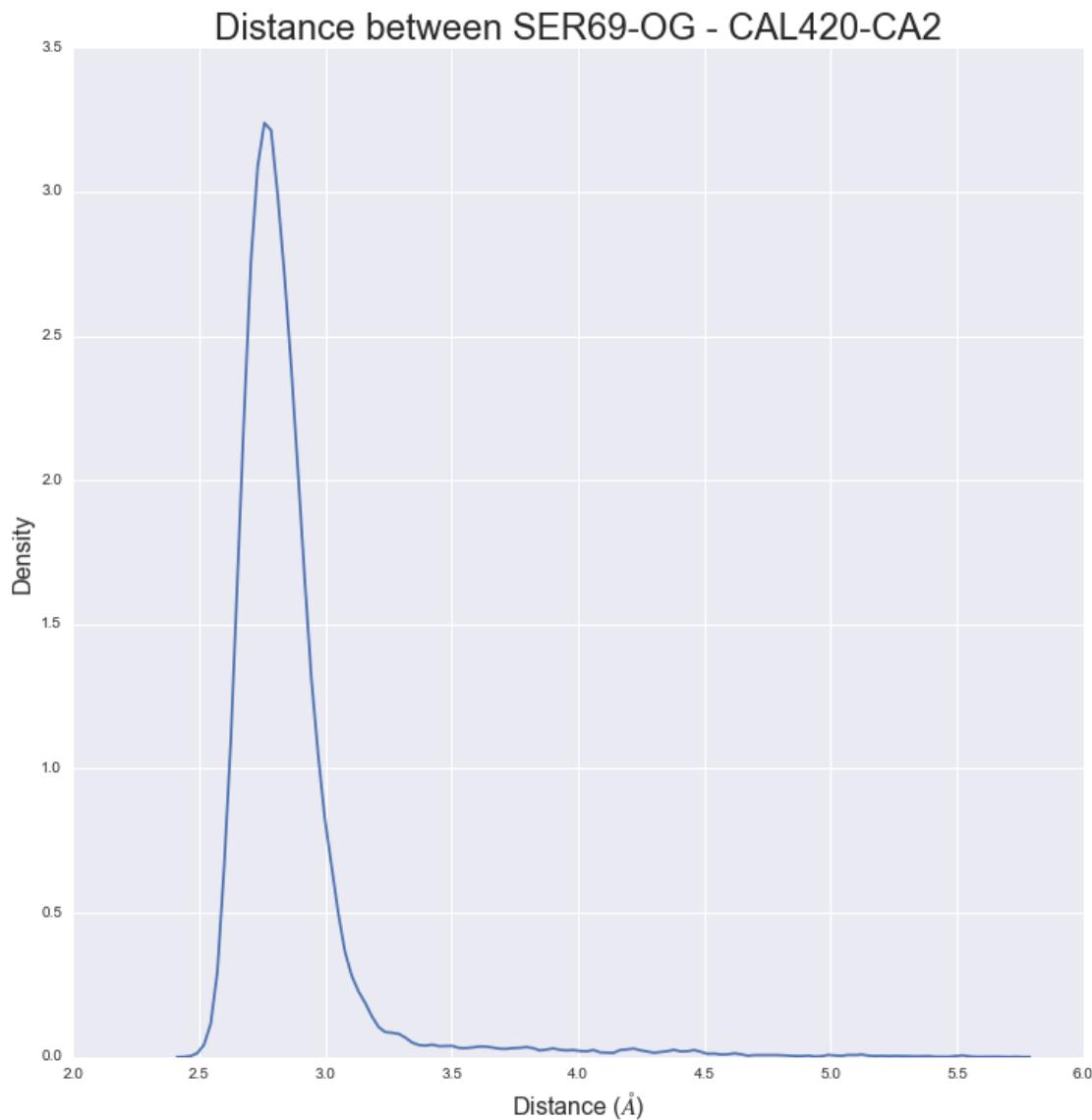
05\_Prod\_troponin\_egcg\_MD2\_000-050\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD2\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD2\_100-150\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD2\_150-200\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_200-250\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_250-300\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_300-350\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_350-400\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_400-450\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_450-500\_run1\_nowater.nc





Total execution time: 4.28 seconds

Total simulation time of all frames: 498.000010986 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1071

Atom2 number: 6810

Calculating distance between following atoms: THR71-OG1 - CAL420-CA2

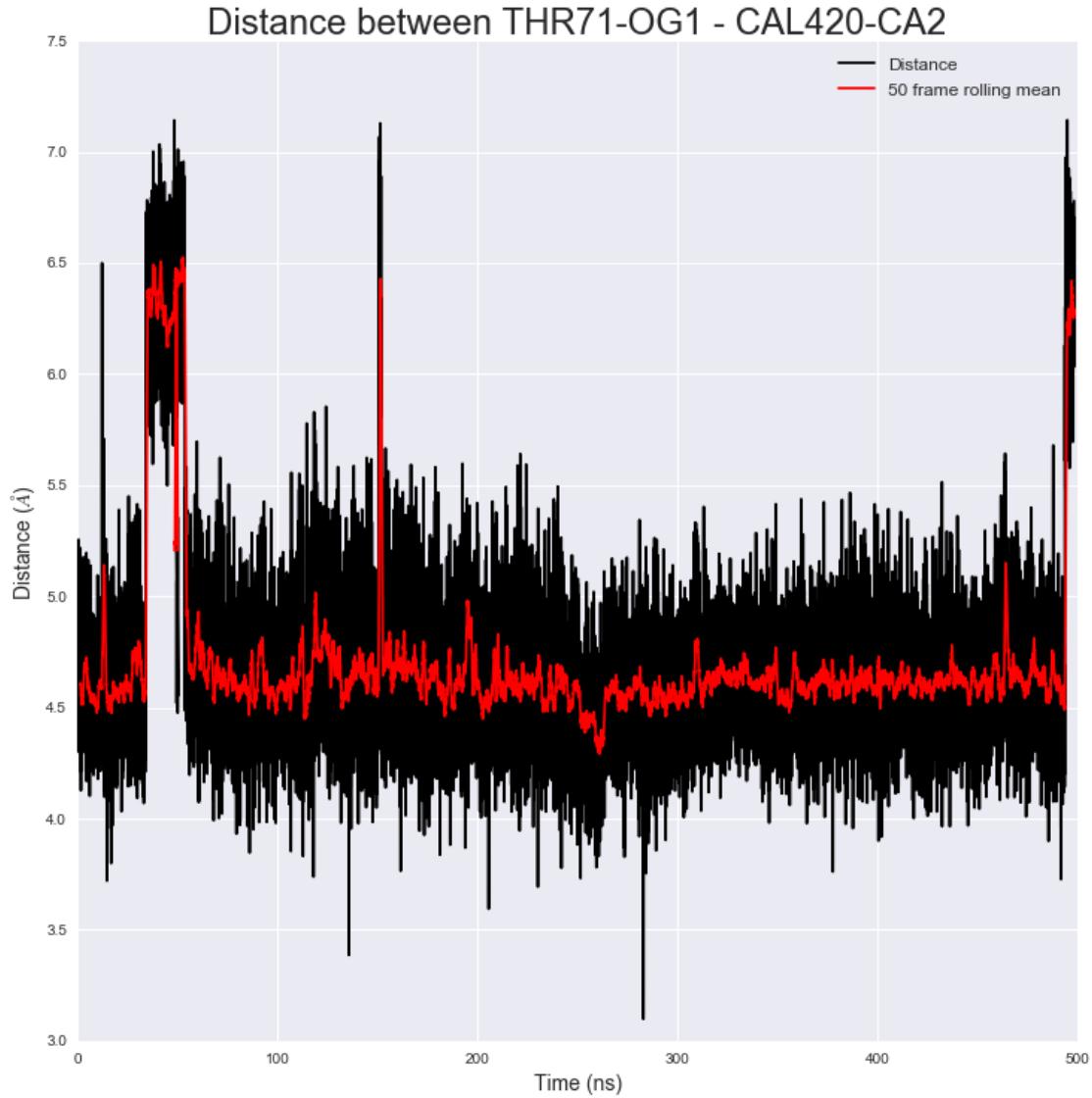
Loading trajectories from the following files:

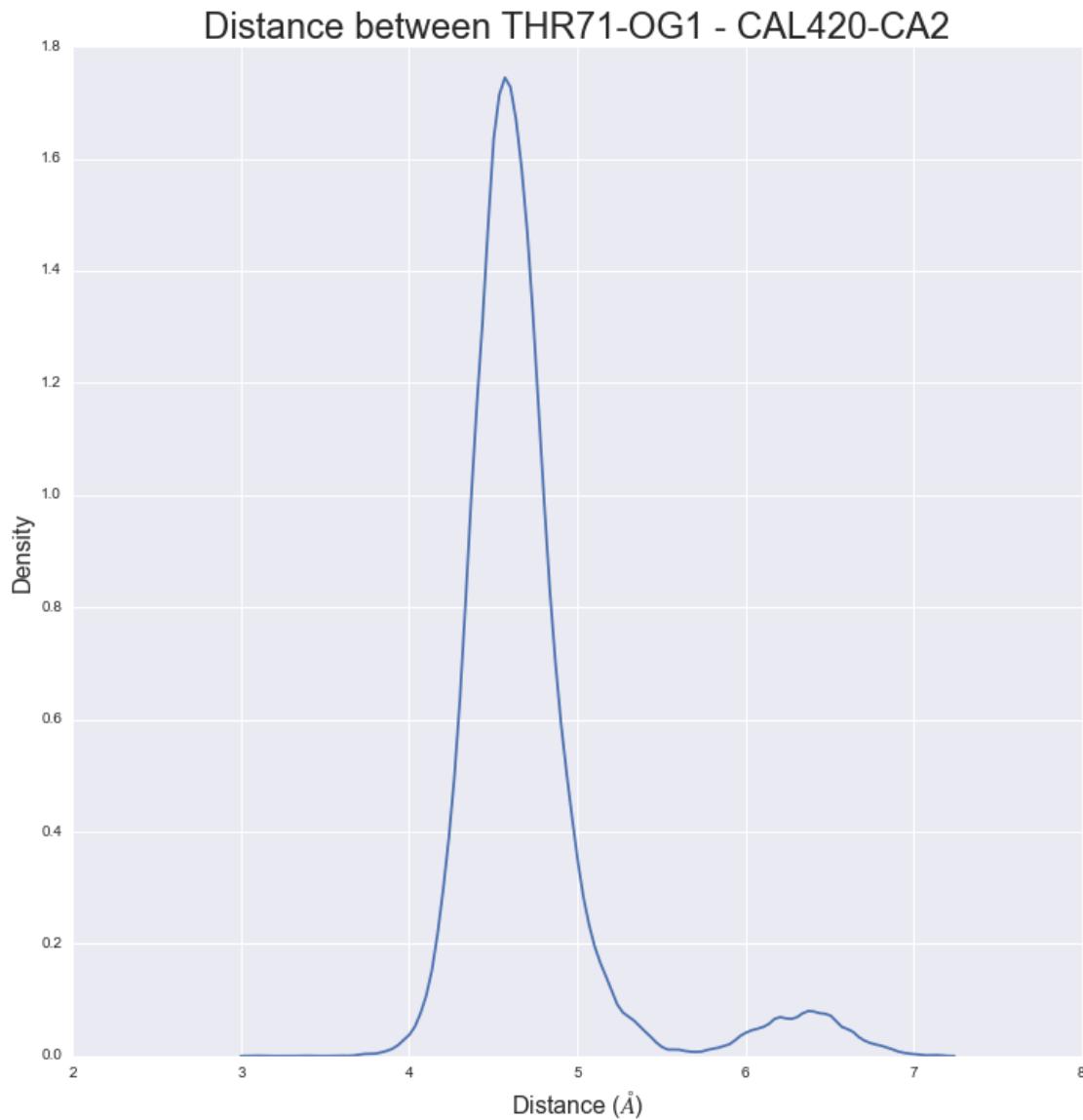
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05\_Prod\_troponin\_egcg\_MD2\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD2\_100-150\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD2\_150-200\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_200-250\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_250-300\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_300-350\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_350-400\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_400-450\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_450-500\_run1\_nowater.nc





Total execution time: 4.05 seconds

Total simulation time of all frames: 498.000010986 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1099

Atom2 number: 6810

Calculating distance between following atoms: ASP73-OD1 - CAL420-CA2

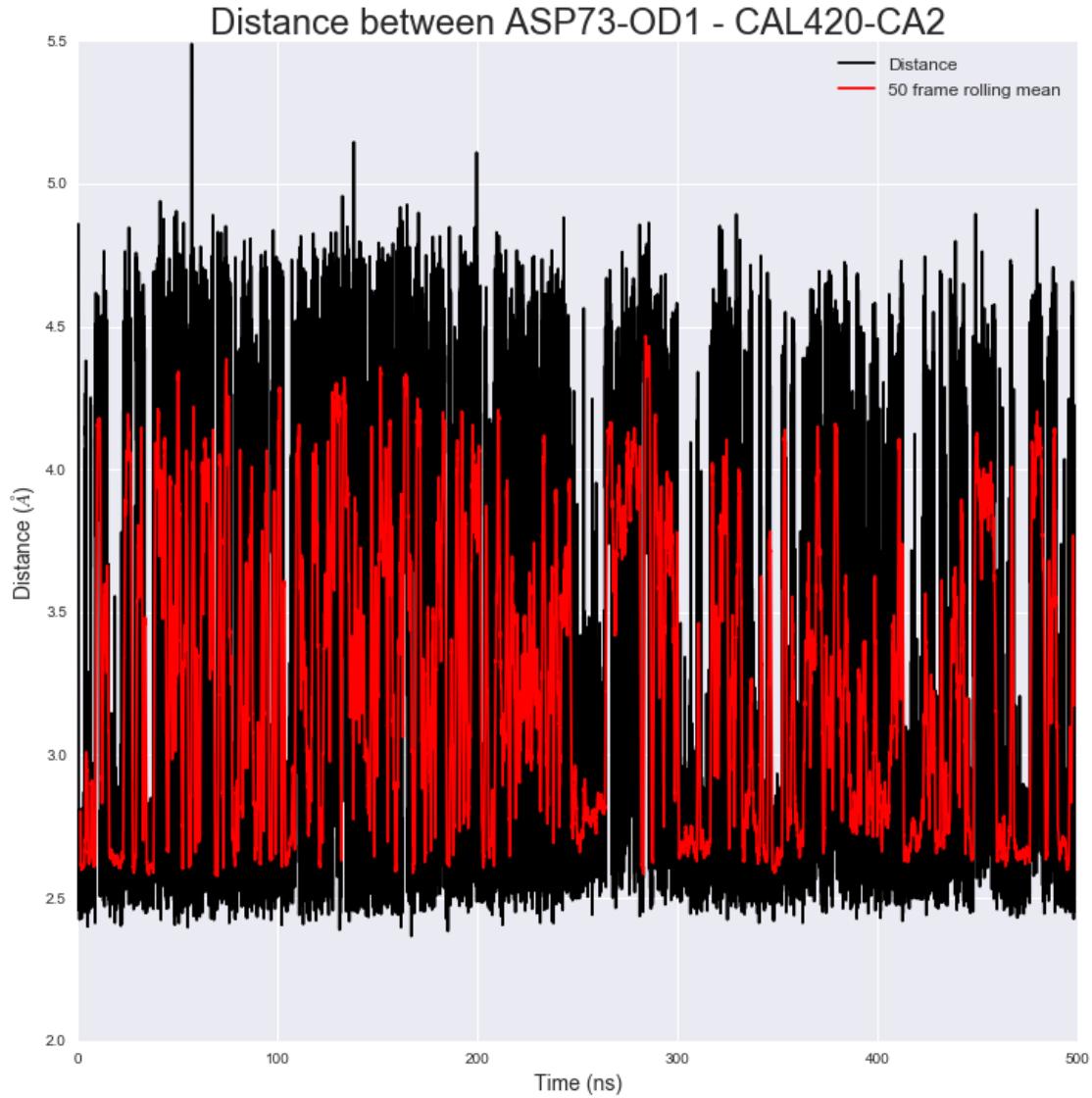
Loading trajectories from the following files:

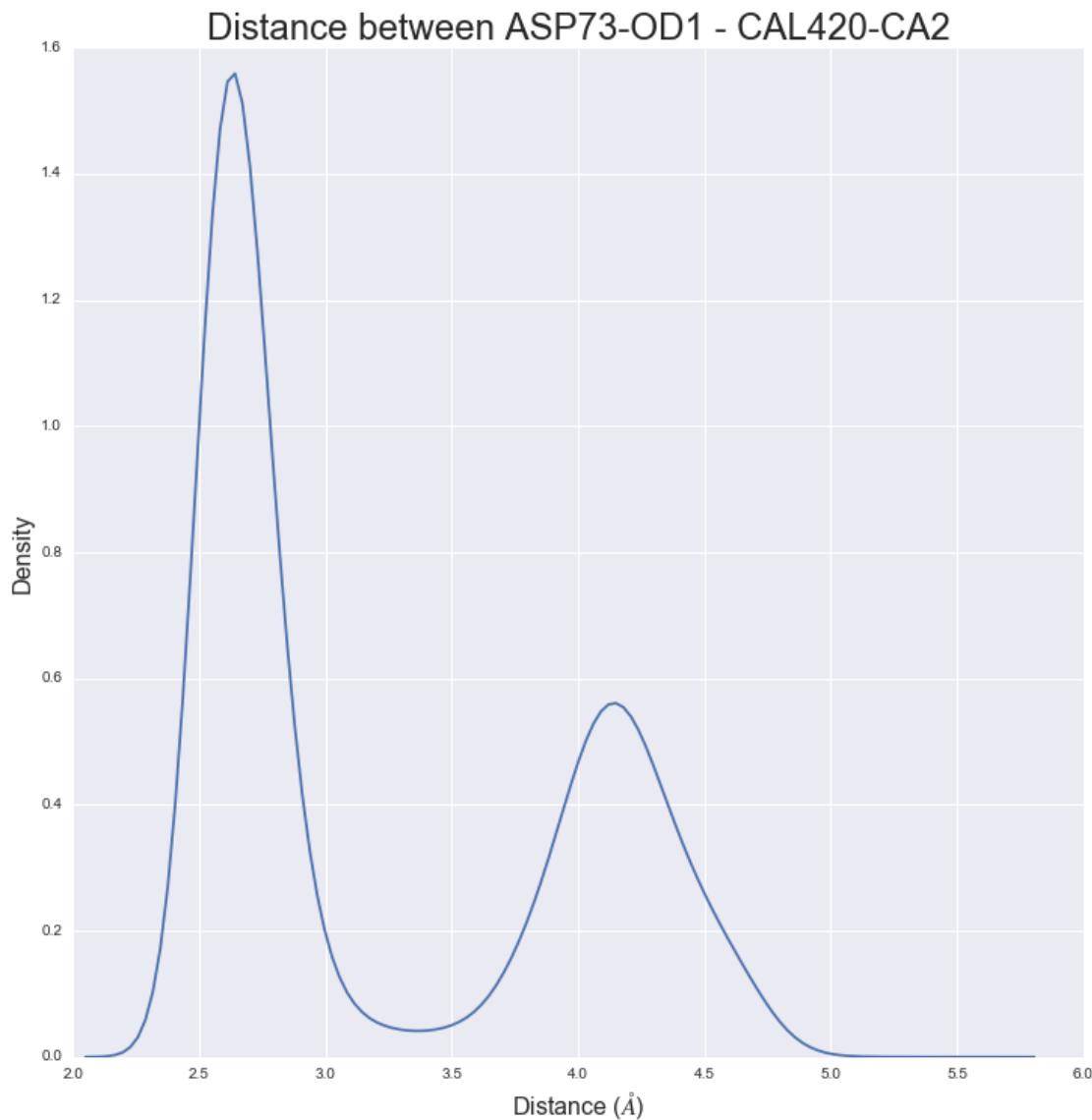
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05\_Prod\_troponin\_egcg\_MD2\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD2\_100-150\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD2\_150-200\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_200-250\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_250-300\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_300-350\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_350-400\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_400-450\_run1\_nowater.nc  
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Total execution time: 4.35 seconds

Total simulation time of all frames: 498.000010986 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1100

Atom2 number: 6810

Calculating distance between following atoms: ASP73-OD2 - CAL420-CA2

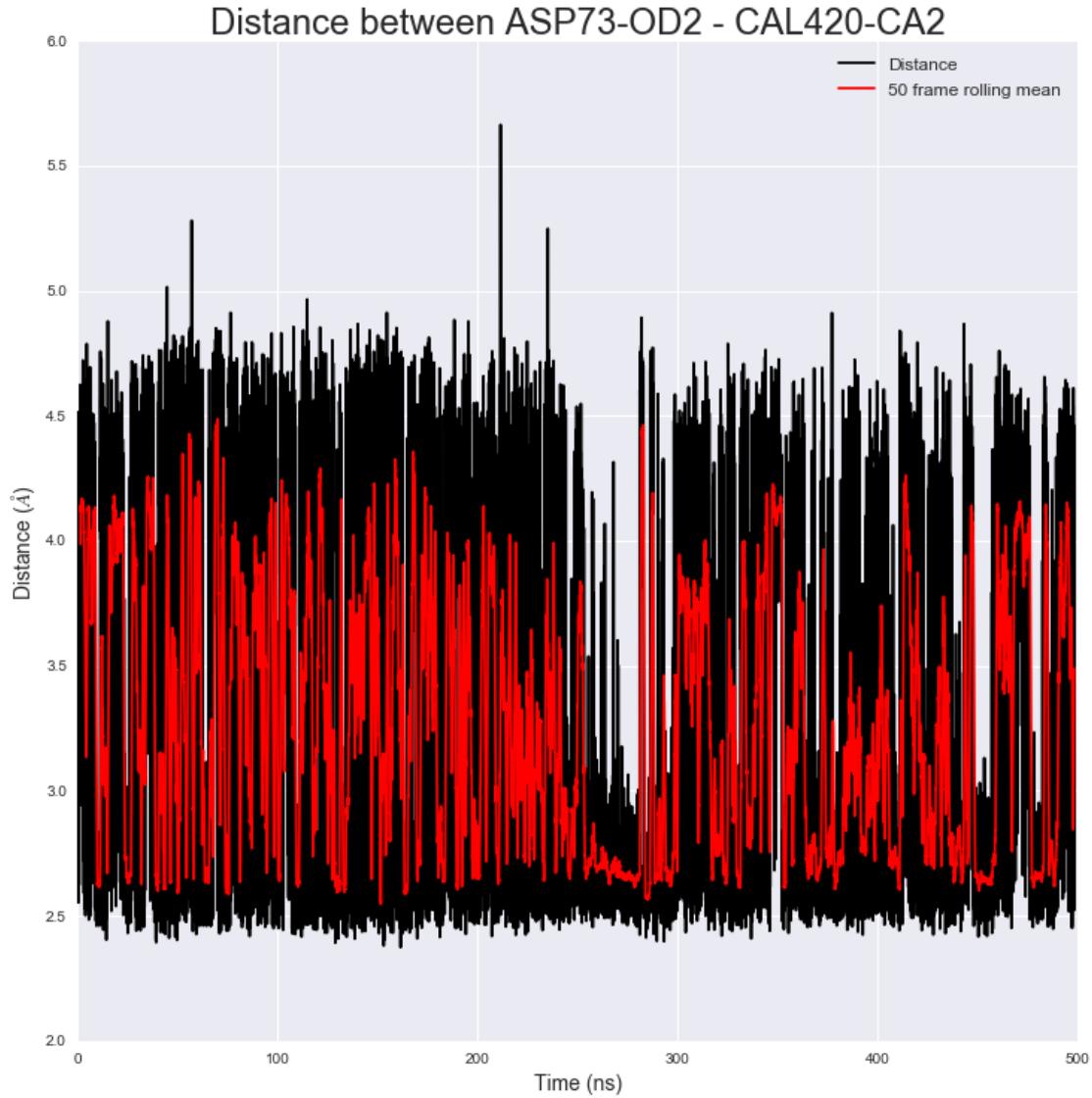
Loading trajectories from the following files:

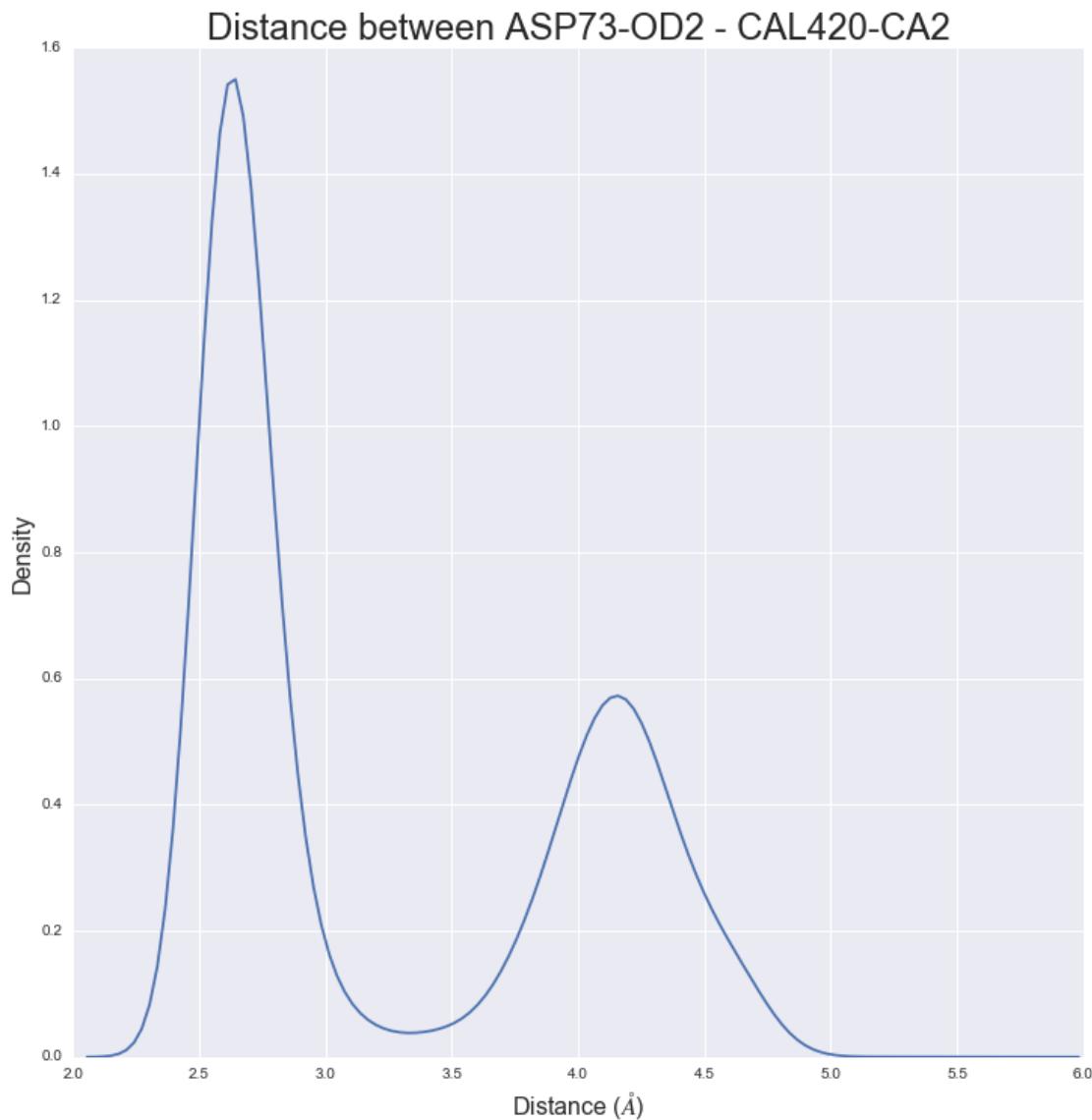
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05\_Prod\_troponin\_egcg\_MD2\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD2\_100-150\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD2\_150-200\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_200-250\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_250-300\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_300-350\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_350-400\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_400-450\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_450-500\_run1\_nowater.nc





Total execution time: 4.37 seconds

Total simulation time of all frames: 498.000010986 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1131

Atom2 number: 6810

Calculating distance between following atoms: ASP75-OD1 - CAL420-CA2

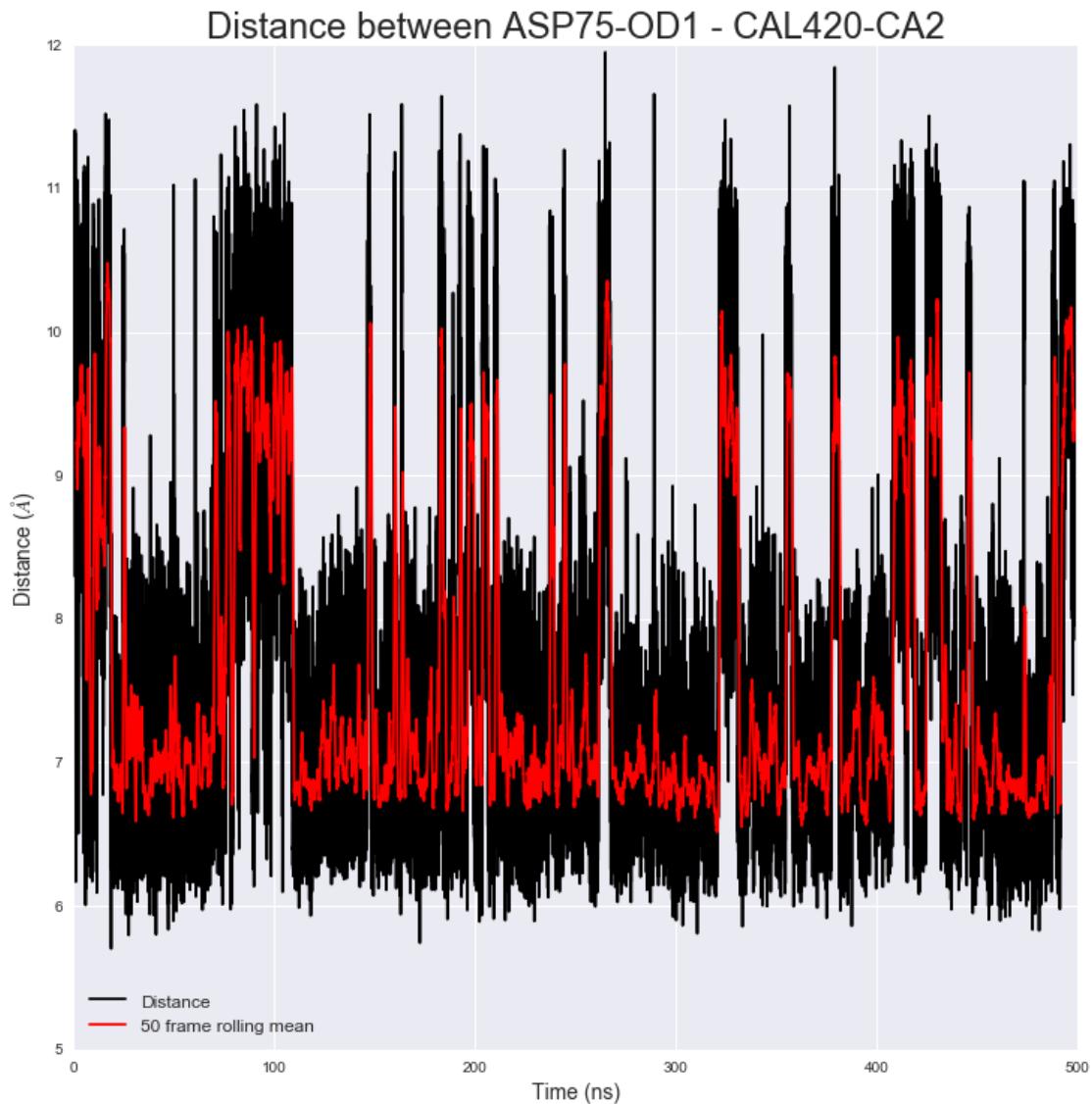
Loading trajectories from the following files:

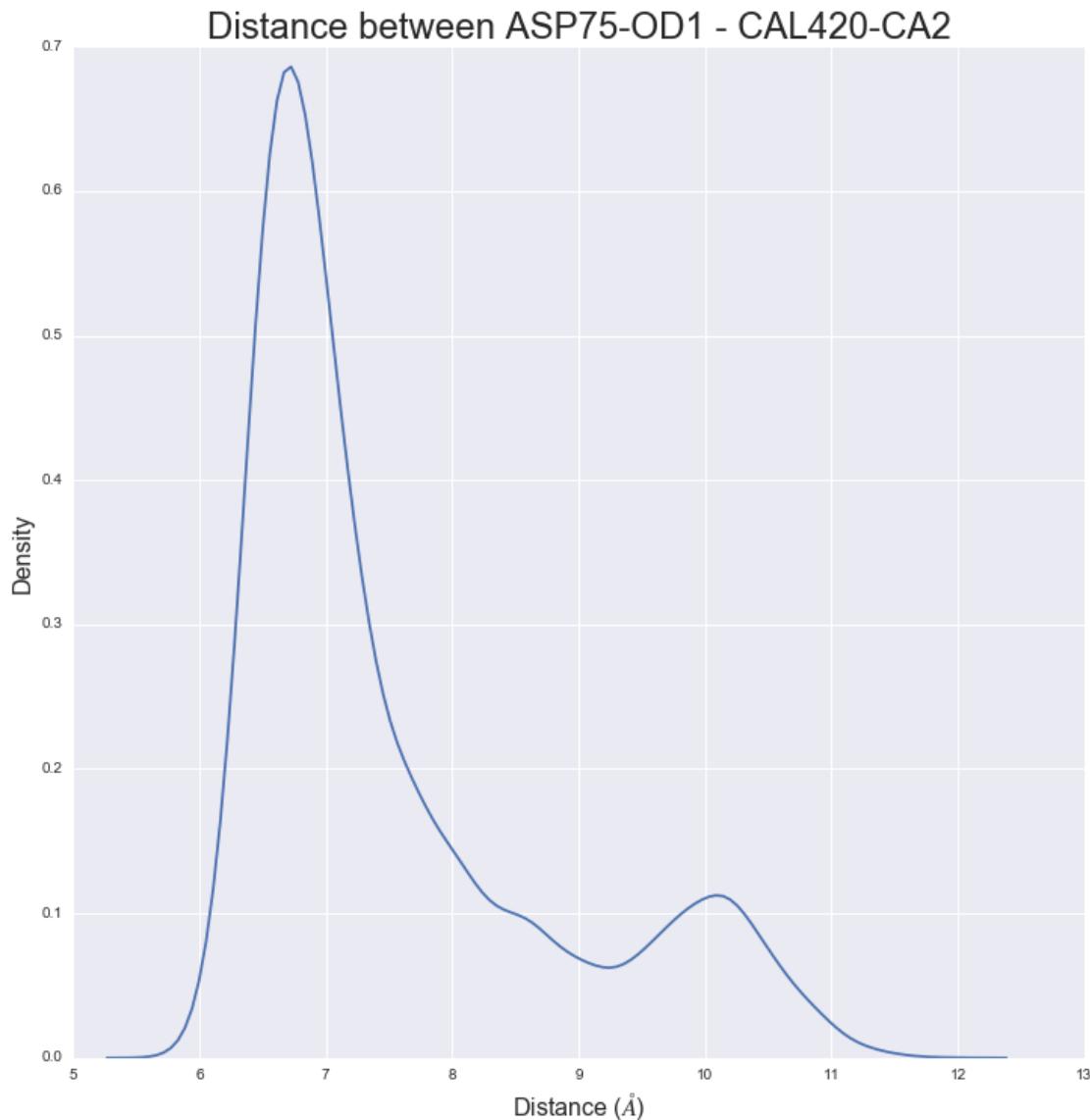
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05\_Prod\_troponin\_egcg\_MD2\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD2\_100-150\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD2\_150-200\_run1\_nowater.nc  
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05\_Prod\_troponin\_egcg\_MD2\_300-350\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_350-400\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_400-450\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_450-500\_run1\_nowater.nc





Total execution time: 4.54 seconds

Total simulation time of all frames: 498.000010986 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1132

Atom2 number: 6810

Calculating distance between following atoms: ASP75-OD2 - CAL420-CA2

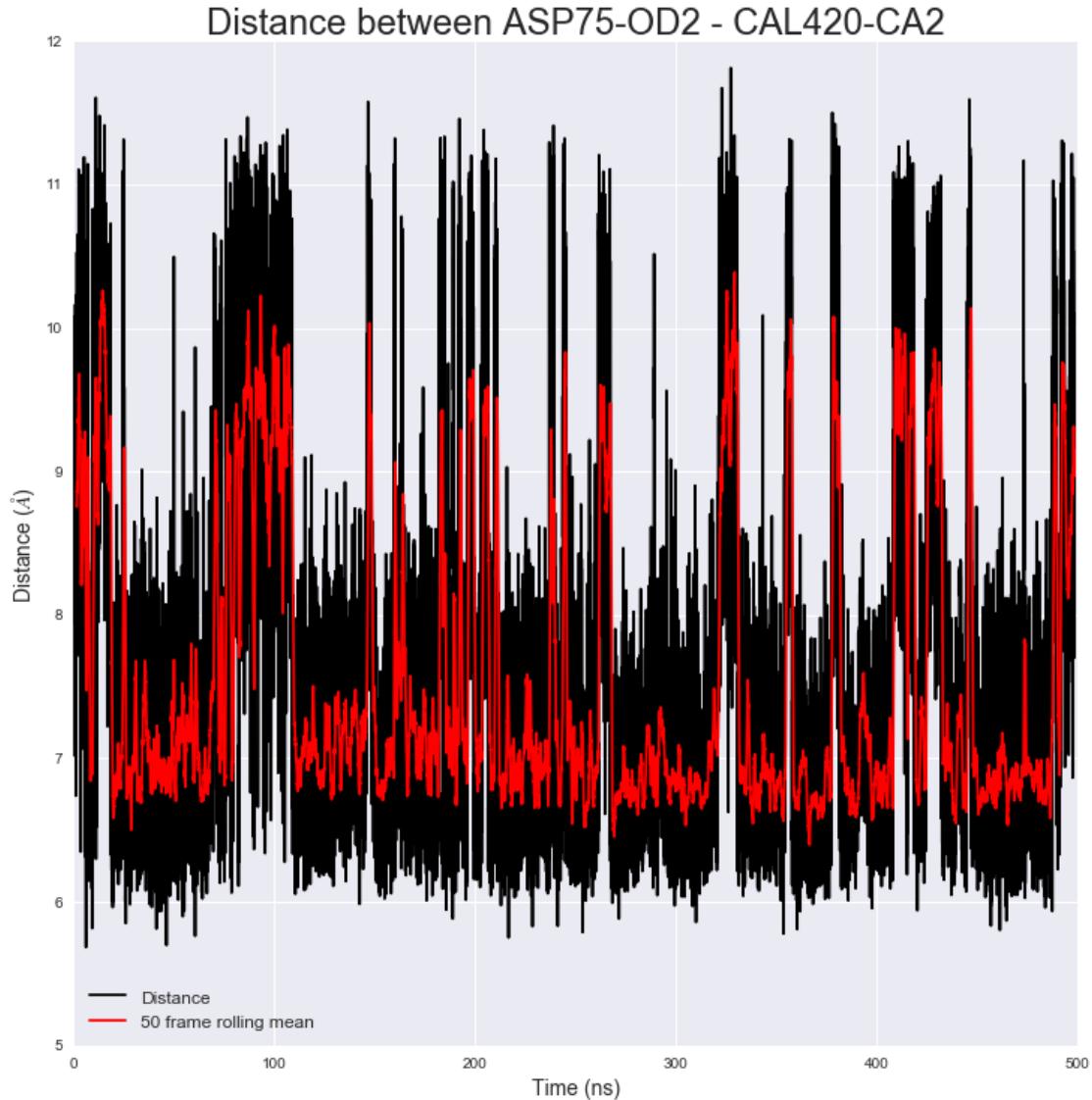
Loading trajectories from the following files:

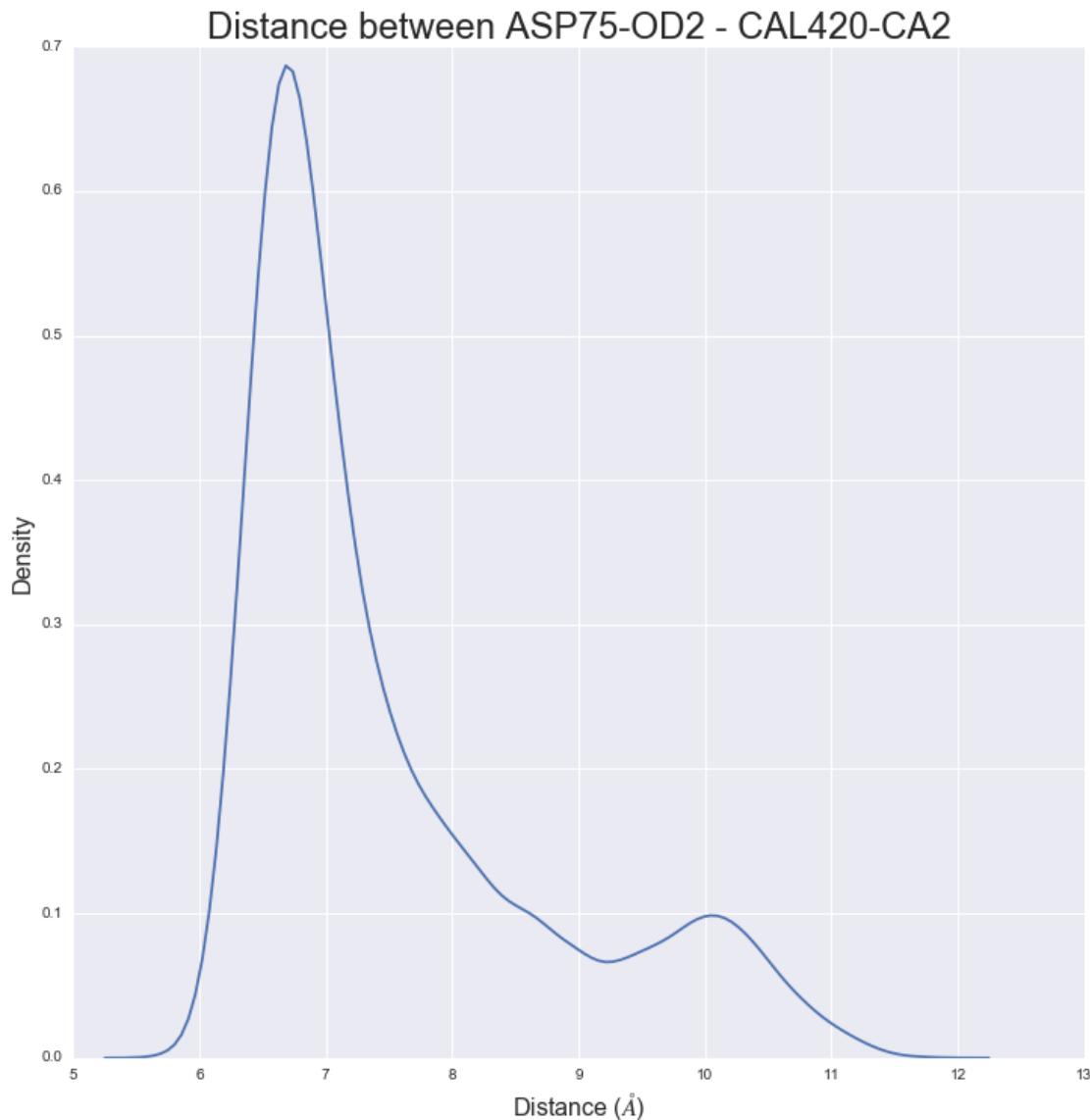
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05\_Prod\_troponin\_egcg\_MD2\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD2\_100-150\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD2\_150-200\_run1\_nowater.nc  
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05\_Prod\_troponin\_egcg\_MD2\_250-300\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_300-350\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_350-400\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_400-450\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_450-500\_run1\_nowater.nc





Total execution time: 4.16 seconds

Total simulation time of all frames: 498.000010986 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1146

Atom2 number: 6810

Calculating distance between following atoms: GLU76-OE1 - CAL420-CA2

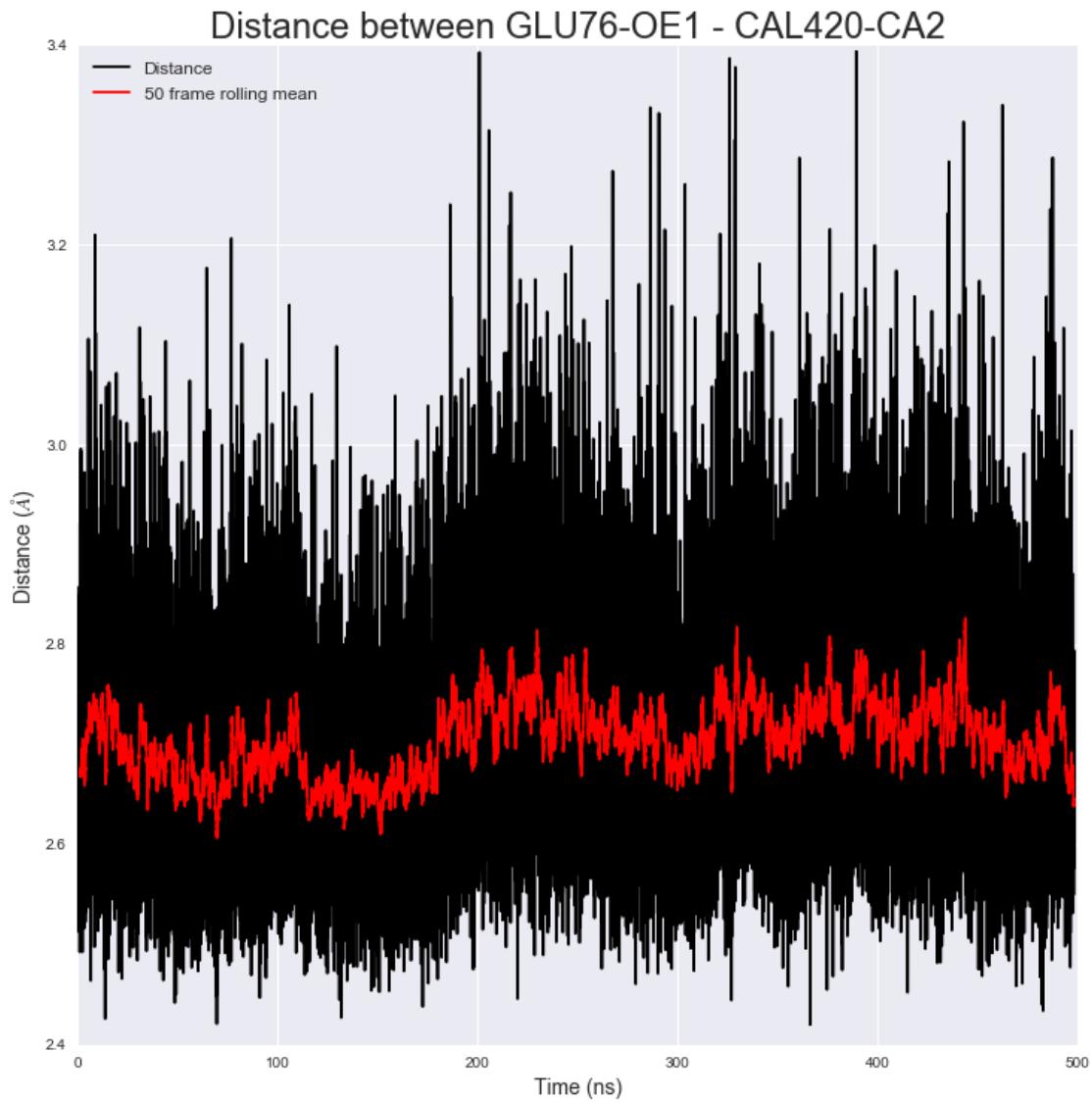
Loading trajectories from the following files:

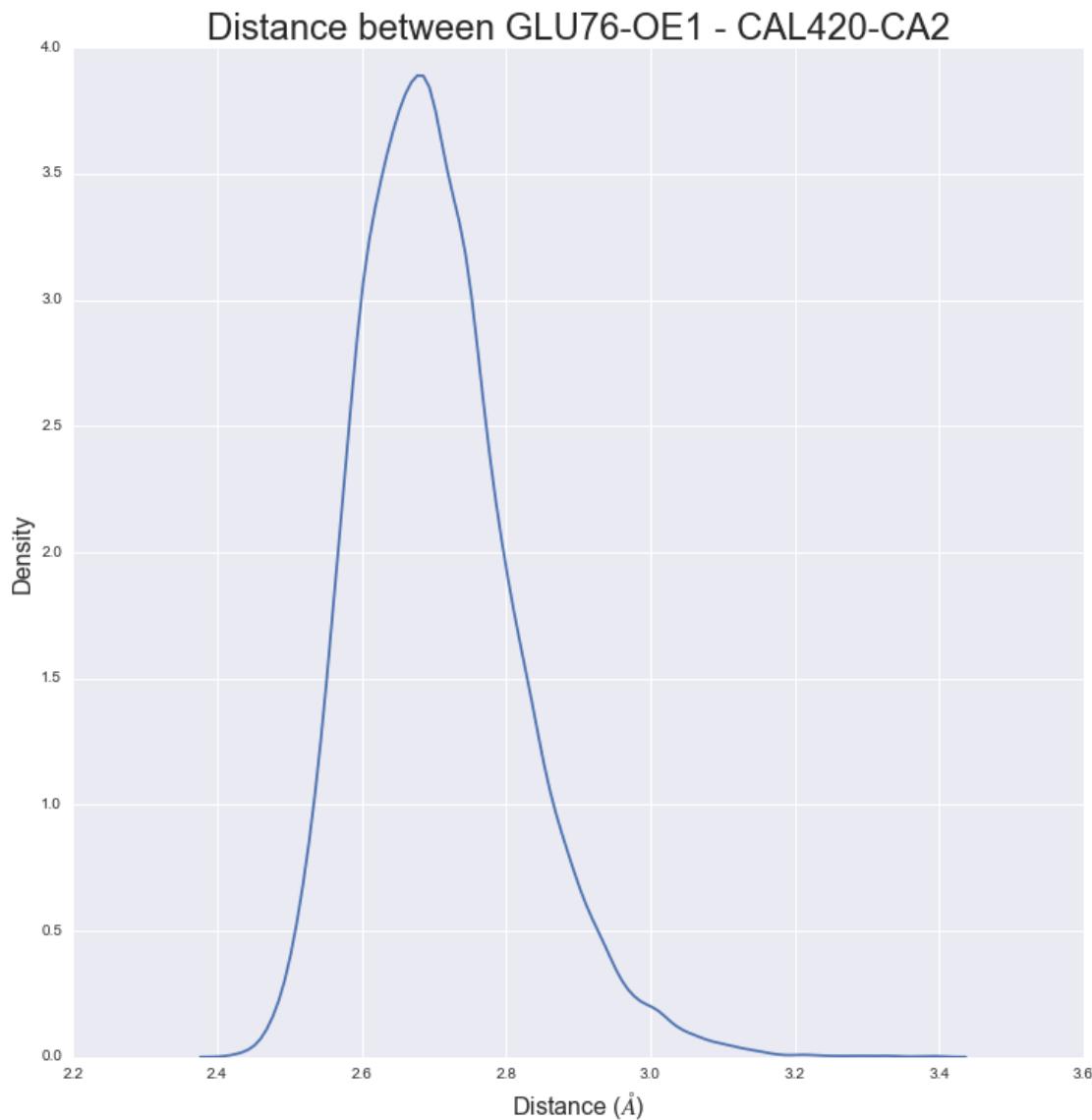
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05\_Prod\_troponin\_egcg\_MD2\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD2\_100-150\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD2\_150-200\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_200-250\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_250-300\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_300-350\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_350-400\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_400-450\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_450-500\_run1\_nowater.nc





Total execution time: 4.31 seconds

Total simulation time of all frames: 498.000010986 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1147

Atom2 number: 6810

Calculating distance between following atoms: GLU76-OE2 - CAL420-CA2

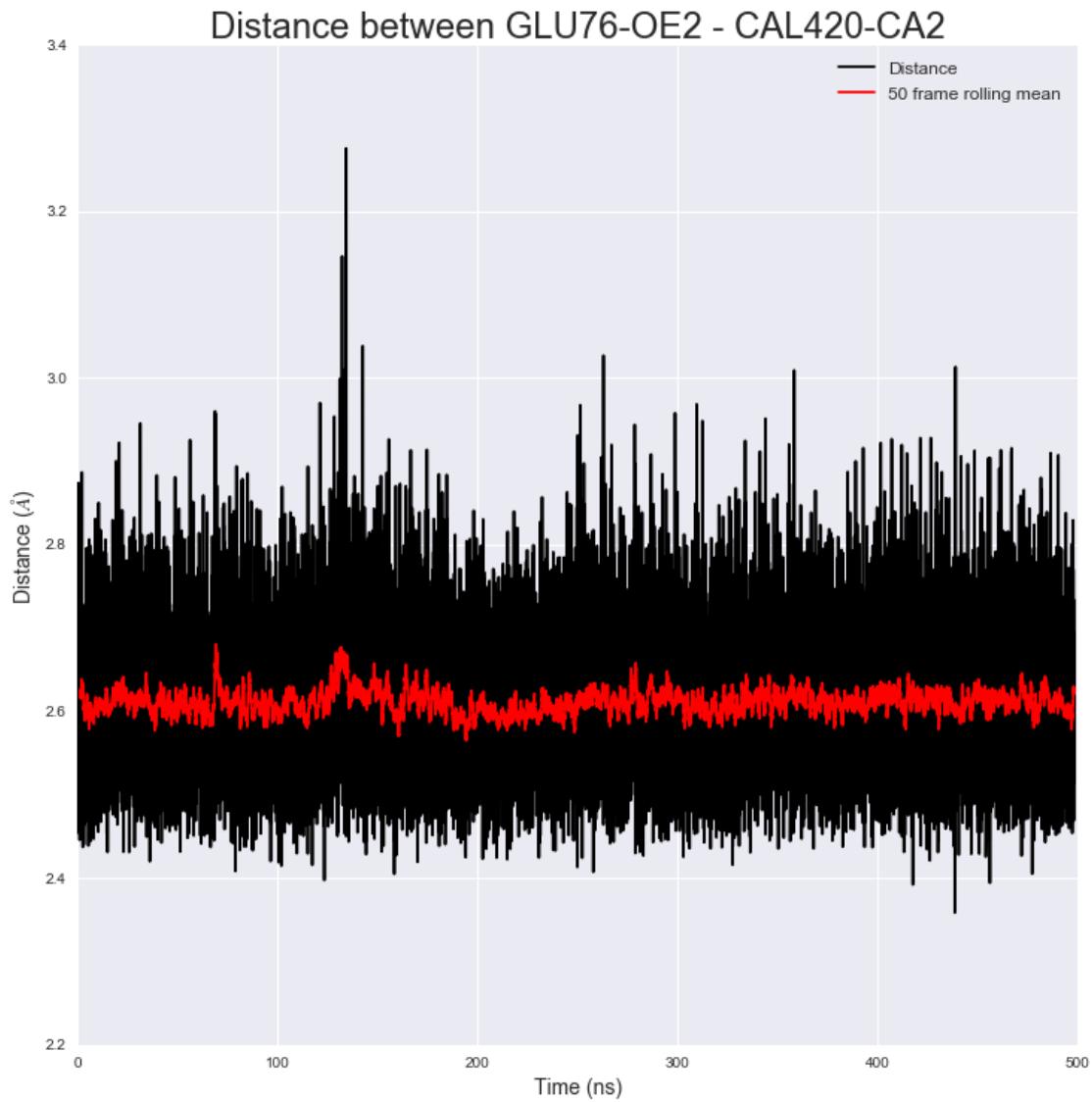
Loading trajectories from the following files:

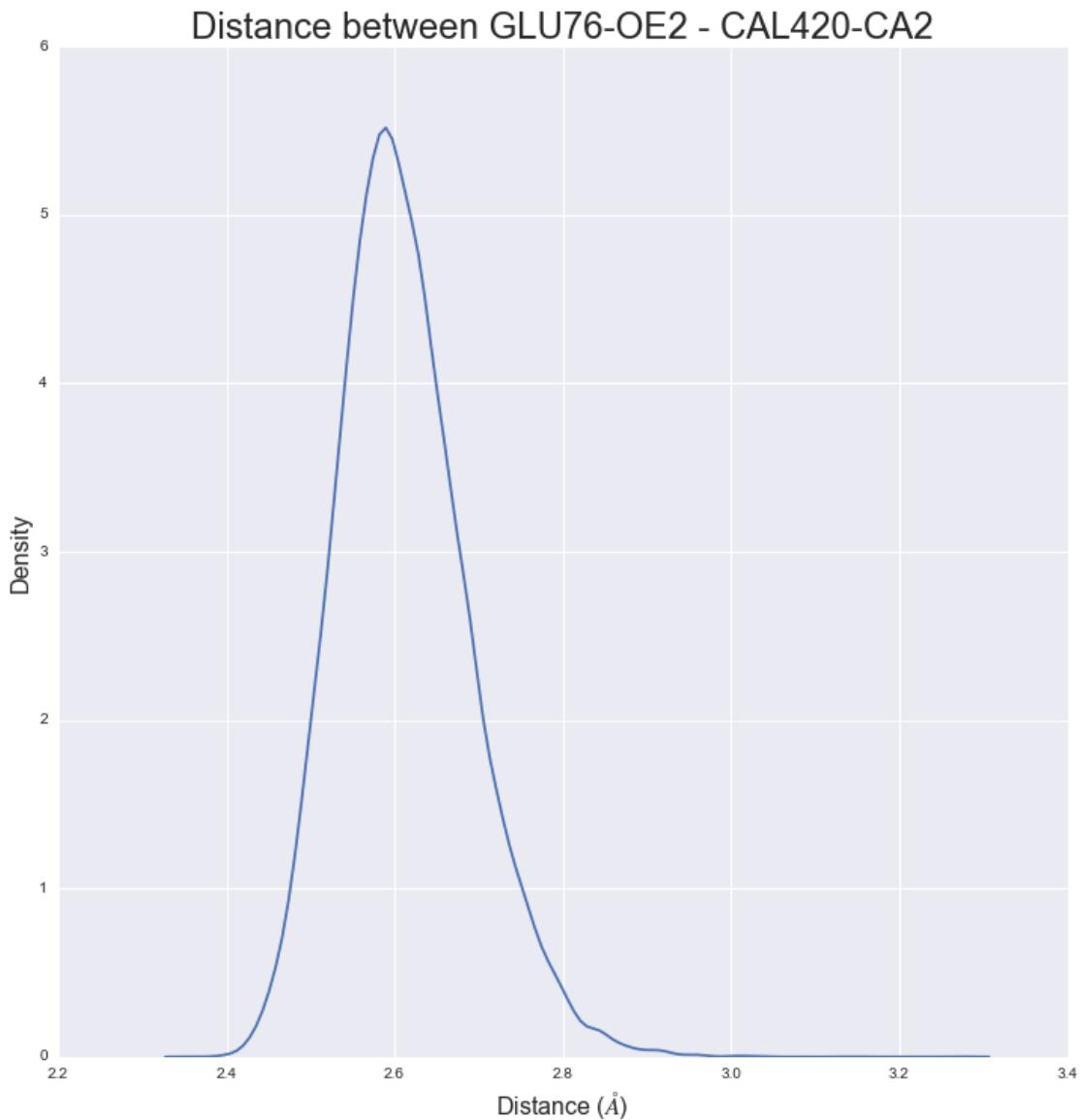
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05\_Prod\_troponin\_egcg\_MD2\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD2\_100-150\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD2\_150-200\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_200-250\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_250-300\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_300-350\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_350-400\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_400-450\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD2\_450-500\_run1\_nowater.nc





Total execution time: 4.21 seconds

Total simulation time of all frames: 498.000010986 nanoseconds

### 0.3 MD3

```
In [15]: topology_MD3 = '/Users/gil_f.hoben/Troponin_md_processed/MD3/run1/troponin_egcg_MD3_nowater.pr
trajectory_MD3 = '/Users/gil_f.hoben/Troponin_md_processed/MD3/run1/Trajectories/'
for atom1 in atom1_list:
    main(topology_MD3, trajectory_MD3, atom1, atom2, verbose = 1)
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The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

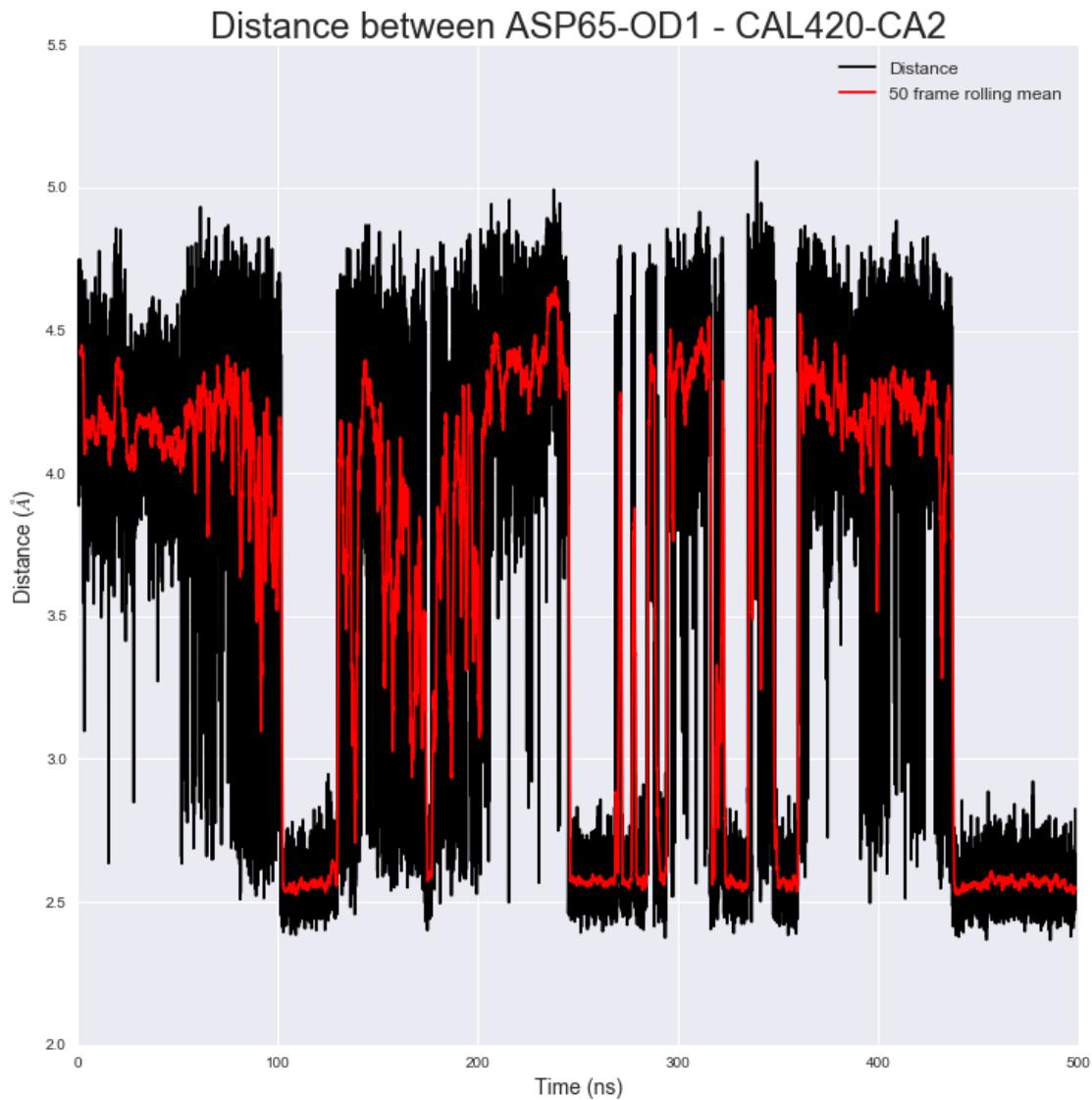
Atom1 number: 1005

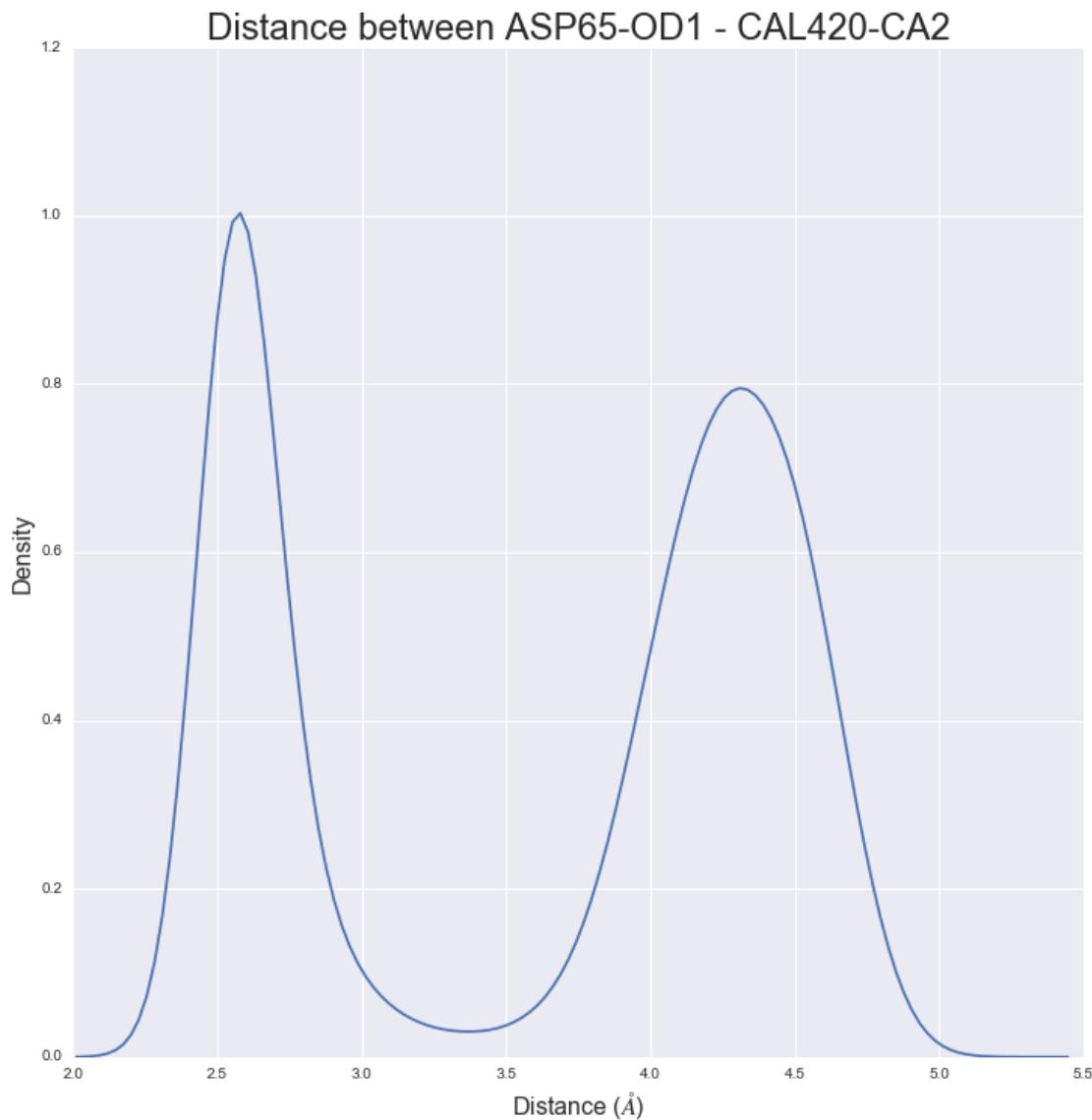
Atom2 number: 6810

Calculating distance between following atoms: ASP65-OD1 - CAL420-CA2

Loading trajectories from the following files:

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05\_Prod\_troponin\_egcg\_MD3\_050-100\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_100-150\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_150-200\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_200-250\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_250-300\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_300-350\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_350-400\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_400-450\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_450-500\_run1\_nowater.nc





Total execution time: 32.56 seconds

Total simulation time of all frames: 498.000010986 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1005

Atom2 number: 6810

Calculating distance between following atoms: ASP65-OD1 - CAL420-CA2

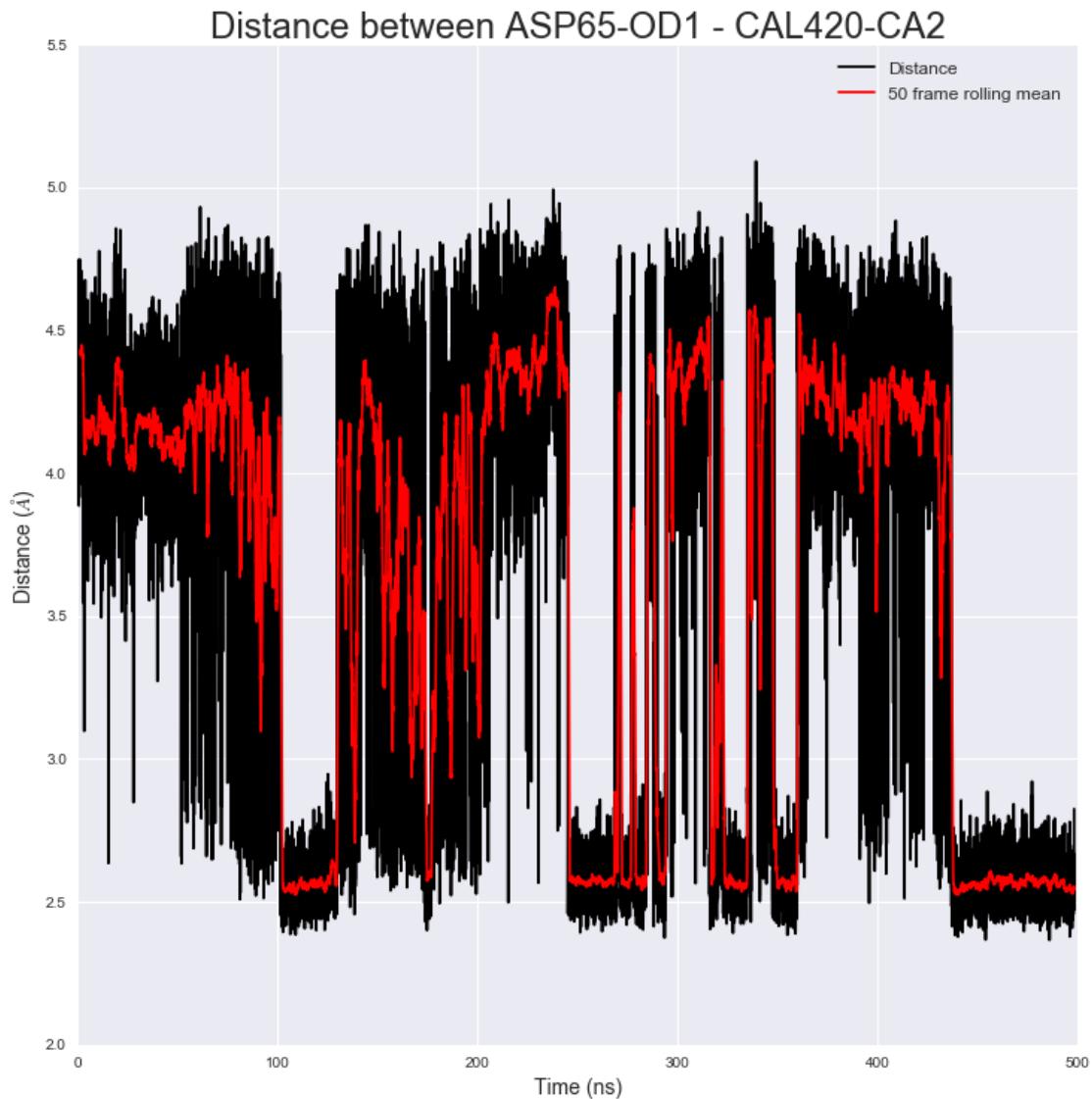
Loading trajectories from the following files:

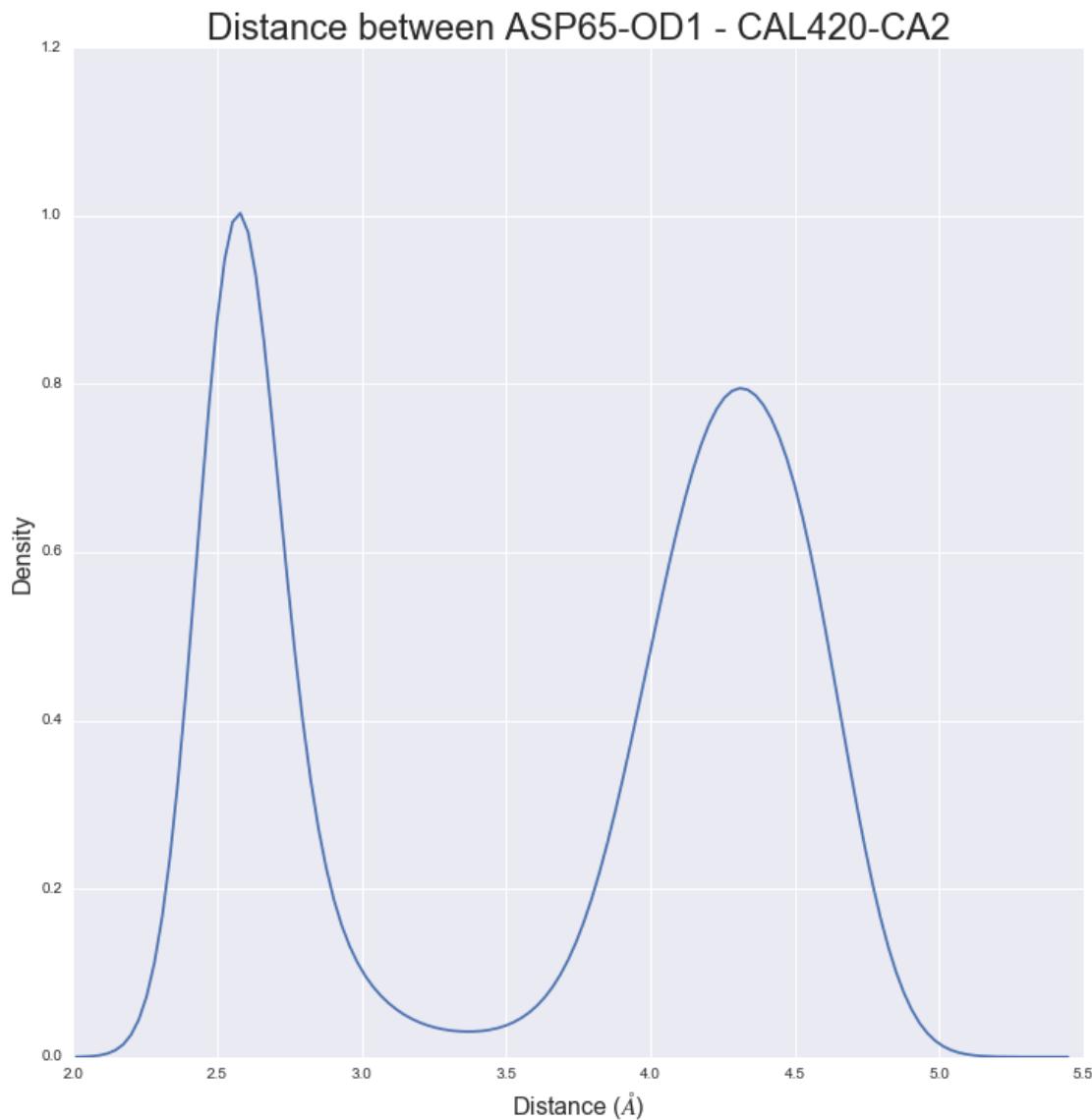
05\_Prod\_troponin\_egcg\_MD3\_000-050\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD3\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD3\_100-150\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD3\_150-200\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_200-250\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_250-300\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_300-350\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_350-400\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_400-450\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_450-500\_run1\_nowater.nc





Total execution time: 23.47 seconds

Total simulation time of all frames: 498.000010986 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1020

Atom2 number: 6810

Calculating distance between following atoms: GLU66-OE1 - CAL420-CA2

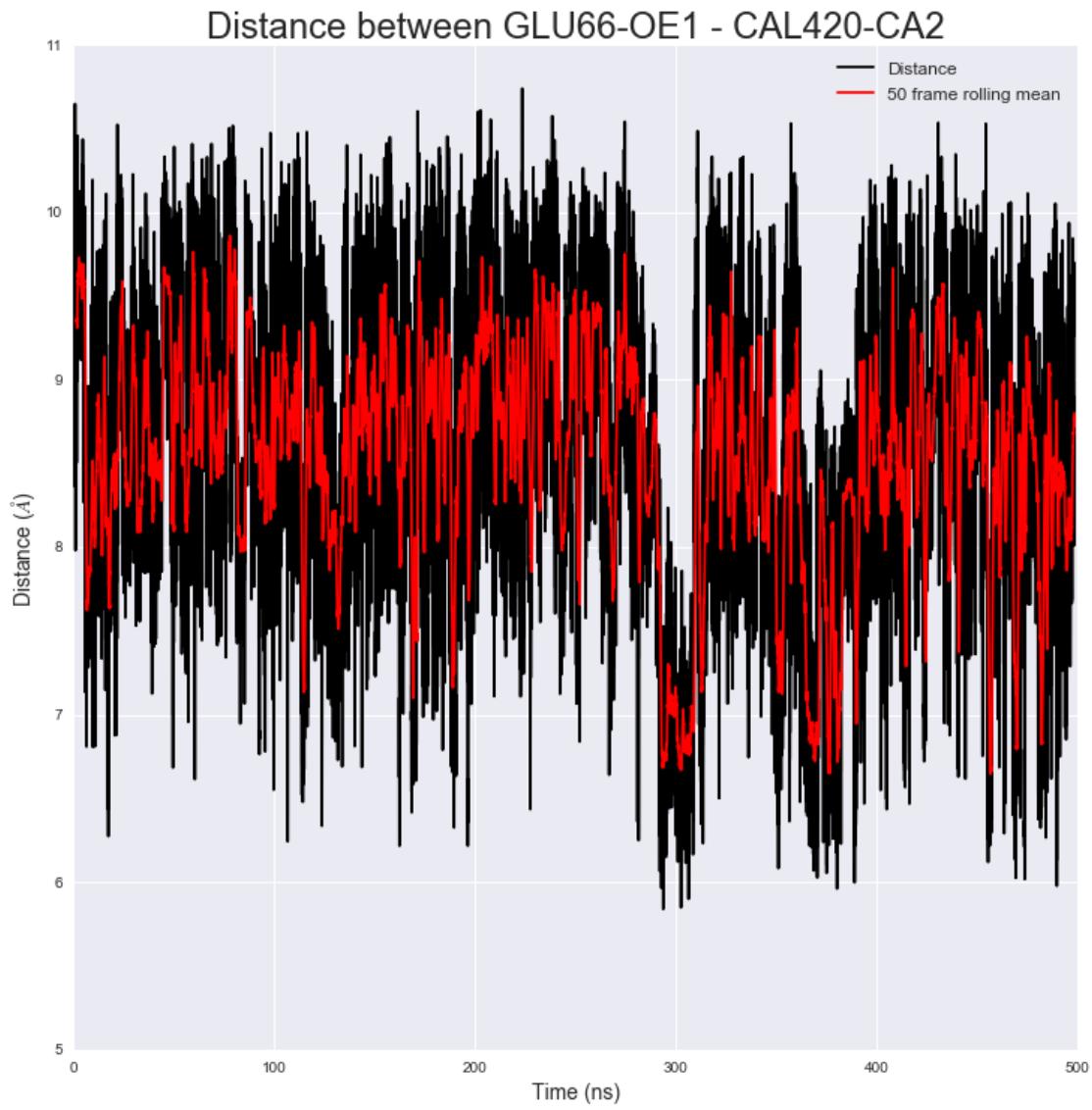
Loading trajectories from the following files:

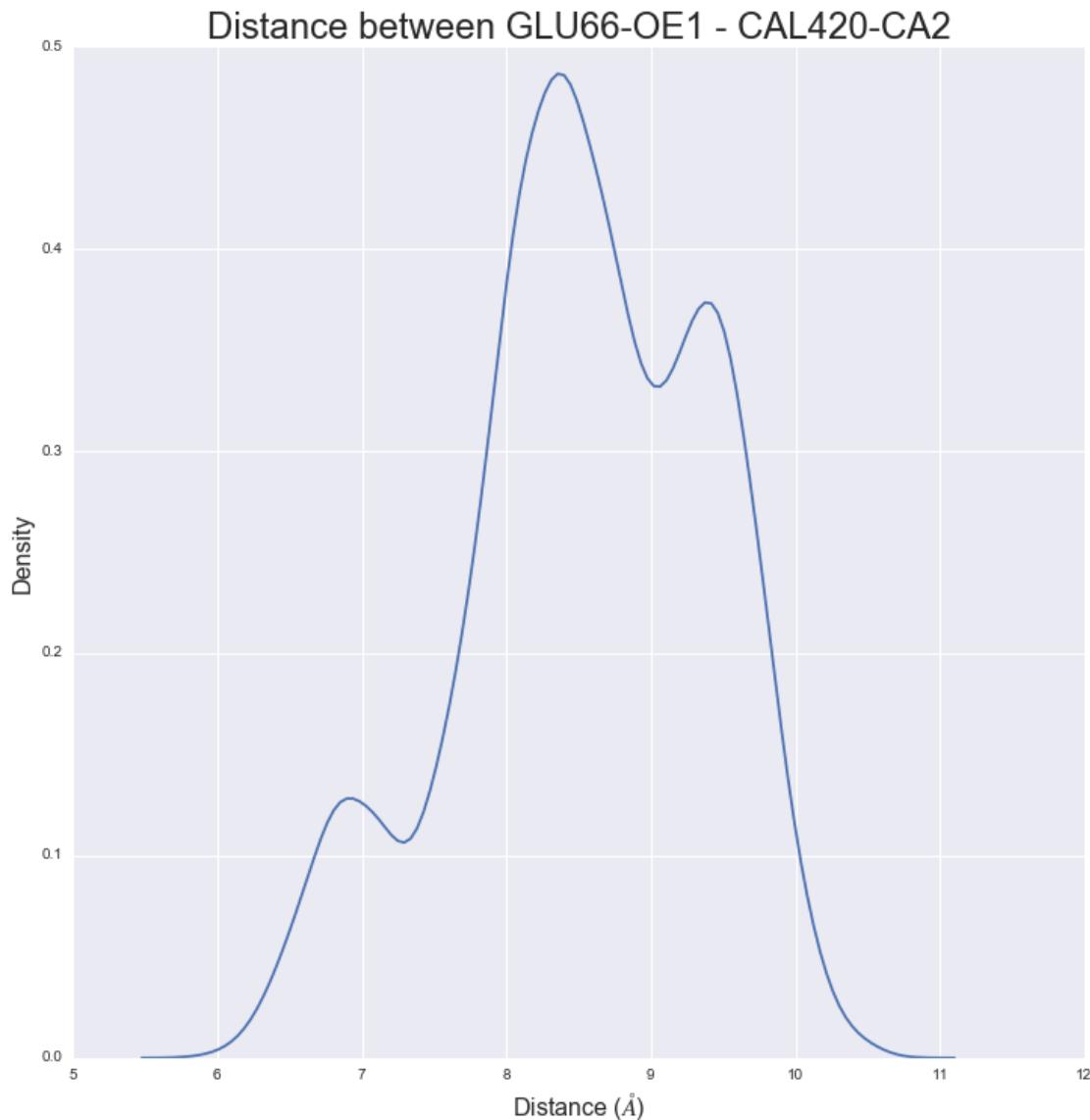
05\_Prod\_troponin\_egcg\_MD3\_000-050\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD3\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD3\_100-150\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD3\_150-200\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_200-250\_run1\_nowater.nc  
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05\_Prod\_troponin\_egcg\_MD3\_300-350\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_350-400\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_400-450\_run1\_nowater.nc  
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Total execution time: 8.80 seconds

Total simulation time of all frames: 498.000010986 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1021

Atom2 number: 6810

Calculating distance between following atoms: GLU66-OE2 - CAL420-CA2

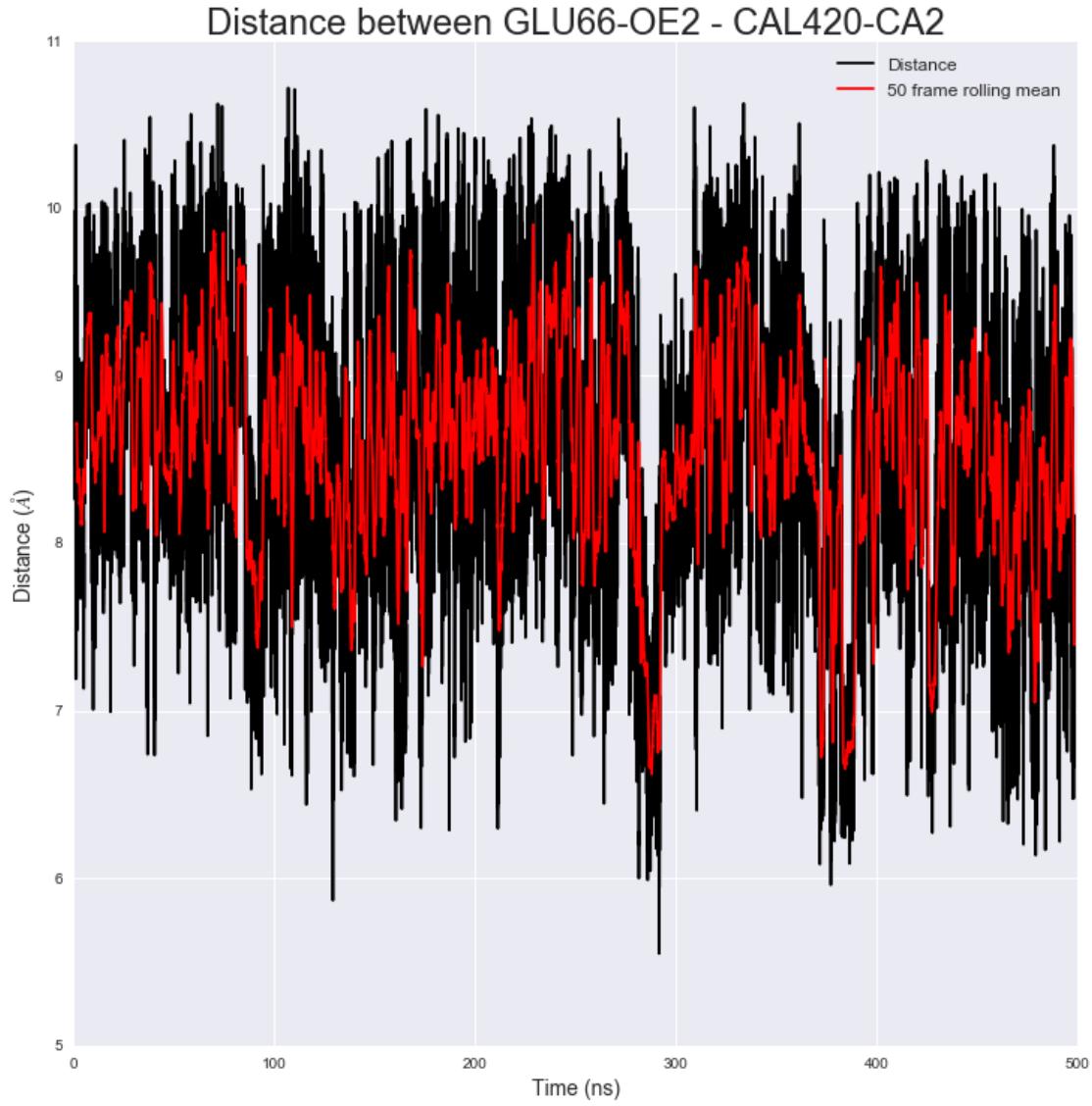
Loading trajectories from the following files:

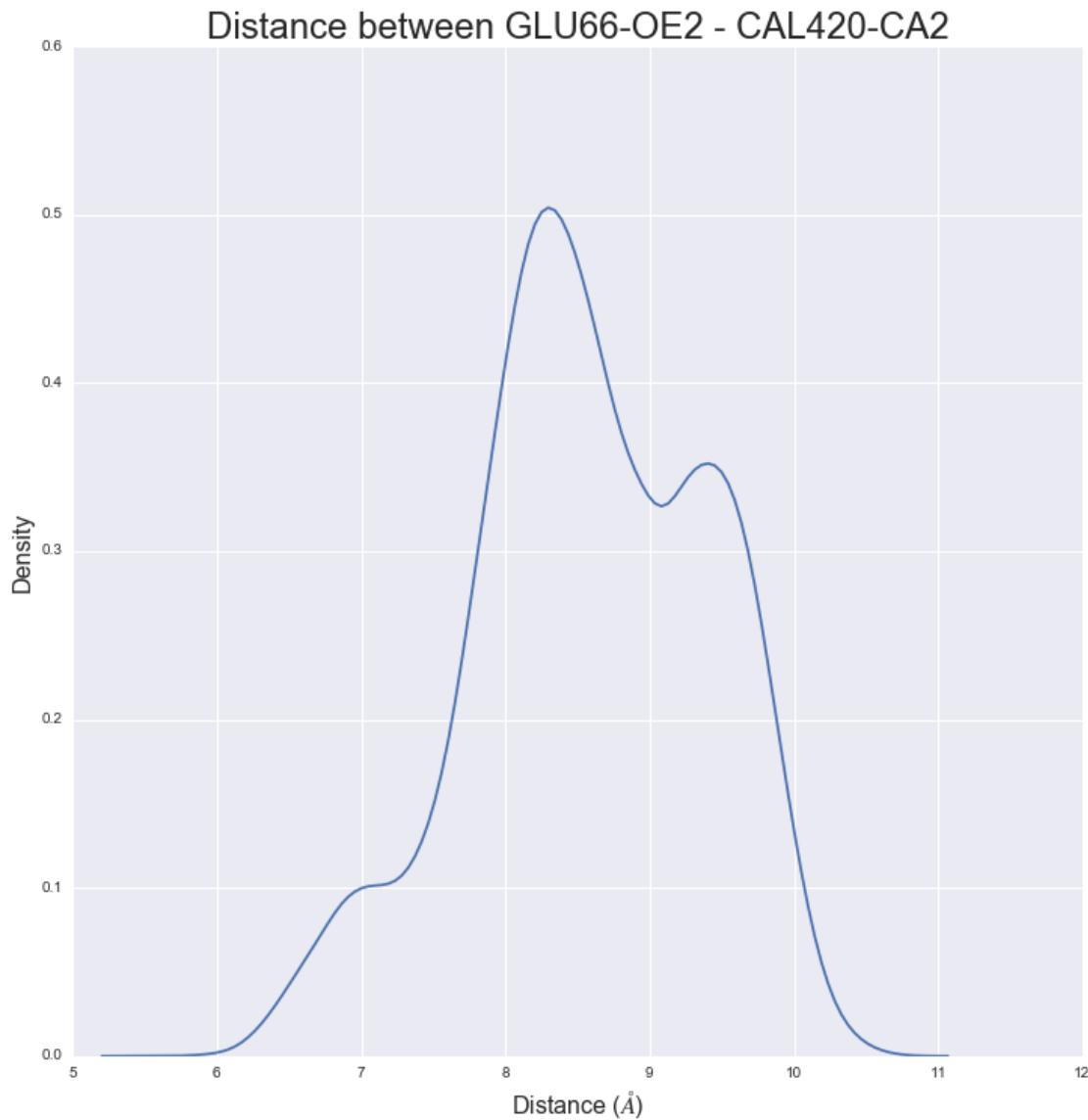
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05\_Prod\_troponin\_egcg\_MD3\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD3\_100-150\_run1\_nowater.nc

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05\_Prod\_troponin\_egcg\_MD3\_250-300\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_300-350\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_350-400\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_400-450\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_450-500\_run1\_nowater.nc





Total execution time: 42.85 seconds

Total simulation time of all frames: 498.000010986 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1032

Atom2 number: 6810

Calculating distance between following atoms: ASP67-OD1 - CAL420-CA2

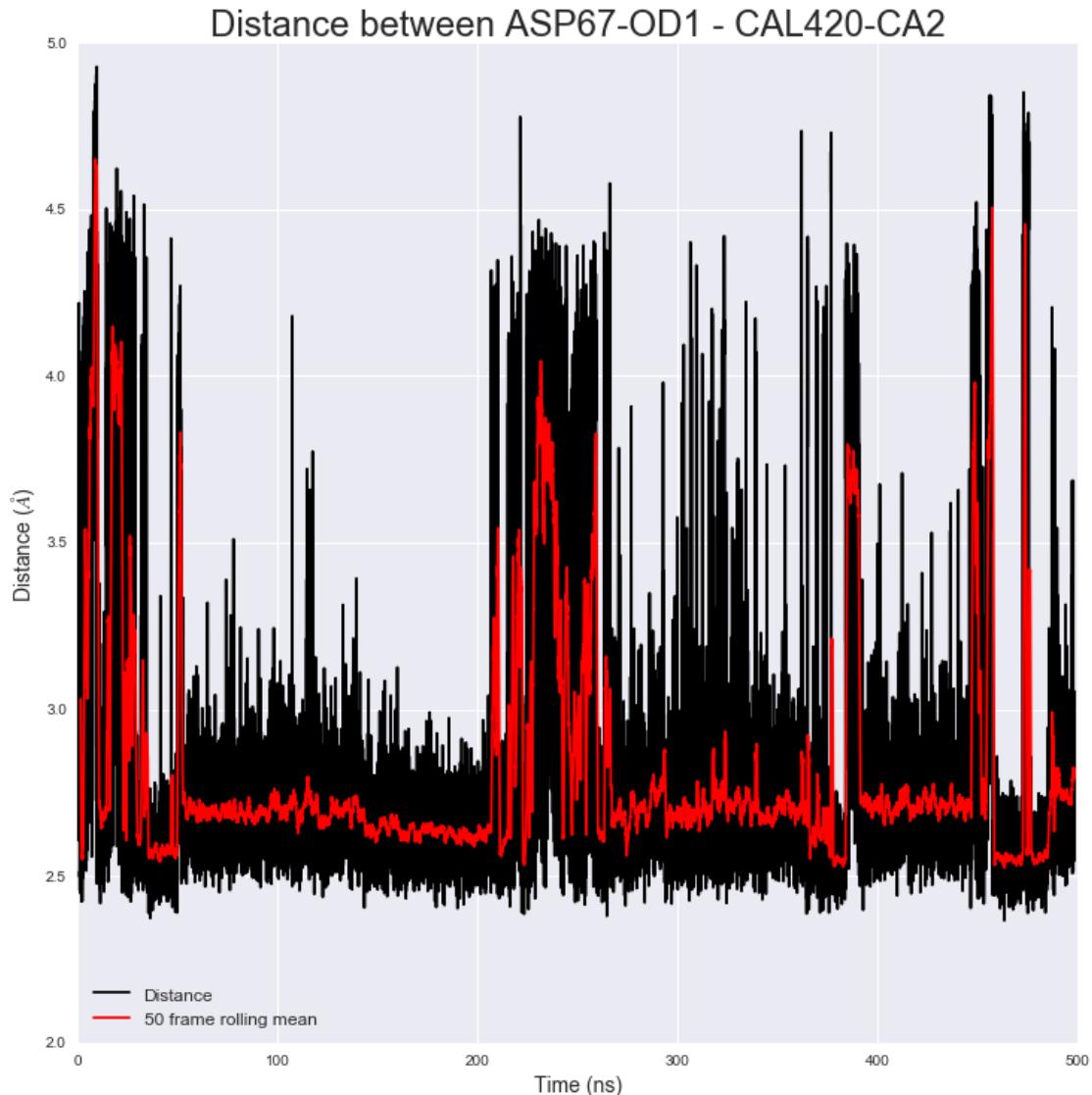
Loading trajectories from the following files:

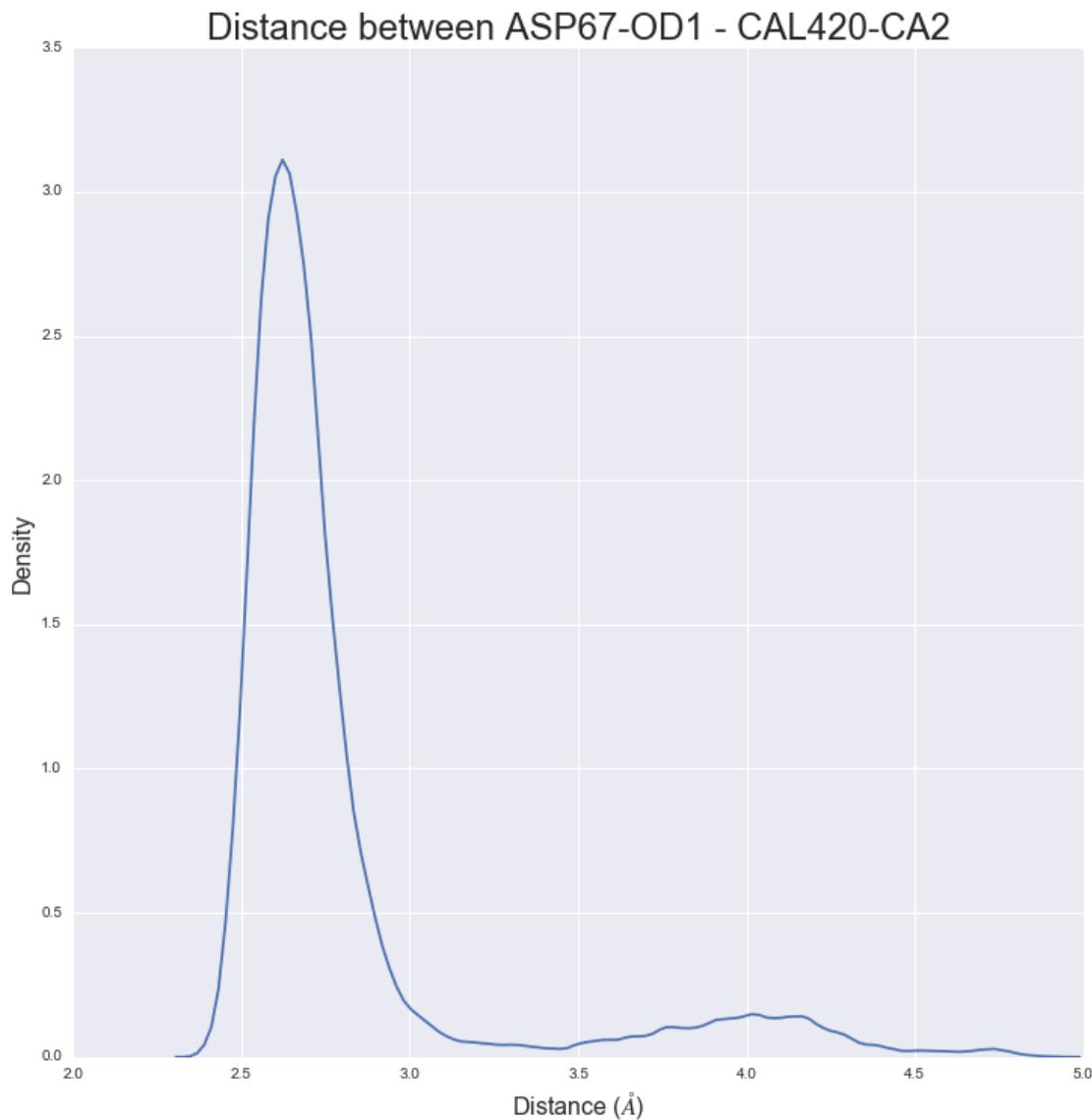
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05\_Prod\_troponin\_egcg\_MD3\_100-150\_run1\_nowater.nc

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05\_Prod\_troponin\_egcg\_MD3\_300-350\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_350-400\_run1\_nowater.nc  
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Total execution time: 55.72 seconds

Total simulation time of all frames: 498.000010986 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1033

Atom2 number: 6810

Calculating distance between following atoms: ASP67-OD2 - CAL420-CA2

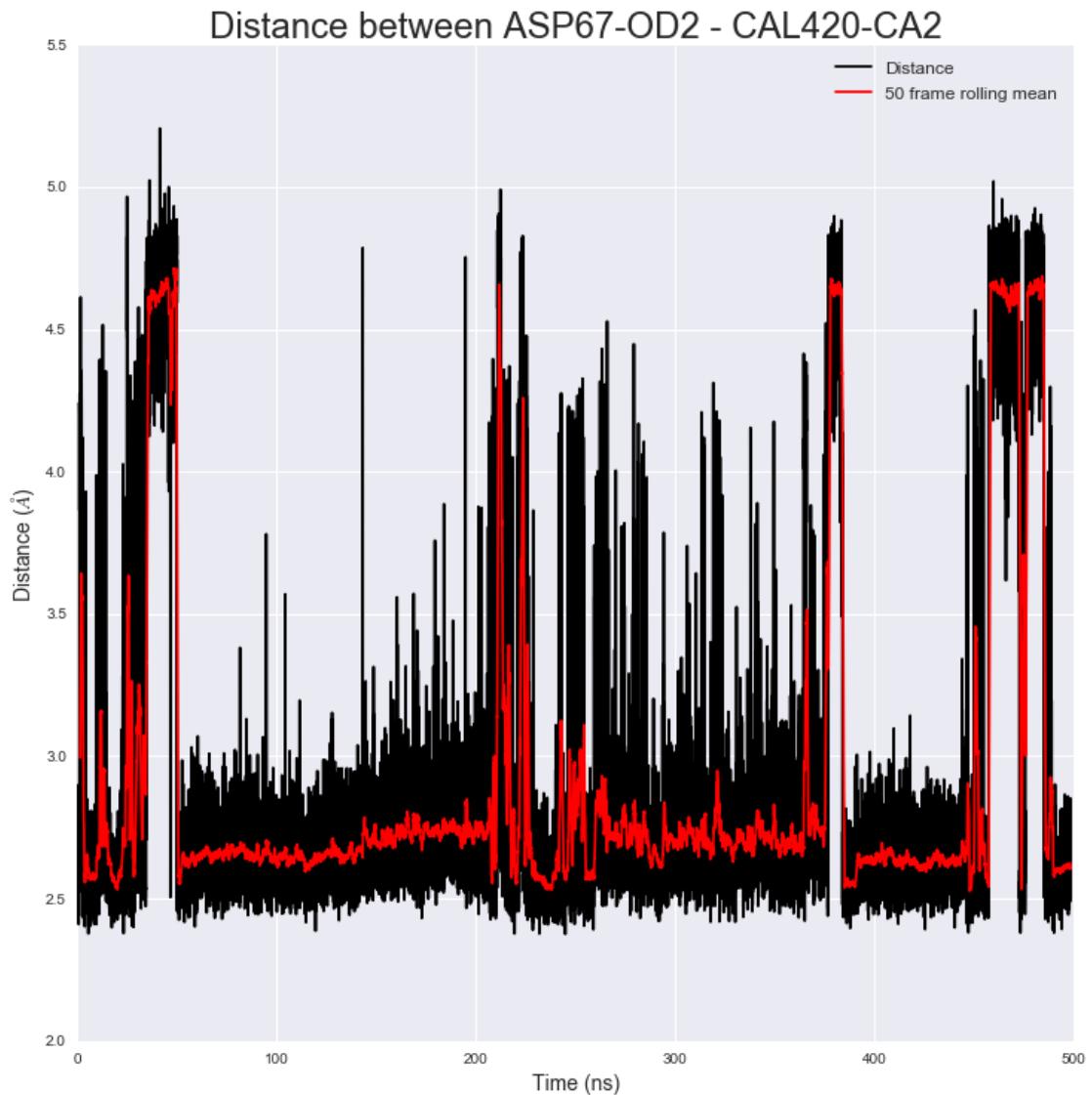
Loading trajectories from the following files:

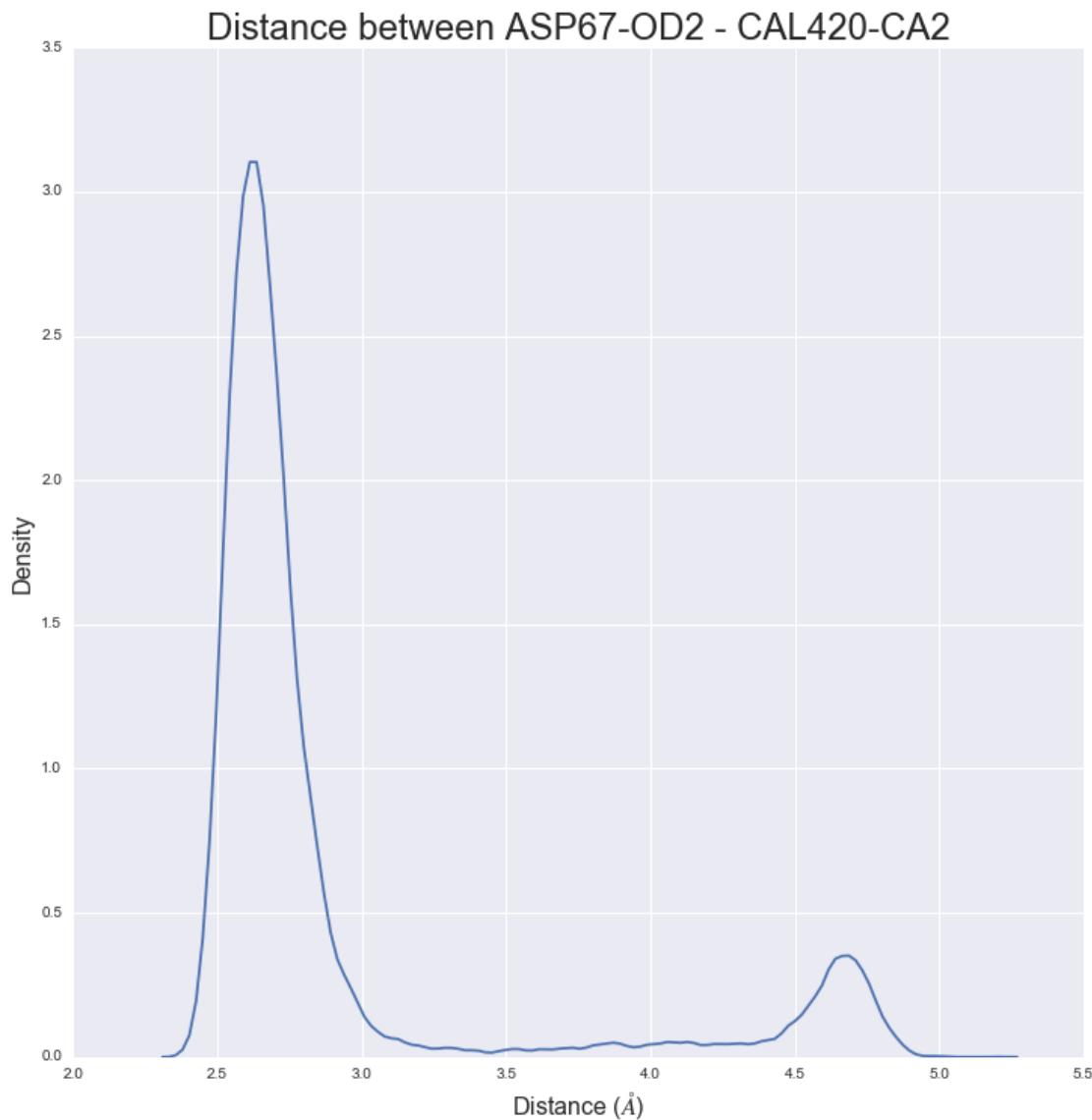
05\_Prod\_troponin\_egcg\_MD3\_000-050\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD3\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD3\_100-150\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD3\_150-200\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_200-250\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_250-300\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_300-350\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_350-400\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_400-450\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_450-500\_run1\_nowater.nc





Total execution time: 36.81 seconds

Total simulation time of all frames: 498.000010986 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1050

Atom2 number: 6810

Calculating distance between following atoms: SER69-OG - CAL420-CA2

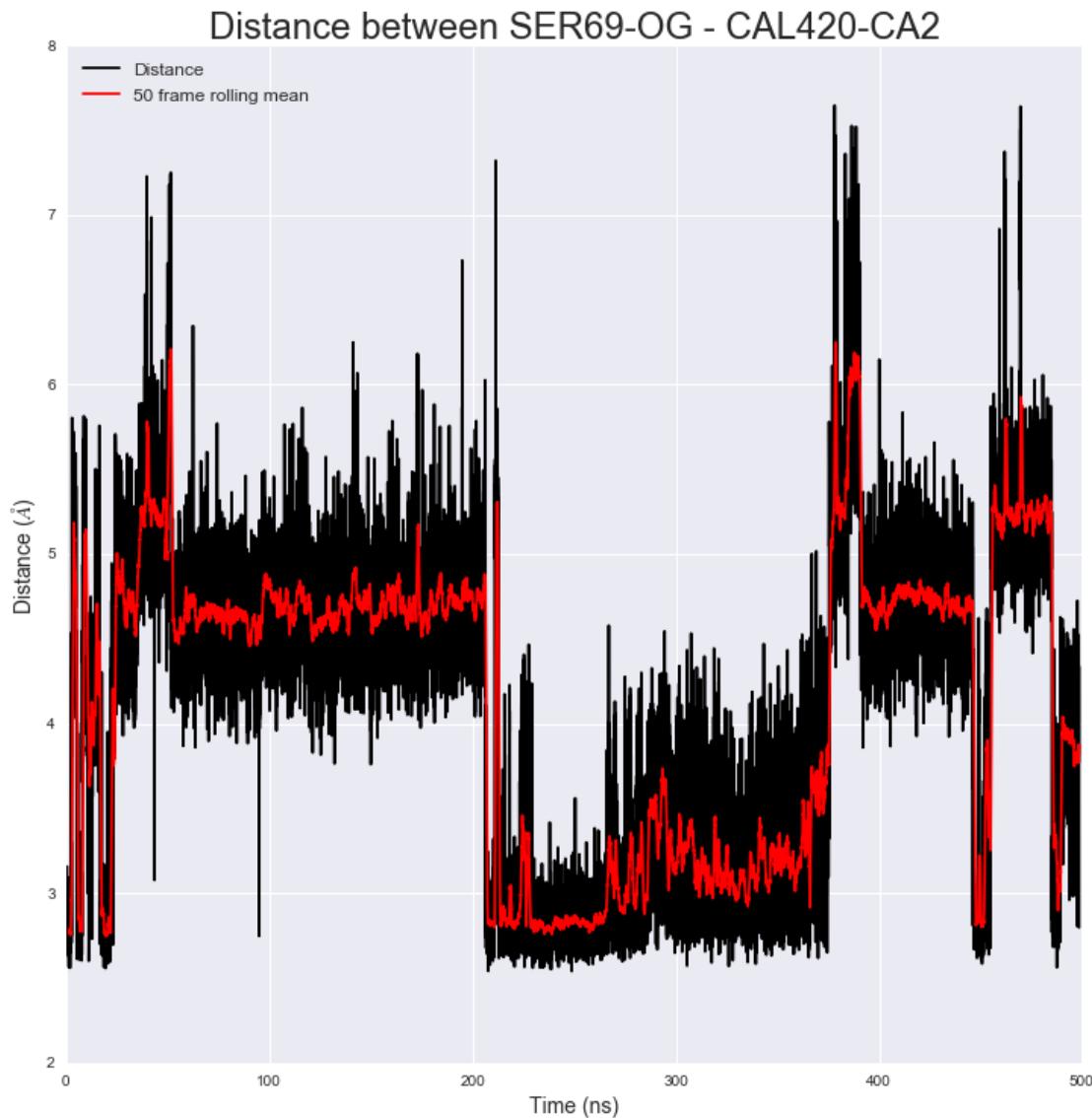
Loading trajectories from the following files:

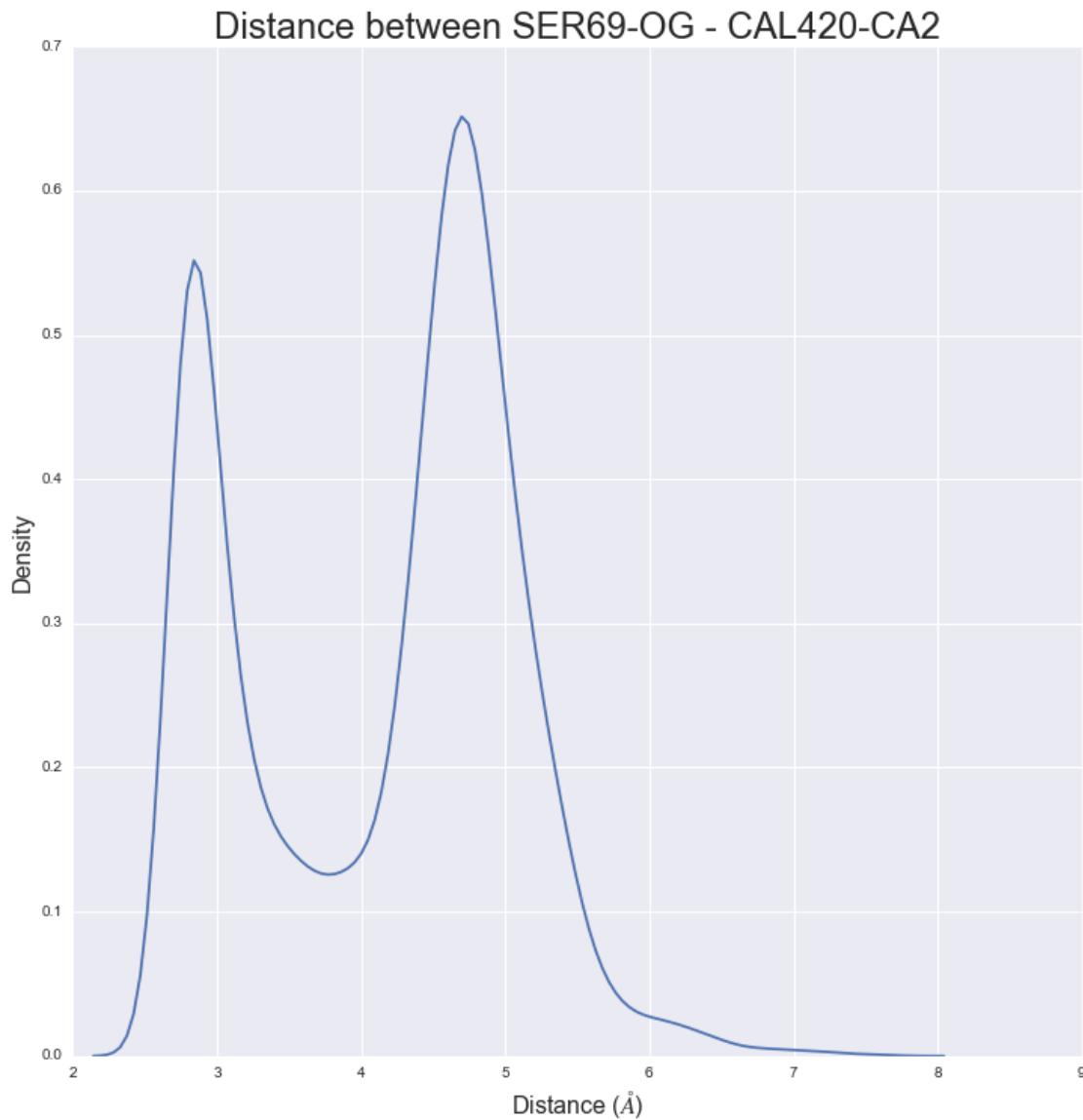
05\_Prod\_troponin\_egcg\_MD3\_000-050\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD3\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD3\_100-150\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD3\_150-200\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_200-250\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_250-300\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_300-350\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_350-400\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_400-450\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_450-500\_run1\_nowater.nc





Total execution time: 32.54 seconds

Total simulation time of all frames: 498.000010986 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1071

Atom2 number: 6810

Calculating distance between following atoms: THR71-OG1 - CAL420-CA2

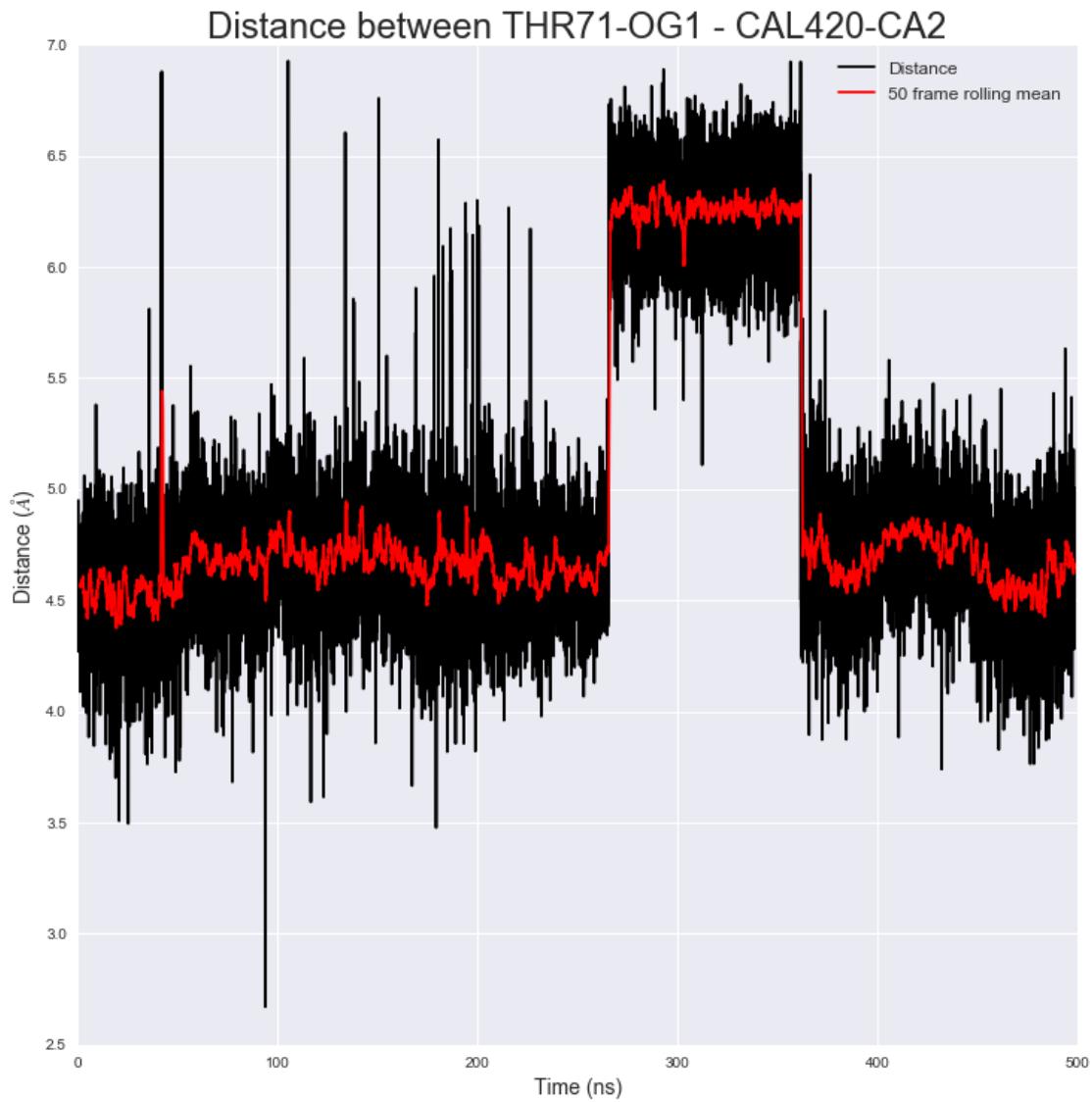
Loading trajectories from the following files:

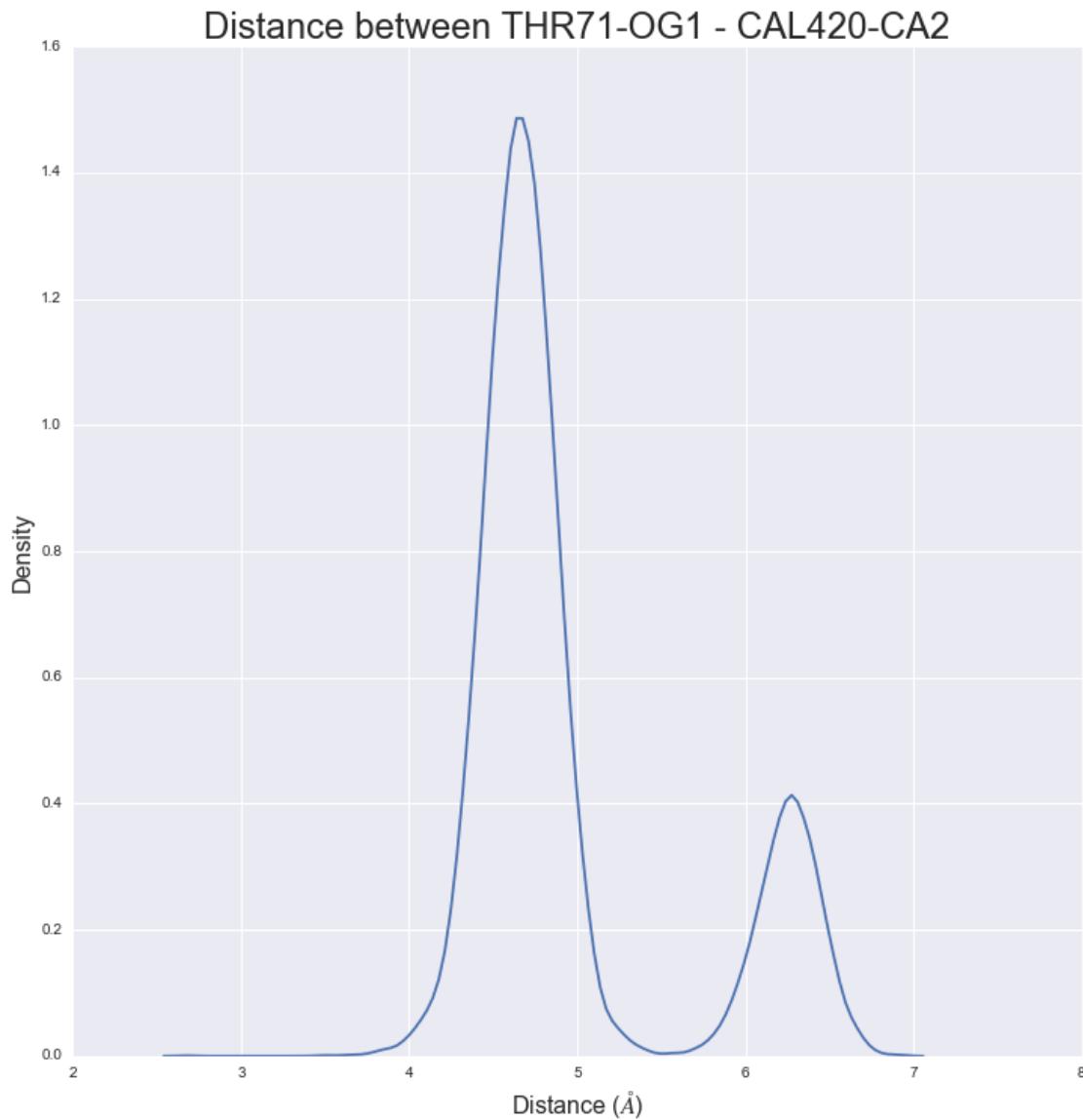
05\_Prod\_troponin\_egcg\_MD3\_000-050\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD3\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD3\_100-150\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD3\_150-200\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_200-250\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_250-300\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_300-350\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_350-400\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_400-450\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_450-500\_run1\_nowater.nc





Total execution time: 33.03 seconds

Total simulation time of all frames: 498.000010986 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1099

Atom2 number: 6810

Calculating distance between following atoms: ASP73-OD1 - CAL420-CA2

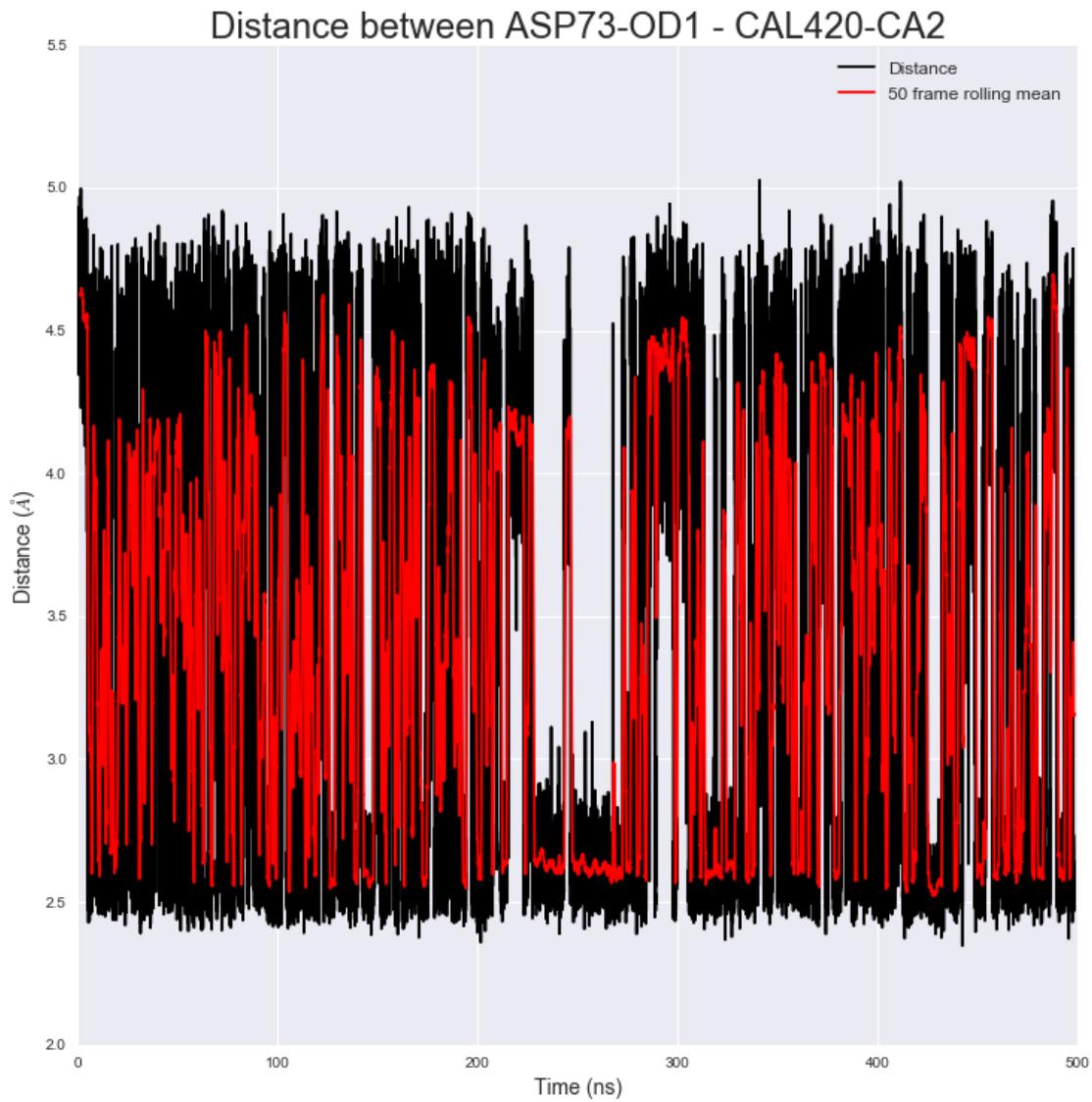
Loading trajectories from the following files:

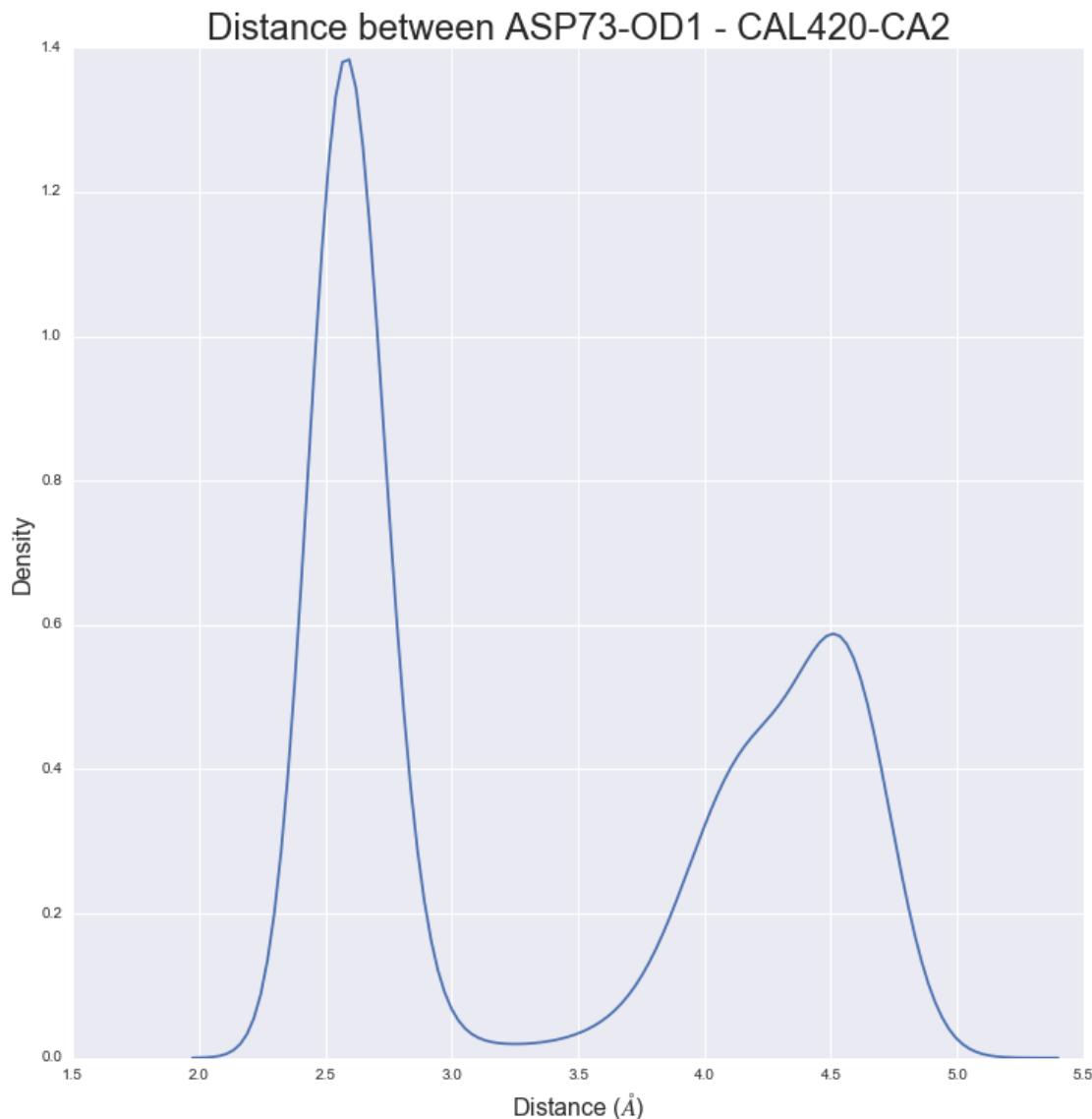
05\_Prod\_troponin\_egcg\_MD3\_000-050\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD3\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD3\_100-150\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD3\_150-200\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_200-250\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_250-300\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_300-350\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_350-400\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_400-450\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_450-500\_run1\_nowater.nc





Total execution time: 31.49 seconds

Total simulation time of all frames: 498.000010986 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1100

Atom2 number: 6810

Calculating distance between following atoms: ASP73-OD2 - CAL420-CA2

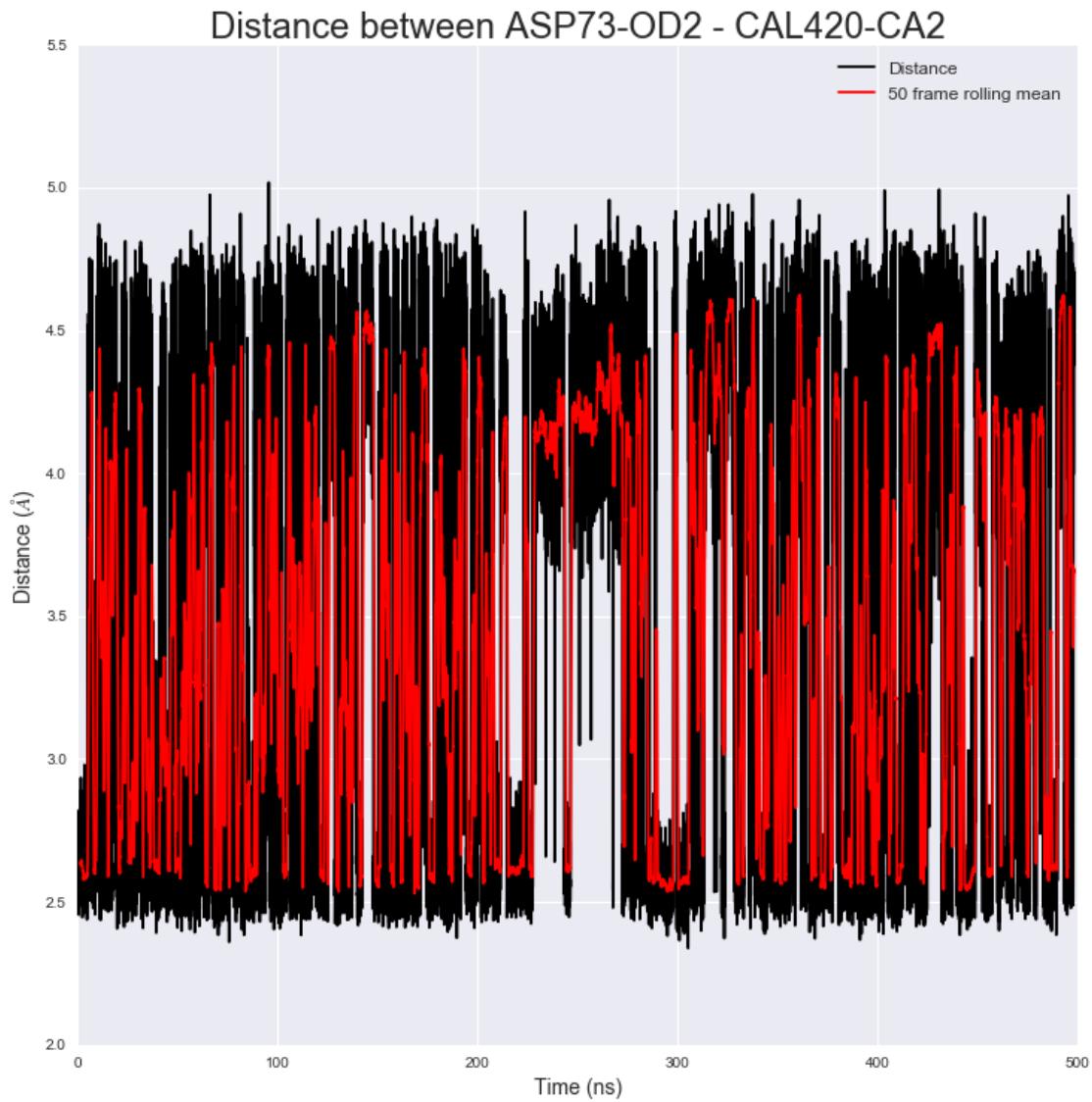
Loading trajectories from the following files:

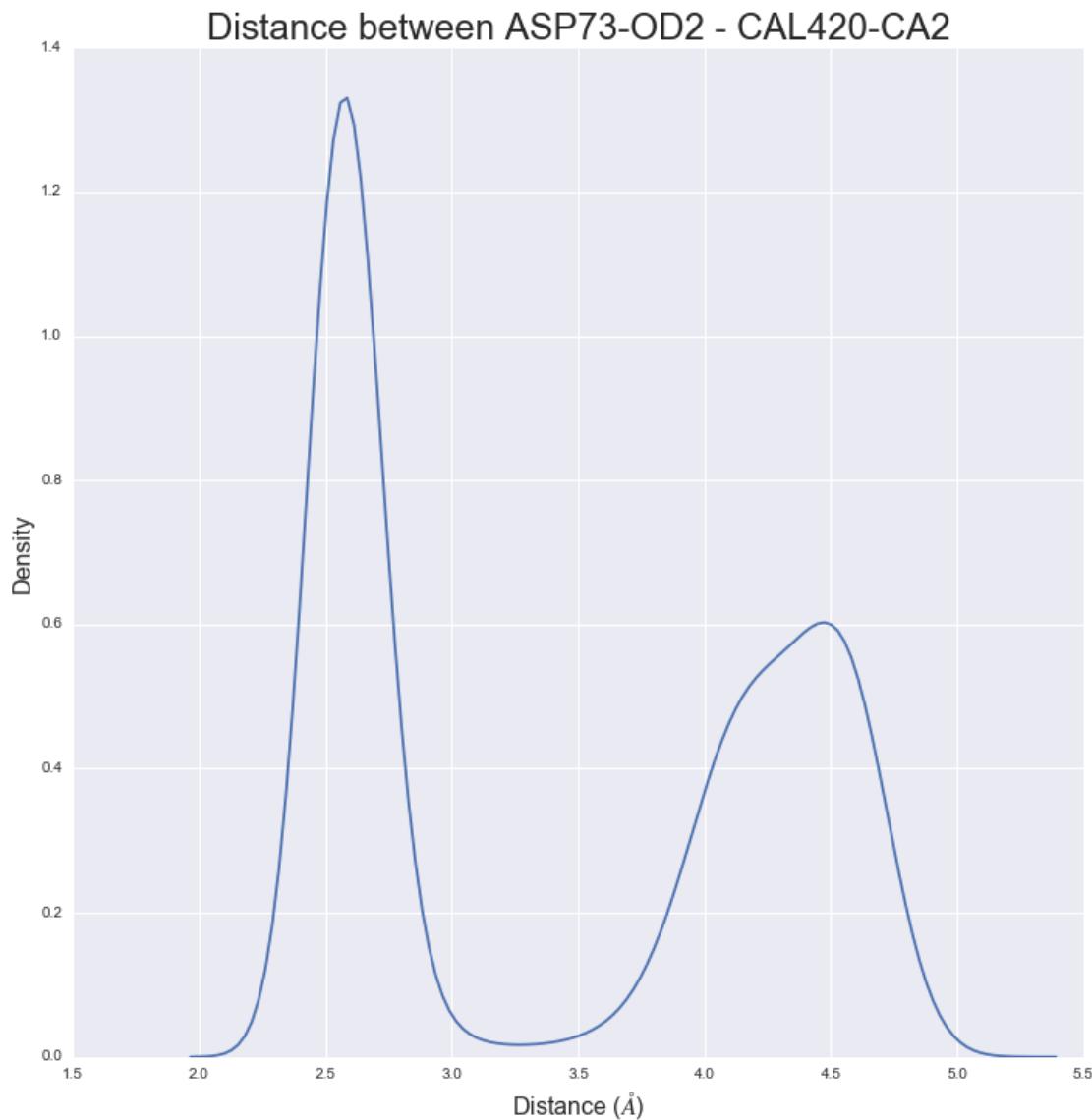
05\_Prod\_troponin\_egcg\_MD3\_000-050\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD3\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD3\_100-150\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD3\_150-200\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_200-250\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_250-300\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_300-350\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_350-400\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_400-450\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_450-500\_run1\_nowater.nc





Total execution time: 28.70 seconds

Total simulation time of all frames: 498.000010986 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1131

Atom2 number: 6810

Calculating distance between following atoms: ASP75-OD1 - CAL420-CA2

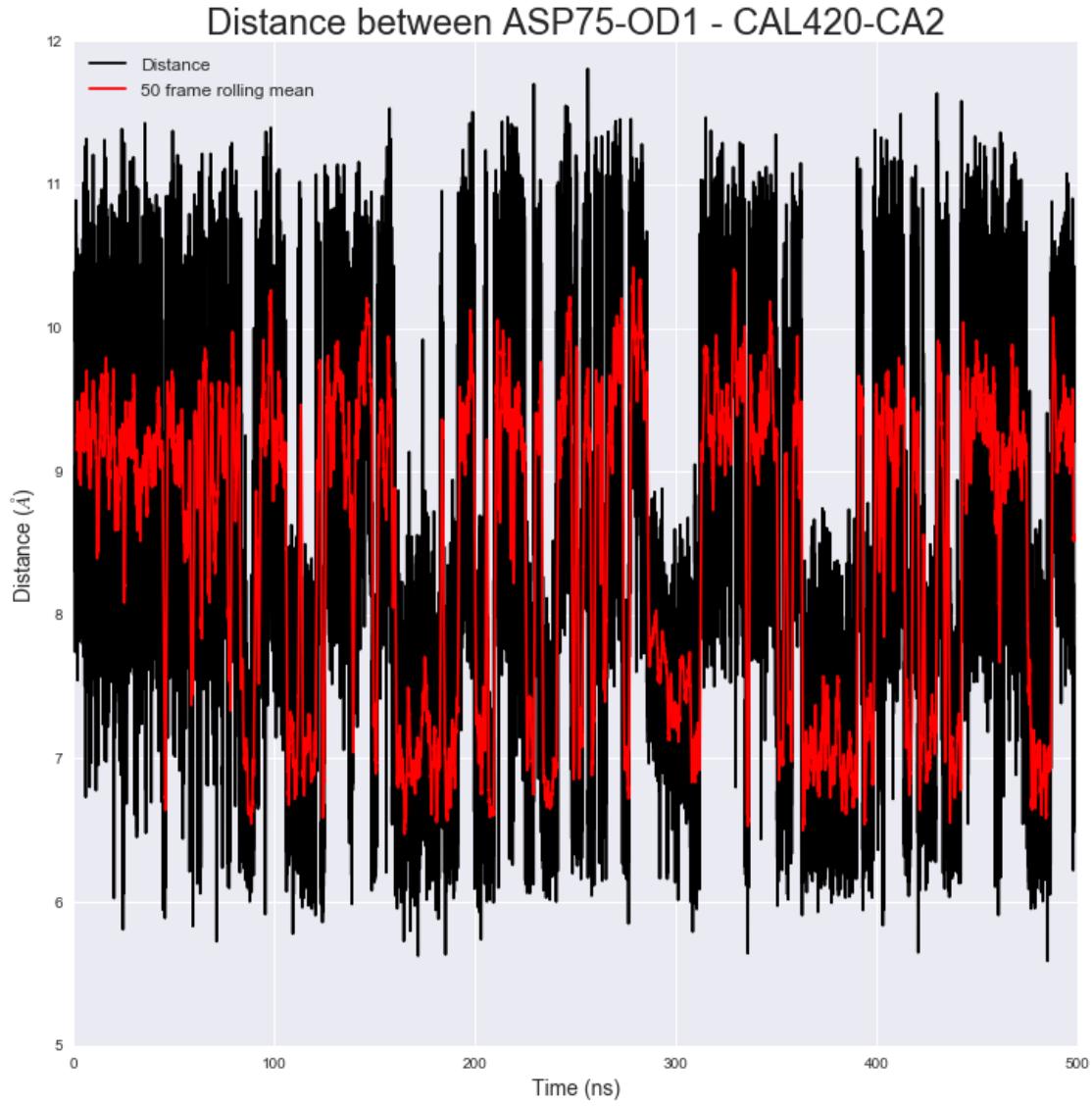
Loading trajectories from the following files:

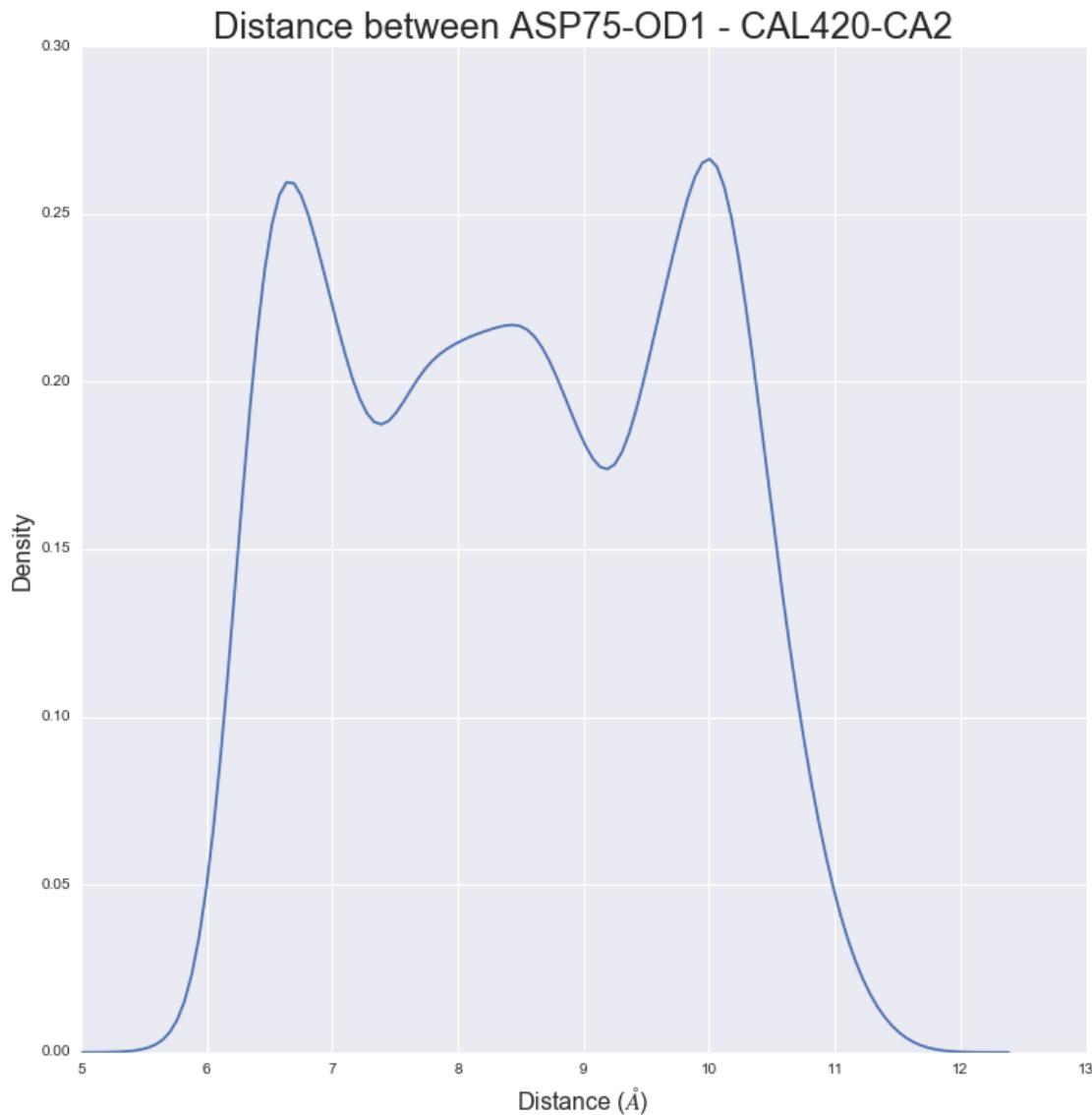
05\_Prod\_troponin\_egcg\_MD3\_000-050\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD3\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD3\_100-150\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD3\_150-200\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_200-250\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_250-300\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_300-350\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_350-400\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_400-450\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_450-500\_run1\_nowater.nc





Total execution time: 39.34 seconds

Total simulation time of all frames: 498.000010986 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1132

Atom2 number: 6810

Calculating distance between following atoms: ASP75-OD2 - CAL420-CA2

Loading trajectories from the following files:

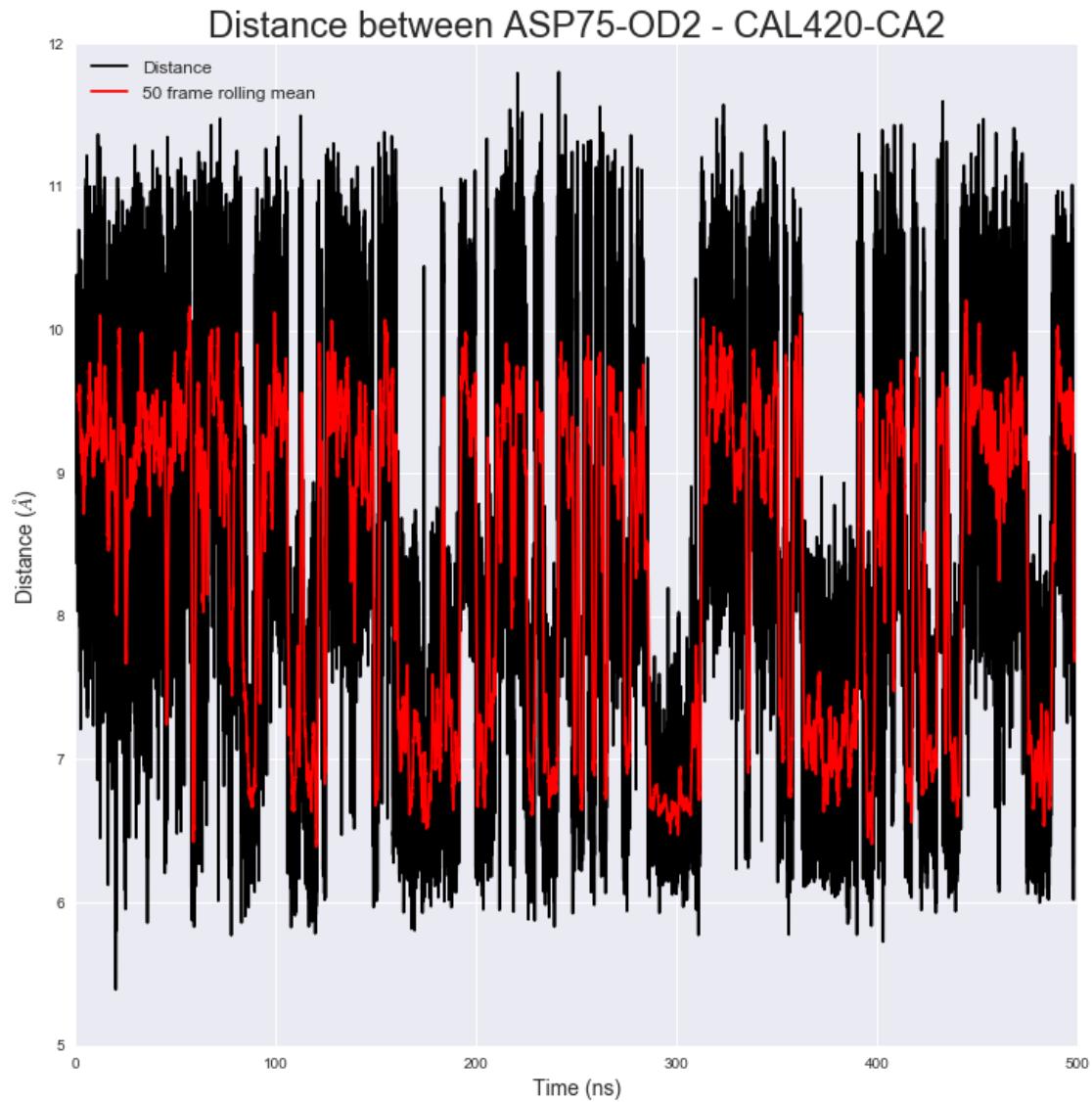
05\_Prod\_troponin\_egcg\_MD3\_000-050\_run1\_nowater.nc

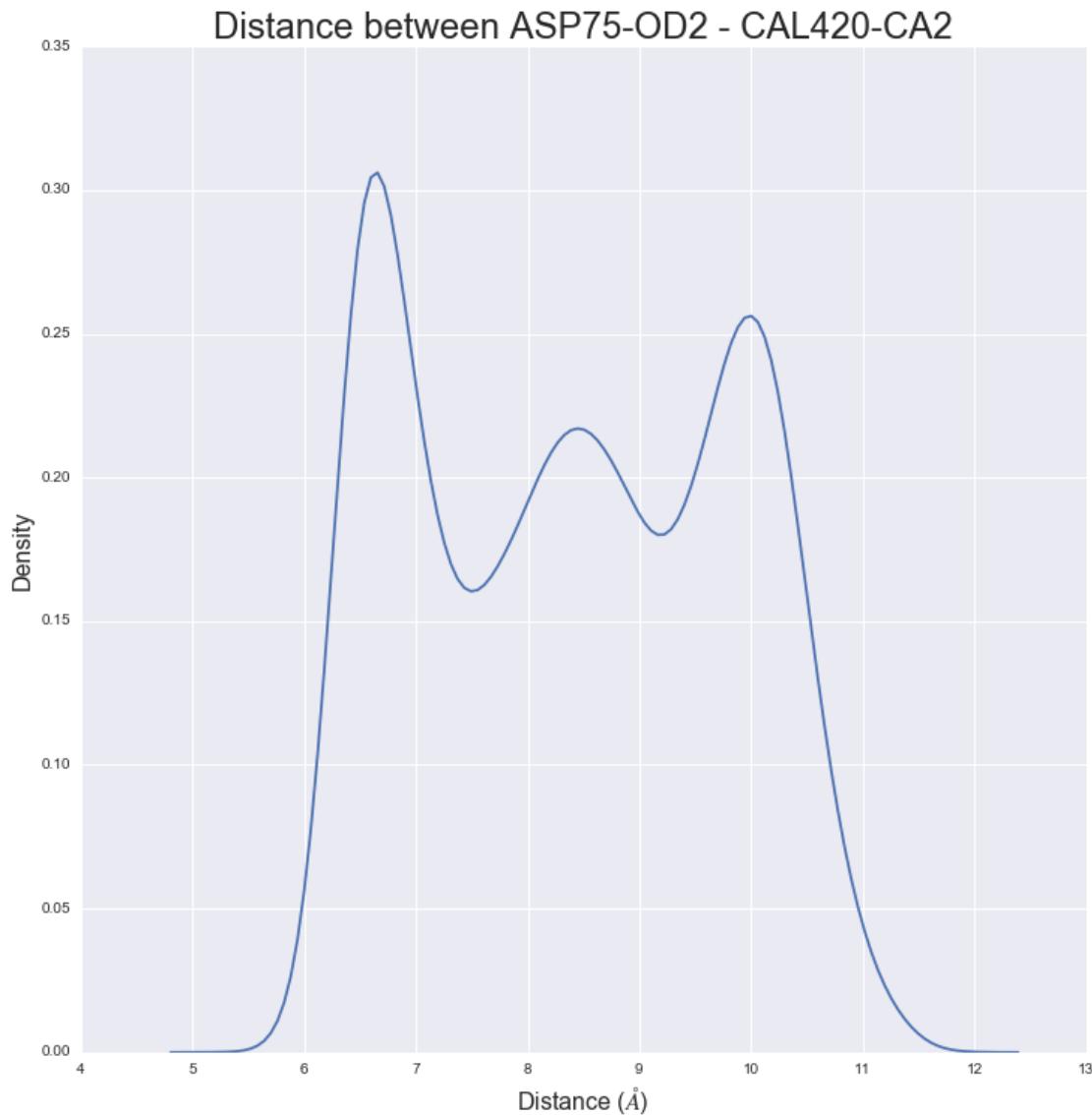
05\_Prod\_troponin\_egcg\_MD3\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD3\_100-150\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD3\_150-200\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD3\_200-250\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_250-300\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_300-350\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_350-400\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_400-450\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_450-500\_run1\_nowater.nc





Total execution time: 38.58 seconds

Total simulation time of all frames: 498.000010986 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1146

Atom2 number: 6810

Calculating distance between following atoms: GLU76-OE1 - CAL420-CA2

Loading trajectories from the following files:

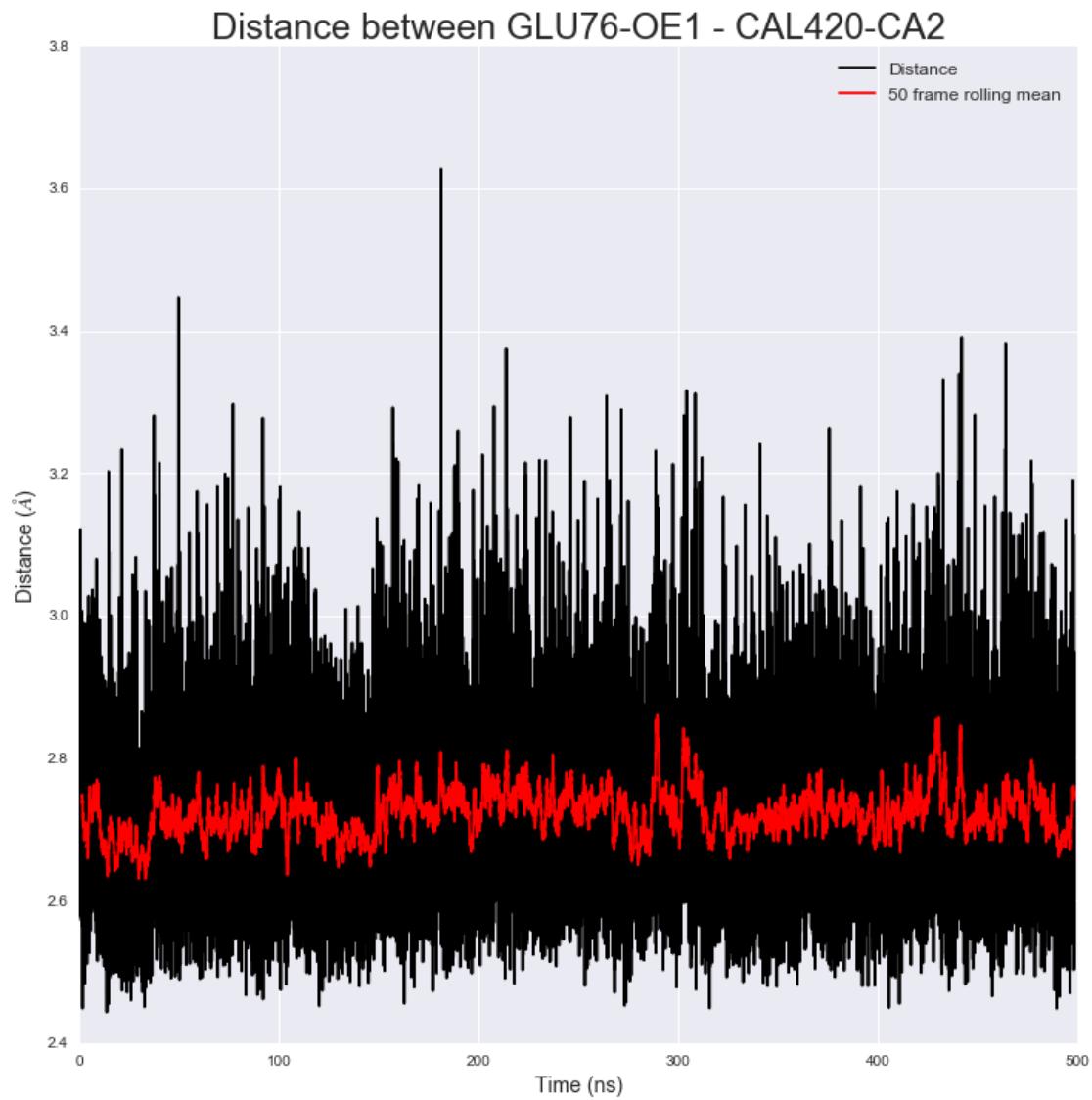
05\_Prod\_troponin\_egcg\_MD3\_000-050\_run1\_nowater.nc

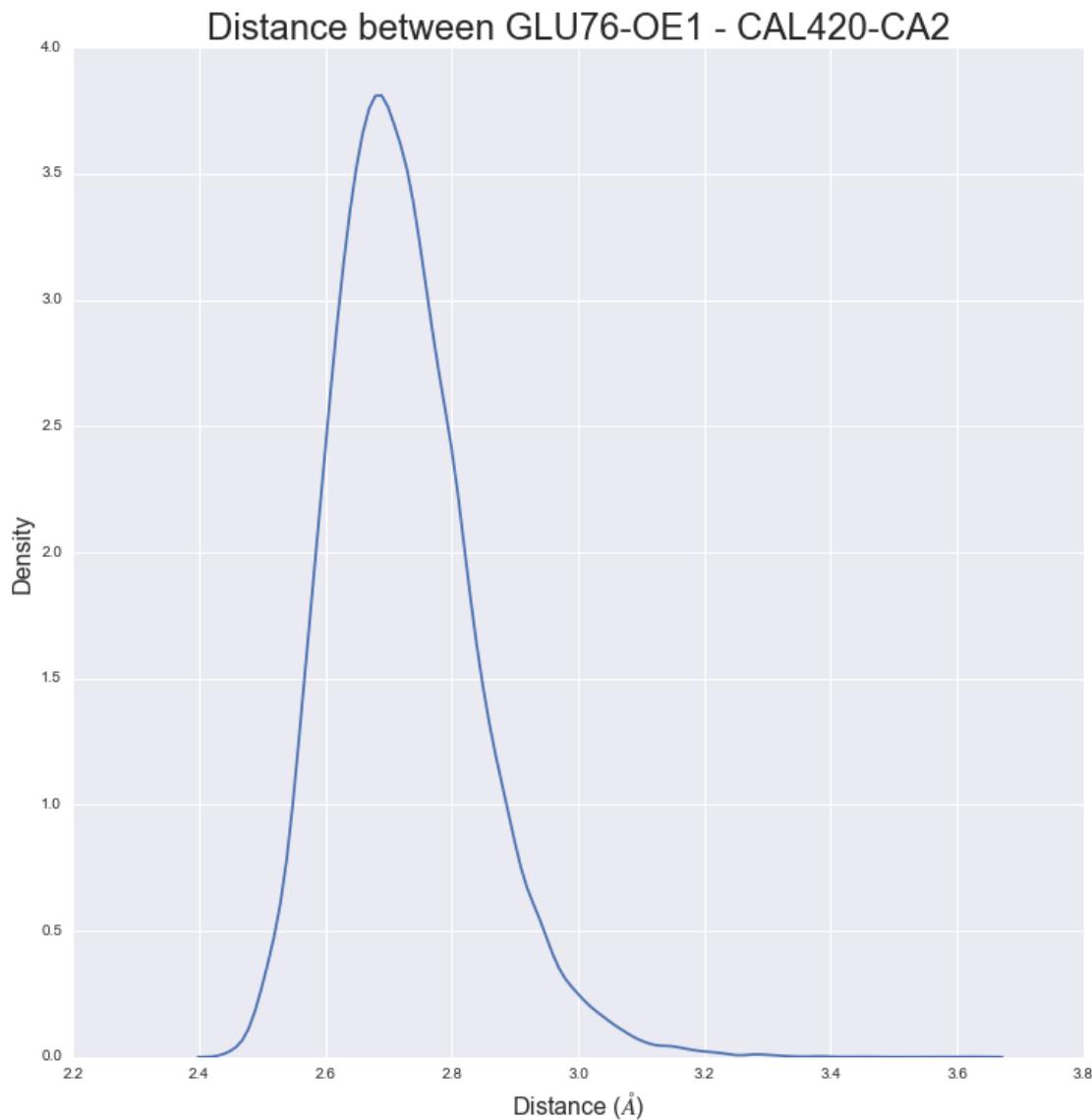
05\_Prod\_troponin\_egcg\_MD3\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD3\_100-150\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD3\_150-200\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD3\_200-250\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_250-300\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_300-350\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_350-400\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_400-450\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_450-500\_run1\_nowater.nc





Total execution time: 39.44 seconds

Total simulation time of all frames: 498.000010986 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1147

Atom2 number: 6810

Calculating distance between following atoms: GLU76-OE2 - CAL420-CA2

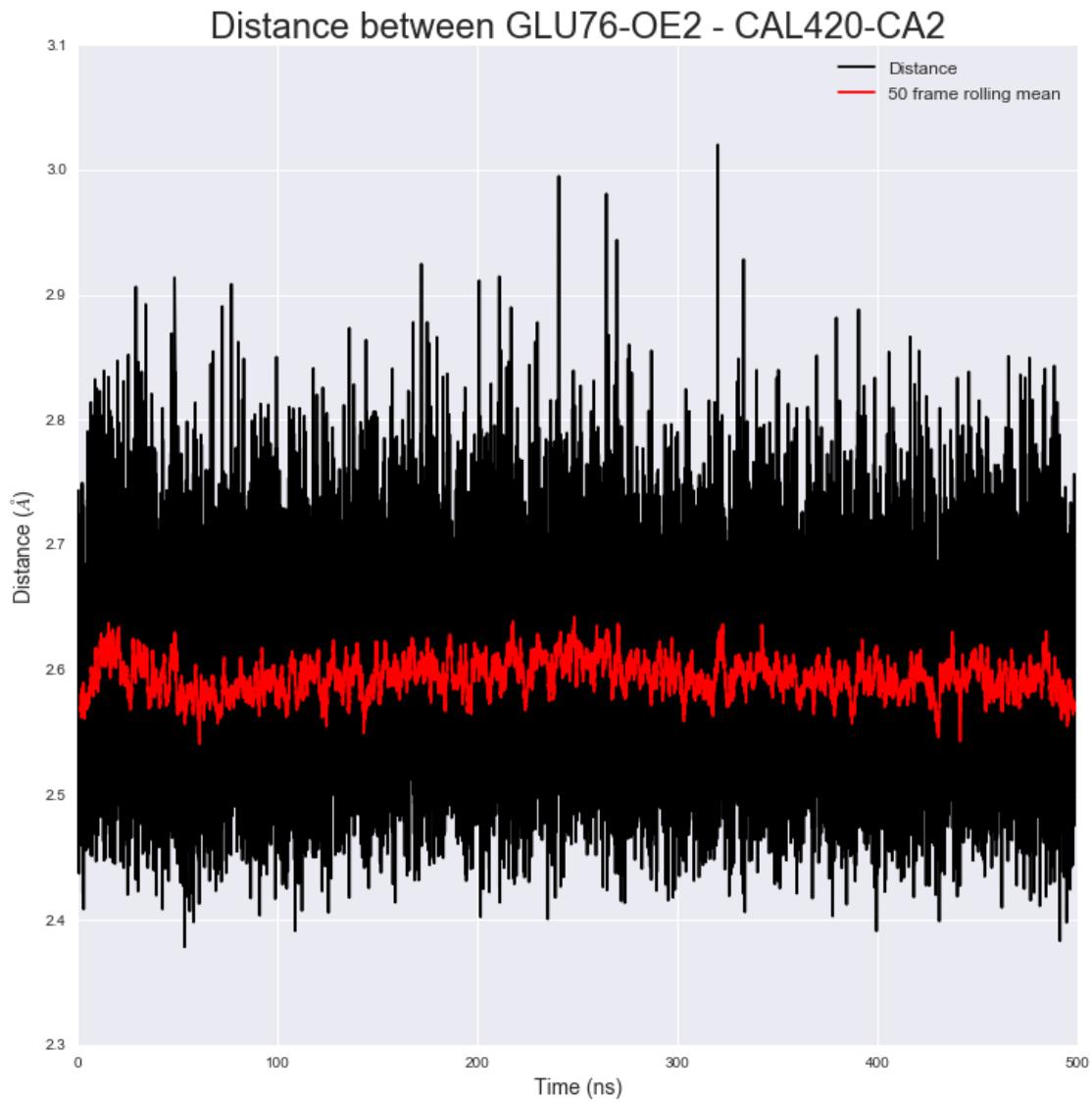
Loading trajectories from the following files:

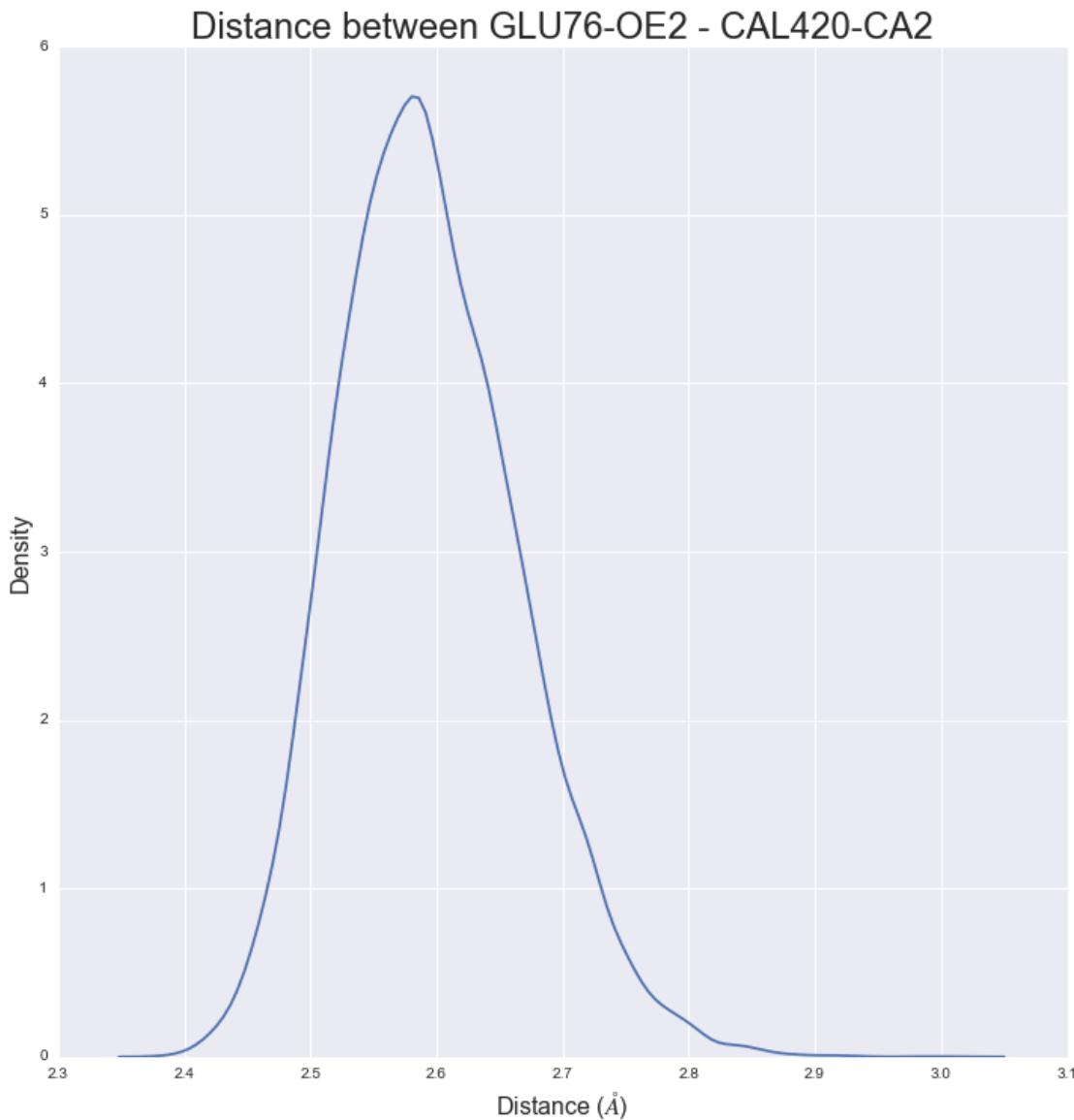
05\_Prod\_troponin\_egcg\_MD3\_000-050\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD3\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD3\_100-150\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD3\_150-200\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_200-250\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_250-300\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_300-350\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_350-400\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_400-450\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD3\_450-500\_run1\_nowater.nc





Total execution time: 24.84 seconds

Total simulation time of all frames: 498.000010986 nanoseconds

#### 0.4 MD4

```
In [11]: topology_MD4 = '/Users/gil_f.hoben/Troponin_md_processed/MD4/run1/troponin_egcg_MD4_nowater.prmtop'
         trajectory_MD4 = '/Users/gil_f.hoben/Troponin_md_processed/MD4/run1/Trajectories/'
```

```
In [12]: for atom1 in atom1_list:
            main(topology_MD4, trajectory_MD4, atom1, atom2, verbose = 1)
```

The following topology file was successfully loaded:  
 <mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1005

Atom2 number: 6810

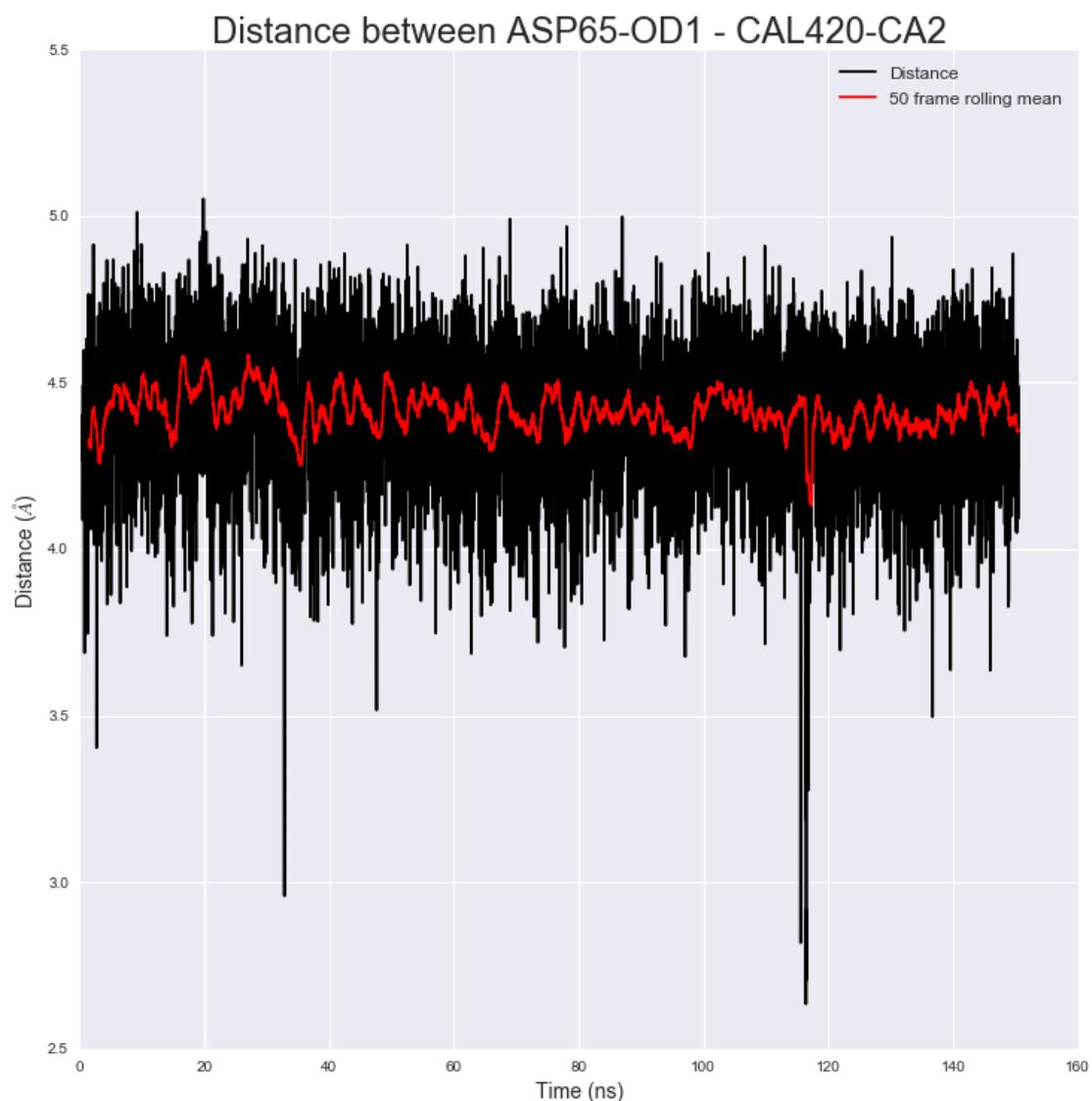
Calculating distance between following atoms: ASP65-OD1 - CAL420-CA2

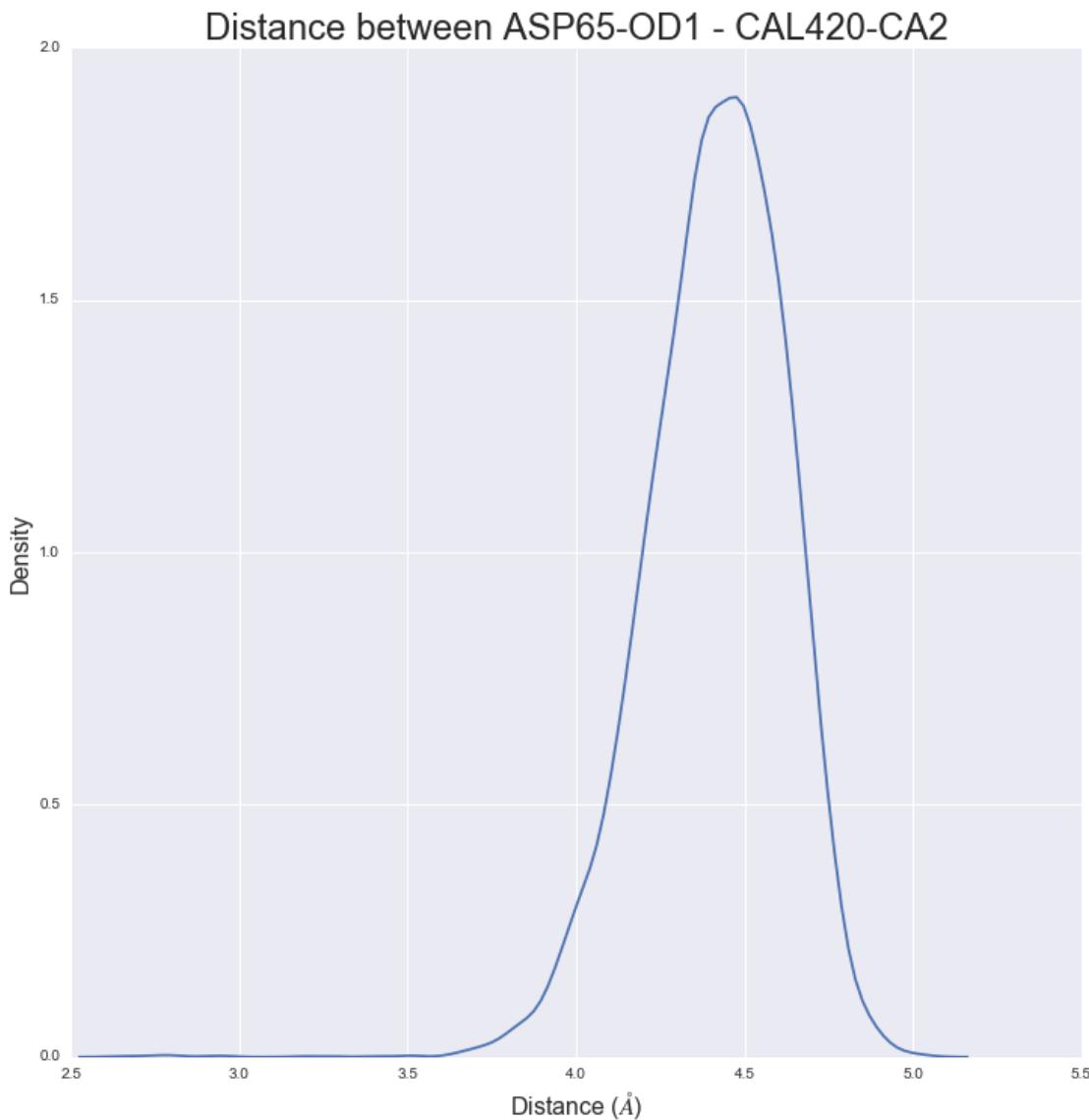
Loading trajectories from the following files:

05\_Prod\_troponin\_egcg\_MD4\_000-050\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD4\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD4\_100-150\_run1\_nowater.nc





Total execution time: 3.21 seconds

Total simulation time of all frames: 149.999995728 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1005

Atom2 number: 6810

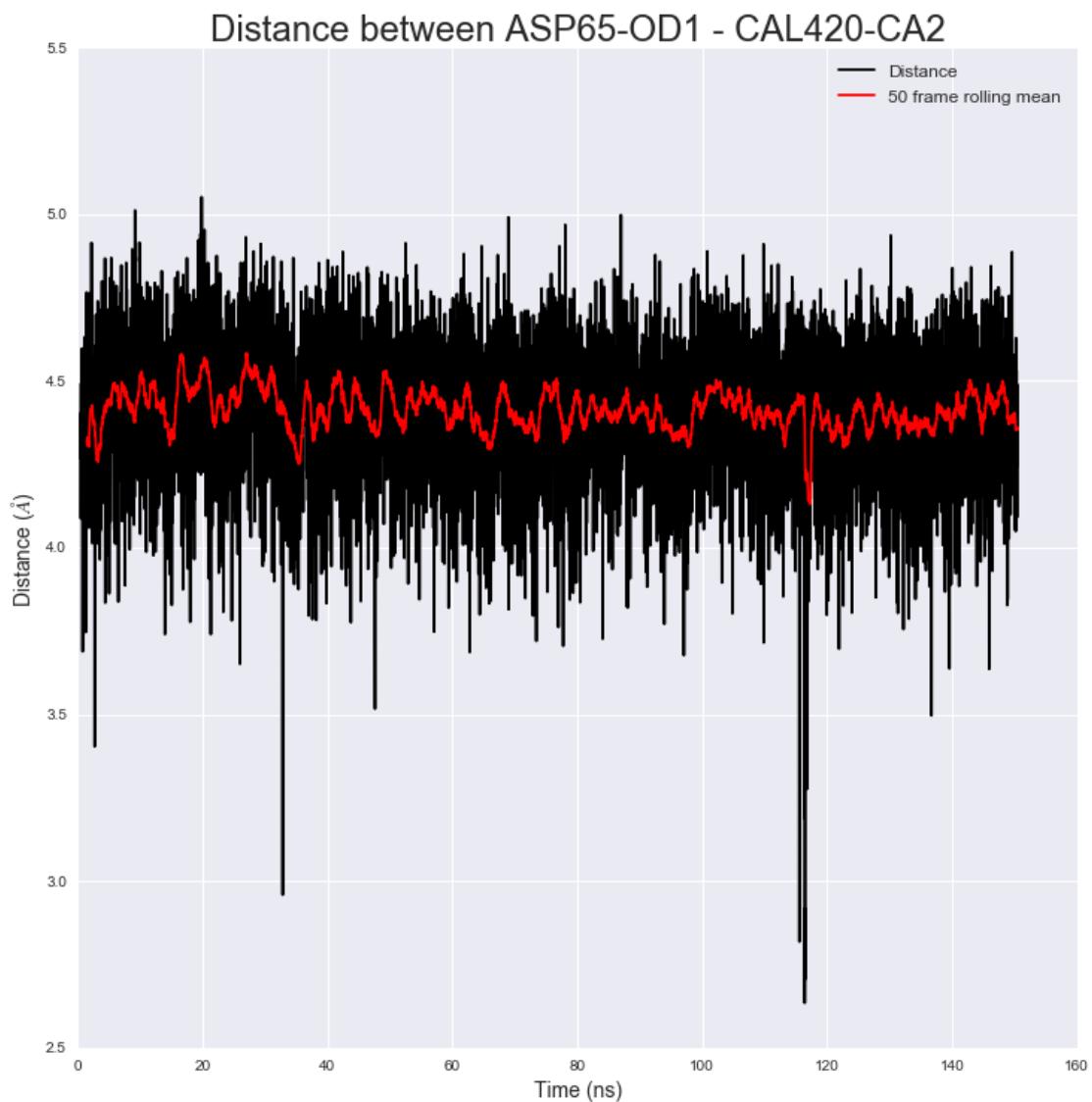
Calculating distance between following atoms: ASP65-OD1 - CAL420-CA2

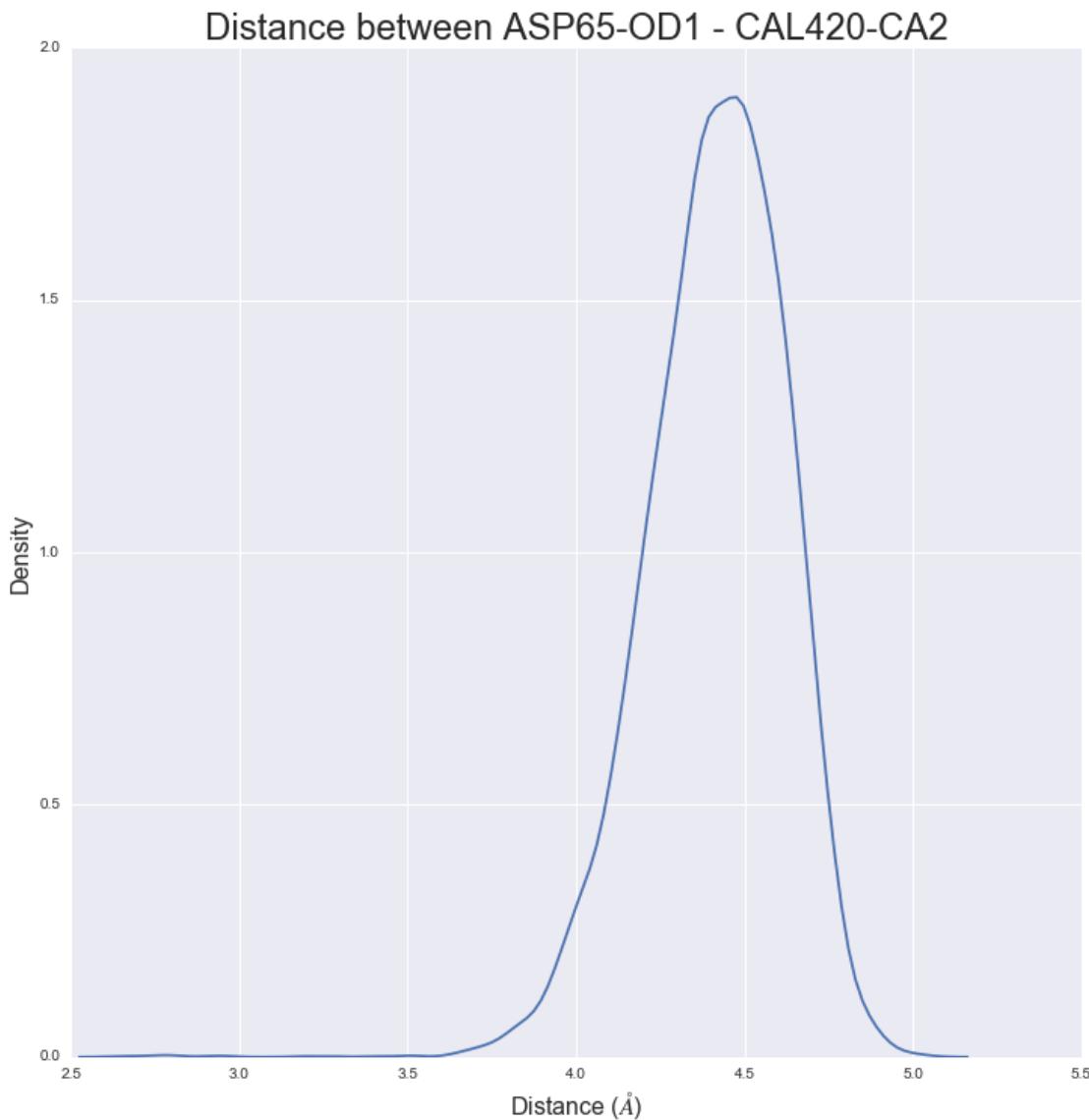
Loading trajectories from the following files:

05\_Prod\_troponin\_egcg\_MD4\_000-050\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD4\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD4\_100-150\_run1\_nowater.nc





Total execution time: 2.07 seconds

Total simulation time of all frames: 149.999995728 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1020

Atom2 number: 6810

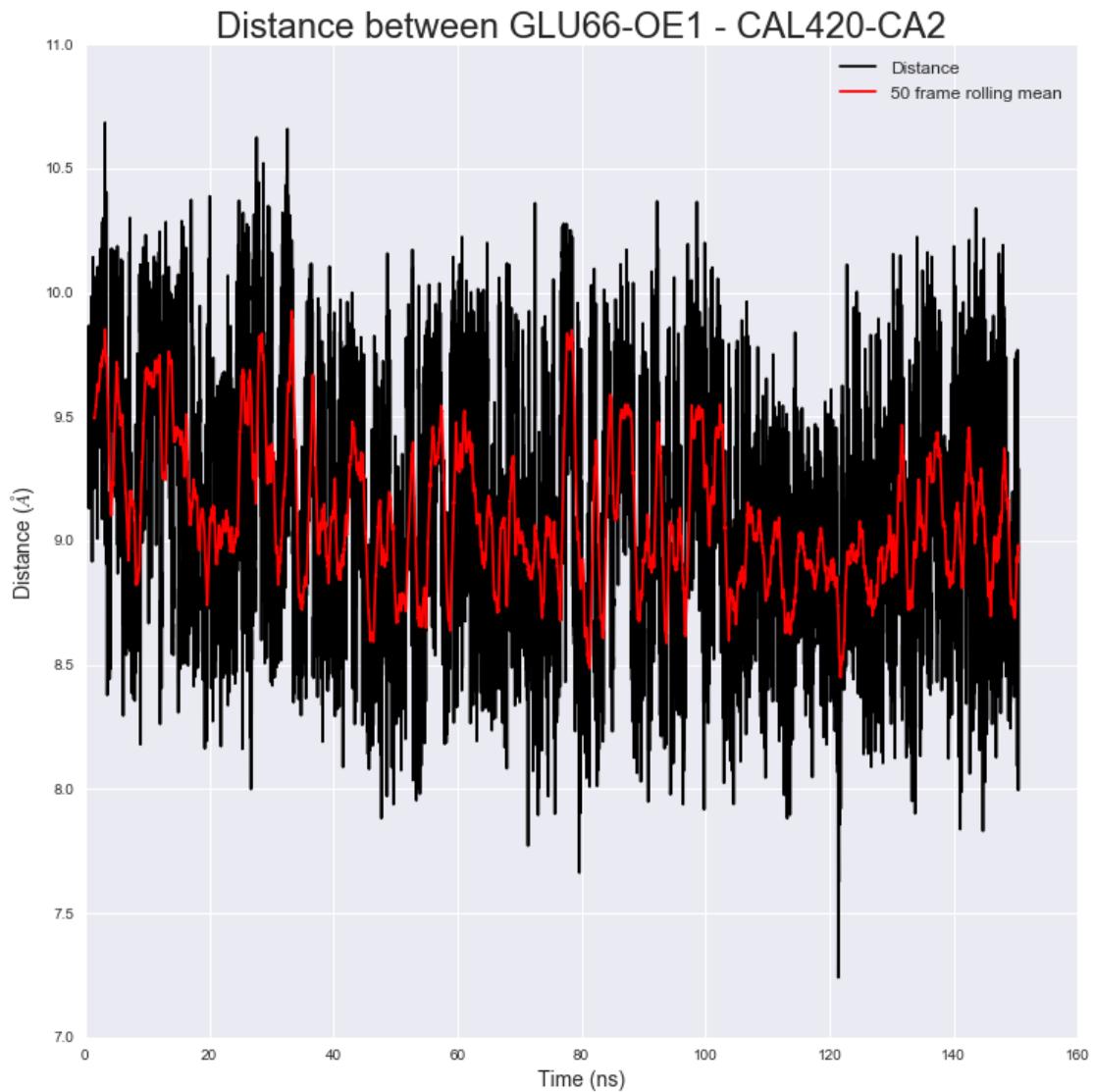
Calculating distance between following atoms: GLU66-OE1 - CAL420-CA2

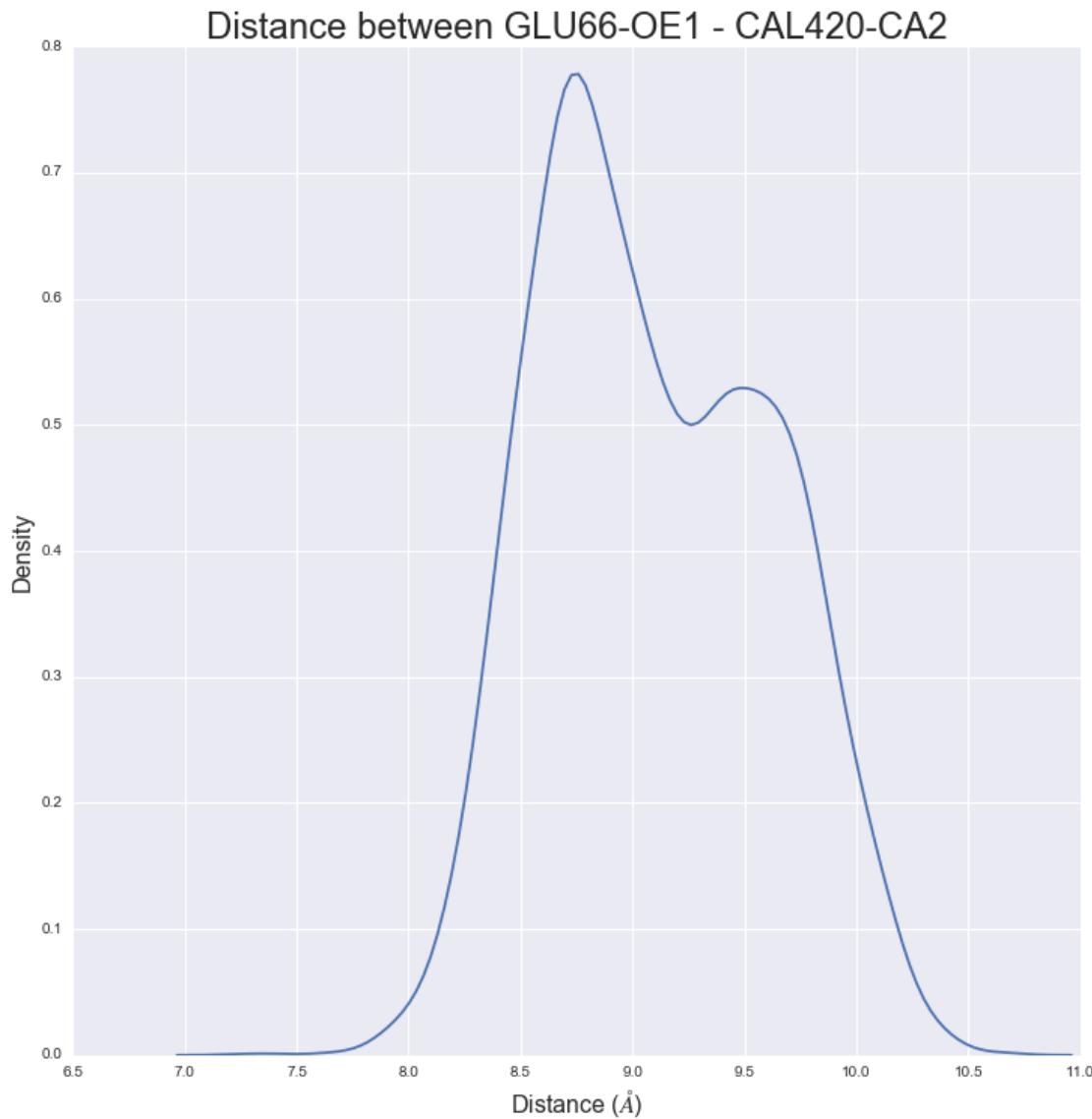
Loading trajectories from the following files:

05\_Prod\_troponin\_egcg\_MD4\_000-050\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD4\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD4\_100-150\_run1\_nowater.nc





Total execution time: 2.39 seconds

Total simulation time of all frames: 149.999995728 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1021

Atom2 number: 6810

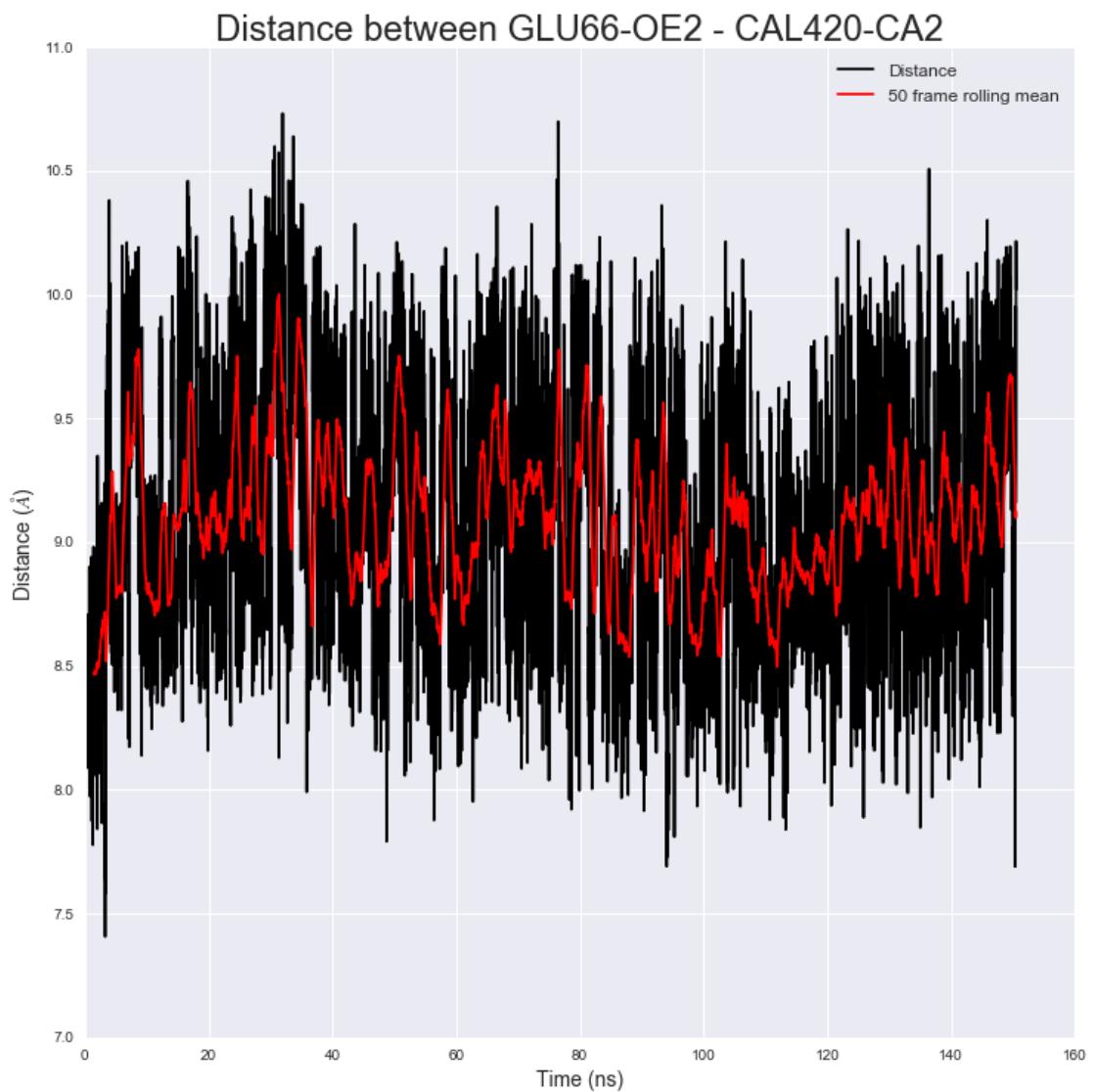
Calculating distance between following atoms: GLU66-OE2 - CAL420-CA2

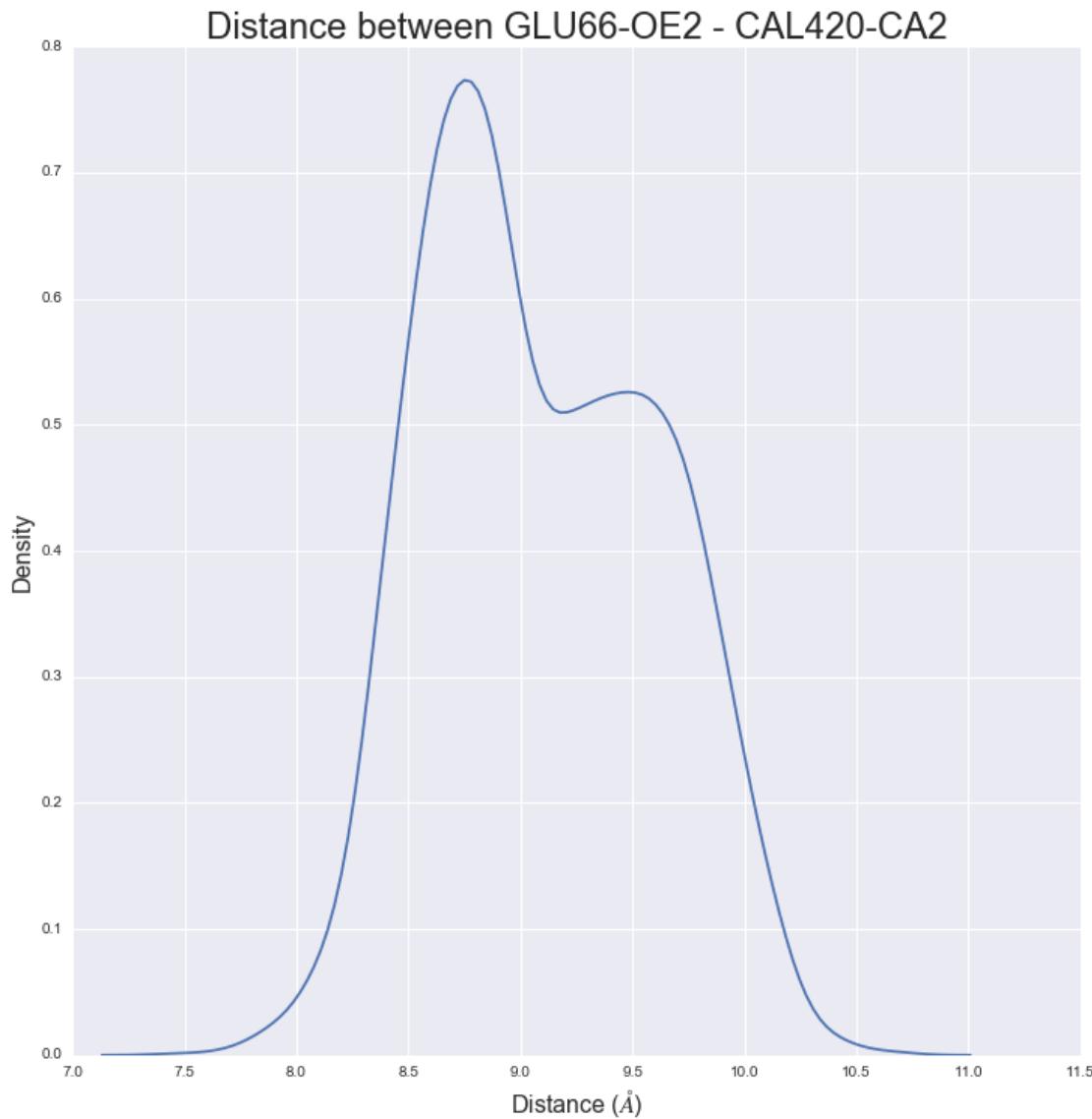
Loading trajectories from the following files:

05\_Prod\_troponin\_egcg\_MD4\_000-050\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD4\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD4\_100-150\_run1\_nowater.nc





Total execution time: 2.20 seconds

Total simulation time of all frames: 149.999995728 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1032

Atom2 number: 6810

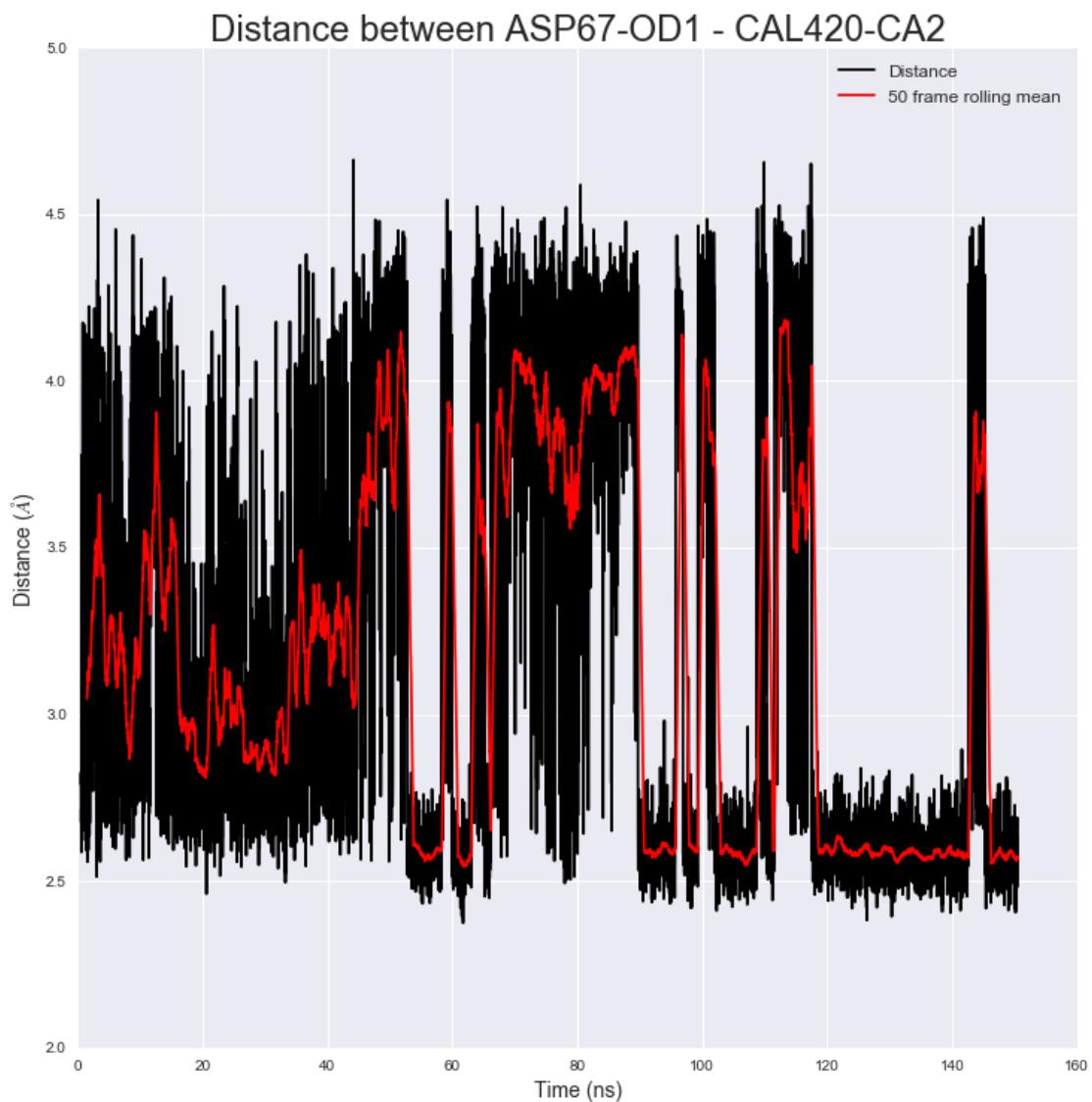
Calculating distance between following atoms: ASP67-OD1 - CAL420-CA2

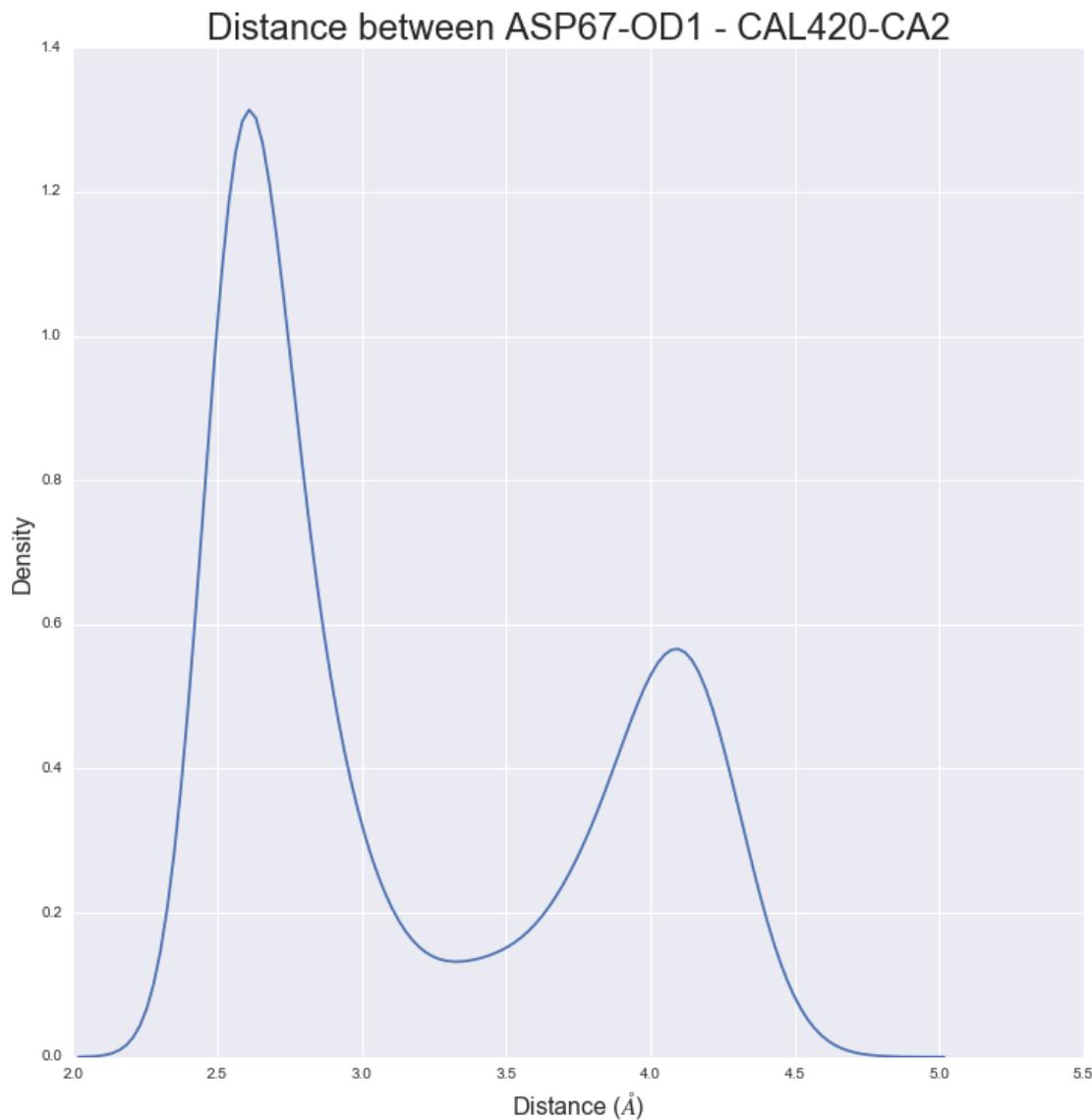
Loading trajectories from the following files:

05\_Prod\_troponin\_egcg\_MD4\_000-050\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD4\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD4\_100-150\_run1\_nowater.nc





Total execution time: 2.16 seconds

Total simulation time of all frames: 149.999995728 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1033

Atom2 number: 6810

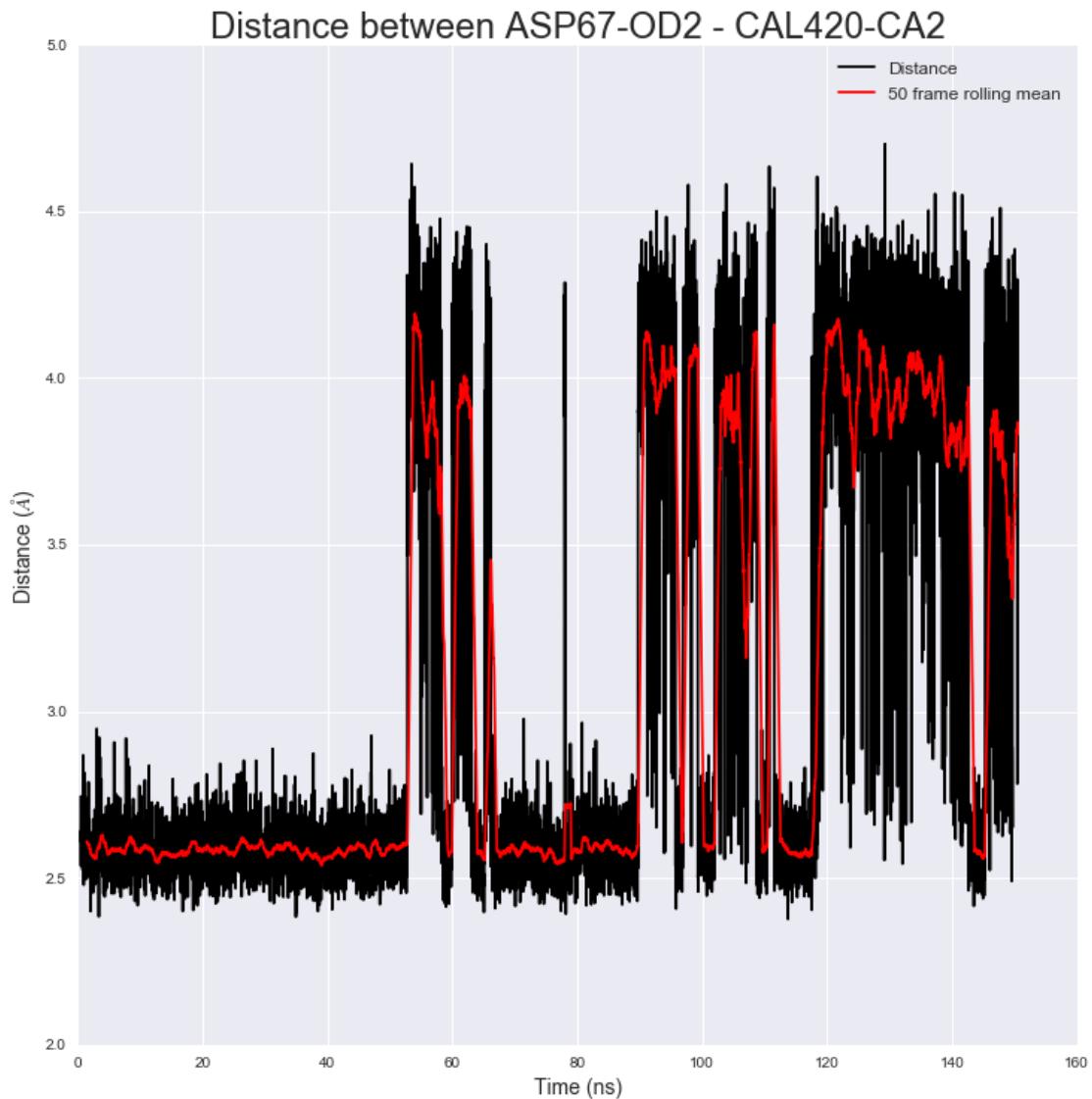
Calculating distance between following atoms: ASP67-OD2 - CAL420-CA2

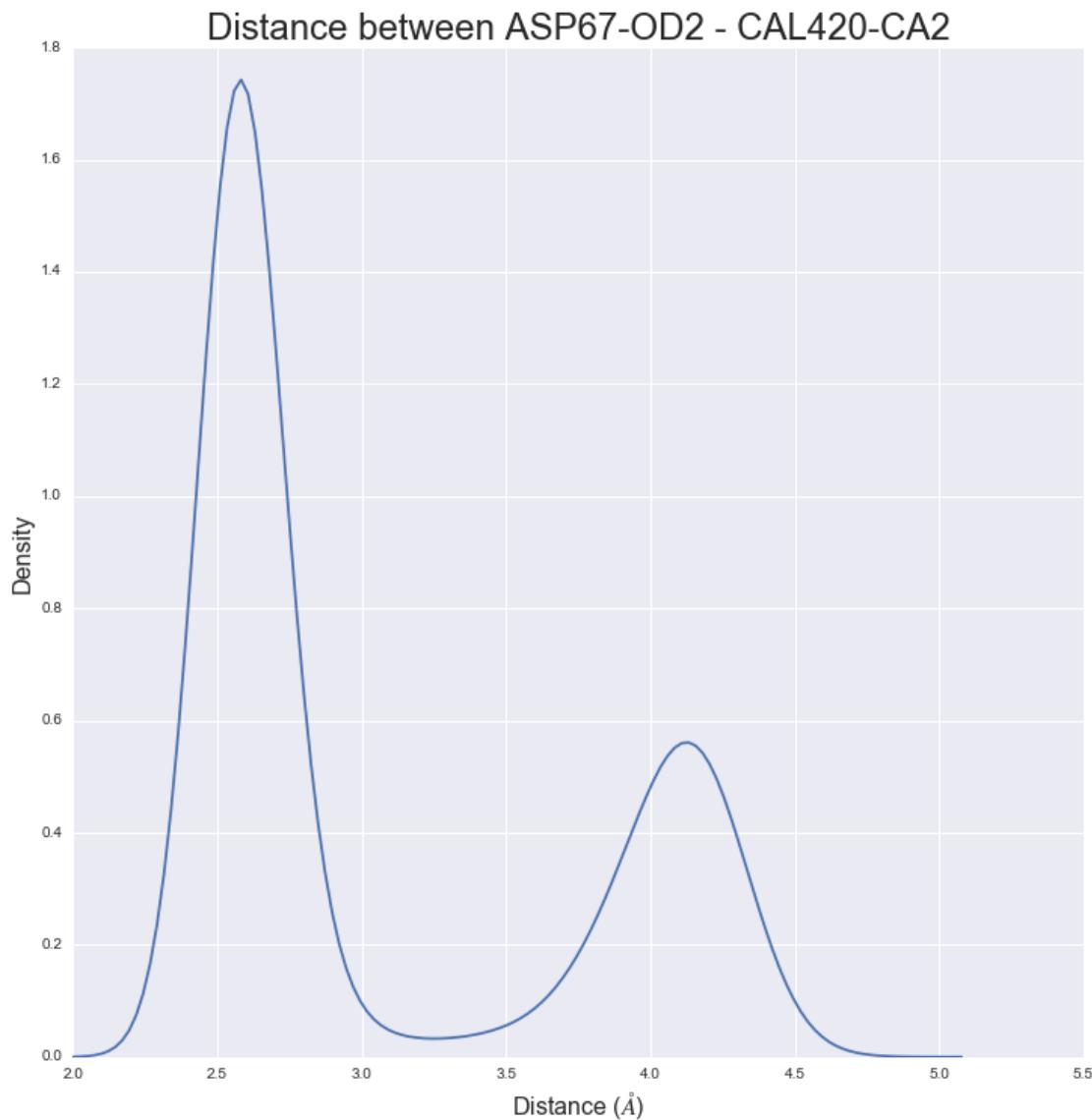
Loading trajectories from the following files:

05\_Prod\_troponin\_egcg\_MD4\_000-050\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD4\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD4\_100-150\_run1\_nowater.nc





Total execution time: 2.47 seconds

Total simulation time of all frames: 149.999995728 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1050

Atom2 number: 6810

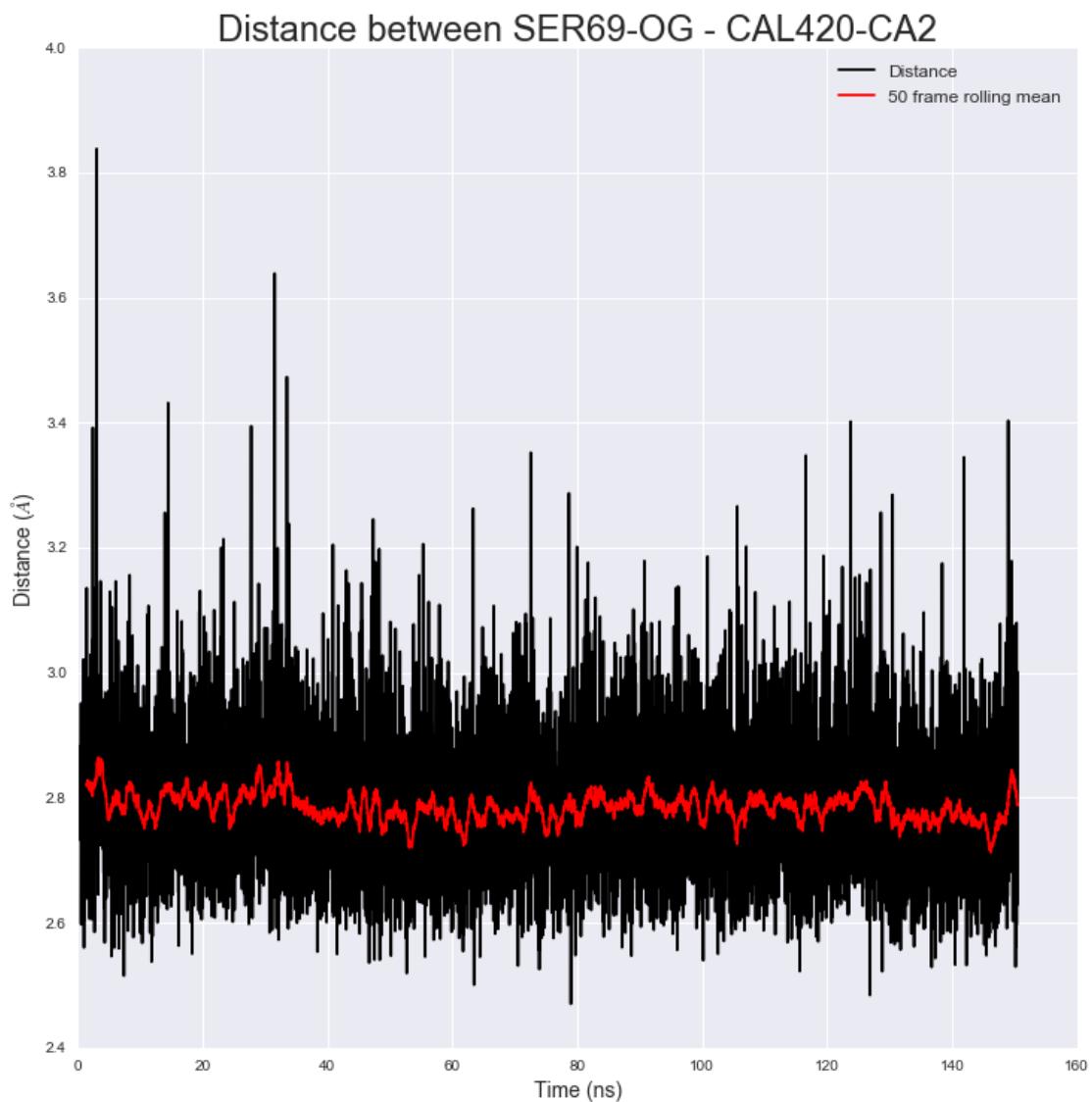
Calculating distance between following atoms: SER69-OG - CAL420-CA2

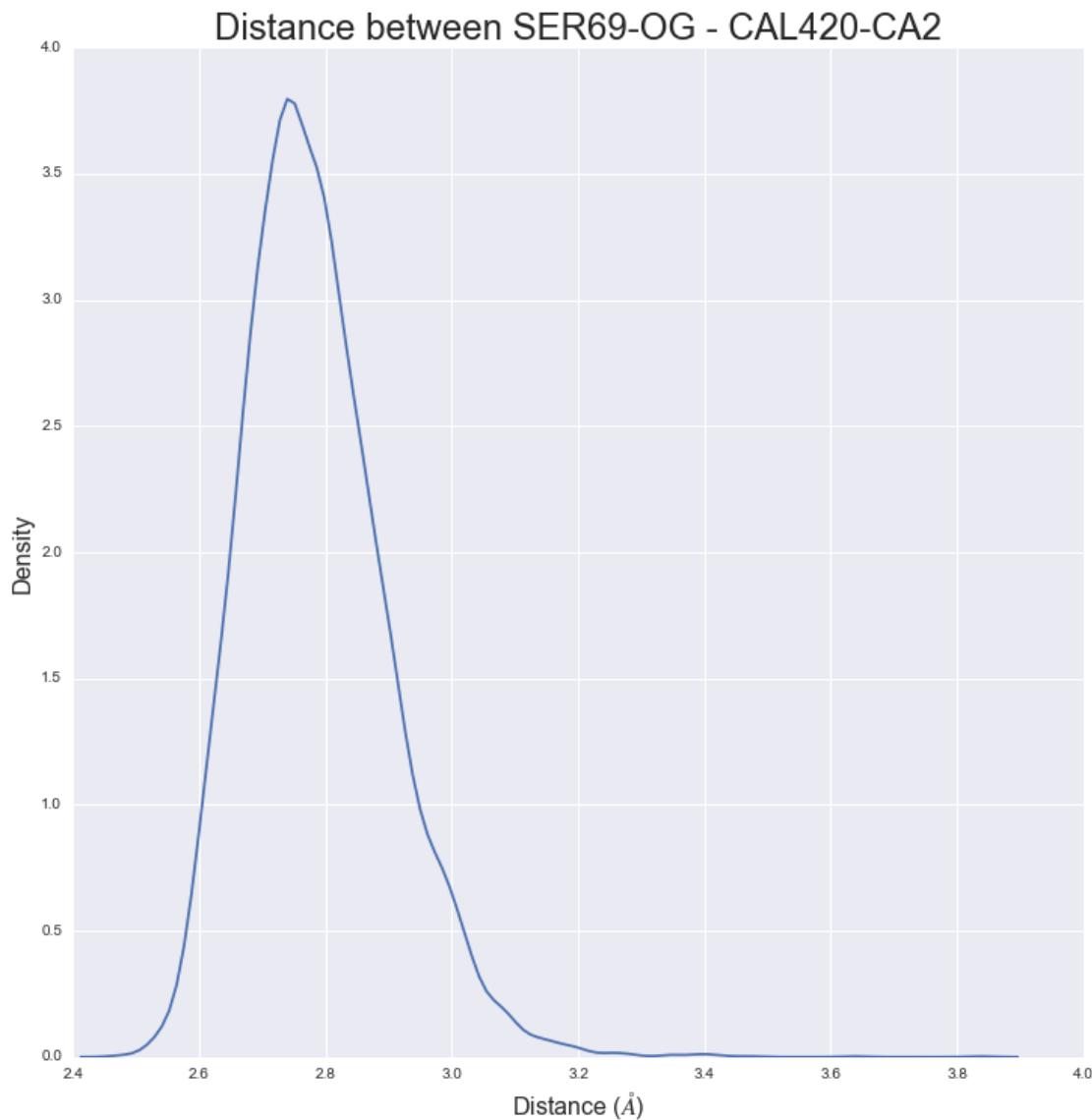
Loading trajectories from the following files:

05\_Prod\_troponin\_egcg\_MD4\_000-050\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD4\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD4\_100-150\_run1\_nowater.nc





Total execution time: 2.11 seconds

Total simulation time of all frames: 149.999995728 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1071

Atom2 number: 6810

Calculating distance between following atoms: THR71-OG1 - CAL420-CA2

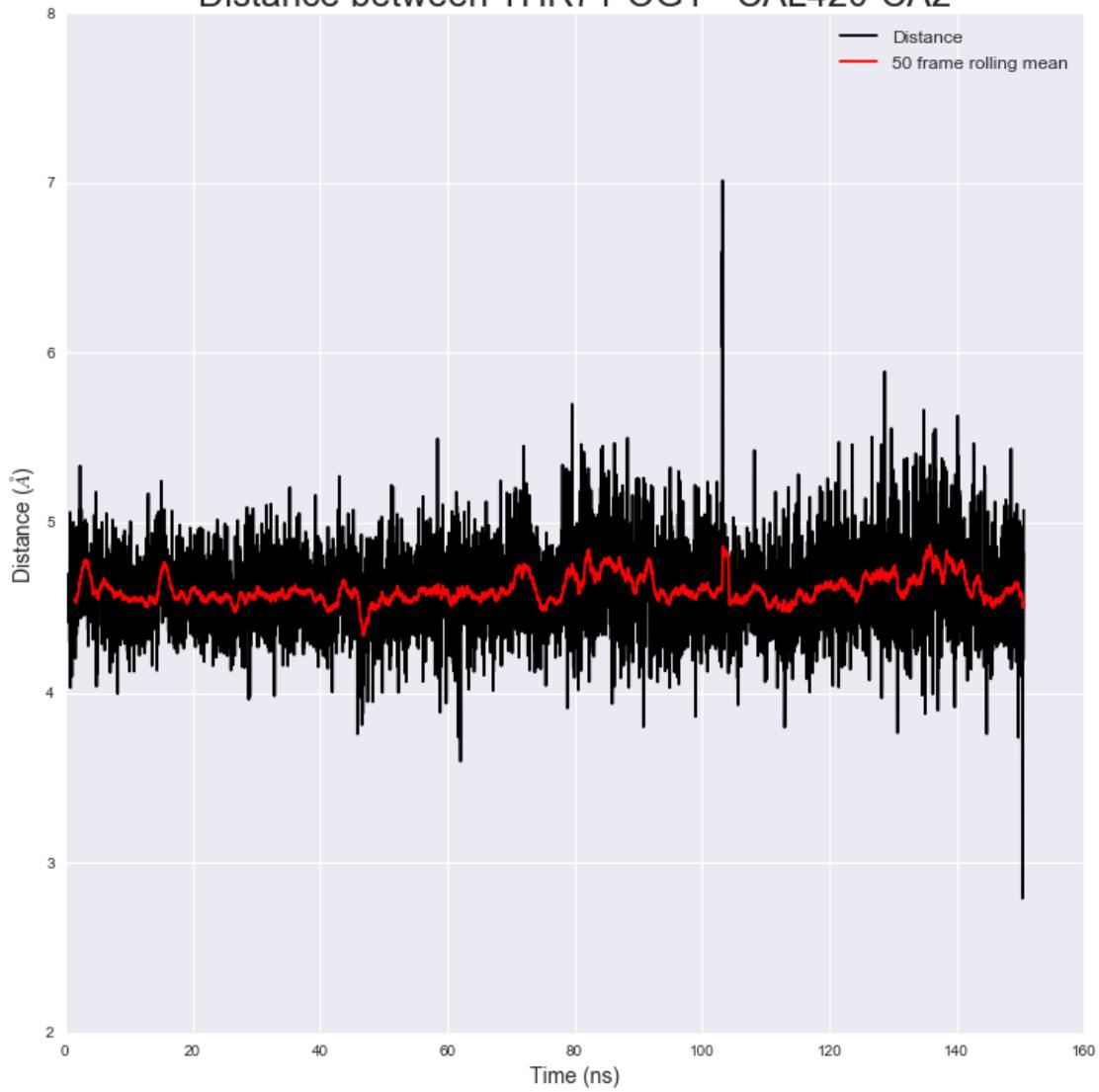
Loading trajectories from the following files:

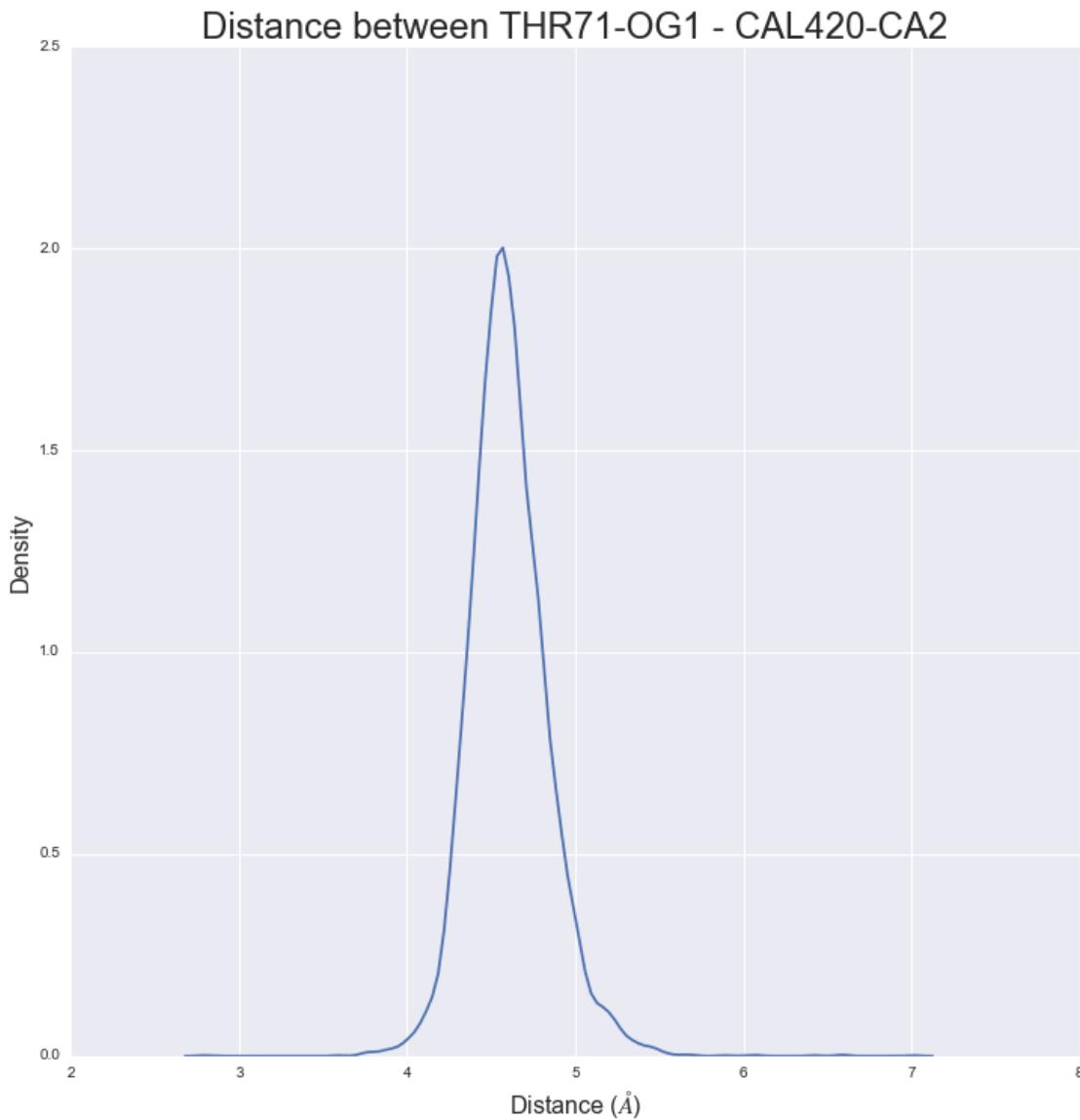
05\_Prod\_troponin\_egcg\_MD4\_000-050\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD4\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD4\_100-150\_run1\_nowater.nc

### Distance between THR71-OG1 - CAL420-CA2





Total execution time: 1.91 seconds

Total simulation time of all frames: 149.999995728 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1099

Atom2 number: 6810

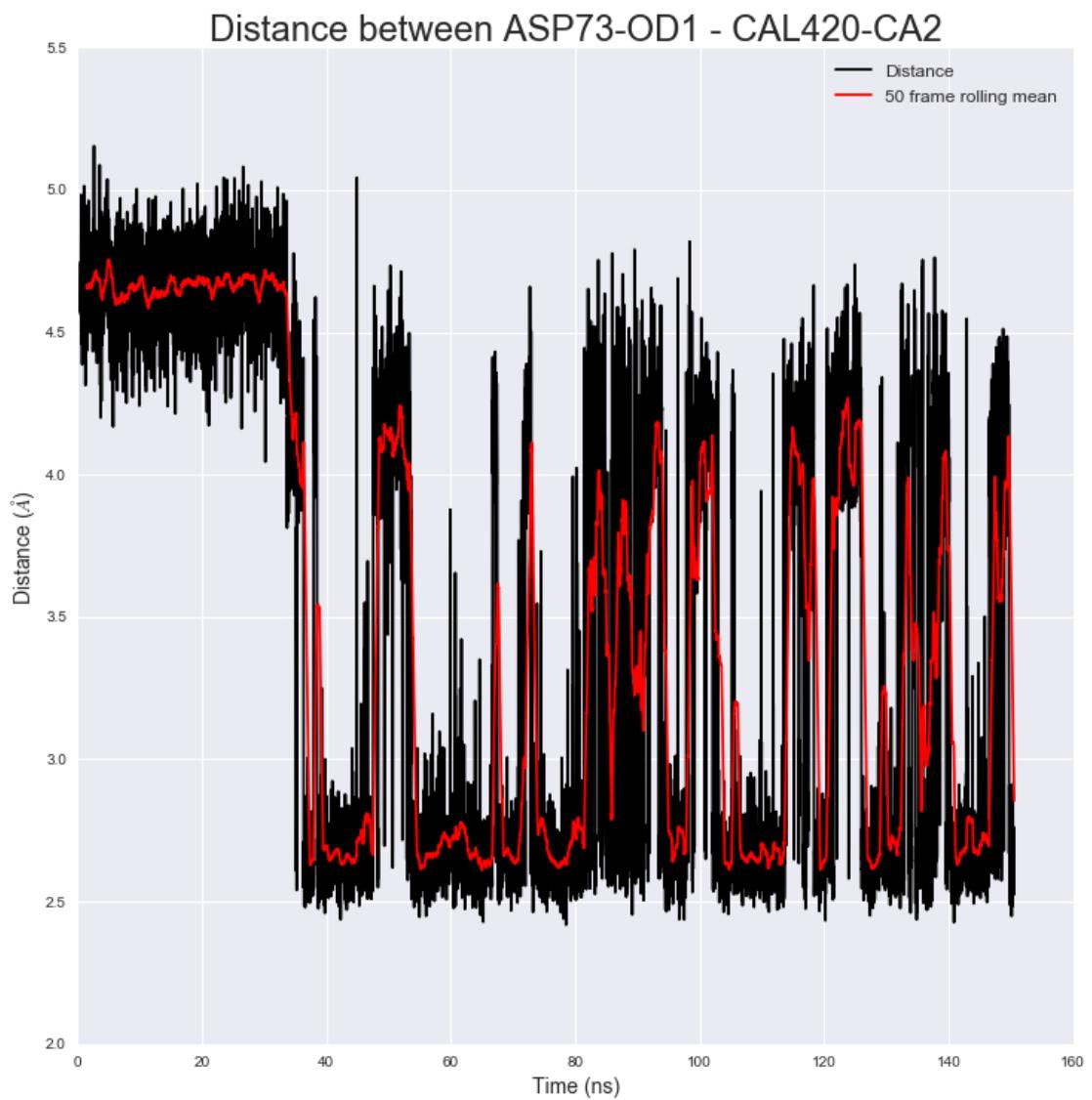
Calculating distance between following atoms: ASP73-OD1 - CAL420-CA2

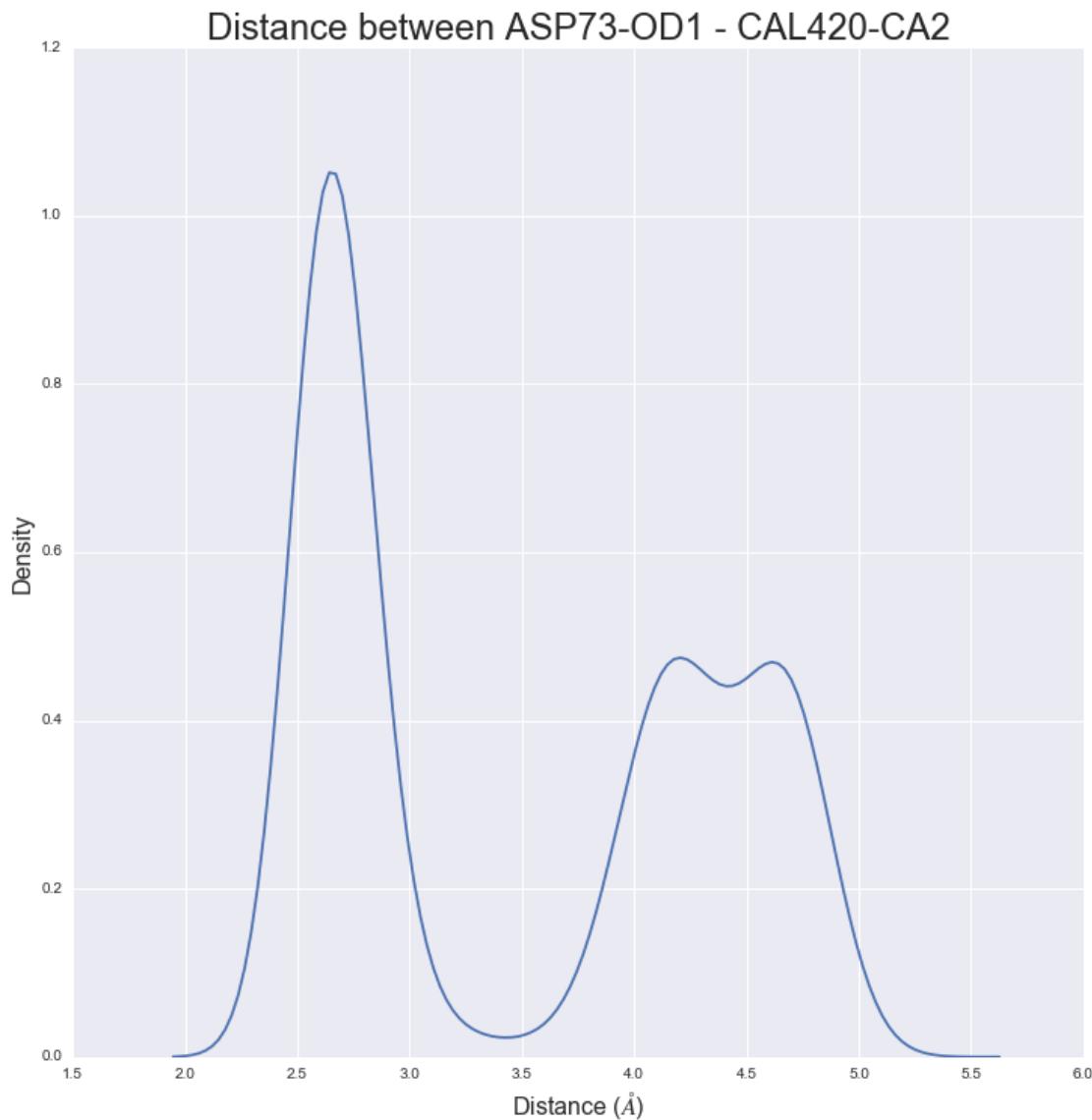
Loading trajectories from the following files:

05\_Prod\_troponin\_egcg\_MD4\_000-050\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD4\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD4\_100-150\_run1\_nowater.nc





Total execution time: 2.22 seconds

Total simulation time of all frames: 149.999995728 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1100

Atom2 number: 6810

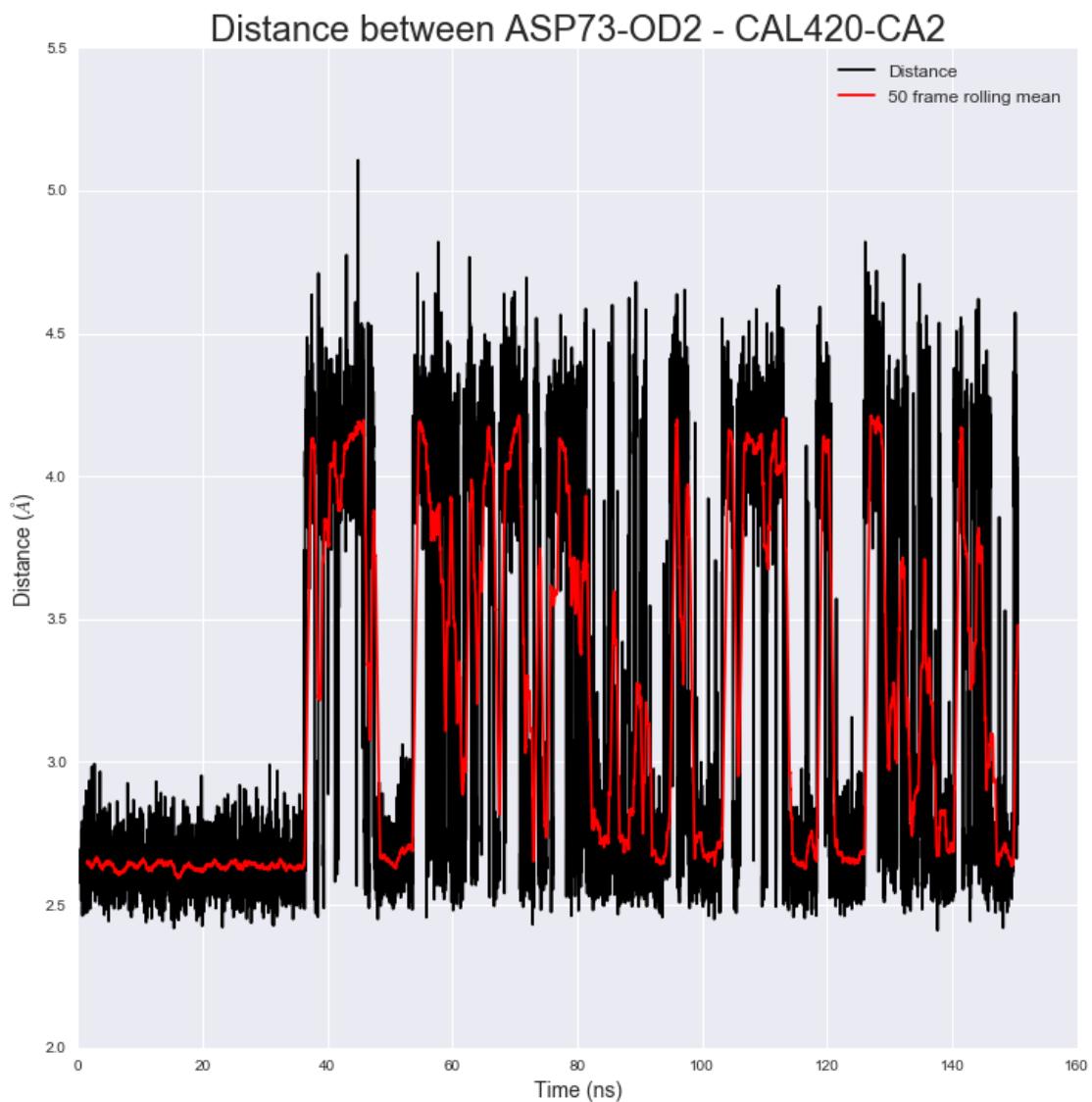
Calculating distance between following atoms: ASP73-OD2 - CAL420-CA2

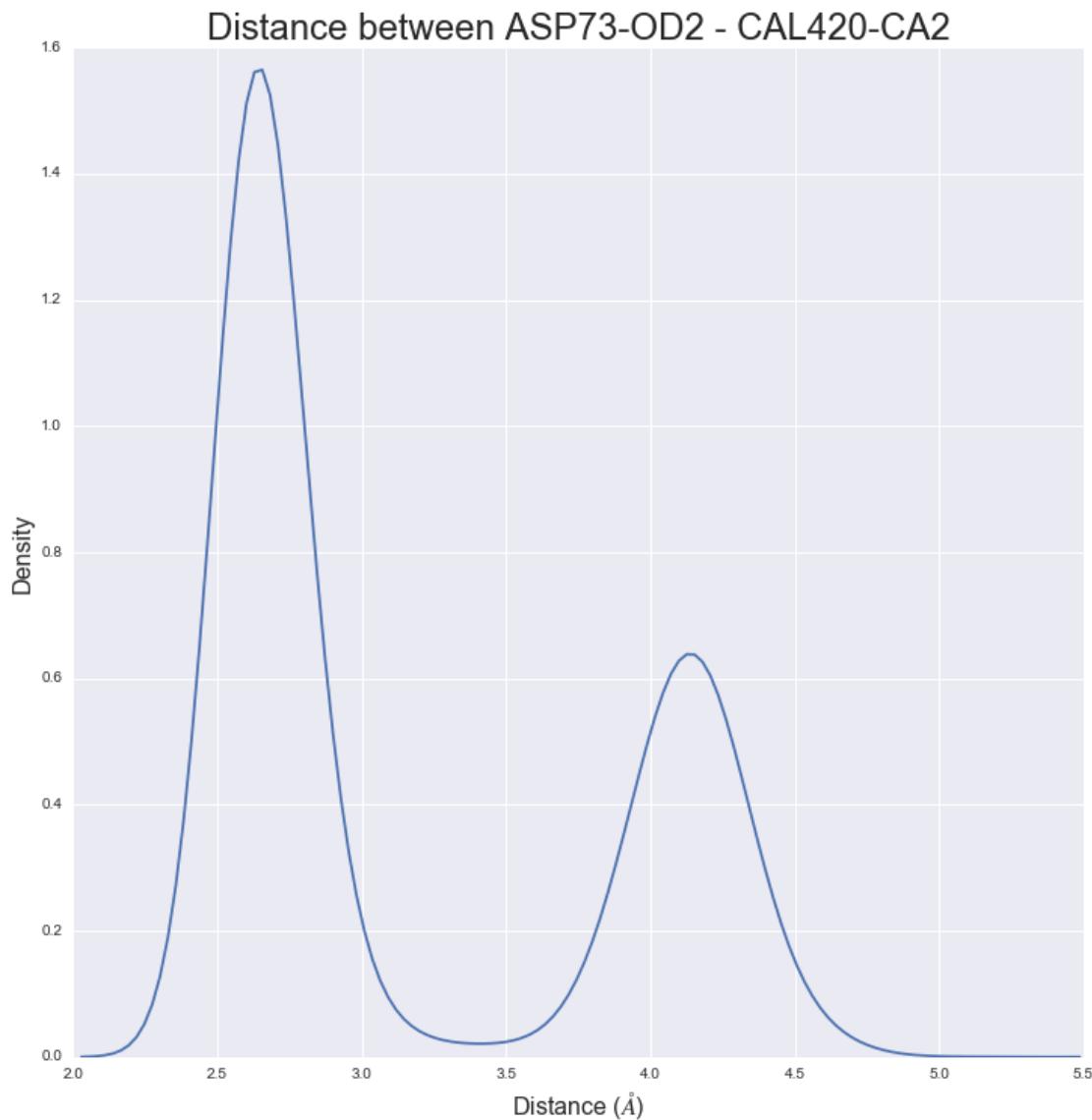
Loading trajectories from the following files:

05\_Prod\_troponin\_egcg\_MD4\_000-050\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD4\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD4\_100-150\_run1\_nowater.nc





Total execution time: 2.09 seconds

Total simulation time of all frames: 149.999995728 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1131

Atom2 number: 6810

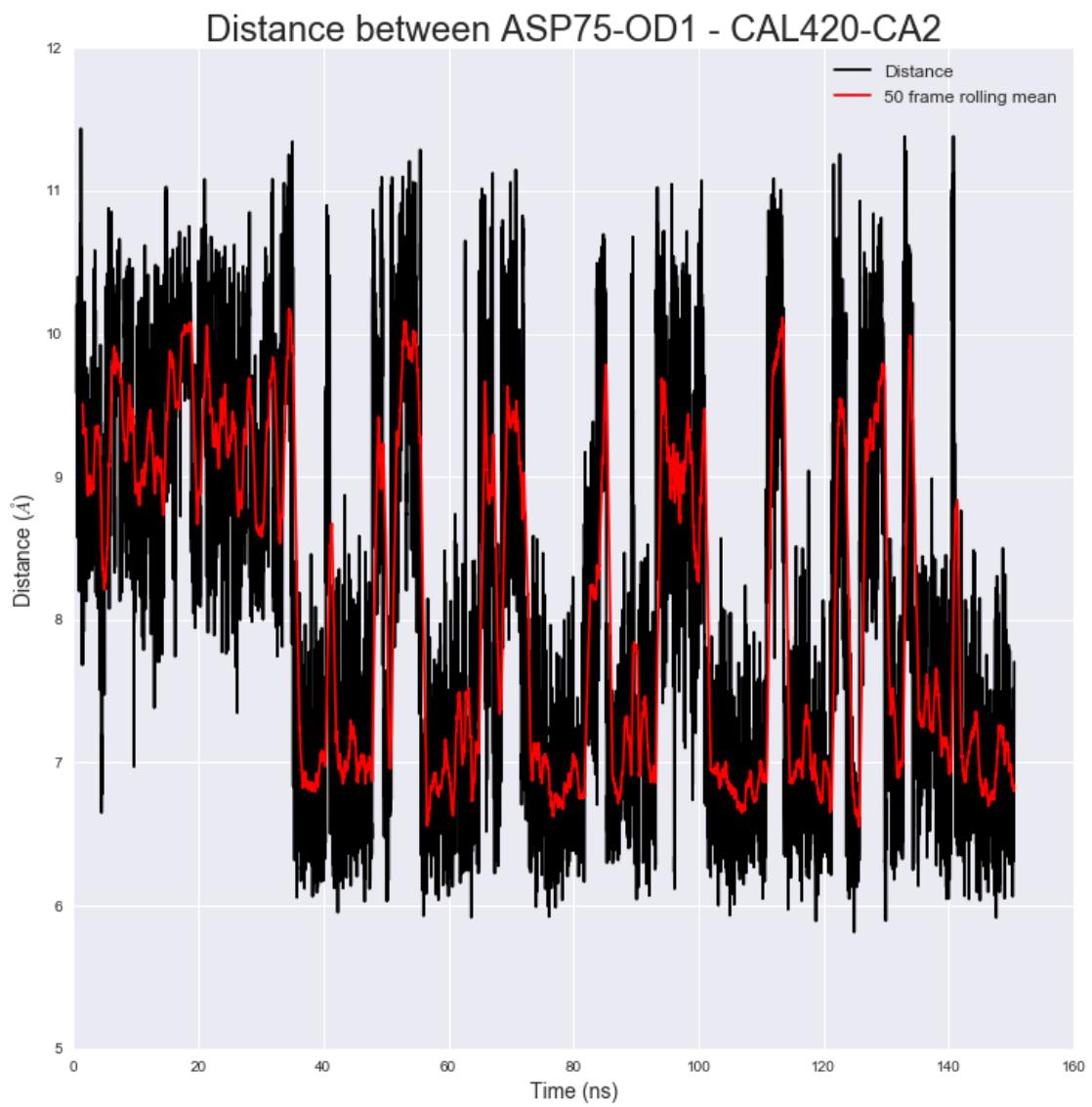
Calculating distance between following atoms: ASP75-OD1 - CAL420-CA2

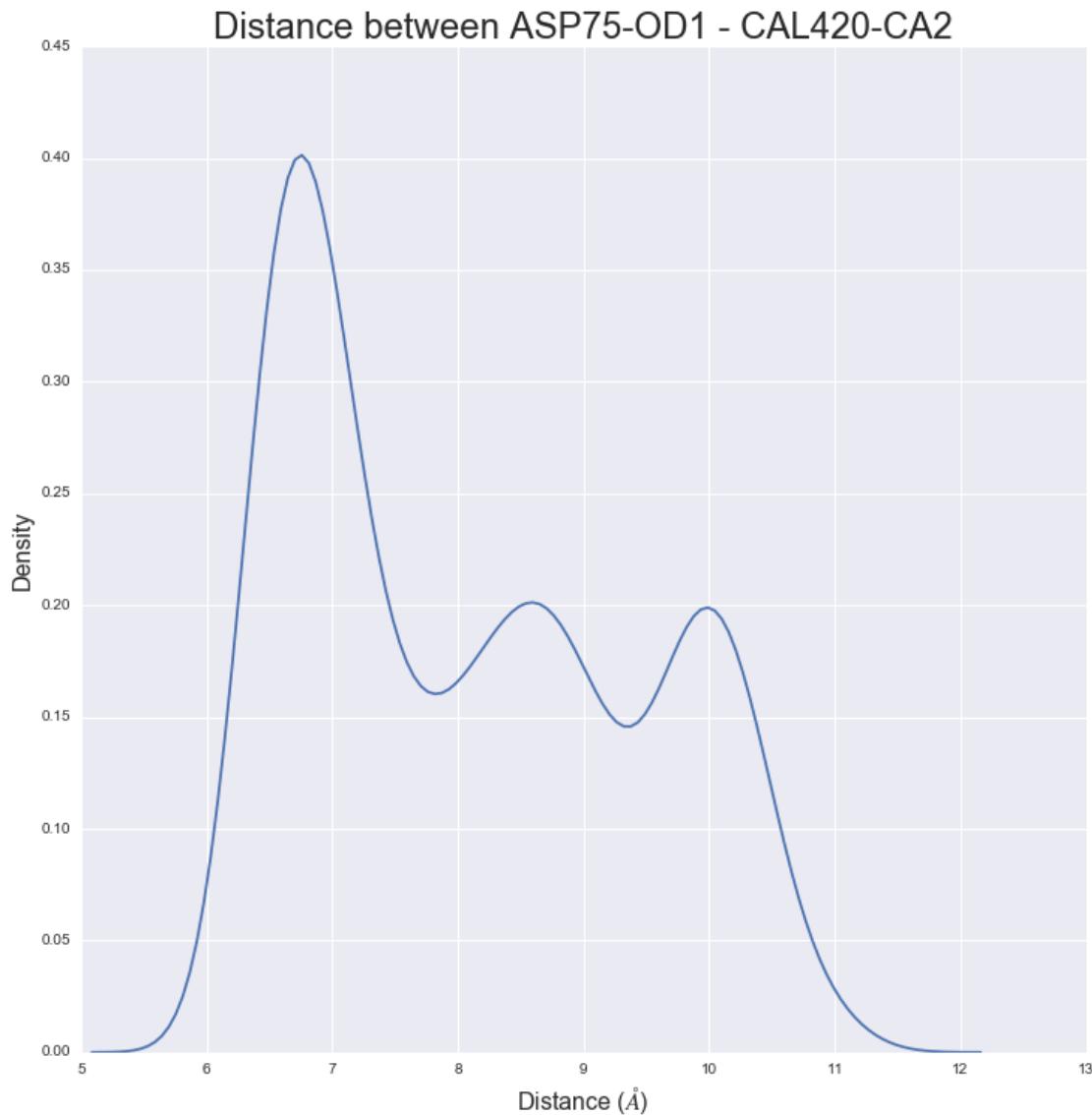
Loading trajectories from the following files:

05\_Prod\_troponin\_egcg\_MD4\_000-050\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD4\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD4\_100-150\_run1\_nowater.nc





Total execution time: 2.13 seconds

Total simulation time of all frames: 149.999995728 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1132

Atom2 number: 6810

Calculating distance between following atoms: ASP75-OD2 - CAL420-CA2

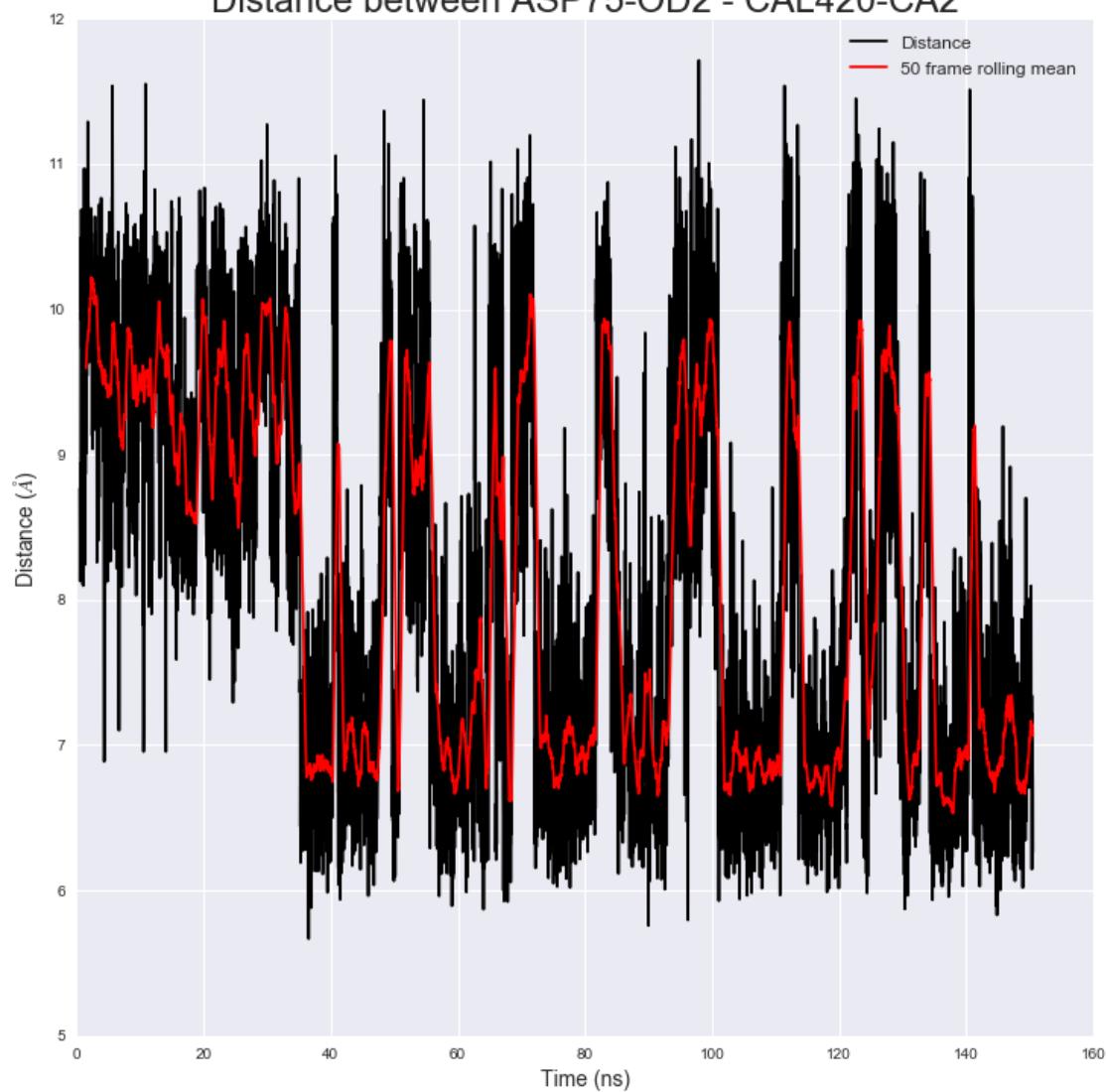
Loading trajectories from the following files:

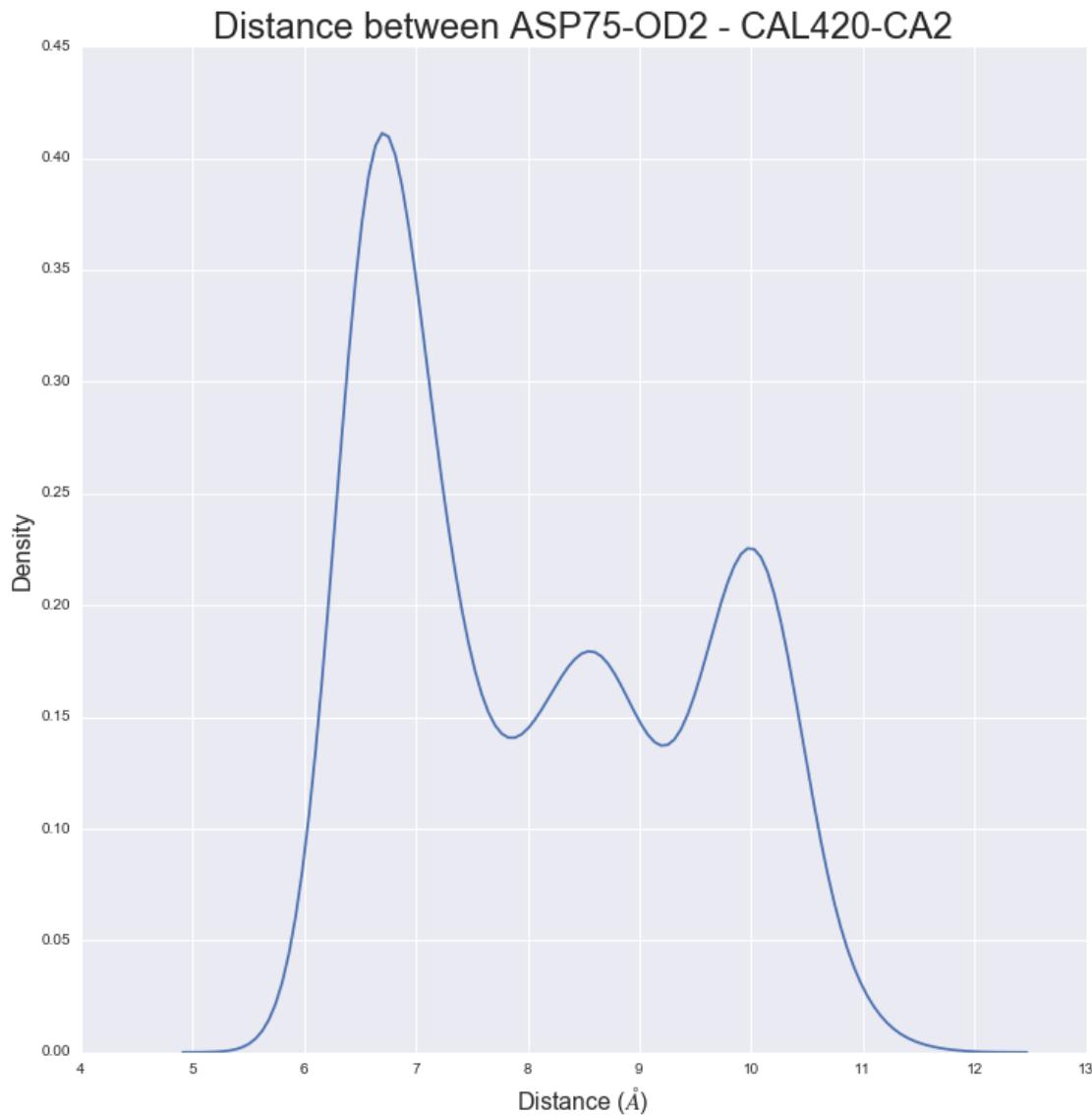
05\_Prod\_troponin\_egcg\_MD4\_000-050\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD4\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD4\_100-150\_run1\_nowater.nc

### Distance between ASP75-OD2 - CAL420-CA2





Total execution time: 2.08 seconds

Total simulation time of all frames: 149.999995728 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1146

Atom2 number: 6810

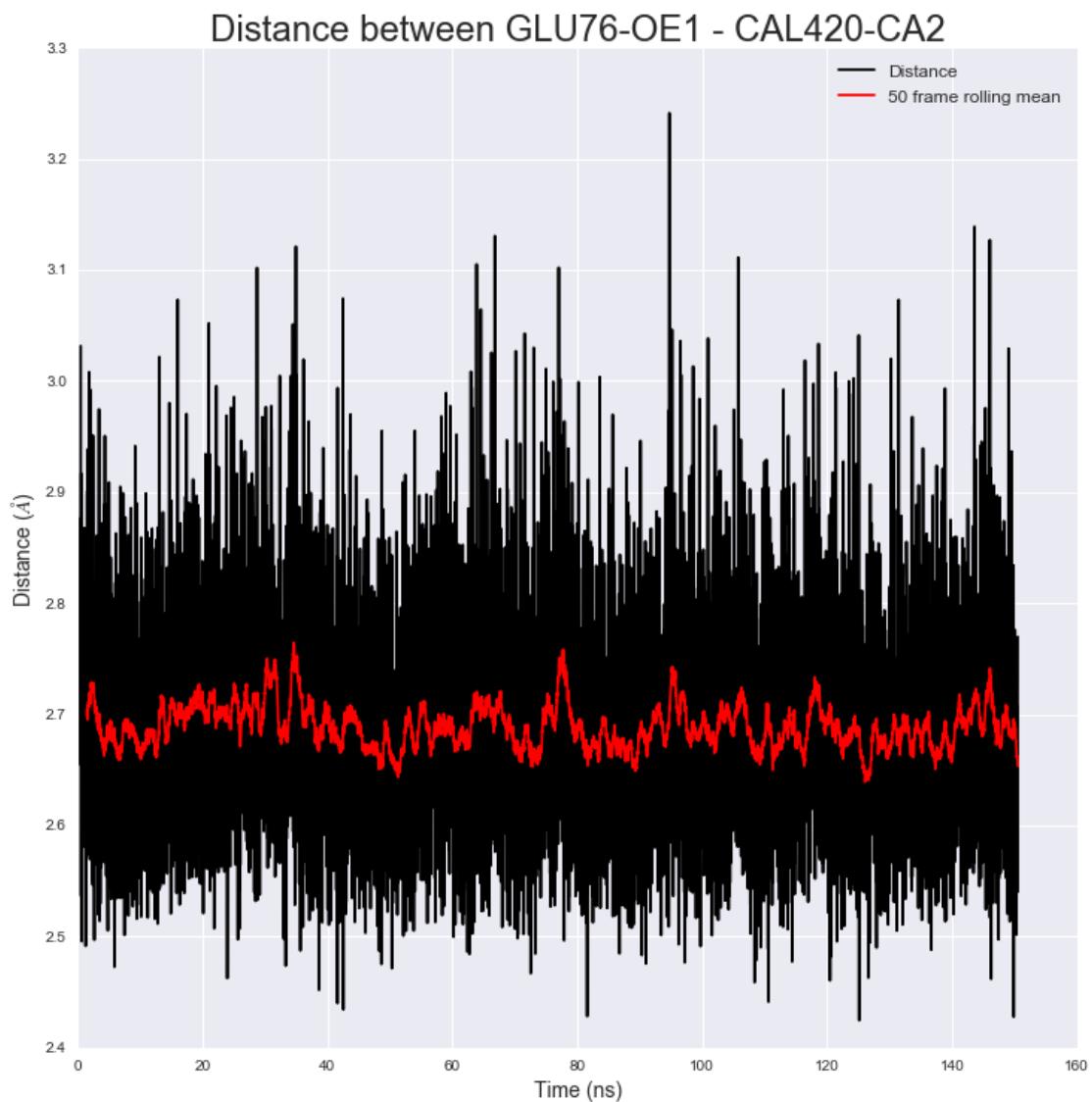
Calculating distance between following atoms: GLU76-OE1 - CAL420-CA2

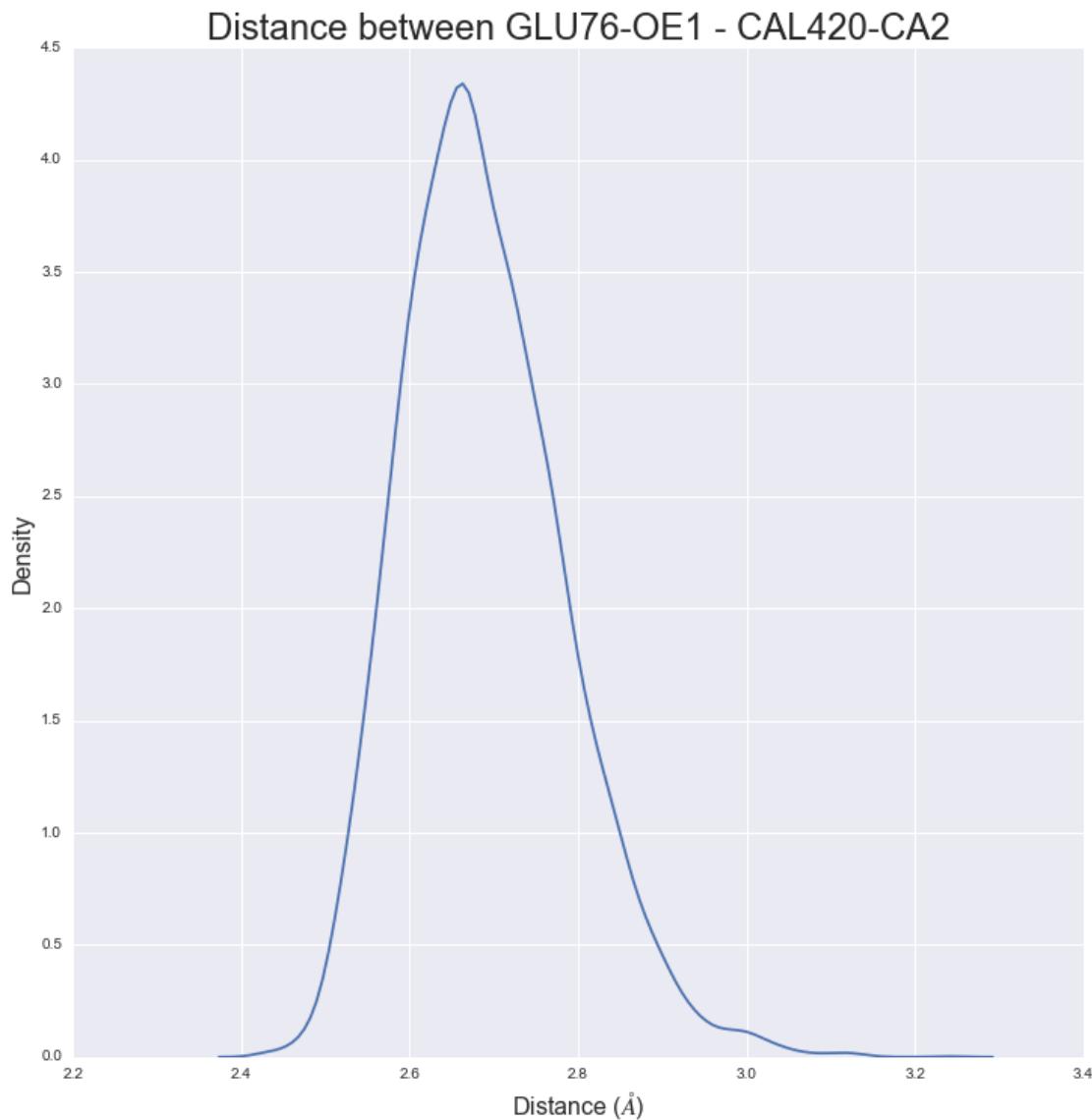
Loading trajectories from the following files:

05\_Prod\_troponin\_egcg\_MD4\_000-050\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD4\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD4\_100-150\_run1\_nowater.nc





Total execution time: 2.20 seconds

Total simulation time of all frames: 149.999995728 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1147

Atom2 number: 6810

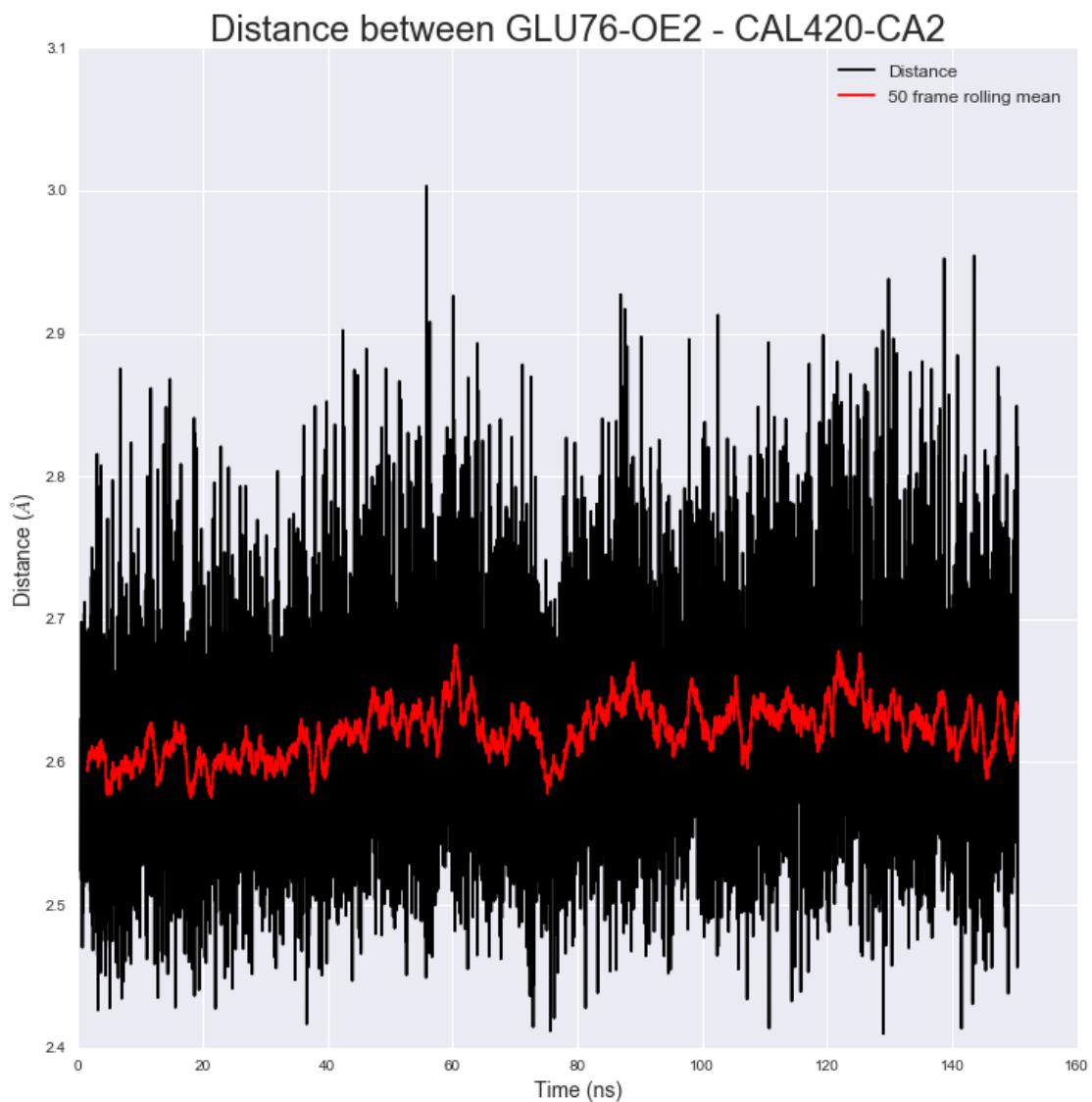
Calculating distance between following atoms: GLU76-OE2 - CAL420-CA2

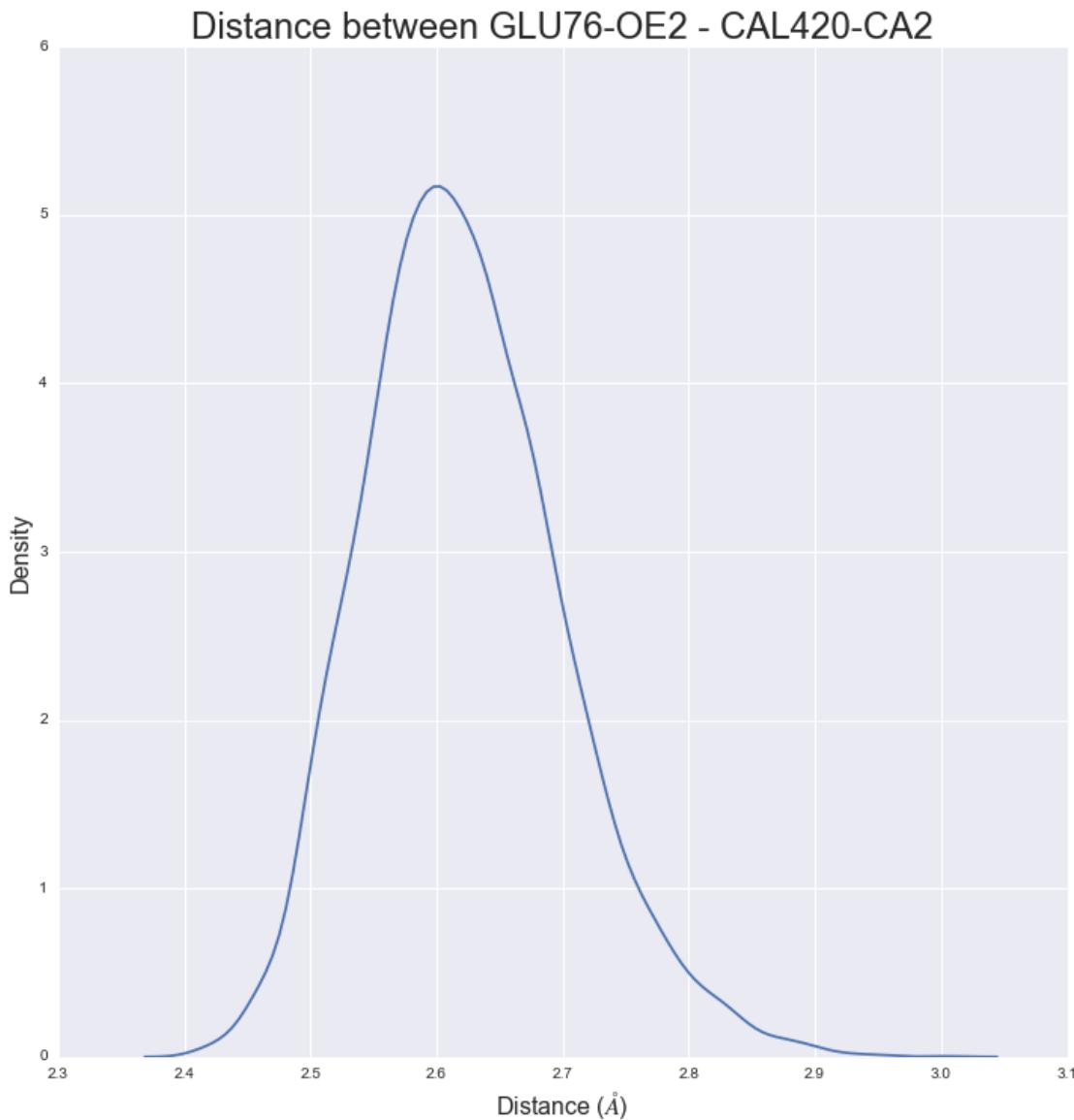
Loading trajectories from the following files:

05\_Prod\_troponin\_egcg\_MD4\_000-050\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD4\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD4\_100-150\_run1\_nowater.nc





Total execution time: 2.33 seconds

Total simulation time of all frames: 149.999995728 nanoseconds

## 0.5 MD5

```
In [13]: topology_MD5 = '/Users/gil_f.hoben/Troponin_md_processed/MD5/run1/troponin_egcg_MD5_nowater.pr
          trajectory_MD5 = '/Users/gil_f.hoben/Troponin_md_processed/MD5/run1/Trajectories/'
```

```
In [14]: for atom1 in atom1_list:
          main(topology_MD5, trajectory_MD5, atom1, atom2, verbose = 1)
```

The following topology file was successfully loaded:  
`<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>`

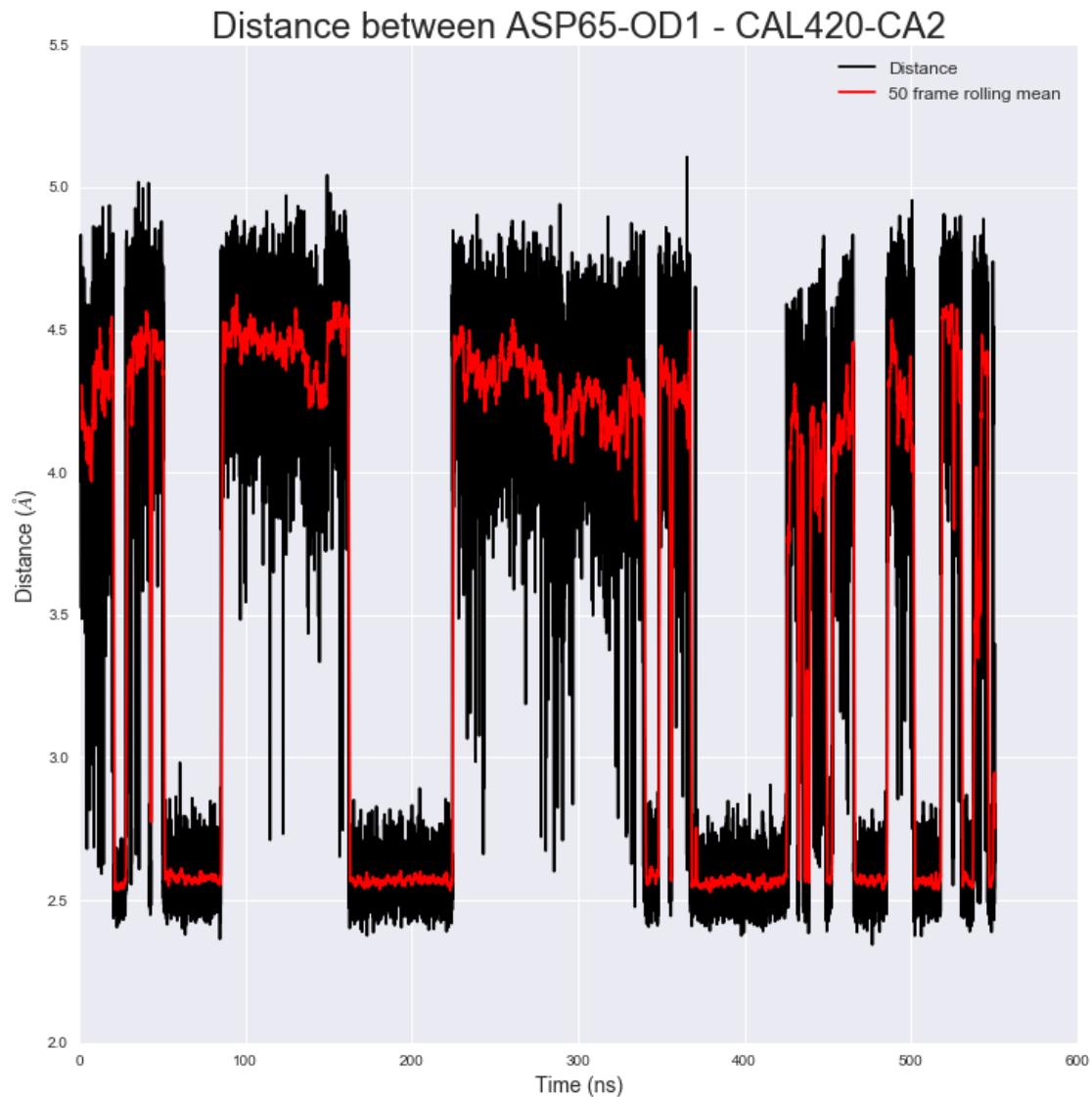
Atom1 number: 1005

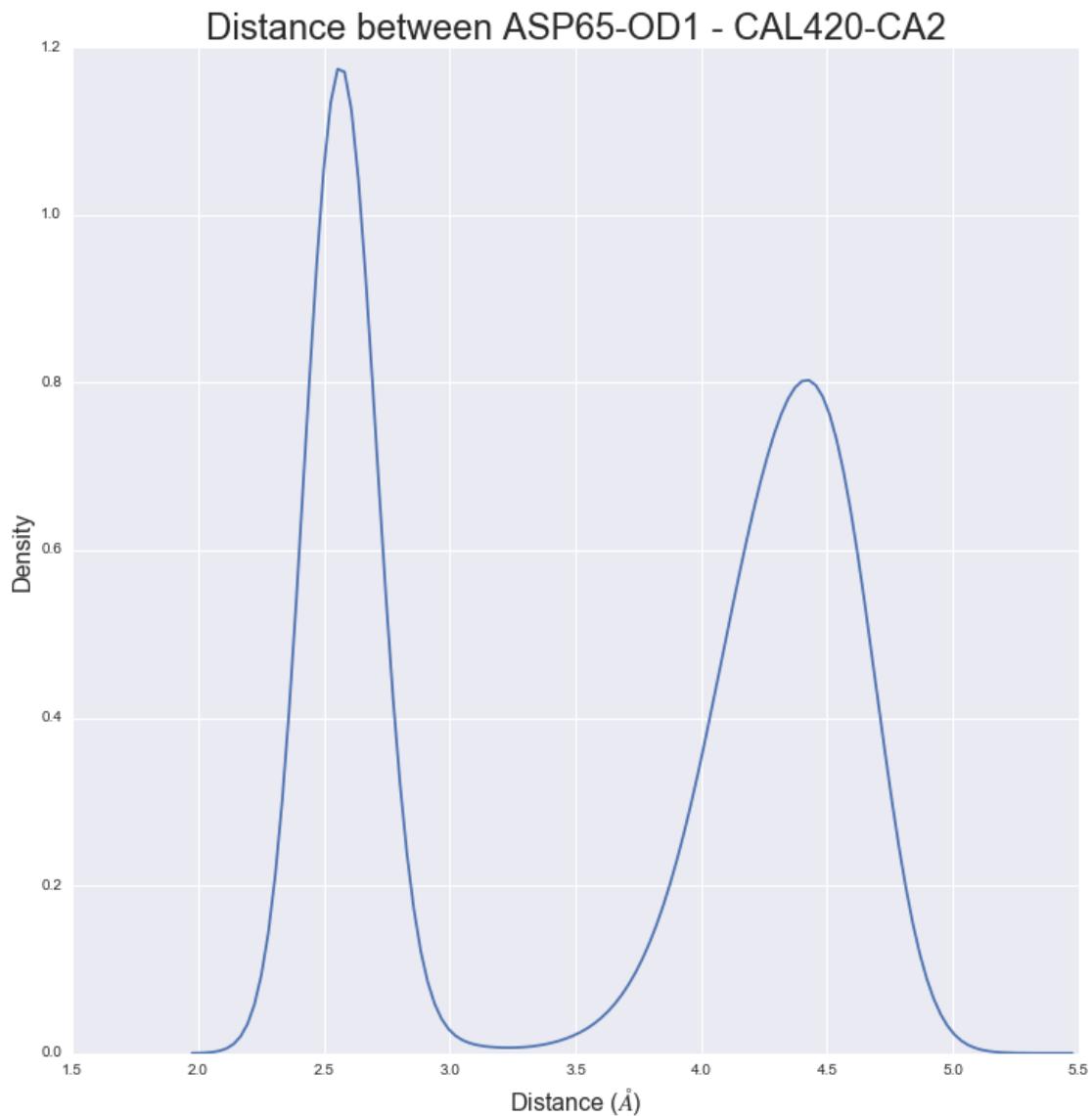
Atom2 number: 6810

Calculating distance between following atoms: ASP65-OD1 - CAL420-CA2

Loading trajectories from the following files:

05\_Prod\_troponin\_egcg\_MD5\_000-050\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_050-100\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_100-150\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_150-200\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_200-250\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_250-300\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_300-350\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_350-400\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_400-450\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_450-500\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_500-550\_run1\_nowater.nc





Total execution time: 7.44 seconds

Total simulation time of all frames: 549.999980469 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1005

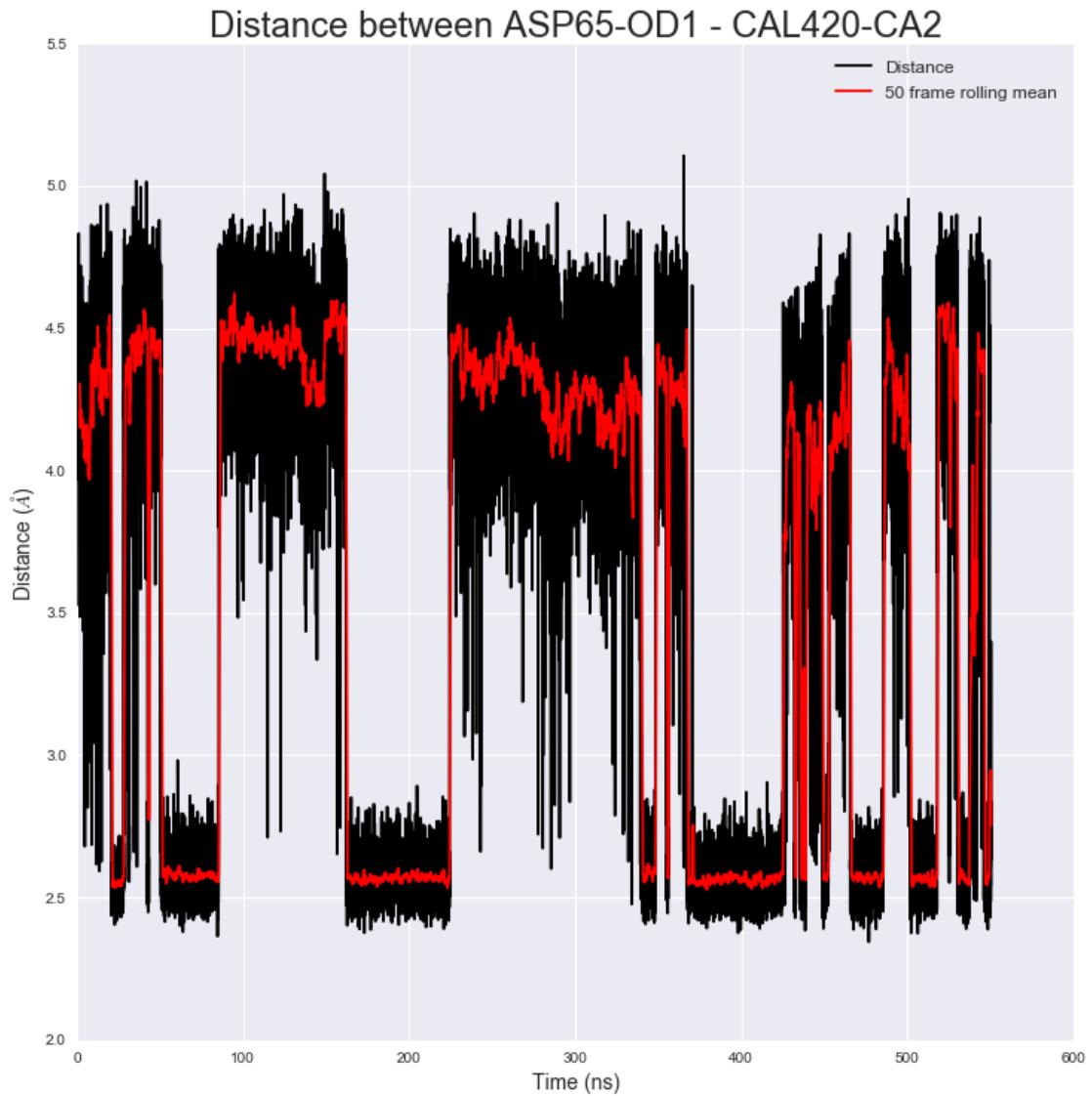
Atom2 number: 6810

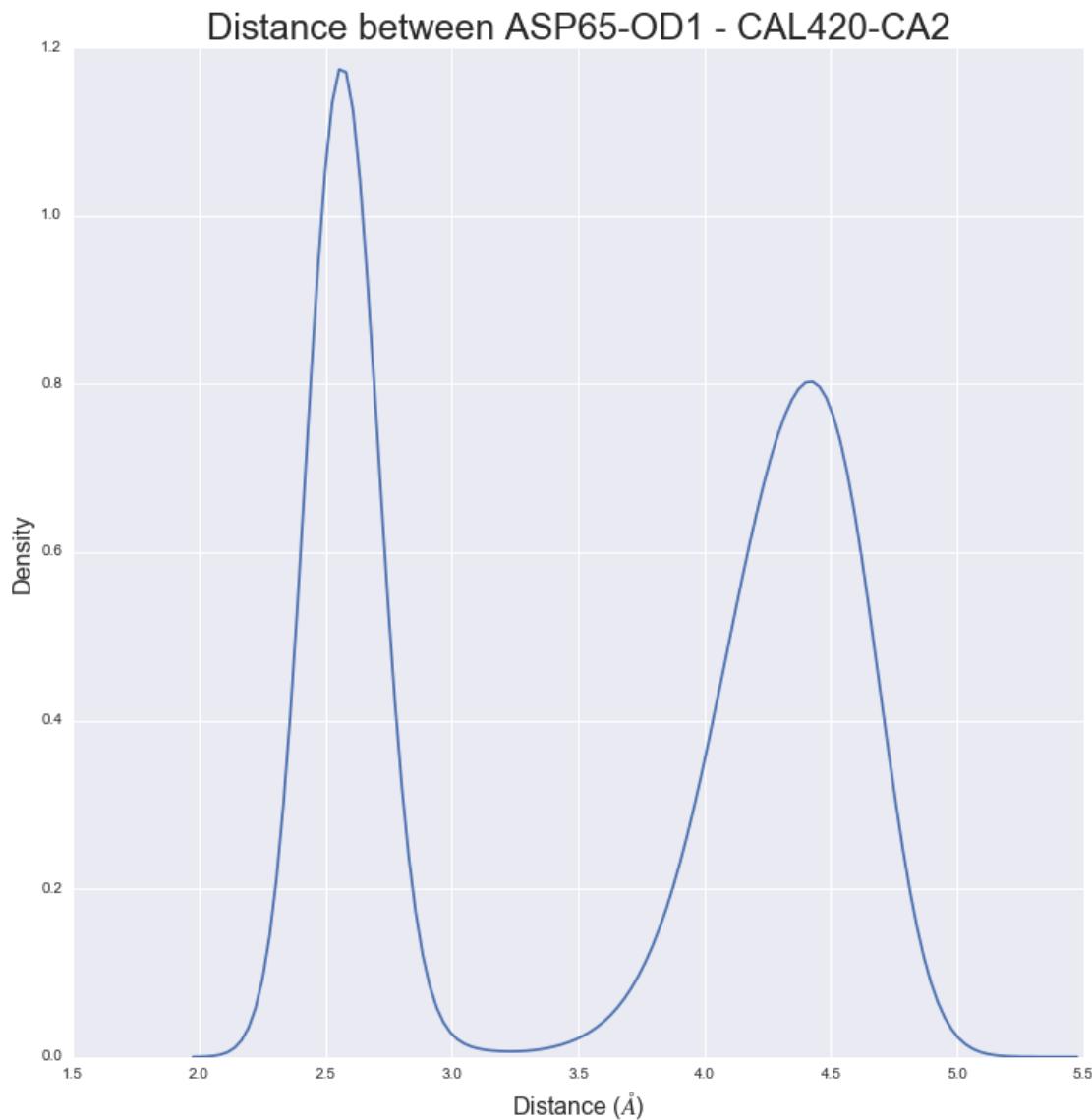
Calculating distance between following atoms: ASP65-OD1 - CAL420-CA2

Loading trajectories from the following files:

05\_Prod\_troponin\_egcg\_MD5\_000-050\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD5\_050-100\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_100-150\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_150-200\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_200-250\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_250-300\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_300-350\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_350-400\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_400-450\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_450-500\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_500-550\_run1\_nowater.nc





Total execution time: 4.94 seconds

Total simulation time of all frames: 549.999980469 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1020

Atom2 number: 6810

Calculating distance between following atoms: GLU66-OE1 - CAL420-CA2

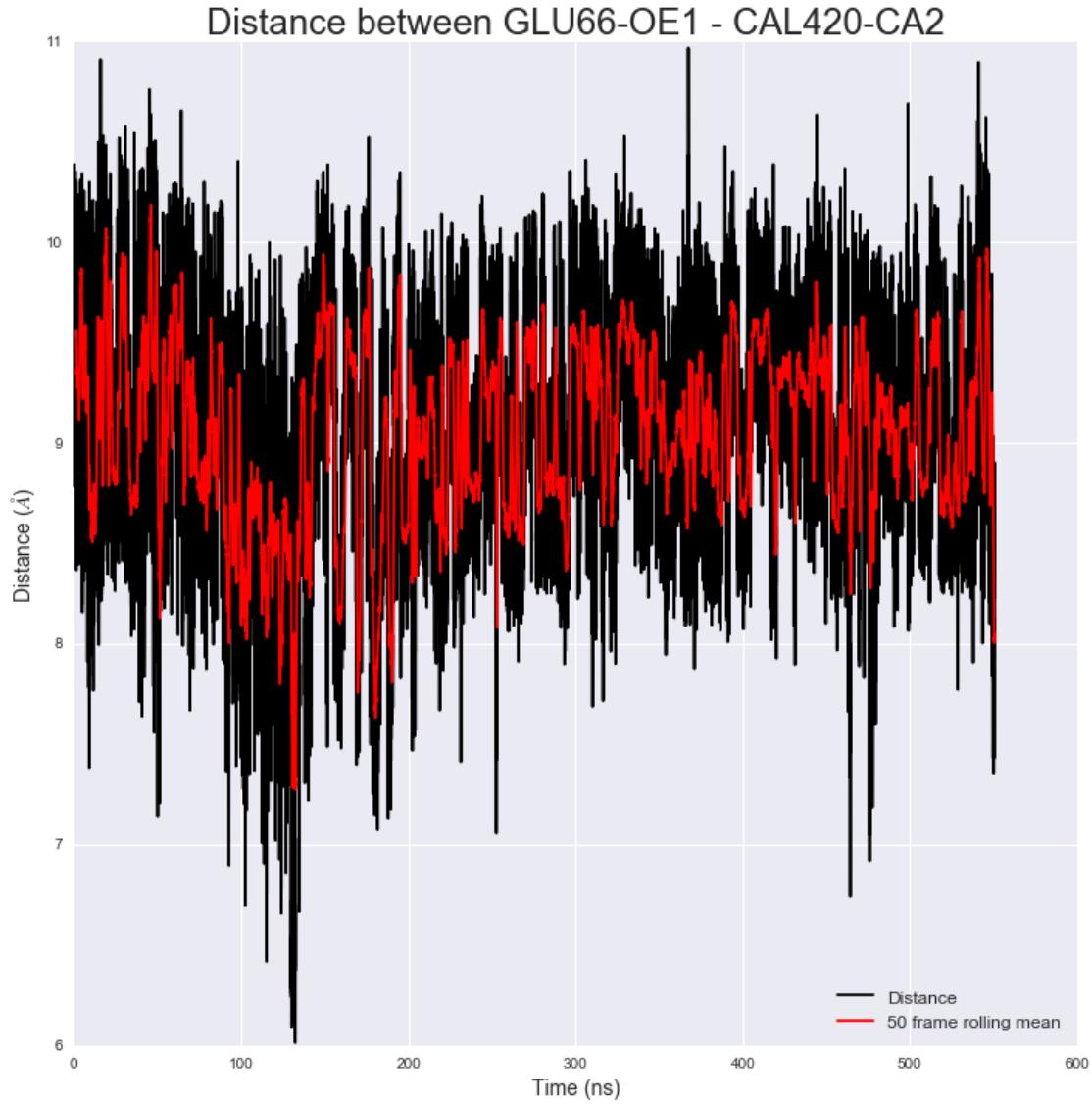
Loading trajectories from the following files:

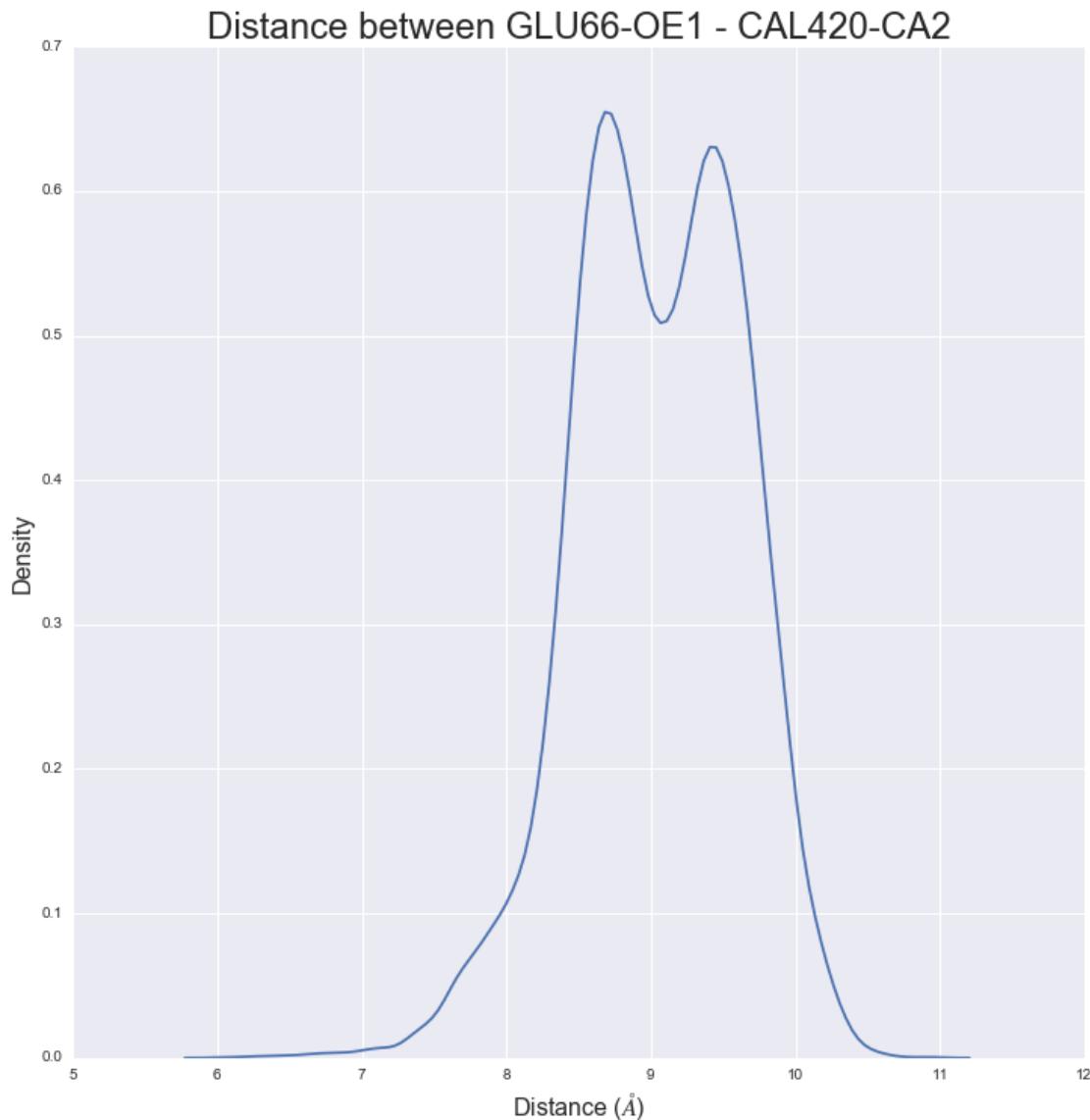
05\_Prod\_troponin\_egcg\_MD5\_000-050\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD5\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD5\_100-150\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD5\_150-200\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_200-250\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_250-300\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_300-350\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_350-400\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_400-450\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_450-500\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_500-550\_run1\_nowater.nc





Total execution time: 4.97 seconds

Total simulation time of all frames: 549.999980469 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1021

Atom2 number: 6810

Calculating distance between following atoms: GLU66-OE2 - CAL420-CA2

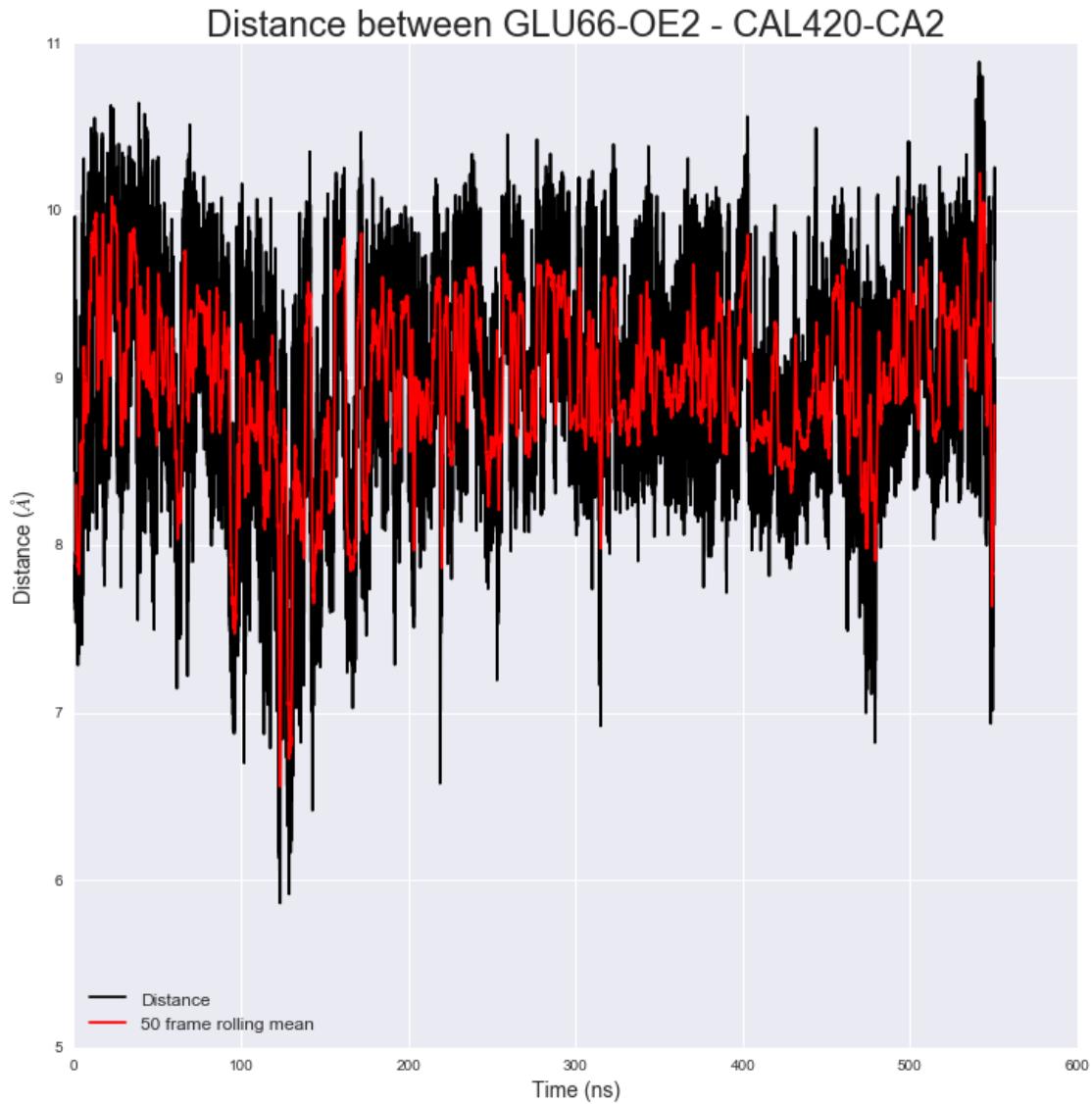
Loading trajectories from the following files:

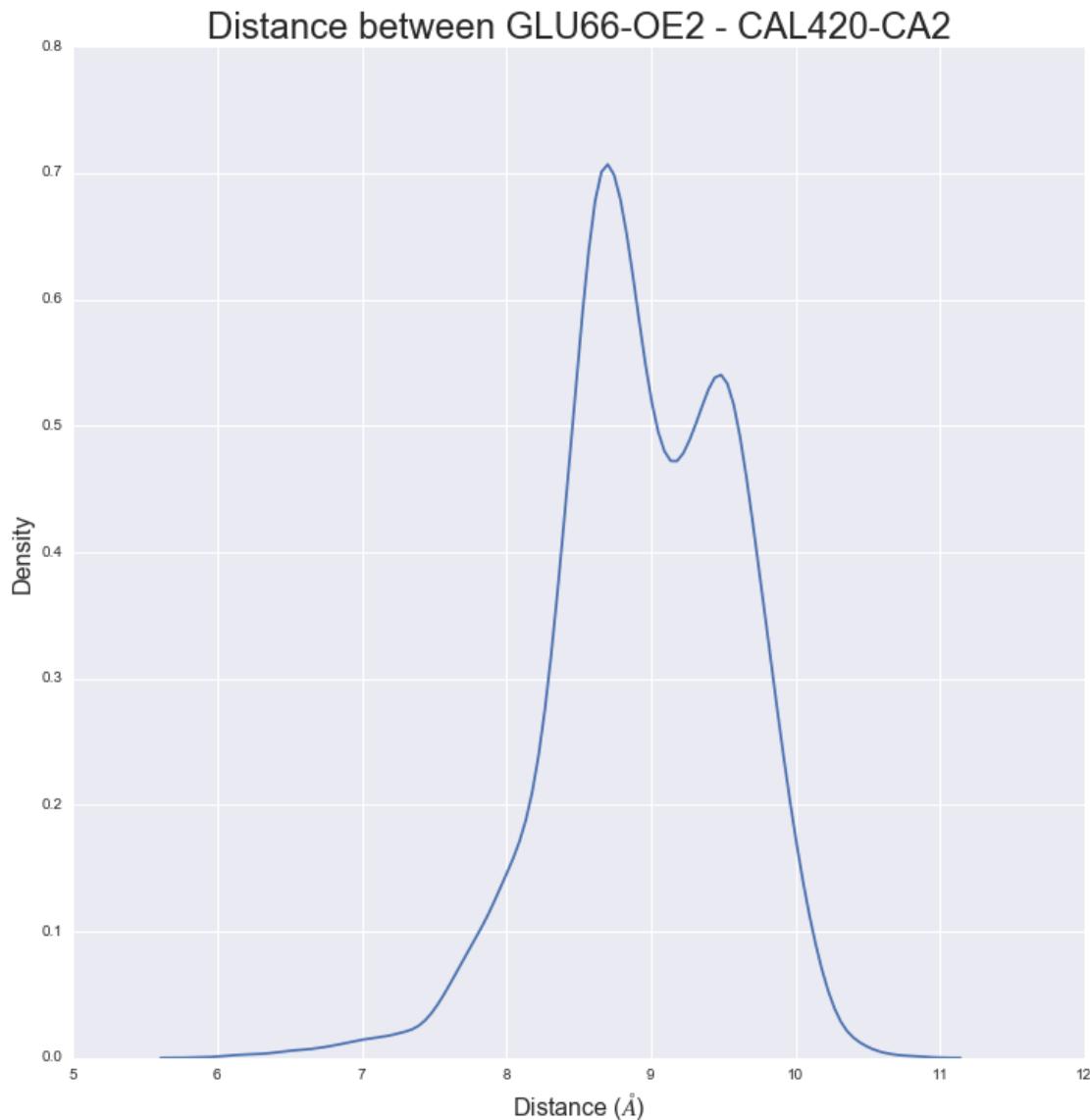
05\_Prod\_troponin\_egcg\_MD5\_000-050\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD5\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD5\_100-150\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD5\_150-200\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_200-250\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_250-300\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_300-350\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_350-400\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_400-450\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_450-500\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_500-550\_run1\_nowater.nc





Total execution time: 4.99 seconds

Total simulation time of all frames: 549.999980469 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1032

Atom2 number: 6810

Calculating distance between following atoms: ASP67-OD1 - CAL420-CA2

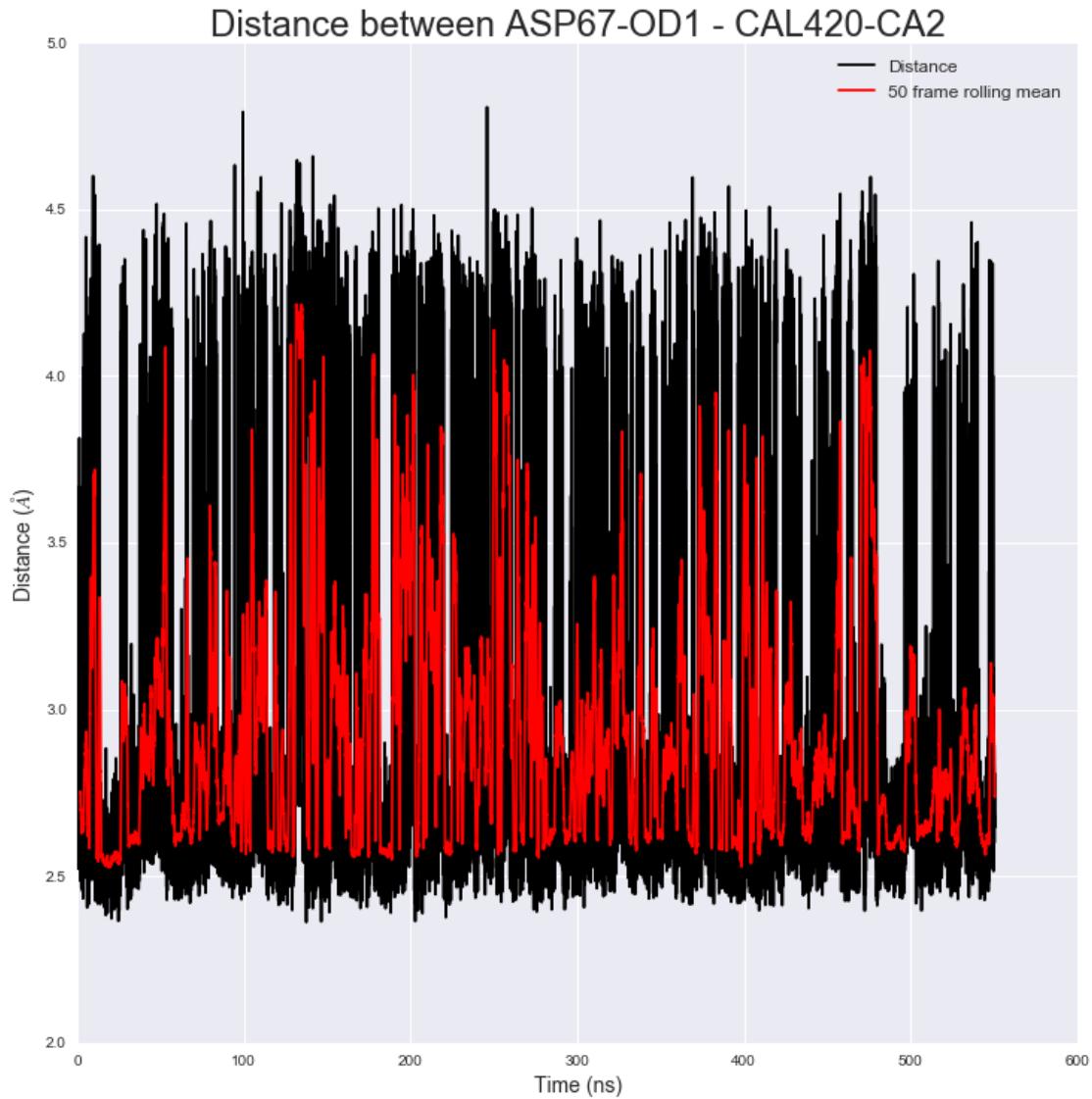
Loading trajectories from the following files:

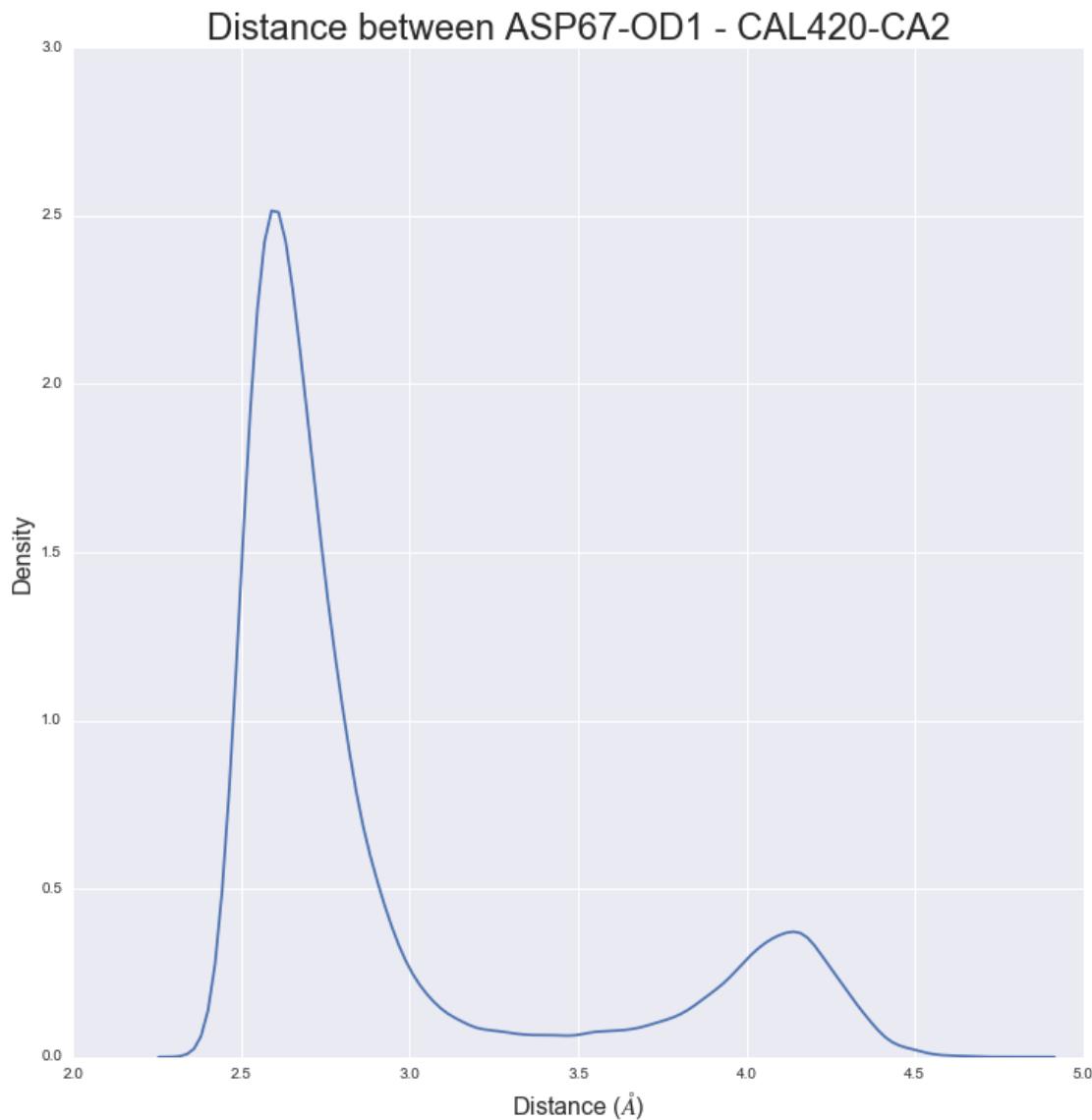
05\_Prod\_troponin\_egcg\_MD5\_000-050\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD5\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD5\_100-150\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD5\_150-200\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_200-250\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_250-300\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_300-350\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_350-400\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_400-450\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_450-500\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_500-550\_run1\_nowater.nc





Total execution time: 4.92 seconds

Total simulation time of all frames: 549.999980469 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1033

Atom2 number: 6810

Calculating distance between following atoms: ASP67-OD2 - CAL420-CA2

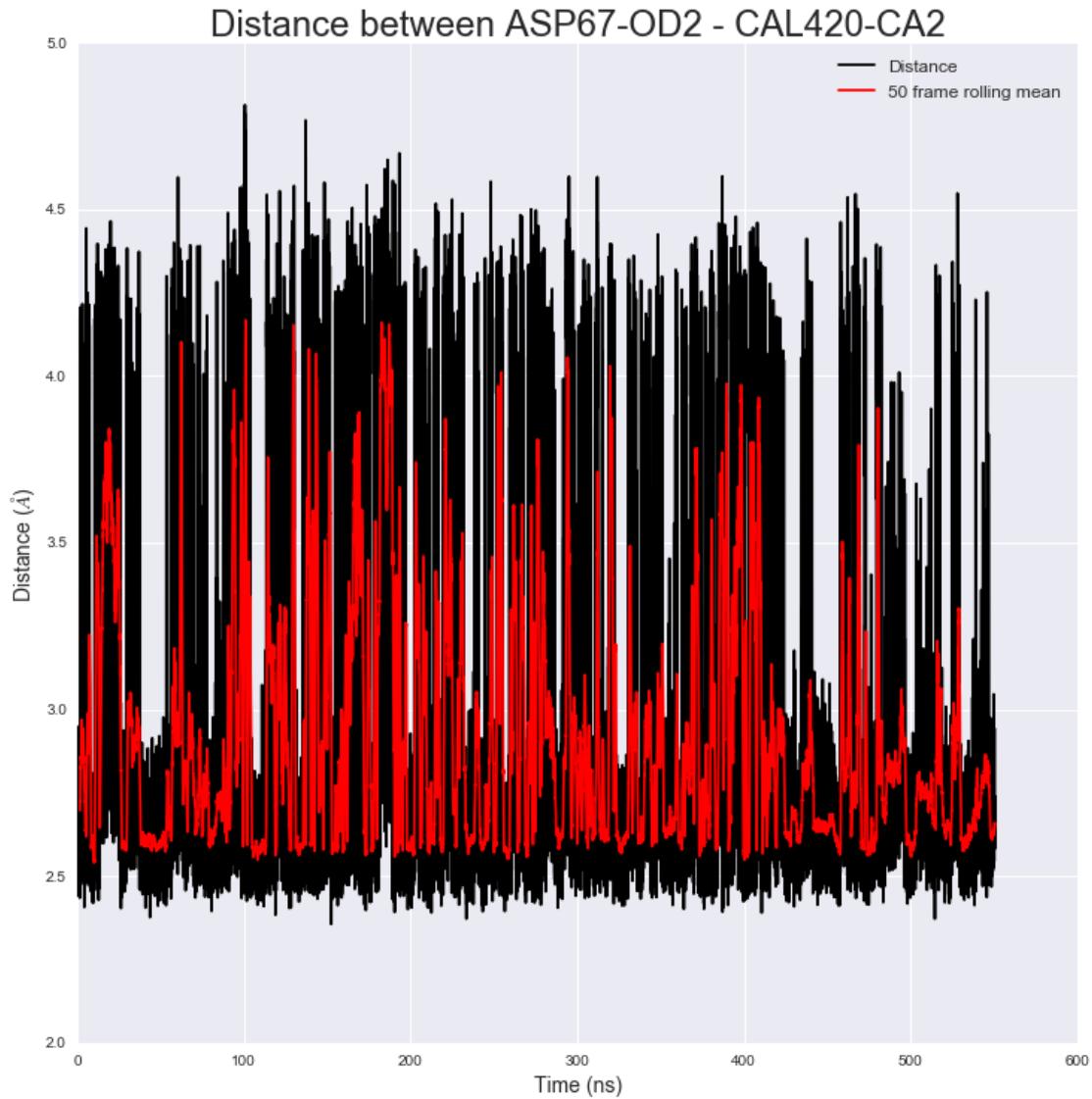
Loading trajectories from the following files:

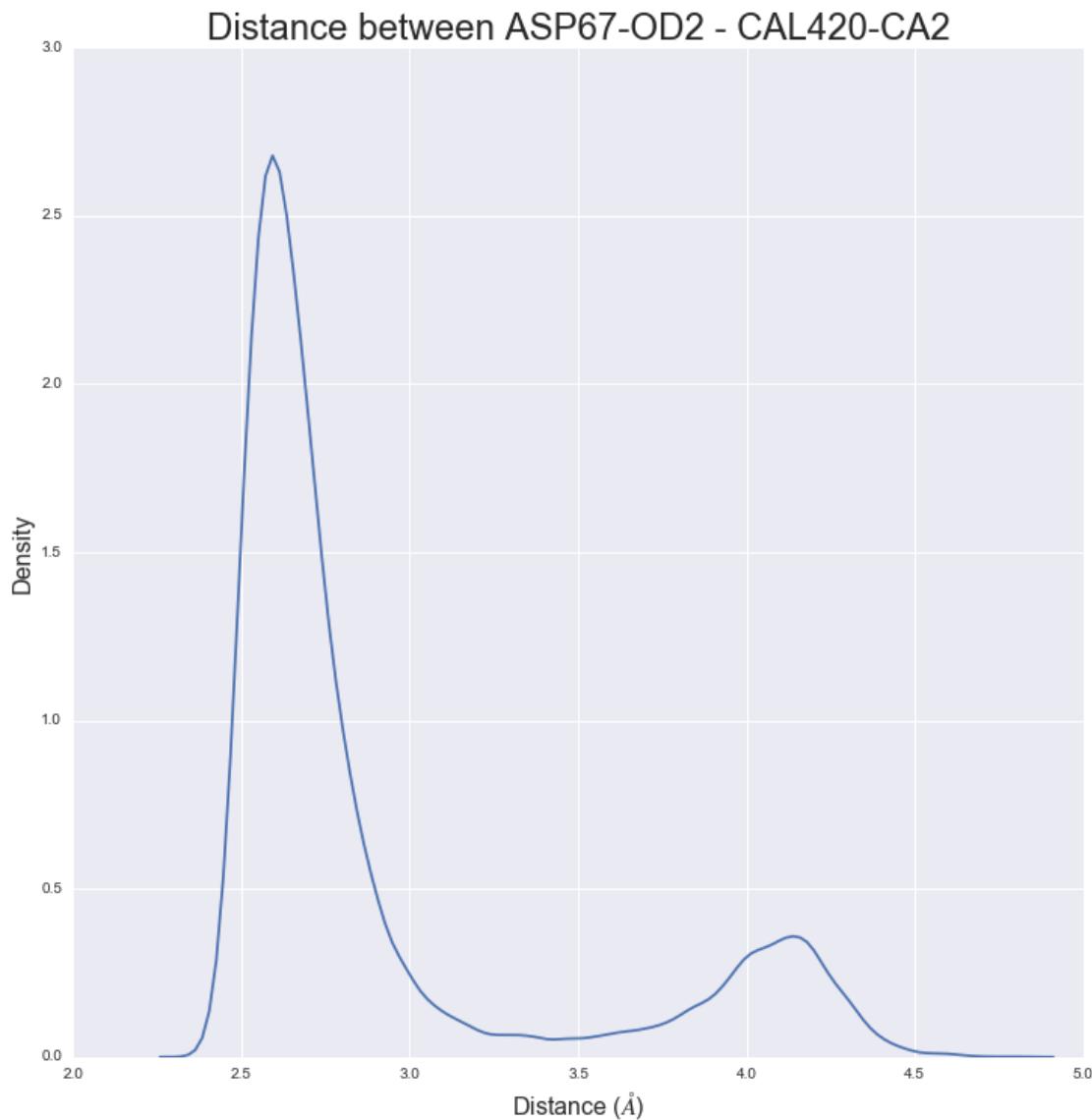
05\_Prod\_troponin\_egcg\_MD5\_000-050\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD5\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD5\_100-150\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD5\_150-200\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_200-250\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_250-300\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_300-350\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_350-400\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_400-450\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_450-500\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_500-550\_run1\_nowater.nc





Total execution time: 4.97 seconds

Total simulation time of all frames: 549.999980469 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1050

Atom2 number: 6810

Calculating distance between following atoms: SER69-OG - CAL420-CA2

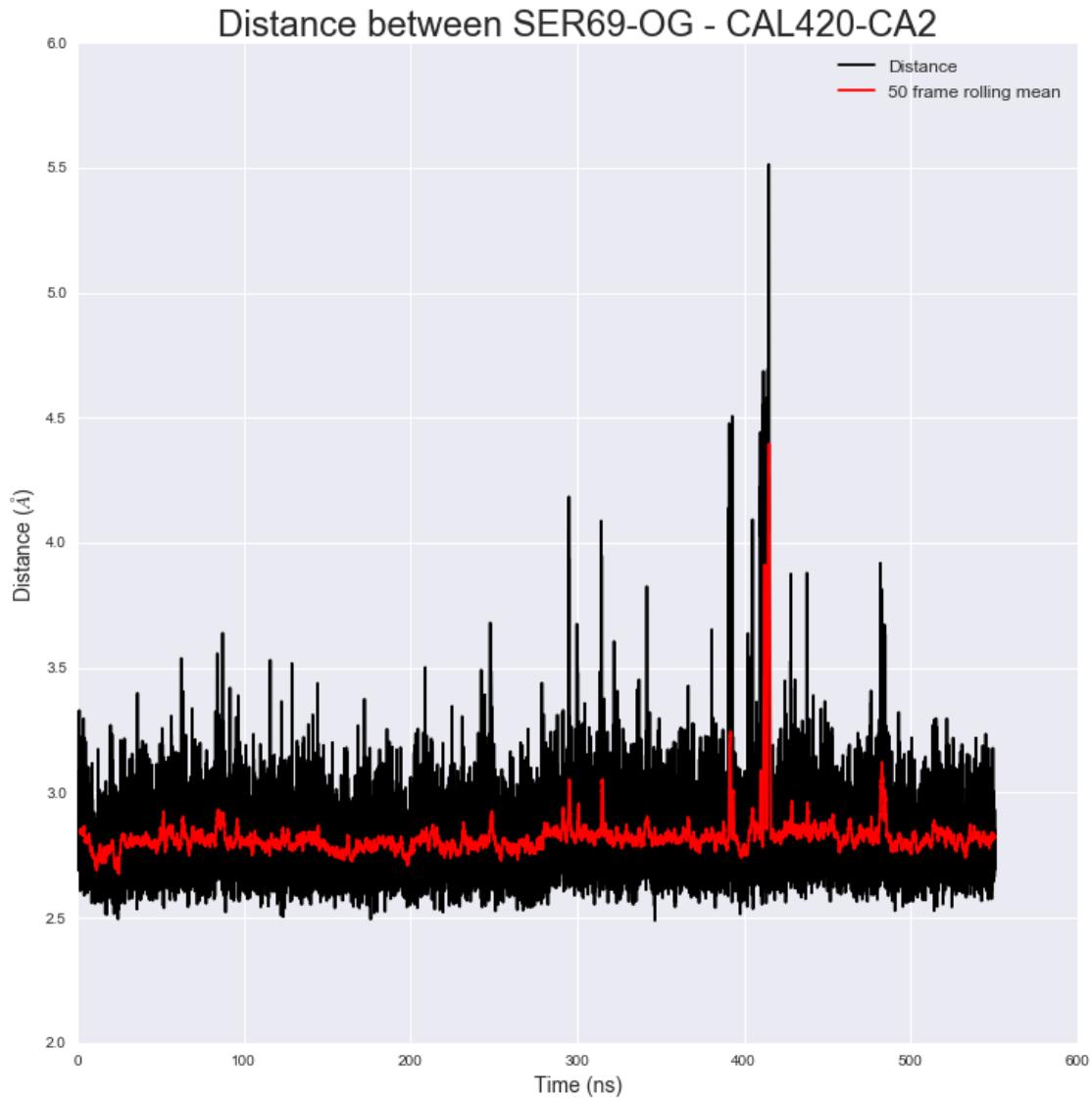
Loading trajectories from the following files:

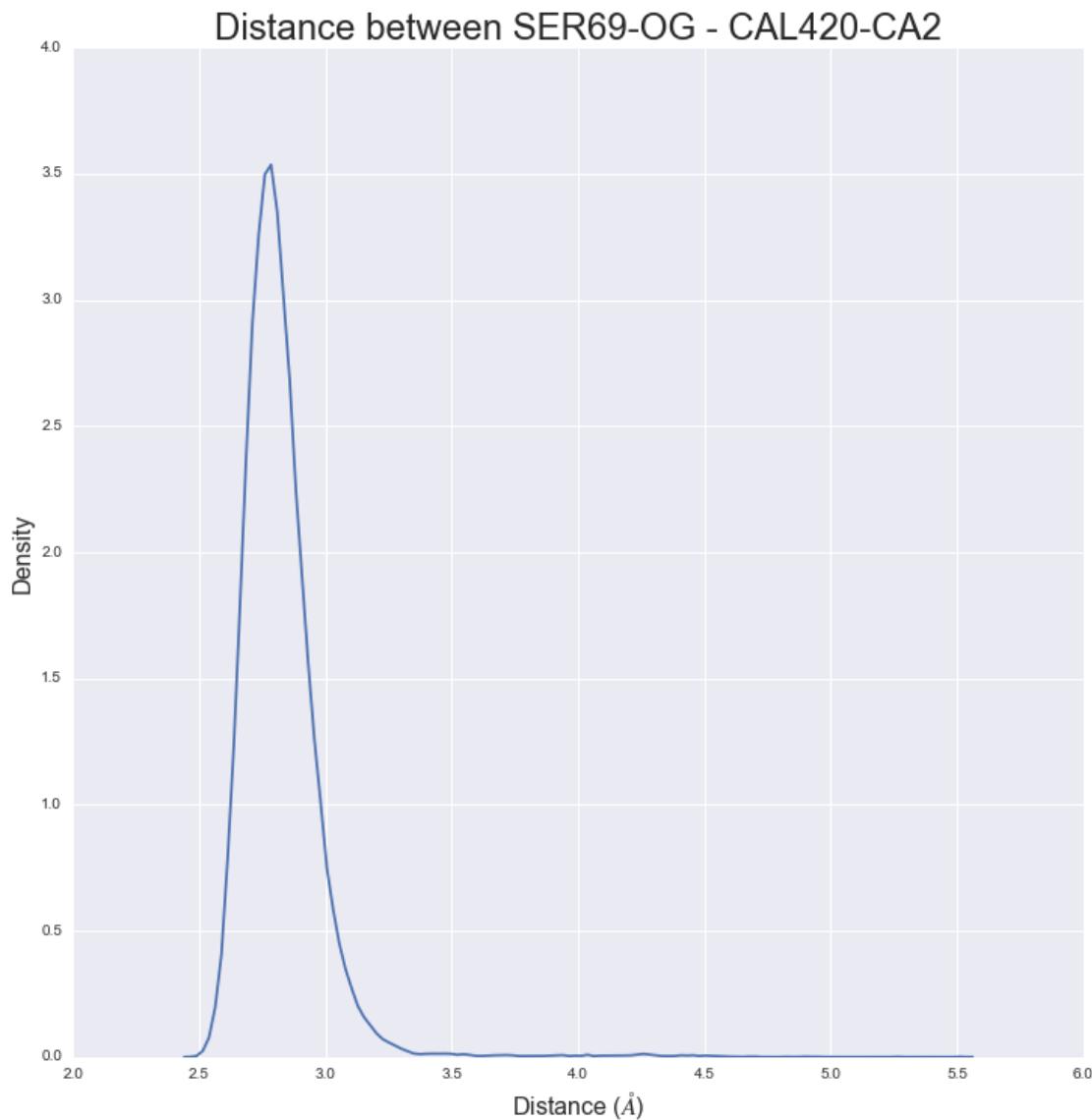
05\_Prod\_troponin\_egcg\_MD5\_000-050\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD5\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD5\_100-150\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD5\_150-200\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_200-250\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_250-300\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_300-350\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_350-400\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_400-450\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_450-500\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_500-550\_run1\_nowater.nc





Total execution time: 4.74 seconds

Total simulation time of all frames: 549.999980469 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1071

Atom2 number: 6810

Calculating distance between following atoms: THR71-OG1 - CAL420-CA2

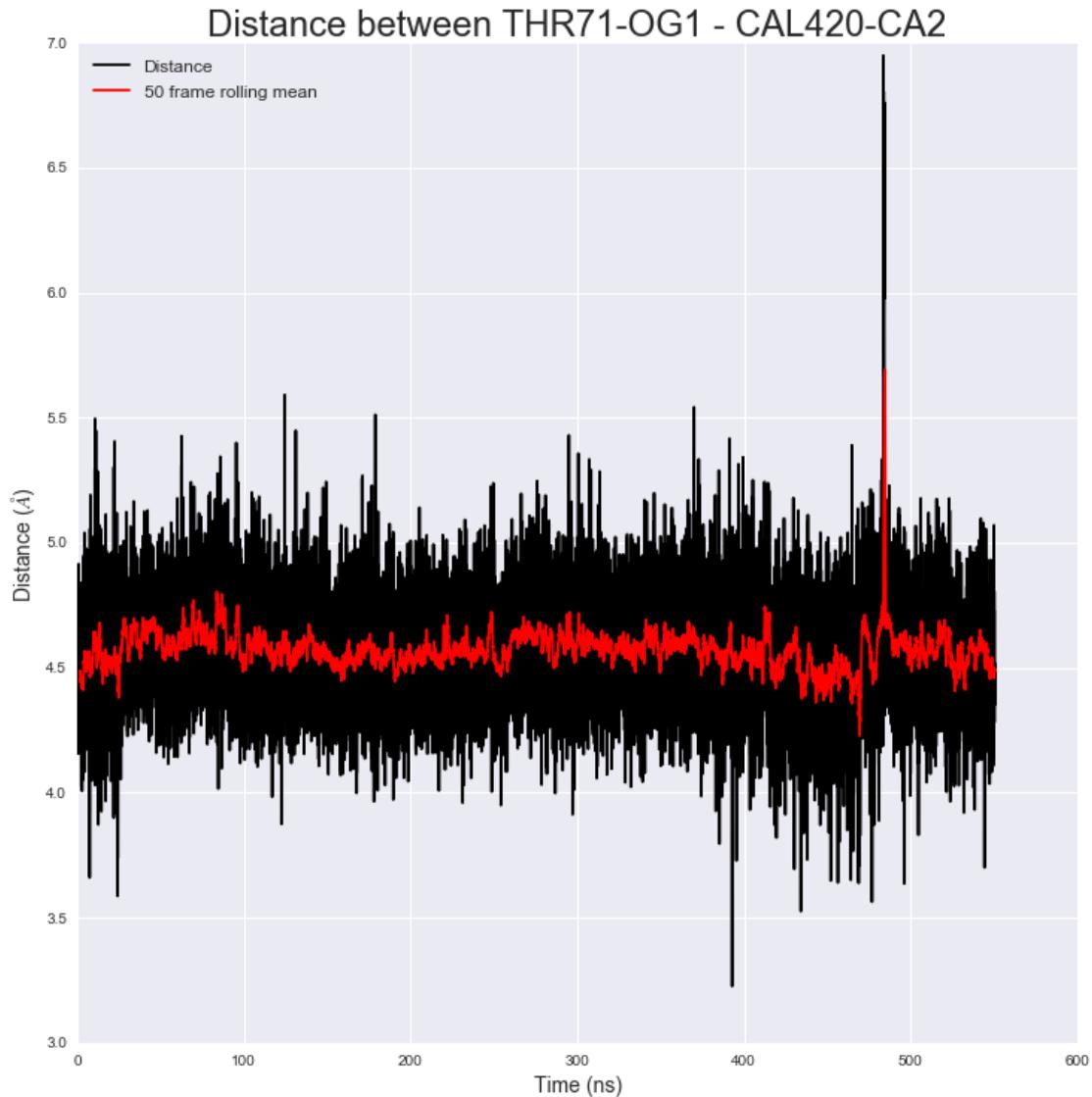
Loading trajectories from the following files:

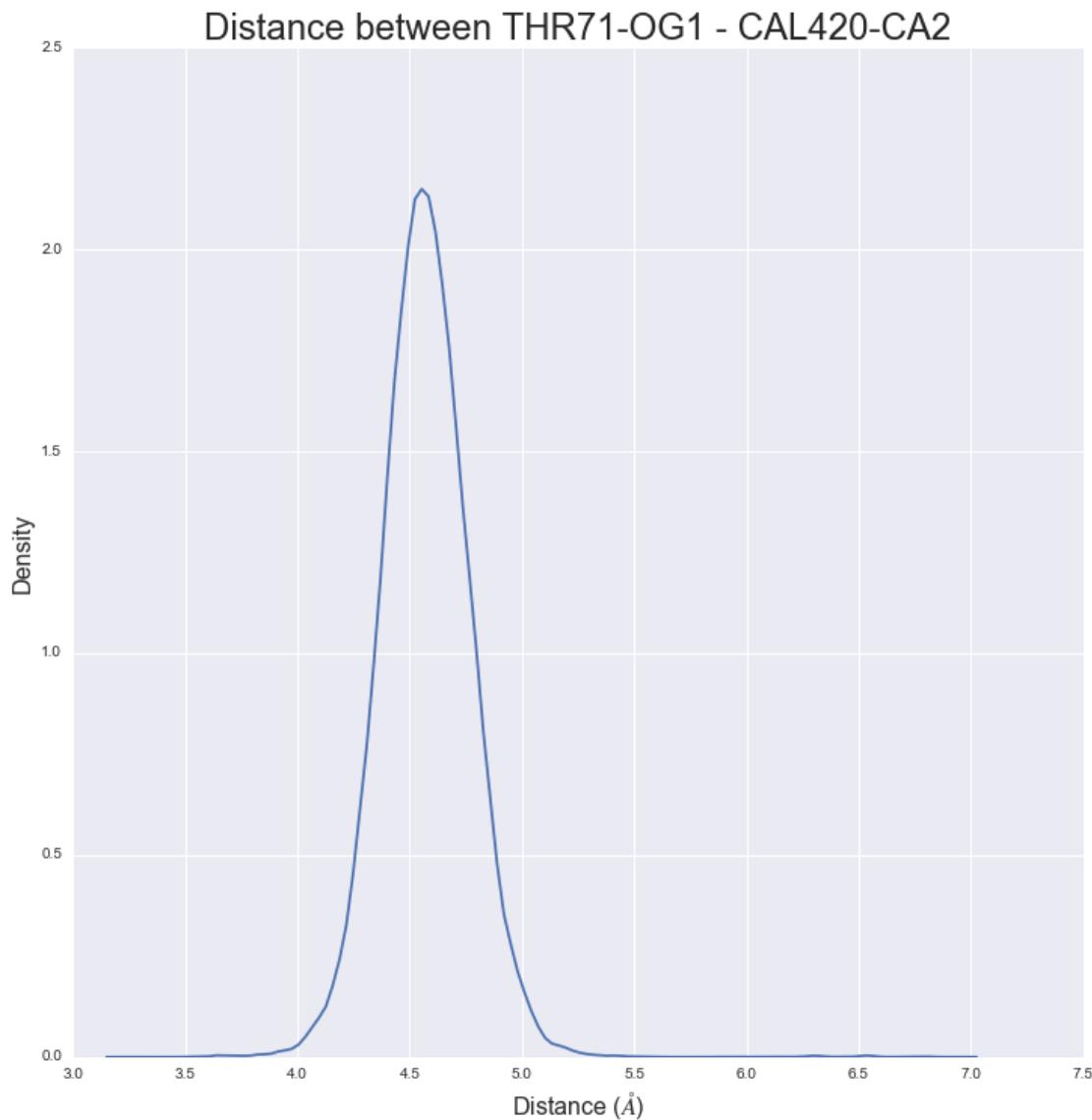
05\_Prod\_troponin\_egcg\_MD5\_000-050\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD5\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD5\_100-150\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD5\_150-200\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_200-250\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_250-300\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_300-350\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_350-400\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_400-450\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_450-500\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_500-550\_run1\_nowater.nc





Total execution time: 4.98 seconds

Total simulation time of all frames: 549.999980469 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1099

Atom2 number: 6810

Calculating distance between following atoms: ASP73-OD1 - CAL420-CA2

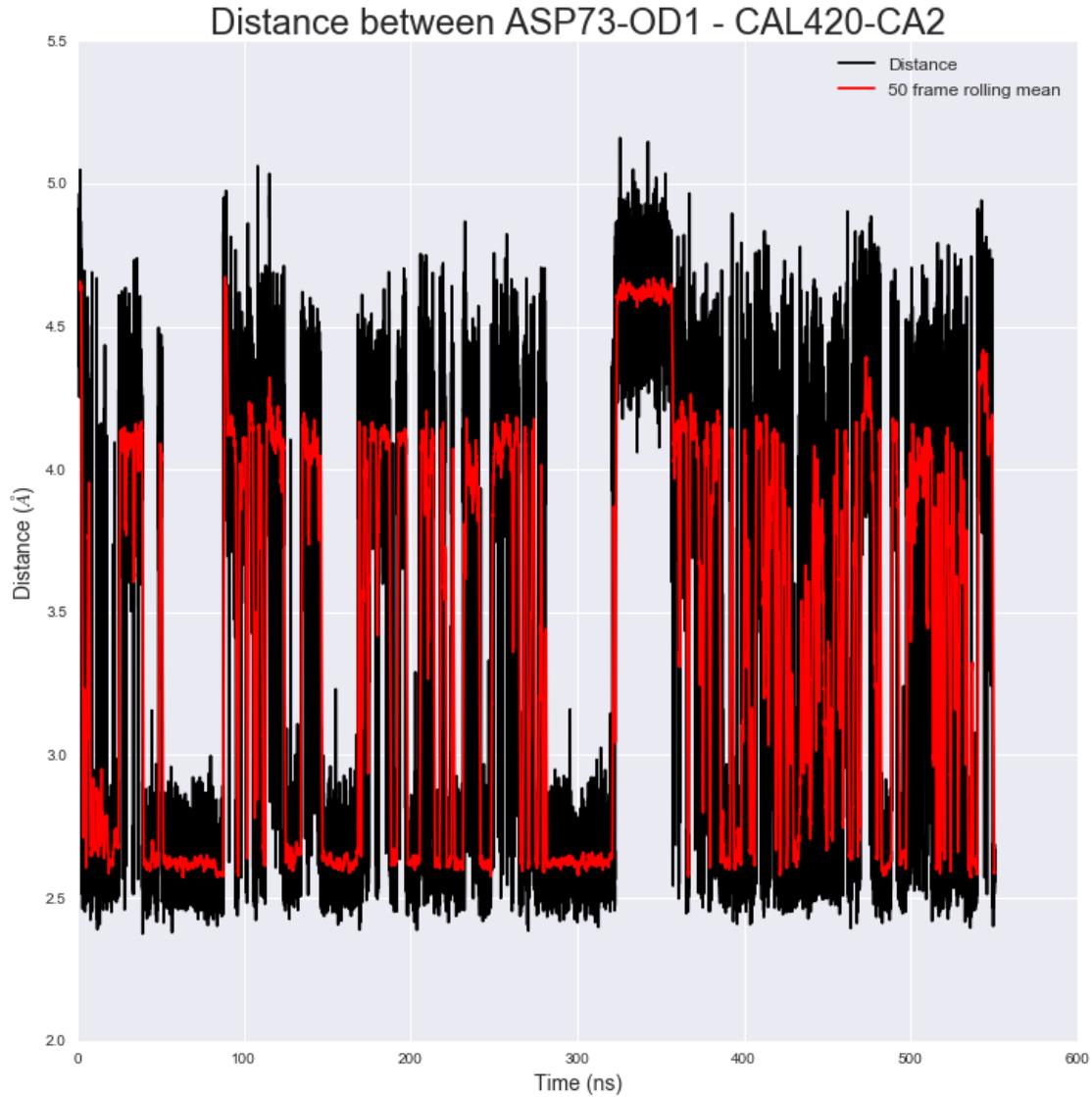
Loading trajectories from the following files:

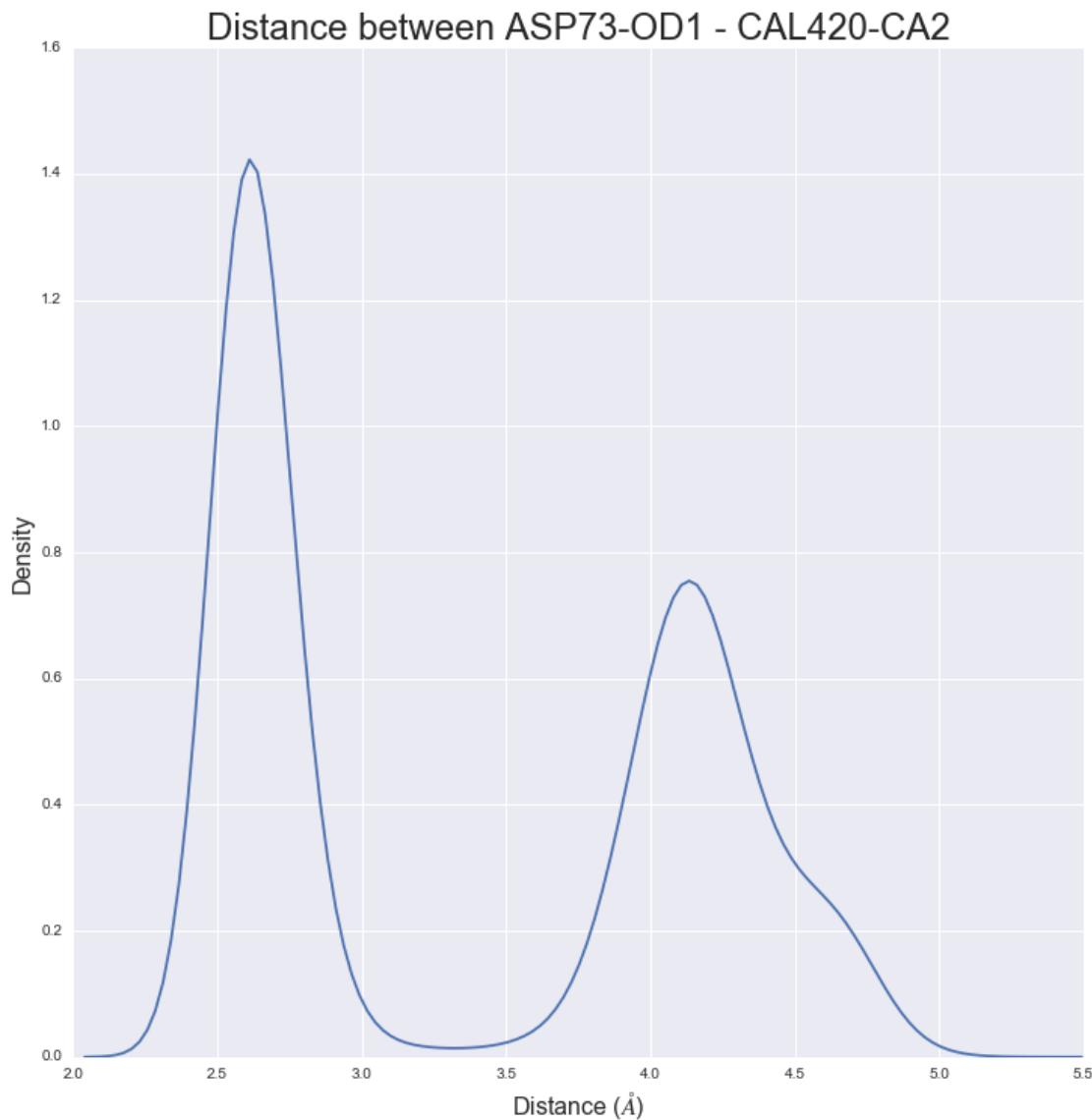
05\_Prod\_troponin\_egcg\_MD5\_000-050\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD5\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD5\_100-150\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD5\_150-200\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_200-250\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_250-300\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_300-350\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_350-400\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_400-450\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_450-500\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_500-550\_run1\_nowater.nc





Total execution time: 4.90 seconds

Total simulation time of all frames: 549.999980469 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1100

Atom2 number: 6810

Calculating distance between following atoms: ASP73-OD2 - CAL420-CA2

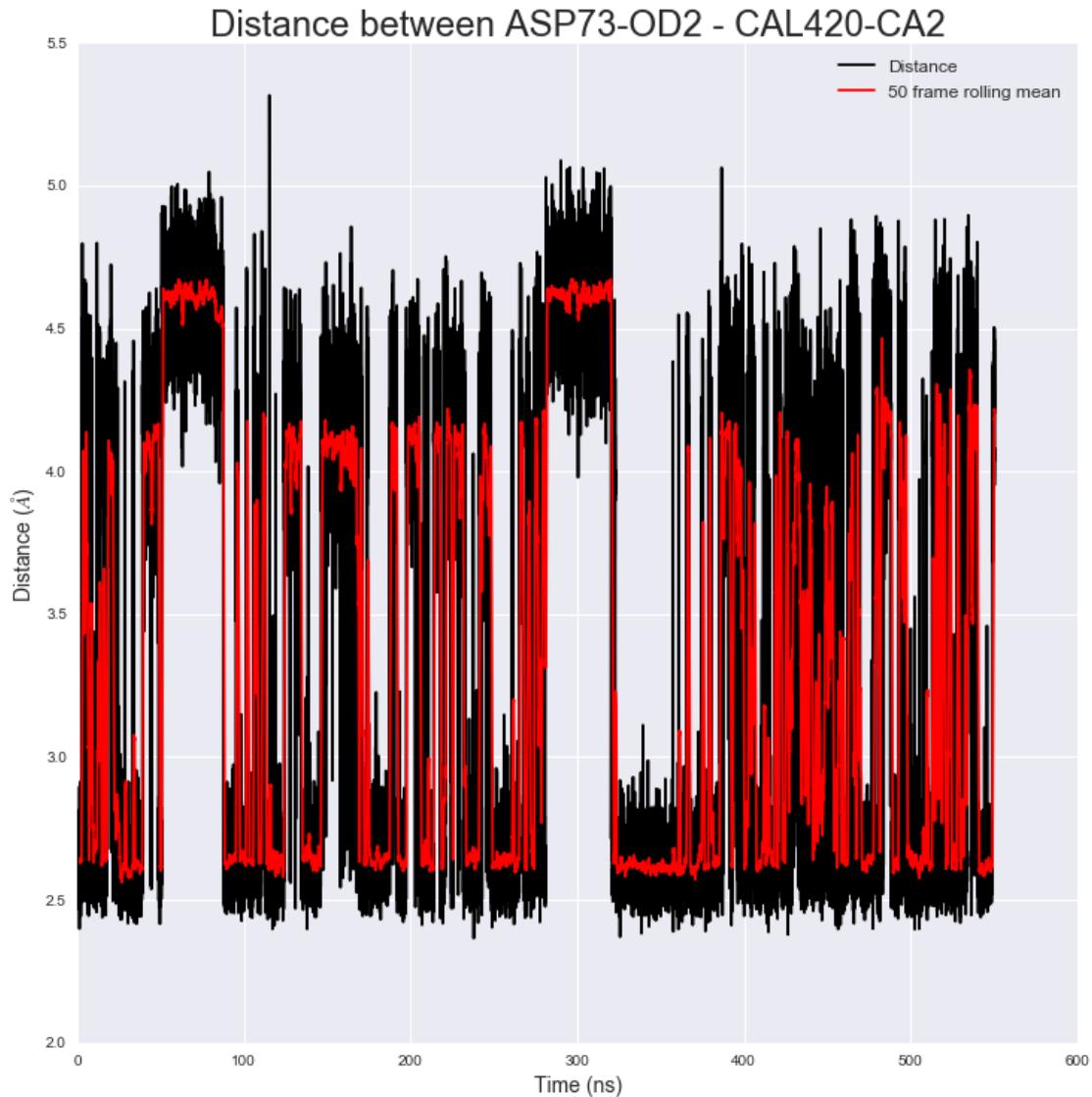
Loading trajectories from the following files:

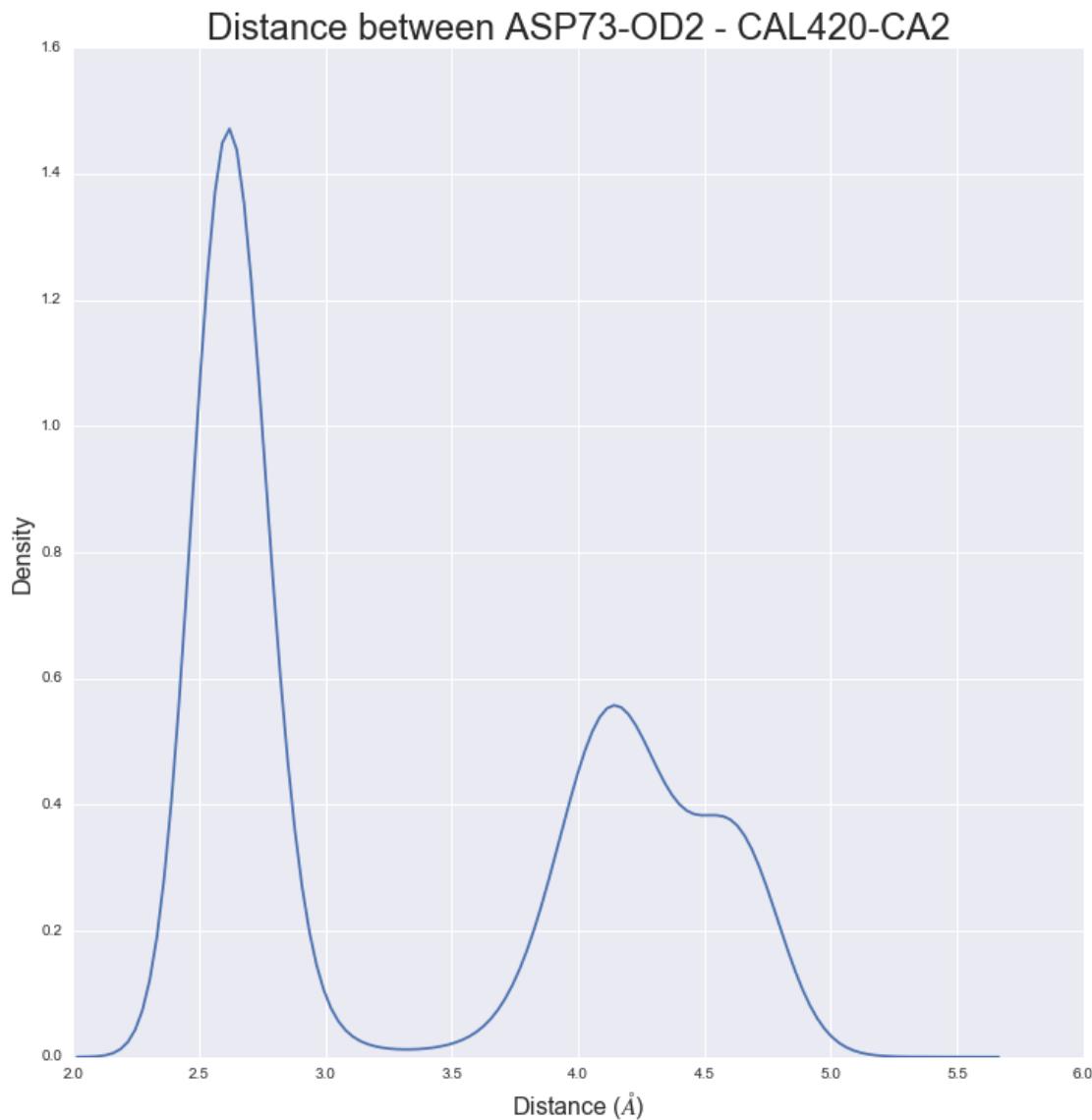
05\_Prod\_troponin\_egcg\_MD5\_000-050\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD5\_050-100\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD5\_100-150\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD5\_150-200\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_200-250\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_250-300\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_300-350\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_350-400\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_400-450\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_450-500\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_500-550\_run1\_nowater.nc





Total execution time: 5.27 seconds

Total simulation time of all frames: 549.999980469 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1131

Atom2 number: 6810

Calculating distance between following atoms: ASP75-OD1 - CAL420-CA2

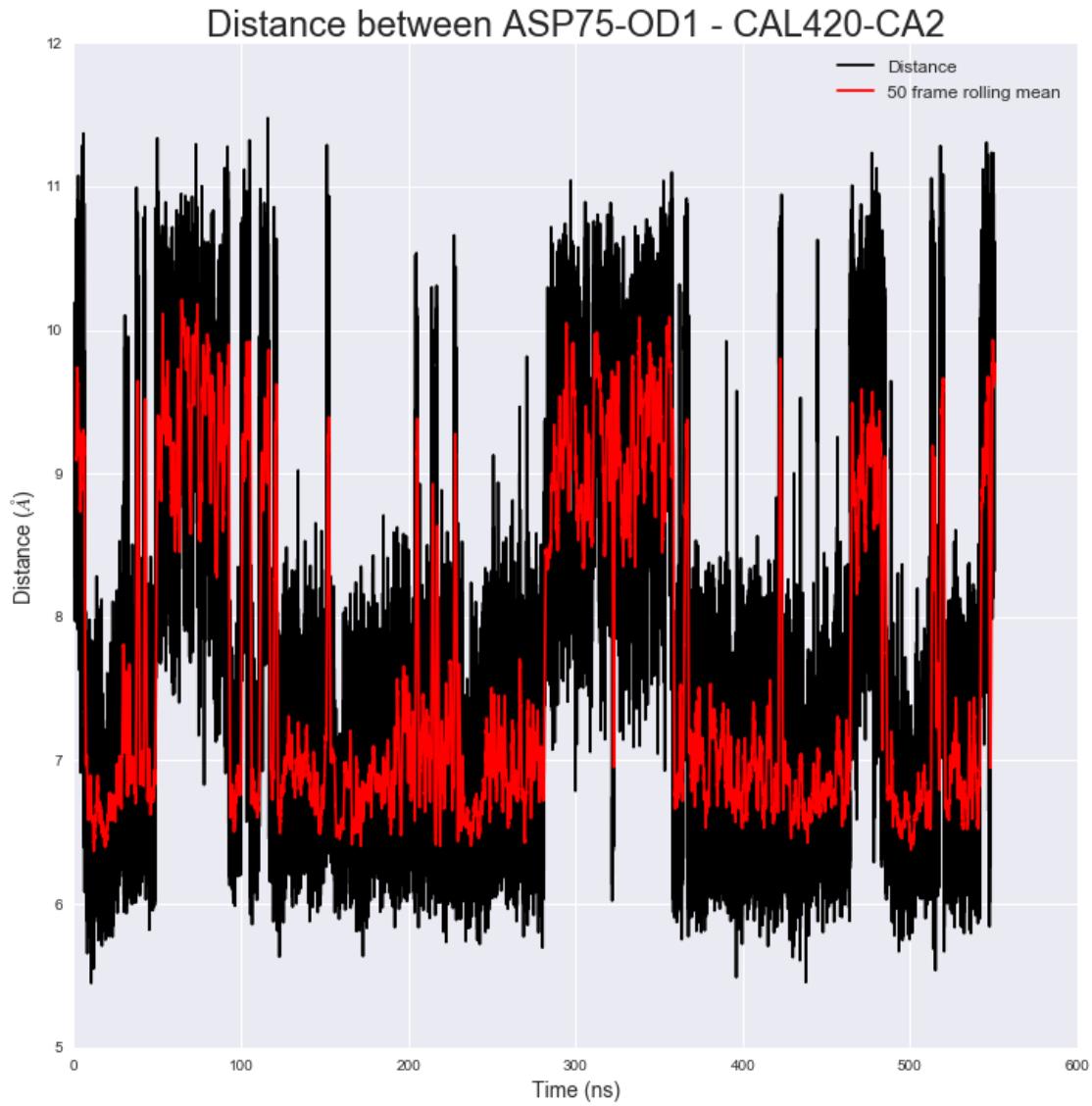
Loading trajectories from the following files:

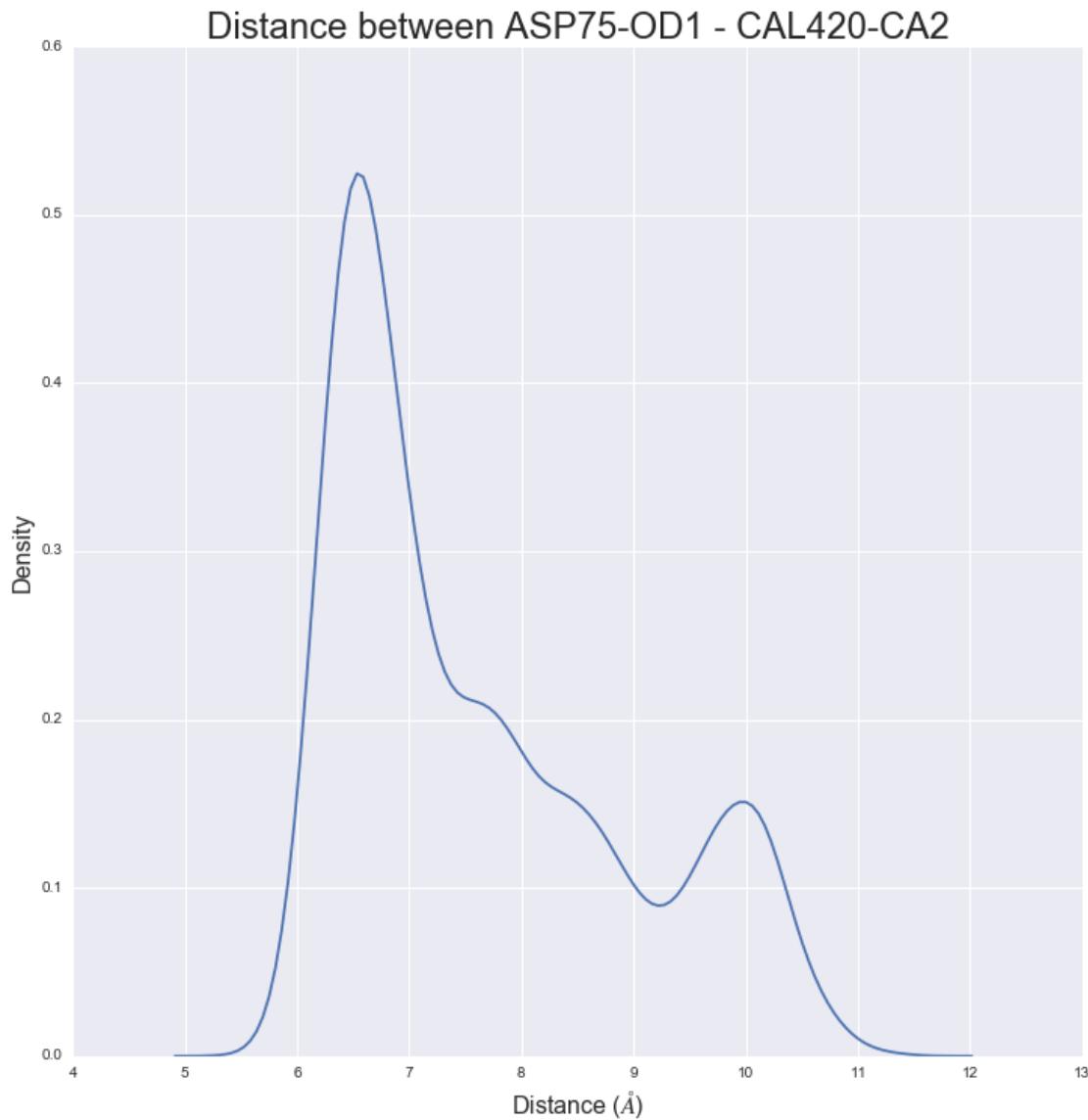
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05\_Prod\_troponin\_egcg\_MD5\_100-150\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD5\_150-200\_run1\_nowater.nc  
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05\_Prod\_troponin\_egcg\_MD5\_250-300\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_300-350\_run1\_nowater.nc  
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05\_Prod\_troponin\_egcg\_MD5\_400-450\_run1\_nowater.nc  
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Total execution time: 5.04 seconds

Total simulation time of all frames: 549.999980469 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1132

Atom2 number: 6810

Calculating distance between following atoms: ASP75-OD2 - CAL420-CA2

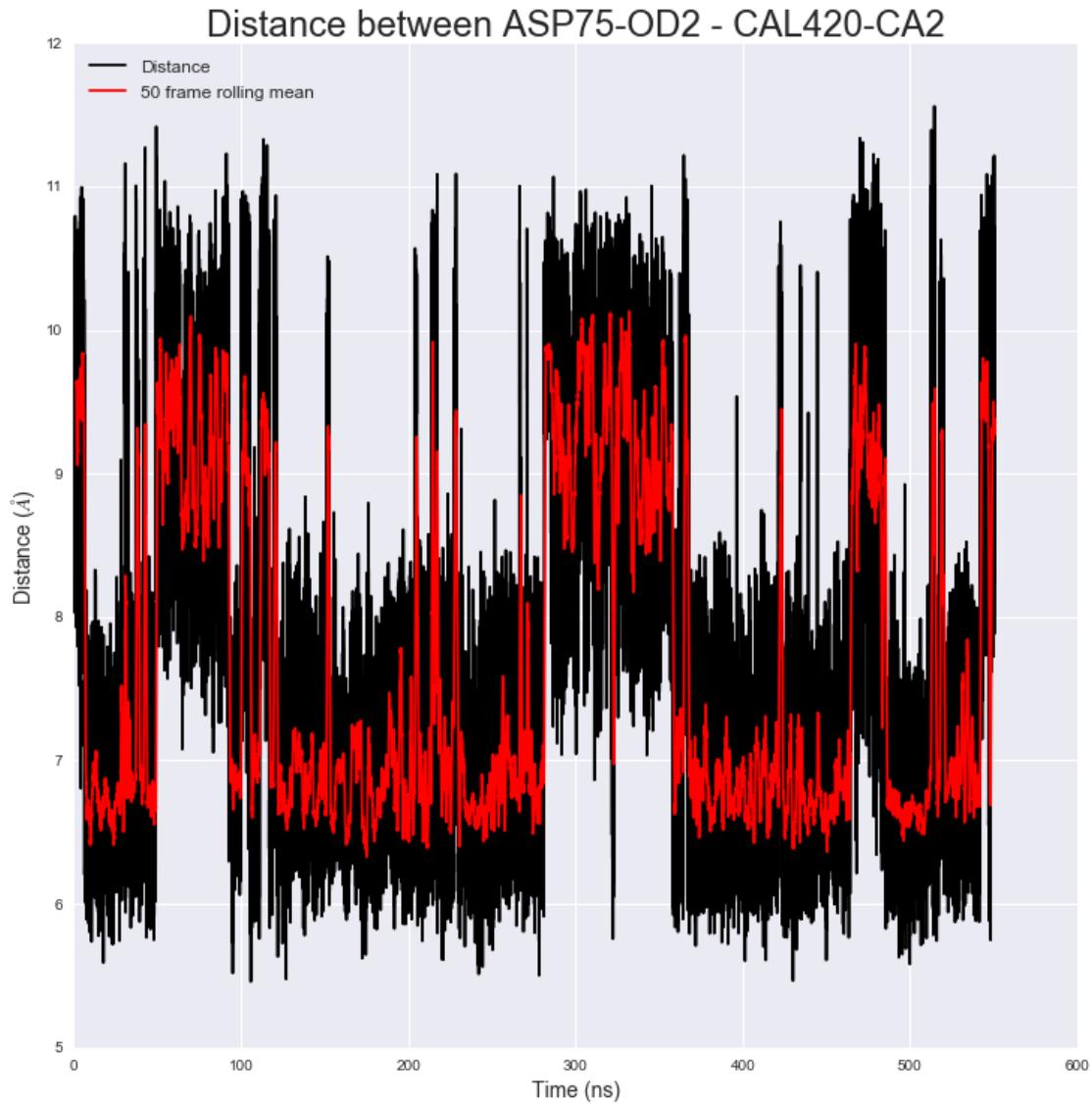
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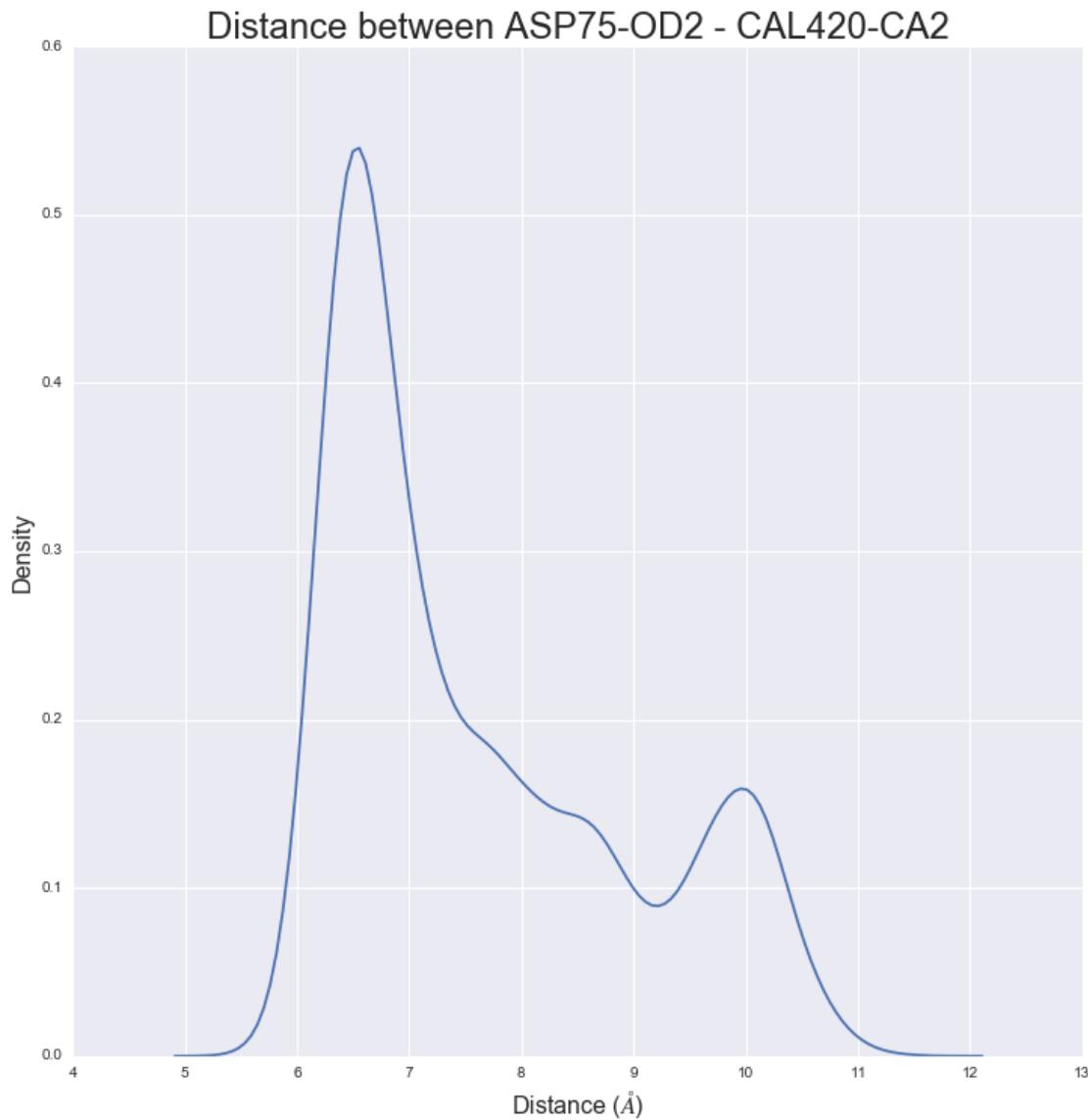
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05\_Prod\_troponin\_egcg\_MD5\_100-150\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD5\_150-200\_run1\_nowater.nc  
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05\_Prod\_troponin\_egcg\_MD5\_300-350\_run1\_nowater.nc  
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05\_Prod\_troponin\_egcg\_MD5\_400-450\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_450-500\_run1\_nowater.nc  
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Total execution time: 5.54 seconds

Total simulation time of all frames: 549.999980469 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1146

Atom2 number: 6810

Calculating distance between following atoms: GLU76-OE1 - CAL420-CA2

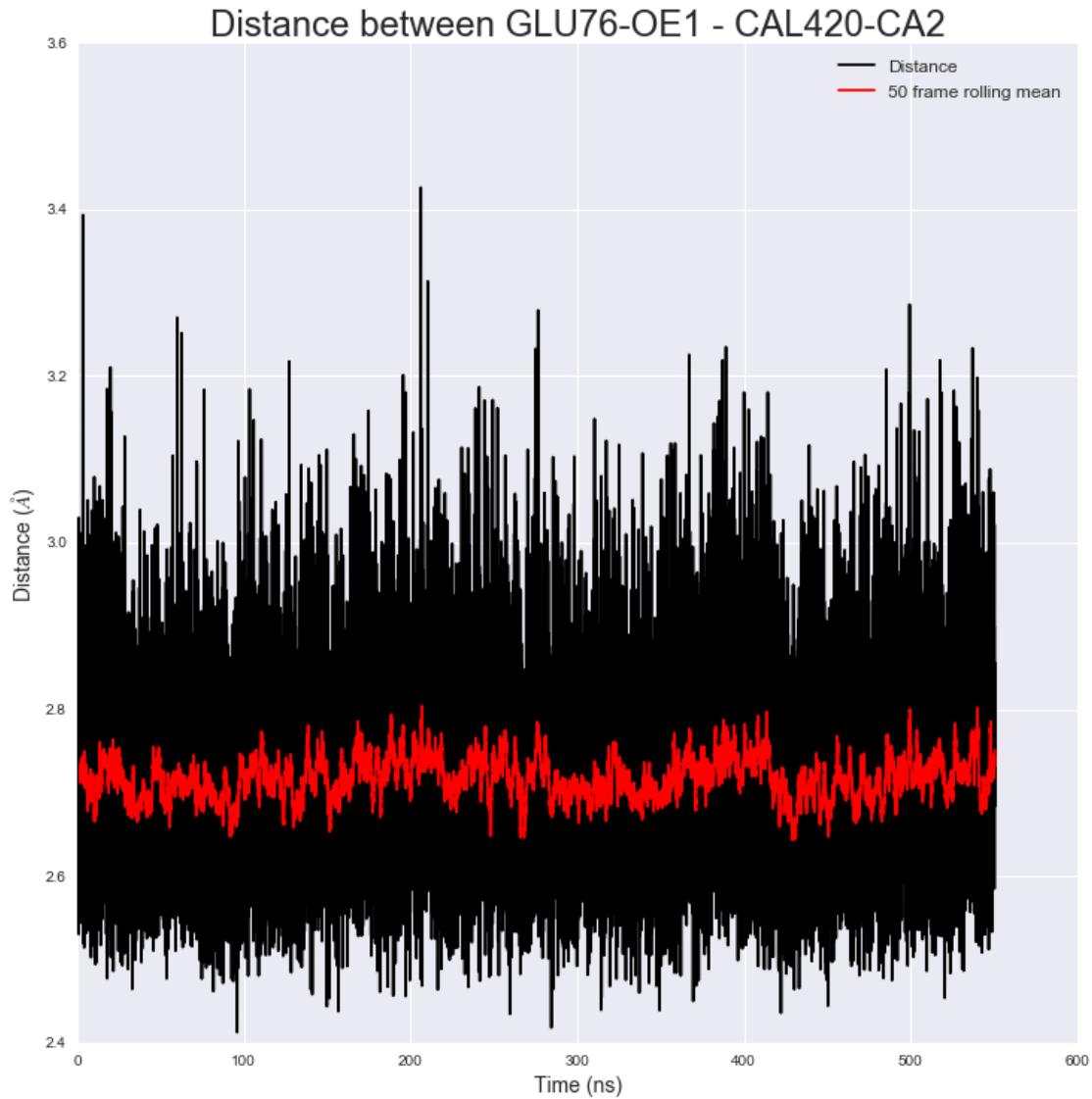
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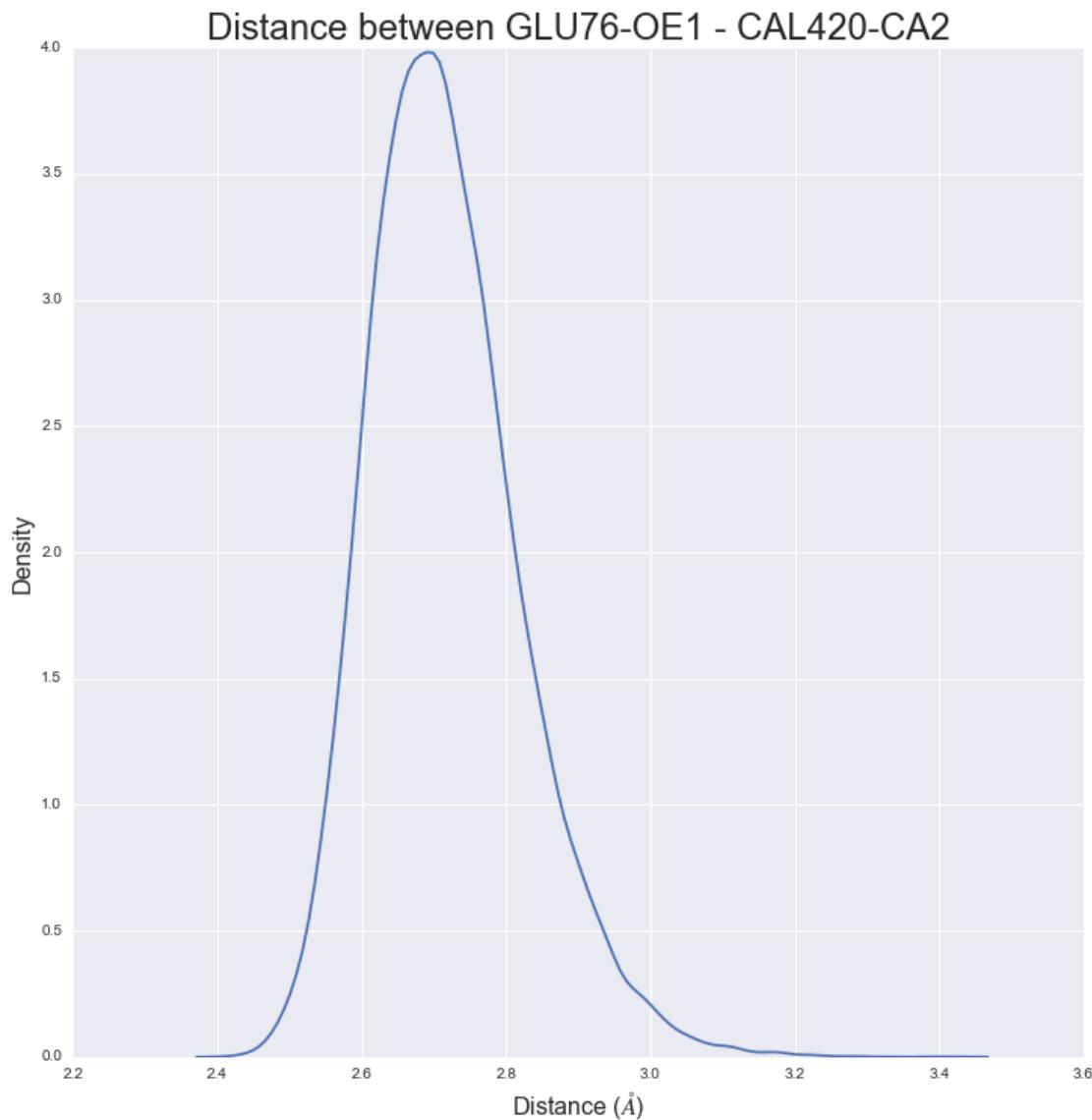
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05\_Prod\_troponin\_egcg\_MD5\_100-150\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD5\_150-200\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_200-250\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_250-300\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_300-350\_run1\_nowater.nc  
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Total execution time: 5.20 seconds

Total simulation time of all frames: 549.999980469 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Atom1 number: 1147

Atom2 number: 6810

Calculating distance between following atoms: GLU76-OE2 - CAL420-CA2

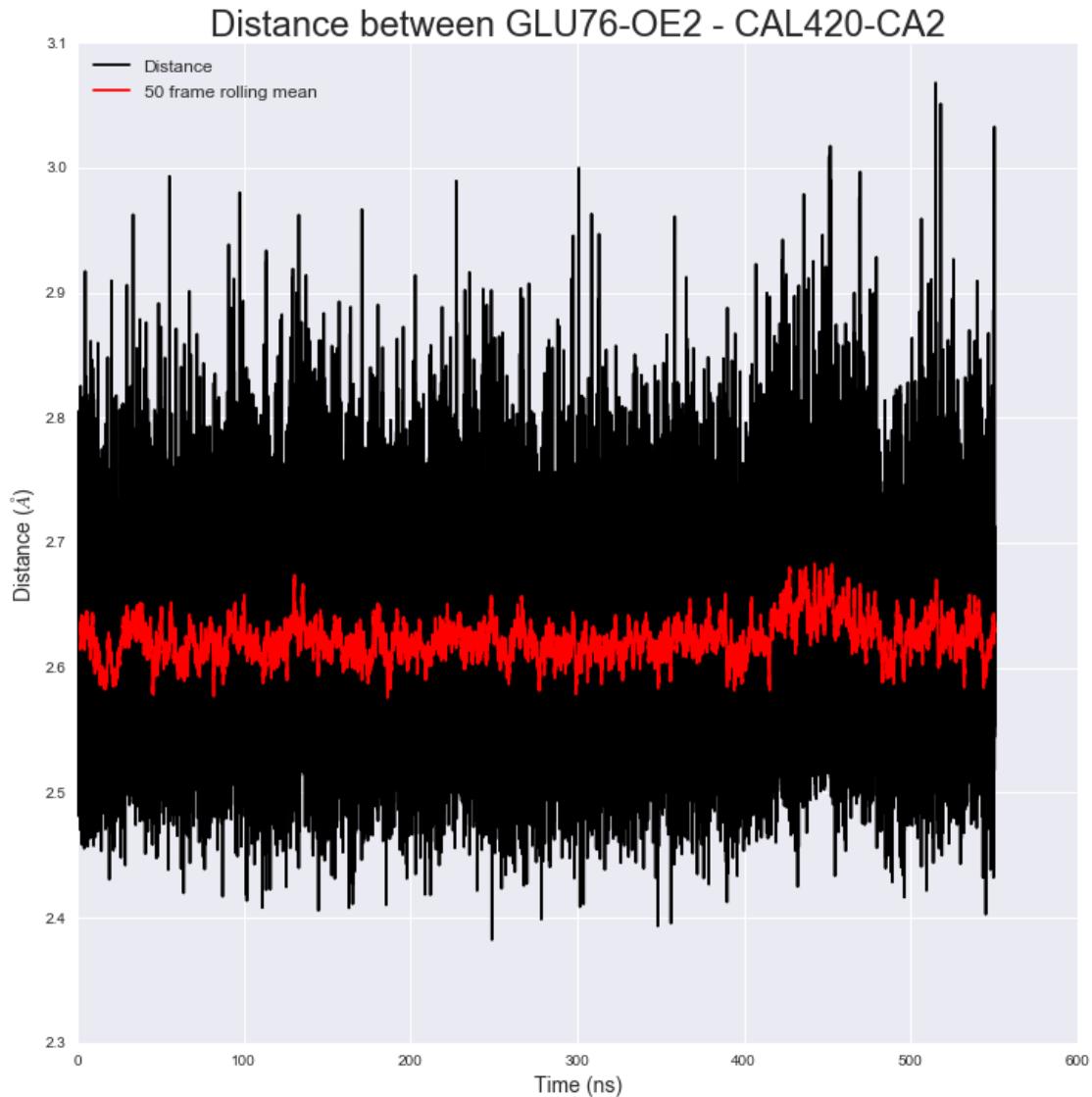
Loading trajectories from the following files:

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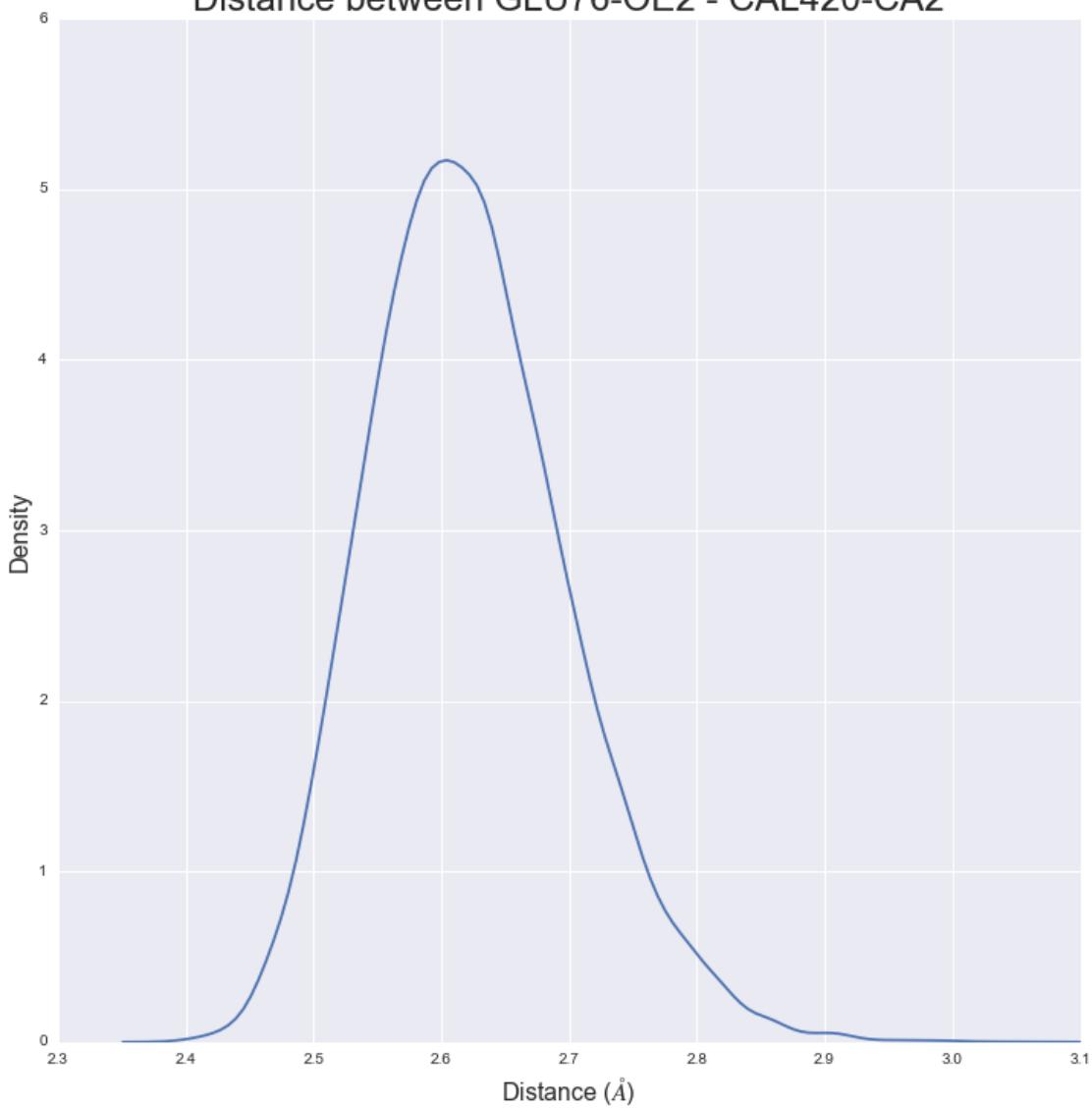
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05\_Prod\_troponin\_egcg\_MD5\_100-150\_run1\_nowater.nc

05\_Prod\_troponin\_egcg\_MD5\_150-200\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_200-250\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_250-300\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_300-350\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_350-400\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_400-450\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_450-500\_run1\_nowater.nc  
05\_Prod\_troponin\_egcg\_MD5\_500-550\_run1\_nowater.nc



### Distance between GLU76-OE2 - CAL420-CA2



Total execution time: 5.27 seconds

Total simulation time of all frames: 549.999980469 nanoseconds

In [ ]: