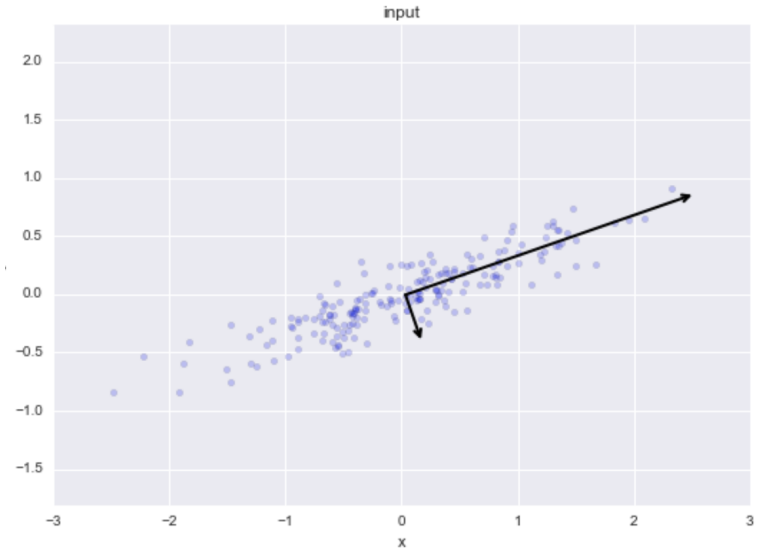
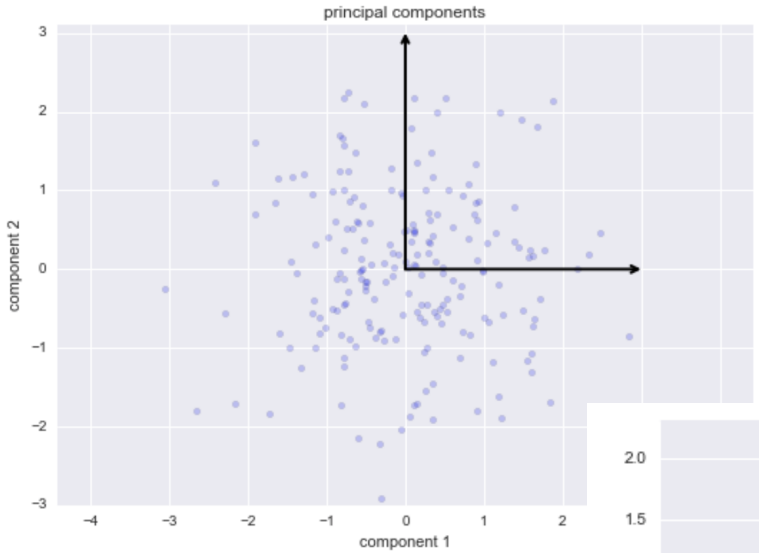
Dimensionality Reduction

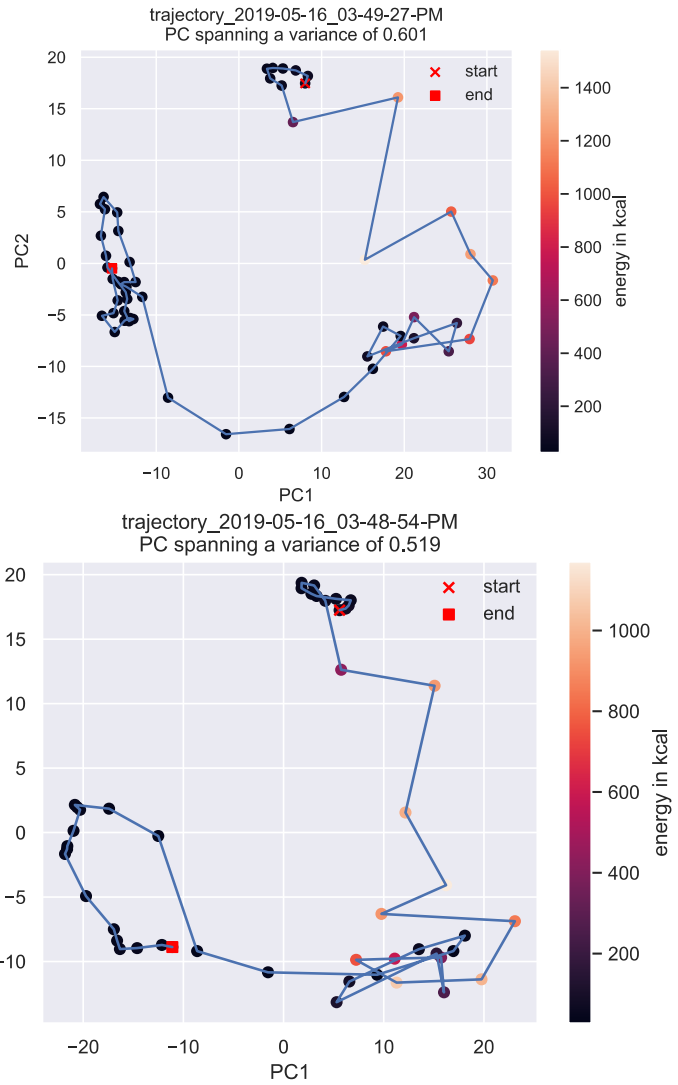
Example PCA plots

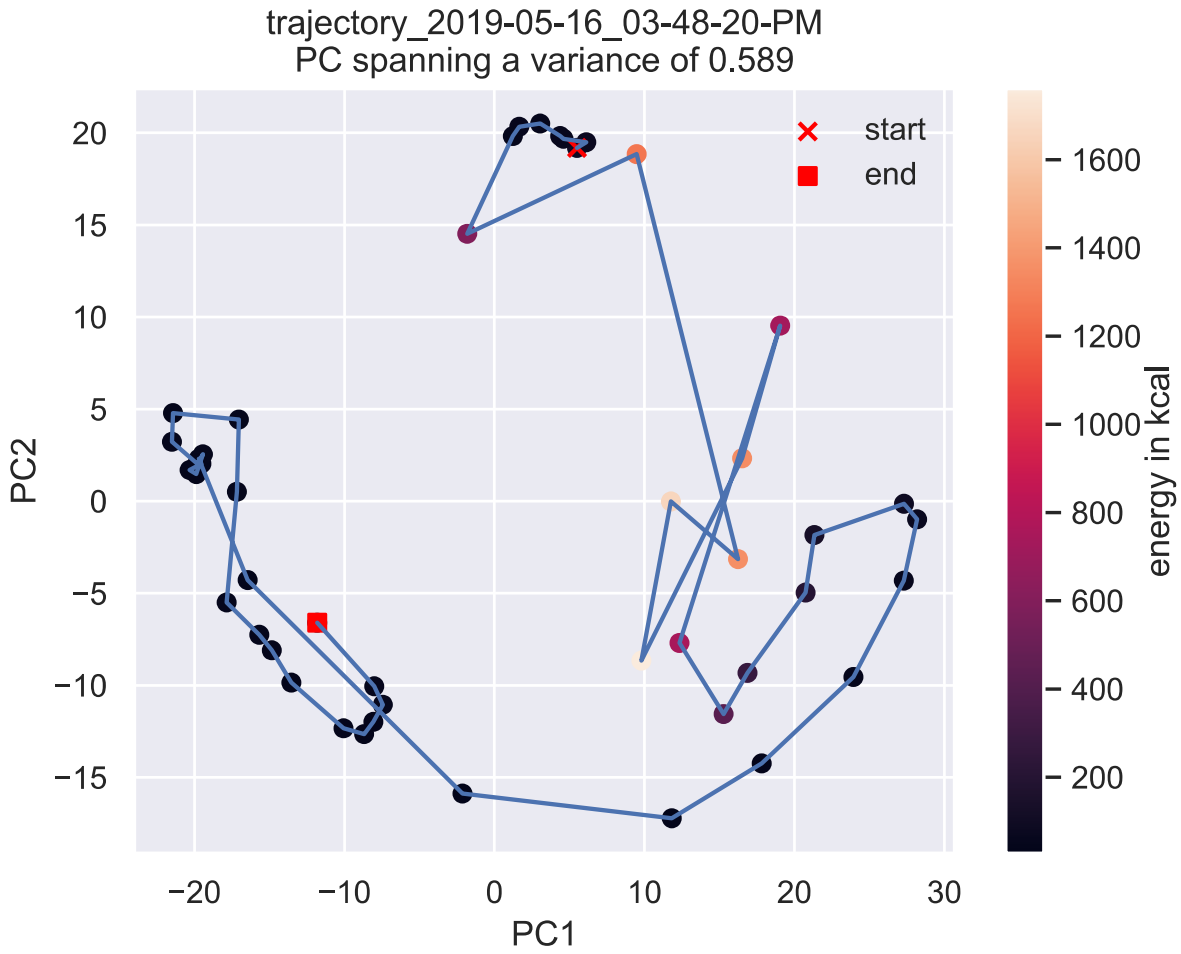


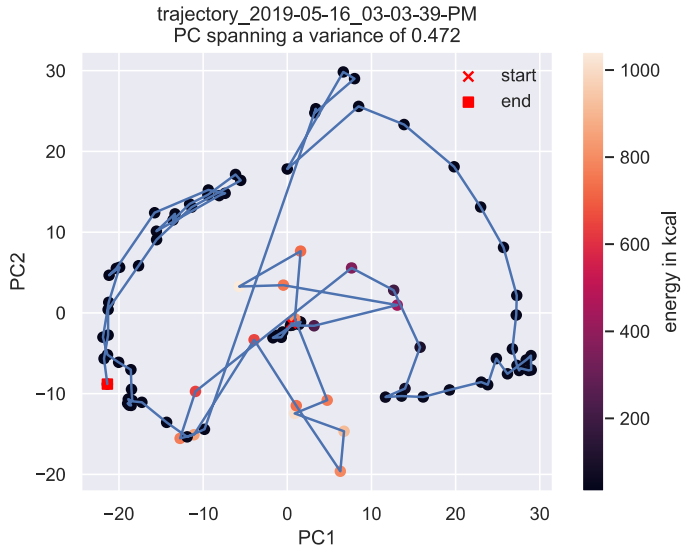


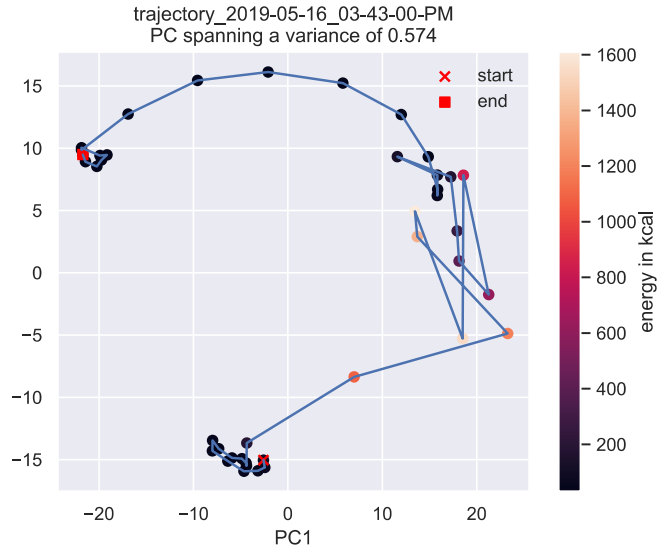
https://jakevdp.github.io/PythonDataScienceHandbook/05.09-principal-component-analysis.html

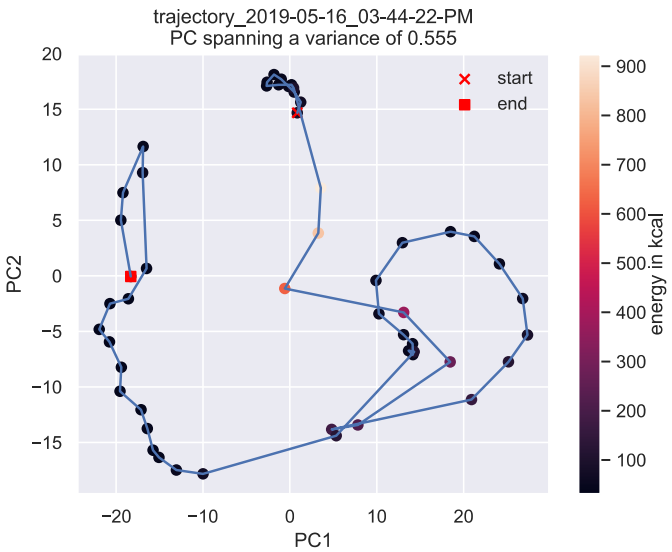
Principal components 1 and 2 with energy

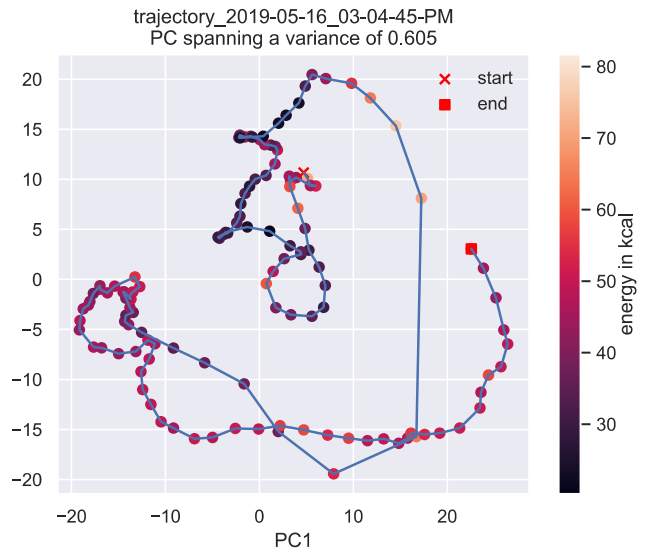


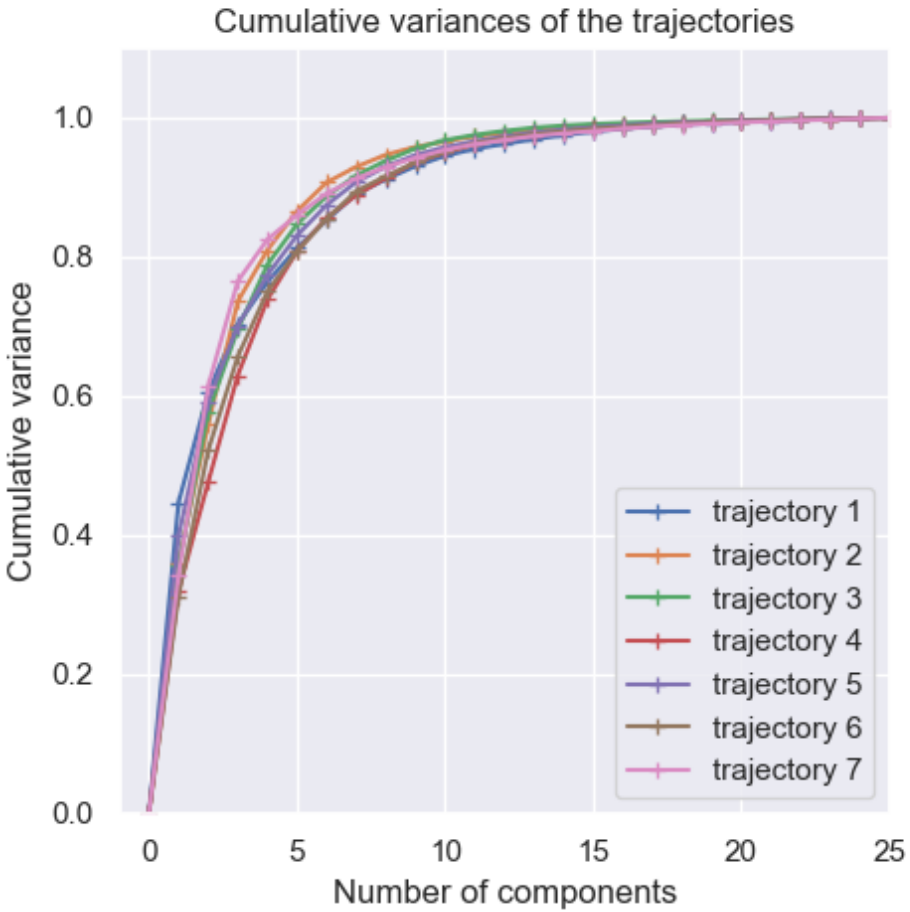


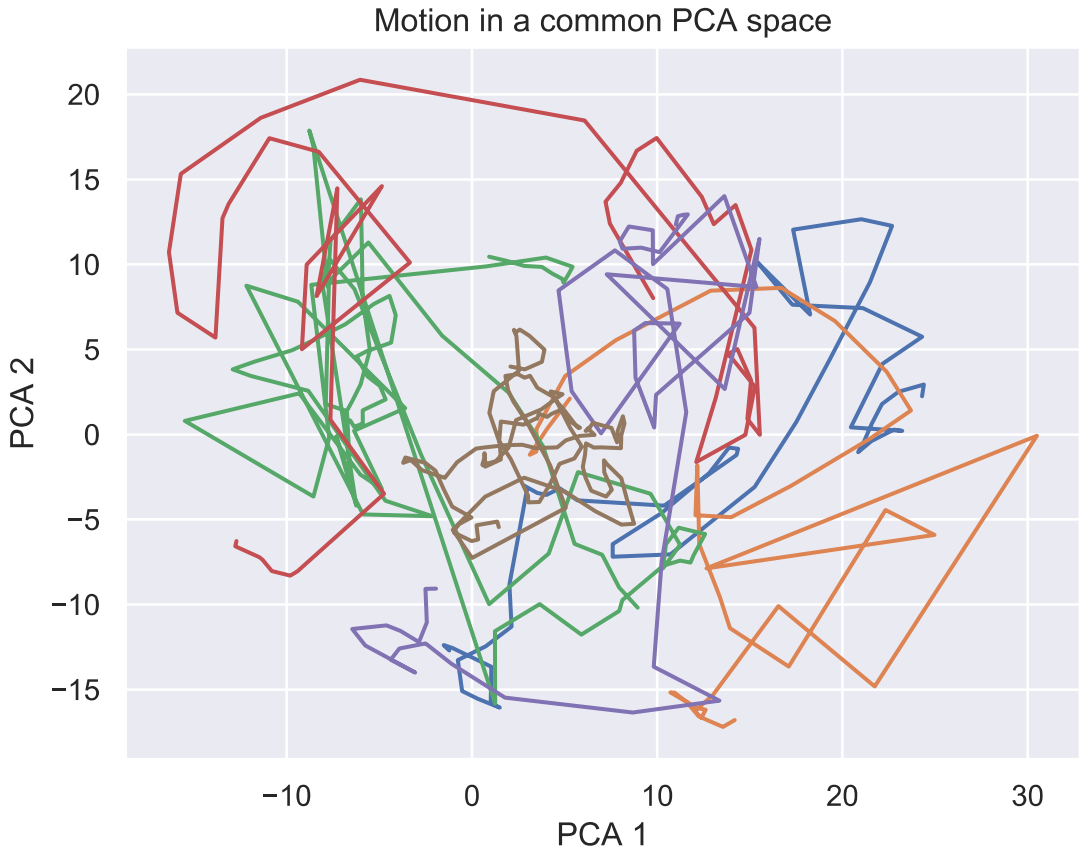

trajectory_2019-05-16_03-03-39-PM
PC spanning a variance of 0.472
start
end
PC1
PC2
energy in kcal


trajectory_2019-05-16_03-43-00-PM
PC spanning a variance of 0.574
start
end
PC1
energy in kcal

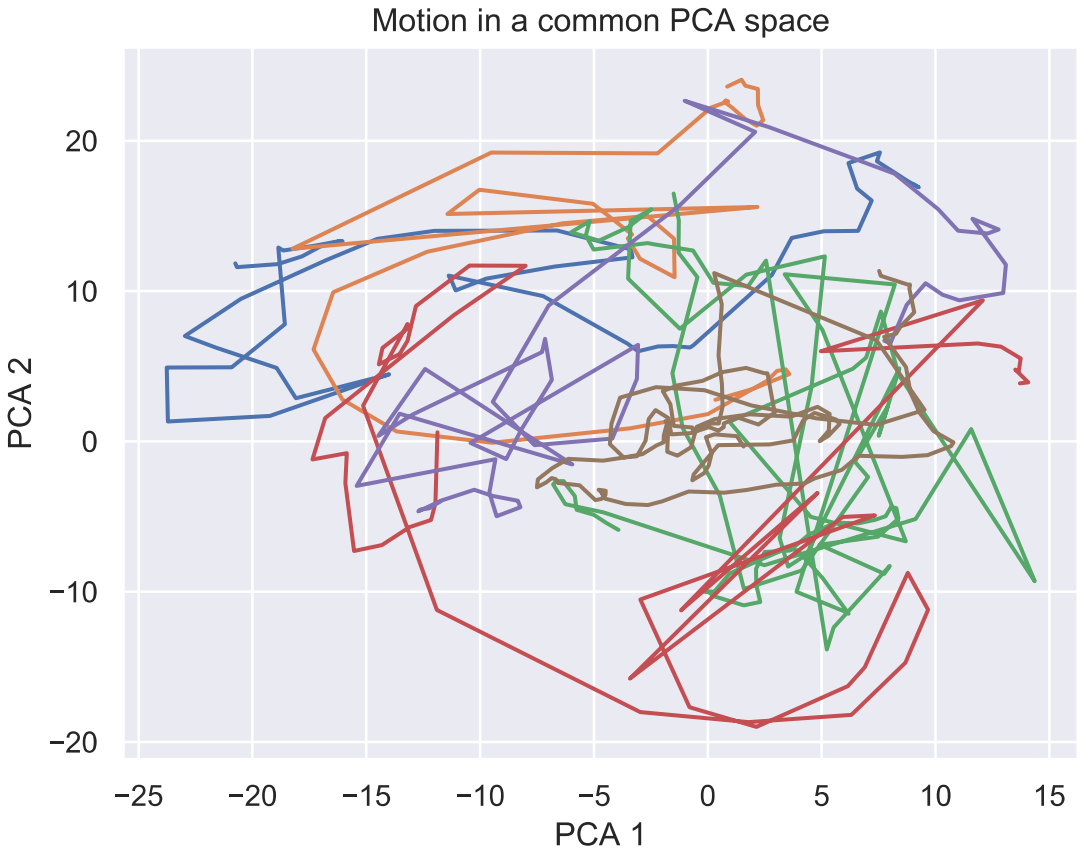

trajectory_2019-05-16_03-44-22-PM
PC spanning a variance of 0.555
start
end
PC1
PC2
energy in kcal


trajectory_2019-05-16_03-04-45-PM
PC spanning a variance of 0.605
start
end
PC1
energy in kcal


Cumulative variances of the trajectories
Cumulative variance
Number of components
trajectory 1
trajectory 2
trajectory 3
trajectory 4
trajectory 5
trajectory 6
trajectory 7

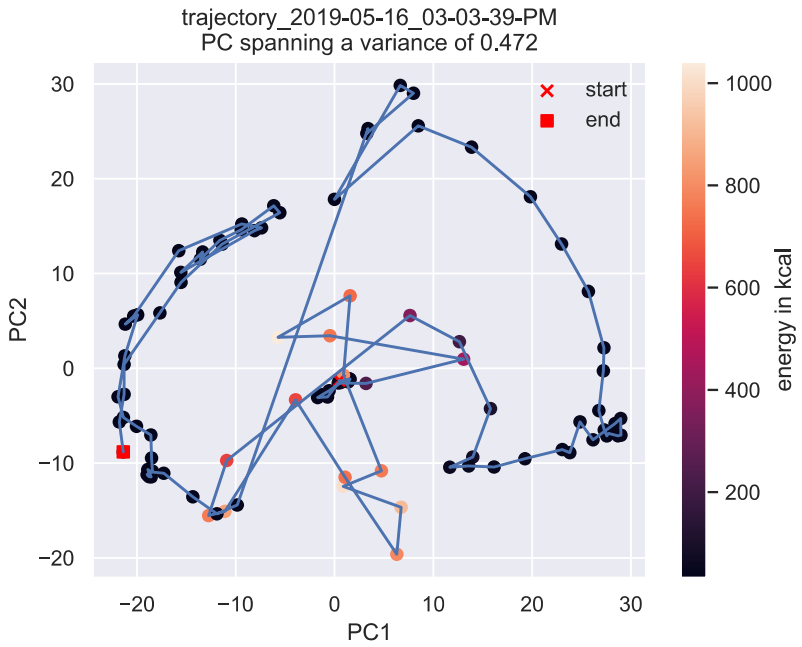


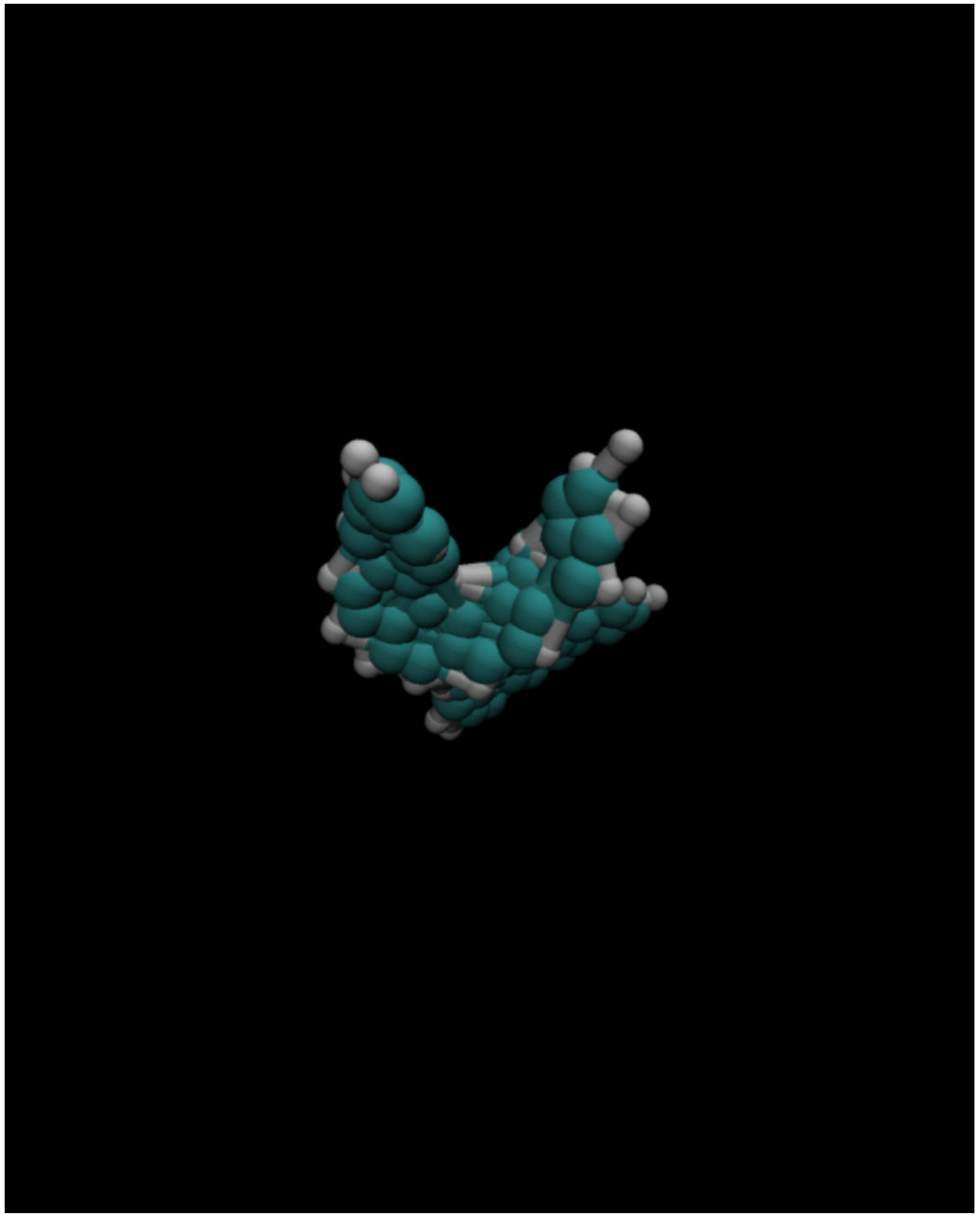
Principal components of individual trajectories



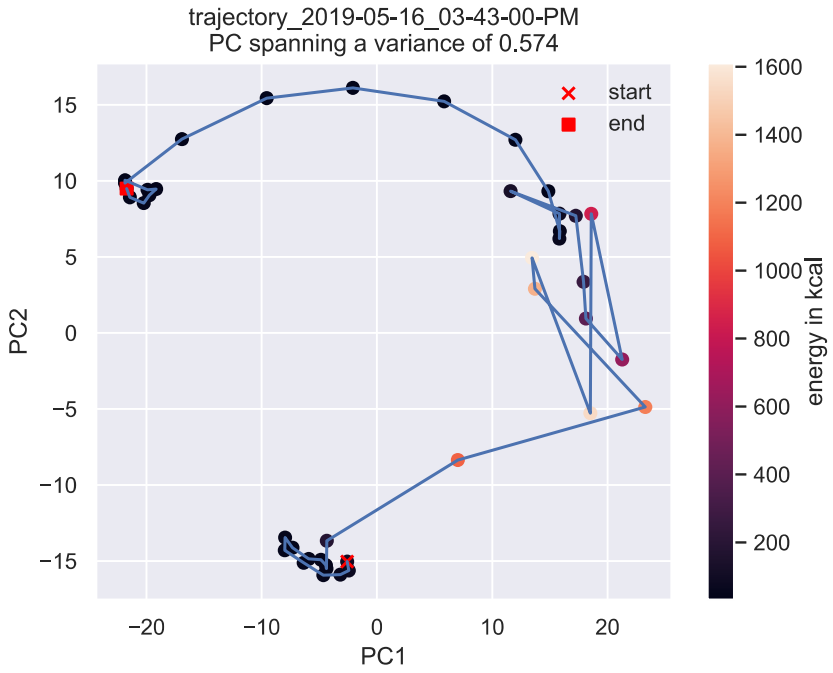
Principal components of combined trajectories

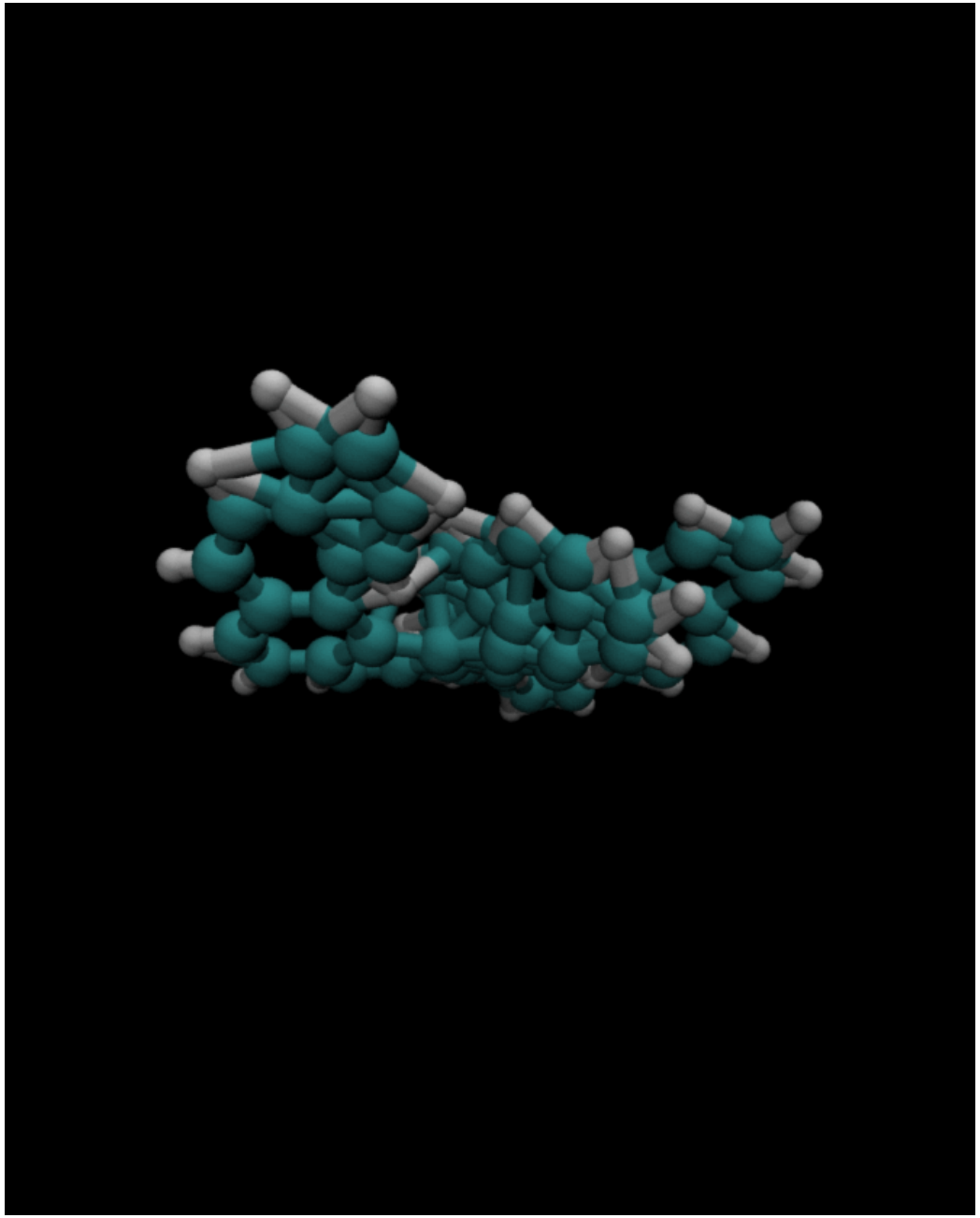
Component 1


trajectory_2019-05-16_03-03-39-PM
PC spanning a variance of 0.472
start
end
PC2
PC1
energy in kcal
30
20
10
0
−10
−20
−20
−10
0
10
20
30
1000
800
600
400
200

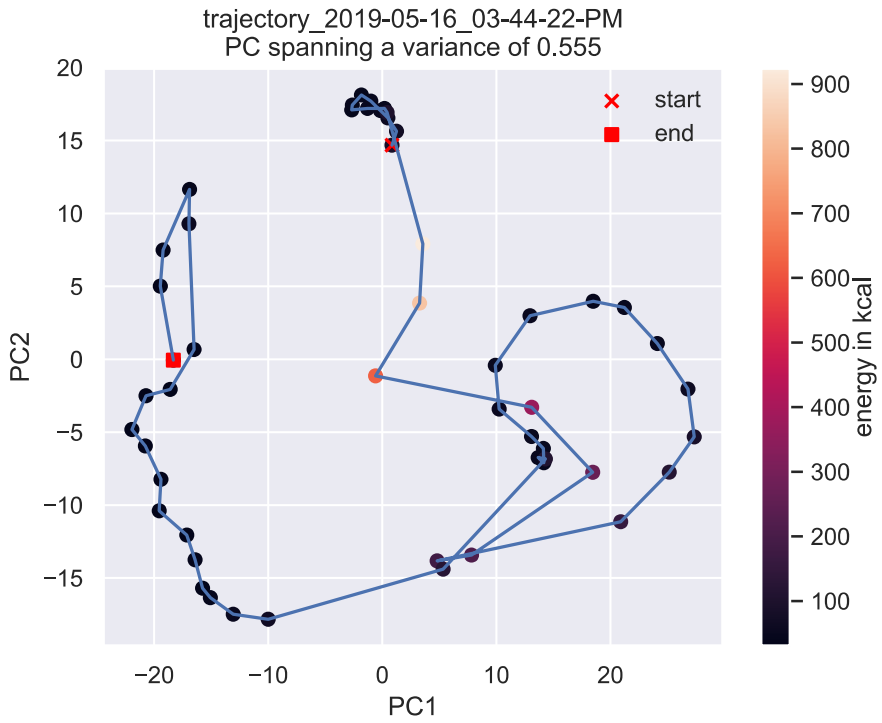
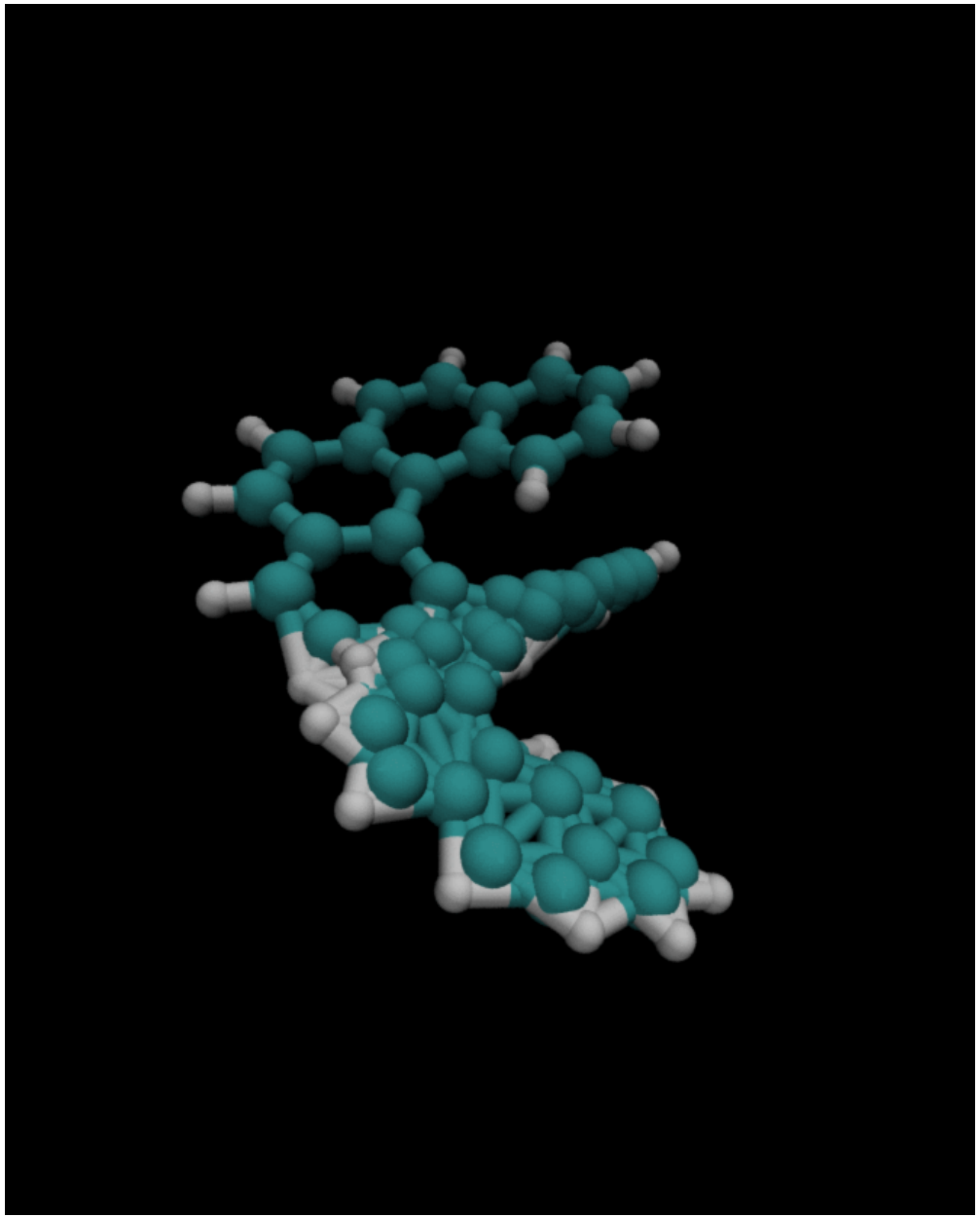


Component 1


trajectory_2019-05-16_03-43-00-PM
PC spanning a variance of 0.574
start
end
PC1
PC2
energy in kcal
15
10
5
0
−5
−10
−15
−20
−10
0
10
20
1600
1400
1200
1000
800
600
400
200



Component 4


trajectory_2019-05-16_03-44-22-PM
PC spanning a variance of 0.555
start
end
PC1
PC2
energy in kcal
20
15
10
5
0
−5
−10
−15
−20
−10
0
10
20
900
800
700
600
500
400
300
200
100