Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Conformational Transition Mechanism of Adenylate Kinase: A Comparison of All-Atom Molecular Dynamics Simulation to Coarse-Grained Methods MUSTAFA TEKPINAR, Yuzuncu Yil University, AHMET YILDIRIM, Siirt University — Adenylate kinase (ADK) performs a large conformational transition between its open and closed conformations. In this transition, order of conformational events can be investigated by molecular dynamics (MD) method. However, MD method requires large-scale computational resources and a significant amount of time to observe a full conformational transition. On the other hand, coarse-grained methods can produce transition pathways in a short amount of time with a questionable accuracy. To assess accuracy of coarse-grained methods, they need to be compared with all-atom models. Due to this reason, we produced a full conformational transition of ADK from closed state to open state by using all-atom classical molecular dynamics. This conformational transition has been compared with 7 coarse-grained methods in terms of order of conformational events. In the end, we evaluated successes and failures of each coarse-grained method.

Mustafa Tekpinar
Yuzuncu Yil University

Date submitted: 15 Nov 2013 Electronic form version 1.4