Abstract Submitted
for the OSS11 Meeting of
The American Physical Society

Computer Simulation Study of the Stability Mechanism of Thermophile, MJ0305[1] HYUNDEOK SONG, THOMAS BECK, University of Cincinnati — Methanococcus jannaschii (MJ) is a methane-producing thermophile, which was discovered in a 2600m-deep Pacific Ocean vent in 1983. It has the ability to thrive at high temperatures and high pressures, which are unfavorable for most life forms. There have been some experiments to study its stability under extreme conditions, but still the origin of the stability of MJ is not exactly known. MJ0305 is MJ's chloride channel protein. The structure of MJ0305 was built by homology modeling. We compared the stability of MJ0305 with mesophilic Ecoli at 300K, 330K, and 360K by computer simulation to test the effects of temperature. Our results show that high temperatures significantly affect the number of salt bridges and hydrogen bonds. High temperatures decreased the average number of hydrogen bonds for Ecoli and MJ0305. Increased salt bridges at 330K make MJ0305 more stable. Network analysis of MJ0305 showed an increase in the number of hubs at high temperatures. In contrast, the number of hubs of Ecoli was decreased at high temperatures. Calculated network entropy is proportional to the number of hubs. Increased network entropy of MJ0305 at 330K implies increased robustness.

[1]NSF, Dr. John Cuppoletti

Hyundeok Song
University of Cincinnati

Date submitted: 10 Mar 2011 Electronic form version 1.4