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The stability mechanism of 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. We have investigated the stability mechanism of MJ0305 by computer simulation. The structure of MJ0305 was built by homology modeling. We compared the stability of MJ0305 with mesophilic Ecoli at 300K, 330K, 360K, and 1atm, 130atm, 260atm by computer simulation to test the effects of both temperature and pressure. Our results show that high temperatures and high pressures significantly affect the salt bridges and hydrogen bonds. High temperatures decreased the average number of hydrogen bonds for Ecoli and MJ0305. However, high pressures at 360K increased the number of salt bridges for Ecoli and MJ0305. The radius of gyration of MJ0305 was decreased at high temperatures. Increased compactness at high temperatures, and Increased salt bridges at high pressures make MJ0305 more stable. This research may have impacts on renewable energy and chemical sensors.

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