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Theoretical simulation of compression of single bovine carbonic anhydrase II molecule by AFM tip KATSUNORI TAGAMI, MASARU TSUKADA, Waseda University, Japan — Based on all-atom force field model called CHARMM, we calculated the force distance curves of the single bovine carbonic anhydrase II molecule adsorbed on the graphite surface in the UHV condition. The AFM tip is modeled by the graphite sheet of monolayer thickness. The force distance curves show the nonlinear feature which can be classified into three regions, i.e., the attractive, weak repulsive, and strong repulsive force regions. We found that in the second region the surrounding alpha helices are compressed while in the third region the core beta sheets are also compressed. This finding indicates that the heterogeniousity in a single protein molecule can be measured by the AFM. We will also discuss the effect of the temperature on the force distance curves.

Katsunori Tagami
Waseda University

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