# 第313回　化学科コロキウムのご案内
# （大学院英語化PT）

**Title:** **Computational approach for understanding protein functions and structures**

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**Date :** **March 8, 2022, 13:30 - 15:00**

**Place:** **ZOOM**

Abstract: We have studied the relation between the protein functions and not only the static but also dynamic structures by using the computational approach. I will report some molecular dynamics study examples. Transmembrane protein CD44 plays an important role on the cell rolling via hyaluronan (HA) binding. The HA binding – unbinding mechanism regulated by the allosteric conformational change under fluid shear stress has also been reported. We therefore investigated HA binding on CD44 HABD by using molecular dynamics (MD) simulation, and I will talk about the details of the HA binding- unbinding mechanism from our MD study. Also, I will report the MD study about the factors which determine the enzyme activity and substrate specificity on the serine protease neuropsin.

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