Evolving through jiggling-wiggling atoms – the functional molecular mechanics of proteins studied by first-principle-based and data-driven methods

by Prof. Lee-Wei Yang,
Department of Life Science, NTHU

Abstract

Atoms constituting proteins are of no exception in matters subject to general physics laws. Life forms evolve through constant motions of proteins such that molecular functional controls are coupled dearly with their intrinsic or perturbed dynamics. Proteins change their conformation to respond external stimuli in order to communicate information across cell membranes, assist essential nanomachines to translate mRNA into proteins, or facilitate substrate uptake for subsequent enzymatic reactions. In this workshop, I will introduce popular first-principle-based and data-driven methods that generate and analyze these seemingly complicate modes of motions to obtain mechanistic insights in protein functions. Examples are given to describe how such techniques can be useful to design antimicrobial peptides and a drug-screening/repurposing platform.