Multi-Scale Simulations of Proteases Point to Evolutionarily Conserved Functional Mechanics Across the Enzyme Family

P. Carloni [1]

Abstract: Nature has used a large variety of protein scaffolds and different chemistry to perform enzymatic peptide hydrolysis. By using a variety of molecular simulation tools, spanning from hybrid QM/MM calculations, to classical MD, coarse-grain calculations, along with structural bioinformatics, we suggest here that proteases have been evolutionarily selected to possess similar functional motions despite the observed fold variations. Thus, during Evolution, Nature has not conserved folds for this biological function (for instance known aspartyl proteases are either beta-dimers or alpha-beta monomers) but it has preserved selected elements with specific mechanical properties.

[1] International School for Advanced Studies (SISSA/ISAS)
via Beirut 4, 34014 Trieste, Italy
carloni@sissa.it