HIV-1 protease functional dynamics can be extracted directly from a diverse set of experimental structures

Abstract:
The conformational changes of structures of proteins and chromatin are related to their functional mechanism. Different conformations of proteins can be related to their functional dynamics. HIV-1 protease, an essential viral enzyme which cleaves the viral peptides to generate the proteins that assemble into a mature virion, attains conformations that enable the structure to recruit substrate, catalyze the substrate, and release the products. To determine the functional dynamics of the protease structure, I studied protease experimental structures from the protein database using principal component analysis and also used normal mode analysis for numerical simulations. I find that the major structural components of the protease homodimer structure perform coordinated moves that can be attributed to its functional mechanism. On the other hand, chromatin is a complex of DNA and proteins which is a DNA packaging unit. I investigated the DNA folding in 30-nm chromatin fiber and its relation to the gene expression. I find that the high and low active genes have distinct nucleosome fiber organizations. The linker length between two nucleosomes in high active genes follows the 10n+5 pattern, whereas the linker length in low active genes follows the 10n pattern.