Signal transduction of the HAMP domain in four helix bundles from Molecular Dynamics
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Many proteins are involved in transmitting signals across membranes and the mechanism has long been a subject of interest. HAMP domain presents in a large number of transmembrane proteins and transduces the external signal across the membrane. Here we perform Molecular Dynamics simulation based on the NMR structure of a HAMP domain reported by Hulko et al. recently. We find that the signal transduction is fast (in picoseconds) and a cooperative process. It not only involves the rotation of the helices, but also the change of the shapes of the helices. X-da packing of the four-helical coiled coil is stabilized over “knobs into holes” packing by the offset of helices.