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Inter-domain communication through intrinsically disordered region (IDR) revealed through the ensemble structure analysis

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The functionally relevant inter-domain communication between the domains linked by intrinsically disordered region was explored by NMR in combination with small angle X-ray scattering. Based on the ensemble structure analyses and the numerical simulations to reproduce the chemical shift changes along with the substrate concentration, we have demonstrated how the domains cooperate to enhance the protein function through the substantially dynamic spatial allocation of the domains. Pin1, a proline cis/trans isomerase, comprises two domains linked by 10-residue IDR, one is the substrate binding domain to recognize pSer/pThr-Pro motif and the other is the enzyme domain that rotates the Pro peptide bond in the motif. The enzyme domain shows very limited affinity to the substrate, but its binding ability was enhanced by two orders of magnitude in the presence of the substrate binding domain linked by IDR; in which the inter-domain fly-casting mechanism plays to keep the substrate bound to Pin1 by tossing and receiving the substrate between the domains, once the substrate is bound to either one of the domains. A new functional aspect of IDR will be addressed.

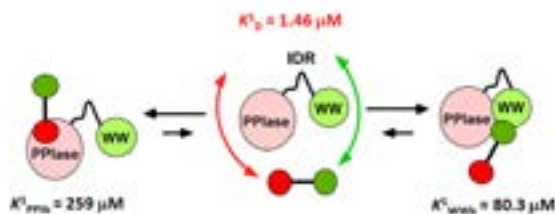


Figure1: Inter-domain substrate migration mechanism to enhance the binding ability of the enzyme domain by 200-fold. In this process, the IDR roles in prompting the domains to efficiently capture the substrate by allowing them for searching the substrate in a wide space, as analogously described as fly-casting.

Biography

Shin-ichi Tate has got his PhD degree from the University of Tokyo in 1993. He has the experience as a visiting Researcher at ETH (Prof. K Wüthrich) and NIH (Dr. A Bax). He has been a Professor in the Department of Mathematical and Life Sciences at Hiroshima since 2006. He is now the Director of the Research Center for the Mathematics on Chromatin live Dynamics (RcMcd), and the Dean of the School of Science in Hiroshima University.

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