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An insight into the evolutionary consequences of reptilian TLRs and their role in host-specific pathogenicity

Toll-Like Receptors (TLRs) are most studied class of Pattern Recognition Receptors (PRRs) which recognize exogenous Pathogen-Associated Molecular Patterns (PAMPs) and endogenous Damage-Associated Molecular Patterns (DAMPs) and are prime sentinels of innate immunity. Reptiles being the non-conventional model organisms remain a under deprived class in the study of structure, function and ligand specificity of TLRs except few studies published very recently. Among them, TLR5 is the only protein sensing receptor playing an inevitable role in the signaling cascade involved in innate immunity by recognizing bacterial flagellin. The unavailability of structural and ligand binding information of this receptor till date; directed us to model its ligand binding domain and docking with flagellin. Presence of several homologous proteins having considerable identity and coverage enabled us to construct a reliable 3D model of TLR5 ligand binding domain of Indo-Asian wall lizard *Hemidactylus flaviviridis* (hfTLR5). Experimentally, solved crystal structure of *Zebrafish* TLR5-N14VLR in complex with *Bacillus subtilis* flagellin (bsflagellin) was used as template to carry out template based molecular docking studies. Comparative analysis of docking energies and protein–ligand interactions of all the ligands revealed that bsflagellin residues interact with hfTLR5 ligand binding domain through hydrogen-bonds and hydrophobic interactions positionally segregated at two interfaces which lie in previously reported potential interacting region of TLR5. The described side chain of hot spot residue bsflagellin 'R89' was found to make maximum contacts and is shown inserted within the cavity formed by hfTLR5 interacting residues. Out of six, three residues of hfTLR5 (H264, G267 and N274) were found to be conserved in almost all the vertebrate classes and four out of six residues of flagellin were found to be identical in flagellins of TLR5 activating bacteria. The complex thus obtained may help us to better understand the functioning of hfTLR5, thereby bridging the gap in the evolution of species-specific host-microbe interactions.

Biography

Soma Mondal Ghorai has completed her PhD from University of Delhi and currently working as Assistant Professor in the Department of Zoology, Hindu College, University of Delhi, India. She has published more than 10 papers in reputed journals and has been actively involved in research in Comparative Immunology.