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In silico characterization of *Plasmodium falciparum* purinergic receptor: A novel chemotherapeutic target

Sonal Gupta
Shiv Nadar University, India

Serpentine receptors with G-protein coupled receptor (GPCR) like seven transmembrane (7 TM) topology are identified in *Plasmodium*. A class of 7 TM receptors known as purinergic receptors binds to purines such as ADP, ATP and UTP and mediates important physiological functions including regulation of calcium signaling. Here we performed *in silico* analysis of *P. falciparum* serpentine receptors and found that one of the *P. falciparum* serpentine receptors, PfSR12 possess nucleotide binding consensus P-loop sequence in addition to seven transmembrane domains. The presence of conserved seven transmembrane domains and a consensus nucleotide binding sequence (P-loop) suggest that PfSR12 is a putative purinergic receptor. On further analysis using docking programs, we found four active binding residues Asn149, Lys150, Asn151 and Gly152 in P-loop of PfSR12, interact with ATP. This work gives insights into the interactions between putative purinergic receptor PfSR12 and its ligand ATP which can be explored in structure based drug designing against malaria.

Biography

Sonal Gupta has completed her PhD in 2013 from International Centre for Genetic Engineering and Biotechnology (ICGEB), New Delhi, India and continued working as Research Associate for about 1.5 years. She is currently working as UGC Postdoctoral Fellow at Shiv Nadar University. Her current project focuses on elucidating signaling pathways in infectious disease like malaria and finding new drug targets against malaria. Her research interest focuses on understanding the role of secondary messengers and downstream effector molecules in parasite growth and invasion. Her current findings in this project have been recently published in *Systems and Synthetic Biology Journal* (Springer).

sonal01g@gmail.com

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