OMICS International
conferenceseries.com

Nasimul Hoda, J Pharma Care Health Sys 2015, 2:5
http://dx.doi.org/10.4172/2376-0419.C1.008

# Pharmaceutical Summit and Expo

**October 08-10, 2015 New Delhi, India**

## Structure guided lead identification of potent *Plasmodium falciparum* phospho-ethanolamine methyltransferase inhibitors

**Nasimul Hoda**
Jamia Millia Islamia, India

Malaria is a leading cause of human deaths affected by parasitic infection in tropical and subtropical reasons. Out of the four plasmodium species responsible for this disease in human *Plasmodium falciparum* is the most deadly. Due to the widespread resistance of the current antimalarial drugs, intense research efforts are focused on identification of new potent antimalarials. We report here, a structure based drug discovery strategy for design and synthesis of a series of potent and novel triazine based antimalarials. The X-ray structure of Plasmodium falciparum phosphoethanolamine methyltransferase (PfPMT) is used as a target as it is unique to the parasite. Trisubstituted triazine and its anlaogs are produced by an inexpensive three to four step synthesis giving excellent yields. Parasite growth inhibition assays further confirmed the activity of the molecules to be in 5 to 0.8 μM range showing selectivity towards the parasite over mammalian cells. Molecular dynamics simulations on the PfPMT-inhibitor complex shed light on the inhibition mechanism for further optimization of the lead compounds.

### Biography

Nasimul Hoda has completed his PhD from Patna University and Postdoctoral studies from IIT Delhi, Supercomputing facility for bioinformatics and computational biology (SCFBIO-IITD). He is the Assistant Professor in Chemistry at Jamia Millia Islamia (Central University). He is working in the field of Drug design and focussing on the development of antimalarial and anti-neurodegenerative agents.

hodanasimul@gmail.com

**Notes:**