Supplementary materials

Binding mode exploration of LuxR-thiazolidinedione analogues, e-pharmacophore based virtual screening in the designing of LuxR inhibitors and its biological evaluation

Sundaraj Rajamanikandan, Jeyaraman Jeyakanthan & Pappu Srinivasan

aDepartment of Bioinformatics, Alagappa University, Karaikudi, TamilNadu.
bDepartment of Animal Health and Management, Alagappa University, Karaikudi, TamilNadu.
Figure 1S: The sequence alignment of LuxR and SmcR generated by ClustalW.

![Sequence Alignment]

Figure 2S: 2D representation of thiazolidinedione analogues used for docking studies.

![Thiazolidinedione Analogues]
Figure 3S: Distance deviation profile of conserved amino acid residues (Asn133 & Gln137) for six LuxR_thiazolidinedione complexes.
Figure 4S: Binding modes of top two lead molecules with LuxR protein a) ChemBridge_5343641, b) ChemBridge_7824888.

Figure 5S: 2D representation of ChemBridge_5343641 used for in vitro assays.
Figure 6S: Inhibitory effect of ChemBridge_5343641 on biofilm formation of *V. harveyi*.