Insights on pH-dependent conformational changes of mosquito odorant binding proteins by molecular dynamics simulations

Manoharan Malini, Fuchs Patrick F.J., Ramanathan Sowdhamini, Offmann Bernard

Supplementary Figures

Supplementary Figure 1. RMSD plots obtained after the least mean square fit of residues of 11- 124 to C-alpha atoms of the different simulation systems. Native pH with ligand (left) pH4.0 with ligand(right). The different duplicates for each simulation system are represented in different colours

CquiOBP1	-VTPRRDAEYPPPELLEALKPLHDICAKKTGVTDEAII	EFSDGKIHEDEKLKCYMNCLFH	59
AgamOBP1	DTTPRRDAEYPPPELLEALKPLHDICLGKTGVTEEA	IKKFSDEEIHEDKLKCYMNCLFH	60
	.*****:***:***:*****		
CquiOBP1	EAKVDDNGDVHLEKLHDSLPNSMHDIAMHMGKRCLY	PEGENLCEKAFWLHKCWKQADPK	119
AgamOBP1	EAKVDDNGDVHLEKLHDSLPSSMHDIAMHMGKRCLY	PEGETLCDKAFWLHKCWKQSDPK	120
	*****.*****.***:*****:***		
CquiOBP1	HYFLV	124	
AgamOBP1	HYFLV	125	

	M		

Supplementary Figure 2. Conservation of mutated residues between AgamOBP1 and CquiOBP1: Sequence alignment of AgamOBP1 and CquiOBP1. The conserved residues mutated by Rusconi et al. (21) in AgamOBP1 are highlighted in a box.

Supplementary Figure 3. Conservation of charged residues in loop 3 and helix 6 that are involved in the conformational twist (indicated by arrows). Shown is the alignment of closest homologues of CquiOBP1 from OS-E/OS-F group from other mosquito species (after Manoharan et al, Genome Biol Evol (2013), 5(1):163-180).

Supplementary Figure 4. RMS fluctuations of ligand atoms at the two different pH conditions. The high pH simulation is represented in black. The low pH simulation is represented in red.