

Supplementary Informations

Flap Dynamics of Plasmepsin Proteases: Proposed Parameters and Molecular Dynamics Insight

Wilson Karubiu^a, Soumendranath Bhakat ^a, Lara McGillewie and Mahmoud E.S. Soliman ^{a*}

^aSchool of Health Sciences, University of KwaZulu-Natal, Westville, Durban-4000, South
Africa

*Corresponding author: Mahmoud E. S. Soliman (email: soliman@ukzn.ac.za)

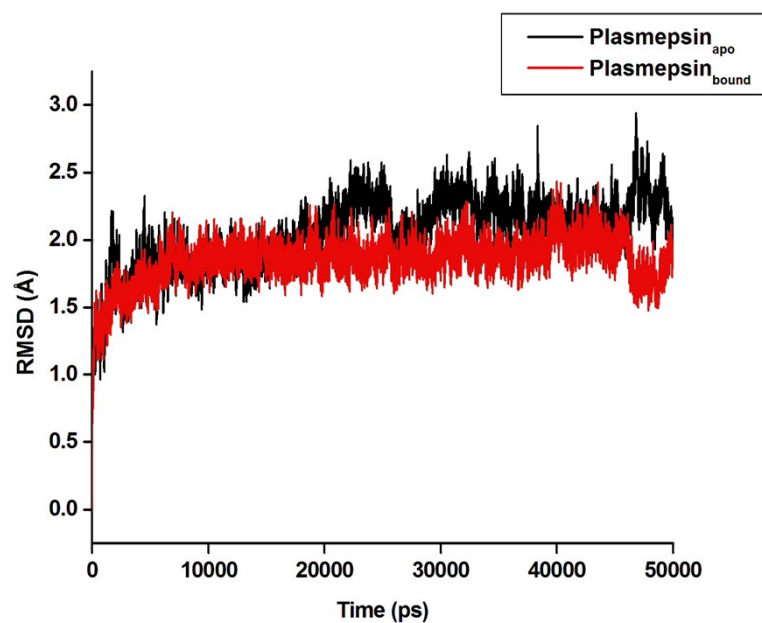


Figure S1. The RMSD fluctuation during the simulation time for both apo (black) and bound (red) conformations. The RMSD was calculated taking in account C- α atoms of the systems.

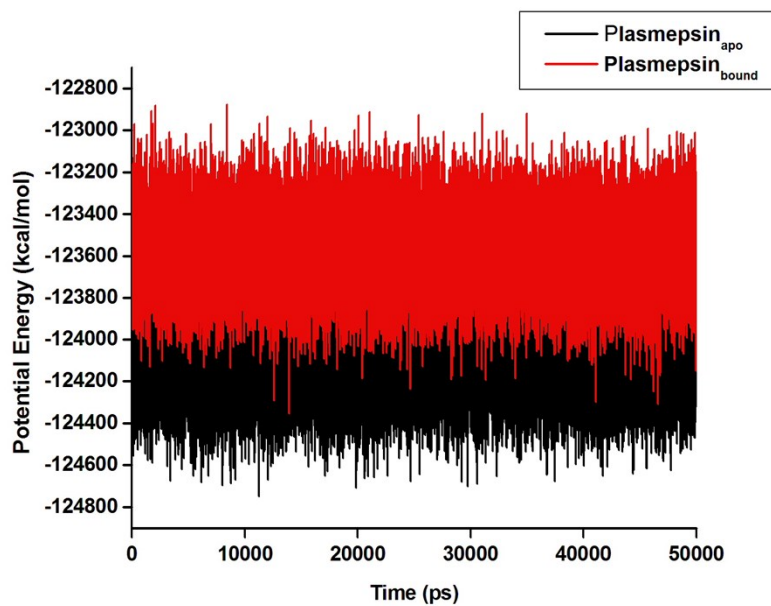


Figure S2. The potential energy fluctuations for both apo (black) and bound (red) conformations during simulation time.

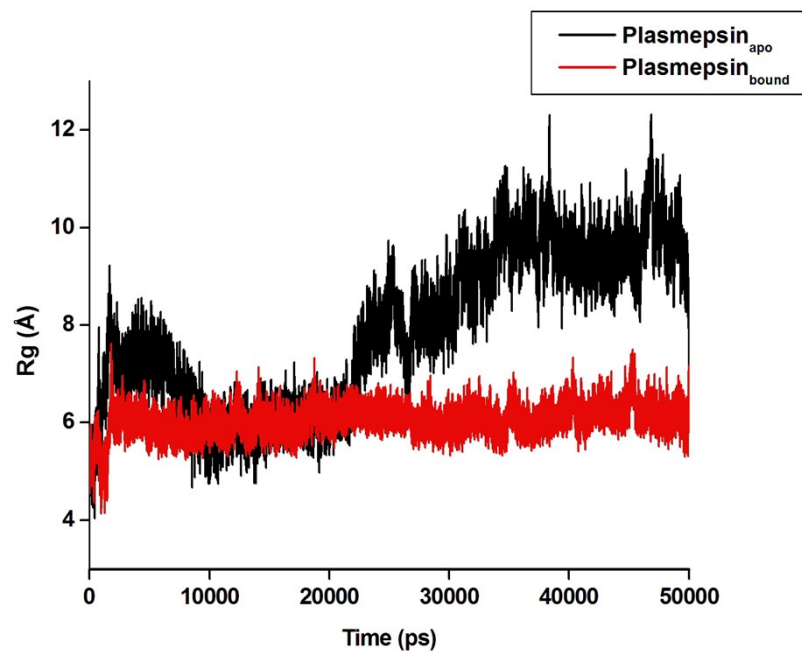


Figure S3. The fluctuation in radius of gyration (Rg) for apo and bound conformations of plasmepsin taking in account C- α atoms of flap tip residues, Val78 and Leu292.