Supplementary Materials

Dual Anti-inflammatory and Selective Inhibition Mechanism of Leukotriene A4 Hydrolase/Aminopeptidase: Insights From Comparative Molecular Dynamics and Binding Free Energy Analyses

Appiah-Kubi Patrick^a and Mahmoud E. S. Soliman^{a*}

^a Molecular Modelling and Drug Design Research Group, School of Health Sciences,
University of KwaZulu-Natal, Westville, Durban 4001, South Africa

*Corresponding author: Mahmoud E. Soliman

email: soliman@ukzn.ac.za

Telephone: +27 0312607413, Fax: +27 031260 779

A

B

S1. The Potential Energy (PE) plots of LT_{AR} , LT_{PEP} and LT_{ARPEP} (**A**) and LT_{AR} and LT_{SC} (**B**) during the molecular dynamic simulation.

A

B

S2. Number of inter-molecular hydrogen bond (Hb) interactions observed during the molecular dynamic simulation for LT_{AR} , LT_{PEP} and LT_{ARPEP} (**A**) and LT_{AR} and LT_{SC} (**B**).

S3. Ligplot showing interactions between PGP (A), SC-57461A (B), ARM1 (C) and the binding sites residues of Leukotriene A4 hydrolase.