Supplementary Information

Alkane monooxygenase study by molecular modelling techniques

Journal of Computer-Aided Molecular Design

Elias Silva dos Santos[1,2] and Elias Ramos de Souza[2,3]

[1]Instituto de Física, Universidade Federal da Bahia, Rua Barão de Geremoabo s/n – Ondina, Salvador, BA, 40.300-000, Brazil

[2]Mosaico Fluido Pesquisa e Inovação ltda, Rua Ewerton Visco, 324, Ed. Holding Empresarial s 102/201, Caminho das Árvores, Salvador, BA, 41820-022, Brazil

[3]Instituto Federal de Educação, Ciência e Tecnologia da Bahia, Rua Emidio dos Santos, s/n –Barbalho, Salvador, BA, 40.301-015, Brazil

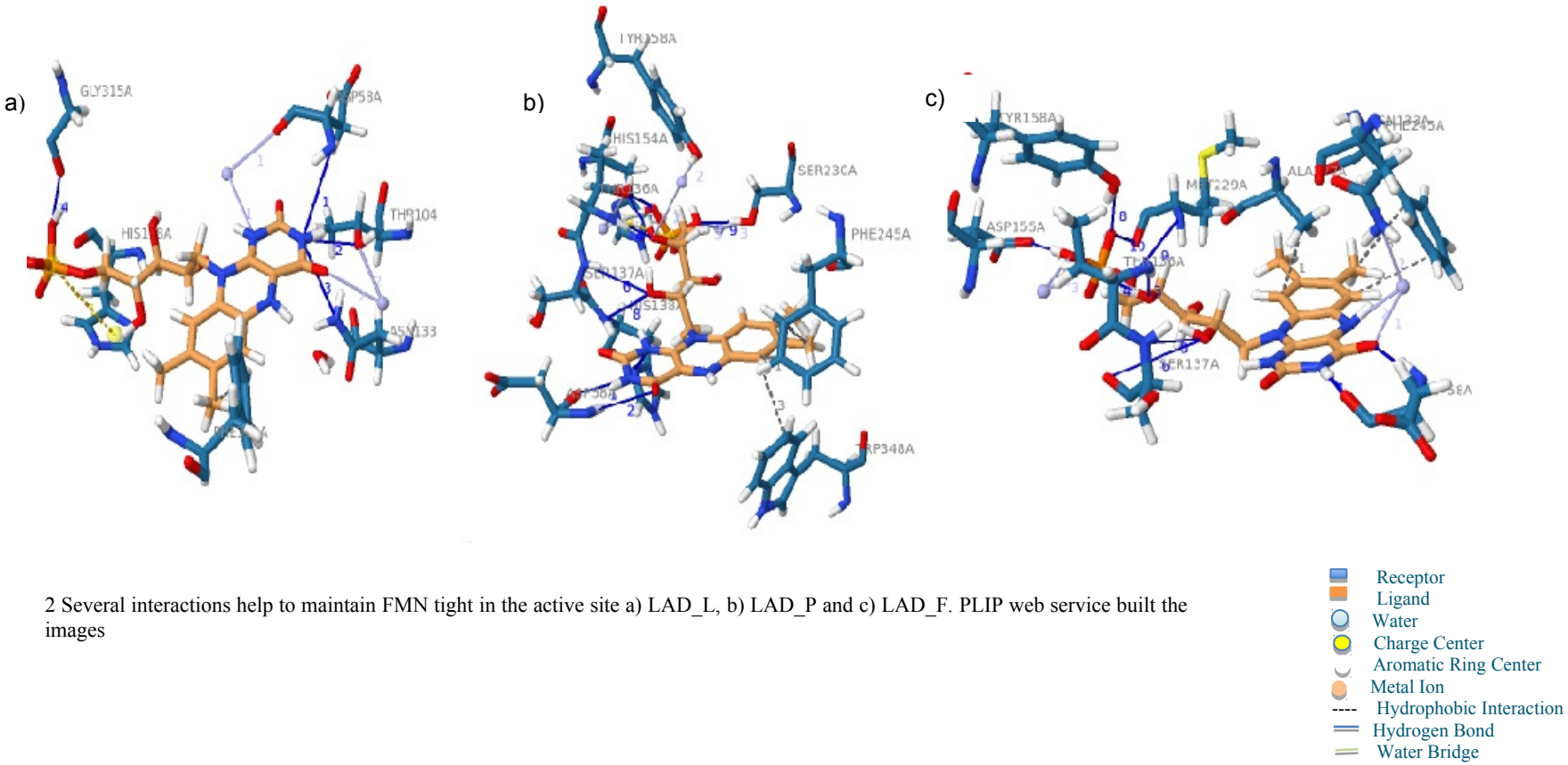
*Corresponding author. Email: eliasss@ufba.br

Phone/Fax: +55 71 32836638/+55 713283 6606

Contents

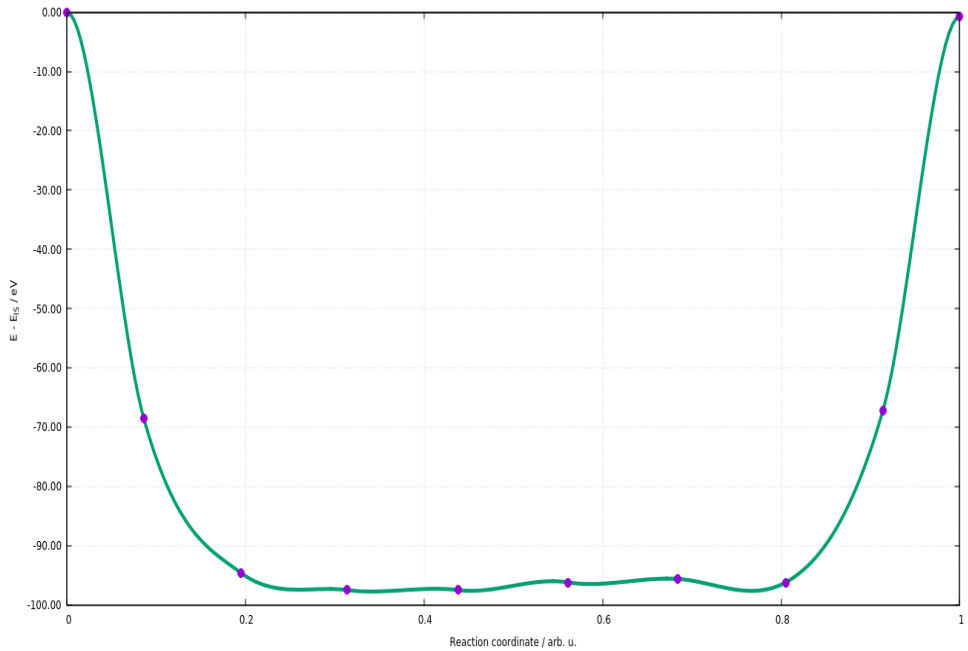
1 Distance of the minimum-energy crossing points between the nearest O (O_2-C_{4a}) to CH (substrate) of LAD_P and LAD_L systems

Distance (nm)	LAD_P	LAD_L
r	0.32	0.33



2 Several interactions help to maintain FMN tight in the active site a) LAD_L, b) LAD_P and c) LAD_F. PLIP web service built the images

Receptor
Ligand
Water
Charge Center
Aromatic Ring Center
Metal Ion
Hydrophobic Interaction
Hydrogen Bond
Water Bridge



3 Energy along reaction pathway for O_2 molecule. The reaction coordinate corresponds to the total distance the O_2 travels between the starting and final points. Gnuplot built the graph.