CERTIFICATE

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The organizing committee certifies that

Dr. Dian Herasari, M.Si.

has contributed as

PRESENTER

at

Virtual International Conference

The 3rd International Conference on Applied Sciences, Mathematics, and Informatics (ICASMI)

"Natural Science, Mathematics, and Informatics in Industrial Revolution (IR) 4.0 toward The Sustainable Development Goals (SDGs)"

Held by Faculty of Mathematics and Natural Sciences, University of Lampung
September 3rd – 4th, 2020, Bandar Lampung, Indonesia

Dr. Eng. Suripto Dwi Yuwono, S.Si., M.T.
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Prof. Dr. Rudy TM Situmeang, M.Sc.
Chairman

INTERNATIONAL CONFERENCE ON APPLIED SCIENCES MATHEMATICS AND INFORMATICS (ICASMI)
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Subject: Letter of Acceptance (LoA)

Dear Madame/Sir,
D Herasari; R Hertadi; F M Warganegara; Akhmaloka

We are happy to inform you that your paper entitled **"Dynamics of Lid lipMNK on Lys229Gln Mutation by Molecular Dynamics Simulation Approach "** is accepted as oral presentation in the **3rd International Conference on Applied Sciences, Mathematics and Informatics (ICASMI)**, that will be held in Online Meeting, 3-4 September 2020.

Please do not hesitate to contact us if you have further questions.

Thank you.

Bandar Lampung, 01 September 2020
Your sincerely,
The Conference Chairman,

Prof. Rudy Situmeang

Dynamics of Lid lipMNK on Lys229Gln Mutation by Molecular Dynamics Simulation Approach

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Abstract. A double lid Manuk lipase (lipMNK) is a local lipase isolated from Manuk crater, Jawa Barat, Indonesia. The catalytic activity of lipMNK is determined by the change in the conformation of lipMNK from a closed lid (c-lipMNK) to an open lid (o-lipMNK). The identification of salt-bridge interactions that stabilize the dynamic changes from c-lipMNK to o-lipMNK has shown several ionic interactions involving lid residues as the responsible interaction. One of them is Asp178 - Lys229, which is an interlid salt-bridge. To obtain more information about the role of the interaction and or the residue, in-silico mutation was carried out. Lys185Gln mutations were performed on the primary structure of c-lipMNK using Pymol. In the mutant structure obtained, then the solvation process is carried out at 20% acetonitrile conditions, parameterization, and molecular dynamics simulations. MD was carried out with an NPT ensemble at 358 K for 40 nanoseconds in 20% acetonitrile. The results showed that Lys229Gln mutation accelerated lid opening movements. Simulations for 40ns in wild type only opened the lid c-lipMNK as far as 3.64 Å and 6.90 Å (for lid A and lid B, respectively), while in the mutant the lid movement distances were 13.82 Å and 18.58 Å (for lid A and lid B, respectively). However, this mutation also shows unfolding in another segment beyond the lid. The existence of this unfolding, for example, can be seen in the change in the distance between the residues of His223 and Glu202, which was originally 14.41 Å further away to 24.47 Å. This suggests that the Asp178 - Lys229 salt bridge has an important role in maintaining the overall stability of the c-lipMNK structure.

Keyword: lipMNK, in-silico mutation, molecular dynamics