



# PROGRAM BOOK

The 2<sup>nd</sup> International Conference on Applied Sciences, Mathematics and Informatics



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RADAR LAMPUNG  
*Selalu Ada yang Baru*



**Abstract.** Chromium(III) complexes have been known to increase insulin absorption and decrease glucose levels in the blood, so Cr(III) complexes can be used as an antidiabetic supplement especially for people with diabetes type 2. The experimentally Cr(III) complexes proven to decrease glucose level, but the role mechanism of Cr(III) complexes in the body until now there is no explain in detail. In this research, the interaction of Cr(III) phenylalanine [Cr(phe)3] with protein tyrosine phosphatase (PTP) was studied by molecular docking. The aims this study was to identify the active site of PTP that binding with those Cr(III) phenylalanine. This research performed by computational calculations Hartree-Fock with basis set 6-31G, the interaction with PTP used the Autodock Vina software. The results showed that [Cr(phe)3] interact with 5 amino acids of PTP, i.e Leu(13), Arg(18), Ser(94), Asp(129) and Tyr(131) with the interaction energy of -6.6 Kcal/mol. The results showed that the interaction Cr(III) phenylalanine with PTP indicate hydrogen bonding with bond length from 1.8Å to 2.9 Å.

**Keywords :** Chromium(III) phenylalanine; PTP; Docking

#### 21. Effect of Mutation on the Dynamics of Lid lipMNK by Molecular Dynamics Approach

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**Abstract.** Manuk Lipase (lipMNK) is a double lid lipase from thermophilic microorganism, *Geobacillus uzonensis*, isolated from Manuk Crater, Garut, West Java, Indonesia. Several studies have demonstrated that the catalytic action of lipase involved the dynamics movement of lid segments from closed to open states upon the substrate binding. The lipMNK conformational dynamics also result in changes in ionic interactions involving residues in lid segment. In this study, the effect of mutation to dynamics of lid lipMNK. was studied at the atomic level by molecular dynamics (MD) simulation. In-silico mutation was performed on the lipMNK primary structure using Pymol software. Next, mutant structure solvated in 20% acetonitrile. MD is done by using AMBER software, force field ff03.r1. temperature 358K for 100 ns simulation. The results showed that dynamics conformation of lid lipMNK involving 3 pairs of salt bridges, Asp178 - Ly2229, Asp182 - Arg179, and Glu189 - Lys185. Mutations in Lys229Gln, Arg179Gln and Lys185Gln, can accelerate the lid opening movement, as can be seen from differences in lid movement distance compared to wild type. Visualization of MD mutant yield structure and distance changes of some reference residues suggest that mutations in these three residues cause unfolding in other segments of lipMNK. This suggests that a salt bridge involving all three residues has an important role in maintaining the stability of lipMNK

structure. These results indicate that lid integrity is not only important for the stability of the lid but is also important for the overall stability of lipMNK structure.

**Keywords :** lipMNK; lid; in silico mutation; molecular dynamics simulation

#### 22. Synthesis 4-piperilmorpholine from piperine

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**Abstract.** Piperine was isolated from black pepper by soxhletation method using a technical ethanol solvent. This compound is used as precursor for the synthesis of 4-piperilmorpholine. The synthesis was carried out via a pre-target piperoilchloride, where the piperine was initially hydrolyzed using KOH ethanolate for 24 hours, added SOCl<sub>2</sub> and then mixed with morpholine at 0-5 ° C. The result of synthesis was obtained 4-piperilmorpholine with yield of 40,80%.

**Keywords :** 4-piperilmorpholine; piperine; soxhletation; hydrolysis

#### 23. Antibacterial Activity of Acetic Extracts of Stem Bark *Swietenia macrophylla* (Meliaceae)

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**Abstract.** Meliaceae is one tropical plant widely spreads in Asia, tropical Africa, and Latin America. This plant family consists of 50 genera and 1400 species. In Indonesia there are about 33 genera and 405 species of Meliaceae. Meliaceae is famous for its wood quality since its wood properties are strong, hard, and resistant to termite attack and therefore it is widely used for furniture and building materials. Beside of its wood quality, this plant is also known as traditional medicines to treat skin irritation, to prevent hypertension, to cure urinary tract infections, and fever. Several of Meliaceae plants widely known in Indonesia especially are *Swietenia macrophylla* ('Mahoni'). Phytochemically, both of species have been reported as sources of secondary metabolites belong to terpenoids and limonoids groups and several isolated compounds have been reported to have important biological activities, such as antibacterial, antifeedant, antimalarial, antiinflammatory, antiviral and insecticide. The samples of *S. macrophylla* stem bark were obtained from Bogor Botanical Gardens, West Java. The isolation of secondary metabolites was carried out by extraction at room temperature (maceration) using acetone solvent, followed by identification of secondary metabolites using various solvent. The antibacterial activity of extracts and isolated compounds were examined against ten pathogenic bacteria including two Gram-(+) bacteria, i.e. *Bacillus subtilis* and *Staphylococcus aureus* and three Gram-(-) bacteria, i.e. *Escherichia coli*, *Salmonella thypi* and *Vibrio choleraeaus*.

**Keywords :** Meliaceae; *Swietenia macrophylla*; antibacterial



# CERTIFICATE

The organizing committee certifies that

*Dian Herasari*

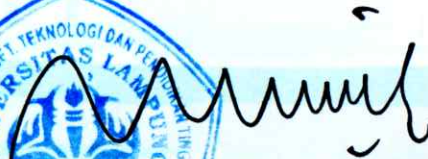
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