STRUCTURE ELUCIDATION OF CHIRAL METABOLITES FROM MICROBIAL TRANSFORMATION OF MEDROXYPROGESTERONE AND ANALYSIS OF THEIR *IN-VITRO* ACETYLCHOLINESTERASE INHIBITORY ACTIVITY VIA MOLECULAR DOCKING

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Fermentation of microorganisms is one of the top sources of drugs and drug leads in the field of natural products. This is because microbial transformation provides sustainable uses of resources under defined culture conditions that are unconstrained by seasonal fluctuations and geographical restrictions. The analysis of literature remarkably demonstrates a relatively small involvement of chiral microbial transformed products as novel neuroactive compounds. In addition, no report on biotransformation of medroxyprogesterone has been published to date. As a part of our ongoing research on microbial transformation of physiologically active steroids, this study aims to discover diverse bioactive metabolites from a single compound. Two chiral microbial transformed products were obtained from the fermentation of medroxyprogesterone with *Cunninghamella elegans*. DFT/B3LYP calculations was later carried out to determine the absolute structure configuration of chiral transformed products. Slight modification to Elllman's method was used for evaluation of acetylcholinesterase (AChE) inhibititory activity of biotransformed compounds, and the binding interactions of compounds were studied by molecular docking. All compounds showed various degree of acetylcholinesterase inhibitory activities. Even though these compounds are not as potent as the standard drug (Eserine IC_{50}: 0.06 µm), they could serve as leads for discovery and biosynthesis of prospective analogues with superior inhibitory activity.

Keywords - Medroxyprogesterone, Microbial Transformation, Chiral, Hydroxylation, Molecular Docking