UNIVERSITI TEKNOLOGI MARA

QUANTUM MECHANICAL STUDY OF UREASE INHIBITION BY ISATIN DERIVED SULPHONYL HYDRAZIDE

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AUTHOR'S DECLARATION

I declare that the work in this thesis was carried out in accordance with the regulations of Universiti Teknologi MARA. It is original and is the results of my own work, unless otherwise indicated or acknowledged as referenced work. This thesis has not been submitted to any other academic institution or non-academic institution for any degree or qualification.

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ABSTRACT

Isatin (1H-indole-2,3-dione) plays a vital role in pharmaceuticals and agriculture due to its unique properties which make Isatin one of the important heterocyclic compounds. Nowadays, fertilizers based on nitrogen compounds are widely used in agriculture. This fertilizer which has a high nitrogen content can cause bacterial urease activity to release an abnormally large amount of ammonia into the air thus, could contaminate the environment, and making it more toxic to other living things. The use of urease inhibitors on this fertilizer can reduce the level of ammonia released into the atmosphere to improve the environment area and improves the nitrogen use efficiency. In this report study, the simulation of the urease inhibition activity was conducted by using one of the quantum molecular models that are known as Geometric, Frequencies, Noncovalent interactions extended Tight Binding (GFN-xTB) to calculate its energies and the result is being studied on the interaction between the urease, 3LA4 a plant urease from jack bean as known as Canavalia ensiformis with the interest inhibitor, that is compound 5 which is isatin derived by sulphonyl hydrazide. Before running the energy calculation, the interest inhibitor needs to do molecular docking into the 3LA4 urease. After that, the extended tight-binding method is used on the urease inhibition activity.

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