***MOLECULAR DOCKING APPROACH, INTERNAL AND EXTERNAL VALIDATION AND PREDICTION OF Sargassum sp. AGAINST CARBONIC ANHYDRASE II***

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***ABSTRACT***

***Background and aims:***

Virtual screening, or insilico screening is a high-performance computational method for analyzing a set of chemical compound databases to identify candidate drug compounds. Research studies demonstrate the potential of compounds present in brown grass using molecular docking research.

Computational molecular docking screening was performed using Molegro Virtual Docker 6.0 (MVD) software. The carbonic anhydrase enzyme was extracted from the protein database (5GMN).

**Methods:**

Molecular docking was performed using Molegro Virtual Docker (MVD) 6.0 at the active site at the active site of the carbonic anhydrase enzyme to predict the activity of the compound. Docking validation was carried out by redocking the natural ligand of the 5GMN enzyme into its active site. Acceptance criteria were determined with a Root Mean Square Deviation (RMSD) value below 2.0 . Validation of the method can be seen from the RMSD value obtained when anchoring the reference ligand to the receptor. RMSD value 1.13 Angstrom (RMSD < 2). MolDock (Grid) Score (scoring function) and MolDock Optimizer (algorithm) show that this method has a high validity value.

**Results.**

This combination was maintained and its toughness was retested using as many as 100 distracting compounds which were tethered together with the training set.

Obtained the best 4 combinations seen from the enrichment factor, EF (1% ;5% ;10% ;20%) of 10.2 ;1.96 ; 4 ; 3, the procedure was further assessed by using the ROC curve value of 0.859, obtained the MolDock Score (Grid) vs MolDock Optimizer method

**Conclusion/Discussion.**

The results showed that all compounds worked relatively well against Polmacoxib as a natural ligand and also had a lower rerank score than Polmacoxib and Celecoxib. From this study, it can be concluded that Trephloroethol, Fukosterol, Eckol, Sargahydroquinic Acid, 7-Phloroeckol, Dieckol, Chlorogenic Acid, Diphlorethohydroxycarmalol, Stigmasterol are estimated to be more potent active ligands than the other 2 training sets. Prediction of the toxicity of stigmasterol compounds is relatively safe with an LD50 value of 866mg/kg and is not hepatotoxic, carcinogenic and cytotoxic and can be further optimized pharmacologically and evaluated clinically.

***Keywords:, carbonic anhydrase, molecular docking,*** ***stigmasterol.***

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