

## RESEARCH ARTICLE

### *Top-Leads from Natural Products for Treatment of Alzheimer's Disease: Docking and Molecular Dynamics Study*

Son Tung Ngo<sup>a</sup> and Mai Suan Li<sup>b\*</sup>

<sup>a</sup>*Institute for Computational Science and Technology, 6 Quarter, Linh Trung Ward, Thu Duc District, Ho Chi Minh City, Vietnam* <sup>b</sup>*Institute of Physics, Polish Academy of Sciences, Al. Lotnikow 32/46, 02-668 Warsaw, Poland*

Since available drugs are not efficient to treat the Alzheimer's disease the search for new leads is of great interest. One of possible ways is to use the Eastern medicine. Because the aggregation of amyloid peptides  $A\beta_{1-40}$  and  $A\beta_{1-42}$  may be responsible for the Alzheimer's disease, we have collected 342 compounds derived from Vietnamese plants and studied their binding affinity to these peptides and their mature fibrils using the docking technique combined with the Molecular Mechanic-Poisson Boltzmann Surface Area method. We predict that five ligands Dracorubin, Taraxerol, Taraxasterol, Hinokiflavone, and Diosgenin may be good candidates to cope with the Alzheimer's disease showing high binding affinity to monomers and mature fibrils of amyloid peptides. Dracorubin and Taraxerol are eventually more promising than Curcumin (diferulom-rthane) which is under clinical trial. Five top-leads can cross the blood-brain barrier as well as well be absorbed by human body.

**Keywords:** Alzheimer, herbs, drug design, docking, MM-PBSA, Blood-brain barrier, HIA.

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\*Corresponding author. Email: masli@ifpan.edu.pl