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Evaluation on the Potential of Ganoderma lucidum Bioactive Compounds as Alpha-Glucosidase Enzyme Inhibitor: A Computational Study

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Abstract
Introduction: Computational simulation study was carried out on bioactive compounds of Ganoderma lucidum (G. lucidum). Methods: Molecular docking and molecular dynamics (MD) simulations were performed. The input files for protein and ligands were retrieved from Protein Data Bank (PDB) and PubChem database. Human maltase-glucoamylase (PDB ID: 3L4Y) is the protein (α-glucosidase enzyme). The ligands are thirteen compounds derived from G. lucidum together with acarbose and miglitol as controls. Results: Docking result showed the lowest binding energy is from Ganomycin B (-7.8 kcal/mol) compared to acarbose and miglitol (-5.0 kcal/mol and -4.4 kcal/mol) respectively. MD simulation showed interaction of 3L4Y-Ganomycin B achieved stable interaction and conformation as follows: root mean square deviation (RMSD) is ± 2.7 Å, average distance of ±1.8 Å and constant hydrogen bonds around 1 - 3. Conclusion: Ganomycin B was found to have good binding affinity, embarking its potential as a potent α-glucosidase inhibitor.

Author Keywords
Ganoderma lucidum; molecular docking; molecular dynamics; protein-ligand binding; α-glucosidase inhibitor

References

- Zaccardi, F, Webb, DR, Yates, T, Davies, MJ.
Pathophysiology of type 1 and type 2 diabetes mellitus: a 90-year perspective
(2016) *Postgrad Med J*, 92 (1084), pp. 63-69.
- Murce, E, Cuya-Guizado, TR, Padilla-Chavarria, HI, França, TCC, Pimentel, AS.
Structure-based de novo design, molecular docking and molecular dynamics of primaquine analogues acting as quinone reductase II inhibitors
(2015) *J Mol Graph Model*, 62, pp. 235-244.
- Seeliger, D, de Groot, BL.
Ligand docking and binding site analysis with PyMOL and Autodock/ Vina
(2010) *J Comput Aided Mol Des*, 24 (5), pp. 417-422.
- Morris, GM, Huey, R, Lindstrom, W, Sanner, MF, Belew, RK, Goodsell, DS, Olson, AJ.
AutoDock4 and AutoDockTools4: Automated docking with selective receptor flexibility
(2009) *J Comput Chem*, 30 (16), pp. 2785-2791.
Dec

- Ibrahim, MA, Bester, MJ, Neitz, AW, Gaspar, ARM.
Rational in silico design of novel α-glucosidase inhibitory peptides and in vitro evaluation of promising candidates
(2018) *Biomed Pharmacother*, 107, pp. 234-242.

- Nguyen, H, Nguyen, T, Le, L.
Computational Study of Glucose-6-phosphate-dehydrogenase deficiencies using Molecular Dynamics Simulation
(2016) *South Asian Journal of Life Sciences*, 4 (1), pp. 32-39.

- Wallace, AC, Laskowski, RA, Thornton, JM.
LIGPLOT: a program to generate schematic diagrams of protein-ligand interactions
(1995) *Protein Eng*, 8 (2), pp. 127-134.

- Van Der Spoel, D, Lindahl, E, Hess, B, Groenhof, G, Mark, AE, Berendsen, HJ.
GROMACS: fast, flexible, and free
(2005) *J Comput Chem*, 26 (16), pp. 1701-1718.

- Quiroga, R, Villarreal, MA.
Vinardo: A Scoring Function Based on Autodock Vina Improves Scoring, Docking, and Virtual Screening
(2016) *PLoS One*, 11 (5), p. e0155183.

- Afriza, D, Suriyah, WH, Ichwan, SJA.
In silico analysis of molecular interactions between the anti-apoptotic protein survivin and dentatin, nordentatin, and quercetin
(2018) *Journal of Physics: Conference Series*, 1073 (3), p. 032001.

- Chen, D, Oezguen, N, Urvil, P, Ferguson, C, Dann, SM, Savidge, TC.
Regulation of protein-ligand binding affinity by hydrogen bond pairing
(2016) *Sci Adv*, 2 (3), p. e1501240.

- Nasution, MAF, Toepak, EP, Alkaff, AH, Tambunan, USF.
Flexible docking-based molecular dynamics simulation of natural product compounds and Ebola virus Nucleocapsid (EBOV NP): a computational approach to discover new drug for combating Ebola
(2018) *BMC Bioinformatics*, 19, p. 419.
(Suppl 14)

- Martínez, L.
Automatic identification of mobile and rigid substructures in molecular dynamics simulations and fractional structural fluctuation analysis
(2015) *PLoS One*, 10 (3), p. e0119264.

- Jusoh, N, Zainal, H, Abdul Hamid, AA, Bunnori, NM, Abd Halim, KB, Abd Hamid, S.
In silico study of carvone derivatives as potential neuraminidase inhibitors
(2018) *J Mol Model*, 24 (4), p. 93.

- Sharma, S, Kumar, P, Chandra, R.
Introduction to molecular dynamics
(2019) *Molecular Dynamics Simulation of Nanocomposites Using BIOVIA Materials Studio, Lammps and Gromacs*, 23, pp. 1-38.

- Hussein, Z, Taher, SW, Gilcharan Singh, HK, Chee Siew Swee, W.
Diabetes Care in Malaysia: Problems, New Models, and Solutions
(2015) *Ann Glob Health*, 81 (6), pp. 851-862.

- Ma, HT, Hsieh, JF, Chen, ST.
Anti-diabetic effects of Ganoderma lucidum
(2015) *Phytochemistry*, 114, pp. 109-113.

- Wang, F, Zhou, Z, Ren, X, Wang, Y, Yang, R, Luo, J, Strappe, P.
Effect of Ganoderma lucidum spores intervention on glucose and lipid metabolism gene expression profiles in type 2 diabetic rats
(2015) *Lipids Health Dis*, 14, p. 49.

- Zhao, XR, Huo, XK, Dong, PP, Wang, C, Huang, SS, Zhang, BJ, Zhang, HL, Ma, XC.
Inhibitory Effects of Highly Oxygenated Lanostane Derivatives from the Fungus Ganoderma lucidum on P-Glycoprotein and α-Glucosidase
(2015) *J Nat Prod*, 78 (8), pp. 1868-1876.

- Zheng, Y, Ley, SH, Hu, FB.
Global aetiology and epidemiology of type 2 diabetes mellitus and its complications
(2018) *Nat Rev Endocrinol*, 14 (2), pp. 88-98.

- Chaudhury, A, Duvoor, C, Reddy Dendi, VS, Kraleti, S, Chada, A, Ravilla, R, Marco, A, Mirza, W.
Clinical Review of Antidiabetic Drugs: Implications for Type 2 Diabetes Mellitus Management
(2017) *Front Endocrinol (Lausanne)*, 8, p. 6.

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