In Silico Study of Flavonoid Interacting with Dopamine D2 Receptor (Poster Presentation) - International Conference on Medicinal Chemistry and Timmerman Award 2013 Universitas Indonesia, 28 - 29th October 2013

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Abstrak

As a prolactin antagonist, dopamine binds to its receptor D2 and suppresses the secretion of prolactin from the pituitary gland. Required ligand that can interact with receptor so that dopamine can no longer bound to its receptor. Ligands empirically derived from plants and have been proven to increase human lactation. In silico study using molecular docking technique to identify ligand interaction with dopamine D2 receptor (PDB: 1I15). The best posing and binding energy (ΔG) were analyzed and ranked to get potential dopamine D2 receptor inhibitor. Binding energy of apigenin, luteolin, kaempferol, quercetin, and myricetin with PDB: 1I15 gives value respectively -5.90, -5.67, -5.64, -5.28, -4.36 kcal/mol. Interaction occurred between the ligand and amino acid residue ASN 192, PRO 204, SER 209 formed hydrogen bonding and hydrophobic interaction with HIS 189.