Automated Docking of Modafinil into 5-Hydroxytryptamine Receptor 1A using Semiempirical Free Energy Force field and Lamarckian Genetic Algorithm

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Docking is used frequently to predict the binding orientation of small molecule drug candidates to their protein targets, in order to in turn predict the affinity and activity of the small molecule. This curtails that docking plays an important role in the lucid design of drugs. Docking is used when Modafinil, referred to as the ligand, is docked into a Serotonin 1A receptor. The ligand was optimized using the software package Spartan8.0, and docked using Autodock. The results of the binding energy were -7.2 KJ/mol, a favorable binding energy.