MOLECULAR DOCKING USING MULTI-AGENT TECHNOLOGY

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Degree of Master of Science in Artificial Intelligence

Department of Computational Mathematics

University of Moratuwa

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Declaration

I declare that this dissertation does not incorporate, without acknowledgment, any material previously submitted for a Degree or a Diploma in any University and to the best of my knowledge and belief, it does not contain any material previously published or written by another person or myself except where due reference is made in the text. I also hereby give consent for my dissertation, if accepted, to be made available for photocopying and for interlibrary loans, and for the title and summary to be made available to outside organization.

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Dedication

I dedicate this thesis to my parents

Mr.Shelton Fernando and Mrs.Hemamalani Fernando.

I hope this achievement will complete the dream that both of you had for me all those many years ago when you choose to give the best education you could.

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Abstract

Traditional computer-based simulators for manual molecular docking for rational drug discovery have been very time consuming and a tedious task. It is evident from the literature that such computer-based solutions have been implemented merely with conventional software technologies. A large body of research publication has shown the power of Multi Agent technology for development of smart fully automated simulators.

In this research, a multi agent-based solution, named as NanoAgent, has been developed to automate the drug discovery process with little human intervention. In this solution, *ligands* and *proteins* are implemented as agents, who pose the knowledge of permitted connections with other agents to form new molecules. The system also includes several other agents for surface determination, cavity finding and energy calculation. These agents autonomously activate and communicate with each other to come up with a most probable structure over the ligands and proteins, which are participating in deliberation. Domain ontology is maintained to store the common knowledge of molecular bindings, whereas specific rules pertaining to the behavior of ligands and proteins are stored in their personal ontologies. Among other operational rules, agents are built with rules pertaining to theories of Poison Boltzmann, Vander Walls, and Monte Carlo, regarding ligands and proteins to calculate the optimal binding energy. Existing, Protein Data Bank (PDB) has also been used to calculate the space required by ligand to bond with the receptor. The drug discovery process of NanoAgent has exemplified exciting features of multi agent technology, including, communication, coordination, negotiation, butterfly effect, self-organizing and emergent behavior. Since agents consume fewer computing resources, NanoAgent has recorded optimal performance during the drug discovery process.

NanoAgent has been tested for the discovery of the known drugs for the known protein targets. It has 80% accuracy by considering the prediction of the correct actual existence of the docked molecules using energy calculations. By comparing the time taken for the manual docking process with the time taken for the molecular docking by NanoAgent, there has been 95% efficiency. The results suggest that the Multi-Agent Systems technology can be successfully applied to automate the manual molecular docking process, which is an inherently complex problem. Further work on this project can be identified as the development of automated solutions for protein-protein docking, which is a hot topic in biochemistry and allied disciplines.

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