



Faculty of Science
Mathematics Department

Bio-Inspiring Computing and its Application in Cheminformatics

A Thesis

Submitted to Department of Mathematics and Computer Science,
Faculty of Science - Menoufia University

In Partial Fulfillment of the requirements for the Master Degree of Science
(M. Sc. in Scientific Computing)

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Summary

Cheminformatics is a multi-disciplinary area includes Mathematics, Statistics and Computer Science to tackle them in Chemistry. In this thesis we try to find the similarity between 2 molecules based on their chemical structure since the similarity in structure refers to similarity in biological activities. Using bio-inspiring techniques and algorithm we proposed a new binary algorithm based on the Whale Optimization Algorithm (WOA) , then we apply it in Feature selection problem to select the 50 best property among 4665 property.

Chapter One: introduces an overview Cheminformatics and its programs.

Chapter Two: discusses the advantages of Swarm Intelligence and survey all methods name.

Chapter Three: presents 2 novel version of Whale Optimization Algorithm (WOA) and applied them in Feature Selection Problem.

Chapter Four: Results compared with 5 other algorithms and 8 statistical criteria.

Chapter Five: proposes an application in Cheminformatics dataset which we converted from SMILES to numbers. .

Chapter Six: provides new ideas and areas for future research topics.