

STUDIES ON THE CORRELATION
BETWEEN MOLECULAR PHYSICAL
PARAMETERS AND PHARMACOLOGICAL
ACTIVITIES OF SELECTED MARINE
NATURAL PRODUCTS

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MASTER OF SCIENCE
UNIVERSITI MALAYSIA TERENGGANU

2012



tesis
RS 160.7 .I8 2012



1100087632
Studies on the correlation between molecular physical parameters
and pharmacological activities of selected marine natural
products / Isrina Mohamad Saleh.

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ISRINA BINTI MOHAMAD SALEH

Thesis Submitted in Fulfilment of the Requirement
for the Degree of Master of Science in the
Faculty of Science and Technology
Universiti Malaysia Terengganu

September 2012

DEDICATION

This thesis is dedicated to my lovely Ibu, Adik and family for their endless love, support and encouragement throughout the course of the thesis.

I also dedicate this thesis to Ayahku who taught me the best kind of knowledge and to all my friends.

Abstract of thesis presented to the Senate of Universiti Malaysia Terengganu in fulfilment of the requirements for the degree of Master of Science

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ISRINA BINTI MOHAMAD SALEH

September 2012

Main Supervisor : Assoc Prof. Ku Halim Ku Bulat, Ph.D.
Co-Supervisor : Juriffah Ariffin, Ph.D.
Faculty : Science and Technology

The aim of this research project is to determine the molecular physical parameters that can be used to predict the pharmacological activities of marine natural products. For this study, fifty marine natural product molecules which had been identified to have biological activities were selected to be evaluated their physical properties using quantum mechanical software package of Gaussian 09 at the theoretical level of Density Functional Theory B3LYP/6-31G(d,p). Amongst the selected parameters are total electronic energy, HOMO, LUMO, energy band gap, dipole moment, zero-point vibrational energy, total enthalpy, total entropy, heat capacity and molar volume. These physical parameters and other added molecular parameters such as molecular mass, and number of selected atoms (H, C, O, Cl, Br) were analyzed using a procedure of principle component analysis in SPSS. The pair-wise factor plots were

employed to see if there exist any correlation between their pharmacological activities and any of the molecular parameters selected. Results showed that these pair-wise factor plots were successfully clustered almost 91% of the selected molecules according to their pharmacological activities. Based on these pair-wise factor plots and also their factor loadings, it can be concluded that anticancer and anti-fungus agents can be categorized according to their molecular mass and total electronic energy. Whilst, anti-malarial can be classified according to their bonding molecular orbital (HOMO) and number of aromatic rings. Meanwhile molecular size and thermodynamics properties can be used to cluster the antibacterial molecules. However, the wide range of antiviral can be grouped together by their dipole moment.

Abstrak tesis yang dikemukakan kepada Senat Universiti Malaysia Terengganu
sebagai memenuhi keperluan untuk Ijazah Sarjana Sains

**KAJIAN TERHADAP KAITAN ANTARA PARAMETER FIZIKAL
MOLEKUL DAN AKTIVITI FARMAKOLOGIKAL HASILAN
SEMULAJADI MARIN YANG TERPILIH**

ISRINA BINTI MOHAMAD SALEH

September 2012

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Tujuan kajian ini adalah untuk mencari parameter fizikal molekul yang boleh digunakan untuk menentukan aktiviti farmakologi sesuatu sebatian semulajadi marin. Dalam kajian ini, lima puluh sebatian semulajadi marin yang telah dikenal pasti mempunyai aktiviti biologi oleh penyelidik terdahulu dipilih untuk ditentukan parameter fizikal dengan menggunakan pakej perisian kuantum mekanik Gaussian 09 pada aras teori B3LYP/6-31G(d,p). Diantara parameter yang dipilih adalah jumlah tenaga elektron, tenaga orbital ikatan tertinggi, tenaga orbital anti-ikatan terendah, perbezaan tenaga jalur, momen dwikutub, tenaga getaran takat-sifar, jumlah entalpi, jumlah entropi, muatan haba dan isipadu molar. Semua parameter fizikal dan parameter molekul tambahan seperti jisim molekul dan bilangan atom (H, C, O, Cl, Br) telah dianalisis dengan kaedah analisis komponen utama menggunakan SPSS versi 16.0. Plot faktor berpasangan telah diaplikasikan untuk melihat jika terdapat

kaitan antara aktiviti farmakologi dengan mana-mana parameter molekul yang terpilih. Dapatan kajian menunjukkan bahawa plot faktor berpasangan telah dapat mengelompokkan 91% daripada molekul yang dipilih mengikut aktiviti farmakologi masing-masing. Berdasarkan plot faktor berpasangan dan juga faktor bebanan, dapat disimpulkan bahawa agen antikanser dan antikulat boleh dikelompokkan berdasarkan jisim molekul dan jumlah tenaga elektronik. Manakala, antimalaria dapat diklasifikasikan mengikut tenaga orbital ikatan tertinggi (HOMO) dan bilangan gelang aromatik. Parameter saiz molekul dan sifat termodinamik boleh digunakan untuk molekul antibakteria. Walaubagaimanapun, molekul antivirus mencakupi kawasan yang agak luas dan dapat dikumpulkan bersama melalui momen dwikutub.