

THEORETICAL STUDIES
ON THE ANTICANCER AGENTS FROM
SELECTED MARINE NATURAL
PRODUCTS

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MASTER OF SCIENCE
UNIVERSITI MALAYSIA TERENGGANU

2013

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

October 2013

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

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August 2013

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The aim of the present study is to find the molecular descriptors responsible for the variety of anticancer activities. In this study, fifty marine natural products molecules, those had confirmed to show anticancer activities experimentally, were selected to be evaluated their physical parameters using quantum mechanical software package Gaussian 09 at the theoretical level of B3LYP/DFT 6-31G (d,p). The outputs of this program such as SCF Energy, molecular orbital energies (LUMO, HOMO, energy band gap), dipole moment and thermodynamics properties (enthalpy, entropy, and free-energy of formation, ZPVE) along with other predictors (molecular mass, number of selected atoms, number of aromatic and number of non-aromatic rings) were then statistically analyzed using statistical software package of SPSS version 20.0 by employing the principle component analysis procedure; taking only into consideration all the factor-loading of greater than 0.30. These four principle components; PC1, PC2, PC3 and PC4 were plotted against each other in the manner pair-wise factor plots. Detailed analysis of this pair-wise factor plots revealed that only PC1 and PC3 can be used significantly to separate some of anticancer molecules

against the rests. Plots of PC1 versus PC2 and PC1 versus PC3 clearly delineate the colon anticancer molecules from lungs and breasts. However, there is still an overlapping between cervix anticancer molecules and the others. For the plots of PC2 versus PC3 and PC3 versus PC4, anticancer of ovary was single-out from the rests along the PC3 component. Based on these results, it can be concluded that colon anticancer can be predicted by molecular mass, molar volume and thermodynamic properties. Meanwhile, ovarian anticancer can be predicted based on molecular orbital properties such as LUMO and energy band gap.

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

**KAJIAN TEORI TERHADAP AGEN ANTIKANSER DARIPADA
BAHAN SEMULAJADI MARIN TERPILIH**

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Tujuan kajian ini adalah untuk mencari sifat fizikal molekul bahan metabolit sekunder dari marin yang boleh digunakan untuk meramalkan sifatnya sebagai agen antikanser. Dalam kajian ini, lima puluh molekul bahan semulajadi marin yang telah terbukti sebagai antikanser secara eksperimen dipilih untuk dinilai sifat fizikalnya dengan menggunakan perisian Gaussian 09 pada tahap teori DFT B3LYP/6-31G(d,p). Hasil bagi program ini adalah seperti tenaga SCF, tenaga orbital molekul (LUMO, HOMO, dan jurang tenaga HOMO/LUMO), momen dwikutub dan sifat termodinamik (entalpi, entropi, dan tenaga bebas pembentukan, dan ZPVE) serta sifat-sifat fizikal lain seperti (jisim molekul, nombor atom, nombor gelang aromatik dan nombor gelang bukan aromatik) dan kemudiannya, dianalisis menggunakan pakej perisian statistik (SPSS) versi 20.0 dengan menggunakan kaedah analisis komponen utama dengan nilai faktor muatan lebih besar daripada 0.30. Komponen utama PC1, PC2, PC3 dan PC4 diplot antara satu sama lain secara berpasangan. Analisis terperinci mengenai plot pengfaktoran berpasangan mendedahkan bahawa hanya komponen utama PC1 dan PC3 boleh digunakan dengan ketara untuk memisahkan kelompok molekul antikanser berbanding yang lain. Plot pengfaktoran

PC1 melawan PC2 dan PC1 melawan PC3 menunjukkan pemisahan antara molekul antikanser kolon dengan molekul antikanser payudara dan paru-paru. Walaubagaimanapun, terdapat pertindihan antara molekul antikanser servik dan molekul paru-paru dan molekul payudara. Bagi plot PC2 melawan PC3 dan PC3 melawan PC4, kelompok antikanser ovari merupakan kelompok tunggal berbanding kelompok antikanser lain sepanjang rantau PC3. Berdasarkan keputusan yang diperolehi, antikanser kolon bagi sesuatu molekul boleh diramalkan berdasarkan jisim molekul, isipadu molar dan sifat-sifat termodinamik. Manakala, antikanser ovari boleh diramalkan berdasarkan sifat orbital molekul LUMO dan jurang tenaga HOMO/LUMO.