CURRENT RESEARCH AND DEVELOPMENT IN BIOTECHNOLOGY ENGINEERING AT IIUM

VOLUME II

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IN SILICO PREDICTION OF ANTICANCER ACTIVITY OF NITROSOUREAS

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ABSTRACT

Computer aided methods provide important tools in academic and industrial research. It accelerates a number of studies in various fields such as in drug discovery and development. Discovery of new drugs with low toxicity and have properties that fulfill the desired criteria as an effective drug become a priority for some scientists. The best models of QSAR were obtained by using semi empirical quantum chemical RM1 method. Heuristic and best multilinear regression methods were applied in order to obtain the best correlation. Three data sets involved were aliphatic nitrosoureas set, chloroethyl substituted nitrosoureas set and carbohydrate substituted nitrosoureas set. Each data set was examined for their effective dose and %ILS properties. However, %ILS properties gave better correlation than dose properties. The first potent nitrosourea from aliphatic nitrosoureas data set has %ILS value of 1575.07, while the second potent nitrosourea from chloroethyl substituted nitrosoureas set has %ILS value of 1894.08. Lastly, the %ILS value obtained for the third potent nitrosourea from carbohydrate substituted nitrosoureas set is 1147.62.

Keywords: Anti-cancer activity, QSAR, nitosourea, *In silico* method.

INTRODUCTION

Many attempts have been done to develop theoretical methods in discovering new drugs. Quantitative structure activity relationship (QSAR) approach has proved as one of the best theoretical methods especially in computational chemistry. The use of QSAR contributes to the discovery of new chemicals with better physical, chemical or biochemical properties and to use them as effective chemicals such as pharmaceuticals and anticancer agents (Ferguson *et al.*, 1997).

Last 40 years, the first QSAR study had been discovered by Hanch and Fujita (Selassie C. D., 2003). This theoretical approach is used to correlate bioactivity and structure of a compound quantitatively. The correlation is then represented as a model mathematical equation. Usually, the right hand side of the equation consists of physicochemical properties of the bioactive compound such as hydrophobicity, electronic effects and steric factors while