STRUCTURE-ACTIVITY STUDIES ON ANTICANCER AGENTS:

AN MLR APPROACH

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ABSTRACT

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Cancer is a disease characterized by abnormal cells growth. Cancer can be treated by chemotherapy which consists of anticancer agents. Quantitative Structure Activity Relationship, QSAR studies provide promising solutions to reduce the cost and time taken for the production of anticancer agents. Here, data from several papers have been re-analyzed using different descriptors. Multiple linear regression (MLR) analysis has been used to determine whether the difference in the choice of descriptors will affect the R^2 value and hence providing a better QSAR model. The evaluation done in this study shows that the R^2 obtained is comparable with the original data. Eleven QSAR models have been developed. Five QSAR models have been accepted as good prediction models as the R^2cv value is more than 0.5. The best QSAR prediction model obtained has the value of R^2 equal to 1 and R^2cv value is 0.93 which consists of eight significant descriptors.

CHAPTER 1

INTRODUCTION

1.2   Cancer diseases

Cancer is a disease characterized with abnormal cell growth also known as carcinoma or malignancy. There are many types of cancer with breast and cervical cancer being the top two most common cancers in Malaysian women (Zarihah *et al.*, 2003). Most cancers can be treated and some cured, depending on the specific type, location, and stage. Once diagnosed, cancer is usually treated with a combination of surgery, chemotherapy and radiotherapy. With more research done, treatments are becoming more specific for different types of cancer. Recently, biological therapy is also used in treating cancer (Giannelli *et al.*, 2008).

As the thought of cancer instills fear and is perceived fatal, more and more research contributing to reducing pain and suffering of cancer victims are going locally and internationally. However, research in drug design and drug synthesis takes time and very expensive.