

UNIVERSITI TEKNOLOGI MARA (UiTM)

**DOCKING OF MOUSE P-GLYCOPROTEIN
(ABCB1a/MDR3) WITH RHODAMINE B AND
VINBLASTINE**

HAZUREEN BINTI MOHD HALIMI

**FACULTY OF PHARMACY
UNIVERSITI TENOLOGI MARA (UiTM)**

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TABLE OF CONTENTS

	Page
TITLE PAGE	
APPROVAL SHEET	i
ACKNOWLEDGEMENT	ii
TABLE OF CONTENTS	Hi
LIST OF FIGURES	vi
LIST OF TABLES	vii
LIST OF ABBREVIATIONS	viii
ABSTRACT	x
CHAPTER ONE (INTRODUCTION)	
1.1 Computational drug design	1
1.2 Molecular docking	1
1.3 P-glycoprotein	2
1.4 Vinblastine	4
1.5 RhodamineB	4
1.6 Statement of Problem	5
1.7 Aim of the study	5

1.8	Hypothesis	6
1.9	Significance of study	6

CHAPTER TWO (LITERATURE REVIEW)

2.1	P-glycoprotein	
2.1.1	Introduction	7
2.1.2	ABCB1	7
2.1.3	Drug binding	8
2.1.4	P-glycoprotein in Blood Brain Barrier	9
2.2	Ligands	
2.2.1	RhodamineB	11
2.2.2	Vinblastine	12
2.3	Molecular Docking	
2.3.1	Introduction	13
2.4	Binding sites	14

CHAPTER THREE (MATERIAL AND METHODS)

3.1	Sequence alignment	
3.1.1	Bioinformatics tools	15
3.2	Binding site prediction	16

ABSTRACT

P-glycoprotein (Pgp) is an ATP-dependent transport protein that is selectively expressed at entry points of xenobiotics. It acts as an efflux pump that prevents xenobiotics from entering sensitive organs. Pgp also plays a key role in the absorption and blood-brain barrier penetration of many drugs. The overexpression of Pgp in cancer cells has been associated with multidrug resistance in tumors. To date, there is still no research has been done to identify the specific amino acid at the binding site in Pgp that vinblastine binds to computationally. Predictions of the binding sites were done using the Q-siteFinder. This study also uses the Autodock software to find the amino acid residues that the vinblastine and rhodamine B interacts with. The results concluded that there are two binding sites predicted from Pgp which are the TM 6 and TM 12. The results also concluded that mouse Pgp interacts with Phe 332, Phe 339, He 336 in TM6. In TM 12, Leu 971, lie 977, Val 978, Gly 980 and Ala 981 were found to have interaction with mouse Pgp. Based on the findings of this study also, it can be concluded that drugs often bind to TM 6 and TM 12 that are important for function. Overall, this study suggested that the Autodock software provides a quick, and inexpensive way of evaluating potential drug efflux problem at the early stages of drug development.