

CONTENTS

a.	Dedication	i
b.	Declaration by Researcher	ī
c.	Certificate from the Research Supervisor.	īī
d.	Acknowledgement	iv
e.	List of Tables	v-vii
f.	List of Figures	viii-xii
g.	Contents	xiii-xiv
1	CHAPTER 1: Introduction	1-9
	1.0 Introduction:	1
	1.1 Acridinecarboxamide, A Class of Anticancer Drug	1
	1.2 Description of DNA-Drug Binding	1
	1.3 Azaacridinecarboxamide, A New Anticancer Agent	2
	1.4 Importance of Drug pK_a	3
	1.5 Objective of Study	5
	References	8
2	CHAPTER 2: Methodology	10-16
	2.1 Introduction	10
	2.2 Electron Correlation	11
	2.3 Basis Set	12
	2.4 Density Functional Theory (DFT)	13
	2.5 JoinMolecules Package	14
	2.6 Comparison of HF/6-31G, HF/6-31G*, HF/6-31G**, DFT and MP2	15
	References	16
3	CHAPTER 3: Ab initio Calculations on the Stacking of 9-aminoacridine with Nucleobases and Watson-Crick Base Pairs.	17-31
	3.1 Introduction	17
	3.2 Methodology	18
	3.3 Results and Discussions	19
	3.4 Conclusion	22
	References	31
4.	CHAPTER 4: Ab initio Study of the Nature of Stacking between aza Analogues of Acridine-4-carboxamides with Sequences of DNA.	32-51
	4.1 Introduction	32
	4.2 Methodology	33
	4.2.1 Models of stacked structures	33
	4.2.2 Calculation of Stacking Interaction	34
	4.3 Results and discussion	34
	4.4 Conclusion	37
	References	51

5.	CHAPTER 5: Evaluation of Efficient Stacking of Aromatic Rings in the Intercalation Between Aza-analogues of Acridine-4-carboxamides and Base Pairs of DNA.	52-75
	5.1 Introduction	52
	5.2 Methodology	53
	5.3 Results and Discussion	54
	5.3.1 Contribution of π - π interaction in chromophore and base pair stacking:	54
	5.3.2 Contribution of π - group interaction and p-s interaction:	55
	5.4 Conclusion	58
	References	74
6.	CHAPTER 6: Evaluation of Stacking Interaction by Chromophore of 9-anilinoacridine with Sequences of DNA.	76-84
	6.1 Introduction	76
	6.2 Methodology	77
	6.3 Results and Discussion	77
	6.4 Conclusion	79
	References	84
7.	CHAPTER 7: Intercalation model of drug between sequences of DNA	85-94
	7.1 Introduction	85
	7.2 Methodology	86
	7.3 Results and discussion	86
	7.4 Conclusion	87
	References	94
8.	CHAPTER 8: Prediction of pK_a From Basicity of Atomic Sites of Drugs	95-109
	8.1 Introduction	95
	8.2 Theory	97
	8.3 Results and Discussion	98
	8.3.1 Sites of protonation	98
	8.3.2 Geometries of protonated drugs	99
	8.3.3 Estimation of pK_a	99
	8.3.4 Complementarity of pK_a values of drugs with physiological environment	100
	8.4 Conclusion	101
	References	109
9.	CHAPTER 9: Is Protonated Chromophore Necessary for Intercalation?	110-117
	9.1 Introduction	110
	9.2 Methodology	111
	9.3 Results and Discussion	111
	9.4 Conclusion	112
	References	117
10.	Chapter 10: Conclusion	118-120
	Appendix 1: List of Publications	A
	Appendix 2: Conversion factors	B