## A STUDY OF PHOTOINDUCED INTERACTIONS OF SOME ACRIDINE DERIVATIVES WITH ORGANIC AMINES AND MACROMOLECULES OF BIOLOGICAL RELEVANCE

THESIS SUBMITTED FOR THE DEGREE OF
DOCTOR OF PHILOSOPHY (SCIENCE)
OF
JADAVPUR UNIVERSITY

## BY BROTATI CHAKRABORTY

CHEMICAL SCIENCES DIVISION

SAHA INSTITUTE OF NUCLEAR PHYSICS

1/AF BIDHANNAGAR

KOLKATA 700064

INDIA

JANUARY, 2012

## **Contents**

List of Abbreviations	i
Thesis Layout	iii
Chapter 1: Prologue	1-64
1.1 Introduction	1
1.2 Acridine derivatives, organic amines and macromolecules of biological relevance — Scope of the thesis	5
1.3 Photoinduced Electron Transfer (PET) and Energy Transfer	9
1.3.1 Photoinduced Electron Transfer	10
1.3.1.1 History of Photoinduced Electron Transfer Reaction	11
1.3.1.2 Energetics	13
1.3.1.3 Theories of Electron Transfer Reactions	15
1.3.1.4 Effect of solvent on electron transfer	24
1.3.1.5 Distance dependence on electron transfer	26
1.3.1.6 Electron transfer in organized systems	28
1.3.1.7 Electron transfer in proteins	29
1.3.1.8 Electron transfer in DNA	33
1.3.2 Resonance Energy Transfer	34
1.4 Magnetic field effect (MFE) on PET reactions	38
1.4.1 Vector spin description of radical ion pairs	40
1.4.2 S-T intersystem crossing and mechanism of magnetic field effect	42
1.4.3 Magnetic field effect on triplet precursors	44
1.4.4 Magnetic field effect on singlet precursors	46
1.5 Host-Guest complex: Supramolecular chemistry	48
References	51
Chapter 2: Materials, Methods & Experimental Techniques	65-75
2.1 Instrumentation	65

2.1.1 UV-vis absorption Spectroscopy	65
2.1.2 Circular Dichroism Spectroscopy	65
2.1.3 <sup>1</sup> H Nuclear Magnetic Resonance Spectroscopy	65
2.1.4 Fluorescence Spectroscopy	65
2.1.5 Fluorescence lifetime measurement	66
2.1.6 Laser Flash Photolysis	69
2.1.7 Isothermal Titration Calorimetry (ITC)	70
2.1.8 Molecular Docking Studies	72
2.2 Reagents and sample preparation	72
2.2.1 Reagents	72
2.2.2 Preparation of samples	74
References	75
Chapter 3: Interaction of Proflavin with aromatic amines in homogeneous	76-91
and heterogeneous media	
3.1 Introduction	76
3.2 Results and discussion	77
3.2.1 Fluorescence study in homogeneous media	77
3.2.2 Fluorescence study in heterogeneous media	79
3.2.3 Laser Flash photolysis and magnetic field effect	81
3.2.3.1 Interaction of DMA with PF <sup>+</sup>	81
3.2.3.2 Interaction of DMDPM with PF <sup>+</sup>	85
3.3 Conclusion	90
References	91
Chapter 4: Interaction of Proflavin with an aliphatic amine in homogeneous	92-105
and heterogeneous media	
4.1 Introduction	92
4.2 Results and discussion	93
4.2.1 Homogeneous medium	93
4.2.2 Heterogeneous medium	94
4.2.3 Laser Flash photolysis and magnetic field effect	96

4.3 Conclusion	104
References	105
Chapter 5: Magnetic field effect on photoinduced electron transfer reactions	106-126
of two acridine derivatives with organic amines in homogeneous medium	
5.1 Introduction	106
5.2 Results and discussion	107
5.2.1 AD-organic amine systems	107
5.2.2 AY-organic amine systems	115
5.3 Conclusion	125
References	126
Chapter 6: Interaction of Proflavin and Acridine Yellow with model proteins	127-166
6.1 Introduction	127
6.2 Results and discussion	129
6.2.1 Preliminary studies on drug-protein interaction	129
6.2.1.1 UV-vis absorption spectroscopy	129
6.2.1.2 Fluorescence Spectroscopy	131
6.2.1.3 Effect of SDS	135
6.2.1.4 Laser Flash Photolysis	135
6.2.2 Study using steady-state and time resolved absorption and fluorescence spectroscopies and MFE to explore PET in drug-protein interaction	138
6.2.2.1 UV-vis absorption spectroscopy	138
6.2.2.2 Circular Dichroism Studies	141
6.2.2.3 Fluorescence Spectroscopy	143
6.2.2.4 Laser flash photolysis and magnetic field effect	150
6.2.2.5 Docking Results	157
6.3 Conclusion	164
References	165
Chapter 7: Host-guest chemistry of Acridine Yellow and Cucurbit [7] uril	167-179
7.1 Introduction	167

Chapter 8: Epilogue	180-181
References	179
7.3 Conclusion	178
7.2.5 Isothermal Titration Calorimetry	175
7.2.4 <sup>1</sup> H NMR study	173
7.2.3 Steady-State Fluorescence Anisotropy	173
7.2.2 Steady-State and Time-Resolved Fluorescence	169
7.2.1 UV-vis absorption	168
7.2 Results and discussion	168

List of publications

Reprints