

LIST OF CONTENTS

ABSTRACT	5
1. INTRODUCTION	7
1.1 NUCLEAR MAGNETIC RESONANCE- SHORT DESCRIPTION	7
1.1.1. COSY	16
1.1.2. TOCSY	19
1.1.3. H 2D J (Homo 2D-J Resolved Spectroscopy)	20
1.1.4. NOESy (Nuclear Overhauser effect spectroscopy)	22
REFERENCES	29
1.2. COMPUTER MODELING-PRINCIPLES	31
REFERENCES	39
1.3. PRINCIPLES OF PROTEIN STRUCTURE	41
REFERENCES	49
2. STRUCTURAL STUDY ON A LOM-AKH PEPTIDE STRUCTURE USING ¹ H NMR TECHNIQUE AND RESTRAINED AND UNRESTRAINED MOLECULAR DYNAMICS SIMULATION	51
2.1. CONFORMATIONAL STUDY ON AN INSECT NEUROPEPTIDE (LOM-AKH-I) OF THE AKH/RPCH -FAMILY BY COMBINED ¹ H NMR SPECTROSCOPY AND MOLECULAR MECHANICS	51
METHODS	53
RESULTS	55
CONCLUSIONS	77
2.2. CONFORMATIONAL STUDIES OF EMP-AKH PEPTIDE USING UNRESTRAIN MOLACULAR DYNAMICS METHOD IN DMSO MIMICKING ENVIRONMENT	79
METHODS	80
RESULTS	81
CONCLUSIONS	85
2.3. CONFORMATIONAL STUDIES OF THE EMP-AKH PEPTIDE USING MOLECULAR AND SIMULATED ANNEALING.DYNAMICS METHODS	87

METHODS	88
RESULTS	90
CONCLUSIONS	113
REFERENCES	115
3. STRUCTURAL STUDY ON AN EMP-AKH PEPTIDE STRUCTURE USING ¹ H NMR TECHNIQUE, RESTRAINED AND UNRESTRAINED MOLECULAR DYNAMICS SIMULATION	117
3.1. CONFORMATIONAL STUDY ON AN INSECT NEUROPEPTIDE OF THE AKH/RPCH-FAMILY BY COMBINED ¹ H NMR SPECTROSCOPY AND MOLECULAR MECHANICS	118
CONCLUSIONS	130
3.2 CONFORMATIONAL STUDIES OF EMP-AKH PEPTIDE USING UNRESTRAIN MOLACULAR DYNAMICS METHOD IN DMSO MIMICKING ENVIRONMENT	131
MATERIALS AND METHODS	131
RESULTS	132
CONCLUSIONS	137
3.3. CONFORMATIONAL STUDY ON AN AKH/RPCH (EMP-AKH) NEUROPEPTIDE IN THE PRESENCE OF SDS MICELLES	139
MATERIALS AND METHODS	139
RESULTS	142
3.4 CONFORMATIONAL STUDIES OF THE EMP-AKH PEPTIDE USING MOLECULAR, LANGEVIN AND SIMULATED ANNEALING DYNAMICS METHODS	151
METHODS	152
RESULTS	154
CONCLUSIONS	180
REFERENCES	181