

# Table of Contents

---

Abstract	(i)
Declaration	(v)
Certificates	(vi)
Acknowledgement	(vii)
Table of Contents	(ix)
List of Figures	(xvi)
List of Tables	(xxiii)
List of Abbreviations	(xxv)
List of Publications	(xxvii)
Conference Proceedings	(xxviii)
<b>CHAPTER 1 : Motivation &amp; outline of the Thesis</b>	<b>1- 4</b>
<b>1.1</b> Motivation of the present work	2
<b>1.2</b> Outline of the thesis	3
<b>CHAPTER 2 : Introduction &amp; review of literature</b>	<b>5-24</b>
<b>2.1</b> Alzheimer's disease	9
2.1.1    Overview of Alzheimer's disease	9
2.1.2    The history of Alzheimer's disease	9
2.1.3    Disease presentation	10
2.1.4    Known factors playing a role for AD	11
2.1.5    Alzheimer's disease diagnosis	12
2.1.6    Amyloid cascade hypothesis: A $\beta$ peptide in cause of AD	13
2.1.7    Production of A $\beta$ peptide from APP	15
2.1.8    Neuronal toxicity of A $\beta_{1-42}$ peptide	15
2.1.9    Monomers of A $\beta_{1-42}$ peptide	15
2.1.10   Dimerization of A $\beta_{1-42}$ peptide	16
2.1.11   Cross-seeding interaction of A $\beta_{1-42}$ peptide and Tau	17
2.1.12   Intrinsic disordered regions in A $\beta_{1-42}$ peptide	19
2.1.13   Oligomers and Fibrils of A $\beta_{1-42}$ Peptide	20
2.1.14   Inhibitors of A $\beta_{1-42}$ peptide aggregation	22

# Table of Contents

---

2.2	Main objectives of the thesis	23
<b>CHAPTER 3 :</b>	<b>Methods</b>	<b>25-45</b>
3.1	Computational Techniques	
3.1.1	Molecular dynamics simulation	26
3.1.1.1	History of simulation	26
3.1.1.2	Theory of molecular dynamics simulation	27
3.1.1.3	Force field	28
3.1.1.4	Long range interactions: Ewald sum	30
3.1.1.5	Dealing with molecules: SHAKE algorithm	31
3.1.1.6	Periodic boundary conditions	31
3.1.1.7	Temperature and pressure computation and control	32
3.1.1.8	Water molecule models	33
3.1.1.9	Molecular dynamics steps	34
3.1.2	Potential of mean force	38
3.1.2.1	Umbrella sampling	38
3.1.2.2	Running the umbrella sampling calculations	39
3.1.2.3	The Weighted Histogram Analysis Method for Free-Energy Calculations	40
3.1.3	PatchDock	41
3.1.4	The molecular mechanics energies combined with the Poisson-Boltzmann or generalized Born and surface area continuum solvation method (MM-PBSA and MM-GBSA)	42
3.1.5	Contact Map Analysis	43
3.1.6	PDBsum	44
3.1.7	Analysis of trajectories	44
<b>CHAPTER 4 :</b>	<b>Investigations on the structural characteristics that seed the aggregation of A<math>\beta</math><sub>1-42</sub> peptide: Insights from molecular dynamics simulations</b>	<b>46-58</b>
4.1	Abstract	47
4.2	Introduction	47

# Table of Contents

---

<b>4.3</b>	Materials & Methods	48
4.3.1	A $\beta_{1-42}$ peptide folding simulation	48
4.3.2	A $\beta_{1-42}$ mutant (Lys 28 to Pro 28) peptide folding simulation	49
4.3.3	A $\beta_{1-42}$ peptide simulation at higher temperature	49
<b>4.4</b>	Results & Discussions	49
4.4.1	Conformational stability of A $\beta_{1-42}$ peptide from the simulation	49
4.4.2	Secondary structure characteristics of A $\beta_{1-42}$ peptide	52
<b>4.5</b>	Conclusions	58
<b>CHAPTER 5 :</b>	<b>Structural characterization of Amyloid <math>\beta_{17-42}</math> peptide dimer by potential of mean force analysis: Insights from molecular dynamics simulations</b>	<b>59-78</b>
<b>5.1</b>	Abstract	60
<b>5.2</b>	Introduction	60
<b>5.3</b>	Materials and Methods	62
5.3.1	Preparation of initial A $\beta_{17-42}$ peptide dimer model	62
5.3.2	Construction of dimer structure using docking	62
5.3.3	PMF calculation	64
5.3.4	Identification of interface residues and hot spot residues	65
<b>5.4</b>	Results & Discussions	65
5.4.1	Free energy analyses of A $\beta_{17-42}$ peptide dimer	65
5.4.2	Conformational dynamics of the optimized A $\beta_{17-42}$ peptide dimer structure from the free energy profile	71
5.4.3	Interaction study of the optimized A $\beta_{17-42}$ peptide dimer structure from the free energy profile	75
5.4.4	C $\alpha$ – C $\alpha$ distance map analysis	77
<b>5.5</b>	Conclusions	78
<b>CHAPTER 6 :</b>	<b>Cross-seeding interactions between Amyloid <math>\beta</math> and Tau protein can enhance aggregation?</b>	<b>79-87</b>
<b>6.1</b>	Abstract	80

# Table of Contents

---

<b>6.2</b>	Introduction	80
<b>6.3</b>	Materials & Methods	81
6.3.1	Preparation of initial $A\beta_{25-35}/A\beta_{25-35}$ homo-dimer; $Tau_{273-284}/Tau_{273-284}$ homo-dimer and $A\beta_{25-35}/Tau_{273-284}$ hetero-dimer	81
6.3.2	PMF calculation	81
<b>6.4</b>	Results & Discussions	82
6.4.1	Free energy analysis of $A\beta_{25-35}$ peptide with $Tau_{273-284}$	82
6.4.2	Protein-Protein interaction study of the optimized $A\beta_{25-35}/Tau_{273-284}$ hetero-dimer and $A\beta_{25-35}/A\beta_{25-35}$ and $Tau_{273-284}/Tau_{273-284}$ homo-dimers from the free energy profile	83
6.4.3	Conformational dynamics of the optimized $A\beta_{25-35}/Tau_{273-284}$ hetero-dimer and $A\beta_{25-35}/A\beta_{25-35}$ and $Tau_{273-284}/Tau_{273-284}$ homo-dimers	85
6.4.4	Residue-Residue interaction profile of the optimized $A\beta_{25-35}/Tau_{273-284}$ hetero-dimer structure	86
<b>6.5</b>	Conclusions	87
<b>CHAPTER 7 :</b>	<b>Examination of the intrinsic disordered regions present in the <math>A\beta_{1-42}</math> peptide</b>	<b>88-96</b>
<b>7.1</b>	Abstract	89
<b>7.2</b>	Introduction	89
<b>7.3</b>	Materials & Methods	90
<b>7.4</b>	Results & Discussions	92
<b>7.5</b>	Conclusions	96
<b>CHAPTER 8 :</b>	<b>Investigation on the interactions stabilizing the <math>A\beta_{1-42}</math> peptide oligomers and <math>A\beta_{1-42}</math> fibril polymorphs</b>	<b>97-118</b>
<b>8.1</b>	Abstract	98
<b>8.2</b>	Introduction	98
<b>8.3</b>	Materials & Methods	100
8.3.1	Preparation of initial monomer structure to construct $A\beta_{1-42}$	100

# Table of Contents

---

	peptide oligomers	
	8.3.2 Construction of A $\beta$ <sub>1-42</sub> peptide oligomer structures	100
	8.3.3 Investigation of interface statistics and interface residues in trimer and tetramer	100
	8.3.4 Interaction study of A $\beta$ <sub>1-42</sub> fibril polymorphs	101
<b>8.4</b>	<b>Results &amp; Discussions</b>	<b>101</b>
	8.4.1 Conformational dynamics of A $\beta$ <sub>1-42</sub> peptide oligomers	101
	8.4.2 Hydrogen bonding and Hydrophobic contact analysis of A $\beta$ <sub>1-42</sub> peptide oligomers	105
	8.4.3 Interface statistics and residue-residue interaction study of A $\beta$ <sub>1-42</sub> peptide oligomers using PDBsum server	109
	8.4.4 Structural characterization of polymorphic A $\beta$ <sub>1-42</sub> fibrils	111
	8.4.5 Interaction studies of polymorphic A $\beta$ <sub>1-42</sub> fibrils	113
<b>8.5</b>	<b>Conclusions</b>	<b>118</b>
<b>CHAPTER 9 :</b>	<b>Inhibition of A<math>\beta</math><sub>1-42</sub> peptide aggregation using short ss- oligonucleotide as polyions: An <i>in silico</i> approach</b>	<b>119-130</b>
<b>9.1</b>	<b>Abstract</b>	<b>120</b>
<b>9.2</b>	<b>Introduction</b>	<b>120</b>
<b>9.3</b>	<b>Materials &amp; Methods</b>	<b>121</b>
	9.3.1 Building ss-oligonucleotide from Nucleic Acid Builder (NAB)	121
	9.3.2 MD Simulation of A $\beta$ <sub>1-42</sub> peptide monomer in presence of ss-oligonucleotide	121
	9.3.3 MD Simulation of A $\beta$ <sub>17-42</sub> peptide dimer in presence of ss-oligonucleotide	121
<b>9.4</b>	<b>Results &amp; Discussions</b>	<b>122</b>
	9.4.1 Effect of ss-oligonucleotide on the conformations of A $\beta$ <sub>1-42</sub> peptide	122
	9.4.2 Secondary structural analysis of A $\beta$ <sub>1-42</sub> monomer in presence of ss-oligonucleotide	122
	9.4.3 Stability of A $\beta$ <sub>1-42</sub> peptide in presence of ss-oligonucleotide	125

# Table of Contents

---

9.4.4	Hydrophobic contacts and hydrogen bonding analysis of $A\beta_{1-42}$ peptide and the ss- oligonucleotide	126
9.4.5	Effect of ss-oligonucleotide on conformations of $A\beta_{17-42}$ peptide dimer	126
9.4.6	Hydrophobic contacts and hydrogen bonding analysis of $A\beta_{17-42}$ peptide dimer and the ss-oligonucleotide	128
9.4.7	Binding energetics of ss-oligonucleotide with $A\beta_{1-42}$ peptide	128
<b>9.5</b>	Conclusions	130
<b>CHAPTER 10 : <i>In silico</i> investigation on the inhibition of <math>A\beta_{1-42}</math> peptide aggregation by <math>A\beta_{1-40}</math> peptide using potential of mean force study</b>		<b>131-147</b>
<b>10.1</b>	Abstract	132
<b>10.2</b>	Introduction	132
<b>10.3</b>	Materials & Methods	133
10.3.1	Computational model of $A\beta_{1-42}/A\beta_{1-40}$ hetero-dimer and $A\beta_{1-42}/A\beta_{1-42}$ homo-dimer	133
10.3.2	Interface residues and hot spot residues identification	133
<b>10.4</b>	Results & Discussions	134
10.4.1	Free energy profile	134
10.4.2	Conformational dynamics of $A\beta_{1-42}/A\beta_{1-42}$ homo-dimer and $A\beta_{1-42}/A\beta_{1-40}$ hetero-dimer	135
10.4.3	Hydrogen bonding analysis of $A\beta_{1-42}/A\beta_{1-40}$ hetero-dimer	137
10.4.4	Conformational dynamics of the lowest energy conformer of the $A\beta_{1-40}/A\beta_{1-42}$ hetero-dimer and $A\beta_{1-42}/A\beta_{1-42}$ homo-dimer using distance restraints	137
10.4.5	Protein-Protein interaction study	141
10.4.6	Estimation of binding free energy of $A\beta_{1-40}$ peptide to $A\beta_{1-42}$ peptide by MM-PBSA method	146
<b>10.5</b>	Conclusions	147

# Table of Contents

---

<b>CHAPTER 11 :</b>	<b>A comparative study to elucidate the inhibitory mechanism of a 6-mer peptide fragment of A<math>\beta</math><sub>1-42</sub> peptide as a potential therapeutic in Alzheimer's disease</b>	<b>148-160</b>
11.1	Abstract	149
11.2	Introduction	149
11.3	Materials & Methods	150
11.3.1	Construction of input files for docking	150
11.3.2	Docking of A $\beta$ <sub>1-42</sub> peptide, A $\beta$ <sub>17-42</sub> fibril and 6-mer peptide	151
11.4	Results & Discussions	152
11.4.1	Binding characteristics of the analogue	152
11.4.2	Effect of the analogue on A $\beta$ <sub>17-42</sub> fibril	154
11.4.3	Potential of mean force for unbinding of the analogue	155
11.4.4	Binding characteristics of the analogue with the A $\beta$ <sub>1-42</sub> monomer	158
11.5	Conclusions	160
<b>CHAPTER 12 :</b>	<b>Summary and Future prospects</b>	<b>161-164</b>
12.1	Overview of results	162
12.2	Future prospects	163
	Bibliography	165
	<b>Publications (first page)</b>	

# List of Figures

---

<b>Figure No.</b>		<b>Page No.</b>
<b>CHAPTER 2</b>		
2.1	Atomic structure and assembly of an amyloid fibril.	6
2.2	Schematic representation of A $\beta$ <sub>1-42</sub> peptide aggregation pathway from monomer to mature fibrils	8
2.3	Nucleation-dependent polymerization model of amyloid aggregation	8
2.4	Normal brain vs Alzheimer's disease brain	10
2.5	Different stages and the associated symptoms in AD	11
2.6	From Amyloid Precursor Protein to Amyloid $\beta$ Peptide: a hypothetical pathway	14
2.7	The 3-D structure of A $\beta$ <sub>1-42</sub> fibril illustrating the intermolecular nature of the inter-strand interaction	21
<b>CHAPTER 3</b>		
3.1	Schematic illustration of the main contribution to the empirical potential energy function	29
3.2	Periodic boundary conditions in two dimensions. The simulation cell (solid) is surrounded by translated copies of itself (dashed)	32
3.3	Schematic flowchart of steps involved in MD Simulation	34
3.4	Schematic representation of TIP3P water model	34
3.5	A schematic one-dimensional energy surface. Minimization methods move downhill to the nearest minimum	35
3.6	A line search is used to locate the minimum in the function in the direction of the gradient	36
<b>CHAPTER 4</b>		
4.1	A) Temperature vs time course of simulation period; B) Potential Energy vs time course of simulation period for A $\beta$ <sub>1-42</sub> peptide structure	51
4.2	Backbone RMSD vs time course of simulation period for the A) A $\beta$ <sub>1-42</sub> peptide with the equilibrated structure as the reference structure; B) A $\beta$ <sub>1-42</sub> peptide with lowest potential energy conformer as the reference structure	51



# List of Figures

---

4.3	B-factor values of C- $\alpha$ atoms as a function of residue number is shown for A $\beta$ <sub>1-42</sub> peptide	53
4.4	Radius of gyration as a function of time course of simulation for the A $\beta$ <sub>1-42</sub> peptide	53
4.5	Secondary structure assignment per residue for the A $\beta$ <sub>1-42</sub> peptide conformer during the time course of simulation period. (The encircled portion in red shows the appearance of $\beta$ -strands in A $\beta$ <sub>1-42</sub> peptide)	53
4.6	Probability score of secondary structure assignment per residue for the average structure of A $\beta$ <sub>1-42</sub> peptide during the time course of simulation period.	55
4.7	Snapshots of A $\beta$ <sub>1-42</sub> peptide wild type at 300 K during the time course of simulation period	55
4.8	Snapshots of A $\beta$ <sub>1-42</sub> peptide mutant at 300 K during the time course of simulation period	57
4.9	Snapshots of intermediates and final configuration of MD simulations of A $\beta$ <sub>1-42</sub> peptide structure at higher temperatures	57

## CHAPTER 5

5.1	Distribution of conformer population of A $\beta$ <sub>17-42</sub> peptide dimer	63
5.2	Potential of mean force as a function of the reaction co-ordinates for the association of the A $\beta$ <sub>17-42</sub> /A $\beta$ <sub>17-42</sub> peptide dimer(in kcal/mol)	66
5.3	Captured snapshots of the A $\beta$ <sub>17-42</sub> peptide dimer at 300 K during the time course of simulation period at varying inter-chain distances in Å	67
5.4	Probability score of secondary structure for each residue of the A $\beta$ <sub>17-42</sub> peptide dimer at 300 K at increasing inter-chain distance	68
5.5	Probability score of secondary structure for each residue of the A $\beta$ <sub>17-42</sub> peptide dimer at 300 K at decreasing inter-chain distance	68
5.6	Backbone RMSD vs time course of simulation period for the A $\beta$ <sub>17-42</sub> peptide dimer in explicit solvent. A) At increasing inter-chain distance; B) At decreasing inter-chain distance	69
5.7	Electrostatic Energy vs time course of simulation period and Van der Waals Energy vs time course of simulation period for the A $\beta$ <sub>17-42</sub> peptide dimer with A) increasing inter-chain distance; B) decreasing inter-chain distance	70

# List of Figures

---

5.8	Captured snapshots of the $A\beta_{17-42}$ dimer at 300 K during the time course of simulation period at constant ( $7.5 \text{ \AA}$ ) inter-chain distances	72
5.9	A) Total Energy vs time course of simulation period; B) Potential Energy vs time course of simulation period for the $A\beta_{17-42}$ peptide dimer at constant inter-chain distance	72
5.10	Total number of A) inter-molecular hydrogen bonds; B) intra-molecular hydrogen bonds vs total number of frames for the $A\beta_{17-42}$ peptide dimer at constant inter-chain distance	72
5.11	The total number of interface residues in $A\beta_{17-42}$ peptide dimer as predicted by the PDBsum server	76
5.12	$C\alpha - C\alpha$ contact probability map (inter-peptide) at 300 K of the $A\beta_{17-42}$ peptide dimer at optimal inter-chain distance	77

## CHAPTER 6

6.1	Potential of mean force as a function of the reaction co-ordinates for the association of the homo- dimer ( $A\beta_{25-35}/A\beta_{25-35}$ & $\text{Tau}_{273-284}/\text{Tau}_{273-284}$ ) and hetero-dimer ( $A\beta_{25-35}/\text{Tau}_{273-284}$ ) (in kcal/mol)	82
6.2	The interface residues showing different interactions as predicted by the PDBsum server of A) $A\beta_{25-35}/A\beta_{25-35}$ homo-dimer; B) $\text{Tau}_{273-284}/\text{Tau}_{273-284}$ homo-dimer; C) $A\beta_{25-35}/\text{Tau}_{273-284}$ hetero-dimer	84
6.3	Snapshots at 300 K during the time course of simulation period at optimal inter-chain distances of A) $A\beta_{25-35}/A\beta_{25-35}$ homo-dimer; B) $\text{Tau}_{273-284}/\text{Tau}_{273-284}$ ; C & D) $A\beta_{25-35}/\text{Tau}_{273-284}$ hetero-dimer	86
6.4	$C\alpha - C\alpha$ contact probability map (inter-peptide) at 300 K of the monomeric units of the A) $A\beta_{25-35}/A\beta_{25-35}$ homo-dimer; B) $\text{Tau}_{273-284}/\text{Tau}_{273-284}$ homo-dimer; C) $A\beta_{25-35}/\text{Tau}_{273-284}$ hetero-dimer at optimal inter-chain distance	87

## CHAPTER 7

7.1	Amyloidogenic residues of $A\beta_{1-42}$ peptide as predicted by AMYLPRED2 software	93
7.2	Disorder Probability Graph for $A\beta_{1-42}$ peptide as predicted by DisEMBL	93
7.3	A) $A\beta_{1-42}$ peptide showing the disordered regions in red color; B) seed structure of $A\beta_{1-42}$ peptide obtained in Chapter 3; C) sequence of $A\beta_{1-42}$ peptide	94

# List of Figures

---

## CHAPTER 8

8.1	Initial structures generated from the M-ZDock server: A) $A\beta_{1-42}$ trimer; B) $A\beta_{1-42}$ tetramer	101
8.2	Snapshots of $A\beta_{1-42}$ trimer at different time intervals of simulation	102
8.3	Time evolution of secondary structure of $A\beta_{1-42}$ trimer at 300 K. A) chain A; B) chain B; C) chain C. The encircled area in blue shows the appearance of $\beta$ -strands	102
8.4	Snapshots of $A\beta_{1-42}$ tetramer at different time intervals of simulation	104
8.5	Time evolution of secondary structure of $A\beta_{1-42}$ tetramer at 300 K. A) chain A; B) chain B; C) chain C; D) chain D. The encircled area in blue shows the appearance of $\beta$ -strands	104
8.6	Total number of inter-molecular hydrogen bonds vs total number of frames for the $A\beta_{1-42}$ trimer during the time course of simulation at 300 K	106
8.7	Total number of hydrophobic contacts vs total number of frames for the $A\beta_{1-42}$ trimer during the time course of simulation at 300 K	106
8.8	Total number of inter-molecular hydrogen bonds vs total number of frames for the $A\beta_{1-42}$ tetramer during the time course of simulation at 300 K	107
8.9	Total number of hydrophobic contacts vs total number of frames for the $A\beta_{1-42}$ tetramer during the time course of simulation at 300 K	107
8.10	Inter-peptide salt-bridge vs total number of frames for A) $A\beta_{1-42}$ trimer; B) $A\beta_{1-42}$ tetramer during the time course of simulation at 300 K	111
8.11	Snapshots of $A\beta_{1-42}$ fibril polymorphs: A) $A\beta_{17-42}$ ; B) $A\beta_{11-42}$ ; C) $A\beta_{MO11-42}$ ; D) $A\beta_{1-42}$	112
8.12	The interface residues and interface plot statistics in $A\beta_{17-42}$ dimer as predicted by PDBsum server	114
8.13	The interface residues and interface plot statistics in $A\beta_{11-42}$ dimer as predicted by PDBsum server	115
8.14	The interface residues and interface plot statistics in $A\beta_{MO11-42}$ dimer as predicted by PDBsum server	116
8.15	The interface residues and interface plot statistics in $A\beta_{1-42}$ dimer as predicted by PDBsum server	117

# List of Figures

---

## CHAPTER 9

- 9.1 Snapshots of A $\beta$ <sub>1-42</sub> peptide in presence of ss-DNA at 300 K during the time course of simulation period 123
- 9.2 Probability score of secondary structure for each residue in the A $\beta$ <sub>1-42</sub> peptide in presence of ss-oligonucleotide 123
- 9.3 Snapshots of A $\beta$ <sub>1-42</sub> peptide at 300 K during the time course of simulation period in presence of 12-mer ss-oligonucleotide 124
- 9.4 Time evolution of secondary structure of A $\beta$ <sub>1-42</sub> peptide in presence of ss-oligonucleotide at 300 K 124
- 9.5 A) Backbone RMSD vs time course of simulation period; B) Radius of Gyration as a function of time course of simulation; C) B-Factor value of C- $\alpha$  atoms for each residue using the backbone atomic fluctuation as a function of amino acids for the A $\beta$ <sub>1-42</sub> peptide in presence of ss-oligonucleotide 125
- 9.6 A) Total number of hydrogen bonds; B) Total number of hydrophobic contacts vs time course of simulation period for the A $\beta$ <sub>1-42</sub> peptide in presence of ss-oligonucleotide. 127
- 9.7 A) Initial structure of A $\beta$ <sub>17-42</sub> dimer-ss-oligonucleotide complex; B) snapshots of A $\beta$ <sub>17-42</sub> dimer at 300 K during the time course of simulation period in presence of ss-oligonucleotide 127
- 9.8 A) Total number of hydrophobic contacts; B) Total number of hydrogen bonds vs time course of simulation period for the A $\beta$ <sub>17-42</sub> dimer in presence of ss-oligonucleotide 129
- 9.9 A) Electrostatic Energy; B) VdWaal Energy vs time course of simulation period for the A $\beta$ <sub>1-42</sub> peptide in presence of ss-oligonucleotide; C) Electrostatic Energy; D) Vdwaal Energy vs time course of simulation period for the A $\beta$ <sub>17-42</sub> dimer in presence of ss-oligonucleotide 129

## CHAPTER 10

- 10.1 Potential of mean force of A $\beta$ <sub>1-42</sub>/A $\beta$ <sub>1-40</sub>hetero-dimer and A $\beta$ <sub>1-42</sub>/A $\beta$ <sub>1-42</sub> homo-dimer (in kcal/mol) as a function of the inter-chain distance (in Å) which is between the center of mass (COM) of the C- $\alpha$  atom of two monomers 134
- 10.2 A) Snapshots of the A $\beta$ <sub>1-42</sub>/A $\beta$ <sub>1-42</sub> homo-dimer; B) snapshots of the A $\beta$ <sub>1-42</sub>/A $\beta$ <sub>1-40</sub>hetero-dimer at 300 K during the time course of simulation period at varying inter-chain distances in Å 136

# List of Figures

---

10.3	Probability score of secondary structure assignment per residue for the average structure of $A\beta_{1-42}$ monomer of the $A\beta_{1-42}/A\beta_{1-42}$ homo-dimer taken from the molecular dynamics simulation trajectory A) increasing inter-chain distance; B) decreasing inter-chain distance	136
10.4	Probability score of secondary structure assignment per residue for the average structure of $A\beta_{1-42}$ monomer of the $A\beta_{1-42}/A\beta_{1-40}$ hetero-dimer taken from the molecular dynamics simulation trajectory A) increasing inter-chain distance; B) decreasing inter-chain distance	138
10.5	Total number of: A) inter-molecular hydrogen bonds; B) intra-molecular hydrogen bonds as a function of time for the $A\beta_{1-42}/A\beta_{1-40}$ hetero-dimer at constant inter-chain distance	138
10.6	Snapshots of $A\beta_{1-42}/A\beta_{1-40}$ hetero-dimer obtained after MD simulation run at constant inter-chain distance (13 Å)	139
10.7	Backbone RMSD vs time course of simulation period for the $A\beta_{1-42}/A\beta_{1-40}$ hetero-dimer complex at the constant distance	139
10.8	RMSF of C- $\alpha$ atoms for each residue using the backbone atomic fluctuation as a function of amino acids for the lowest energy conformer $A\beta_{1-42}/A\beta_{1-40}$ hetero-dimer	140
10.9	A) Total Energy; B) Potential Energy vs time course of simulation period for the $A\beta_{1-42}/A\beta_{1-40}$ hetero-dimer at constant inter-chain distance	142
10.10	Time dependence distance between Asp23 and Lys28 of: A) lowest energy conformer $A\beta_{1-42}/A\beta_{1-40}$ hetero-dimer; B) lowest energy conformer $A\beta_{1-42}/A\beta_{1-42}$ homo-dimer	142
10.11	A) The interface residues; B) the interface plot statistics of lowest energy conformer of $A\beta_{1-42}/A\beta_{1-42}$ homo-dimer at constant distance	143
10.12	A) The interface residues of lowest energy conformer $A\beta_{1-42}/A\beta_{1-40}$ hetero-dimer; B) the interface plot statistics of the lowest energy conformer $A\beta_{1-42}/A\beta_{1-40}$ hetero-dimer at constant distance	144
10.13	The interface residues of the $A\beta_{1-42}/A\beta_{1-42}$ homo-dimer showing different interactions as predicted by the PDBsum server	145
10.14	A). VdWaals; B) Electrostatic Energy vs time course of simulation period for the $A\beta_{42}/A\beta_{40}$ hetero- dimer after MD simulation run at constant inter-chain distance	146

## CHAPTER 11

## List of Figures

---

11.1	Structure of A) the initial A $\beta_{1-42}$ monomer/analogue 6 complex; B) the initial A $\beta_{17-42}$ fibril/analogue 6 complex with the highest atomic contact energy and surface area score obtained from PatchDock server	153
11.2	Conformational dynamics of A $\beta_{17-42}$ fibril in presence of analogue 6 at different time course of simulation at 300 K	154
11.3	Conformational dynamics of A $\beta_{17-42}$ fibril in presence of analogue 5 at different time course of simulation at 300 K	155
11.4	Potential of mean force of A $\beta_{1-42}$ monomer/reference peptide and A $\beta_{1-42}$ monomer / analogue 6 (in kcal/mol) as a function of the inter-chain distance (in Å)	156
11.5	Snapshots of A $\beta_{1-42}$ monomer/analogue 6 complex at different inter-chain distances during the potential of mean force analysis at 300 K	157
11.6	Snapshots of A $\beta_{1-42}$ monomer/reference peptide complex at different inter-chain distances during the potential of mean force analysis at 300 K	157
11.7	Contact map analysis showing residue-residue interactions in the global minima structure of: A) A $\beta_{1-42}$ monomer/reference peptide complex; B) A $\beta_{1-42}$ monomer/analogue 6 complex	159
11.8	LigPlot analysis showing the interactions as predicted by the PDBsum server of the global minima structure of: A) A $\beta_{1-42}$ monomer/reference peptide complex; B) A $\beta_{1-42}$ monomer/analogue 6 complex	159

# List of Tables

<b>Table No.</b>		<b>Page No.</b>
<b>CHAPTER 2</b>		
2.1.	Neurodegenerative diseases linked to protein misfolding	7
<b>CHAPTER 5</b>		
5.1	The inter-chain distances between the monomeric units of A $\beta$ <sub>17-42</sub> peptide dimer	64
5.2	Inter-molecular hydrogen bonding analysis of A $\beta$ <sub>17-42</sub> peptide dimer	73
5.3	Intra-molecular hydrogen bonding analysis of A $\beta$ <sub>17-42</sub> peptide dimer	74
5.4	Interface Statistics of A $\beta$ <sub>17-42</sub> peptide dimer as provided by the PDBsum server	76
<b>CHAPTER 6</b>		
6.1	The inter-chain distances for the homo-dimer A $\beta$ <sub>25-35</sub> /A $\beta$ <sub>25-35</sub> ; Tau <sub>273-284</sub> /Tau <sub>273-284</sub> and the hetero-dimer A $\beta$ <sub>25-35</sub> /Tau <sub>273-284</sub>	82
6.2	The interface plot statistics of the homo-dimers (A $\beta$ <sub>25-35</sub> /A $\beta$ <sub>25-35</sub> , Tau <sub>273-284</sub> /Tau <sub>273-284</sub> ) and hetero-dimer (A $\beta$ <sub>25-35</sub> /Tau <sub>273-284</sub> ) as predicted by the PDBsum server	84
<b>CHAPTER 7</b>		
7.1	Hot spots of A $\beta$ <sub>1-42</sub> peptide as predicted by AGGRESCAN.AA: amino acid; a <sup>4</sup> v: a <sup>3</sup> v average; HSA: hot spot area; NHSA: normalized HSA; a <sup>4</sup> vAHS: a <sup>4</sup> v average in the Hot Spot	95
<b>CHAPTER 8</b>		
8.1	Secondary structural analysis of A $\beta$ <sub>1-42</sub> peptide oligomers	103
8.2	Inter-molecular hydrogen bonding analysis of A $\beta$ <sub>1-42</sub> trimer	105
8.3	Inter-molecular hydrogen bonding analysis of A $\beta$ <sub>1-42</sub> tetramer	108
8.4	The interface plot statistics of the A $\beta$ <sub>1-42</sub> trimer as predicted by the PDBsum server	110
8.5	The inter-peptide salt bridge analysis of the A $\beta$ <sub>1-42</sub> trimer as predicted by the PDBsum server	110
8.6	The interface plot statistics of the A $\beta$ <sub>1-42</sub> tetramer as predicted by the PDBsum server	110
8.7	The inter-peptide salt bridge analysis of the A $\beta$ <sub>1-42</sub> tetramer as	110

# List of Tables

---

predicted by the PDBsum server

## CHAPTER 10

- 10.1 Binding free energy of  $A\beta_{1-40}$  peptide to  $A\beta_{1-42}$  peptide in the hetero-dimer system and  $A\beta_{1-42}$  to  $A\beta_{1-42}$  in the homo-dimer system 146

## CHAPTER 11

- 11.1 Docking result of the 6-mer peptides with  $A\beta_{1-42}$  monomer and  $A\beta_{17-42}$  fibril respectively 153



# List of Abbreviations

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Å	:	Angstrom
A $\beta$	:	Amyloid Beta
ACE	:	Atomic contact Energy
AD	:	Alzheimer's Disease
AFM	:	Atomic Force Microscopy
APP	:	Amyloid Precursor Protein
ApoE	:	Apolipoprotein E
ATP	:	Adenosine Triphosphate
BPTI	:	Bovine Pancreatic Trypsin Inhibitor
CG	:	Coarse-grained
CD	:	Circular Dichroism
CHC	:	Central Hydrophobic Core
COM	:	Centre of Mass
CMA	:	Contact Map Analysis
CVD	:	Cardiovascular Diseases
3-D	:	3-Dimensional
DM2	:	Diabetes Mellitus type 2
DMD	:	Discrete Molecular Dynamics
DNA	:	Deoxyribonucleic Acid
EM	:	Electron Microscopy
FAD	:	Familial AD
FFT	:	Fast Fourier Transform
FTD	:	Frontotemporal Dementia
FTIR	:	Fourier-transform Infrared Spectroscopy
GB	:	Generalized Born
HbP	:	Hidden beta propensity
IDP	:	Intrinsically Disordered Protein
IDR	:	Intrinsically Disordered Region
IM-MS	:	Ion Mobility Mass Spectrometry
LTP	:	Long-term Potentiation
MD	:	Molecular Dynamics
MRI	:	Magnetic Resonance Imaging
MTBR	:	Microtubule Binding Region
ns	:	nanosecond
NAB	:	Nucleic Acid Builder
NFT	:	Neurofibrillary Tangles
NIA	:	National Institute on Ageing
NMR	:	Nuclear Magnetic Resonance Spectroscopy
ps	:	picosecond
PB	:	Poisson-Boltzmann
PDB	:	Protein Data Bank
PET	:	Positron Emission Tomography
PMF	:	Potential of Mean Force
PSC	:	Pairwise Shape Complementarity
PSEN	:	Presenilin
RC	:	Reaction Coordinate
REMD	:	Replica Exchange Molecular Dynamics
R <sub>g</sub>	:	Radius of Gyration

# List of Abbreviations

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RMSD	:	Root Mean Square Deviation
RMSF	:	Root Mean Square Fluctuation
SPC	:	Simple Point Charge
SP	:	Senile Plaques
ss	:	Short single-stranded
TEM	:	Transmission Electron Microscopy
TIP3P	:	Transferable Intermolecular Potential Three-point
US	:	Umbrella Sampling
UV	:	Ultra Violet
VMD	:	Visual Molecular Dynamics
WHAM	:	Weighted Histogram Analysis Method

# List of Publications

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**This thesis is partly based on the following original communications:**

1. Dutta, M., & Mattaparthi, V.S.K. In silico Investigation on the Inhibition of A $\beta$ 42 Aggregation by A $\beta$ 40 peptide by Potential of Mean Force study. *Journal of Biomolecular Structure and Dynamics*, **2017**. DOI: 10.1080/07391102.2017.1296783.
2. Dutta, M., Chutia, R., & Mattaparthi, V.S.K. Structural Characterization of Amyloid  $\beta$ 17-42 Dimer by potential of mean force analysis: Insights from Molecular Dynamics Simulations. *Proteins & Peptide Letters*, 24(7): 650-660, **2017**.
3. Dutta, M., & Mattaparthi, V.S.K. Inhibition of A $\beta$  1–42 peptide aggregation using short ss-oligonucleotide as polyions: an in silico approach. *Journal of Biomolecular Structure and Dynamics*, 35(7): 1401-1406, **2017**.
4. Dutta, M., Chutia, R., & Mattaparthi, V.S.K. Cross-seeding interaction between Amyloid  $\beta$  and Tau protein can enhance aggregation, *Current Biotechnology*, 6(3): 273-279, **2017**.
5. Dutta, M., Deb, A., & Mattaparthi, V.S.K. Investigations on the Structural Characteristics that Seed the Aggregation of Amyloid-1-42 Peptide: Insights from Molecular Dynamics Simulations. *Current Proteomics*, 13(3): 172-178, **2016**.
6. Dutta, M., and Mattaparthi, V.S.K. A comparative study to elucidate the inhibitory mechanism of a 6-mer fragment of Amyloid- $\beta$ 42 peptide as a potential therapeutic in Alzheimer's disease: Insights from Molecular Dynamics Simulations. *Current Science*, **2017**.(Recently accepted)
7. Dutta, M., and Mattaparthi, V.S.K. A Computational Approach to Understand the Interactions Stabilizing the A $\beta$ 1-42 Peptide Oligomers. *3 Biotech*, 2017. (Manuscript communicated)

**In addition, this thesis also contains unpublished data.**

# Conference Proceedings

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- **Dutta, M., & Mattaparthi, V.S.K.** Structural Characterization of Amyloid  $\beta_{17-42}$  Dimer by potential of mean force analysis: Insights from Molecular Dynamics Simulations. International conference on “Advances in Biotechnology & Biotherapeutics” held at Sathyabama University on 8<sup>th</sup> -10<sup>th</sup> March, 2017.
- **Dutta, M., & Mattaparthi, V.S.K.** Study on the  $A\beta_{1-42}$  peptide dimerization process using molecular dynamics simulation. International conference on "Exploring Mechanisms in Biology: Theory and Experiment" organized by the Molecular Graphics and Modelling Society (MGMS) on the 25th-27th. November 2015, A\*STAR, Singapore.
- **Dutta, M., & Mattaparthi, V.S.K.** Inhibition of  $A\beta$  aggregation in Alzheimer disease using the poly-ion short single stranded DNA: an *in silico* study. 19th Conversation: Albany, June 9-13, 2015 at Albany, New York.
- **Dutta, M., & Mattaparthi, V.S.K.** Amyloid  $\beta$  peptide folding simulation to trace out the seed structure responsible for aggregation. International conference on Mathematical and Computational Biology held at the Indian Institute of Technology (IIT), Kanpur, India.
- **Dutta, M., & Mattaparthi, V.S.K.** Conformational dynamics of Amyloid beta peptide in water. International conference on “Disease biology and therapeutics” held at The Institute of Advanced Study in Science & Technology (IASST), Guwahati, India.
- Organized and **attended lecture series** on “Recent Advances in Mathematical and Computational Biology” held on 18th -19th October, 2014 jointly organized by National Network for Mathematical and Computational Biology (NNMCB) Govt. of India, and Tezpur University, Assam, India.