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List of Abbreviations

Å	:	Angstrom
Aβ	:	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
Rg	:	Radius of Gyration

List of Abbreviations

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

This thesis is partly based on the following original communications:

1. Dutta, M., & Mattaparthi, V.S.K. In silico Investigation on the Inhibition of Aβ42 Aggregation by Aβ40 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 β17-42 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 Aβ 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 β 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-β42 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 Aβ1-42 Peptide Oligomers. *3 Biotech*, 2017. (Manuscript communicated)

In addition, this thesis also contains unpublished data.

- **Dutta, M., & Mattaparthi, V.S.K.** Structural Characterization of Amyloid β_{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^{th}-10^{th} 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 Aβ 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 β 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.