

**COMPUTATIONAL ANALYSIS OF SEVEN
MYOSIN XI PROTEINS (XI-A to XI-G) IN
*ARABIDOPSIS THALIANA***



By:

Sidra Toor

ID: 15004140009

SUPERVISOR:

Dr. Nouman Rasool

**DEPARTMENT OF CHEMISTRY
SCHOOL OF SCIENCE
UNIVERSITY OF MANAGEMENT AND TECHNOLOGY,
LAHORE, PAKISTAN.**

2017

**COMPUTATIONAL ANALYSIS OF SEVEN MYOSIN XI
PROTEINS (XI-A to XI-G) IN *ARABIDOPSIS THALIANA***

Submitted to University of Management and Technology

Lahore

In partial fulfillment of the requirements

For the award of degree of

**MASTER OF SCIENCE
IN
CHEMISTRY**

BY

SIDRA TOOR

ID

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 5 | 0 | 0 | 4 | 1 | 4 | 0 | 0 | 0 | 9 |
|---|---|---|---|---|---|---|---|---|---|---|

SESSION: 2015-2017

**DEPARTMENT OF CHEMISTRY
SCHOOL OF SCIENCE
UNIVERSITY OF MANAGEMENT AND TECHNOLOGY,
LAHORE, PAKISTAN.**

DECLARATION

I **Sidra Toor** d/o Sardar Ahmed ID: **15004140009**, Session 2015-2017 hereby declare that the matter printed in the thesis titled “**COMPUTATIONAL ANALYSIS OF SEVEN MYOSIN XI PROTEINS (XI-A to XI-G) IN *ARABIDOPSIS THALIANA***” is my own work and has not yet been printed, published and submitted as research work, thesis or publication in any form in any university, research institution etc. in Pakistan or abroad.

Dated:

Sidra Toor

DEDICATION

*I dedicate this thesis
to
my Parents, without their prayers
I would never be able
to
work hard and gain this achivement.*

SUMMARY

Arabidopsis is widely used in the field of plant research. Arabidopsis thaliana emerged as a model organism for plant biologists in early nineties. Myosins belong to a super family of molecular motor proteins that occur in probably all eukaryotic cells. These proteins are actively involved in trafficking of cell organelles, including the endoplasmic reticulum, mitochondria, peroxisomes, golgi stacks, and endomembrane vesicles. Myosins are also involved in signal transduction in cell. The present study aims at the analysis of physio-chemical properties of seven myosin XI (XI-A, XI-B, XI-C, XI-D, XI-E, XI-F, and XI-G), their functions, binding sites, sub cellular locations, secondary and tertiary structures prediction. Phylogenetic analysis, molecular simulation and molecular docking will be conducted through using different bioinformatics tools to study the characteristics of these proteins.

ACKNOWLEDGEMENT

All praise to **Almighty Allah**, who allowed me and has provided me qualities to complete some study perform and to donate to respectable subject of knowledge.

This dissertation identifies the investigation perform performed at School of Science, University of Management and Technology, Lahore under the direction of **Dr. Nouman Rasool** to whom I'm very indebted for direction, indicating the niche, full time support, advice, help and suggestions. His bits of guidance, discussions, recommendations and remarks were generally supply of enthusiasm and zeal for me. He's generally wonderful, sort, generally prepared to greatly help pupils for understanding and study and needed suffering for the duration of my research. I'm very obliged to him for his security, persistence, immense understanding and important time. I can not need dreamed having a much better supervisor and teacher for my study perform and thesis.

Finally, I'm poor and deficient in language to get acceptable phrases to state my thoughts with tearful eyes for my supportive **Parents** who shown me to get the first faltering step, to talk the initial term and influenced me for the duration of of my entire life, whose arms are usually elevated for wishes which created me effective atlanta divorce attorneys subject of my life. They reinforced me to reach resources in my own academic endeavors and different spheres of life. Their time and evening wishes permit me to participate larger some ideas of living, resolving every one of issues and increased my ethical to complete my goals.

Sidra Toor

TABLE OF CONTENTS

| | |
|---|-----------|
| DECLARATION..... | i |
| DEDICATION..... | ii |
| SUMMARY..... | iii |
| ACKNOWLEDGMENTS..... | iv |
| TABLE OF CONTENTS..... | v |
| LIST OF FIGURES..... | vii |
| LIST OF TABLES..... | viii |
| | |
| 1 Introduction..... | 2 |
| 1.1 Arabidopsis thaliana ----- | 2 |
| 1.2 Motor proteins ----- | 3 |
| 2 Literature Review..... | 10 |
| 3 Materials and Methods..... | 24 |
| 3.1 Sequence Retrieval and Alignment ----- | 24 |
| 3.2 Physio-chemical properties analysis----- | 24 |
| 3.3 Prediction of sub cellular localization ----- | 24 |
| 3.4 Motif and gene structure analysis ----- | 24 |
| 3.5 Phylogenetic analysis----- | 24 |
| 3.6 Secondary Structure and binding site Prediction----- | 25 |
| 3.7 Binding site prediction ----- | 255 |
| 3.8 Homology modeling ----- | 25 |
| 3.9 Molecular Dynamics----- | 26 |
| 3.10 Molecular Docking ----- | 26 |
| 4 Results..... | 29 |
| 4.1 Physio-chemical properties of Arabidopsis thaliana myosin proteins----- | 29 |

| | | |
|----------|---|------------|
| 4.2 | Sub cellular and chromosomal location of Arabidopsis thaliana myosin proteins ----- | 30 |
| 4.3 | Analysis of Arabidopsis thaliana myosin XI proteins ----- | 31 |
| 4.4 | Sequence alignment and phylogenetic tree ----- | 31 |
| 4.5 | Secondary Structure ----- | 39 |
| 4.6 | Homology modelling ----- | 42 |
| 4.7 | Molecular Dynamics and Simulation ----- | 47 |
| 4.8 | Molecular Docking ----- | 54 |
| 4.8.1 | Docking with Myosin XI-A ----- | 54 |
| 4.8.2 | Docking with Myosin XI-B ----- | 63 |
| 4.8.3 | Docking with Myosin XI-C ----- | 71 |
| 4.8.4 | Docking with Myosin XI-D ----- | 79 |
| 4.8.5 | Docking with Myosin XI-E ----- | 88 |
| 4.8.6 | Docking with Myosin XI-F ----- | 96 |
| 5 | Discussion..... | 115 |
| 6 | Conclusion..... | 122 |
| 7 | References..... | 124 |

LIST OF FIGURES

| | |
|--|-------------------------------------|
| Figure 1.1: Plant of Arabidopsis thaliana | 4 |
| Figure 1.2: Class XI Myosin (Li, 2008)..... | 6 |
| Figure 4.1: Motif analysis for six myosin proteins | 31 |
| Figure 4.2: Phylogentic tree for six Myosin XI proteins | 32 |
| Figure 4.3: Sequence alignment of Myosin XI seven proteins | 39 |
| Figure 4.4: Secondary structure of MyosinXI-A | 39 |
| Figure 4.5: Secondary structure of MyosinXI-B | 40 |
| Figure 4.6: Secondary structure of MyosinXI-C | 40 |
| Figure 4.7: Secondary structure of MyosinXI-D | 40 |
| Figure 4.8: Secondary structure of MyosinXI-E..... | 41 |
| Figure 4.9: Secondary structure of MyosinXI-F..... | 41 |
| Figure 4.10: Secondary structure of MyosinXI-G | 41 |
| Figure 4.11: Tertiary structure of Myosin XI-A..... | 43 |
| Figure 4.12: Tertiary structure of Myosin XI-B | 44 |
| Figure 4.13: Tertiary structure of Myosin XI-C | 44 |
| Figure 4.14: Tertiary structure of Myosin XI-D..... | 45 |
| Figure 4.15: Tertiary structure of Myosin XI-E..... | 45 |
| Figure 4.16: Tertiary structure of Myosin XI-F..... | 46 |
| Figure 4.17: Tertiary structure of Myosin XI-G | 46 |
| Figure 4.18: Gyration plot for XI-A | 47 |
| Figure 4.19: RMSD graph for XI-A | 48 |
| Figure 4.20: RMSD plot for XI-B..... | 48 |
| Figure 4.21: Gyration plot for XI-B..... | 49 |
| Figure 4.22: RMSD plot for XI-C..... | Error! Bookmark not defined. |
| Figure 4.23: Gyration plot for XI-C..... | 50 |
| Figure 4.24: RMSD plot for XI-D | 49 |
| Figure 4.25: Gyration plot for XI-D | 51 |
| Figure 4.26: RMSD plot for XI-E..... | 50 |
| Figure 4.27: Gyration plot for XI-E..... | 52 |
| Figure 4.28: RMSD plot for XI-F | 51 |
| Figure 4.29: Gyration plot for XI-F | 53 |
| Figure 4.30: RMSD plot for XI-G | 53 |
| Figure 4.31: Gyration plot for XI-G | 54 |

LIST OF TABLES

| | |
|---|-----|
| Table 4.1: Physio-chemical properties of Arabidopsis thaliana myosin XI proteins . | 29 |
| Table 4.2: Subcellular localization of Arabidopsis thaliana myosin XI proteins | 30 |
| Table 4.3: Characteristics of secondary structures of Arabidopsis thaliana myosin proteins..... | 42 |
| Table 4.4: Molecular docking results of 24 compounds against Myosin XI-A..... | 55 |
| Table 4.5: Molecular docking results of 24 compounds against Myosin XI-B..... | 63 |
| Table 4.6: Molecular docking results of 24 compounds against Myosin XI-C..... | 71 |
| Table 4.7: Molecular docking results of 24 compounds against Myosin XI-D..... | 80 |
| Table 4.8: Molecular docking results of 24 compounds against Myosin XI-E..... | 88 |
| Table 4.9: Molecular docking results of 24 compounds against Myosin XI-F | 97 |
| Table 4.10: Molecular docking results of 24 compounds against Myosin XI-G..... | 106 |

CHAPTER 1

INTRODUCTION

1 INTRODUCTION

1.1 *Arabidopsis thaliana*

Arabidopsis thaliana, an annual plant which has a place with family Brassicaceae, has a common physical look as different plants of the family show up. It has single essential root which delivers little parallel roots (Meinke *et al.*, 1998). At its development organize plant picks up tallness around 20-25 cm. It has single stem which bears blooming at development. At the base of the plant, leaves frame a rosette having green to violet shading. Leaves are secured with unicellular hairs (trichomes). How huge leaves fluctuates between 1.5 to 5 cm altogether and 2 to 10 mm in width (Figure 1.1). Blooms are organized on corymb, having 3mm distance across. The natural product is 5-20 mm long in the best possible execution of siliqua and every siliqua contains 20-30 seeds (Meinke *et al.*, 1998). *Arabidopsis thaliana* developed as model life form for plant researcher around 25 years back (Meinke *et al.*, 2009) and after that plant has been utilized broadly in the field of plant inquire about. Noteworthy highlights which made this plant as model living being were littler size, short germination period and impervious to natural burdens. Encourage subsequent to the sequencing of its genome it turned into the customary reference in the field of plant science (Meinke *et al.*, 2009).

Cell association requires managed load transport along cytoskeletal components. Myosin V engines are among without a doubt the most saved organelle engines and have now been very much portrayed in both yeast and mammalian frameworks (Donovan and Bretscher, 2015). Engine proteins fit in with three primary families, kinesins, dyneins and myosins (Vale, 2003). The enormous occasion of kinesins and

dyneins is to carry on as the engine of microtubule fibres whereas myosin follows up on actin (Vale *et al.*, 2003). The significant capacity of intracellular motility in plants is repositioning of organelles, charge conveyance and cytosol development. Charge conveyance involves on transportation of particles from the site of the blend to the site of the target. It likewise contains the take-up of substances from outside and exchange to cytoplasmic organelles mindful reusing or utilize. Directional development of engine proteins is required for the control and upkeep of fluctuated organic wonders through the age of thought process drive. Repositioning of cell organelles can be utilized to do metabolic changes under different natural conditions i.e change in light power or pathogenic assault. The exemplary occurrence of light force might be the translocation of chloroplast into cell space that is utilized to advance the photosynthetic action at the cell level (Sato *et al.*, 2001). In plants, intracellular development is happened by free dispersion along cytoskeleton fibres and the cytoskeleton grids are exceedingly elements in nature.

1.2 Motor proteins

Among individuals from myosin XI proteins, every part performs recognize work. Additionally, full length XI-K yellow fluorescent protein (YFP) is related to endomembrane trafficking along F-actin (Peremyslov *et al.*, 2012). These proteins tie with ATP, hydrolyze it to produce power and development alongside actin fibres (Ito *et al.*, 2009). Myosin XI-K is connected with the endoplasmic reticulum and effectively takes an interest in its redesigning and development (Sparkes, 2010; Ueda *et al.*, 2010). Myosin proteins additionally help to determine the phone capacities like cell motility, film transportation, muscle constriction, cytokinesis and flag