MOLECULAR DYNAMICS-GUIDED MODIFICATION OF AFPIV 3D STRUCTURE TO IMPROVE ICE BINDING INTERACTION

By

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Thesis Submitted to the School of Graduate Studies, Universiti Putra Malaysia, in Fulfilment of the Requirements for the Degree of Doctor of Philosophy

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Abstract of thesis presented to the Senate of Universiti Putra Malaysia in fulfilment of the requirement for the degree of Doctor of Philosophy

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Chairman : Associate Professor Siti Nurbaya Oslan, PhD
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Exotic properties of antifreeze proteins (AFPs) and antifreeze peptides have currently been widely used in cryopreservation due to their special functions; ice crystal growth inhibition (IRI) and thermal hysteresis (TH). Chemical synthesis of AFPs and their natural protein (wild-type) are uneconomical and time consuming. Moreover, some AFPs have low function naturally (less activity) to be used in cryopreservation where the cells can be damaged due to formation of ice crystals and toxicity of cryoprotectants. Thus, this study aims to design a new AFP from the wild-type with improved activity using molecular dynamics (MD) guidance. In this *in-silico* study, the modified afp1m from yeast was fused to multi-helices of AFPIV from fish. A new linker was designed to boost the ice interaction of AFPIV and make it more cost-effective. The newly designed model was designated as AFP1m3. The present of the new linker has improved the interaction between the ice lattice and AFP1m3, thus make it more economical for further practical utilizations. Various bioinformatics tools such as Expasy Protparam, PepWheel, SWISS-MODEL, Phyre2, ERRAT, PROCHECK and ProQ were used to analyze the physicochemical, functional and structural properties of this newly designed AFP (AFP1m3) model. Furthermore, MD simulation with GROMACS software for 100 ns, was conducted to evaluate the interaction between ice and the new mutant. The primary structure analysis showed that AFP1m3 is hydrophobic in nature due to the high content of non-polar residues. The secondary structure analysis revealed that this protein was fully helix by using PepWheel tool. The results of the 3D structure model by excluding SWISS-MODEL and Phyre2 demonestrated that AFP1m3 had the best model by these modelling tools with QMEAN of -0.23, confidence of 98.2% and coverage score of 23% as well as Ramachandran value of around 96%, had the best model. In addition, the analysis of the predicted model validity proved that AFP1m3 was extremely a good model according to ProQ tool criteria. Analysis of MD simulation results illustrated that AFP1m3 had more rigidity according to its proper helical structure, better interaction with ice due to its

stability of hydrogen bonds which mimic the freezing and thawing temperatures in cryopreservation condition at -8 and 25 ºC and high activity regarding to the low rate of ice growth at three different temperatures. This study may shed light on application of newly designed AFPIV in cryopreservation at low concentration. The conclusion can be drawn that the AFP1m3 improved its anti-freeze properties with better ice interaction (high activity) at a lower cost to meet medical applications especially in cryopreservation of cells and tissues.

Abstrak tesis yang dikemukakan kepada Senat Universiti Putra Malaysia sebagai memenuhi keperluan untuk ijazah Doktor Falsafah

PENGUBAHSUAIAN BERPANDU DINAMIK MOLEKUL STRUKTUR 3D AFPIV UNTUK MENINGKATKAN INTERAKSI IKATAN AIS

Oleh

ESKANDARI AZADEH HASSAN

Februari 2023

Pengerusi : Profesor Madya Siti Nurbaya Oslan, PhD
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Sifat eksotik protein antibeku (AFP) dan peptida antibeku kini telah digunakan secara meluas dalam pengawetan krio kerana fungsi khasnya; perencatan pertumbuhan kristal ais (IRI) dan histerisis haba (TH). Sintesis kimia AFP dan protein semulajadinya (jenis liar) adalah tidak ekonomik dan memakan masa. Selain itu, sesetengah AFP mempunyai fungsi rendah secara semula jadi (kurang aktiviti) untuk digunakan dalam pengawetan krio di mana sel boleh rosak akibat pembentukan hablur ais dan ketoksikan krioprotektan. Oleh itu, kajian ini bertujuan untuk mereka bentuk AFP baharu daripada jenis liar dengan aktiviti yang dipertingkatkan menggunakan panduan dinamik molekul (MD). Dalam kajian dalam siliko ini, afp1m yang diubah suai daripada yis telah dicantumkan kepada pelbagai heliks AFPIV daripada ikan. Penyambung baharu telah direka untuk meningkatkan interaksi ais AFPIV dan menjadikannya lebih kos efektif. Model yang direka bentuk baru telah ditetapkan sebagai AFP1m3. Kehadiran penyambung baharu telah menambah baik interaksi antara kekisi ais dan AFP1m3, sekali gus menjadikannya lebih menjimatkan untuk kegunaan praktikal selanjutnya. Pelbagai alat bioinformatik seperti Expasy Protparam, PepWheel, SWISS-MODEL, Phyre2, ERRAT, PROCHECK dan ProQ telah digunakan untuk menganalisis sifat fizikokimia, fungsian dan struktur model AFP (AFP1m3) yang direka bentuk baharu ini. Tambahan pula, simulasi MD dengan perisian GROMACS selama 100 ns, telah dijalankan untuk menilai interaksi antara ais dan mutan baharu. Analisis struktur primer menunjukkan bahawa AFP1m3 bersifat hidrofobik kerana kandungan sisa bukan kutub yang tinggi. Analisis struktur sekunder mendedahkan bahawa protein ini adalah heliks sepenuhnya dengan menggunakan alat PepWheel. Keputusan model struktur 3D dengan mengecualikan SWISS-MODEL dan Phyre2 menunjukkan bahawa AFP1m3 mempunyai model terbaik dengan alat pemodelan ini dengan QMEAN sebanyak -0.23, keyakinan 98.2% dan skor liputan 23% serta nilai Ramachandran sekitar 96%, mempunyai model terbaik. Di samping itu, analisis kesahan model yang diramalkan membuktikan bahawa AFP1m3 adalah model

yang sangat baik mengikut kriteria alat ProQ. Analisis keputusan simulasi MD menggambarkan bahawa AFP1m3 mempunyai lebih ketegaran mengikut struktur heliksnya yang betul, interaksi yang lebih baik dengan ais kerana kestabilan ikatan hidrogennya yang meniru suhu beku dan pencairan dalam keadaan kriopreservasi pada -8 dan 25 ºC dan aktiviti yang tinggi mengenai kadar pertumbuhan ais yang rendah pada tiga suhu berbeza. Kajian ini mungkin memberi penerangan tentang penggunaan AFPIV yang baru direka bentuk dalam pengawetan krio pada kepekatan rendah. Kesimpulannya boleh dibuat bahawa AFP1m3 meningkatkan sifat anti-bekunya dengan interaksi ais yang lebih baik (aktiviti tinggi) pada kos yang lebih rendah untuk memenuhi aplikasi perubatan terutamanya dalam pengawetan krio sel dan tisu.

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LIST OF ABBREVIATIONS

°C	Degree centigrade
%	Percentage
>	Greater than
<	Lesser than
&	And
α	Alpha
β	Beta
∆Gs	Surface free energy changes
∆Gv	Free energy changes
∆H	Change in enthalpy
∆S	Change in enthalpy of the system
3D	3-Dimensional
Å	Angstrom
AFGP	Antifreeze glycoprotein
afp1	Antifreeze peptide 1
Afp1	Antifreeze protein type I from *Glaciozyma Antarctica*
afp1m	Antifreeze peptide 1m
AFP1m1	Antifreeze protein 1m1
AFP1m2	Antifreeze protein 1m2
AFP1m3	Antifreeze protein 1m3
AFP1m4	Antifreeze protein 1m4
afp4m	Antifreeze peptide 4m
AFPI	Antifreeze protein type I
AFPII	Antifreeze protein type II
AFPIII	Antifreeze protein type III

AFPIV	Antifreeze protein type IV
AFPs	Antifreeze proteins
AL	Atomic level
AMBER	Assisted Model Building with Energy Refinement
CHARMM	Chemistry at Harvard Macromolecular Mechanics
CPAs	Cryoprotectant agent/agents
DIS	Dynamic ice shaping
DMSO	Dimethyl sulphoxide
DNA	Deoxyribonucleic acid
dNMR	Dynamic NMR
FITC	Fluorescein isothiocyanate
GROMACS	Groningen machine for chemical simulations
Hecs	Human embryonic stem cells
HPLC	High pressure liquid chromatography
hypAFPs	Hyperactive AFPs
IBPs	Ice binding proteins
IRI	Ice recrystallization inhibition
Kcal	Kilocalorie
KDa	Kilo Dalton
L-J	Lenard Jones
MD	Molecular dynamics
Mg	Milligram
Ml	Milliliter
mM	Millimolar
mol	Mole
N	Nitrogen
N	Number of molecules

NCBI	National Center of Biotechnology Information
NMR	Nuclear magnetic resonance
NPS	Network Protein Sequence
ns	Nanosecond
O	Oxygen
PBC	Periodic boundary condition
PDB	Protein Data Bank
PIR-PSD	Protein Information Resource Protein Sequence Database
PME	Particle Mesh Ewald
P-P	Protein-protein
Ps	Picosecond
PVP	Poly vinyl pyrolidone
QMEAN	Qualitative Model Energy Analysis
R	Rate
R	Radius
RMSD	Root mean square deviation
SHS	Shorthorn sculpin
SMART	Simple Modular Architecture Research Tool
SOPMA	Self-Optimized Prediction Method
TH	Thermal hysteresis
Tm	Melting temperature
TrEMBL	Translated European Molecular Biology Laboratory
UniProt	Universal Protein Resource
V	Volume
W-P	Water-protein
W-W	Water-Water
ΔEint	Change of interaction energy

ΔT	Change in Temperature
Δt	Change of distance
Ω	Molar volume of ice

CHAPTER 1

INTRODUCTION

Various methods of cryopreservation recently are highly demanded due to effective procedures of this technique which plays a crucial role in cell biology and regenerative medicine although, it is not so convincing to be established (Jang *et al.,* 2017). Cryoprotectant (CPA) is a technically-derived term invented to define any chemical that can be added and used with cells, tissues before storage at freezing which produces a high survival rate post-thaw as compared with its absence. CPA is an important feature in cryopreservation application. One of the main cells permeable CPA that used vastly in cell suspension within cryopreservation method is dimethyl sulfoxide (DMSO) (Morgan *et al*., 2016; Bender 2016; Lewis *et al*., 2016).

DMSO can enter the cells under cryopresavation techniques and decrease cell injuries through in unfrozen solutions via reducing the concentration of electrolytes thus, may surrounding the cells at different temperatures hence, reducing the formation of ice growth, osmotic shock and cell shrinkage within freezing procedure (Whaley *et al*., 2021; Bui *et al.*, 2017). All methods in cryopreservation showed that the survival of cells with availability of DMSO decreased dramatically due to its cytotoxicity and internal signaling inhibition (Higuchi *et al*., 2016; Faiella *et al*., 2016).

Utilization of current form of standard DMSO which is applied in freezing suspensions is improper in freezing conditions through the evidences of 2- and 3-D network experience with various modes that occurred in cryoinjuries (Whaley *et al*., 2021; Erol *et al*., 2021). Therefore, for future diagnosis and therapies based on cell and tissues development of novel CPA instead of DMSO is inevitable.

Many studies revealed that proline (Moradi *et al*., 2021), antifreeze proteins (AFPs) (Panch *et al*., 2019) trehalose (Anjoz *et al*., 2021) and sucrose (Anjoz *et al*., 2021), can be used naturally in the cell suspension within cryopreservation methods and can be replaced or limited instead of DMSO (Slitcher *et al.,* 2018). Recently AFPs have shown as a potent CPA due to their special properties of ice recrystallization inhibition (IRI) and their attachment to the cell membranes to stabilize them or ice nucleation alters (Biggs *et al*., 2017; Biggs *et al*., 2019). In thawing process growth of ice crystals may lead to formation of large ice that causing cell injuries which is a major troubling and have significant contribute to cell death.

There are several applications of AFPs that can be utilized widely in industry, agriculture and medicine. Cryopreservation is one of the medical utilization of AFPs. These methods using in cell, organs and tissues are well applied in animals or even plants by using some CPA such as DMSO, poly vinyl pyrolidone

(PVP) and glycerol. The freezing and thawing cycle is harmful for the cells and tissues in this regard. Therefore, for cytosol dehydration and reduce the formation of ice crystals intracellularly, the high concentration of CPAs is highly required however, using of the high concentration of these materials are extremely toxic for the tissue and cells (Ali *et al*. 2021; Murray *et al*., 2022). There are many researches around using of AFPs in cryopreservation of the organs and cells according to its unique properties. Researches have focused on type III and I of AFPs using in cryopreservation of the cells and tissues successfully (Kim *et al.*, 2017). However, there is not any research around AFPIV from fish and its application in industry or medicine. So far, all AFPIV derived from fish however, the study over them are still unknown. The most researches have conducted on AFPIV from longhorn sculpin fish (Deng et al., 1998) and this is the reason of selecting this type of AFP from fish for further study in this research.

Lately the new sort of protein in Longhorn sculpin fish revealed that was fully different in comparison with other AFPs. This protein is enrichment with glutamine and glutamate amino acids that consists of 108 amino acids with molecular weight of nearly 12 kDa that is much greater than other identified AFP from sculpin fish. Greatly, the structure of a protein is completely helices with a number of α-helical folds which the hydrophobic residues are located in front of the interior while, the 4 amphipathics are organized with the polar sides (Petzold *et al*., 2009). In fact, this protein (LS-12) was contrived from growing the ice crystals and formed the trapezohedral hexagonal shape (Hew *et al.*, 1980). The protein characters are also difference in enactment with previous types of this special protein, LS-12, can be classified as type four of antifreeze proteins (AFPIV) (Zhao *et al*., 1998). Various problems have risen because of this revelation. However, the low concentration of this AFP occurred in these fishes, the main role of this protein would not be as antifreeze. Previous studies proved that LHS from New Brunswick seas cannot protect them from freezing conditions due to blood low level of AFPIV (Deng *et al*., 1998).

Glaciozyma antarctica an Antarctic yeast (Turchetti *et al*., 2011), can produce an 18 kDa AFP with low sequence identity to other AFPs (UniProtKB accession code D0EKL2). Secondary structure prediction of full sequence of AFP was adapted the α-helical structures that have small sequences of amino acids, therefore several peptide segments were designed based on native AFPs that showed α-helical secondary structure. It is believed that *G. antarctica* can express eight AFP genes with various types but at the present only one gene related to the AFP type I (AFPI) has been identified completely. (UniProtKB accession code D0EKL2). The secondary structure of AFP from *G.antarctia* is consisting of three beta- sheets and four alpha helices. The region which is responsible for ice recrystallization inhibition is the α-helical structures and can bind to the hydrophobic face of ice crystals (Turchetti *et al*., 2014; Shah *et al*., 2012). It is accepted that small peptides segments can be used as a molecular tool to intimate as AFPs. Researchers found that the thermal hysteresis (TH) analysis which were done on *G. antarctica* antifreeze peptides activity are as follows: peptide 1m, peptide 4m, peptide 3, respectively. The most amphipathic peptide in nature is 1m accompanied by 4m and at last is peptide 3 (Shah *et al*.,

2012). The structure of antifreeze protein 1m (afp1m) contains 25 amino acids replacing Leu19 with Glu (L19E) which increase stability.

Apart from all excremental and theoretical aspects of protein identifications and analysis, several computational investigations online servers and molecular dynamics (MD) simulations are available to approach new opportunities and obtain experimental as well as expanding scientific thoughts extremely quick. Using computational tools and effective servers provide a cost-effective way for researchers to find out and understand the structural features and physicochemical properties of a protein, even may lead to gain for the successful design of many biological experiments during a short period of time. Furthermore, many tools are available to analyze several protein physicochemical properties as well as their functional characterizations. Various experimental studies related to AFPs have been reported within time to time rather than computational analysis of AFPs (Kumar *et al*., 2018). Therefore, recently scientists have been tried to study and design the antifreeze protein structures and study over them through computational techniques.

1.1 Problem statement

Using natural cryoprotectants recently is attracted by the scientists due to their unique properties. The biopreservation CPAs are classified as AFPs however, some of this proteins in this group such as AFPIV have low activities according to their TH measurement (0.5 ^{0}C at 2mM concentration). AFPIV from longhorn sculpin fish (LHS) is recently discovered but its activity is extremely low due to its structural function. Moreover, current techniques in cryopreservation are harmful for the cells, tissues and organs related to the intracellular and extracellular formation of ice crystals and their cytotoxicity in cell cryopreserved high concentration. Therefore, they induce major problems within this method.

1.2 Hypothesis and Objectives

The hypothesis of the current research is implying that the computational study could prove this newly designed multi-helices AFP with high ice interactions and activity that can be utilized as a CPA to maintain the cells integrity at low concentration. These can be achieved using the flowing objectives:

I. To design a new multi-helices structure from fish and yeast
II. To analyze the primary, secondary and tertiary models of the newly designed AFPIV multi-helices using bioinformatics tools
III. To evaluate the models of the newly designed AFPIV with molecular dynamics simulation
IV. To elucidate the rate of ice crystals and assess of freezing and thawing temperatures of the newly designed AFPIV which mimic the cryopreservation application *via* molecular dynamics simulation.

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