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In-Silico Comparative Study on Millets Peptide Inhibiting Fat Mass and Obesity-Associated Protein

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Abstract - Over and undernutrition are generally perceived as lifestyle or diet related disorders. Apart from these external contributors, certain genes and proteins have been studied to plays a vital role in maintaining the metabolic state of an individual. One such gene is the fat mass and obesity-associated (FTO) protein- an m6A RNA demethylase, responsible for regulating energy homeostasis. This protein has been found to be strongly associated with obesity and related metabolic disorders. Targeting FTO with small-molecule inhibitors has shown promise as a therapeutic approach to manage obesity. The study employs a comprehensive computational strategy to identify bioactive peptides acting as potential natural inhibitors of the FTO protein derived from three millet species— finger millet (**Eleusine coracana**), pearl millet (**Pennisetum glaucum**), and foxtail millet (**Setaria italica**). Bioactive peptides were curated from published literature focusing on millet seed proteins. Their physicochemical properties were assessed using PepCalc to evaluate stability and solubility. Subsequently, three-dimensional structures of the peptides were predicted using the I-TASSER server to generate high-confidence models for docking. Molecular docking analyses were conducted using ClusPro to examine peptide-FTO binding affinities and interaction poses. The crystal structure of human FTO (retrieved from the Protein Data Bank) served as the docking target. Top-performing peptide-FTO complexes were further taken for molecular dynamics (MD) simulations to evaluate the dynamic behavior and stability of the interactions. Key parameters such as RMSD, RMSF, and hydrogen bond profiles were analyzed over the course of the simulations. Our results show that several millet-derived peptides bind strongly and stably to the FTO protein, with favorable docking scores and sustained hydrogen bonding at its active site. These findings highlight the potential of millet peptides as natural FTO inhibitors for developing functional foods or nutraceuticals to combat obesity.

Keywords: FTO protein, millet-derived peptides, foxtail millet, finger millet, pearl millet, molecular docking, GROMACS, I-TASSER, ClusPro, PepCalc

1. Introduction

Cereal grains (including wheat, rice, barley, rye, oat, millet and corn) have been a part of human diet for a long period of time. They contribute to maximum portions of an individual's diet, acting as the ultimate source of both macro and micro-nutrients. Compared to other cereals, millets are nutrient-dense comprising a richer micronutrient profile with bioactive flavonoids which tends to fulfil the critical health demands [1]. Millet proteins exclusively contain essential amino acids, majorly the sulphur-containing ones e.g., methionine and cysteine. Among other cereals, millets are placed sixth, accounted for 1.3% of entire cereal production. They are minor and perennial grains of the *Poaceae* family, serving as the prime food source in the tropical and arid regions of the world. Apart from the nutritional value, it is bestowed with the medicinal value as well, which is conferred by of vitamins, minerals, and bioactive compounds that are present in it. Due to their high nutritional value, these archeological staples have been coined as nutricereals. Millets, containing two categories as major and minor millets. After unravelling the nutritional aspects, several scientific evidence also suggests the therapeutic values of millets. The studied impacts are reduction in progression of prediabetes, improved glycemic control, maintained BMI,

alleviated cardiovascular risks, etc [2],[3],[4]. Apart from the resistant starch (RS) and being a gluten free choice, the phytochemicals like proanthocyanidins present in the grain and bran of the millets have been found to possess anti-obesity effects by inducing satiety.

Millets, like finger millet (Eleusine coracana L.), pearl millet (Pennisetum glaucum L.), and foxtail millet (Setaria italica) are nutrient-dense ancient grains traditionally cultivated in arid and semi-arid regions of India and Africa. These grains are increasingly recognized for their rich nutritional profiles, resilience to climate stress, and health-promoting properties. As modern diets struggle with lifestyle disorders and nutrient deficiencies, finger, pearl, and foxtail millets offer a valuable solution, serving as functional foods that support health and sustainable food systems. These millets are excellent sources of energy, carbohydrates, proteins, and dietary fiber. Pearl millet provides approximately 361 kcal/100g, with 12% protein, 67% carbohydrates, 2.3% fiber, and 4.8% fat. It also contains high levels of resistant starch and both soluble and insoluble dietary fibers, which support gut health and glucose metabolism [5]. In comparison, finger millet provides 321 kcal/100g, with 7.2g protein, 66.8g carbohydrates, 1.9g fat, and a high fiber content of 11.18g, making it especially beneficial for blood sugar control and bowel regularity. The starch in pearl millet (65.8–75.3g/100g) is slightly higher than in finger millet, but both have distinct advantages due to their slowly digestible carbohydrates, promoting a low glycemic response. Millets are notable for their high protein content and favourable amino acid profiles like foxtail millet, it contains a comparatively higher level of protein, i.e., 12.3g per/100g. Pearl millet protein content ranges from 8–24%, containing all essential amino acids, particularly leucine, isoleucine, valine, and lysine. Fermentation and germination enhance its in vitro protein digestibility (up to 84%) [6].

Finger millet also has an exceptional essential amino acid ratio (44.7%), exceeding the FAO reference pattern. It is especially rich in lysine, methionine, threonine, and sulfur-containing amino acids, which are typically low in other cereals, making it a valuable dietary addition for improving protein quality in plant-based diets . Though generally low in fat, both millets contain health-promoting unsaturated fatty acids. Pearl millet contains 4.8% fat, with 75% being unsaturated, including oleic, linoleic, and linolenic acids, and a favorable omega-3 content. Finger millet, with 1.3–1.8% fat, also includes beneficial polyunsaturated fatty acids. Despite its lower fat content, its lipid profile (including linoleic and alpha-linolenic acid) plays a supportive role in cardiovascular and neural health.

All three millets are micronutrient-rich, but finger millet especially stands out. It contains 344–398 mg of calcium per 100g, making it the richest plant-based source of calcium, vital for bone development [7]. It also provides iron (4.6–5.4 mg), magnesium (161 mg), phosphorus (283 mg), and potassium (408 mg). Pearl millet contains iron (up to 8 mg/100g), zinc (3.1 mg), magnesium, and B-complex vitamins including thiamine, riboflavin, niacin, and folic acid. These are mostly concentrated in the aleurone and germ layers, and processing methods like fermentation and germination help improve their bioavailability. Finger and pearl millet are high in dietary fiber, which enhances gut motility, regulates blood glucose, and promotes satiety. Finger millet contains up to 21.1% dietary fiber, with 11% insoluble and 2% soluble fiber, making it one of the highest among cereals. Pearl millet contains around 15% dietary fiber, higher than wheat, and includes arabinoxylans and β-glucans, known for their prebiotic potential. Millets are rich in bioactive compounds such as polyphenols, flavonoids, and tannins, which impart antioxidant, anti-inflammatory, antidiabetic, and anticarcinogenic properties [8].

Finger millet contains phenolic acids like gallic, ferulic, and p-coumaric acids, and flavonoids such as quercetin and proanthocyanidins. Pearl millet is rich in phenolic acids (147.8 mg/100g), tocopherols, and phytates, which in small amounts can also play protective roles. Other than compounds like phytates, flavonoids and tannins can, many possible compounds can be of therapeutic interest to us. Thus, we aim to find such molecules for their future applications.

Fat mass and obesity-associated protein (FTO) is an m6A RNA demethylase that has been implicated in the development of obesity and metabolic disorders [9]. The protein influences multiple aspects of energy homeostasis and fat metabolism, making it a central player in the pathogenesis of obesity. Genetic variations in FTO affect appetite and satiety, while FTO's enzymatic activity impacts adipocyte function and energy expenditure, ultimately contributing to the development and maintenance of excess body weight and fat mass. Inhibition of FTO activity has emerged as a promising therapeutic strategy to manage obesity. Bioactive peptides were curated from published literature focusing on millet seed proteins. Their physicochemical properties were assessed using PepCalc to evaluate stability and solubility. Subsequently, three-dimensional structures of the peptides were predicted using the I-TASSER [10] server to generate high-confidence models for docking.

Molecular docking analyses were conducted using ClusPro to examine peptide-FTO binding affinities and interaction poses. The crystal structure of human FTO (retrieved from the Protein Data Bank) served as the docking target. Top-performing peptide-FTO complexes were further subjected to molecular dynamics (MD) simulations using GROMACS [11], [12] tool to evaluate the dynamic behavior and stability of the interactions. Key parameters such as RMSD, RMSF, and hydrogen bond profiles were analyzed over the course of the simulations. Our results show that several millet-derived peptides bind strongly and stably to the FTO protein, with favorable docking scores and sustained hydrogen bonding at its active site.

2. Materials and Methods

2.1. Protein

The three-dimensional crystal structure of FTO protein from Homo sapiens (PDB ID: 4IDZ) was obtained from the RCSB Protein Data Bank (Fig 1). The selected structure consists of 495 amino acids in chain A and has a resolution of 2.46 Å, making it suitable for molecular interaction studies.

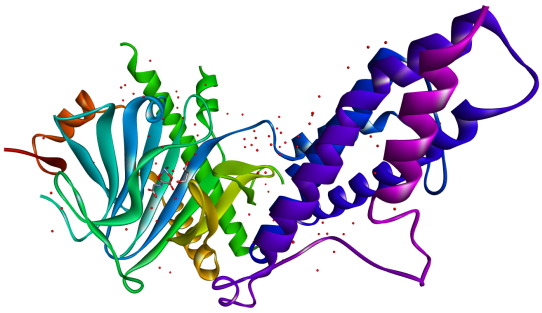


Fig 1: FTO protein structure 4IDZ.pdb

2.2. Peptide Collection

Bioactive peptides were systematically collected through a literature-based approach, focusing on peer-reviewed research articles reporting peptide sequences derived from seed storage proteins of three millet species: **finger millet (Eleusine coracana)**, **foxtail millet (Setaria italica)**, and **pearl millet (Pennisetum glaucum)**. The selection was based on peptides with known or predicted bioactivities relevant to metabolic health. F**inger millet**, two peptides—**TSSSLNMAVRGGLTR** (Fig 2(a)) and **STTVGLGISMRSASVR (Fig 2(b))**—were retrieved from the study [13] , which explored protein hydrolysates for their nutraceutical properties. P**earl millet**, one peptide—**SDRDLLGPNNQYLPK (Fig 2(c))**—was extracted from the work of Himani Agrawal, which analyzed functional peptides derived from pearl millet proteins using enzymatic hydrolysis and mass spectrometry[9]. **Foxtail millet**, the peptides **EDDQMDPMAK (Fig 2(d))** and **QNWDFCEAWEPCF (Fig 2(e))** were selected from research conducted by Hongbing Chen and Shuai Hu, where bioactive peptides were identified through a combination of in silico prediction and experimental validation [14]. These curated peptides served as the basis for subsequent computational evaluations, including physicochemical characterization, structural modeling, molecular docking, and molecular dynamics simulations to assess their potential as FTO inhibitors.

2.3. Peptide Physicochemical Properties

The physicochemical properties of the collected peptides, including molecular weight, net charge, hydrophobicity, and isoelectric point (pI), were computed using the PepCalc.com web tool. These parameters provided initial insights into the stability, solubility, and potential bioactivity of the peptides.

Table 1: Peptide Physiochemical Properties

Sl.	Number of residues	Molecular weight (g/mol)	Iso-electric point	Net charge at pH 7	Estimated solubility
(a)	Finger Millet Peptide-1 (15)	1549.76	12.1	2	Good water solubility
(b)	Finger Millet Peptide-2 (16)	1621.86	12.1	2	Poor water solubility
(c)	Pearl Millet Peptide-1 (15)	1729.89	6.51	0	Good water solubility
(d)	Foxtail Millet Peptide-1 (10)	1179.28	3.32	-3	Good water solubility
(e)	Foxtail Millet Peptide-2 (13)	1674.81	0.65	-3.1	Poor water solubility

2.4. Peptide Structure Prediction

The three-dimensional (3D) structures of the bioactive peptides collected from finger millet, foxtail millet, and pearl millet were predicted using the **I-TASSER** [10]**. T**he model with the **highest C-score r**egardless of its rank was selected for downstream molecular docking and simulation studies.

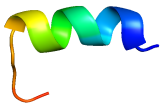
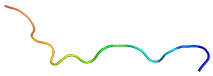
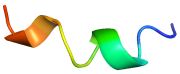
Fig 2 (a)	Fig 2 (b)	Fig 2 (c)	Fig 2 (d)	Fig 2 (e)
				

Fig. 2 (a-e): Structure of the peptides used in the study.

2.5. Molecular Docking

To investigate the interaction potential of millet-derived peptides with the fat mass and obesity-associated (FTO) protein, molecular docking studies were performed using the **ClusPro protein–protein docking server**, a widely used tool for modeling peptide–protein interactions [15],[16]. Preparation of FTO protein is carried out using **UCSF ChimeraX** [17]. The structure was refined by **removing heteroatoms and water molecules**, followed by **the addition of hydrogen atoms** to stabilize the protein for docking simulations. Any **missing residues** were identified and accounted for to ensure completeness and structural integrity of the target. Peptides were prepared by adding **Hydrogen atoms** to ensure accurate representation of potential bonding interactions during docking. Further, molecular docking was performed using the **ClusPro protein–protein docking server as it has been depicted in the adjacent figure**. ClusPro performs rigid-body docking through **Fast Fourier Transform (FFT)-based sampling** and clusters them based on the lowest energy poses. The server evaluates docking poses using a weighted scoring function that approximates the binding energy. Docking results were ranked by **cluster size** and **binding energy score**, with the most populated and energetically favorable clusters selected for further analysis. The image shows the 3D interactions of the peptide with FTO. These peptide–FTO complexes were then subjected to molecular dynamics simulations to assess the stability and persistence of the interactions using LigPlot+ [18].

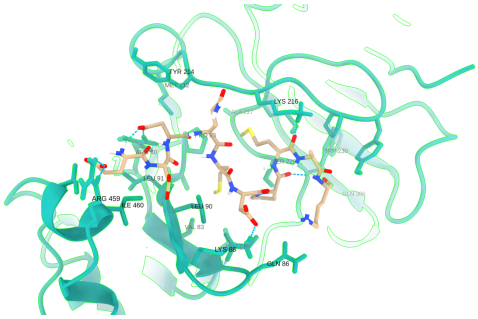


Figure 3 showing the 3D interactions of the peptide.

2.6. Molecular Dynamics Simulation

To validate the docking results and assess the stability of the peptide-FTO complexes, molecular dynamics simulations were conducted using GROMACS (GROningen MAchine for Chemical Simulations) [12], [11]. The systems were solvated, energy-minimized, equilibrated, and subjected to production runs to monitor the behavior of the complexes over time. To assess the conformational stability of the FTO–peptide complexes, Root Mean Square Deviation (RMSD) of the backbone atoms was calculated over a 100 ns molecular dynamics simulation. RMSD is a crucial parameter that provides insight into the extent of structural deviation from the initial conformation and serves as a key metric for evaluating system equilibration and structural integrity over time. Furthermore, root-mean-square fluctuation (RMSF), radius of gyration, hydrogen bond interactions, and binding free energies were analysed.

3. Results

The computational analysis identified several peptides from foxtail millet, finger millet, and pearl millet with favorable binding affinity towards the FTO protein. The docking scores and simulation trajectories indicated stable interactions, with some peptides forming consistent hydrogen bonds with the active site residues of FTO. These findings suggest that millet-

derived peptides have the potential to act as natural inhibitors of FTO, supporting their use in developing functional foods or therapeutics targeting obesity.

Fig 3 (a): Finger Millet 1
Binding Energy: -821.6, H-Bonds: 5

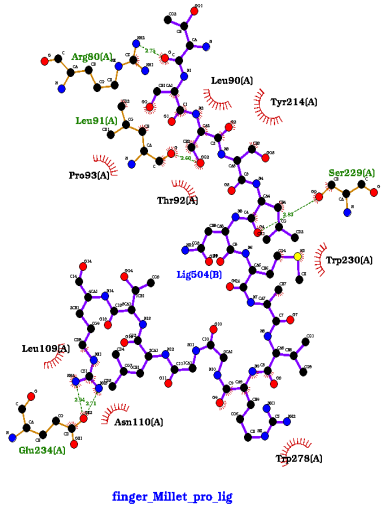


Fig 3 (b) Finger Millet 2
Binding Energy: -912.8, H-Bonds: 4

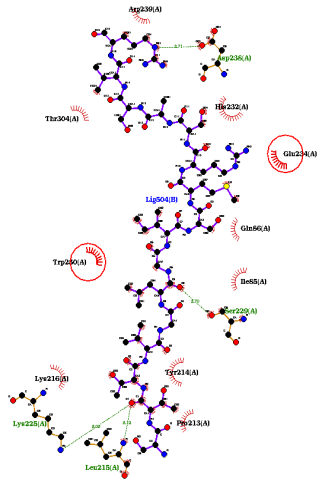


Fig 3 (c) Pearl Millet
Binding Energy : -655.8, H-Bonds: 3

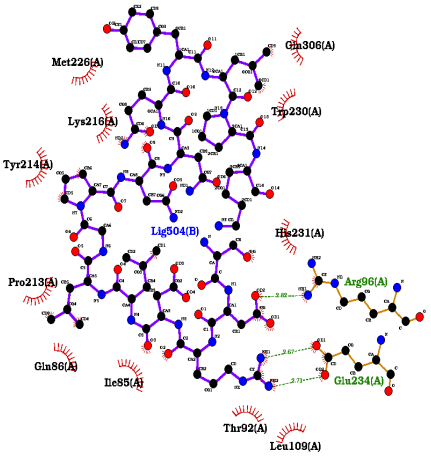


Fig 3 (d) Foxtail Millet-1
Binding Energy : -607, H-Bonds : 5

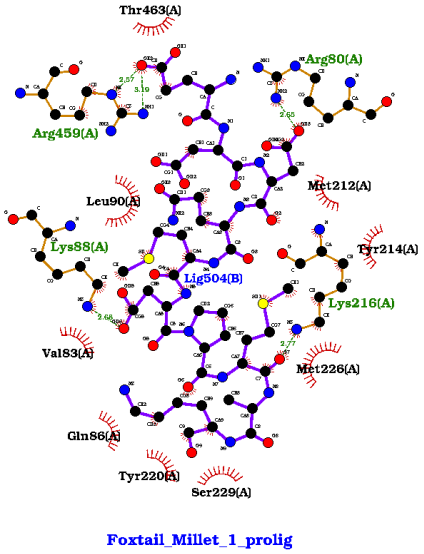


Fig 3 (e) Foxtail Millet-2
Binding Energy: -1133.4, H-Bonds: 3

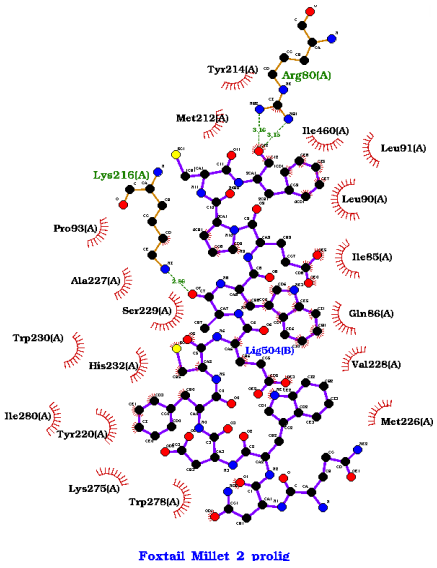


Fig 3: Amino acid interactions with peptides:

Fig 3 (a): Arg80, Leu90, Tyr214, Leu91, Tyr214, Pro93, Ther92, Ser229, Trp230, Trp278l, Asn110, Leu109.
Fig 3 (b): Arg239, Thr304, Asp238, His232, Glu234, Trp280, Gln86, Ile85, Ser229, Tyr214, Pro213, Leu215, Lys225, Lys216
Fig 3 (c): Met226, Gln306, Trp230, His231, Arg96, Glu234, Leu109, Thr92, Ile85, Gln86, Pro213, Tyr214, Lys216
Fig 3 (d): ArgA59, Thr463, Arg80, Met212, Tyr214, Lys216, Met226, Ser229, Tyr220, Gln86, Val83, Lys88, Leu90

Fig 3 (e): Tyr214, Met212, Ile460, Leu91, Leu90, Lys216, Ile85, Pro93, Ala227, Ser229, Gln86, Trp230, His232, Val228, Ile280, Tyr220, Met226, Lys275, Trp278

3.1 Molecular Dynamics Simulation Analysis of FTO-Peptide Complexes

3.1.1 RMSD Analysis

As illustrated in Fig 4(a), all peptide-bound FTO complexes underwent a characteristic RMSD stabilization phase within the first 20–30 ns, followed by consistent fluctuations, indicating that the systems reached equilibrium and remained dynamically stable. Among the complexes, **Finger Millet_1** (black) exhibited the highest RMSD values (~1.4–1.5 nm), implying greater structural deviation and flexibility. **Foxtail Millet_2** (blue) showed moderate RMSD levels (~0.8–1.0 nm), reflecting a stable yet relatively dynamic interaction. In contrast, **Foxtail Millet_1** (green), **Finger Millet_2** (red), and **Pearl Millet** (yellow) maintained lower RMSD values (~0.5–0.7 nm), denoting high conformational stability. Notably, the **Pearl Millet** complex remained consistently stable throughout the simulation, with minimal fluctuations, indicating strong peptide binding and low conformational drift. Similarly, **Finger Millet_2** showed compact behavior with RMSD values remaining under 0.6 nm. These findings suggest that millet-derived peptides, particularly from **pearl** and **foxtail millet**, form stable complexes with the FTO protein. The RMSD profiles highlight how sequence-specific interactions can influence structural dynamics and protein stability.

3.1.2 RMSF Analysis

Root Mean Square Fluctuation (RMSF) analysis was conducted to evaluate the residue-wise flexibility of the FTO backbone in response to peptide binding. As shown in Fig 4(b), all complexes exhibited RMSF values between 0.1 and 0.35 nm for most residues, indicating a largely stable backbone conformation. Key fluctuations were observed at the N-terminal region (~residues 1–20), especially in **Foxtail Millet_2** (blue), which exceeded 0.5 nm due to typical terminal flexibility. Minor peaks were also observed in loop regions around residues 180–190, 260–270, and 340–360, particularly in **Pearl Millet** (yellow) and **Finger Millet_2** (red) complexes. Higher mobility was noted at the C-terminal end (~residues 500–520), with **Finger Millet_2** showing the most pronounced fluctuation above 0.5 nm. The core region (residues 100–400) remained highly stable across all peptide-bound systems, with RMSF values under 0.2 nm. These results suggest that millet-derived peptides preserve the structural integrity of the FTO protein while permitting moderate flexibility in specific functional regions.

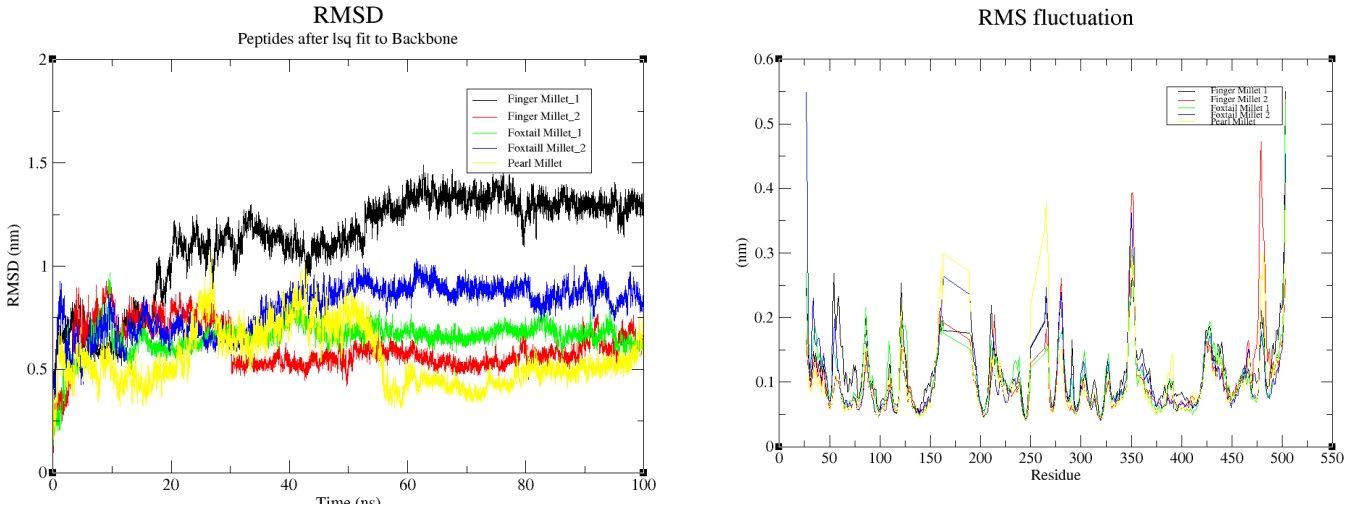


Fig 4 (a-b): FTO Protein-Millets Peptide RMSD and RMSF

3.1.3 Radius of Gyration (Rg) Analysis

The radius of gyration (Rg) was calculated to evaluate the compactness and folding behavior of the peptide-bound FTO protein. As shown in Fig 4(c), all complexes maintained stable Rg values between 2.5 nm and 2.65 nm throughout the simulation. **Pearl Millet** (yellow) exhibited the highest average Rg (~2.63–2.66 nm), suggesting a slightly more extended protein conformation. **Foxtail Millet_1** and **Foxtail Millet_2** (green and blue) showed higher early-stage fluctuations but stabilized at ~2.6–2.63 nm. **Finger Millet_1** and **Finger Millet_2** (black and red) maintained lower Rg values (~2.52–2.57 nm), indicating more compact protein structures. These results demonstrate that peptide binding does not induce significant unfolding and that the structural compactness of FTO is maintained, reinforcing the stability of the modeled peptide–protein complexes.

3.1.4 Total Energy Analysis

Total energy analysis was performed to examine the thermodynamic stability of the peptide–FTO complexes. As shown in Fig 4(d), all systems reached energetic equilibrium early in the simulation and remained within narrow energy ranges. **Pearl Millet** (yellow) displayed the most stable energy profile (−6.10 × 10^5 kJ/mol), indicating strong and favourable peptide binding. **Foxtail Millet** peptides (green and blue) had slightly lower energies (−6.15 to −6.20 × 10^5 kJ/mol), reflecting even more energetically stable interactions. **Finger Millet** peptides (black and red) showed slightly higher energies (~−6.05 to −6.10 × 10^5 kJ/mol) but remained stable throughout. The consistency of energy values supports the structural and dynamic observations and suggests that millet-derived peptides contribute to the stability of FTO complexes, with **foxtail** and **pearl millet** peptides showing the most favourable binding profiles.

Fig 4 (c)

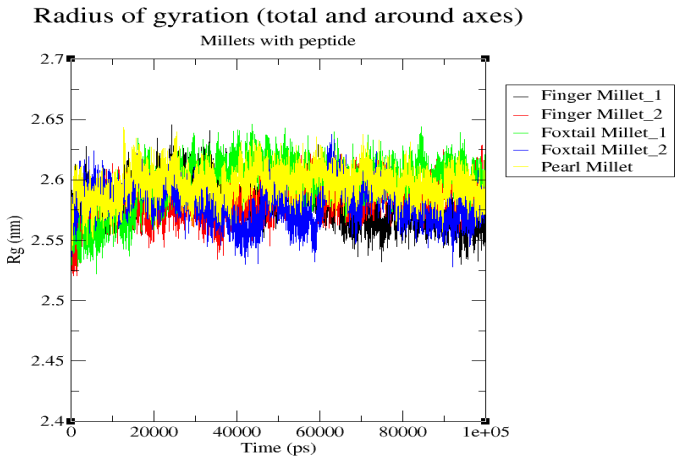


Fig 4 (d)

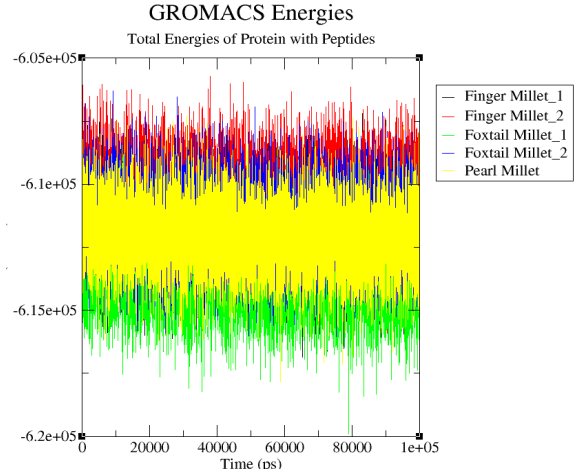


Fig 4 (c-d): FTO Protein-Millets Peptide "Radius of Gyration" and "Total Energies"

3.1.5 Hydrogen Bond Analysis

Hydrogen bonding interactions were assessed over the 100 ns simulation to quantify the binding affinity and interaction stability between FTO and the millet-derived peptides. A donor-acceptor distance cutoff of 0.35 nm was applied. As depicted in Fig 4(e), **Finger Millet_2** (red) consistently formed the highest number of hydrogen bonds, averaging 10–15 and peaking near 18. **Finger Millet_1** (black) also showed a strong interaction profile with 10–14 bonds. **Foxtail Millet_1** (green) and **Pearl Millet** (yellow) formed moderate numbers of hydrogen bonds (6–10), while **Foxtail Millet_2** (blue) exhibited the fewest (2–6), suggesting weaker or more transient interactions. These results highlight the variability in binding strength among the peptides and suggest that **Finger Millet_2** and **Pearl Millet** are particularly effective in establishing stable hydrogen-bonded networks with the FTO protein.

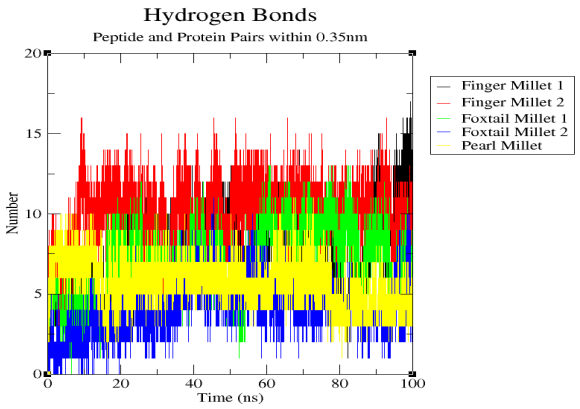


Fig 4 (e): FTO Protein-Millets Peptide "H-Bonds"

4. Conclusion

This study utilized a comprehensive computational approach to identify millet-derived peptides as potential inhibitors of the FTO protein, a key player in obesity. Peptides from finger, foxtail, and pearl millet were modeled using I-TASSER and docked to FTO via ClusPro, revealing stable interactions. GROMACS-based molecular dynamics simulations confirmed the structural stability and binding affinity of the complexes. Pearl millet and finger millet 2 peptides showed the highest stability, with minimal RMSD and RMSF values, consistent Rg, and persistent hydrogen bonding. These findings highlight the therapeutic potential of millet peptides as natural FTO inhibitors, warranting further experimental validation.

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