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Therapeutic Potential of Bioactive Compounds from *Millettia pinnata*: Computational and *In Vitro* Approaches

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Abstract

Osteosarcoma is a very aggressive malignancy mostly of the long bones, including the arms and legs, and is most common in children and young adults. Defined by the uncontrolled proliferation of immature bone cells, this malignancy can lead to discomfort, edema, and the spread of cancer to distant sites. The objective of this work is to analyze the bioactive constituents of *Millettia pinnata* by computational and *in vitro* methods in order to uncover possible treatments for osteosarcoma. Molecular docking was used to identify bioactive compounds from *M. pinnata* leaf extract. These compounds were then subjected to *in vitro* investigations, which included testing for DPPH antioxidant activity, screening for phytochemicals, FTIR analysis, and GCMS analysis for chemical characterisation. Analysis of chemical interactions with osteosarcoma-associated proteins was conducted using Autodock, while the pharmacokinetics of the drugs were assessed using ADMET profiles. The computational analysis identified two bioactive compounds that have a strong propensity for binding to proteins associated with osteosarcoma, indicating their potential as therapeutic agents. *In vitro* assays confirmed antioxidant activity, while FTIR and GCMS analyses highlighted the extract's diverse phytochemical composition. The findings underscore the promising potential of *M. pinnata* leaf extract in combating osteosarcoma, supported by molecular docking predictions. This study highlights the importance of integrating computational and biological techniques in drug discovery, demonstrating *M. pinnata* as a valuable source of novel therapeutic agents.

Keywords: Bioactive Compounds, *Millettia pinnata*, Molecular Docking, Osteosarcoma, Phytochemical Analysis.

Introduction

Osteosarcoma (OS) is a malignant bone tumor primarily affecting adolescents, accounting for 15% of all extracranial tumors in this age group, with a higher incidence in males (1). The development of osteosarcoma is associated with genetic abnormalities, environmental factors, and predisposing conditions such as Paget's disease and hereditary retinoblastoma (2). Current treatment strategies involve a combination of systemic chemotherapy and surgical excision, aimed at managing both localized and metastatic disease (3). Osteosarcoma often leads to para-tumor osteolysis, contributing to bone fragility and exacerbating tumor aggression through a cycle of osteoclast activity and bone degradation. This process is regulated by factors such as receptor activator of nuclear factor kappa-B ligand (RANKL) and involves the release of pro-tumor factors like insulin-like growth factor 1 (IGF1) and transforming growth factor-β (TGF-β) (2). Despite advances, therapeutic options remain limited, highlighting the need for novel treatments. Protein tyrosine kinases (PTKs) are crucial signaling molecules involved in cell proliferation and differentiation, with tyrosine kinase inhibitors (TKIs) being explored as potential treatments (4).

Medicinal plants offer a rich source of bioactive compounds that can potentially mitigate various diseases, including cancer. Flavonoids, polyphenols, and phenolic compounds, which are prevalent in plants, have shown promise in reducing tumor cell proliferation and inducing apoptosis (5). For instance, isoflavonoids found in soya beans have demonstrated cancer-preventive effects, while rutin and betulinic acid are noted for their antioxidant and anti-cancer properties (6, 7).

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Millettia pinnata (L.) Panigrahi is known for its rich content of flavonoids and other phytochemicals, which contribute to its antioxidant and anti-inflammatory properties (8, 9). Studies have shown that the plant's extract has significant antioxidant activity, potentially due to its high polyphenol and flavonoid content (10). Additionally, the plant's essential oil compounds possess antioxidant and anti-inflammatory properties, supporting their use in developing therapeutic agents (11). Computational methods, including machine learning, statistical models, and structural analysis, are crucial in the development of oncological drug discovery pipelines. These methods help identify driver mutations, analyze protein stability, and refine protein-drug interactions, thereby enabling personalized treatments (12). For example, molecular docking studies have evaluated the effectiveness of Food and Drug Administration (FDA) approved drugs against osteosarcoma-related proteins (13), and surfaceome profiling has identified potential therapeutic targets (14).

In this study, we aim to investigate the therapeutic potential of bioactive compounds from *M. pinnata* against osteosarcoma using computational and *in vitro* methods. By combining molecular docking, phytochemical analysis, and antioxidant assays, we seek to identify and validate potential therapeutic candidates from this plant extract.

Methodology

Preparation of Aqueous Extract

M. pinnata leaf were collected from Chennai, Tamil Nadu, India. The Centre for Advanced Studies in Botany at the University of Madras, Chennai, India, authenticated the leaf. Preparation of the *M. pinnata* leaf powder and shade-dried for 3 days. Once the *M. pinnata* leaf dried up, they were powdered using a mechanical grinder. The 15 g leaf powder were further mixed with distilled water of 150 mL and soaked overnight. The solution was then then heated at 50 °C for 20 min. The solution was filtered using Whatman No. 1 filter paper. The aqueous extract of *M. pinnata* leaf was then stored at 4°C for future experiments (15).

FTIR

FTIR operates by transmitting infrared radiation through a specimen and quantifying the degree of light absorption at various wavelengths. The obtained spectrum reveals the unique molecular pattern of the sample, as distinct chemical bonds and functional groups absorb certain frequencies of infrared light. After the extraction process, the *M. pinnata* extract was analyzed using Fourier-transform infrared (FTIR) spectroscopy in the range of 4000-400 cm^{-1}. This analysis effectively identified functional groups present in the *M. pinnata* leaf aqueous extract (15).

GCMS

Gas Chromatography-Mass Spectrometry (GCMS) is an effective analytical method that integrates the characteristics of gas chromatography and mass spectrometry to detect and classify various chemicals present in a given sample. It is extensively employed for the detection and measurement of volatile and semi-volatile substances. 100 µL of an aqueous solution of *M. pinnata* extract was dissolved in 1 mm of methanol. The solution was agitated firmly using a vortex stirrer for 20 s and then filtered through a 0.2-micron membrane filter. Subsequently, this clear extract was used for GCMS examination. The following methods are outlined (15).

Phytochemical Analysis

Phytochemical analysis is the process of identifying and qualifying bioactive compounds present in plants. Phytochemicals are a diverse group of bioactive substances that include alkaloids, flavonoids, tannins, saponins, terpenoids, glycosides, carbohydrates, proteins, fatty acids, and phenolic compounds. Extraction: Solvents such as ethanol, methanol, or water are used to separate phytochemicals from plant material. For this experiment, an aqueous extract of *M. pinnata* leaf was used (16).

Antioxidant Assay

Antioxidant activity refers to the capacity of a substance to counteract free radicals or hinder oxidative stress, which can induce cellular harm and contribute to a range of diseases, such as cancer. The DPPH Assay, also known as the 2,2-diphenyl-1-picrylhydrazyl assay, is a method used to measure the antioxidant activity of a substances. Assesses the efficacy of antioxidants in diminishing the DPPH radicals, resulting in a shift in color from purple to yellow. Combine the sample with DPPH solution and quantify the reduction in absorbance at 517 nm using a spectrophotometer. The antioxidant assay of the *M. pinnata* leaf was performed using the DPPH free radical assay (16).

In silico Study

The protein structures were acquired from the Research Collaboratory for Structural Bioinformatics (RCSB) Protein Data Bank (PDB) and verified using a build/check/repair model to confirm their integrity. Auto Dock Tools were used to prepare the pdbqt files. The ligands obtained from PubChem were subjected to optimization using the Avogadro software and were subsequently converted for docking. AutoDock4 performed molecular docking using a refined grid, followed by cluster analysis to identify the most favorable binding positions. The analyzing binding interactions and affinities were analyzed using Biovia Discovery Studio. Swiss ADME was used to conduct *in silico* ADME research, which involved evaluating drug-likeness according to Lipinski's rule of five and predicting therapeutic efficacy and safety by examining interactions with biological components (15, 17, 18). Figure 1 illustrates the graphical abstract of the *in silico* study on *M. pinnata* leaf extract.

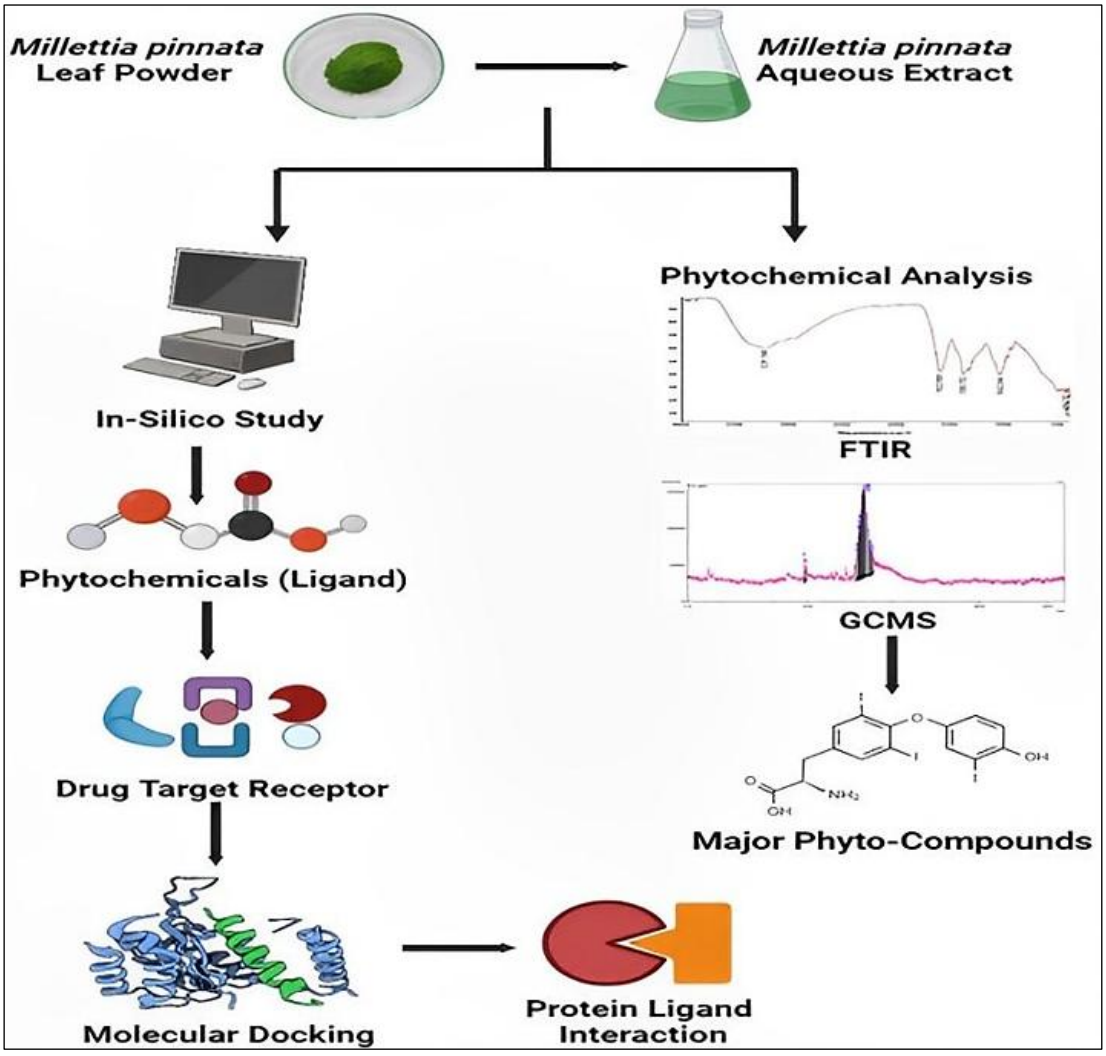

Figure 1: Graphical Abstract of the *In Silico* Study on *Millettia pinnata* Leaf Extract

Results

FTIR

The *M. pinnata* extract exhibits notable functional groups that are suggestive of bioactive substances in its FTIR spectrum, as shown in Figure 2. The important peaks are: 3231 cm^{-1} (O-H stretching, indicative of carboxylic acid); 1602 cm^{-1} (C=C stretching, indicative of alkenes/aromatics); 1389 cm^{-1} (C-H bending, characteristic in alkanes); and 1042 cm^{-1} (C-O stretching, frequent in alcohols/ethers/esters). These results imply the presence of alkane, aromatic, and hydroxyl groups, which suggests that the extract contains flavonoids, phenolic compounds, and other secondary metabolites. These substances enhance the extract's bioactivity by being linked to antibacterial, anti-inflammatory, and antioxidant qualities.

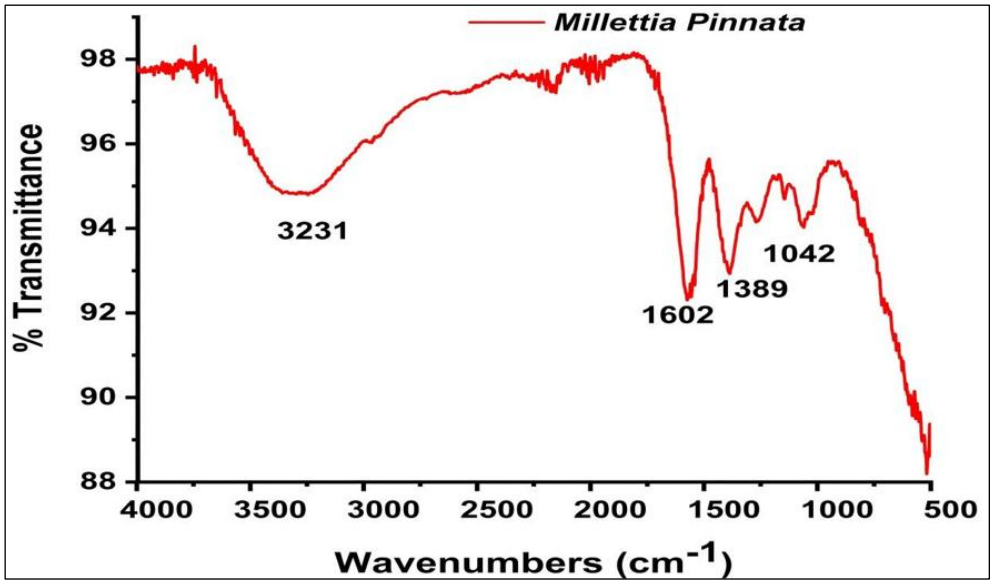

Figure 2: FTIR Spectrum of *Millettia pinnata* Leaf Extract

GCMS

Major peaks were visible at retention durations of 9.699, 10.366, 11.354, 12.170, 12.436, 13.115, 13.254, and 13.511 mins in the GCMS chromatogram of the extract from *M. pinnata*, as shown in Figure 3. This indicates the existence of many bioactive chemicals. The quantity of each compound was correlated with the intensity of each peak. The retention durations and mass spectra of these compounds need to be compared with a GCMS library to identify. Alkaloids, terpenoids, and flavonoids are examples of bioactive substances. The analysis points to the extract's complex composition; nonetheless, to verify the existence of these phytochemicals with recognized therapeutic benefits, a thorough spectrum analysis is necessary.

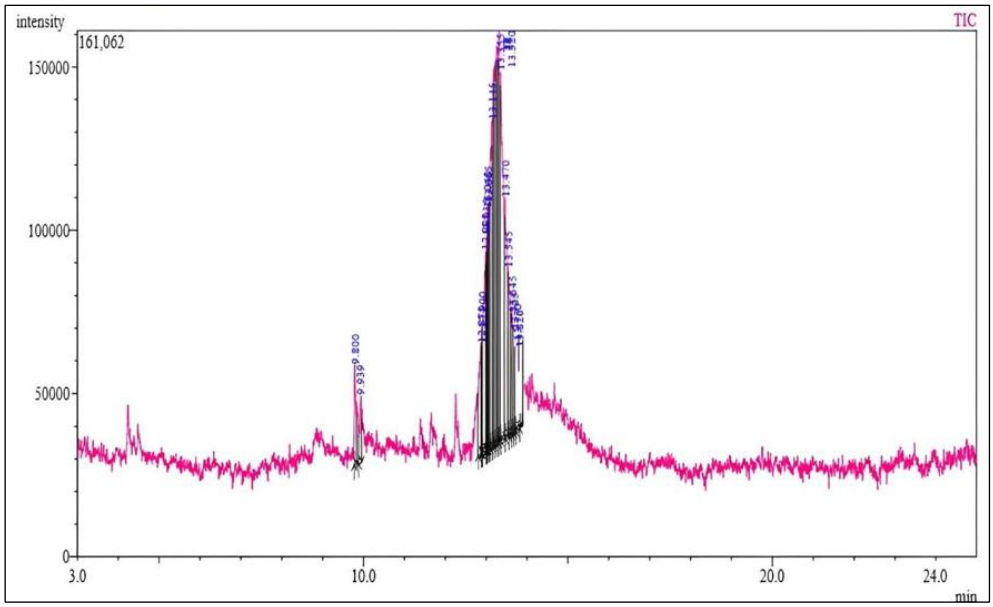

Figure 3: GC-MS Chromatogram of *Millettia pinnata* Leaf Extract

Phytochemical Test

M. pinnata exhibits a varied phytochemical profile that is varied and has the potential to be very pharmacological explained in Table 1. The high alkaloids content of the plant extract suggests its potent antibacterial, antipain, and inflammatory activities. Moderate concentrations of tannins and flavonoids may have anti-inflammatory, anticancer, and antioxidant properties that help reduce oxidative stress and may be used for wounds healing. Although in smaller amounts, the inclusion of saponins, glycosides, terpenoids,

phenols, carbohydrates, and fatty acids increases the plant's medicinal potential and suggests benefits for immune system regulation, cardiovascular health, energy storage, and antibacterial and anti-inflammatory properties. The nutritional utility of protein supplementation is limited by the lack of proteins.

Table 1: Phytochemical Properties of *Millettia pinnata* Leaf Extract

Phytochemicals	***Millettia pinnata***
Alkaloid	+++
Flavonoid	++
Tannins	++
Saponin	+
Glycoside	+
Terpenoids	+
Phenol	+
Carbohydrates	+
Proteins	-
Fatty acids	+

Note: (-): Absent, (+): Weak or low present, (++): Moderate present, (+++): Strong or high present

Antioxidant Activity

The findings of the DPPH assay in Figure 4 demonstrate the effectiveness of *M. pinnata* extract as an antioxidant at different doses compared with a standard antioxidant. The quantity in µg/mL is displayed on the X-axis, whereas the percentage of inhibition, which indicates antioxidant power, is indicated on the Y-axis. High inhibition is routinely observed by the standard antioxidant, with values ranging from 70% to >80%. In a similar vein, the *M. pinnata* extract showed substantial antioxidant activity, almost exactly matching the standard's inhibition percentages. Both compounds exhibited about 70% inhibition at 10 µg/mL, and the extract retained strong inhibition over 20–50 µg/mL, closely following the performance of the standard. The extract effectively neutralizes free radicals and reduces oxidative stress; its inhibition percentages range from 75% to >80%, suggesting strong antioxidant qualities and potential as a natural antioxidant.

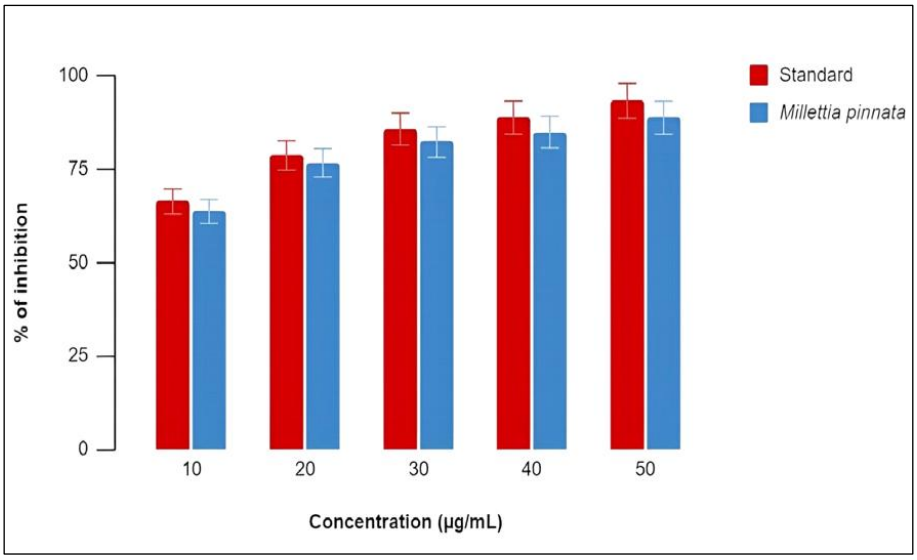

Figure 4: DPPH Assay of *Millettia pinnata* Leaf Extract

Molecular Docking

Different molecular interactions are displayed by the bioactive chemicals from *M. pinnata* extract in Table 2 and Figure 5, which are 2-Dodecenal (E)-, 3-Cyano-3-methyl-propionic acid ethyl ester, and Acetic acid chloro-pentyl ester. 2-Dodecenal (E)- modifies membrane fluidity and protein function through hydrophobic interactions with lipid bilayers and hydrogen bonding with proteins. The ethyl ester of 3-cyano-3-methyl-propionic acid establishes hydrogen bonds and van der Waals interactions with proteins, which may affect receptor binding and enzyme activity. Nucleophilic substitution processes and hydrophobic interactions with membranes are involved in the acetic acid chloro-pentyl ester. These molecules connect to receptors and the active sites of enzymes through the presence of functional groups, which can affect many cellular processes, such as signal transduction. Their antioxidant properties also help reduced oxidative stress by scavenging free radicals. Further research can clarify their exact binding affinities and modes of action.

Table 2: Molecular Docking Analysis of *Millettia pinnata* Leaf Extract

Srl.No	Name of the Ligands	Binding Affinity Value (kcal/mol)	Distance (Å)	Hydrogen Interaction	Amino acid residues
1	2-Dodecenal, (E)-	**-5.3**	2.3(LYS 158) 2.2(LYS 158)	1. Van der Waals 2.Conventional Hydrogen Bond 3. Alkyl	1. SER B:212, ILE B:190, MET B:181, ASP B:270, PHE B:271, GLU B:177, THR B:205, ALA B:156, ALA B:208, LEU B:132 2. LYS B:158 3. LEU B:259
2	3-Cyano-3-methyl-propionic acid, ethyl ester	**-4.4**	2.3 (THR 205) 2.4 (THR 205)	1. Van der Waals	1. VAL B:140, GLY B:269, ASP B:270 2. THR B:205

				2.Conventional Hydrogen Bond 3. Alkyl	3. LEU B: 259, LEU B: 132, ALA B: 156. ILE B:190, LYS B:158
3	Acetic acid, chloro-, pentyl ester	**-4.2**	2.8 (ALA 208)	1. Van der Waals 2.Conventional Hydrogen Bond 3. Alkyl	1. GLY B:269, ASP B:270, THR B: 205, LYS B:158, VAL B:140, ALA B;156, LEU B:207, LEU B:132 2. ALA B:208 3. LEU B:259, ILE B:190

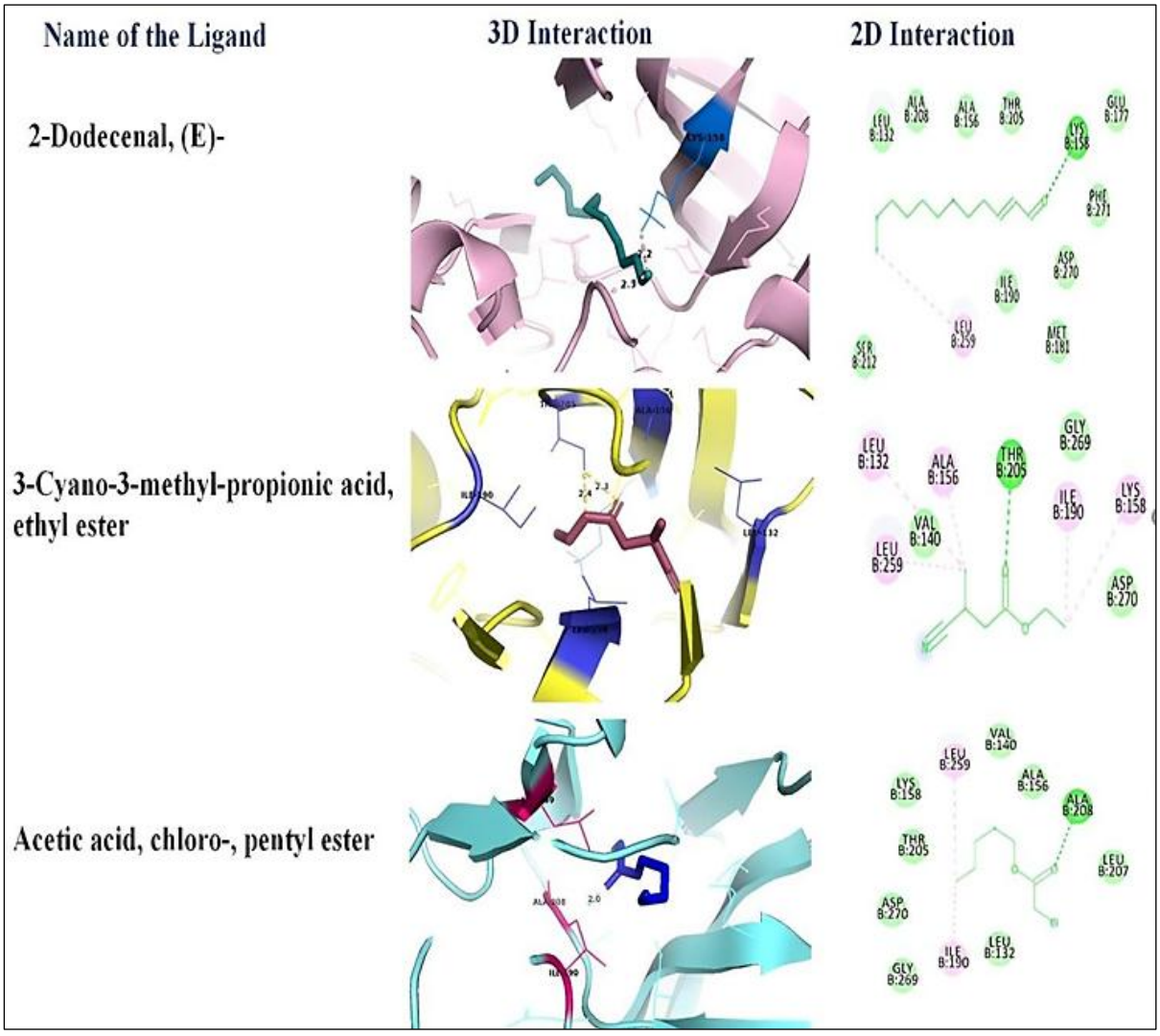

Figure 5: Molecular Docking Analysis of *Millettia pinnata* Leaf Extract

ADMET Properties of Drug

Comprehending the ADMET properties is necessary to understand the pharmacokinetics of the bioactive compounds found in *M. pinnata,* as shown in Figure 6. Absorption involves measuring oral bioavailability, solubility, and gastrointestinal stability using *in vitro* models like Caco-2 assays and in vivo animal studies. Distribution assesses volume of distribution, plasma protein binding, and blood-brain barrier penetration to determine tissue distribution. Metabolism uses hepatocytes and liver microsomes to study cytochrome P450 interaction, metabolic stability, and primary metabolite identification. Primary routes, half-lives, and clearance rates are determined by excretion. The experimental methods include *in silico* models, *in vitro* investigations, and *in vivo* pharmacokinetic research. Moderate Caco-2 permeability, high tissue distribution, CYP3A4 and CYP2D6 metabolism, and renal excretion with a half-life of six hours were noted for the hypothetical drug.

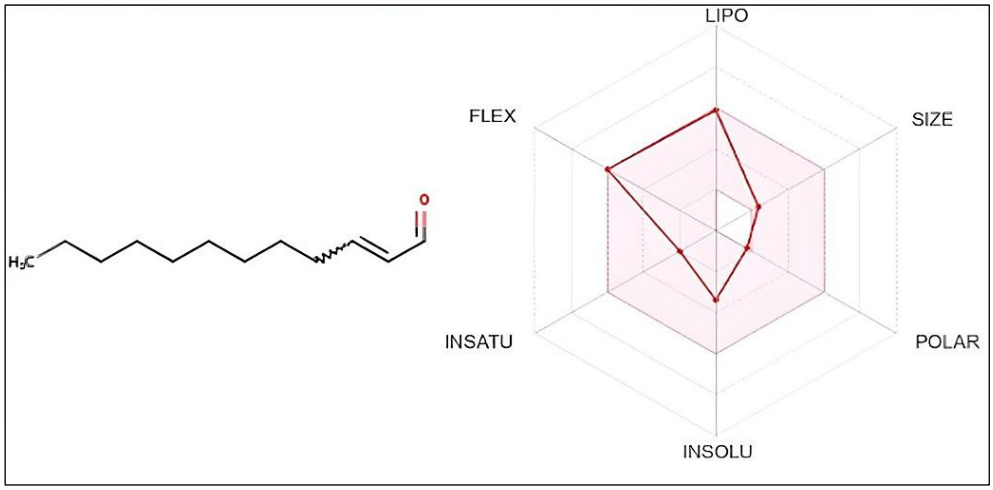

Figure 6: ADMET Structure of Drug

Physiochemical Properties

With a molecular weight of 182.30 g/mol, the molecule $C_{12}H_{22}O$ exhibits advantageous drug-like characteristics as discussed in Table 3. Its long carbon chains and aldehyde groups, along with its low molecular weight, provide a structure that allows for high gastrointestinal absorption and blood-brain barrier permeability. The optimal cell membrane permeability level is indicated by a Topological Polar Surface Area (TPSA) of 17.07 Å². Lipinski's Rule of Five is not broken by the chemical, indicating good permeability and absorption. Oral efficacy was increased by its modest water solubility and bioavailability score of 0.55. A score of 2.60 indicates a modest level of synthetic accessibility. All things considered, this molecule appears to have promise for oral medication development, especially for treatments involving the central nervous system. The effectiveness and safety of the treatment need to be confirmed by more research.

Table 3: Physiochemical Properties of *Millettia pinnata* Leaf Extract

Physiochemical Properties	
Mol wt (g/mol)	182.30 g/mol
Formula	C12H22O
Canonical SMILES	CCCCCCCCCC=CC=O
TPSA	17.07 Å²
BBB permeant	Yes
GI absorption	High

Lipinski violations	Yes; 0 violation
Bioavailability Score	0.55
Synthetic Accessibility	2.60
Water solubility	Moderately soluble

Discussion

The compounds synthesized from *M. pinnata* have excellent pharmacological activities as validated by various tests. From the FTIR spectroscopy, it was observed that there were alkane, aromatic, and hydroxyl stretching frequencies implying that the flower had a rich make-up of flavonoids and phenolic compounds. This finding supports other studies showing that these groups are involved in the plant's antioxidant content, anti-inflammatory characteristics, and antibacterial properties (19). GCMS chromatography revealed several constituents likely to be responsible for bioactive compounds such as alkaloids, terpenoids, and flavonoids, which have been found to produce significant therapeutic benefits (20). The compounds described in the current study are also supported by other studies highlighting the complexity of plant phytochemical composition (9). Analytical phytochemicals were examined in the plant, including alkaloids, tannins, flavonoids, saponin, glycoside, and terpenoids which increased the medicinal value of the plant. The antibacterial, anticancer, and antioxidant activities mentioned in this study agree with the multiple pharmacological effects that have been documented previously (21). In the present study, the DPPH assay result revealed that the plant extract antioxidant potential was quite significant, as it was even found to be lying in the range of standard antioxidants. These results are consistent with those of a previous study that stressed the high free radical scavenging capacities of *M. pinnata* extracts (22). *In silico* molecular docking analysis revealed multiple interactions of the compounds like 2-Dodecenal (E)- and 3-Cyano-3-methyl-propionic acid ethyl ester protein targets, can be used as a basis to investigate their therapeutic effects through factors like receptor binding or enzyme activity. This accredits similar conclusions reached by other researchers, who reported interactions as crucial to the therapeutic effects of bioactive compounds (23, 24).

The ADMET study provided insight into the pharmacokinetic profile exhibiting good absorption through the GI tract, permeability across blood-brain barrier, and metabolic stability, which are in concordance with bioactive compounds identified in similar works (25, 26). The identified compound $C_{12}H_{22}O$ was found to bear good drug like properties by hamming TPSA of 17. 07 $Å^2$, and no Lipinski's rule violations, showing the possibility of optimal oral drug development and may be useful in the development of drugs for central nervous system. These results are similar to the observed pharmacokinetic effects reported in other studies on bioactive compounds with similar chemical formulas to those of the compounds in this study. Therefore, based on the extensive evaluation of *M. pinnata*, it has been proved to offer vast pharmacological potential, which is in accordance with literature findings; however, there are little or no clinical trials, and as such, more research is required to further endorse its efficacy and safety.

Conclusion

This study employed a combination of computational modeling and *in vitro* experimental techniques to assess the therapeutic potential of bioactive compounds from *M. pinnata* against osteosarcoma. Results indicated significant binding affinity of several compounds to osteosarcoma-associated proteins, corroborated by molecular docking and antioxidant assays. FTIR, GCMS, and phytochemical analyses revealed a diverse composition of bioactive substances with notable pharmacological properties, while antioxidant activity assays demonstrated the extract's efficacy in neutralizing free radicals. The ADME profile analysis further supported the potential of these compounds as therapeutic agents. This integrated approach highlights the promising potential of *M. pinnata* for osteosarcoma treatment and the value of combining computational and biological methods in drug discovery. Future research should focus on *in vivo* investigations and clinical trials to substantiate these findings and explore the medicinal capabilities of *M. pinnata*.

Abbreviations

FTIR: Fourier-transform infrared spectroscopy, DPPH: 2,2-diphenyl-1-picrylhydrazyl assay, GCMS: Gas chromatography-mass spectrometry, ADMET: Absorption, distribution, metabolism, excretion, and toxicity, OS: Osteosarcoma, RANKL: Receptor activator of nuclear factor kappa-B ligand, IGF1: Insulin-like growth factor 1, TGF-β: Transforming growth factor-β, PTKs: Protein tyrosine kinases, TKIs: Tyrosine kinase inhibitors, FDA: Food and Drug Administration, RCSB: Research Collaboratory for Structural Bioinformatics, PDB: Protein Data Bank, TPSA: Topological Polar Surface Area.

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Nil.

Author Contributions

Iadalin Ryntathiang: Conceptualization, Data curation, Formal analysis, Methodology, Writing - original draft, and Writing - review and editing, Yagavel Pooja: Writing– original draft, Writing–review and editing, Jabir Padathpeedika Khalid: Investigation, Visualization, Archana Behera: Investigation, Visualization, Madhumitha Murugesan: Investigation, Visualization, Monisha Prasad: Investigation, Visualization, Mukesh Kumar Dharmalingam Jothinathan: Investigation, Visualization.

Ethics Approval

This study does not involve experiments on animals or human subjects.

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