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The Computer Aided Drug Design Studies of Medicinal Plants and their Derivatives with Fat Mass and Obesity Associated Protein

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ABSTRACT

Purpose: *This study aimed to predict the binding affinity, orientation, and physical interaction between medicinal plant such as Myristica fragrans, Tamarindus indica, Piper nigrum, Zingiber officinale, Murraya konini, Oryza sativa and fat mass and obesity-associated protein.*
Methods: *The mechanism of medicinal plant and protein association was explored by molecular docking, a bioinformatic tool. The association results were compared with the reported results of the anti-obesity drug such as liraglutide, semaglutide and with the flavonoids. Mcule tools were used for the molecular docking of medicinal plant with fat mass and obesity associated protein. PyMol and Discovery Studio Visualizer was used to visualize the results of this docking.*
Result: *The binding affinity of medicinal plant was higher than the liraglutide, semaglutide and flavonoids such as Daidzein, Exemestane, Kaempherol, Letrozole, And Rutin.*
Novelty: *In this study, the medicinal plant can alleviate obesity by interacting with the fat mass and obesity-associated protein. This inhibitory interaction was more significant as compared to other reported phytochemicals and drugs.*

Keywords: *AutoDock Vina, Binding Affinity, Medicinal plant, Molecular Docking*

INTRODUCTION

OBESITY

Obesity refers to an abnormally high proportion of total body fat. It results from less physical work and more mental work existing in our present day living and working conditions. High cost of conventional drugs, relatively high incidence of toxicity and side effects, unavailability of orthodox drugs in many rural areas and clinical limitation especially in the management of some chronic diseases are some of the risks in case of modern medicine. Hence Indian traditional herbal medicine which provides an effective solution without side effects for this possible risk is preferred here. According to the World Health Organization (WHO), approximately 80% of the world's population currently uses herbal medicines in healing different ailments. Among the estimated 400,000 plant species, only 6% have been studied for biological activity, and about 15% have been investigated phytochemically [1,2]. This shows a need for planned activity guided phyto-pharmacological evaluation of herbal drugs. This article is aimed to provide an overview of research work done on 20 anti obese plants with more emphasis on solvent used to extract, dosage administered, active principle identified and biochemical parameters employed to validate anti-obese effect of each plant.

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MEDICINAL PLANT

Myristica fragrans

It belongs to the family Myristicaceae. It is an aromatic tree. The plant is a native of Moluccas, now cultivated in many tropical countries of both hemispheres. In India, it is grown in Tamil Nadu. The ethanolic extract of this plant extract demonstrated significant hypolipidaemic effects in experimentally induced hyperlipidaemia in rabbits. It lowered the lipoprotein lipid levels, total cholesterol, LDL cholesterol and triglycerides. HDL cholesterol was not significantly affected. Total cholesterol, HDL and LDL: HDL ratios were also significantly lowered. It lowered the level of total cholesterol in the heart and liver and demonstrated platelet antiaggregatory activity[3].Seed extract administration reduced both total and LDL cholesterol, lowered the cholesterol/ phospholipid ratio and elevated the decreased HDLratio significantly in hypercholesterolemic rabbits. This extract also prevented the accumulation of cholesterol, phospholipids and triglycerides in liver, heart and aorta and dissolved atheromatous plaques of aorta. Fecal excretion of cholesterol and phospholipid were significantly increased in these rabbits[4].

Tamarindus indica

It belongs to the family Fabaceae. It is a large tropical tree. It is cultivated and naturalized in the tropics throughout the world. Oral administration of aqueous pulp extract of this plant resulted in a dose dependent decrease in body weigh of rats. The decrease in body weight may be attributed to the reduction in food and water intake caused by chemicals that affect brain centers involved in satiety and hunger or could have inhibited digestive enzymes or decreased bioavailability of nutrient caused by ant nutritional factors present in plant extract. Dose dependent decrease in body weight could also be attributed to the presence of anti-nutritional factors like saponins in the extract. Though the rats were fed with diet with adequate protein, the plant extract might not have allowed proper absorption of protein which could account for the decreased body weight. The aqueous pulp extract of the plant at 2700-4500mg/kg dose had lowered body weight, serum cholesterol and low-density lipoprotein. It had significantly increased triglycerides and high density lipoproteins[5].

Piper nigrum

It belongs to the family Piperaceae. It is a branched climbing perennial shrub. It is cultivated in the hot and moist parts of India, Ceylon and other tropical countries. Piperine is the active principle found in this plant. Piperine supplementation at 40 mg piperine/kg body weigh significantly ($P < 0.05$) reduced the levels of plasma total cholesterol, low density lipoprotein (LDL), very low-density lipoprotein (VLDL) and the activity of 3-hydroxy 3-methyl glutaryl coenzyme A (HMG CoA) reductase in the liver, heart

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and aorta, VLDL and significantly ($P < 0.05$) elevated the levels of plasma and tissue lipoprotein lipase (LPL) and plasma lecithin cholesterol acyl transferase (LCAT) in high fat diet fed male wistar rats. Simultaneous supplementation of piperine significantly ($P < 0.05$) enhanced fecal excretion of bile acids and neutral sterols implying that piperine can prevent the accumulation of plasm a lipids andlipoproteins significantly by modulating the enzymes of lipid metabolism[6].

Zingiber officinale

It belongs to the family Zingiberaceae. It is a rhizomatous perennial herb. This is a native of tropical Asia, but is now grown as a commercial in Latin America and Africa as well as South EastAsia. Aqueous extract of at 0.4 ml/kg body weight showed significant decrease in plasma glucose and cholesterol in rats fed with 99% growers mash and 1% cholesterol. Same results were obtained when rats were subjected to an aqueous extract of and at 1ml/Kg body weight[7]. Ethanolic extract of ginger (200mg/kg) lowered serum triglycerides, lipoproteins, phospholipids as well as serum and tissue cholesterol. In addition rats receiving ginger extract with cholesterol showed a lower degree of atherosclerosis.Ginger extract consumption reduced plasma cholesterol, inhibited LDL oxidation and attenuated development of atherosclerosis in atherosclerotic, apolipoprotein E-deficient mice[8].

Murraya koenigii

Murraya koenigii (M. koenigii) (L) Spreng (Family: Rutaceae) is usually known as “curry leaves”. The tropical and subtropical regions in the world have large distributions of M. koenigii [9]. Among the 14 global species belonging to the genus of Murraya, only two, M. koenigii and M. paniculate, are available in India. M. koenigii is more important due to its huge spectrum of traditional medicinal properties. For centuries, this plant has been used in diverse forms and holds a place of pride in Indian Ayurvedic medicine, known as “krishnanimba” [10]. Different parts of M. koenigii, such as its leaves, root, bark, and fruit, are known to promote various biological activities. Aromatic bioactive constituents in the leaves of M. koenigii retain their flavor and other qualities, even after drying [11,12,13,14,15,16]. M. koenigii leaves are slightly bitter in taste, pungent in smell, and weakly acidic. They are used as antihelminthics, analgesics, digestives, and appetizers in Indian cookery [17,18]. The green leaves of M. koenigii are used in treating piles, inflammation, itching, fresh cuts, dysentery, bruises, and edema. The roots are purgative to some extent. They are stimulating and used for common body aches. The bark is helpful in treating snakebites [19,20]. The essential oil extracted from M. koenigii leaves is reported to possess anti-oxidative, hepatoprotective [21,22,23,24], antimicrobial, antifungal [25,26,27], anti-inflammatory, and nephroprotective activities in animal models [28,29,30]. The medicinal properties of M. koenigii have been accredited to several chemical constituents of different carbazole alkaloids and other important

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metabolites, like terpenoids, flavonoids, phenolics, carbohydrates, carotenoids, vitamins, and nicotinic acid from different parts of the M. koenigii plant.

Oryza sativa

Oryza sativa has a high anthocyanin content in the colored bran and high phenolic content in the husk. Biologically active compounds in plants are available as dietary supplements and cosmetics. To expand the utilization of natural resources, PES1CMU will be a natural remedy for skin hyperpigmentation and aging. Cell-free tyrosinase inhibition and scavenging assays were used to screen all extracts, including PES1CMU-rice bran oil (RBO), PES1CMU-defatted rice bran (DFRB), and PES1CMU-husk (H). PES1CMU extracts were first examined in IBMX-stimulated B16 cells and H2O2-induced fibroblasts. The results exhibited that PES1CMU-DFRB was the most effective inhibitor of mushroom tyrosinase, intracellular melanin production (fold change of 1.11 ± 0.01), and tyrosinase activity (fold change of 1.22 ± 0.10) in IBMX-stimulated B16 cells. Particularly, PES1CMU-DFRB showed a comparable whitening effect to the standard arbutin with no significant difference ($p > 0.05$). Moreover, PES1CMU-DFRB and PES1CMU-H demonstrated strong scavenging activities. After accelerated cell aging caused by H2O2 exposure in fibroblasts, the levels of malondialdehyde production in all PES1CMU-treated fibroblasts were comparable with those of standard l-ascorbic acid ($p > 0.05$). Besides, PES1CMU-DFRB and PES1CMU-H treatment significantly inhibited collagen degradation against MMP-2 compared to l-ascorbic acid-treated cells ($p > 0.05$). PES1CMU rice-processing wastes (DFRB and H) could become potential natural sources for dermatocosmetic constituents in skin anti-aging and whitening products[31].

REVIEW OF LITERATURE

Damayanti CA, and their group. In year 2023.Carried out study on Computational Insight into Anti-Obesity Effects of Indonesian Phytobiotics to GLP1R (Glucagon-Like Peptide 1 Receptor) Protein in Anas javanica.

Mojosari ducks (Anas javanica) is native Indonesia laying ducks was a egg producing type with quite high egg production, must be maintain body weight to propotional condition as laying duck. If the body weight surpasses normal, it can lead to obesity and reduce the eggs quality. One of the proteins closely related to obesity and hyperglycemia is GLP1R (Glucagon-Like Peptide 1 Receptor). The increase in GLP1R activity by one of the compounds that have been widely researched is loureirin B. Interaction between loureirin B and GLP1R increases insulin production in the body so that hyperglycemia and body weight can be controlled properly. Exploration of phytobiotic compounds from Indonesia is needed to find the substitution of loureirin B as an anti-obesity agent. According to the findings of in silico study (protein modeling and molecular docking), cynaroside (-9.2 kcal/mol), 14-Deoxy-11,12-didehydroandrographolide (-9.1 kcal/mol), rutin (-8.8 kcal/mol), andrographidine E (-8.6 kcal/mol), and cianidanol (-7.8 kcal/mol) had stronger binding affinity than loureirin B (-7.4 kcal/mol). Andrographidine E, derived from the plant Andrographis paniculata, is the best candidate for GLP1R agonist. The binding affinity that Andrographidine E has is lower than control compounds, so it is easier for bonds to occur between proteins and such compounds. In addition, the interacting amino acids do not have unfavourable bonds that make it more stable than other candidates. Results from clinical

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studies show that the use of A. paniculata can reduce glucose levels[32].

Mengrong Cheng, and their group in China carried out Computational analyses of obesity associated loci generated by genome-wide association studies.
Genome-wide association studies (GWASs) have discovered associations of numerous SNPs and genes with obesity. However, the underlying molecular mechanisms through which these SNPs and genes affect the predisposition to obesity remain not fully understood. Aims of our study are to comprehensively characterize obesity GWAS SNPs and genes through computational approaches. For obesity GWAS identified SNPs, functional annotation, effects on miRNAs binding and impact on protein phosphorylation were performed via RegulomeDB and 3DSNP, miRNASNP, and the PhosSNP 1.0 database, respectively. For obesity associated genes, protein-protein interaction network construction, gene ontology and pathway enrichment analyses were performed by STRING, PANTHER and STRING, respectively[33].

Lavanya Prabhakar and Dicky John Davis G in Chennai, Tamil Nadu, India carried out study on Computational study of potential inhibitors for fat mass and obesity-associated protein from seaweed and plant compounds.
Over the past three decades, with substantial changes in lifestyle, the tendency to gain weight has increased, which is resulting in significant consequences affecting an individual's well-being. The fat mass and obesity-associated (FTO) gene is involved in food intake and energy expenditure and plays a crucial role in regulating homeostasis and controlling energy expenditure by hindering signals that generate from the brain. Edible seaweeds have been shown to enhance satiety owing to their health benefits. Methods: Extensive screening of plant-derived anti-obesity compounds and seaweed compounds was conducted and validated for ADME properties and toxicity prediction. Further, the top ranked compounds were docked against the FTO protein to identify potential inhibitors and were subjected to molecular dynamic simulation studies to understand the binding stability of ligand protein complex. Finally, MM/PBSA studies were performed to calculate the binding free energy of the protein-ligand complexes[34].

Ji-Hyuk Park, Wona Jee, and their group, in Republic of Korea carried out study on Timosaponin A3 Induces Anti-Obesity Effects In Vitro and In Vivo
Obesity is a serious global health challenge, closely associated with numerous chronic conditions including type 2 diabetes. Anemarrhena asphodeloides Bunge (AA) known as Jimo has been used to address conditions associated with pathogenic heat such as wasting-thirst in Korean Medicine. Timosaponin A3 (TA3), a natural compound extracted from AA, has demonstrated potential therapeutic effects in various disease models. However, its effects on diabetes and obesity remain largely unexplored. We investigated the anti-obesity and anti-diabetic properties of TA3 using in vitro and in vivo models. TA3 treatment in NCI-H716 cells stimulated the secretion of glucagonlike peptide 1 (GLP-1) through the activation of phosphorylation of protein kinase A catalytic subunit (PKAc) and 5′ -AMP-activated protein kinase (AMPK). In 3T3-L1 adipocytes, TA3 effectively inhibited lipid accumulation by regulating adipogenesis and lipogenesis. In a high-fat diet (HFD)-induced mice model, TA3 administration significantly reduced body weight gain and food intake. Furthermore, TA3 improved glucose tolerance, lipid profiles, and mitigated hepatic steatosis in HFD-fed mice. Histological analysis revealed that TA3 reduced the size of white adipocytes and inhibited adipose tissue generation. Notably, TA3 downregulated the expression of lipogenic factor, including fattyacid synthase (FAS) and sterol regulatory element-binding protein 1c

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(SREBP1c), emphasizing its potential as an anti-obesity agent. These findings revealed that TA3 may be efficiently used as a natural compound for tackling obesity, diabetes, and associated metabolic disorders, providing a novel approach for therapeutic intervention[35].

Manobharathi V1, Surya C, and their group in Perambalur carried out study on Pshytochemical Screening and Antiobesity Activity of morinda citrifolia leaves extract

Natural medicines have been the only option for the prevention and treatment of human diseases for thousands of years. Morinda citrifolia, popularly known as noni, is widely utilized in traditional medicine. Many components of the noni tree, including the roots, leaves, and seeds, are used in these traditions. The leaves of M. citrifolia have been utilized in a variety of commercial products marketed for their health benefits. The study was designed to investigate the phytochemical screening and antioxidant properties of M. citrifolia. Thereby, we tested the extract from M. citrifolia leaves obtained by hydro distillation against fungi and bacteria. Herewith, M.Citrifolia leaf Powder Extract was prepared with three different solvents of Ethanol, Methanol and water were obtained for further testing of qualitative Phytochemical Analysis. Moreover, the leaf extract was prepared by conventional extraction method and it was assessed with minimum inhibitory concentration (MIC) against clinical isolate of Ecoli. Anti-fungal activity of M. citrifolia leaves extract against penicilium was tested in vitro. The antioxidant activity of these extract was evaluated by reducing the DPPH radical. Antioxidant Activity of DPPH radical scavenging Activity IC50 205µg. This M.Citrifolia demonstrated excellent anti-obesity and antioxidant potential with pancreatic lipase inhibitory effect (21.7 ± 1.3%). It is concluded that the flavonoids and phenols especially alkaloides are the major compounds in M. Citrifolia leaves which possess more Antioxidant, Antibacterial, Antifungal and Antiobesity activities of ethanolic extract of M. citrifola leaves[36].

Hyuck Kim1, Jihwan Lee2, and their group in Korea carried out study on Anti-obesity effects of two herbal extracts in C57BL/6N mice fed high-fat diet

The objective of this study was to investigate the anti-obesity effects of adding Momordica charantia (MC) and Chrysanthemum zawadskii var. latilobum (CZ) extracts to drinking water on obesity-induced mice. A total of 84 eight-week-old C57BL/6N male mice with an initial body weight (BW) of 28.11 ± 1.39 g were used in this study. All treatments were fed a highfat diet for d 28. Mice were randomly divided into seven drinking treatments (six replicate each treatment) based on the initial BW. Treatments are as follows: control (CON), normal tap water, MC 1, CON with 1% MC aqueous extract, MC 2, CON with 2% MC aqueous extract, CZ 1, CON with 1% CZ aqueous extract, CZ 2, CON with CZ aqueous extract (2%), MCZ 1, CON with 1% MC aqueous extract and 1% CZ aqueous extract, MCZ 2, CON with 2% MC aqueous extract and 2% CZ aqueous extract. During the entire period, the CZ 1, MCZ 1, and MCZ 2 significantly decreased ($p < 0.05$) gain to feed than CON. The CON significantly higher ($p < 0.05$) water intake than other treatments on d 0 to 14. The MCZ 1 significantly decreased ($p < 0.05$) relative (ratio of absolute organ weight to BW) organ weights, including retroperitoneal white adipose tissue (RWAT) weight and inguinal white adipose tissue (IWAT) weight, compared to CON. In conclusion, our study suggests that there was no significant difference in the antiobesity effects between MC and CZ, and MCZ 1 has synergistic effects by regulating adipose tissue[37].

Doaa Salah Eldin Abdelfattah, Mervat A. Fouad and their group from Egypt carried out study on Anti-Obesity Effect of Combining White Kidney Bean Extract, Propolis Ethanolic Extract and CrPi3 on Sprague-Dawley Rats Fed a High-Fat Diet

Obesity has been associated with the occurrence and prevalence of various chronic metabolic

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diseases. The management of obesity has evolved to focus not only on reducing weight, but also on preventing obesity-related complications. Studies have shown that bioactive components in natural products like white kidney bean extract (WKBE), propolis ethanolic extract (PEE), and chromium picolinate (CrPi3) showed anti-obesity properties. However, no studies have examined the outcomes of combining any of these nutraceutical supplements. We compared the effects of HFD supplemented with WKBE, WKBE+PEE, or WKBE+PEE+CrPi3 against control and obese groups using Sprague-Dawley rats fed a 45% high-fat diet as an in vivo model. Nutritional parameters, biochemical parameters, and biomarkers of cardiovascular disease, liver function, kidney function, and gut health were among the comparable effects. Our findings showed that combining the three nutraceutical supplements had a synergetic effect on reducing weight gain, food utilization rate, abdominal fat, serum lipids, arterial and hepatic lipids, risk of cardiovascular disease, and blood glucose level, in addition to improving renal function and gut microbiota. We attributed these effects to the α-amylase inhibitor action of WKBE, flavonoids, and polyphenol content of PEE, which were potentiated with CrPi3 resulting in a further reduction or normalization of certain parameters[38].

Kumaraswamy Athesh, Nayagam Agnel Arul John, and their group from Tiruchirappalli Tamil Nadu, India carried out study on Protective Effect of Dolichos biflorus Seed Extract on 3T3-L1 Preadipocyte Differentiation and High-Fat Diet-Induced Obesity in Rats

Obesity is known to be one of the severe health issues worldwide, as its prevalence continues to rise as well as its association with other chronic diseases worsens. Even though various approaches have been underway to prevent or treat obesity, alternative approaches are in need to combat this chronic condition because of the unsatisfactory efectiveness and adverse side efects of the existing approaches. Dolichos biforus L. seeds have been employed as a weight-loss treatment in folk medicine. Considering the necessity to develop a safe alternative remedy to rising obesity, the current investigation has been set up to assess the antiobesity potential and the mode of action of the aqueous seed extract of D. biforus (ASEDB) in a cell line (3T3-L1) and high-fat diet (HFD)-induced rats. Forinvitro studies, 3T3-L1 cell lines were cultured in Dulbecco's modifed Eagle medium (DMEM) augmented with adipogenic-inducing medium and the infuence of the extract (10 µg/mL–500 µg/mL) on 3T3-L1 adipocyte viability, adipogenesis, and lipolysis was assessed. An in-vitro study revealed maintenance of cell viability, reduced triglycerides (TG) accumulation, and promoted lipolysis in 3T3-L1 cells by ASEDB. Following in-vitro analysis, the HFD-induced obese rats were treated with ASEDB at diferent concentrations (100 mg/kg, 200 mg/kg, and 300 mg/kg) for 60 days and the efect was evaluated through various anthropometric and biochemical parameters. Te fndings revealed a signifcant decrement in total body weight, organ weights, fat pad weights, and restoration of abnormal levels of glucose, leptin, insulin, lipid markers, and antioxidant system to normal by ASEDB treatment. Also, pancreatic lipase inhibition analysis of ASEDB revealed a modest level of inhibition with an IC50 value of 213.3 µg/mL. All these fndings exposed that ASEDB possesses pronounced antiobesity potential and exhibits its protective efect by suppressing food intake, reducing fat digestion and absorption, limiting adipogenesis, enhancing lipolysis, and alleviating oxidative stress[39].

Kamlesh Kumar Bhutani, Rahul Birari and Kausik Kapat from Punjab, India carried out study on Potential Anti-obesity and Lipid Lowering Natural Products: A Review

Obesity has reached epidemic proportions globally, with more than 1 billion adults overweight - at least 300 million of them clinically obese. In Ayurveda, obesity is called

'medoroga'. The detailed features and treatments of the disease have been described in an old Ayurvedic text, Charak and Sushrut Samhita. There are some native plants that are commonly used for the treatment of obesity in Ayurveda. Unfortunately, only few medications are available in the market, with side effects and unacceptable efficacy. With the current view that botanical drugs can be developed faster and more cheaply than conventional single entity pharmaceuticals, the review mainly focuses on the rationality of their use with appropriate literature data support[40].

Joanne A Rathbone, Tegan Cruwys and Jolanda Jetten from Australia carried out study on Non-stigmatising alternatives to anti-obesity public health messages: Consequences for health behaviour and well-being

This project investigated how alternative non-stigmatising public health messages influence people's health behaviours and well-being, relative to traditional stigmatising weight-loss messages. We conducted three experimental studies (total N=1281) that compared traditional weight-loss messages to weight-neutral messages (Study 1), weight-inclusive messages (Study 2) and size acceptance messages (Study 3). Results revealed that public health messages have differential effects on health behaviours and well-being, depending on the audience's BMI or perceived weight. However, campaigns that challenge weight stigma and promote body positivity have positive effects on some psychological indicators of health and well-being for people of all body sizes[41].

Abdelaziz Ghanemi , Mayumi Yoshioka and Jonny St-Amand from Canada carried out study on In Vitro Mimicking of Obesity-Induced Biochemical Environment to Study Obesity Impacts on Cells and Tissues

Obesity represents a heavy burden for modern healthcare. The main challenge facing obesity research progress is the unknown underlying pathways, which limits our understanding of the pathogenesis and developing therapies. Obesity induces specific biochemical environments that impact the different cells and tissues. In this piece of writing, we suggest mimicking obesity-induced in vivo biochemical environments including pH, lipids, hormones, cytokines, and glucose within an in vitro environment. The concept is to reproduce such biochemical environments and use them to treat the tissue cultures, explant cultures, and cell cultures of different biological organs. This will allow us to clarify how the obesity-induced biochemistry impacts such biological entities. It would also be important to try different environments, in terms of the compositions and concentrations of the constitutive elements, in order to establish links between the effects (impaired regeneration, cellular inflammation, etc.) and the factors constituting the environment (hormones, cytokines, etc.) as well as to reveal dose-dependent effects. We believe that such approaches will allow us to elucidate obesity mechanisms, optimize animal models, and develop therapies as well as novel tissue engineering applications[42].

Shirin Hasani-Ranjbar, Neda Nayebi,and their group from Tehran, Iran. carried out study on A systematic review of the efficacy and safety of herbal medicines used in the treatment of obesity.

This review focuses on the efficacy and safety of effective herbal medicines in the management of obesity in humans and animals. PubMed, Scopus, Google Scholar, Web of Science, and IranMedex databases were searched up to December 30, 2008. The search terms were "obesity" and ("herbal medicine" or "plant", "plant medicinal" or "medicine traditional") without narrowing or limiting search elements. All of the human and animal studies on the effects of herbs with the key outcome of change in anthropometric measures

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such as body weight and waist-hip circumference, body fat, amount of food intake, and appetite were included. In vitro studies, reviews, and letters to editors were excluded. Of the publications identified in the initial database, 915 results were identified and reviewed, and a total of 77 studies were included (19 human and 58 animal studies). Studies with Cissus quadrangularis (CQ), Sambucus nigra , Asparagus officinalis , Garcinia atroviridis , ephedra and caffeine, Slimax (extract of several plants including Zingiber officinale and Bofutsushosan) showed a significant decrease in body weight. In 41 animal studies, significant weight loss or inhibition of weight gain was found. No significant adverse effects or mortality were observed except in studies with supplements containing ephedra, caffeine and Bofutsushosan. In conclusion, compounds containing ephedra, CQ, ginseng, bitter melon, and zingiber were found to be effective in the management of obesity. Attention to these natural compounds would open a new approach for novel therapeutic and more effective agents[43].

B.Pushpa Latha, I. Rama Manohar Reddy,and their group from Tirupati, A.P.India carried out study on Medicinal Plants and Their Derivatives as Potential Source in Treatment of Obesity.

Since the time immemorial plants have been in use as sources of medicine throughout the world. The demand for plant-based medicines is ever growing as crude or processed products from plants have less or no adverse effects. The present review covers the taxonomy, habitat, distribution, extraction and identification of active principle of potential medicinal plants used in obesity treatment. The different biochemical markers used to evaluate the anti-obese effect of each plant is also considered[44].

Muhammad Zeeshan Ahmed, Shahzeb Hameed, and their group, from Pakistan carried out study on In Silico Molecular Docking Analysis of Limonene with The Fat Mass and Obesity-Associated Protein by Using Autodock Vina

Purpose: This study aimed to predict the binding affinity, orientation, and physical interaction between limonene and fat mass and obesity-associated protein. Methods: The mechanism of limonene and protein association was explored by molecular docking, a bioinformatic tool. The association results were compared with the reported results of the anti-obesity drug such as orlistat and with the flavonoids. AutoDock Vina tools were used for the molecular docking of limonene with fat mass and obesity associated protein.

PyMol and Discovery Studio Visualizer was used to visualize the results of this docking. Result: The binding affinity of limonene was higher (Least negative G) than the orlistat and flavonoids such as Daidzein, Exemestane, Kaempherol, Letrozole, And Rutin. Novelty: In this study, the limonene can alleviate obesity by interacting with the fat mass and obesity-associated protein. This inhibitory interaction was more significant as compared to other reported phytochemicals and drugs[45].

Udhaya Kumar. S, Senior Research Fellow, Bithia Rajan from Vellore, Tamil Nadu, India carried out study on Comparison of potential inhibitors and targeting fat mass and obesity-associated protein causing diabesity through docking and molecular dynamics strategies

Genome-wide association studies (GWAS) have identified an association between polymorphisms in the FTO gene and obesity. The FTO: rs9939609, an intronic variant, is considered a risk allele for developing diabesity in homozygous and heterozygous forms. This study aimed to investigate the molecular structure of the available inhibitors specific to

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the FTO mutations along with the rs9939609 variant. We identified the best-suited inhibitor molecules for each mutant type containing the rs9939609 risk allele. Missense mutations unique to obesity and containing the risk allele of rs9939609 were retrieved from dbSNP for this study. Further stability testing for the mutations were carried out using DynaMut and iStable tools. Three mutations (G187A, M223V, and I492V) were highly destabilizing the FTO structure. These three mutants and native FTO were docked with each of the nine-inhibitor molecules collected from literature studies with the help of PyRx and AutoDock. Further structural behavior of the mutants and native FTO were identified with molecular dynamics simulations and MM-PBSA analyses, along with the 19complex inhibitor compound. We found the compound 19complex exhibited better binding interactions and is the top candidate inhibitor for the M223V and I492V mutants. This study provided insights into the structural changes caused due to mutations in FTO, and the binding mechanism of the inhibitor molecules. It could aid in developing antiobesity drugs for treating patients with mutations and risk alleles predisposing to obesity[46].

METHODOLOGY

Software and Databases

All the software and databases used in this study are freely available for the use in academic purposes. The PDB (https://www.rcsb.org/) is used to download the 3D structure of the protein. PubChem (https://pubchem.ncbi.nlm.nih.gov/) is used to download the 3D structure of ligands. Python 3.9.1 (https://www.python.org/downloads/) was downloaded and used for language purposes. Discover Studio (https://discover.3ds.com/discovery-studio-visualizer-download) was downloaded and used for molecular visualization, sharing, and analyzing the protein and ligand in modeling studies.

MGLTools (https://ccsb.scripps.edu/projects/visualization/) was downloaded and used for the analysis and visualization of biomolecular systems. Mcule (https://mcule.com/apps/1-click-docking/) was downloaded and used for the virtual screening of proteins and ligand interaction. PyMol (https://pymol.org/2/) was downloaded and used for the visualization of docking results.

Preparation of Receptor File

The 3D structure of the FTO (3LFM) protein (receptor) was downloaded from the PDB. Open the protein file in the Discovery Studio and removed all the molecules other than protein, such as water molecules and ligands, and then saved the file in the .pdb extension.

Grid Setting and File Preparation

The MGLTools were used for setting the grid parameter on the receptor. The protein file with .pdb extension was opened into the MGLTools, polar hydrogen atoms were added in the protein molecule, and then selected the protein as a macromolecule was saved in .pdbqt file. Then added the ligand, set the torsion angle, and saved the ligand in the .pdbqt file.

Preparation of Conf .txt File

The conf .txt file was prepared in such a way that all the center axes and size axes of the set grid were written with the receptor, ligand, and output files extension.

Docking

The AutoDock Vina performed the molecular docking between receptor and ligand according to the procedure described by Trott et al. (2009) and Vina et l. (2020) [47,48]. The results

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were visualized in PyMol and Discovery Studio.

RESULT AND DISCUSSION

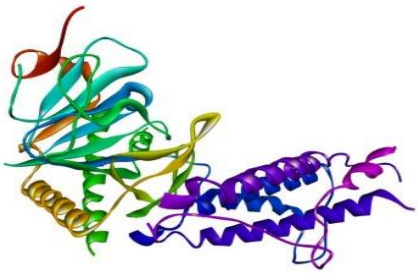
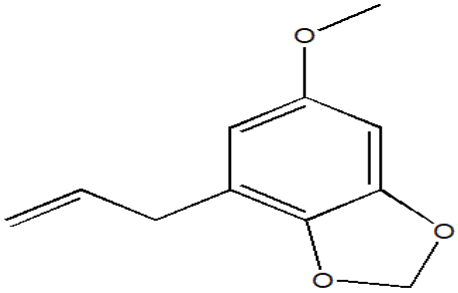


Figure 1. 3D structure of the FTO protein used as a receptor for the molecular docking



7-Allyl-5-methoxy-1,3-benzodioxole

Figure 2. The structural formula of Myristicin used as a ligand for the molecular docking

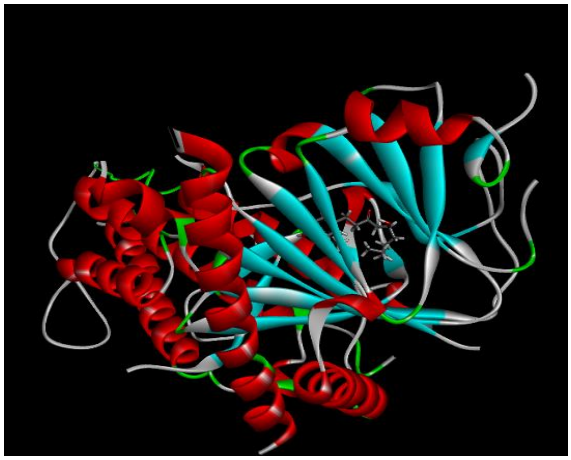
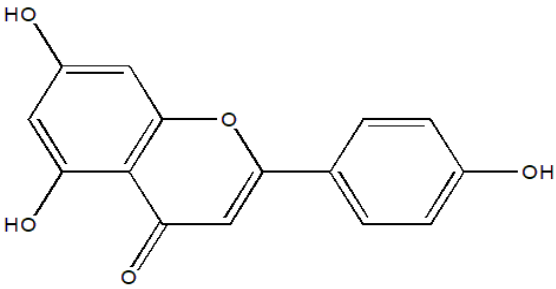


Figure 3. Showing the molecular docking between the FTO protein (receptor) in blue, white, red, and green colors and myristicin (ligand) in grey color.



5,7-dihydroxy-2-(4-hydroxyphenyl)chromen-4-one

Figure 4. The structural formula of Apigenin used as a ligand for the molecular docking

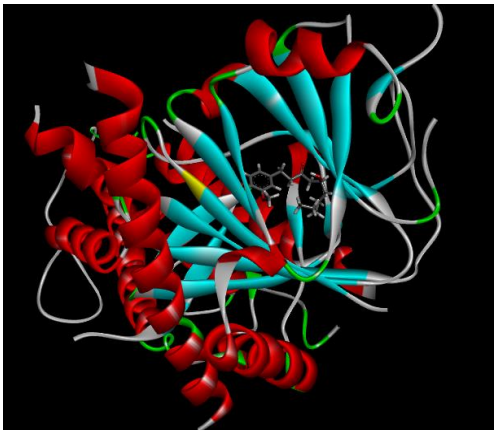
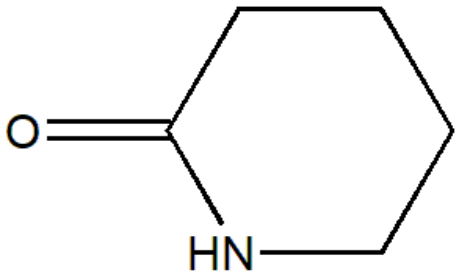


Figure 5. Showing the molecular docking between the FTO protein (receptor) in blue, white, red, and green colors and Apigenin(ligand) in grey color.



Piperidin-2-one

Figure 6. The structural formula of 2-Piperidinone used as a ligand for the molecular docking

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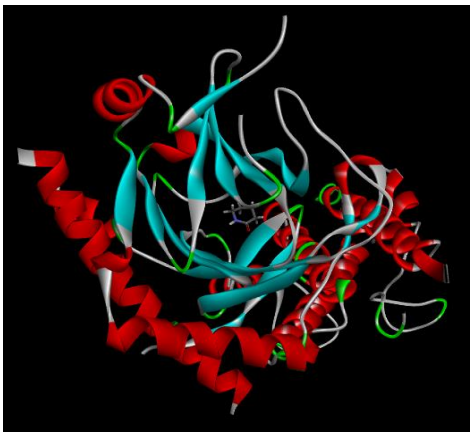
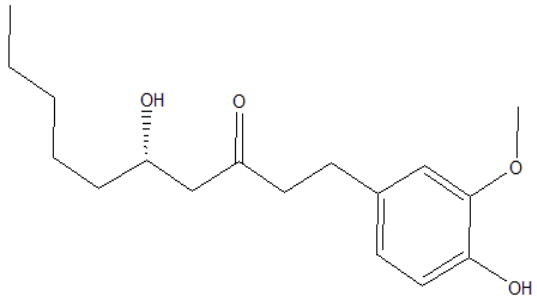


Figure 7. Showing the molecular docking between the FTO protein (receptor) in blue, white, red, and green colors and 2-Piperidinone(ligand) in grey color.



(5S)-5-Hydroxy-1-(4-hydroxy-3-methoxyphenyl)decan-3-one

Figure 8. The structural formula of 6-Gingerol used as a ligand for the molecular docking

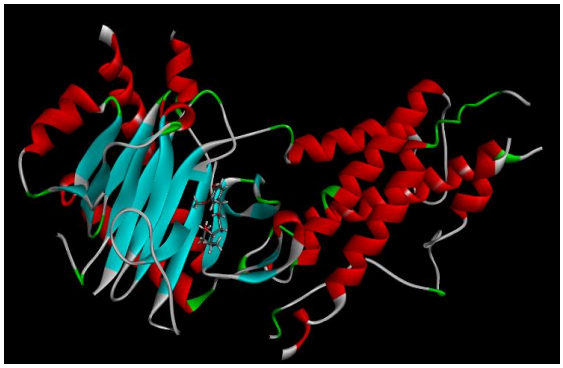
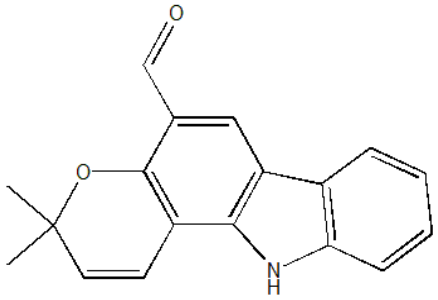


Figure 9. Showing the molecular docking between the FTO protein (receptor) in blue, white, red, and green colors and 6-Gingerol(ligand) in grey color.



3,3-dimethyl-11H-pyrano[3,2-a]carbazole-5-carbaldehyde

Figure 10. The structural formula of Murrayacin used as a ligand for the molecular docking

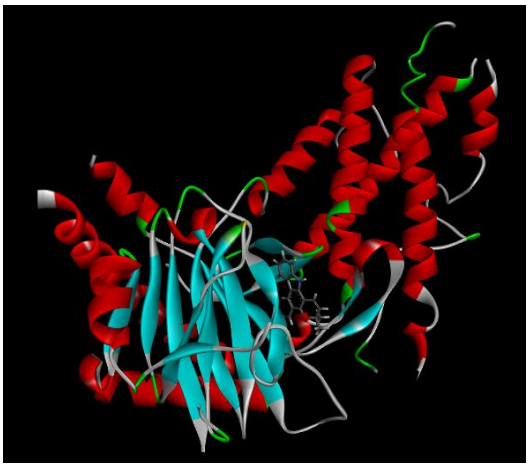
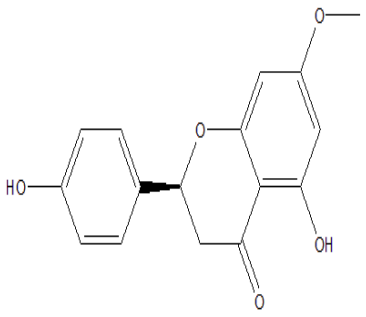


Figure 11. Showing the molecular docking between the FTO protein (receptor) in blue, white, red, and green colors and Murrayacin(ligand) in grey color.



(2S)-5-Hydroxy-2-(4-hydroxyphenyl)-7-methoxy-2,3-dihydro-4H-1-benzopyran-4-one

Figure 12. The structural formula of Sakuranetin used as a ligand for the molecular docking

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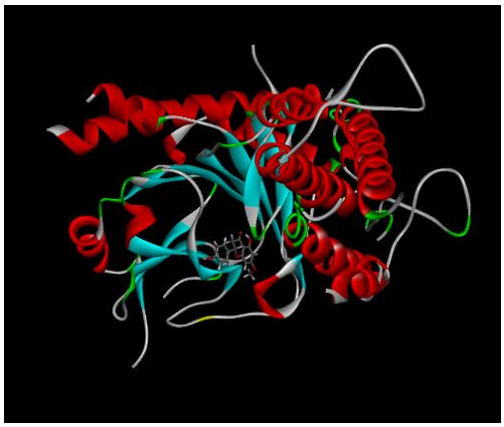

Figure 13. Showing the molecular docking between the FTO protein (receptor) in blue, white, red, and green colors and Sakuranetin(ligand) in grey color.

Table 1: Showing Structure and it Energy

Sr.no.	Structure	Energy
1	Myristicin	12.3701
2	Apigenin	-3.69183
3	2-Piperidinone	2.74307
4	6-Gingerol	-0.247235
5	Murrayacin	32.4726
6	Sakuranetin	16.8412

CONCLUSION

The study confirmed the inhibitory effect of medicinal plant with FTO protein. The inhibition of protein is associated with a decrease in obesity and other associated metabolic disorders. Moreover, the docking results of Medicinal plant were also compared with phytochemical inhibitors for FTO to prove the better results of docking. The interaction between the Medicinal plant and FTO should be confirmed through in vitro studies and better understand the mechanism.

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