PASS ANALYSIS AND MOLECULAR DOCKING OF LIMONENE IN ESSENTIAL OIL EXTRACTED FROM THE PEPPER MINT PLANT

Tukhtayev Sardor Anvarjon o‘g‘li
Teacher of Bukhara innovative education and medical university
Adizova Shoira Toirovna
Teacher of Bukhara innovative education and medical university
Amonov Mukhammad Murod o‘g‘li
Teacher of Bukhara innovative education and medical university
Homitova Gulnoza Zaynidin qizi
Teacher of Asian international university

Annotation. This article analyzes limonene, one of the main components of essential oil extracted from the composition of the pepper mint plant, which grows locally on the territory of Uzbekistan, through modern chemical computer programs and evaluates its pharmacological properties.
Keywords. Protein, ligand, PASS online program, n-sulfanyl-2-indole carboxamide ligands, PPAR gamma protein (Peroxisome Proliferator-Activated Receptor Gamma), CB-Dock2 online server.
Аннотация. В данной статье с помощью современных химических компьютерных программ анализируется лимонен — один из основных компонентов эфирного масла, извлекаемого из состава растения мяты перечной, произрастающего на территории Узбекистана, и оцениваются его фармакологические свойства.
Ключевые слова. Белок, лиганд, онлайн-программа PASS, лиганды n-сульфанил-2-индолкарбоксамида, белок PPAR гамма (рецептор, активируемый пролифераторами пероксисом гамма), онлайн-сервер CB-Dock2.
Annotatsiya. Ushbu maqolada O‘zbekiston hududida mahalliy sharoitda o‘sadigan qalampir yalpiz o‘simligi tarkibidan olinadigan efir moyining asosiy tarkibiy qismlaridan biri bo‘lgan limonen zamonaviy kimyoviy kompyuter dasturlari orqali tahlil qilinadi va uning farmakologik xususiyatlariga baho beriladi.
Kalit so‘zlar. Protein, ligand, PASS onlayn dasturi, n-sulfanil-2-indol karboksamid ligandlari, PPAR gamma oqsili (Peroksisoma proliferator-faollashtirilgan retseptor gamma), CB-Dock2 onlayn serveri.

Research objective: To study the biological activity of limonene through the PASS online program, one of the main components of the peppermint plant, as

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well as its biological activity using limonene as a ligand, in relation to the PPAR protein, one of the nuclear receptors that plays a crucial role in regulating glucose and lipid metabolism. PPAR gamma protein-useful for drugs used in the treatment of type 2 diabetes and other metabolic disorders.

Research materials and methods: The substance needed to carry out this work is limonene, one of the main components of essential oil obtained from the pepper mint plant. Initially, the biological activlog of limonene was studied through the online program PASS. Also, the interaction of limonene with PPAR gamma protein using the CB-Dock2 online server was studied in the molecular docking Method [1].

Results of the study: The biological activity of Menton was predicted using the PASS – computer program. This program PASS (Prediction Activity Structure Substances-predicting activity based on the structure of substances) Russian scientists V.V. Poroikov, D.A. Created by the Filimonov [6]. Through the PASS program, we can see 89.6% antienzymatic properties of limonene as a retinol dehydrogenase inhibitor, and when the study results are observed, we can see 93.4% carminative, that is, 96.1% against excessive gas formation in the body.

The pepper mint plant, which is needed to carry out this work, was harvested from the territory of the Romitan District of the Bukhara region. Drying the raw materials was carried out in a shaded place at room temperature [1,2] separation of essential oil from plant raw materials was carried out in a traditional hydrodistillation method.The extracted essential oil contains more than 10 separate components, one of which is limonene [3]. We studied the obtained limonene, the interaction of one of the nuclear receptors with the PPAR protein using the CB-Dock2 online server [4,5].

Limonene has been found to exhibit high levels of capillary wall strengthening, antienzematic, anti-inflammatory activity, the results of the analysis are shown in Table 1.

Table 1.

Pa	Pi	Biological activity	
0,961	0,001	Carminative	Softening gas in the digestive tract

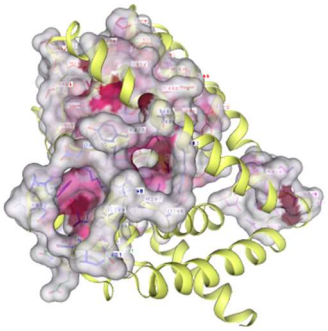
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	0,000	Retinol dehydrogenase inhibitor	Retinol dehydrogenase inhibitor
0,896	0,005	Antieczematic	Antieczematic
0,881	0,001	Alpha-pinene-oxide decyclase inhibitor	Alpha-pinene-oxide decyclase inhibitor
0,816	0,007	Apoptosis agonist	Apoptosis agonist
0,812	0,010	Antineoplastic	Antineoplastic
0,799	0,010	CYP2C substrate	CYP2C substrate

Using the CB-Dock2 online server, ligand interaction gaps of the protein were initially traced, with 5 active gap centers of 6138 , 285, 176, 160, and 156 Å (Figure 1). The ligand and protein were then loaded onto the server and molecular docking was carried out.[7].

1- picture

Active center ID	Space size (Å^3)	center (x, y, z)	Space size (x, y, z)
C1	6138	24, -10, 2	24, 29, 26
C2	285	15, 15, -5	11, 7, 6
C3	176	17, 1, 29	10, 7, 4
C4	160	6, -2, -1	9, 8, 11
C5	156	23, 13, 4	6, 8, 6

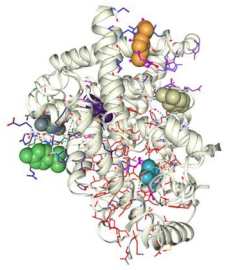


1-figure. Space search results

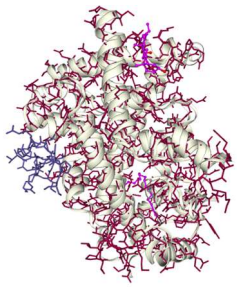
Activity with energies of -3.3, -5.0; -4.6 -4.2, and -4.1 kcal/mol was observed, respectively, to the aforementioned gaps from protein-ligand interactions (Figure 2). The results show that the volume is the largest and the smallest gap has higher ligand activity.

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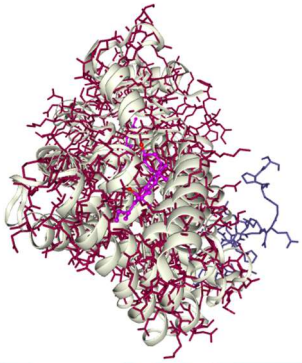
Active center ID	Activity energy	Space size (Å^3)	center (x, y, z)	Docking size (x, y, z)
C1	-3.3	6138	24, -10, 2	24, 29, 26
C2	-5.6	285	15, 15, -5	11, 7, 6
C3	-4.6	176	17, 1, 29	10, 7, 4
C4	-4.2	160	6, -2, -1	9, 8, 11
C5	-4.1	156	23, 13, 4	6, 8, 6



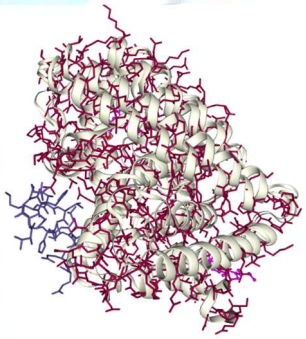
2-figure . Results of activity in spaces



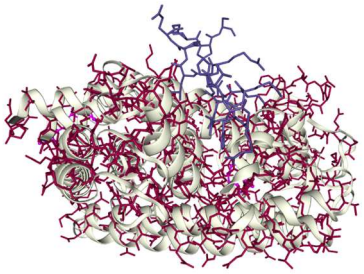
C1



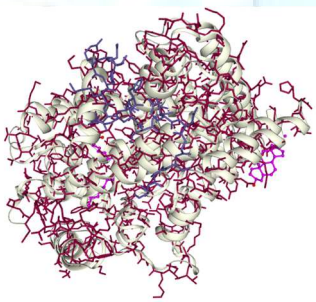
C2



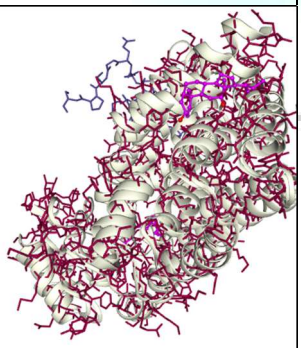
C3



C4



C5



Total

Figure 3. Ligand interaction to the sought spaces of the protein

For the 5 spaces in the protein mentioned above, it was found that the following order shows an active center of a row of amino acids:

Chain A for space C1: ILE281 CYS285 ARG288 LEU330 LEU333 VAL39 LEU340 ILE341 SER342 MET348 LEU353 MET364

Chain A for C2 space: LYS319 TYR320 GLY321 HIS323 GLU324 ASP396 ARG397 PRO398 ARG443 GLN444 VAL46 THR447 LEU476 TYR477

Chain A for C3 space: ASN312 ASP313 VAL315 THR316 LYS319 TYR320 PRO398 GLY399 LEU401 ASP475 Chain B: GLU602 ARG603 HIS604

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Chain A for C4 space: ASN312 ASP313 VAL315 THR316 LYS319 TYR320 PRO398 GLY399 LEU401 ASP475 Chain B: GLU602 ARG603 HIS604

Chain A for C5 space: TYR219 LYS230 ALA231 ARG234 VAL372 ASN375 ALA376 LEU377 GLU378 LEU379 ASP380 ASP381 SER382 HIS425 GLU427 SER428 LEU431 LYS434

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