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# Pass Analysis and Molecular Docking of Menton in Essential Oil Extracted From the Pepper Mint Plant

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**Abstract:**

This article analyzes Menton, 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 software, TRPM8, CB-Dock2 online server.

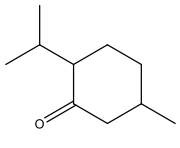
**Research objective**: To study the biological activity of Menton through the online program pass, one of the main components of the peppermint plant, as well as its biological activity using Menton as a ligand, in relation to the TRPM8 protein, a member of M subfamily of the transient receptor potential cation channel.

**Research materials and methods**: the substance needed to carry out this work is Mentone, one of the main components of essential oil obtained from the pepper mint plant. Initially, Menton's biological activlog was studied through the online program PASS. Also, the interaction of Menton with TRPM8 protein, a member of the M subfamily of the transient receptor potential cation channel, 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 that menthol's antienzematic properties are active at 94.8% when the results of research are observed against carminative yani excessive gas formation in the body, with a result of 91.7%. .

Mentone 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.

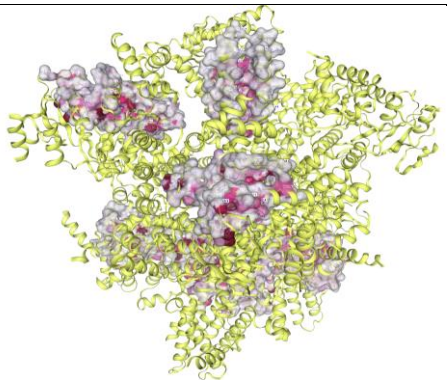
**Table 1.**

| Formula and name of the substance | Pa | Pi | Biological activity |
|---|---|---|---|
|  (MENTHON) | 0,948 | 0,001 | Carminative |
| | 0,917 | 0,004 | Antieczematic |
| | 0,896 | 0,006 | Ubiquinol-cytochrome-c reductase inhibitor |
| | 0,866 | 0,004 | Vasoprotector |
| | 0,860 | 0,007 | Acylcarnitine hydrolase inhibitor |
| | 0,837 | 0,006 | Alkylacetylglycerophosphatase inhibitor |
| | 0,839 | 0,017 | Testosterone 17beta-dehydrogenase (NADP+) inhibitor |

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, along with menthol, is the menthon, which occupies the top ingredient [3]. We studied the obtained Mentone, the interaction of the temporal receptor potential cation channel with the protein TRPM8, a member of subfamily M, using the CB-Dock2 online server [4,5].

Using the CB-Dock2 online server, ligand interaction gaps of the protein were initially traced, with 5 active gap centers of 439-85, 66-31, 55-35, 47-13, and 32-93 Å3 (Figure 1). The ligand and protein were then loaded onto the server and molecular docking was carried out.

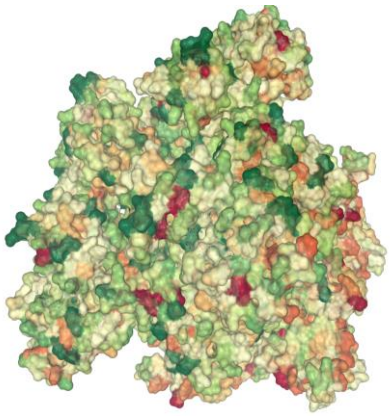
| Active center ID | Space size ($Å^3$) | center (x, y, z) | Space size (x, y, z) |
|---|---|---|---|
| **C1** | 43985 | 125, 149, 177 | 30, 30, 30 |
| **C2** | 6631 | 138, 138, 90 | 20, 20, 28 |
| **C3** | 5535 | 177, 143, 105 | 30, 30, 29 |
| **C4** | 4713 | 170, 142, 170 | 28, 21, 24 |
| **C5** | 3293 | 140, 98, 101 | 26, 28, 21 |



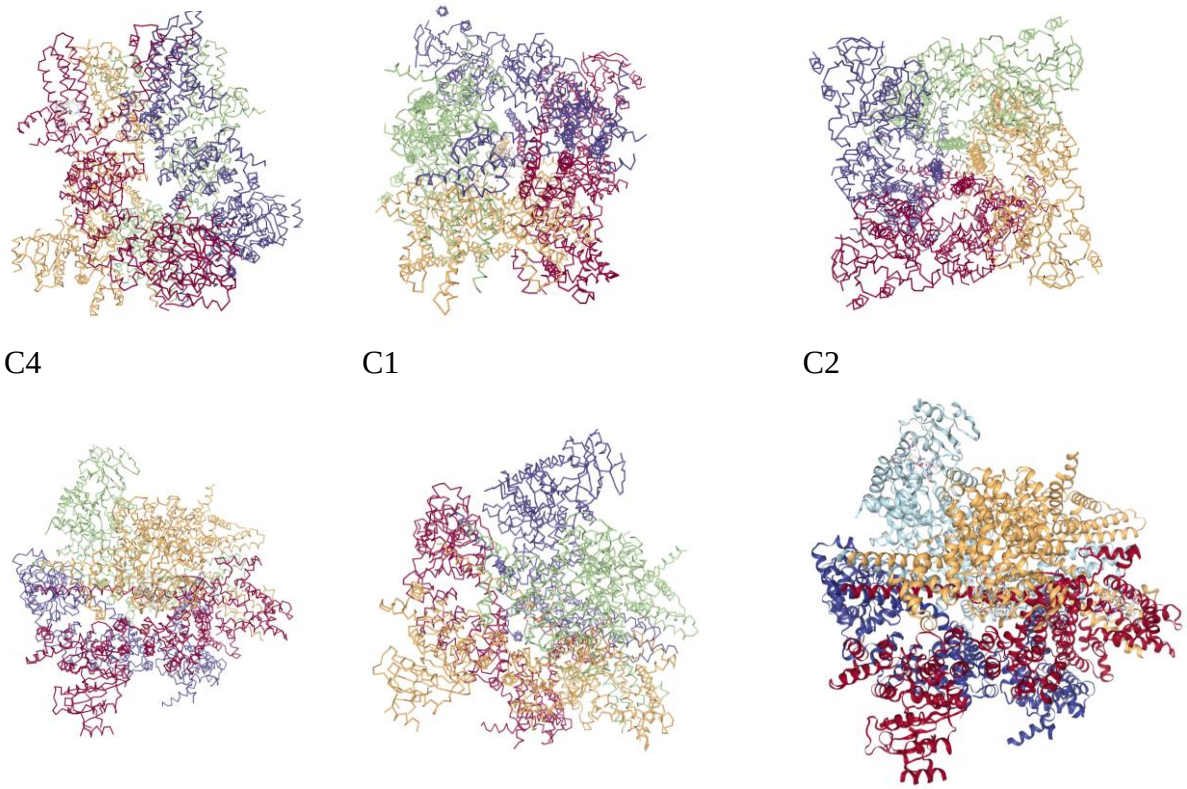
1-figure. Space search results

Activity with energies of -7.0, -5.9; -5.7; -5.7; -5.7 and -5.6 kcal/mol was observed, respectively, from the protein and ligand interactions to the aforementioned gaps (Figure 2). The results show that the volume is the largest and the smallest gap has higher ligand activity.

| Active center ID | Activity energy | Space size (Å$^3$) | center (x, y, z) | Docking size (x, y, z) |
|---|---|---|---|---|
| **C4** | -7.0 | 4713 | 170, 142, 170 | 33, 26, 29 |
| **C1** | -5.9 | 43985 | 125, 149, 177 | 35, 35, 35 |
| **C2** | -5.7 | 6631 | 138, 138, 90 | 25, 25, 33 |
| **C3** | -5.7 | 5535 | 177, 143, 105 | 35, 35, 34 |
| **C5** | -5.6 | 3293 | 140, 98, 101 | 31, 33, 26 |



2-figure . Results of activity in spaces



C4 C1 C2

C3 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 C4 space:** PHE738 ASN741 VAL742 PHE744 TYR745 TYR772 ALA773 VAL775 PHE776 LEU778 PHE779 ASP781 GLU782 GLN785 LEU797 TRP798 MET801 ASP802 LEU806 PHE809 ILE810 ILE813 LEU841 ARGE842 LEU843 ile844 His845 Ile846 ILE857 LEU860 GLN861 LEU1001 GLU1004 TYR1005 ARG1008 PHE1013

**Chain A for C1 space:** LEU965 SER966 ILE969 LEU970 ASN973 **Chain C:** ILE746 LEU749 LEU750 ALA753 TYR836 THR840 LEU843 **Chain D:** MET801 LEU841 ILE844 ILE857 LEU860 GLN861 VAL867 PHE870 LEU871 PHE874 ALA875 VAL876 MET878 VAL879 GLY882 VAL883 GLN886 TRP896 PHE900 TYR908 MET911 PHE912 VAL972 LEU975 PHE979

**Chain A for C2 space:** PHE1082 LEU1085 ASP1086 LEU1089 LEU1092 LYS1093 LEU1096 Chain B: PHE1082 LEU1085 ASP1086 LEU1089 LEU1092 LYS1093 LEU1096 Chain C: PHE1082 LEU1085 ASP1086 LEU1089 leu1092 LYS1093 LEU1096 chain D: PHE1082 LEU1085 ASP1086 LEU1089 LEU1092 LYS1093 LEU1096

**Chain A for C3 space**:ASN449ASP450 Chain B: ILE146 SER147 VAL148 THR149 GLY150 ALA152 ASN154 PHE155 ALA156 LEU157 LYS158 MET161 ARG162 LYS163 GLY182 THR184 ILE214 ALA215 ALA216 MET219 VAL2220 TYR251 GLY269 HIS270 pro271 Thr272 VAL273 GLU274 Ala275 ARG278 ASN279 GLU282 CYS303 GLN306 GLY307 GLY308 GLU311 THR312 ALA315 THR318 SER332 GLY333 GLN34

**Chain C for C5 space**: ILE146 SER147 VAL148 THR149 GLY150 LYS153 LEU180 THR181 GLY182 GLY183 THR184 ILE214 ALA215 ALA216 MET219 VAL220 TYR251 GLY269 HIS270 PRO271 THR272 VAL273 GLU274 ALA275 ARG278 ASN279 GLU282 cys303 GLU311 THR312 ALA315 THR318

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