



QALAMPIR YALPIZ O'SIMLIGIDAN AJRATIB OLINGAN EFIR MOYI TARKIBIDAGI LIMONENNING PASS ANALIZI VA MOLEKULYAR DOKINGI

Homitova Gulnoza Zaynidin qizi

*Osiyo Xalqaro Universiteti kimyo fani
o'qituvchisi 100000, O'zbekiston Respublikasi,
Buxoro sh., Gijduvan 74. Osiyo Xalqaro
Universiteti*

Annotatsiya: Ushbu maqolada O'zbekiston hududida mahalliy holda o'sadigan Qalampir yalpiz o'simligi tarkibidan ajratib olingan efir moyining asosiy komponentlaridan biri Bo'lgan limonenning zamonaviy kimyoviy kompyuter dasturlari orqali tahlil qilinib, uning farmakologik xususiyatlari baholangan.

Kalit so'zlar: Oqsil, ligand, PASS online dasturi, N-sulfanil-2-indol karboksamid ligandlari, PPAR gamma oqsili (Peroxisome Proliferator-Activated Receptor Gamma), CB-Dock2 online server.

Tadqiqot maqsadi: Qalampir yalpiz o'simligining asosiy tarkibiy qismlaridan biri bo'lgan limonenning PASS onlayn dasturi orqali biologik faolligini, shuningdek limonendan ligand sifatida foydalanib biologik faolligini, glyukoza va lipid metabolizmini tartibga solishda hal qiluvchi rol o'ynaydigan yadro retseptorlaridan biri PPAR oqsiliga nisbatan o'rganish. PPAR gamma oqsili- 2-toifa diabet va boshqa metabolik kasalliklarni davolashda ishlatiladigan dorilar uchun foydalidir.

Tadqiqot materiallari va usullari: Ushbu ishni olib borish uchun kerak bo'lgan modda qalampir yalpiz o'simligidan olingan efir moyining asosiy komponentlaridan biri bo'lgan limonen hisoblanadi. Dastlab limonenning biologik faollogini PASS onlayn dasturi orqali o'rganildi. Shuningdek, limonenning CB-Dock2 onlayn serveri yordamida PPAR gamma oqsili bilan o'zaro ta'siri molekulyar doking usulida o'rganildi [1].

Tadqiqot natijalari: Mentonning biologik faolligini PASS – kompyuter dasturi yordamida bashorat qilindi. Bu dastur PASS (Prediction Activity Structure Substances – Moddalarning tuzilishiga asosan faolligini bashorat qilish) Rossiyalik olimlar V.V. Poroikov hamda D.A. Filimonovlar tomonidan yaratilgan [6].PASS dasturi orqali limonenning tadqiq qilish natijalari kuzatilganda 96,1 % da karminativ yani organizmda ortiqcha gaz hosil bo'lishiga qarshi , 93,4 % natija bilan retinol degidrogenaza ingibitori sifatida, 89,6 % antienzematik xossalarini ko'rishimiz mumkin. .

Limonen yuqori darajada kapilyar devorlarini mustahkamlovchi, antienzematik, yallig'lanishga qarshi faollikni namoyon qilishi aniqlandi, tahlil natijalari 1-jadvalda keltirilgan.



All Pa>Pi Pa>0,3 Pa>0,7

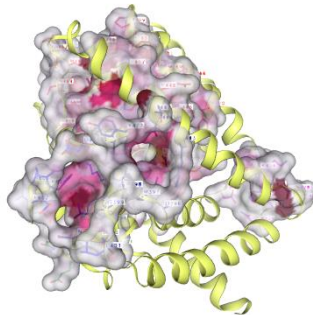
0,961	0,001	Carminative	Ovqat hazm qilish traktidagi gazni yumshatish
0,934	0,000	Retinol dehydrogenase inhibitor	Retinol degidrogenaza ingibitori
0,896	0,005	Antieczematic	Antienzematik
0,881	0,001	Alpha-pinene-oxide decyclase inhibitor	Alfa-pinen-oksidi detsiklaza ingibitori
0,816	0,007	Apoptosis agonist	Apoptoz Agonisti
0,812	0,010	Antineoplastic	Antineoplastik
0,799	0,010	CYP2C substrate	CYP2C substrat

Ushbu ishni olib borish uchun kerak bo'lgan qalampir yalpiz o'simligi yer ustki qismi xomshyolari Buxoro viloyati Romitan tuman hududidan yig'ib olindi. Xomshyoni quritish xona haroratida soya joyda olib borildi [1,2] O'simlik xomshyosidan efir moyini ajratish ananaviy gidrodistillash usulida olib borildi. Ajratib olingan efir moyi tarkibida 10 dan ziyod alohida komponentlar bo'lib ulardan biri limonen [3]. Biz olingan limonenni, yadro retseptorlaridan biri PPAR oqsili bilan CB-Dock2 onlayn serveri yordamida o'zaro ta'sirini o'rgandik [4,5].

CB-Dock2 onlayn serveri yordamida dastlab oqsilning ligand bilan ta'sirlashish bo'shliqlari izlandi, bunda 43985,6631, 5535, 4713 va 3293 Å³ hajmdagi 5 ta faol bo'shliq markazi aniqlandi (1-rasm). So'ng ligand va oqsil serverga yuklanib, molekulyar dokingi amalga oshirildi.[7]

1-rasm

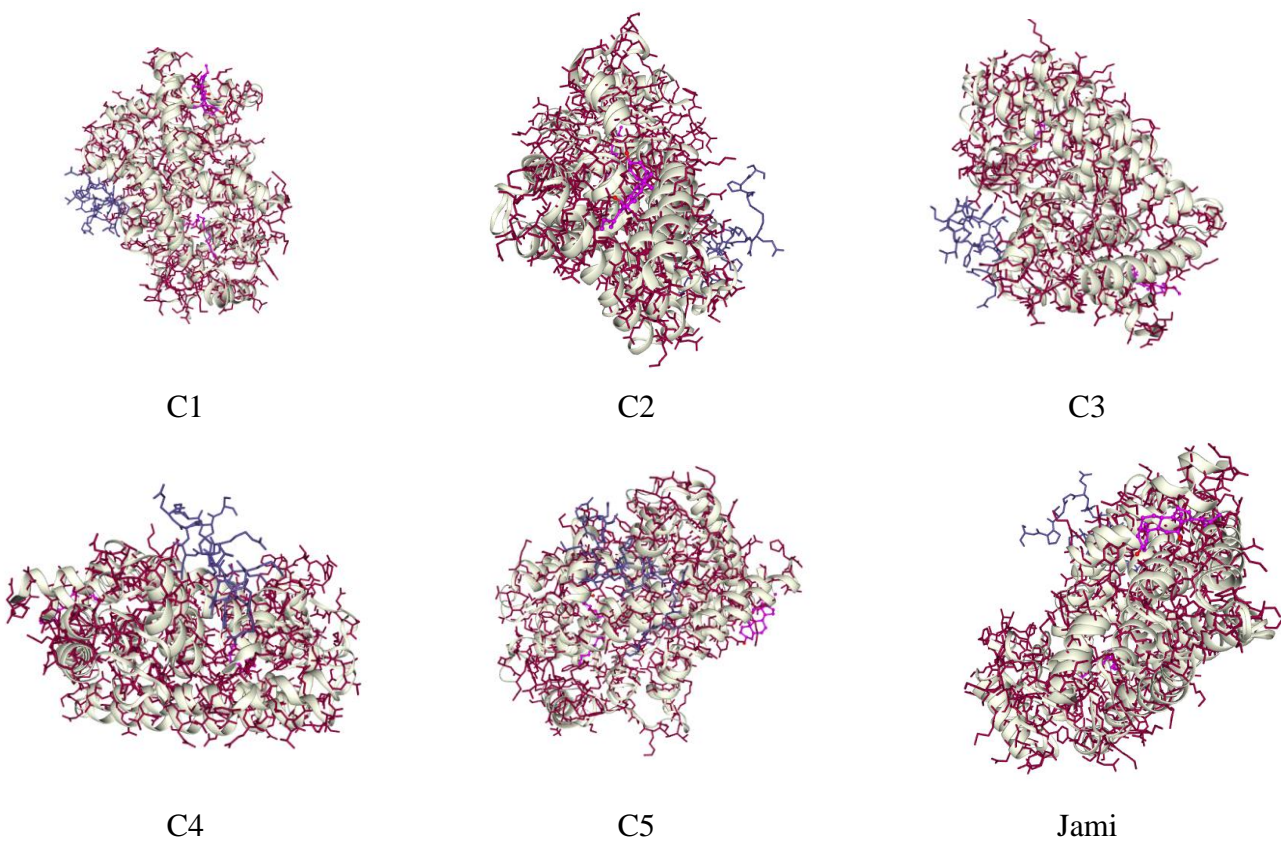
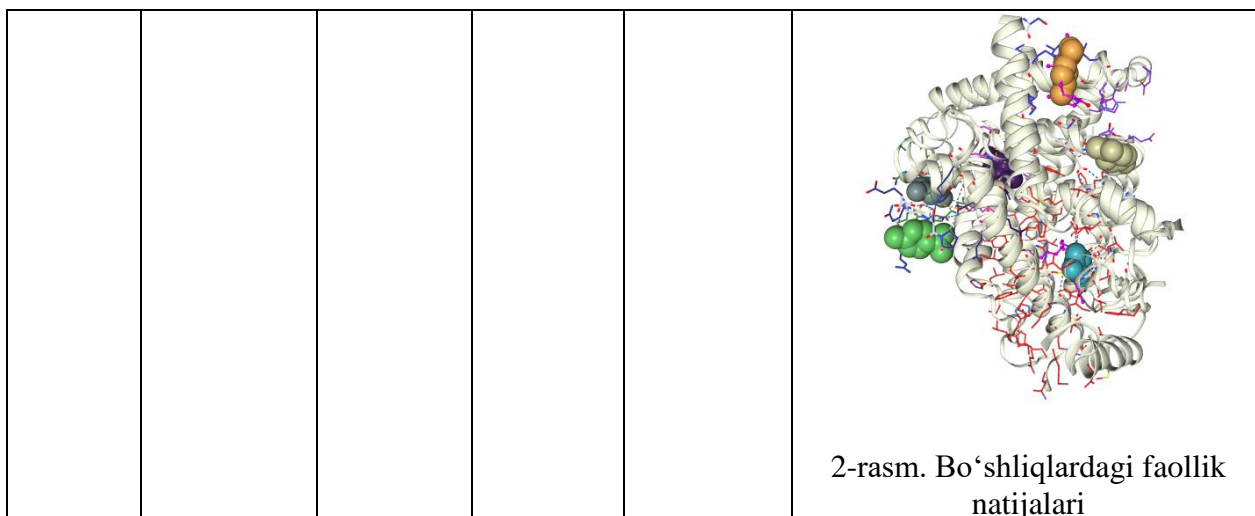
Faol markaz ID	Bo'shliq hajmi (Å ³)	Markaz (x, y, z)	Bo'shliq hajmi (x, y, z)
C1	6138	24, -10, 2	24, 29, 26
C2	285	15, 15, -5	11, 7, 6
C3	176	17, 1, 29	10, 7, 4
C4	160	6, -2, -1	9, 8, 11
C5	156	23, 13, 4	6, 8, 6



1-rasm. Bo'shliqlarni qidirish natijalari

Oqsil va ligandning o'zaro ta'siridan yuqoridagi keltirilgan bo'shliqlarga mos ravishda -3.3, -5.0; -4.6 -4.2 va -4.1 kcal/mol energiyaga ega faollik kuzatildi (2-rasm). Natijalar shuni ko'rsatadiki hajmi eng katta va eng kichik bo'shliqda ligandning faolligi yuqori bo'ladi.

Faol markaz ID	Faollik energiyasi	Bo'shliq hajmi (Å ³)	Markaz (x, y, z)	Docking hajmi (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



3-rasm. Oqsilning izlangan bo'shliqlariga ligandning o'zaro ta'siri

Yuqorida ta'kidlangan oqsil tarkibidagi 5 ta bo'shliq uchun quyidagi tartibda aminokislotalar qatori faol markaz namoyon etishi aniqlandi:

C1 bo'shliq uchun Chain A: ILE281 CYS285 ARG288 LEU330 LEU333 VAL339 LEU340 ILE341 SER342 MET348 LEU353 MET364

C2 bo'shliq uchun Chain A: LYS319 TYR320 GLY321 HIS323 GLU324 ASP396 ARG397 PRO398 ARG443 GLN444 VAL446 THR447 LEU476 TYR477



C3 bo'shliq uchun Chain A: ASN312 ASP313 VAL315 THR316 LYS319 TYR320 PRO398 GLY399 LEU401 ASP475 **Chain B:** GLU602 ARG603 HIS604

C4 bo'shliq uchun Chain A: ASN312 ASP313 VAL315 THR316 LYS319 TYR320 PRO398 GLY399 LEU401 ASP475 **Chain B:** GLU602 ARG603 HIS604

C5 bo'shliq uchun Chain A: TYR219 LYS230 ALA231 ARG234 VAL372 ASN375 ALA376 LEU377 GLU378 LEU379 ASP380 ASP381 SER382 HIS425 GLU427 SER428 LEU431 LYS434

FOYDALANILGAN ADABIYOTLAR

1. Avezov H. T., Homitova G. Z. Efir moylarining tavsifi, ularning ananaviy olinish usullari //Новости образования: исследование в XXI веке. – 2023. – Т. 2. – №. 15. – С. 800-814
2. Homitova, G. (2023). QALAMPIR YALPIZ (MENTHA PIPERITA.L) ASOSIY KOMPONENTI SIFATIDA MENTOLNI ANIQLASH USULLARI. *Interpretation and Researches*, 1(19). <https://interpretationandresearches.uz/index.php/iar/article/view/1566>
3. K.V. peter Handbook of herbs and spices. Volume 1 Woodhead Publishing Limited- 2012.-C-408
4. Morris G. M., Lim-Wilby M. Molecular docking //Molecular modeling of proteins. – 2008. – C. 365-382.
5. Liu, Yang, et al. "CB-Dock2: Improved protein–ligand blind docking by integrating cavity detection, docking and homologous template fitting." *Nucleic acids research* 50. W1 (2022): W159-W164.
6. Filimonov D. A. et al. Prediction of the biological activity spectra of organic compounds using the PASS online web resource //Chemistry of Heterocyclic Compounds. – 2014. – Т. 50. – С. 444-457
7. Zainidinovna, H. G. (2024). Pass Analysis and Molecular Docking of Menton in Essential Oil Extracted From the Pepper Mint Plant. *Innovative: International Multidisciplinary Journal of Applied Technology* (2995-486X), 2(9), 249-252.