TA'LIM VA RIVOJLANISH TAHLILI ONLAYN ILMIY JURNALI

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MENTHA PIPERITA.L O‘SIMLIGIDAN AJRATIB OLINGAN EFIR MOYI TARKIBIDAGI PULEGONNING PASS ANALIZI VA MOLEKULYAR DOKINGI

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Annotatsiya: *Ushbu maqolada O‘zbekiston hududida mahalliy holda o‘sadigan Qalampir yalpiz (Mentha piperita.L) o‘simligi tarkibidan ajratib olingan efir moyining asosiy komponentlaridan biri Bo‘lgan pulegonning zamonaviy kimyoviy kompyuter dasturlari orqali tahlil qilinib, uning farmakologik xususiyatlari baholangan.*

Kalit so’zlar: *Oqsil, ligand, PASS online dasturi, CYP2E1 fermenti, Pulegon, CB-Dock2 online server.*

Tadqiqot maqsadi: Qalampir yalpiz o’simligining asosiy tarkibiy qismlaridan biri bo’lgan pulegonning PASS onlayn dasturi orqali biologik faolligini, shuningdek pulegondan ligand sifatida foydalanib biologik faolligini, metabolizmga uchratadigan fermentlar, masalan, jigarda joylashgan sitokrom P450 oilasi fermentlari (ayniqsa, CYP2E1) bilan yaxshi o‘zaro ta’sir qiladi. Bu fermentlar pulegonni toksik metabolitlar (masalan, mentofuran) ga aylantiradi.

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 pulegon hisoblanadi. Dastlab pulegonni biologik faollogini PASS onlayn dasturi orqali o‘rganildi. Shuningdek, pulegonning CB-Dock2 onlayn serveri yordamida CYP2E1 fermenti 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 pulegonning tadqiq qilish natijalari kuzatilganda 93.7 % da karminativ yani organizmda ortiqcha gaz hosil bo’lishiga qarshi , 88.6 % antienzimatik, 84.2% testosteron 17 betta-degidrogenaza –NADP+ ingibitori xossalarini ko’rishimiz mumkin.

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

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

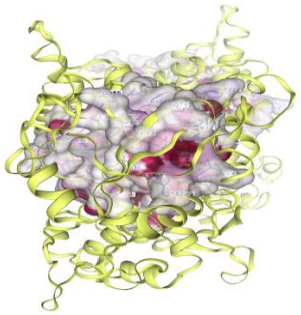
0,937	0,001	Carminative	Karminativ
0,886	0,006	Antieczematic	Antienzimatik
0,842	0,016	Testosterone 17beta-dehydrogenase (NADP+) inhibitor	NADP+ ingibitori
0,833	0,022	Ubiquinol-cytochrome-c reductase inhibitor	Ubixinon sytoxrom-c ingibitori
0,792	0,005	Pterin deaminase inhibitor	Pterin deaminaza inhibitori
0,801	0,021	CYP2J substrate	CYP2J substrati
0,782	0,003	Mannan endo-1,4-beta-mannosidase inhibitor	Mannan endo-1,4-beta-mannosidaza inhibitori
0,783	0,022	Antiseborrheic	Antiseboreik

Ushbu ishni olib borish uchun kerak bo‘lgan qalampir yalpiz o‘simligi yer ustki qismi xomshyolari Buxoro viloyati Romitan tuman hududidan yig’ib olingan. Xomashyoni quritish xona haroratida soya joyda olib borildi [1,2] O‘simlik xomashyosidan efir moyini ajratish ananaviy gidrodistillash usulida olib borildi.Ajratib olingan efir moyi tarkibida 10 dan ziyod alohida komponentlar bo’lib ulardan biri pulegon [3]. Biz olingan pulegonni CYP2E1 fermenti 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 2194,1963,1853,1115,1098 $Å^3$ hajmdagi 5 ta faol bo‘shliq markazi aniqlandi (1-rasm). So‘ng ligand va oqsil serverga yuklanib, molekulyar dokingi amalga oshirildi.

1-rasm

Faol markaz ID	Bo’shliq hajmi ($Å^3$)	Markaz (x, y, z)	Bo’shliq hajmi (x, y, z)
C1	2194	57, 35, 14	25, 16, 12
C2	1963	37, 30, 6	18, 18, 17
C3	1853	5, 0, 39	18, 22, 17
C4	1115	36, 50, 7	22, 11, 20
C5	1098	1, -16, 33	15, 15, 9



1-rasm. Bo‘shliqlarni qidirish natijalari

Oqsil va ligandning o‘zaro ta’siridan yuqoridagi keltirilgan bo‘shliqlarga mos ravishda -6,2, -6,1; -5,8 -5,6 va -5,3 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.

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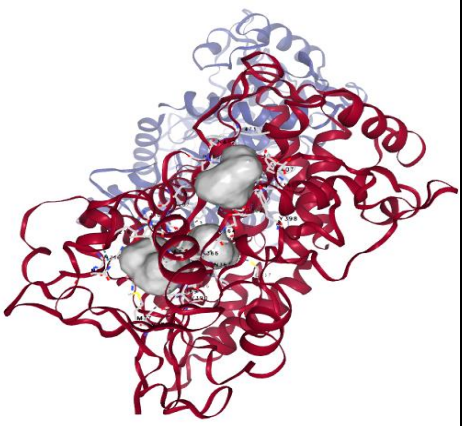
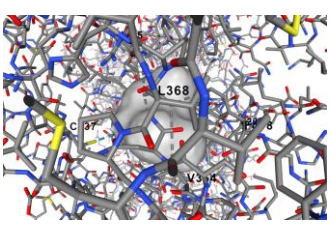
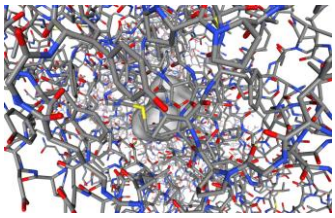
Faol markaz ID	Faollik energiyasi	Bo'shliq hajmi (Å^3)	Markaz (x, y, z)	Docking hajmi (x, y, z)
C2	-6.2	1963	37, 30, 6	23, 23, 17
C3	-6.1	1853	5, 0, 39	23, 27, 17
C5	-5.8	1098	1, -16, 33	17, 17, 17
C1	-5.6	2194	57, 35, 14	30, 17, 17
C4	-5.3	1115	36, 50, 7	27, 17, 25



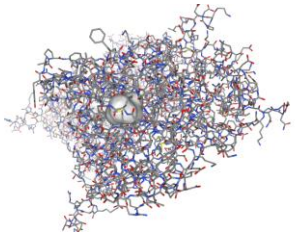
2-rasm. Bo‘shliqlardagi faollik natijalari



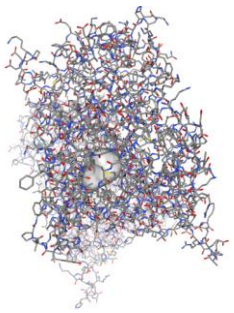
C2



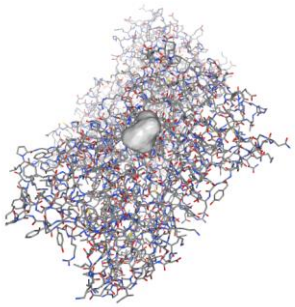
C3



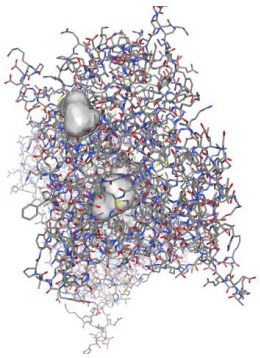
C5



C1



C4



Jami

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:

C2 bo‘shliq uchun Chain A: ARG100 ILE114 ILE115 PHE116 ARG126 PHE207 ASP295 LEU296 PHE298 ALA299 GLU302 THR303 THR304 THR307 GLN358 ILE361 LEU363 VAL364 ASN367 LEU368 LEU393 PRO429 PHE430 SER431 ARG435 VAL436 CYS437 ALA438 GLY439 ALA443 LEU447 PHE478

C3 bo‘shliq uchun Chain B: ARG100 ILE114 ILE115 PHE116 ARG126 PHE207 ASP295 LEU296 PHE298 ALA299 GLU302 THR303 VAL364 ASN367 LEU368 LEU393 PRO429 PHE430 SER431 ARG435 VAL436 CYS437 ALA438 GLY439 PHE478

C5 bo‘shliq uchun Chain B: LEU48 ILE53 PRO54 PHE57 LEU70 VAL72 GLN75 MET77 GLY101 ASP102 LEU103 PRO104 LEU210 GLN216 ASN219 ASN220 PRO222 SER366 ASN367 LEU368 PRO369 GLU371 GLY386 VAL388 VAL390 GLY477 PHE478

C1 Bo‘shliq uchun Chain A: LEU48 ILE53 PHE57 LEU70 VAL72 MET77 ASP102 LEU103 LEU210 GLN216 ASN219 ASN220 SER366 ASN367 LEU368 PRO369 VAL388 VAL390 GLY477 PHE478

C4 bo‘shliq uchun Chain A: ASN52 PRO54 LYS55 THR58 TYR310 PHE360 ILE361 THR362 PRO365 ASP394 SER395 TYR398 GLU407 LEU471 SER472 PRO473 ILE476 CYS480

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