TA'LIM VA RIVOJLANISH TAHLILI ONLAYN ILMIY JURNALI

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# N-ASETYLPROKAINAMID (4-ASETAMIDO-N-(2-(DIETYLAMINO) ETYL) BENZAMID) NING GEM OQSILI BILAN MALEKULAR DOCKINGI

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***Annotatsiya:*** *Ushbu maqolada tibbiyotda membranani barqarorlashtiruvchi faollikka ega bo'lgan, natriy ionlarining kiruvchi tez oqimini ingibit qiladigan, 0 fazada depolarizatsiya tezligini pasaytiradigan atriyal va qorincha miokardining qo'zg'aluvchanligini pasaytirish, shuningdek ta'sir potentsialining samarali refrakter davrining davomiyligini oshiradigan eng mashhur savdo nomi "Prokainamid" ning asosiy tarkibiy qismi bo'lgan N-asetylprokainamidning zamonaviy kimyoviy kompyuter dasturlari orqali tahlil qilinib, uning farmakologik xususiyatlari baholangan.*

***Kalit so'zlar:*** *Oqsil, ligand, GEM, N-asetylprokainamid CB-Dock2 online server*

**Tadqiqot maqsadi**: N-asetylprokainamiddan ligand sifatida foydalanib GEM oqsiliga nisbatan biologik faolligini o‘rganish. Membranani barqarorlashtiruvchi faollikka ega bo'lgan, natriy ionlarining kiruvchi tez oqimini ingibit qiladigan, 0 fazada depolarizatsiya tezligini pasaytish xususiyatiga ega bo'lgan N-atsetilprokainamid Gem oqsili bilan o'zaro tasiri juda barqaror ekanligidan foydalanib uni o'za munosabatini o'rganish.

Tadqiqot materiallari va usullari: Ushbu ishni olib borish uchun kerak bo‘lgan modda N-prokainamid hisoblanadi. CB-Dock2 onlayn serveri yordamida GEM oqsili bilan o‘zaro ta’siri molekulyar doking usulida o‘rganildi.

**Tadqiqot natijalari:**

N-Prokainamid - 4-asetamido-N-(2-(dietylamino)etyl)benzamid- dan foydalangan holda GEM oqsili bilan o‘zaro ta’sirini CB-Dock2 onlayn serveri yordamida o‘zaro ta’sirini o‘rgandik [4,5,7].

CB-Dock2 onlayn serveri yordamida dastlab oqsilning ligand bilan ta’sirlashish bo‘shliqlari izlandi, bunda 1134,714,167,117 va 110 Å hajmdagi 5 ta faol bo‘shliq markazi aniqlandi (1-rasm). So‘ng ligand va oqsil serverga yuklanib, molekulyar dokingi amalga oshirildi.

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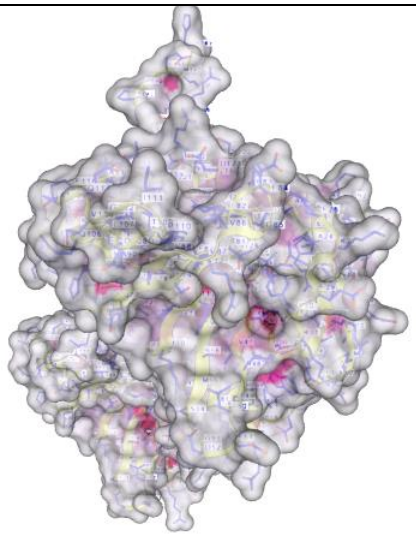
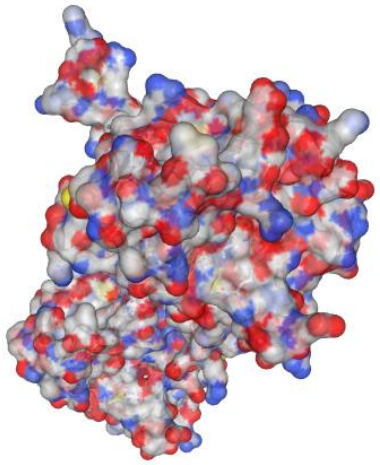
| Faol markaz ID | Bo'shliq hajmi (Å$^3$) | Markaz (x, y, z) | Bo'shliq hajmi (x, y, z) |
|---|---|---|---|
| C1 | 1134 | 24, 212, 136 | 16, 19, 9 |
| C2 | 714 | 7, 200, 102 | 16, 10, 16 |
| C3 | 167 | -2, 177, 85 | 9, 7, 9 |
| C4 | 117 | -10, 183, 86 | 5, 12, 11 |
| C5 | 110 | 29, 216, 118 | 7, 6, 7 |



1-rasm. Bo‘shliqlarni qidirish natijalari

Oqsil va ligandning o‘zaro ta’siridan yuqoridagi keltirilgan bo‘shliqlarga mos ravishda -5.6 , -5.5; -5.3; -5.0 va -4.7 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) |
|---|---|---|---|---|
| C2 | -5.6 | 714 | 7, 200, 102 | 23, 23, 23 |
| C5 | -5.5 | 110 | 29, 216, 118 | 23, 23, 23 |
| C3 | -5.3 | 167 | -2, 177, 85 | 23, 23, 23 |
| C1 | -5.0 | 1134 | 24, 212, 136 | 23, 23, 23 |
| C4 | -4.7 | 117 | -10, 183, 86 | 23, 23, 23 |



2-rasm. Bo‘shliqlardagi faollik natijalari

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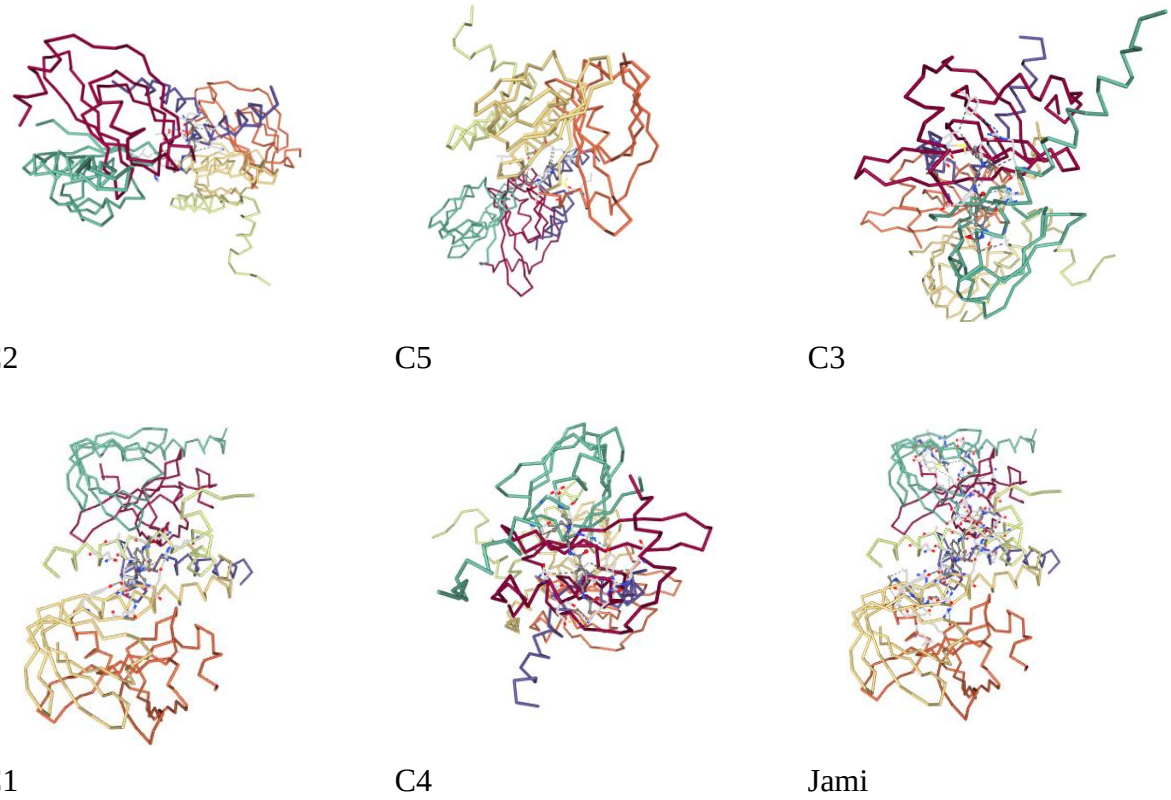


**3-rasm. Oqsilning izlangan bo‘shliqlariga ligandning o‘zaro ta’siri**

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**: ALA24 SER25 GLU26 LYS27 ASN28 GLN66 **ChainB**:HIS83 GLU84 GLY85 ARG87 ILE125 **Chain F**: GLU195 GLN198 ALA199 MET201 LYS202 ARG203 GLY206 ASP207 SER208 ALA209 ALA210 LYS211 GLN213 ALA214 ALA217

**C5 bo‘shliq uchun Chain C**: GLN13 ILE16 TYR17 LEU35 HIS76 ARG79 GLU80 LYS81 LEU82 MET83 HIS84 LEU85 PHE86 **Chain D**: ARG57 ALA60 ALA61 GLU64 ARG65 ARG68 SER69 LEU71 ALA72 MET73 VAL74 **Chain E**: LYS211 SER222

**C3 bo‘shliq uchun Chain A**: GLN13 ASP14 TYR15 ILE16 TYR17 LYS18 LEU35 HIS76 ARG79 GLU80 LEU82 MET83 HIS84 LEU85 PHE86 **Chain B**: ARG57 ALA60 ALA61 GLU64 ARG65 ARG68 LEU71 ALA72

**C1 bo‘shliq Chain C**: MET5 LYS6 LYS7 GLY8 PRO9 TRP12 PRO39 VAL40 SER41 ALA42 ASN43 MET61 GLY62 HIS63 **Chain D**: ARG59 THR95 ASP96 LEU97 ASP98 VAL99 ALA100 ASN101 TYR103 CYS121 **Chain E**: ARG196 ARG197 GLU200 MET201 ARG203 LEU204 GLN213 GLU216 ALA217 GLN220

**C4 bo‘shliq uchun Chain A**: LEU10 GLN13 ASP14 TYR15 ILE16 TYR17 LYS18 GLU73 GLY74 HIS76 ARG79 GLU80 MET83 **Chain B**: ALA61 LEU62 GLU64 ARG65 ARG68

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