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Nitroreductase of the Nitrofural Molecule Molecular Docking with an Enzyme

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Abstract:

In this article, pharmaceuticals with the help of modern information resources protein of the nitrofural molecule contained in furatsilin drug, which is important for industry effect with natural enzymes was considered.

Keywords: Nitrofural molecule, CB-Dock2 online server, NAD(P)H- nitroreductase enzyme, ligand activity, heads.

Introduction: Furatsilin, which is one of the drugs needed to carry out this work Antimicrobial agent, gram-positive and gram-negative bacteria (including Staphylococcus spp. Activity against Streptacocus spp., Escherichia coli Clostridiiumperfringes) has been determined. Other has a different mechanism of action compared to chemotherapeutic agents: microbial flavoproteins - restores the nitro group, the resulting reactive amino derivatives, including those of higher proteins to cell death by changing the conformation of ribosomes and other molecules brings. We take into account that nitrofural, which is the main chemical composition of furatsilin interaction of the molecule with NAD(P)H-nitroreductase enzyme using CB-Dock2 online server we studied its effect [1,2].Using the CB-Dock2 online server, the binding sites of the protein with the ligand were first searched, where 787, 786, 767, 763 and 650 Å3 5 centers of active voids in the volume were determined (Fig. 1). After ligand and protein were uploaded to the server and molecular docking was performed.

An active center ID	Space volume (Å3)	Center (x, y, z)	Space size
C1	787	83, 41, 171	13, 15, 10
C2	786	27, 7, 163	15, 24, 22
C3	767	49, 45, 157	17, 12, 9
C4	763	63, 34, 166	15, 12, 21
C5	650	94, 60, 166	13, 14, 8

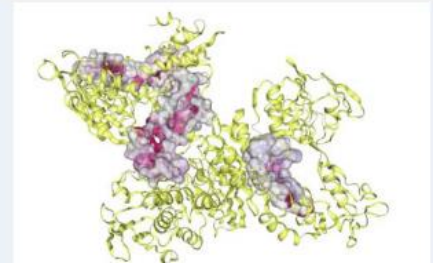

Figure 1. Search results for spaces

5.1, -4.8, respectively, to the above-mentioned spaces from the interaction of protein and ligand; -4.7;Activity with energies of -4.4 and -4.0 kcal/mol was observed (Figure 2). The results show that the size of the the activity of the ligand is high in the largest and smallest space.

Active center	*Activity Energy*	*Space volume*	*Center (x, y, z)*	*Docking volume (x, y z)*
C1	-5.1	787	83, 41, 171	16, 16, 16
C3	-4.8	767	49, 45, 157	22, 16, 16
C4	-4.7	763	63, 34, 166	16,16.26
C5	-4,4	650	94,60,166	16,16,16
C2	-4,0	786	27,7,163	16,29,27

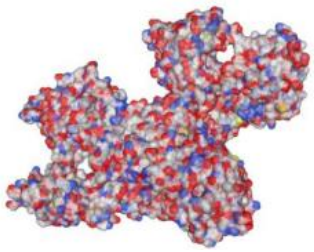

Figure 2. Search results for spaces

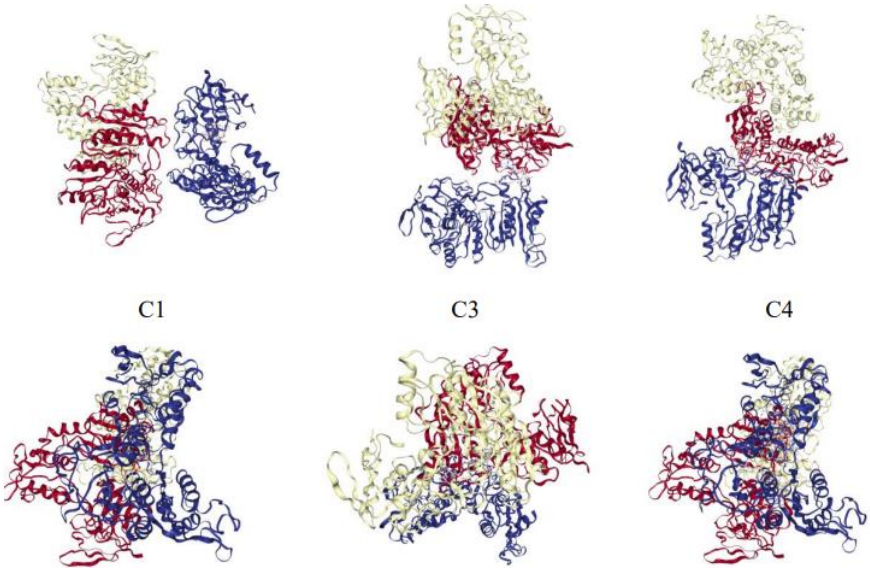

Figure 3. The interaction of the ligand with the desired spaces of the protein

Amino acids in the following order for the 5 spaces in the enzyme NAD(P)H- nitroreductase It was found that the active center exhibits:

Chain C for space C1: : ILE9 GLY10 GLY12 ALA13 ALA14 GLY15 PHE34 GLU35 ALA36 ALA80 GLU81 VAL82 ALA109 ASN110 GLY111 ALA112 SER113 ASN245 LEU248 ALA278 GLY279 ASP280 VAL281 PRO296 LEU297 ALA298 GLY301 ASN302

Chain B for space C2: TYR158 ARG186 SER187 HIS286 THR289 VAL293 TRP294

VAL295 PRO296 LEU297 LEU323 GLY324 THR325 ALA326 LYS337 GLY339 LEU340 GLU344 GLU348

Chain A for space C3: TRP263 ASN265 GLU266 LYS267 GLN269 ARG285 THR289

GLY290 ARG291 ARG292 GLU316 HIS318

Chain C: ILE288 THR289 ARG291 GLU348 GLY349 TYR350 ASP351 ASP379 GLU381

Chain A for space C4*:* ILE288 THR289 GLU348 GLY349 TYR350 ASP351 ASP379 ASN380 GLU381 THR382

Chain C: TRP263 ASN265 GLU266 LYS267 GLN269 ARG285 THR289 GLY290 ARG291 ARG292 GLU316 HIS318

Chain C for space C5: PHE128 THR129 ALA130 ASP131 LEU132 ASP135 ALA136 ILE139 ARG140 MET143 GLU144 LYS145 VAL148 MET163 ALA166 PHE167 GLN170 LYS172 ILE237

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