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Research Article

A study on the interaction and inhibition effect of some natural compound ligands with the 5p21 cancer receptor

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Abstract – Some spices that we consume with foods in daily life add taste and aroma to meals eaten. These spices are also very important for health. In this study, the interaction of the compounds (Carvacrol,Capsaicin,Curcumin), the main active ingredients in some spices, consumed very frequently in some societies, with 5p21, an important cancer receptor, has been determined by the chemical calculation method, and the interaction points and possible bonds that could be formed at the molecular level has been investigated to elucidate the mechanism.

Keywords – 5p21, Carvacrol,Capsaicin,Curcumin and Docetaxel

Introduction

The PDB ID of the target protein anti-cancer and oncogene protein downloaded from the Protein Data Bank (PDB) is 5P21 (1, 2). Black Pepper (Piperine) suppresses cell growth and proliferation and Carvacrol in thyme may induce apoptosis (3). Capsaicin, a bioactive phytocompound found in red hot peppers, inhibits the proliferation of various cancerous cells (4). In this study, the interaction and inhibition effects of the main important compounds in some spices that we use in daily food consumption with the 5P21 oncogene receptor as ligands were investigated by chemical calculation method.

Materials and Method

In this study, docking (5-8), a chemical calculation method that gives results very close to experimental data and allows us to detect interactions and interaction points at the molecular level, whose accuracy and

reliability have been confirmed by different studies, was used in the determination of effective ligand compounds for the 5p21 cancer receptor.

Results and Discussions

The docking scores and Ki related to the interaction of some active ingredients in spice as ligands, for inhibiting 5p21 oncogene receptor are given in Table 1 (5-8).

Table 1. The interaction of important active substances as ligands with 5p21 oncogene receptor

Docking scores of Ligands / Reseptör (5p21**)**	**Free Energy of Binding (kcal/mol)**	**Inhibition Constant, Ki**
Carvacrol	-4.61	419.67 mM
Capsaicin	-5.80	56.15 uM
Curcumin	-6.64	13.56 uM
Docetaxel	-8.85	328.16 nM

In Table 1, the interactions of the ligands determined according to docking scores and Ki values with 5p21 receptor are listed from largest to smallest; Docetaxel > Curcumin > Capsaicin > Carvacrol. Docetaxel (DTX) is one of the most important drugs of the drug group called taxoids used in cancer treatment. (9). As an effective ligand, the intermolecular bonds formed as a result of the interaction of Curcumin with 5p21 oncogene reseptör are given in Table 2 (5-8).

Table 2. Curcumin, as an effective ligand, intermolecular bonds and energy values (kcal/mol) formed as a result of its interaction with 5p21 oncogene receptor

hydrogen bonds	**polar**	**Hydrophobic**	**other**
THR35 (-0.4756)	SER17 (-0.8447)	PRO34 (-1.6543)	LYS147 (-0.8592)
	ASP119 (-0.3891)	TYR32 (-1.2824)	ASP30 (-0.8222)
	LYS16 (-0.383)	PHE28 (1.0843)	LYS117 (-0.7794)
			LEU120 (-0.3297)

As an effective ligand, the hydrogen bond formed by the interaction of Curcumin with 5p21 oncogene receptor is given in Figure 1 (5-8).

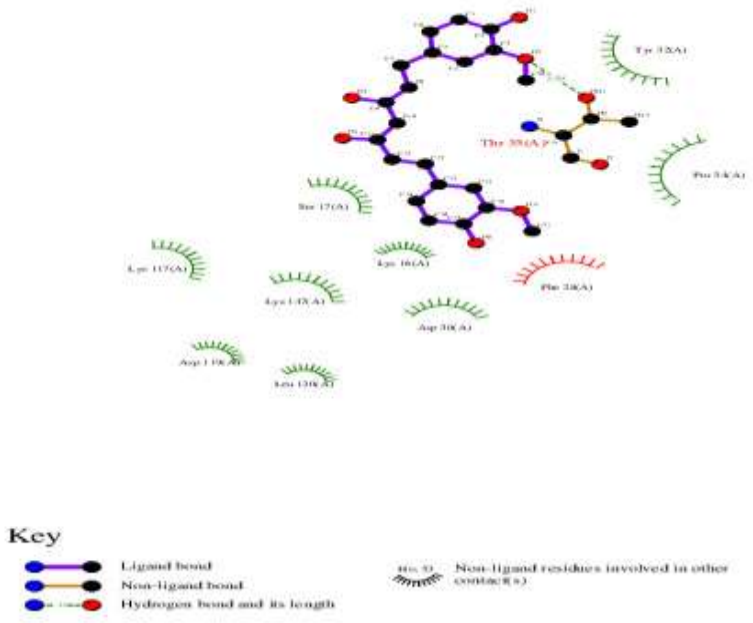

Figure 1. The hydrogen bond formation of Curcumin with 5p21 oncogene receptor

The intermolecular bonds formed as a result of the interaction of Curcumin with 5p21 oncogene receptor are given in Table 3 (5-8).

Table 3. The intermolecular bonds formed as a result of the interaction of Curcumin with 5p21 oncogene receptor

hydrogen bonds	polar	hydrophobic	other
THR35 (-0.4756)	SER17 (-0.8447)	PRO34 (-1.6543)	LYS147 (-0.8592)
	ASP119 (-0.3891)	TYR32 (-1.2824)	ASP30 (-0.8222)
	LYS16 (-0.383)	PHE28 (1.0843)	LYS117 (-0.7794)
			LEU120 (-0.3297)

As an effective ligand, Curcumin 's interaction points with 5p21 oncogene receptor are given in Figure 2 (5-8).

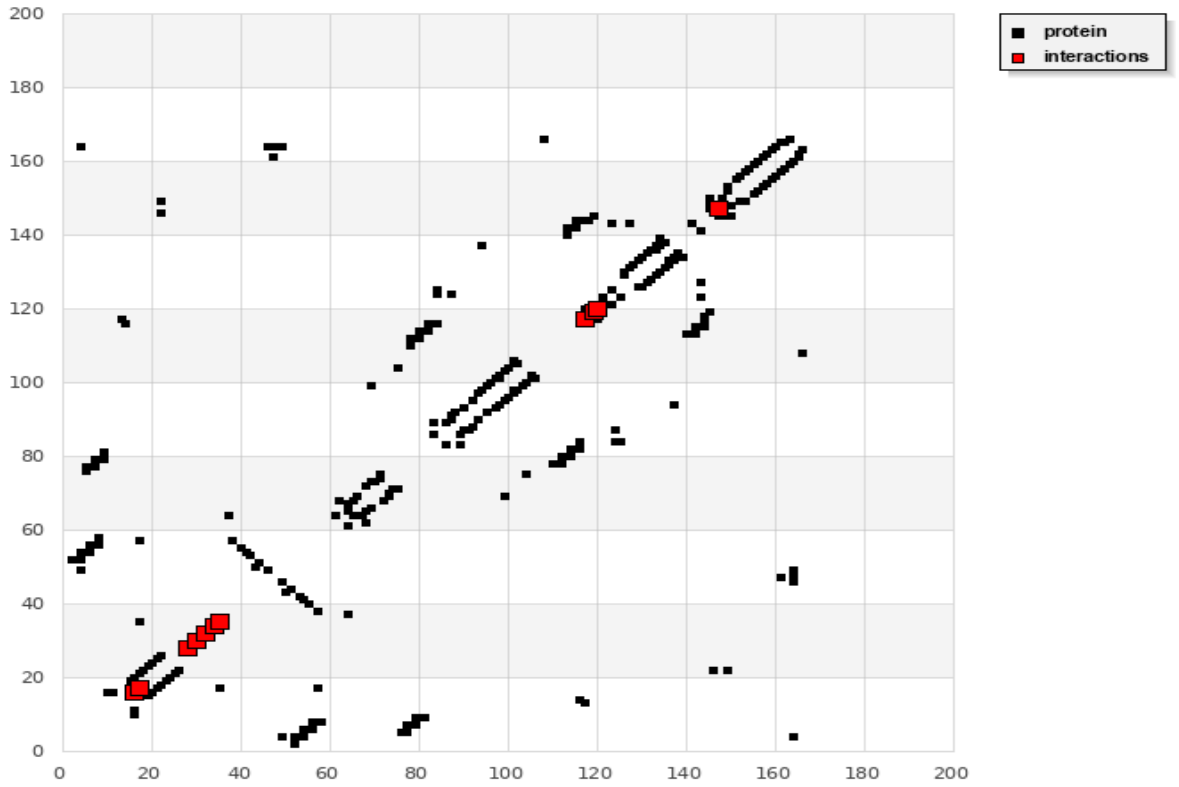

Figure 2. Curcumin 's interaction points with 5p21 oncogene receptor

In Figure 2, Curcumin 's interaction points with 5p21 oncogene receptor effective ligand 16: LYS17: SER28: PHE30: ASP32: TYR34: PRO35: THR117: LYS119: ASP120: LEU147: LYS.

As an effective drug ligand, the intermolecular bonds formed as a result of the interaction of Docetaxel with 5p21 oncogene receptor are given in Table 4.

Table 4. The effective drug ligand, the intermolecular bonds formed as a result of the interaction of Docetaxel with 5p21 oncogene receptor

Polar	**hydrophobic**	**other**
LYS117 (-1.2968)	TYR32 (-2.3564)	LYS16 (-0.7621)
ASP30 (0.3558)	PRO34 (-1.0877)	THR35 (-0.7163)
	PHE28 (-0.8819)	SER17 (-0.4307)
	ALA18 (-0.3528)	

As an effective drug ligand, Docetaxel 's interaction points with 5p21 oncogene receptor are given in Figure 3 (5-8).

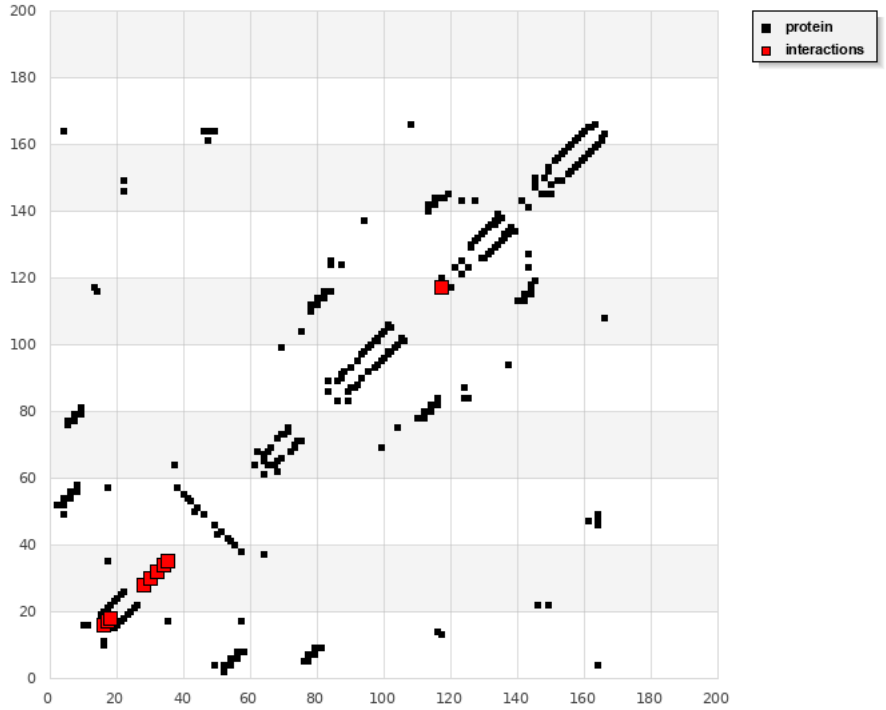

Figure 3. The effective drug ligand, Docetaxel 's interaction points with 5p21 oncogene receptor

In Figure 3, Docetaxel's interaction points with 5p21 oncogene receptor effective ligand 16: LYS17: SER18: ALA28: PHE30: ASP32: TYR34: PRO35: THR117: LYS.

In the discovery of a new drug, it is important to understand the mechanism of the effect of the determined active ingredients on 5p21 target molecule receptors to determine the bonds that may form at the molecular level and the interaction points, as confirmed by similar studies (10-15).

Conclusion

The selected molecules (Carvacrol,Capsaicin,Curcumin and Docetaxel) have a significant effect on inhibiting the 5p21 oncogene cancer receptor and gave results very close to the drug active ingredient in terms of interaction. Considering the intermolecular bonds and interaction points, it can be concluded that the selected ligands are highly effective against the cancer receptor oncogene protein. The data obtained here are original in terms of preventing waste of time and materials, and are also important in guiding experimental and clinical studies.

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