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Research Article

Molecular docking data of piperine with Bax, Caspase 3, Cox 2 and Caspase 9

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Abstract:
Several apoptotic signalling proteins such as Bax, Caspase 3, Cox 2 and Caspase 9 are known to be associated with colorectal cancer (CRC). It is of interest to study the interaction of these proteins with piperine a known drug candidate. We document the binding energy, hydrogen bond interaction and hydrophobic interaction between the piperine and apoptotic proteins for further consideration.

Keywords: Piperine, molecular docking, Bax, Caspase 3, Cox 2 and Caspase 9

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Background:
Apoptosis (programmed cell death) and its associated signalling proteins are linked to drug discovery in cancer **[1-3]**. Several apoptotic signalling proteins such as Bax **[4]**, Caspase 3 **[5],** Cox 2 **[6]** and Caspase 9 **[7]** are known to be associated with colorectal cancer (CRC). It is of interest to study the interaction of these proteins with piperine a known drug candidate **[8].**

Methodology:
Preparation of receptors structures for docking:
The data for 3D structures of proteins **[9]** for BAX (PDB ID: 4S0O), caspase-3 (PDB ID: 5I9B), cox-2 (PDB ID: 1CX2), caspase-9 (PDB ID: 2AR9) were used in this study.

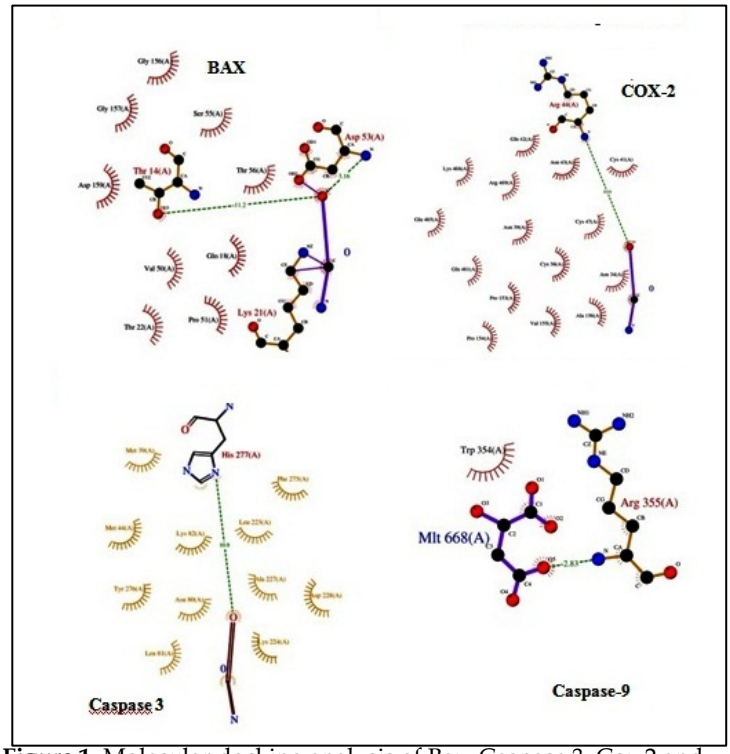

Figure 1: Molecular docking analysis of Bax, Caspase 3, Cox 2 and Caspase 9 with piperine is shown.

Ligand preparation:
Data for piperine was downloded from the pubchem database in SDF format and it was transformed as PDB file format using the Online Smile Translator. Energy minimizations of ligands were completed using the ChemBio 3D Ultra 12.0 using standard protocols.

Molecular docking:
Molecular docking of piperine with Bax, Caspase 3, Cox 2 and Caspase 9 was completed using PatchDock **[10,11]** using standard procedures. The interaction between piperine and Bax, Caspase 3, Cox 2 and Caspase 9 was analyzed using Ligplot (https://www.ebi.ac.uk/thornton-srv/software/LIGPLOT/).

Table 1: The molecular docking analysis data of BAX, COX-2 Cas 3 and Cas 9 with piperine

S. No	Protein name	Score Kcal/mol	ACE	Residues	Ligand Atom	H-bond distance	No of non-bonded interaction
1	Bax	3824	-108.98	THR 14	OG-O	3.30	72
				ASP 53	N-O	3.16	
2	Caspase 3	4174	-187.40	HIS 277	ND-O	2.70	48
3	Cox 2	5042	-219.53	ARG44	N-O	2.49	63
4	Caspase 9	4988	-114.31	ARG 355	N-O	2.83	10

Results and Discussion:
BAX, Cox-2 and Caspase 3 and 9 docked with piperine having scores 3824, 5042, 4174 & 4988 kcal/mol respectively (**Table 1**). The table also provides data for interacting residues with respective atomic contacts. The interaction of Bax **[12, 13]**, Cox 2 **[14],** Caspase 3, and Caspase 9 **[15]** with piperine is illustrated in **Figure 1.** The interactions shows optimal binding features [16-17] for further consideration of piperine as a potential drug candidate in colon cancer research and development.

Conclusion:
The molecular docking analysis data of selected colon cancer linked proteins such as BAX, COX-2 Cas 3 and Cas 9 with piperine is reported for further consideration.

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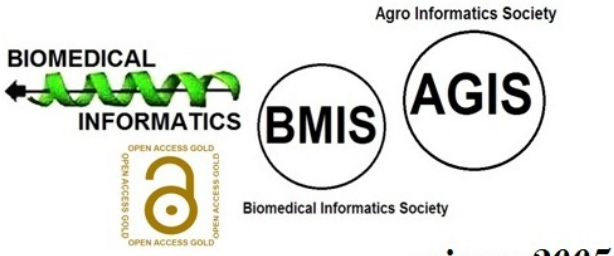

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