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Screening and Molecular Docking the Bioactive Constituent of Brassica Oleraceacapitata to Confirm the Anti-Lipid Peroxidation Effect of Phytol to Resolve Peptic Ulcer

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Abstract:-Lipid peroxidation is one of the significant risk factors for Peptic ulcer disease. Peroxisome Proliferator-Activated Receptor Gamma (PPAR Gamma), a lipid metabolism-regulating receptor, is a substantial target for lipid peroxidation. Pioglitazone is the standard drug used for treatment. This drug has a lot of side effects, but bioactive constituents in the herbs will aid the body in its healing process. The bioactive constituents present in the plants, and their products can resolve peptic ulcers by terminating lipid peroxidation. Brassica oleraceacapitata is a leafy vegetable traditionally used to treat peptic ulcers. Gas Chromatography and Mass Spectroscopy studies have been carried out to identify the bioactive constituents in the leaves of Brassica oleraceacapitata. The Maceration method has been adopted to extract bioactive components with ethanol as an extraction solvent. The chromatogram revealed a total of 77 bioactive constituents. Developing a drug candidate with therapeutic activity is a long and tedious and expensive process. Molecular docking is a powerful tool in the field of drug discovery. Molecular docking is easy, time-saving and cost-effective in determining the binding methods and affinities and predicts the small molecule behavior in the targeted protein binding site. Phytol, an anti-oxidant identified from the ethanolic extract of Brassica oleraceacapitata, has been used as a ligand for Peroxisome Proliferator-Activated Receptor Gamma (PPAR Gamma), and molecular docking has been carried out. The glide energy of the Phytol- PPAR gamma receptor is (-40.70 kcal/mol). Our present study shows that Phytol exhibits binding affinity with the PPAR gamma receptor, which pave the way to develop a new drug from Brassica oleraceacapitata.

Keywords*: PPAR Gamma receptor, lipid peroxidation, Brassica oleraceacapitata, Pioglitazone, Phytol.*

1. Introduction

Peptic Ulcer is an inflammatory disease in the gastrointestinal mucosae due to the imbalance between the defensive and aggressive factors. Lipid peroxidation is a harmful factor disturbing the gut immune system, resulting in peptic ulcers. Oxidation of dietary fat, usage of non-steroidal anti-inflammatory drugs, consumption of alcohol and the pathogenic bacteria Helicobacter Pylorus are the critical sources of lipid peroxidation [1,2]. Lipid peroxidation is a chain process that will continue till the termination products are produced. The end product inhibits gene expression. Peroxisome proliferator-activated receptor (PPAR) gamma receptor is a crucial regulator of lipid metabolism. PPAR Gamma receptor is a nuclear hormone receptor that functions as a transcription factor [3]. Regulation of the PPAR Gamma receptor heals peptic ulcer [4]. Thiazolidinedione drugs such as Pioglitazone are prescribed for peptic ulcers [5]. When an agonist binds to a PPAR gamma receptor, it activates the receptor and protects against peptic ulcer [6]. PPAR gamma receptor is activated by anti-oxidants [7], certain dietary fatty acids [8] and Thiazolidinedione drugs [9]. Synthetic drugs address only the symptoms caused by specific diseases and these drugs will create a lot of side effects. But herbs will aid the body in its

healing process [10]. Hence activating the PPAR gamma receptor by the bioactive constituents identified from the plants and their products have beneficial effects in resolving peptic ulcer.

Brassica oleraceacapitata, a leafy vegetable, is traditionally used for treating peptic ulcers. It exhibits anti-oxidant and anti-inflammatory properties. Some studies demonstrated Brassica oleraceacapitata's antiulcer properties for rats [11–13]. Combined traditional and scientific knowledge about plants provides a new way in the field of pharmacology to develop new drugs. The presence of bioactive constituents in the plants resolves the disease. The bioactive mixture was prepared with ethanol as an extraction solvent using the maceration method. The individual bioactive component in the ethanolic extract mixture has been identified by gas chromatography and mass spectroscopy technique using the instrument Perkin Elmer Clarus580 available at SRM University, Kattankulathur, Chennai (India). The receptor protein will not interact with all the molecules it encounters; but only with one or a few molecules. Hence, determining binding modes and affinity between the bioactive constituent and the receptor helps design therapeutic interventions. But, experimentally determining the protein-ligand complex's structureis difficult and costly. Computational methods such as Molecular docking are easy, time-saving and cost-effective in determining the binding methods and affinities [14]. It hints at the strength of the ligand and receptor protein interaction.

In the present study, the ethanolic extract of the leaves of Brassica oleraceacapitata was prepared by the maceration method and GC-MS studies were done for the ethanolic extract. The potential molecule identified from the extract was selected to target the PPAR gamma receptor for molecular docking studies.

PPAR gamma receptor has activation function-1, DNA binding region and ligand binding region. Binding a ligand to the ligand binding region will activate the PPAR gamma receptor, which cures peptic ulcers. Some amino acids in the binding site of the PPAR gamma receptor play a key role in triggering the receptor. Tyr473, His449, Cys285, Arg288, Tyr327, and Leu330 are the amino acids pivotal in activating the receptor [15] and Ile341 stabilizes the beta-sheet [16].

2. Materials and Methods

2.1 Sample preparation

As a part of the research is oriented to identify the bioactive constituents of Brassica oleracea, the leaves of Brassica oleracea have been separated and washed thoroughly in tap water. The leaves were air-dried and the windows were kept open, allowing little light to prevent microbes from growing. The leaves turned daily, and the dried leaves were ground well to increase surface area. The maceration method has been subjected to an extraction process with ethanol as solvent. Ten grams of the powdered sample were soaked in 200ml ethanol for Three days. The mixture was stirred daily using the magnetic stirrer for Twenty minutes with 500 rotations/min. On the fourth day, the extract was filtered through Whatman no.1 filter paper and the filtrate was kept at room temperature for the evaporation of ethanol. The sample after the evaporation of ethanol has been collected for GC-MS studies.

2.2 Gas Chromatography and mass spectroscopy studies

A fully automated gas chromatograph Perkin Elmer Clarus580, has vaporized and separated the bioactive mixture. The sample is introduced in the splitless mode in the online injection system. The gas chromatography instrument is equipped with FID and TCD detectors to collect and measure the concentration of the ions present in the sample.

Molecular docking uses advances in bioinformatics to determine the binding affinity between the protein and the ligand by computational method. A molecular docking study on the bioactive constituent of the leaves of Brassica oleraceacapitata provides a way in the field of pharmacology to develop a new drug.

2.3 Molecular docking

Glide (Schrodinger maestro module), available in the Centre for Advanced Studies in Crystallography & Biophysics, University of Madras, Chennai, has been utilized for the docking analysis of the present work. In molecular docking, ligand preparation and protein preparation are the initial steps.

2.4 Ligand preparation

From the PubChem database, the input structures of Phytol have been downloaded. For preparing the ligand, the "LigPrep" module has been used. Using OPLS 2005 force field, Ligand energy has been minimized.

2.5 Protein preparation

Protein structure was downloaded from Protein Data Bank (PDB). The proteins downloaded for the study were PPAR Gamma agonist (PDB ID:5Y2O). Protein preparation has been done using the protein preparation wizard, and the protein to be docked has been pre-processed initially. During pre-processing, the water molecules not involved in ligand binding and non-interacting ligands were eliminated. The force field OPLS 2005 has been used for optimizing and minimizing the Pre-processed proteins.

2.6 Induced fit docking

Molecular docking was carried out through Induced fit docking. The optimized energy protein was uploaded in the Maestro environment. A grid box that covers the binding site was generated using Glide's "Receptor generation wizard." The self-docking ligand and the cross-docking ligand were uploaded onto the binding site. Docking was carried out in the extra precision (XP) mode. For each ligand, Twenty poses were selected. The docked complexes were visualized using two- dimensional LigPlot images.

2.7 Docking validation

Molecular docking results are validated by determining the root mean square deviation value for the re-docked (or) self-docked and cross-docked ligands. RMSD values are determined using a molecular graphics system PyMol (TM)2.3.3. The protein structure complexed with a ligand was re-docked in its binding site. The bioactive component identified from Brassica oleraceacapitata was cross-docked in the protein binding site. The docking is achieved by retrieving the protein structure of the PPAR gamma receptor available in the protein data bank (PDB ID: 5Y2O) and the docked complexes stored in the PDB file format. The protein structure from the protein data bank and the PDB file format is opened in PyMol. Using the comment "Align" both the structures are aligned, and the RMSD value is displayed. RMSD value gives information about the deviation of the re-docked and cross-docked ligands with the co-crystal of general conformation.

3. Results and Discussion

3.1 Ligand selection

Bioactive constituents from the ethanolic extract of Brassica oleraceacapitata have been identified by GC-MS studies for the present study. Totally 77 bioactive compounds have been recognized. All the bioactive components are presented in Table 1 and their corresponding chromatogram is illustrated in Figure 1.

Table 1Chromatogram of ethanolic extract of leaves of Brassica oleraceacapitata.

Sl.no	RT (min)	Compound name	Mol. Wt	Formula	Prob%	Area%
1.	2.64	Ethanethioamide	75	C_2H_5NS	16.8	0.07
2.	2.97	Acetic acid	60	$C_2H_4O_2$	82.2	3.37
3.	3.12	Acetol	74	$C_3H_6O_2$	76.8	0.82
4.	3.41	Triethylamine	101	$C_6H_{15}N$	70.0	2.11
5.	3.89	2-propenoic acid,2-propenyl ester	112	$C_6H_8O_2$	44.8	0.44
6.	4.39	Methyl pyruvate	102	$C_4H_6O_3$	84.1	0.51
7.	4.56	Pyrrolidine,2-butyl-1-methyl-	141	$C_9H_{19}N$	75.8	0.18
8.	4.67	Glycolaldehyde dimethyl acetal	106	$C_4H_{10}O_3$	40.4	1.37
9.	5.16	Furfural	96	$C_5H_4O_2$	79.6	1.21

10	5.76	2-Furanmethanol	98	$C_5H_6O_2$	76.1	0.39
11.	5.97	α -Angelica lactone	98	$C_5H_6O_2$	27.6	0.17
12.	6.37	4-cyclopentene-1,3-dione	96	$C_4H_4O_2$	93.9	0.51
13.	8.76	2-Furancarboxaldehyde,5-methyl-	110	$C_6H_6O_2$	95.7	1.68
14.	9.27	2,4-Dihydroxy-2,5-dimethyl-3(2H)-furan-3-one	144	$C_6H_8O_4$	97.8	0.82
15.	13.74	2,5-Dimethyl-4-hydroxy-3(2H)-furanone	128	$C_6H_8O_3$	82.2	1.11
16.	17.41	Pyranone	144	$C_6H_8O_4$	91.2	11.98
17.	19.29	5-hydroxymaltol	142	$C_6H_6O_4$	83.5	1.20
18.	22.23	5-hydroxymethylfurfural	126	$C_6H_6O_3$	94.5	11.28
19.	23.26	Indole	117	C_8H_7N	27.0	0.62
20.	24.00	p-Vinyl guaiacol	150	$C_9H_{10}O_2$	61.1	1.50
21.	25.76	Octa amide, N-(2-mercaptoethyl)-	203	$C_{10}H_{12}NOS$	16.9	1.86
22.	27.52	Tetradecane	198	$C_{14}H_{30}$	36.0	0.27
23.	30.47	1-Undecanol	172	$C_{11}H_{24}$	6.8	0.19
24.	32.45	4-Fluoro-2-trifluoromethylbenzoic acid,2-ethylhexyl ester	320	$C_{16}H_{20}F_4O_2$	25.1	0.05
25.	34.13	3',5'-Dimethoxyacetophenone	180	$C_{10}H_{12}O_3$	28.6	0.24
26.	34.65	3',5'-Dimethoxyacetophenone	180	$C_{10}H_{12}O_3$	24.2	6.02
27.	35.59	Hexadecane	226	$C_{16}H_{34}$	12.2	0.53
28.	41.94	Tetra decanoic acid	228	$C_{14}H_{28}O_2$	83.8	0.29
29.	42.87	Octadecane	254	$C_{18}H_{38}$	16.7	0.37
30.	43.09	5,5,8a-Trimethyl-3,5,6,7,8,8a-hexahydro-2H-chromene	180	$C_{12}H_{20}O$	29.6	0.74
31.	43.82	1H-Indole-3-acetonitrile	156	$C_{10}H_8N_2$	65.3	0.23
32.	44.45	2-Pentadecanone,6,10,14-trimethyl-	268	$C_{18}H_{36}O$	72.3	0.14
33.	45.31	Pentadecanoic acid	242	$C_{15}H_{30}O_2$	76.7	0.25
34.	47.93	Palmitoleic acid	254	$C_{16}H_{30}O_2$	21.5	0.11
35.	48.35	Dibutyl phthalate	278	$C_{16}H_{22}O_4$	29.3	1.48
36.	49.05	n-Hexadecanoic acid	256	$C_{16}H_{32}O_2$	72.2	8.76
37.	49.39	Hexadecanoic acid, ethyl ester	284	$C_{18}H_{36}O_2$	75.5	0.42
38.	49.49	Eicosane	282	$C_{20}H_{42}$	28.8	0.15
39.	49.69	Coumatetralyl isomer-2 ME	306	$C_{20}H_{18}O_3$	14.5	0.16
40.	50.86	i-propyl 14-methylhexadacanoate	312	$C_{20}H_{40}O_2$	28.7	0.31
41.	51.25	Trans-13-octadecenoic acid	282	$C_{18}H_{34}O_2$	6.6	0.06
42.	51.67	Heptadecanoic acid	270	$C_{17}H_{34}O_2$	68.0	0.12
43.	52.61	10-octadecenoic acid, methyl ester	296	$C_{19}H_{36}O_2$	7.6	0.07
44.	52.99	Phytol	296	$C_{20}H_{40}O_2$	71.5	0.22

Sl.no	**RT**	**Compound name**	**Mol. Wt**	**Formula**	**Prob%**	**Area%**

	(min)					
45.	53.58	Cis-Vaccenic acid	282	$C_{18}H_{34}O_2$	9.4	0.09
46.	54.83	9,12-octadecadienoic acid (Z, Z)	280	$C_{18}H_{32}O_2$	16.2	8.78
47.	54.97	Octadecanoic acid	284	$C_{18}H_{36}O_2$	78.6	1.36
48.	56.52	9,12-octadecadienoic acid (Z, Z)	280	$C_{18}H_{32}O_2$	11.5	0.05
49.	56.79	i-propyl 16-methyl-octadecanoate	340	$C_{22}H_{44}O_2$	25.4	0.11
50.	57.26	Cis-10-Nonadecenoic acid	296	$C_{19}H_{36}O_2$	36.8	0.70
51.	57.89	i-propyl 11,12-methylene-octadecanoate	338	$C_{22}H_{42}O_2$	11.0	0.06
52.	59.18	5,8,11-Heptadecatrienoic acid, methyl ester	278	$C_{18}H_{30}O_2$	11.8	0.10
53.	59.79	Ethyl stearate,9,12-diepoxy	340	$C_{20}H_{36}O_4$	10.4	0.18
54.	60.32	Eicosanoic acid	312	$C_{20}H_{40}O_2$	65.8	0.26
55.	61.10	Tetracosane	338	$C_{24}H_{50}$	17.4	0.11
56.	63.31	2-Monopalmitin	330	$C_{19}H_{38}O_4$	47.9	0.11
57.	63.51	1-Heneicosyl formate	340	$C_{22}H_{44}O_2$	4.3	0.13
58.	63.73	Eicosane	282	$C_{20}H_{42}$	12.0	0.39
59.	64.08	2-Monopalmitin	330	$C_{19}H_{38}O_4$	70.4	1.29
60.	64.96	Phthalic acid, di(2-propylpentyl) ester	390	$C_{24}H_{38}O_4$	23.9	0.08
61.	65.55	Docosanoic acid	340	$C_{22}H_{44}O_2$	45.7	0.12
62.	66.26	Eicosane	282	$C_{20}H_{42}$	17.3	0.33
63.	67.73	Butyl 9,12-octadecadienoate	336	$C_{22}H_{40}O_2$	10.3	0.05
64.	68.59	β-Monoolein	356	$C_{21}H_{40}O_4$	43.1	1.25
65.	71.04	Eicosane	282	$C_{20}H_{42}$	8.6	0.19
66.	71.66	Squalene	410	$C_{30}H_{50}$	47.8	0.05
67.	72.46	Hexacosylheptafluorobutyrate	578	$C_{30}H_{53}F_7O_2$	4.9	0.05
68.	73.33	Tetratriacontane	478	$C_{34}H_{70}$	16.5	0.96
69.	74.79	Cholesta-4,6-dien-3-ol, (3β)	384	$C_{27}H_{44}O$	55.2	0.07
70.	74.98	1-Heptacosanol	396	$C_{27}H_{56}O$	4.1	0.76
71.	76.86	Cholesta-4,6-dien-3-ol, (3β)	384	$C_{27}H_{44}O$	73.8	0.41
72.	77.61	15-Nonacosanone	422	$C_{29}H_{58}O$	96.5	3.13
73.	78.16	Hexadecane-1,2-diol	258	$C_{16}H_{34}O_2$	22.6	1.39
74.	80.73	Hexadecane-1,2-diol	258	$C_{16}H_{34}O_2$	11.0	0.27
75.	81.28	Campesterol	400	$C_{28}H_{48}O$	66.9	3.32
76.	82.27	Stigmasterol	412	$C_{29}H_{48}O$	73.8	0.15
77.	84.65	γ-Sitosterol	414	$C_{29}H_{50}O$	87.4	9.31

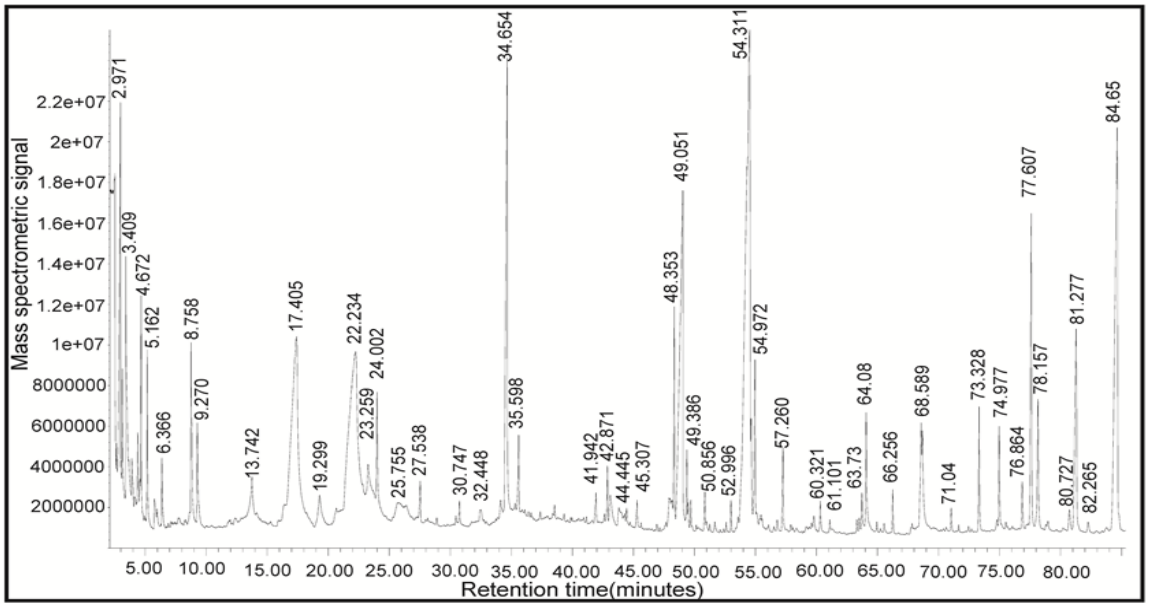

Figure 1 Chromatogram of ethanolic extract of leaves of Brassica oleraceacapitata.

Based on the biological activity in achieving the beneficial effect of resolving peptic ulcers, saturated and polyunsaturated fatty acids and anti-oxidants are gaining attention. The saturated fatty acids, n-Hexadecanoic acid, tetra decanoic acid, Pentadecanoic acid, Heptadecanoic acid, Octadecanoic acid, and Docosanoic acid are identified in the ethanolic mixture. But they don't have any beneficial effect on terminating lipid peroxidation. But they increase the LDL level. Hence are not considered for further studies. The unsaturated fatty acids such as 9,12-octadecadienoic acid (Z, Z), Trans-13-octadecenoic acid, and Palmitoleic acid are identified in the mixture. Even though the unsaturated fatty acids are the natural activators of the PPAR gamma receptor, they will undergo lipid peroxidation [17]. Hence, they are also not considered for molecular docking studies. Anti-oxidants play an important role in terminating the lipid peroxidation chain reaction. Phytol is an anti-oxidant identified in the ethanolic extract of leaves of Brassica oleraceacapitata at a retention time of 52.99 minutes and has been considered for molecular docking studies. The drug-likeness properties of Phytol and the co-crystal Pioglitazone are verified by applying Lipinski's Rule of Five.

3.2 Drug-likeness properties

The drug-likeness properties are tested using Lipinski's Rule of five. The Rule is applied for the bioactive constituent Phytol identified in the ethanolic extract of leaves of Brassica oleraceacapitata along with the co-crystal Pioglitazone. Lipinski's Rule of Five states that a molecule with molecular weight≤ 500, Log P ≤ 5, HBD ≤ 5, and HBA ≤ 10 behaves like a drug. The bioavailability problem occurs if the molecule controversies more than one Rule [18].

Table 2 Lipinski's Rule of Five for Phytol and the co-crystal Pioglitazone.

Molecule	Lipinski's Rule of Five			
	MW	Log P	HBD	HBA
Phytol	296.5	8.2	1	1
Pioglitazone (co-crystal)	356.4	3.8	1	5

MW: Molecular weight; **Log P:** Log of octanol-water partition coefficient; **HBD:** Hydrogen bond donor; **HBA:** Hydrogen bond acceptor.

Applying Lipinski's Rule of Five to Phytol indicates that it is effective via oral availability and satisfies the drug-likeness property. Hence it can be developed as a drug.

3.3 Molecular Docking studies

For molecular docking of the bioactive constituents of the leaves of Brassica oleraceacapitata, the 3-dimensional structural data of the PPAR Gamma receptor bound with Pioglitazone available in the protein data bank (PDB ID:5Y2O) with a resolution of 1.80A° were utilized [19]. A ligand pioglitazone, within its crystalline structure, and the ligand, Phytol identified from Brassica oleraceacapitata were docked in the binding site of the PPAR Gamma receptor.

3.4 Interaction of Phytol within the binding site of PPAR gamma receptor

Phytol is cross docked within the binding site of the PPAR gamma receptor. The agonist binding caused a conformational change in the protein, forming the Phytol- PPAR gamma complex. The two-dimensional interaction image of the phytol-pioglitazone complex is presented in Figure 2.

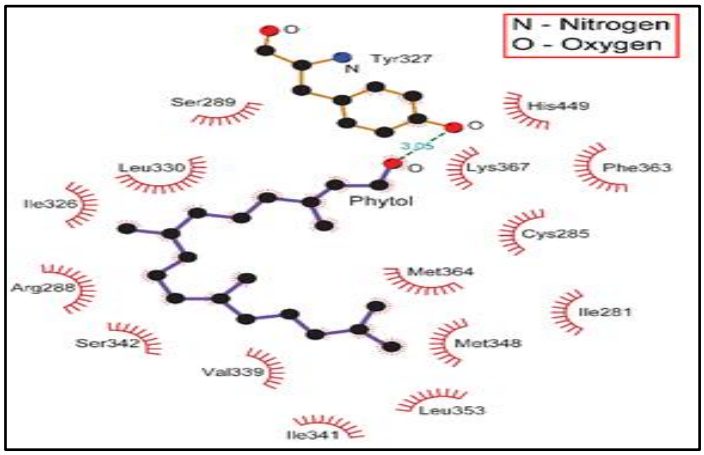

Figure 2 Interaction image of Phytol with PPAR Gamma receptor.

The following observations are made from the two-dimensional interaction pictures:
Hydrogen bonds, hydrophobic interactions and π-stacking play an essential role in protein-ligand formation [20]. Hydrogen bonds are facilitators of protein-ligand interactions [21]. Hydrophobic interactions are crucial in stabilizing the ligand at the binding site [22]. π-stacking occurs between the amino acid and the ligand ring [23]. In the case of the PPAR gamma-Phytol complex, the hydroxyl group of Phytol makes hydrogen bonding with the residues Tyr327. Thetyrosyl group of Tyr donates its hydrogen atom to Phytol's hydroxyl group, and the bond distance between the Tyr327 and the hydroxyl group of Phytol is 3.05A°. Phytol also makes hydrophobic interactions with the amino acids His 449, Ile281, Cys285, Arg288, Ser289, Leu330 and Leu333. These amino acids are responsible for the activation of the receptor. It also interacts with the residues of beta-sheetLeu340, Ile341 and Ser342. The interaction with the residues of the beta-sheet indicates the accessibility of Phytol into the binding site by stabilization of the beta-sheet. These interactions of Phytol with the amino acids in the binding site of the PPAR gamma receptor indicate the presence of Phytol within the receptor and receptor-Phytol complex formation takes place by hydrogen bonding and hydrophobic interactions. Hence, Phytol is also acting as an agonist. The docking score for Phytol- pioglitazone complex is -8.28 and the glide energy o for the complex is -40.70 kcal/ mol.

3.5 Interaction of Pioglitazone (co-crystal) within the binding site of PPAR gamma receptor

The interaction image of the pioglitazone-PPAR gamma receptor complex is shown in Figure 3.

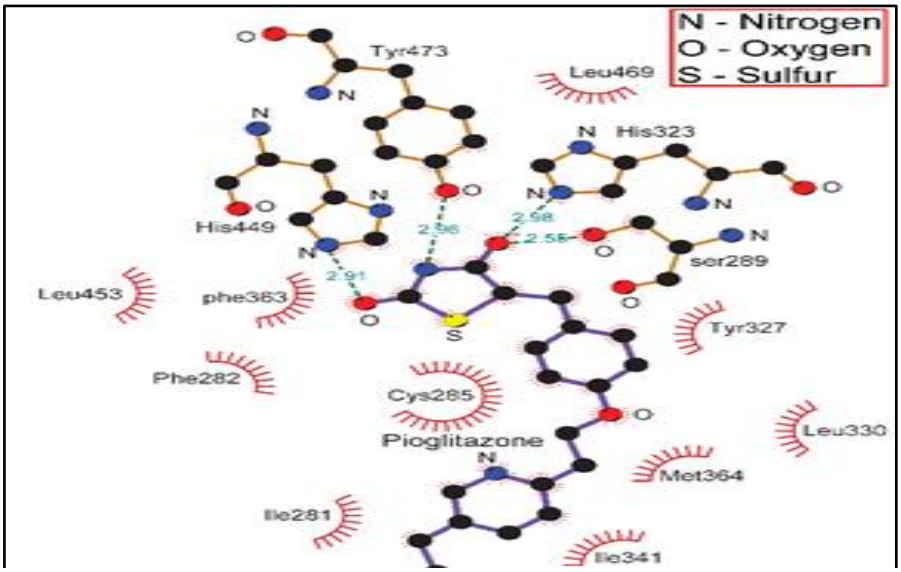

Figure 3 Interaction image of Pioglitazone with PPAR Gamma receptor.

Pioglitazone makes hydrogen bonding with the residues Tyr473, His449, His323 and Ser289. The bond distance between Pioglitazone and the amino acids Tyr473, His449, Ser289 and His323 are 2.96A°, 2.91A°, 2.58A° and 2.98A°. Pioglitazone makes hydrophobic interaction with the Ile281, Phe282, Cys285, Tyr327, and Leu330 of ligand binding region and with the beta-sheet residue Ile341. Pioglitazone directly interacts with the amino acids Tyr473 and Leu469 in the ligand-binding pocket and acts as an agonist. The docking score for Pioglitazone-PPAR Gamma complex is -10.88, and the glide energy for the complex is determined as -55.56 kcal/mol. The docking score and the glide energy of Phytol and Pioglitazone are presented in Table 3.

Table 3 Docking score and Glide energy of the bioactive constituent and the co-crystal.

Compound	Docking score (Kcal/mol)	Glide energy (Kcal/mol)	Hydrogen bonding
Phytol	-8.28	-40.70	Tyr 327 (O-H…O)
Pioglitazone (co-crystal)	-10.88	-55.56	(O…N-H) Tyr473 His449 (N-H…O) His323 (N-H…O) Ser289 (O-H…O)

The ability of the ligand to interact with the receptor is determined by its glide energy values. The negative value of the Glide energy represents the reaction's spontaneity, and spontaneous reaction makes it easier for the ligand to interact with the target receptor. From the above Table, it is inferred that Phytol exhibits a higher negative value and that ligands can easily bind with the receptor.

Molecular docking has been validated by determining the Root Mean Square Deviation between the co-crystallized Pioglitazone docked to the PPAR gamma receptor binding pocket and the original molecule. The RMSD value of the co-crystalline molecule is 0.110A° and that of Phytol is 0.118 A°. Docking validations are acceptable only if the RMSD value is less than 2 A° [24]. The RMSD values are within the excellent range, indicating the molecular docking process's validity.

The molecular docking studies suggest that Phytol targets the PPAR gamma receptor, a critical path to peptic ulcer. Hence, the bioactive constituent of the leaves of Brassica oleraceacapitata can be studied in detail, which will pave a new way in the field of pharmacology to develop drugs.

4. Conclusion

The leaves of Brassica oleraceacapitata is traditionally used for treating peptic ulcer. The GCMS studies on the ethanolic extract of leaves of Brassica oleraceacapitata showed 77 bioactive constituents. Based on its anti-ulcerogenic, anti-oxidant, and drug-likeness properties, Phytol has been considered for molecular docking studies. Phytol exhibits binding affinity towards the PPAR gamma receptor, an essential target for lipid peroxidation-induced peptic ulcer. The glide energy provides an idea about the strength of the protein-ligand interaction. This is helpful in pharmacology to develop drugs from the leaves of Brassica oleraceacapitata.

Acknowledgment

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