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Molecular Docking Study of Active Compounds in White Radish (*Raphanus sativus* L.) on Cyclooxygenase-2 (COX-2) Receptor as an Anti-Inflammatory Agent

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ABSTRACT

Inflammation is a natural endogenous response to injury, infection, or external stimuli, and it plays a critical role in the pathogenesis of various diseases, including arthritis and osteoarthritis. Despite their effectiveness, the long-term use of *nonsteroidal anti-inflammatory drugs* (*NSAIDs*) often leads to several adverse effects, particularly gastrointestinal complications. Therefore, it is crucial to explore safer alternative therapies. This study aimed to evaluate the potential of bioactive compounds found in white radish (*Raphanus sativus* L.) as alternative anti-inflammatory agents using *in silico* molecular docking analysis against the cyclooxygenase-2 (*COX-2*) enzyme. Molecular docking simulations were performed using AutoDock Vina software, with the *COX-2* structure obtained from the Protein Data Bank (PDB ID: 4PH9). The docking results indicated that glucoraphanin and squalene exhibited strong binding affinities with binding energies of –8.53 kcal/mol and –8.62 kcal/mol, respectively. Glucoraphanin was found to form hydrogen bonds with key active site residues similar to the interaction observed with ibuprofen, a standard *NSAID*. Meanwhile, squalene predominantly engaged in hydrophobic interactions with the enzyme. These findings suggest that glucoraphanin and squalene have the potential to act as effective *COX-2* inhibitors and could serve as safer alternatives to conventional *NSAIDs*. However, further *in vitro* and *in vivo* studies are essential to validate their therapeutic potential and safety profiles.

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INTRODUCTION

The enzyme COX-2 or *Prostaglandin Endoperoxide Synthase-2* forms prostaglandins as inflammatory mediators. Among the inflammatory diseases (e.g., osteoarthritis, inflammatory bowel diseases, arthritis), a significant percentage of the population is affected [1]–[3]. As a first-line treatment for these diseases, NSAIDs are also an option. However, when taking NSAIDs chronically, their usage can also result in GI ulceration and bleeding [4]–[6]. Most people experience problems with the digestive tract. NSAIDs cause more than 90% of such ulcers, and 25% of NSAID users develop PUD (Peptic Ulcer Disease) [7], [8]. Also, in elderly age (>65 years), NSAID use has been associated

with increased cardiovascular risk events [1]–[3].

Inflammation is the body's natural reaction to injury, foreign invaders, or worn-out cells, warning us that something might be awry with health. Inflammation is typically red, from increased blood flow to the area. Also, the inflammatory response may lead to edema due to extravasation of further cellular and fluid contents from blood vessels into surrounding tissue [9]–[11]. Plants have been used for medicinal purposes for thousands of years. Because they are pharmacologically active due to the presence of phytochemicals, such as various chemical compounds, many possess strong anti-inflammatory activity [12]–[14]. Relevant examples of that include the alkaloid colchicine [12], the triterpenoid saponin escin [15], the methoxy phenol capsaicin [16], the lignan bicyclol [17], the monoterpene borneol, and the flavonoid quercetin [15]. In the amelioration of pathological status, however, these phytochemicals are frequently accomplished by targeting the molecular pathways that prevent inflammation, i.e., they reduce the levels of pro-inflammatory cytokines and other modulators or activate the anti-inflammatory pathways, such as the increase in the levels of anti-inflammatory cytokines [18], [19].

The provision of anti-inflammatory agents that exhibit minimal side effects is a new strategy, and natural products from plants are used here. White radish (*Raphanus sativus* L.) is one of the candidate plants reported as medicinal plants that could be the object of research due to its phytochemical properties that lead to health. The roots and the leaves are the principal sources of nutrients and phytochemicals. Predominant classes are fat and lipophilic substances (6.4%), terpenes and their characteristic derivatives (8.2%), non-flavonoid polyphenols (8.4%), flavonoids (38.8%), and glucosinolates and hydrolysis compounds (5.6%) [20]–[22]. According to a recent study, *Raphanus sativus* is highly nutritious and contains bioactive phytochemicals that are beneficial for health and have anti-inflammatory activity [20].

In silico research, including molecular docking, to evaluate the potential of natural compounds as therapeutic agents has been gaining popularity [23]–[25]. The novel knowledge gained in this work will further proteomics studies and aid in developing novel bioinformatics approaches. From the viewpoint of organic compound synthesis, enzyme-ligand interactions would contribute to exploring a new synthesis method [26]–[28]. Molecular docking studies can model the interaction between the active compounds and the specific target enzyme (like COX-2). In another study, computational tools were also successfully used to reveal the potential of the compounds of white radish to be anti-insomnia drugs [30].

Accordingly, the present investigation attempts to unveil the power of the active compounds of the white radish by the molecular docking method to inhibit the COX-2 enzyme, which can be further used as a safer and more effective substitute for anti-inflammatory drugs. It has been reported that some phyto-compounds also have anti-inflammatory activity against COX-2; however, less work was done with the compounds of white radish in particular [31].

So far, no docking analysis has been reported on glucoraphanin and squalene isolated from white radish as a reference NSAID on COX-2 active sites through PDB ID: 4PH9. Hopefully, this study can be used as evidence to enlighten potential active anti-inflammatory chemical constituents in white radish with the purpose of rational application for safe and effective anti-inflammatory medicine in the clinic. This indicates that additional molecular investigations of the active constituents and the COX-2 enzyme in white radish are warranted.

METHODS

1. Materials and Tools

The hardware used in this work is an HP notebook (model: tbokri2l) with AMD Ryzen 5 5500U with Radeon Graphics, processor speed 2.10 GHz, 8.00 GB RAM, 64-bit OS with x64-based processor. Software tools used in the present study include AutoDock Vina, Avogadro, OpenBabel, Discovery Studio 2021 Client, and PyMOL. Furthermore, data mining screening was conducted through the PDB website (https://www.rcsb.org/) and the PubChem website (https://pubchem.ncbi.nlm.nih.gov/).

The receptor (macromolecule) selected in this study is Cyclooxygenase-2 (COX-2) with code 4PH9, downloaded from the PDB (Protein Data Bank). The white radish (*Raphanus sativus* L.) based ligand compounds (4-vinyl-2-methoxyphenol, 2,4-dimethylphenol, violaxanthin, squalene, glucoraphanin, and ibuprofen as a reference compound) were downloaded in SDF format from the PubChem website.

2. Ligand Preparation

The receptor and ligand molecules were modeled utilizing BIOVIA Discovery Studio. After optimization, the ligand file was redocked using the "pdbqt" protocol. This conversion, implemented through AutoDock Tools, included adding hydrogen atoms and assigning rotatable bonds to be non-rotatable. The "pdbqt" file was stored on the C drive of a Windows system [32].

3. Preparation of Receptor 4PH9

Human Cyclooxygenase-2 Bound Mefenamic Acid Structure (PDB ID: 4PH9) was obtained online from (https://www.rcsb.org/). The resolution of the protein was 1.81 Å. The PDB file was converted to "pdbqt" format, and hydrogens were added using AutoDock Tools. This prepared receptor structure was uploaded with the prepared ligand to define the docking grid box.

Table 1. Grid box coordinates and sizes.

Indicator	Size
Current total grid points per map	68921
Number of points in the x-dimension	40
Number of points in the y-dimension	40
Number of points in the z-dimension	40
Spacing (angstrom)	0.992
X center	13.578
Y center	23.024
Z center	25.205

4. Grid Box Determination

The grid box was placed over the active site coordinates of the COX-2 (4PH9) enzyme using AutoDock Tools. Care was taken to ensure the whole ligand was within the boundaries of the grid box, a key factor for good docking. The dimensions of the grid box are shown in Table 1.

5. Molecular Docking Process with Autodock Vina

The generated "pdbqt" files of ligand and protein were copied into the Vina working directory. A Vina setup file was defined using Notepad, specifying receptor and ligand file names, grid box size, and center coordinates. Molecular docking was performed using Vina on the command prompt. After docking, the binding free energy (kcal/mol) and root mean square deviation (RMSD) were noted.

Table 2. Distribution of ADMET predictors in pkCSM [4]

Pharmacokinetic parameter	Predictor (code)	Unit	Requirement value
	Water solubility (A1)	log mol/L	-
	Caco2 permeability (A2)	log Papp in 10−6cm/s	>0.9
	Intestinal absorption (human) (A3)	% Absorbed	>30%
Absorbs	Skin Permeability (A4)	log Kp	≥ -2.5
	P-glycoprotein substrate (A5)	Yes/No	-
	P-glycoprotein I inhibitor (A6)	Yes/No	-
	P-glycoprotein II inhibitor (A7)	Yes/No	-
	VDss (human) (D1)	log L/kg	≥ -0.15
Distribution	Fraction unbound (human) (D2)	Fu	-
	BBB permeability (D3)	Log BB	≥ -1
	CNS permeability (D4)	Log PS	≥ -3
	CYP2D6 substrate (M1)	Yes/No	-
	CYP3A4 substrate (M2)	Yes/No	-
	CYP1A2 inhibitor (M3)	Yes/No	-
Metabolism	CYP2C19 inhibitor (M4)	Yes/No	-
	CYP2C9 inhibitor (M5)	Yes/No	-
	CYP2D6 inhibitor (M6)	Yes/No	-
	CYP3A4 inhibitor (M7)	Yes/No	-
Excretion	Total Clearance (E1)	log ml/min/kg	The higher, The better
	Renal OCT2 substrate (E2)	Yes/No	-
	AMES toxicity (T1)	Yes/No	-
	Max tolerated dose (human) (T2)	log mg/kg/day	-
	hERG I inhibitor (T3)	Yes/No	-
	hERG II inhibitor (T4)	Yes/No	-
Toxicity	Oral Rat Acute Toxicity (LD50) (T5)	mol/kg	-
	Oral Rat Chronic Toxicity (LOAEL) (T6)	log/kg bw/day	-
	Hepatotoxicity (T7)	Yes/No	-
	Skin Sensitisation (T8)	Yes/No	-
	T. T.Pyriformis toxicity (T9)	log ug/L	< 0.5
	Minnow toxicity (T10)	log mM	> -0.3

6. Analysis of Molecular Docking Results

Docking results were interpreted by evaluating the binding affinities of various poses in the Log.txt file. RMSD values were also checked to validate docking accuracy. An RMSD value less than 2 Å indicated successful docking, while values greater than 2 Å suggested that the ligand and receptor did not dock properly and the results were unreliable.

7. Visualization of Docking Results

The analysis of the interaction between the receptor and ligand was conducted through the utilization of Discovery Studio Visualizer and PyMOL. This analysis included the examination of amino acid residues depicted in a two-dimensional format [5].

8. Prediction of ADMET using pkCSM

Further studies, such as ADMET prediction, followed the molecular docking results of the screened compounds with the receptor. ADMET profile analysis was used to verify whether the compounds of white radish (*Raphanus sativus* L.) had favorable properties or undesired effects regarding Absorption, Distribution, Metabolism, Excretion, and Toxicity, using the pkCSM web server [35]. This methodology improves the drug development potential by estimating the pharmacokinetics of bioactive molecules. It is integrated into the nominal stage, prospect stage, optimization stage, candidate stage, and further stages of development [36].

RESULTS AND DISCUSSION

1. Receptor Preparation

The protein used as input in this experiment is COX-2 (Cyclooxygenase-2) with resolution PDB ID: 4PH9, an enzyme responsible for the production of prostaglandins and related to inflammatory and pain processes. The 4PH9 structure was obtained from the Protein Data Bank (https://www.rcsb.org/), and the cofactor of its bound drug, ibuprofen, was separated through BIOVIA Discovery Studio software.

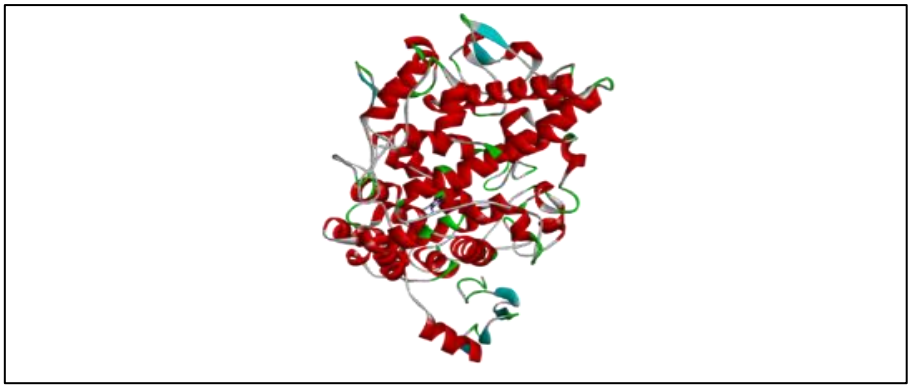


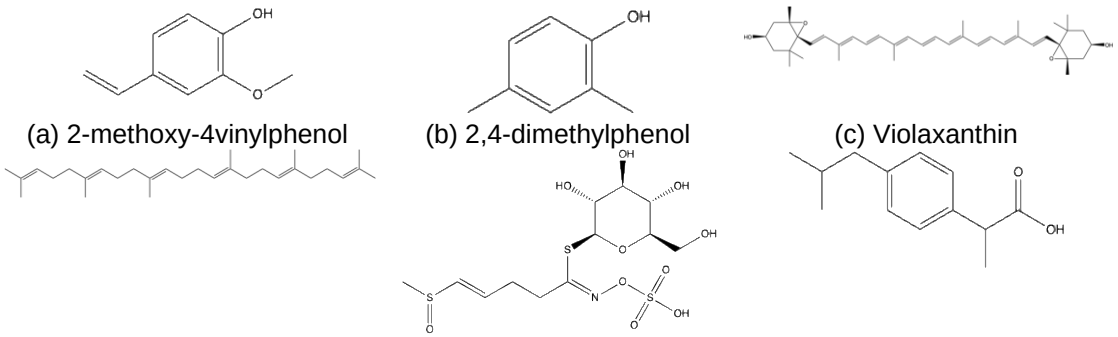
Figure 1. Protein Cyclooxygenase-2 (COX-2) PDB ID: 4PH9

Water molecules in the receptor structure were also deleted to prevent inappropriate hydrogen interactions that could affect simulation results [38]. The structure of COX-2 was re-processed during receptor preparation for docking simulation by adding non-polar hydrogen atoms only, using AutoDock Tools. The aim was to better describe molecular interactions in the simulation, particularly hydrophobic interactions, and avoid artifacts arising from superfluous polar charges [39].

2. Ligand Preparation

The following abbreviations were used in the index list: HSI: hepatosomatic index; PS: plasma and serum; SGR: specific growth rate; TRI: triiodothyronine T_3; T_4: thyroxine; xanthophyll; tocopherol; ROA: rise of action; NOAEL: no observed adverse

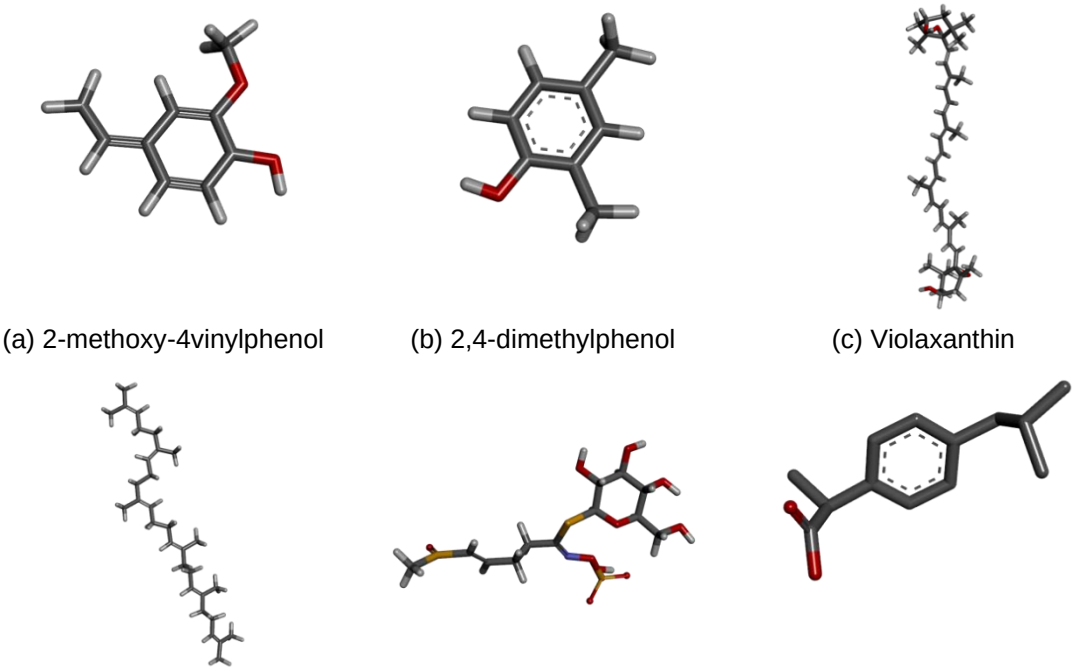
effect level; GAR: growth after recovery; SGRD: standardized growth ratio; CDI: chronic dietary intake.



(a) 2-methoxy-4vinylphenol (b) 2,4-dimethylphenol (c) Violaxanthin

(d) Squalene (e) Glucoraphanin (f) Ligand Protein (Ibuprofen)

Figure 2. The 2D structure of compounds docked to the cyclooxygenase-2 (COX-2) protein (PDB ID: 4PH9)



(a) 2-methoxy-4vinylphenol (b) 2,4-dimethylphenol (c) Violaxanthin

(d) Squalene (e) Glucoraphanin (f) Ligand Protein (Ibuprofen)

Figure 3. The 3D structure of compounds docked to the cyclooxygenase-2 (COX-2) protein (PDB ID: 4PH9)

These compounds were drawn in two-dimensional (2D) configuration with ChemDraw Professional 16.0. Then, geometry optimization was carried out with Chem3D, using the MMFF94 (Merck Molecular Force Field) and MMFF94s force field, importing the structure to obtain a more stable minimum energy conformation. Protonation or proton charge addition was performed using the Gasteiger algorithm for better charge distribution and more accurate electrostatic interactions between ligand and receptor in the docking process, predicting better binding affinity [40]. Hydrogen atoms

were added to mimic biological conditions in the human body (pH ≈ 7). After completing the optimization, all compounds were saved in .pdb format for virtual screening based on molecular docking against the Cyclooxygenase-2 (COX-2) receptor (PDB ID: 4PH9).

3. Method Validation

Before molecular docking, the first step following ligand and receptor preparation is a delicate phase of the validation method of molecular docking by re-docking the native ligand and receptor based on the relevant PDB receptor code [41]. The RMSD value reveals the binding status between the ligand in the cavity and the protein. When the RMSD value is less than the normal value of < 2.0 Å, as a rule of thumb, the molecular docking result is considered reasonable [42].

According to the validation results, the position of the grid box (x; y; z) was determined to be (13.578; 23.024; 25.205), with a corresponding size of 40 × 40 × 40 grid steps. The docking binding energy was recorded at −8.35 kcal/mol, together with the inhibition constant of 761.48 µM, and the RMSD of 0.858 Å, validating the docking protocol with the threshold RMSD value of < 2.0 Å

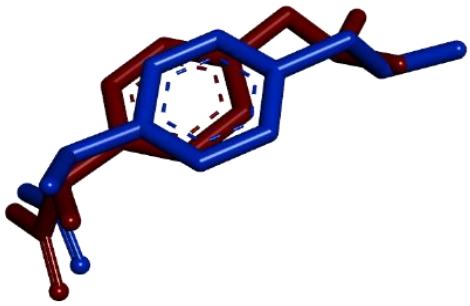


Figure 4. Superimposition of the COX-2 ligand-protein complex (PDB ID: 4P9H) with ibuprofen. (Blue: before re-docking & Purple: after re-docking).

4. Molecular Docking Results

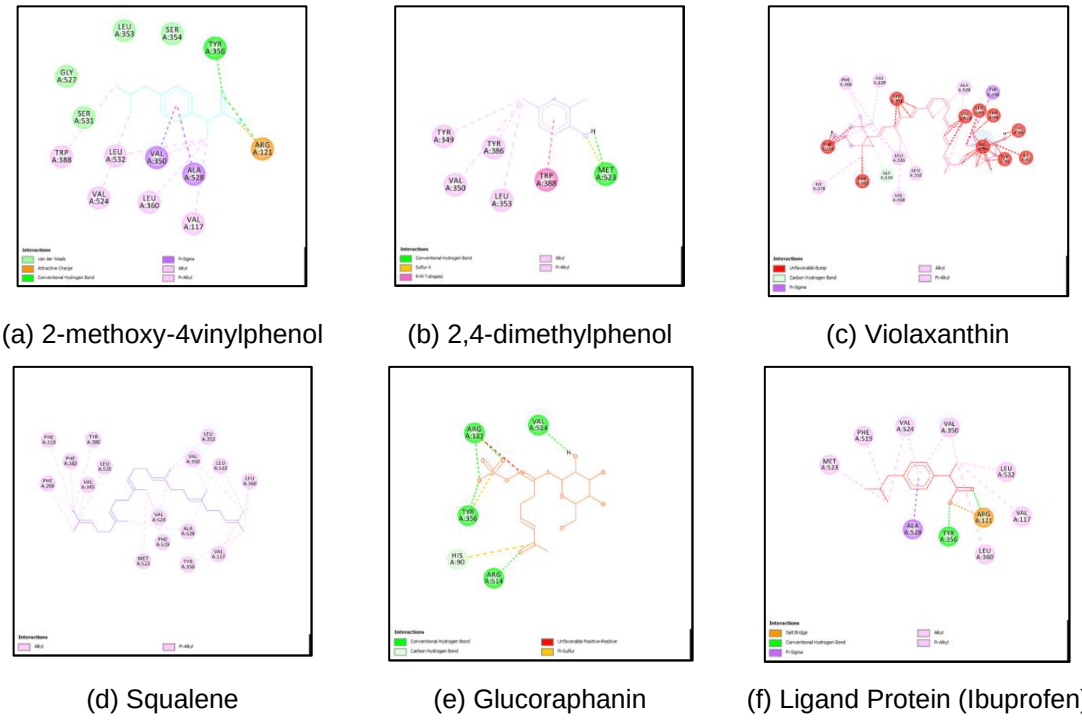
Molecular docking was carried out using the Lamarckian Genetic Algorithm with 100 independent docking runs [43]. The results of molecular binding revealed that glucoraphanin and squalene exhibited the lowest binding energy values of −8.53 kcal/mol and −8.62 kcal/mol, respectively, while their inhibition constants were 563.59 µM and 480.17 µM, respectively. These values were slightly lower than the control compound, ibuprofen, which had a binding energy of −8.35 kcal/mol and an inhibition constant of 761.48 µM [44].

Additionally, structural studies on the compounds 2-methoxy-4-vinylphenol and 2,4-dimethylphenol were conducted. 2-methoxy-4-vinylphenol exhibited a binding energy of −5.32 kcal/mol and a Ki value of 126.68 µM. In comparison, 2,4-dimethylphenol exhibited a binding energy of −5.08 kcal/mol and a Ki value of 187.64 µM, indicating a moderate interacting potential [43].

In contrast, violaxanthin exhibited an anomalous binding energy of +956924.25 kcal/mol, and the Ki value could not be achieved, suggesting that violaxanthin may not be a suitable ligand for binding to the COX-2 receptor studied in the present work

Table 3. Docking results of compounds against the 4P9H receptor.

No.	Compound	Run	Binding energy (kcal/mol)	Ki (μm)
1	2-methoxy-4vinylphenol	16	-5,32	126.68
2	2,4-dimethylphenol	46	-5,08	187.64
3	Violaxanthin	40	+956924,25	n/a
4	Squalene	82	-8,62	480,17
5	Glucoraphanin	21	-8,53	563,59
6	Ligand Protein (Ibuprofen)	36	-8,35	761,48

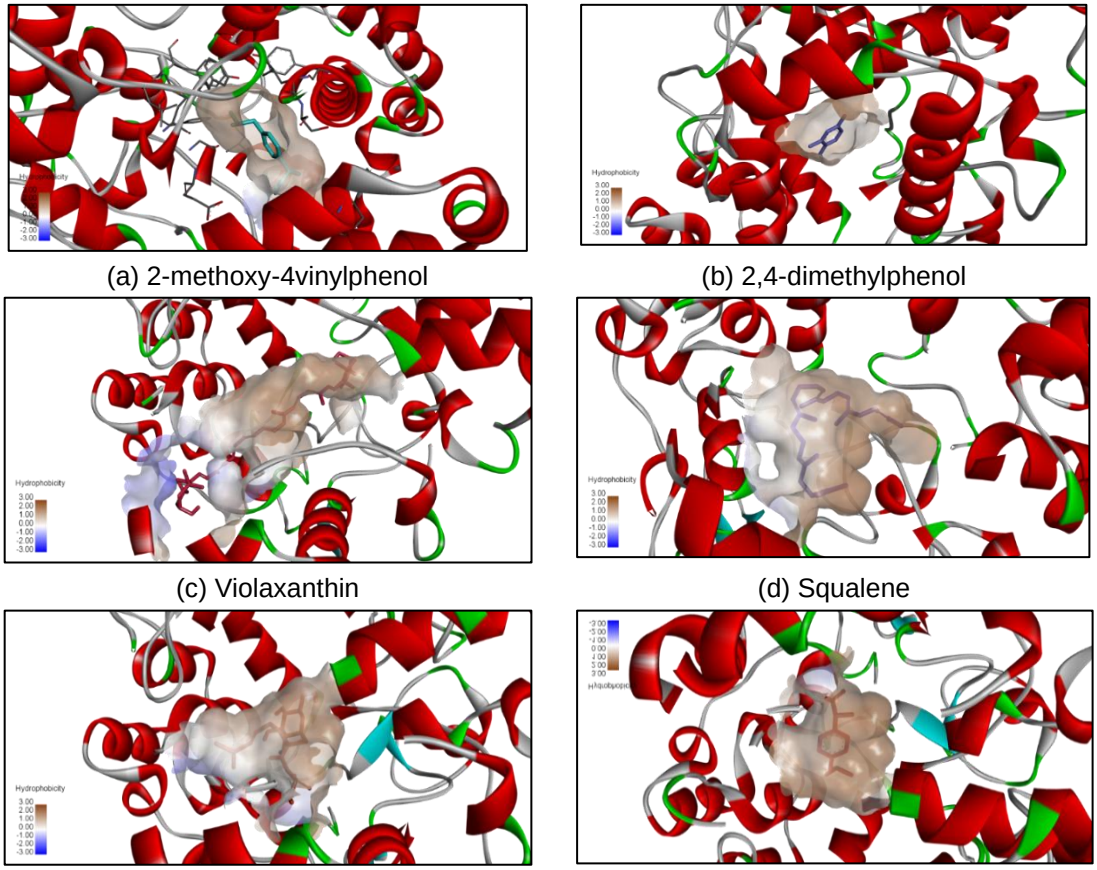


(a) 2-methoxy-4vinylphenol (b) 2,4-dimethylphenol (c) Violaxanthin

(d) Squalene (e) Glucoraphanin (f) Ligand Protein (Ibuprofen)

Figure 5. The bonding interactions formed in the compound (a) 2-methoxy-4vinylphenol, (b) 2,4-dimethylphenol, (c) Violaxanthin, (d) Squalene, (e) Glucoraphanin, (f) Ligand Protein.

The lower the Ki value, the greater the possibility that the compound forms a stable complex with the receptor [45]. A good Ki value is typically within the nanomolar range. Based on binding energy and inhibition constants, glucoraphanin and squalene showed better prospects as COX-2 receptor inhibitors than the standard ibuprofen [46].



(a) 2-methoxy-4vinylphenol (b) 2,4-dimethylphenol

(c) Violaxanthin (d) Squalene

(e) Glucoraphanin (f) Ligand Protein (Ibuprofen)

Figure 6. The results of molecular docking analysis (a) 2-methoxy-4-vinylphenol, (b) 2,4-dimethylphenol, (c) Violaxanthin, (d) Squalene, (e) Glucoraphanin, (f) Ligand Protein (Ibuprofen).

5. Visualization of Ligand-Receptor Interactions

According to the ligand-protein interaction analysis after docking, ibuprofen showed good interaction with target protein COX-2 via hydrogen bonding with amino acid residues *TYR A:356* and *ARG A:121*, and hydrophobic interaction with *MET A:523*, *PHE A:519*, *VAL A:524*, *VAL A:350*, *LEU A:532*, *VAL A:117*, *LEU A:360*, and *ARG A:121*. Hydrogen bonding with these residues is critical in holding the ligand in the active site and is consistent with the binding seen with other NSAID drugs.

In addition, compared to ibuprofen, glucoraphanin showed hydrogen bonds with *ARG A:121* and *VAL A:524*, and hydrophobic interactions with *TYR A:356*, *HIS A:90*, and *ARG A:514*. These interactions indicate that glucoraphanin has a similar binding mode to ibuprofen, especially involving the participation of *ARG A:121* and *TYR A:356*.

Squalene, on the other hand, did not form hydrogen bonds but interacted with several residues solely through hydrophobic contacts (*PHE A:206*, *PHE A:210*, *PHE A:382*, *TYR A:356*, *TYR A:386*, *LEU A:353*, *LEU A:360*, *LEU A:532*, *LEU A:535*, *VAL A:117*, *VAL A:345*, *VAL A:350*, *VAL A:524*, *ALA A:528*, *MET A:523*, *PHE A:519*). Although such hydrophobic interactions may stabilize the protein-ligand complex, the lack of hydrogen bonding suggests potentially

lower binding affinity of squalene compared to ibuprofen and glucoraphanin.

The binding site of glucoraphanin largely overlaps with that of the positive control ibuprofen, suggesting a high probability for glucoraphanin to form a stable protein-ligand complex. On the contrary, squalene, which relies solely on hydrophobic interactions, may form less stable complexes and require additional evaluation to confirm its inhibitory effectiveness.

Table 4. Analysis of hydrogen bonds, hydrophobic interactions, and unfavorable interactions

No	Compound	Hydrogen Bonding	Hydrophobic Bonding	Unfavorable Interactions
1	2-methoxy-4-vinyl phenol	TYR A:356, ARG A:121	TRP A:388, LEU A:532, VAL A:524, VAL A:350, LEU A:360, ALA A:528, VAL A:117, ARG A:121	
2	2,4-dimethylphenol	MET A:523	TYR A:349, VAL A:350, TYR A:386, LEU A:353, TRP A:388, MET A:523	
3	Violaxanthin	GLY A:534	PHE A:206, VAL A:229, ALA A:528, TYR A:536, LEU A:532, LEU A:535, VAL A:350, ILE A:378, PHE A:210, VAL A:524, HIS A:90	SER A:531, PHE A:210, PHE A:382, TYR A:91, HIS A:90, ILE A:92, VAL A:89, THR A:94, LEU A:93, VAL A:524
4	Squalene		PHE A:206, PHE A:210, PHE A:382, TYR A:356, TYR A:386, LEU A:353, LEU A:360, LEU A:532, LEU A:535, VAL A:117, VAL A:345, VAL A:350, VAL A:524, ALA A:528, MET A:523, PHE A:519	
5	Glucoraphanin	ARG A:121, VAL A;524, TYR A:356, HIS A:90, ARG A:514	TYR A:356, HIS A:90	ARG A:121
6	Ibuprofen	TYR A:356, ARG A:121	MET A:523, PHE A:519, VAL A:524, VAL A:350, LEU A:532, VAL A:117, LEU A:360, ARG A;121	

According to the docking results, violaxanthin formed hydrogen bonds with *GLY A:534* and several hydrophobic contacts with residues *PHE A:206*, *VAL A:229*, *ALA A:528*, *TYR A:536*, *LEU A:532*, *LEU A:535*, *VAL A:350*, *ILE A:378*, *PHE A:210*, *VAL A:524*, and *HIS A:*. However, several steric clashes (bad bumps) were observed with residues *HIS A:90*, *SER A:531*, *PHE A:210*, *PHE A:382*, *TYR A:91*, *ILE A:92*, *VAL A:89*, *THR A:94*, *LEU A:93*, and *VAL A:524*,

indicating misalignment within the binding site.

Such a high binding energy of violaxanthin (+956924.25 kcal/mol) suggests kinetic instability or thermodynamic non-spontaneity. Generally, the more negative the binding energy, the stronger and more stable the binding; an unreasonably high positive energy implies that the ligand cannot properly bind the active site [47]. This is supported by the lack of an inhibition constant (Ki) for violaxanthin, indicating no significant inhibition [48].

Compared to ibuprofen, which shows hydrogen-bond interactions with essential residues *ARG A:121* and *TYR A:356*, violaxanthin shows difficulties stabilizing within the binding pocket. Although ibuprofen exhibits good binding energy and appropriate interaction patterns, violaxanthin appears to suffer from steric clashes, resulting in a high binding energy [49].

Therefore, despite many hydrophobic residues, the high binding energy and absence of inhibition constant for violaxanthin suggest that it is not an ideal ligand for the target protein [50]. Structural optimization or ligand modification would be necessary to relieve steric hindrance and improve binding affinity [51].

6. ADMET Analysis

Based on the docking results, ADMET analysis was performed for the two best-performing compounds, squalene and glucoraphanin. All predictions were made using the pkCSM web server based on the SMILES representation of the compounds. Squalene shows very high oral absorption in the intestine despite its poor water solubility; however, skin permeation and Blood-Brain Barrier (BBB) penetration are poor. Its metabolism is predominantly via the *CYP3A4* enzyme [52]. Squalene does not significantly inhibit other CYP enzymes but can potentially inhibit P-gp II. It exhibits a small volume of distribution and only a small unbound fraction in plasma, indicating that squalene is mostly associated with plasma proteins. Regarding toxicity, squalene has low mutagenic, hepatotoxic, and skin-sensitization risks [53]. However, it can block the hERG II ion channel, possibly affecting cardiac rhythm at high concentrations. Squalene shows low acute toxicity in rats and aquatic organisms but exhibits a slow excretion rate, suggesting prolonged residence in the body.

Glucoraphanin is poorly soluble in water and exhibits low permeability across the intestine, skin, and BBB. It shows poor oral absorption, low volume of distribution, and a low unbound plasma fraction. Its metabolism is mainly via the *CYP3A4* enzyme system without significantly inhibiting other CYP enzymes. Glucoraphanin is not associated with significant risks of mutagenesis, hepatotoxicity, or skin reactions, and shows a higher maximum tolerated dose in humans. However, it poses an environmental risk due to its toxicity toward certain aquatic organisms [54].

Table 5. Prediction of ADMET parameters from molecular docking results of the squalene and glucoraphanin compound.

Name Model	Squalene	Glucoraphanin
A1	-8.401	-2.338
A2	1.193	-681
A3	89.002	0
A4	-2.763	-2.735
A5	No	Yes
A6	No	No
A7	Yes	No
D1	0.35	-564
D2	0	692
D3	965	-1.761
D4	-935	-3.913
M1	No	No
M2	Yes	No
M3	No	No
M4	No	No
M5	No	No
M6	No	No
M7	No	No
E1	1.791	0.39
E2	No	No
T1	No	No
T2	-533	1.225
T3	No	No
T4	Yes	No
T5	1.893	2.197
T6	911	3.136
T7	No	No
T8	No	No
T9	438	285
T10	-3.275	5.557

CONCLUSION

Molecular docking analysis using the constituents of white radish to examine their anti-inflammatory effects revealed that glucoraphanin and squalene showed a strong binding affinity with the COX-2 enzyme. The pattern of interaction of glucoraphanin is similar to that of ibuprofen, while squalene depends more on hydrophobic interactions. These two agents have the potential to be selective COX-2 inhibitors.

This research offers novel clues about using white radish compounds in anti-inflammatory therapy. Both glucoraphanin and squalene exhibit higher binding affinity than the control ibuprofen, which could be more effective in the modulation of inflammation.

In addition, this result offers a way to exploit the active ingredients in white radish further. As the mode of action of these compounds is clarified, future investigations can help promote their efficacy as anti-inflammatory agents by fine-tuning their design for COX-2 affinity and efficiency

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