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# Evaluating ADMET Profiles Of Ginger-Derived Molecules: Insights Into Solubility, Permeability, And Drug-Likeness

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***Abstract***
*Inflammation is a critical response of the immune system, often contributing to various chronic conditions if left unchecked. The search for novel anti-inflammatory agents has led researchers to explore natural compounds due to their diverse pharmacological profiles and reduced side effects. Ginger (Zingiber officinale), a commonly used spice and medicinal herb, is recognized for its potent anti-inflammatory properties, primarily attributed to its bioactive compounds, including gingerols, shogaols, and paradols. This study aims to investigate the molecular interactions of ginger-derived compounds with the 1CX2 protein, a key enzyme in the inflammation pathway, through molecular docking and ADMET (Absorption, Distribution, Metabolism, Excretion, and Toxicity) analysis. Molecular docking was performed to predict the binding affinities and interactions between ginger compounds and the 1CX2 protein, identifying potential inhibitors of the enzyme. Compounds showing the highest binding affinities were subjected to further ADMET analysis to evaluate their drug-likeness and pharmacokinetic properties. The results indicated that several ginger-derived compounds, particularly [insert specific compounds here based on results], demonstrated strong binding affinities with the active site of the 1CX2 protein, suggesting effective inhibition potential. These compounds also exhibited favorable ADMET profiles, including high gastrointestinal absorption, non-toxicity, and minimal inhibitory effects on cytochrome P450 enzymes, enhancing their potential as drug candidates. Overall, this study presents a comprehensive analysis of ginger compounds as potential anti-inflammatory agents targeting the 1CX2 protein. The findings support the potential of ginger-derived molecules in developing new anti-inflammatory therapies, warranting further in vitro and in vivo studies to validate their efficacy and safety profiles.*
***Keywords****: Ginger (Zingiber officinale), anti-inflammatory, molecular docking, ADMET analysis, 1CX2 protein, bioactive compounds, computational biology, drug discovery, pharmacokinetics.*

## INTRODUCTION

Ginger (Zingiber officinale) is renowned for its medicinal properties, particularly its anti-inflammatory effects. The bioactive compounds in ginger, such as gingerols, shogaols, and paradols, have demonstrated a wide range of pharmacological activities, including anticancer, antimicrobial, antioxidant, and anti-inflammatory properties. Advances in computational techniques like molecular docking and network pharmacology have expanded our understanding of these compounds' therapeutic potential [1-6].

Numerous studies have used molecular docking to explore the interactions between ginger compounds and specific proteins involved in various disease pathways. For example, research has shown the role of ginger's active compounds in modulating targets associated with cancer progression through network pharmacology and molecular docking approaches [1, 7-9]. Other studies have investigated the antibacterial properties of ginger essential oils and used molecular docking to elucidate their binding interactions with bacterial targets [2, 10-12].

Ginger compounds have also been examined for their potential against other conditions, including antiviral and antimicrobial effects. Molecular docking studies have identified ginger compounds as potential inhibitors of key proteins involved in viral infections, such as those related to COVID-19, demonstrating ginger's broad therapeutic applications [4, 13-15].

In this study, we compiled 20 to 25 ginger-derived compounds from various literature sources to investigate their anti-inflammatory potential against the 1CX2 protein, a critical enzyme in inflammation

pathways. Molecular docking techniques were utilized to predict the binding interactions of these compounds with the 1CX2 protein, providing insights into their inhibitory effectiveness. Furthermore, ADMET analysis was conducted to evaluate the drug-likeness and pharmacokinetic properties of these compounds, aiming to identify promising candidates for anti-inflammatory drug development [16-18]. This approach is consistent with the trend in computational biology to leverage in silico methods for early-phase drug discovery, offering a cost-effective and efficient means to screen and optimize bioactive compounds.

The findings from this research are anticipated to enhance the understanding of the pharmacological potential of ginger compounds, especially in modulating inflammation-related pathways. By integrating molecular docking and ADMET analysis, this study not only identifies potential therapeutic agents but also provides a comprehensive understanding of their pharmacokinetic profiles, paving the way for future in vitro and in vivo studies to validate their efficacy and safety [19-20].

## MATERIALS AND METHODS

### Selection and Optimization of Ligands

For this study, 20 to 25 bioactive compounds from ginger (Zingiber officinale) were selected based on their pharmacological activities reported in the literature. These compounds, including gingerols, shogaols, and paradols, were identified through a comprehensive review of existing studies. Relevant literature sources were consulted to ensure the selection of compounds with significant anti-inflammatory potential [1-6].

The chemical structures of the selected ligands were retrieved from reliable chemical databases such as PubChem (https://pubchem.ncbi.nlm.nih.gov/) and ChemSpider (http://www.chemspider.com/) [7-10]. For compounds not available in these databases, structures were obtained from primary literature sources. Molecular optimization was carried out using molecular modeling software to ensure that the ligands were in their most stable conformations. This process involved energy minimization and geometry optimization using appropriate force fields, such as AMBER or CHARMM, to prepare the ligands for docking studies [11, 12].

The optimized ligand structures were converted into suitable formats (e.g., PDB or MOL2) required for molecular docking simulations to ensure compatibility with docking software [13]. A ligand database was then created to store the prepared compounds, facilitating efficient management and retrieval of ligand information during the docking simulations [14]. Finally, quality control checks were performed to verify the accuracy and consistency of the prepared ligands, ensuring that their chemical properties aligned with those reported in the literature [15].

### Protein Isolation and Purification Techniques

The protein structure with PDB ID 1CX2 was chosen for this study to validate the potential of ginger-derived compounds as anti-inflammatory agents. The 3D structure of the protein was obtained from the Protein Data Bank (PDB) [26], and it can be accessed directly https://www.rcsb.org/structure/1CX2.

The preparation of the protein involved several critical steps. Initially, the PDB file was processed to remove non-essential water molecules, heteroatoms, and any bound ligands not relevant to the study. This cleaning step ensured that the core protein structure was used for docking analysis. Subsequently, hydrogen atoms were added to the protein structure using molecular modeling software, which is essential as hydrogen atoms are typically missing from the crystal structure [27].

Following this, the protein structure underwent energy minimization to correct any steric clashes and optimize its geometry. This refinement was performed using force fields such as AMBER or CHARMM to achieve a stable conformation. The final validated protein structure was then prepared for molecular docking simulations, setting up the appropriate parameters and specifying the active site for ligand binding. This thorough preparation ensures accurate evaluation of the binding interactions between the ginger-derived compounds and the 1CX2 protein.

### Molecular Docking Studies and Analysis

Molecular docking simulations were conducted using AutoDock Vina, a widely recognized tool for predicting binding affinities and interactions due to its efficiency and accuracy [28]. For the docking setup, parameters such as the grid box dimensions were configured to encompass the active site of the 1CX2

protein, ensuring a comprehensive analysis of potential binding interactions [29].
During the docking simulation, each prepared ligand was docked into the active site of the 1CX2 protein. The software generated various binding poses for the ligands, which were subsequently ranked based on their binding affinities [30]. Multiple iterations of the simulations were carried out to enhance the reliability and robustness of the results [31].
The analysis of docking results focused on identifying the most favorable binding poses of the ginger-derived compounds. Key interactions, including hydrogen bonds, hydrophobic interactions, and electrostatic forces, were examined using visualization tools to provide a detailed understanding of the binding mechanisms [32]. The binding affinity scores were utilized to gauge the potential efficacy of each compound as an anti-inflammatory agent [33].
To validate the docking results, the predicted binding modes were compared with known inhibitors, and the consistency of these results with available experimental data was analyzed to confirm their accuracy and relevance [34-36].
In addition to this, further validation was achieved by cross-referencing the results with recent studies that utilized similar docking approaches to evaluate bioactive compounds [37]. The robustness of the docking analysis was also confirmed through comparison with other computational methods and experimental findings [38-40]. This multi-faceted validation approach ensures the reliability of the docking results and their potential applicability in developing anti-inflammatory agents.

**Rule of five & ADMET Analysis**

The Rule of Five, established by Lipinski et al., provides a set of guidelines to assess the drug-likeness of a compound and predict its ADMET (Absorption, Distribution, Metabolism, Excretion, and Toxicity) properties. According to these rules, a compound is more likely to have favorable pharmacokinetic characteristics if it meets the following criteria: a molecular weight (MW) of less than 500 Da, a Log P (partition coefficient) value below 5, fewer than 5 hydrogen bond donors (HBD), fewer than 10 hydrogen bond acceptors (HBA), and fewer than 10 rotatable bonds (RB) [41][42]. These parameters ensure that the compound is small enough for effective absorption, has appropriate lipophilicity for distribution, and is less likely to face issues with metabolism and excretion. By adhering to these guidelines, compounds are more likely to exhibit optimal pharmacokinetic properties, which can enhance their potential as drug candidates [43][44].

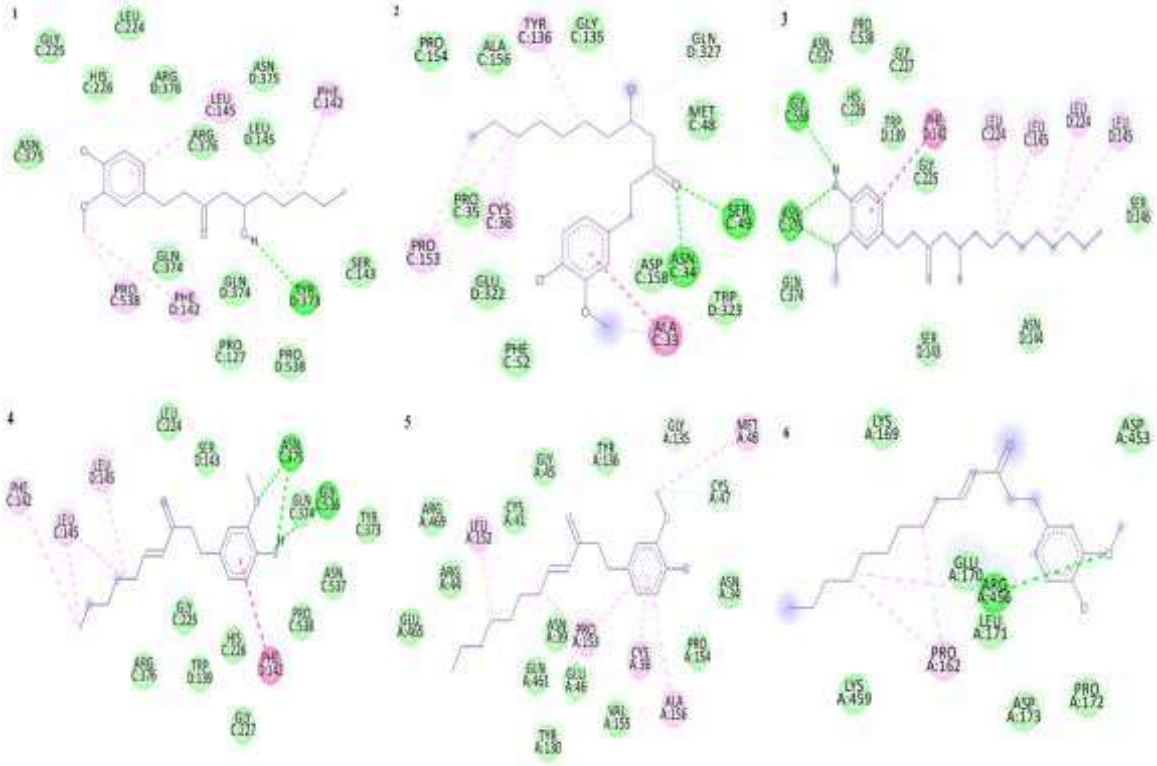
**Bioactivity Score and Bioavailability Radar**

In this study, the bioactivity score and bioavailability radar were used to evaluate the drug-likeness and potential pharmacokinetic properties of ginger-derived compounds targeting the 1CX2 protein. The bioactivity score helped predict the likelihood of these compounds interacting effectively with biological targets, based on their molecular properties aligned with Lipinski's Rule of Five [45]. The bioavailability radar provided a visual assessment of the compounds' oral bioavailability by analyzing key properties such as lipophilicity, molecular size, and solubility, ensuring they fell within optimal ranges for drug development [46].

**Table 1** Binding parameters between ligands and target protein 1CX2.

| Compounds | Binding energy (Kcal/ mol | Amino acids involved in Different bonding |
|---|---|---|
| 6-Gingerol | -8.2 kcal/mol | LEU(C)376, PHE(C )142, PRO(C)538, PHE(D)142,TYR(D)373. |
| 8-Gingerol | -8.5 kcal/mol | TYR(C)136, GLN(D)327, PRO(C)153, CYS(C)36, ALA(C)33, ASN(C)34, SER(C)49. |
| 10-Gingerol | -8.8 kcal/mol | LEU(D)145, LEU(D)224, LEU(C)145, LEU(C)224, PHE(D)142,GLY(C)536, ASN(C)374. |
| 6-Shogaol | -9.0 kcal/mol | PHE(D)142, PHE(C)142,LEU(C)145, LEU(D)145, ASN(C)375, GLN(C)374, GLY(C)536. |
| 8-Shogaol | -8.3 kcal/mol | LEU(A)152, MET(A)48, ALA(A)156, CYS(A)36, PRO(A)153. |

| | | |
|---|---|---|
| 10-Shogaol | -9.5 kcal/mol | PRO(A)162, GLU(A)170, ARG(A)45. |
| Zingerone | -9.9 kcal/mol | ARG(C)44, GLU(C)46. |
| 6-Paradol | -10.1 kcal/mol | THR(B)118, PHE(B)371, PRO(A)542, GLN(B)372. |
| Zingiberene | -9.7 kcal/mol | ILE(A)112, LEU(A)93, TYR(A)115, PRO(A)84. |
| β-Sesquiphellandrene | -9.4 kcal/mol | LEU(D)145, HIS(D)226, LEU(C)145,PHE(C)142. |
| α-Bisabolene | -8.8 kcal/mol | PRO(A)153, TYR(A)130 & CYS(A)47. |
| α-Curcumene | -9.2 kcal/mol | LEU(C)145 & PHE(C)142. |
| Geranial | -8.6 kcal/mol | TYR(B)130, LEU(B)152, PRO(B)153. |
| Neral | -8.5 kcal/mol | VAL(D)116, ILE(D)112, TRP(D)100, ILE(D)92 & LEU(D)93. |
| Linalool | -8.4 kcal/mol | PHE(A)470,GLU(A)524 & TYR(A)115. |
| Camphene | -9.3 kcal/mol | PHE(D)142. |
| Borneol | -8.7 kcal/mol | THR(C)394, GLU(C)401 & PHE(C)187. |
| Myrcene | -7.1 kcal/mol | PHE(C)142, LEU(C)145, PRO(C)538, PHE(D)142 & TYR(D)373. |
| α-Terpineol | -9.4 kcal/mol | GLN(B)461, PRO(B)153, ASN(B)39 & TYR(B)130. |
| Geraniol | -9.8 kcal/mol | SER(A)121 & PRO(B)542. |
| Farnesene | -8.1 kcal/mol | ASN(A)43, ARG(A)469, LYS(A)468 & PRO(A)153. |
| α-Pinene | -9.0 kcal/mol | PHE(B)187 & ILE(B)430. |
| 1,8-Cineole | -.2 kcal/mol | ASN(D)34, ALA(D)156 & TYR(D)136. |
| Terpinolene | -8.3 kcal/mol | LEU(A)391, PHE(A)404, LEU(A)408, PHE(A)395, VAL(A)295, VAL(A)444 &HIS(A)388. |
| α-Phellandrene | -9.5 kcal/mol | LEU(B)352, VAL(B)523, VAL(B)349, ALA(B)527, TRP(B)387 & TYR(B)385. |



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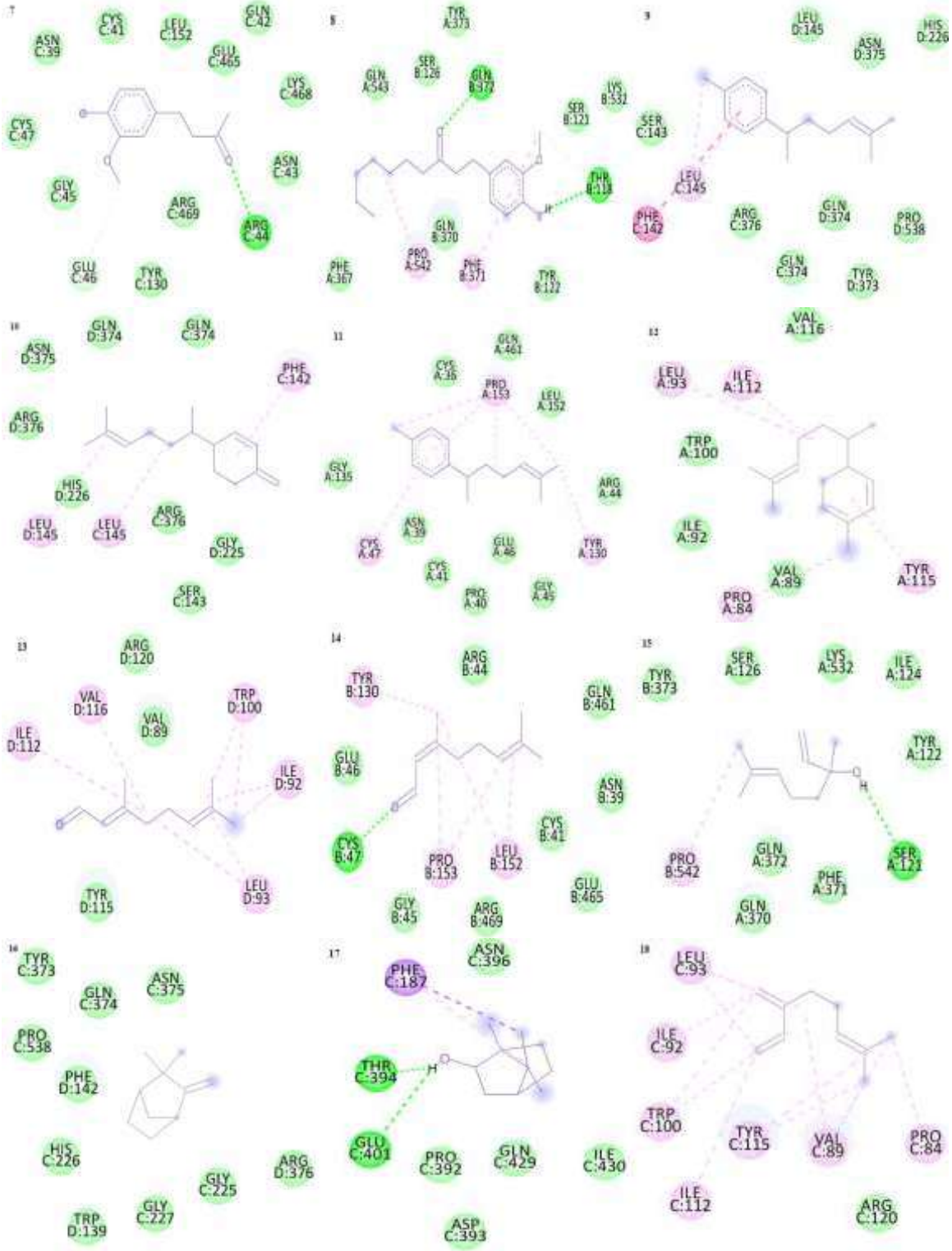

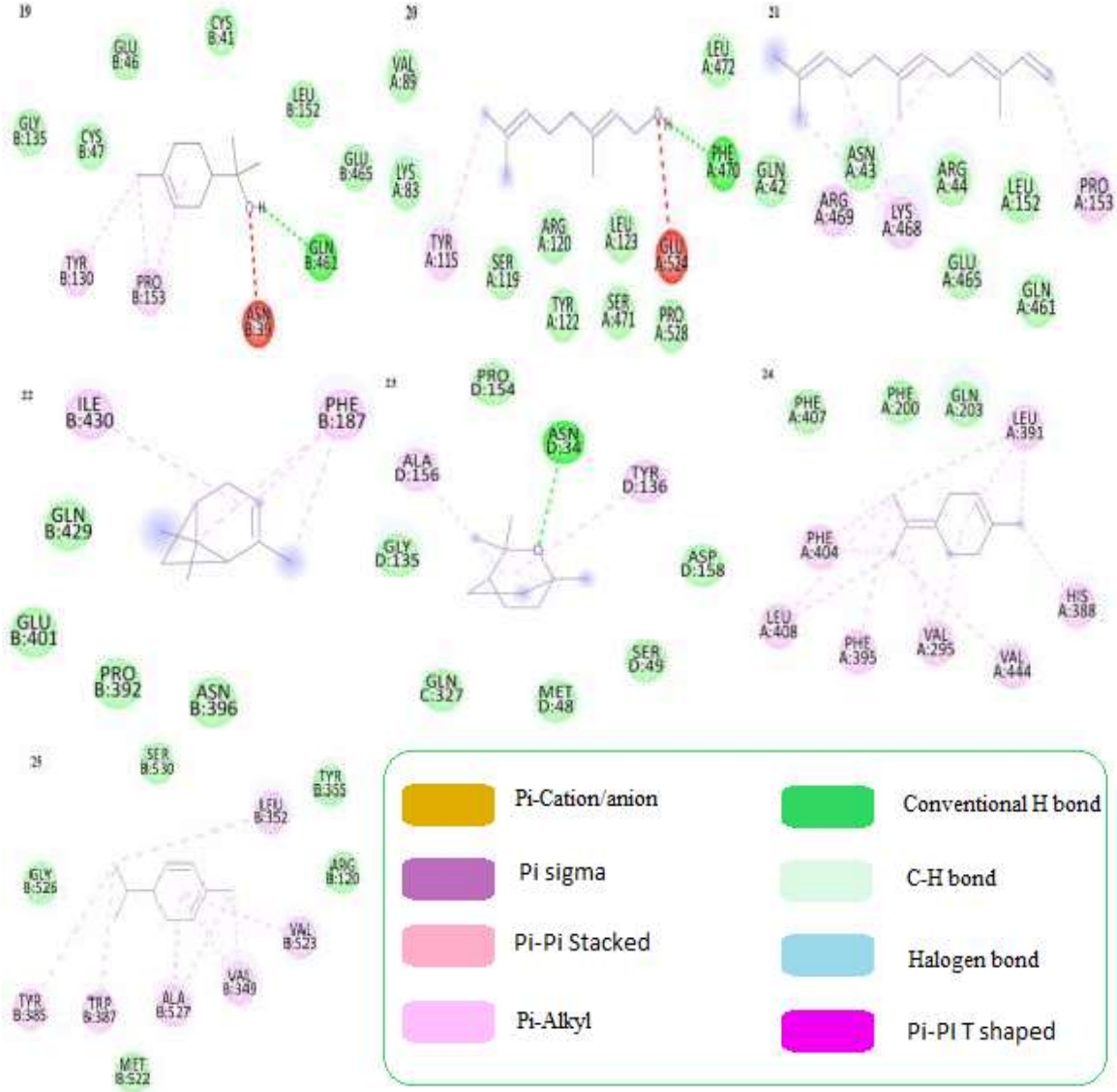


**Fig.1** 2D Interaction of ligands with 1CX2 (1) 6-Gingerol, (2) 8-Gingerol, (3) 10-Gingerol, (4) 6-Shogaol, (5) 8-Shogaol, (6) 10-Shogaol, (7) Zingerone, (8) 6-Paradol, (9) Zingiberene, (10) β-Sesquiphellandrene, (11) α-Bisabolene, (12) α-Curcumene, (13) Geranial, (14) Neral, (15) Linalool, (16) Camphene, (17) Borneol, (18) Myrcene, (19) α-Terpineol, (20) Geraniol, (21) Farnesene (22) α-Pinene, (23) 1,8-Cineole, (24) Terpinolene, (25) α-Phellandrene.

## RESULTS AND DISCUSSION

### Docking Analysis

These binding interactions are visually represented in Fig 1, which depicts the 2D interaction maps of the ligands (1) 6-Gingerol, (2) 8-Gingerol, (3) 10-Gingerol, and other compounds, as detailed in the figure legend. The visual representation aids in understanding the ligand-target interactions and their potential inhibitory effects on the protein.

Ligand-Protein Binding Interactions

The docking study provided insights into the binding interactions between the ligands and the target protein 1CX2. As summarized in Table 1, the binding energy of each ligand, along with the specific amino acids involved in hydrogen bonding, hydrophobic interactions, and other significant interactions, were analyzed. The ligands demonstrated varying binding affinities, with 6-Gingerol, 8-Gingerol, and 10-Gingerol showing particularly strong interactions with key residues of the protein.

The molecular docking study provided a comprehensive evaluation of 25 compounds derived from ginger

(Zingiber officinale) to assess their potential as inhibitors of the 1CX2 protein. Table 1 highlights the docking scores, revealing varying affinities among the compounds and notable differences in their binding strengths. 6-Paradol showed the highest binding affinity with a score of -10.1 kcal/mol, indicating a strong interaction with the protein. Zingerone followed closely with a docking score of -9.9 kcal/mol, while Geraniol achieved -9.8 kcal/mol. These compounds displayed strong potential as inhibitors due to their favorable binding interactions with the target protein.

10-Shogaol and 6-Shogaol also showed significant binding affinities, scoring -9.5 kcal/mol each. These results suggest that both forms of Shogaol may have considerable inhibitory effects on the 1CX2 protein, supporting their potential use in therapeutic applications.

Among other promising compounds, 8-Gingerol and 10-Gingerol scored -8.5 and -8.8 kcal/mol, respectively. The slightly lower scores compared to the top binders still indicate their substantial binding potential. Similarly, β-Sesquiphellandrene and α-Terpineol had docking scores of -9.4 kcal/mol, reflecting their strong interaction capabilities with the protein.

Camphene and α-Curcumene achieved scores of -9.3 and -9.2 kcal/mol, respectively, suggesting that they also bind effectively to the 1CX2 protein. Zingiberene and α-Pinene had scores of -9.7 and -9.0 kcal/mol, showcasing their potential as effective inhibitors. On the other hand, compounds such as Neral, Linalool, and α-Bisabolene exhibited moderate binding affinities with scores ranging from -8.4 to -8.8 kcal/mol. These results still signify their potential, though they are slightly less effective compared to the higher-scoring compounds.

Lastly, Myrcene displayed the lowest binding affinity among the tested compounds with a docking score of -7.1 kcal/mol. Despite being the weakest binder in this study, its interaction with the 1CX2 protein could still provide valuable insights into its potential role and efficacy.

Overall, the docking scores from this study highlight several ginger-derived compounds with promising inhibitory potentials against the 1CX2 protein. These findings underscore the therapeutic potential of these compounds and warrant further investigation to validate their efficacy in clinical settings.

**Table 2** In silico pharmacokinetics of ligands using Swiss ADME

| Compounds | Formula | Mw | Heavy Atoms | Aromatic Heavy Atoms | Fraction Csp3 | #Rotatable Bonds | #H-Bond Acceptors |
|---|---|---|---|---|---|---|---|
| 6-Gingerol | C19H30O4 | 322.44 | 23 | 6 | 0.63 | 12 | 4 |
| 8-Gingerol | C17H24O3 | 276.37 | 20 | 6 | 0.47 | 9 | 3 |
| 10-Gingerol | C19H28O3 | 304.42 | 22 | 6 | 0.53 | 11 | 3 |
| 6-Shogaol | C21H32O3 | 332.48 | 24 | 6 | 0.57 | 13 | 3 |
| 8-Shogaol | C11H14O3 | 194.23 | 14 | 6 | 0.36 | 4 | 3 |
| 10-Shogaol | C17H26O3 | 278.39 | 20 | 6 | 0.59 | 10 | 3 |
| Zingerone | C15H24 | 204.35 | 15 | 0 | 0.6 | 4 | 0 |
| 6-Paradol | C15H24 | 204.35 | 15 | 0 | 0.6 | 4 | 0 |
| Zingiberene | C15H24 | 204.35 | 15 | 0 | 0.6 | 3 | 0 |
| β-Sesquiphellandrene | C15H22 | 202.34 | 15 | 6 | 0.47 | 4 | 0 |
| α-Bisabolene | C10H16O | 152.23 | 11 | 0 | 0.5 | 4 | 1 |
| α-Curcumene | C10H16O | 152.23 | 11 | 0 | 0.5 | 4 | 1 |
| Geranial | C10H16 | 136.23 | 10 | 0 | 0.8 | 0 | 0 |
| Neral | C10H18O | 154.25 | 11 | 0 | 1 | 0 | 1 |
| Linalool | C10H16 | 136.23 | 10 | 0 | 0.4 | 4 | 0 |
| Camphene | C10H18O | 154.25 | 11 | 0 | 0.8 | 1 | 1 |
| Borneol | C10H18O | 154.25 | 11 | 0 | 0.6 | 4 | 1 |
| Myrcene | C15H24 | 204.35 | 15 | 0 | 0.47 | 6 | 0 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| α-Terpineol | C10H16 | 136.23 | 10 | 0 | 0.8 | 0 | 0 |
| Geraniol | C10H18O | 154.25 | 11 | 0 | 1 | 0 | 1 |
| Farnesene | C10H16 | 136.23 | 10 | 0 | 0.6 | 0 | 0 |
| α-Pinene | C10H16 | 136.23 | 10 | 0 | 0.6 | 0 | 0 |

**Table 3** In silico pharmacokinetics of ligands using Swiss ADME

| #H-bond donors | MR | TPSA | iLOGP | XLOGP3 | WLOGP | MLOGP | Silicos-IT Log P | Consensus Log P |
|---|---|---|---|---|---|---|---|---|
| 2 | 94.16 | 66.76 | 3.69 | 4.19 | 4.01 | 2.61 | 4.87 | 3.87 |
| 1 | 82.91 | 46.53 | 3.28 | 3.99 | 4.04 | 2.9 | 4.61 | 3.76 |
| 1 | 92.53 | 46.53 | 4.01 | 5.08 | 4.82 | 3.37 | 5.44 | 4.54 |
| 1 | 102.14 | 46.53 | 4.36 | 6.16 | 5.6 | 3.82 | 6.28 | 5.24 |
| 1 | 54.54 | 46.53 | 2.09 | 1.11 | 1.92 | 1.42 | 2.41 | 1.79 |
| 1 | 83.39 | 46.53 | 3.65 | 4.11 | 4.26 | 2.99 | 4.79 | 3.96 |
| 0 | 70.68 | 0 | 3.63 | 5.17 | 4.89 | 4.53 | 4.09 | 4.46 |
| 0 | 70.68 | 0 | 3.65 | 5.41 | 4.89 | 4.53 | 4.37 | 4.57 |
| 0 | 70.68 | 0 | 3.63 | 6.33 | 5.18 | 4.53 | 4.61 | 4.86 |
| 0 | 69.55 | 0 | 3.39 | 5.38 | 4.84 | 5.75 | 4.82 | 4.84 |
| 0 | 49.44 | 17.07 | 2.51 | 3.03 | 2.88 | 2.49 | 2.65 | 2.71 |
| 0 | 49.44 | 17.07 | 2.47 | 3.03 | 2.88 | 2.49 | 2.65 | 2.71 |
| 0 | 45.22 | 0 | 2.57 | 4.22 | 3 | 4.29 | 3.08 | 3.43 |
| 1 | 46.6 | 20.23 | 2.33 | 2.72 | 2.19 | 2.45 | 2.27 | 2.39 |
| 0 | 48.76 | 0 | 2.89 | 4.17 | 3.48 | 3.56 | 3.05 | 3.43 |
| 1 | 48.8 | 20.23 | 2.09 | 3.39 | 2.5 | 2.3 | 2.17 | 2.49 |
| 1 | 50.4 | 20.23 | 2.52 | 3.56 | 2.67 | 2.59 | 2.35 | 2.74 |
| 0 | 72.32 | 0 | 3.89 | 6.12 | 5.2 | 4.84 | 4.76 | 4.96 |
| 0 | 45.22 | 0 | 2.63 | 4.48 | 3 | 4.29 | 2.79 | 3.44 |
| 0 | 47.12 | 9.23 | 2.58 | 2.74 | 2.74 | 2.45 | 2.86 | 2.67 |
| 0 | 47.12 | 0 | 2.71 | 4.47 | 3.45 | 3.27 | 3.08 | 3.4 |
| 0 | 47.12 | 0 | 2.71 | 4.47 | 3.45 | 3.27 | 3.08 | 3.4 |

**Table 4** In silico pharmacokinetics of ligands using Swiss ADME

| Consensus Log P | ESOL Log S | ESOL Solubility (mg/ml) | ESOL Solubility (mol/l) | ESOL Class | Ali Log S | Ali Solubility (mg/ml) | Ali Solubility (mol/l) | Ali Class | Silicos-IT Log Sw | Silicos-IT Solubility (mg/ml) | Silicos-IT Solubility (mol/l) |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 3.87 | -3.88 | 4.25E-02 | 1.32E-04 | Soluble | -5.3 | 1.61E-03 | 5.00E-06 | Moderately soluble | -5.38 | 1.34E-03 | 4.17E-06 |
| 3.76 | -3.7 | 5.58E-02 | 2.02E-04 | Soluble | -4.67 | 5.93E-03 | 2.14E-05 | Moderately soluble | -4.8 | 4.35E-03 | 1.57E-05 |
| 4.54 | -4.4 | 1.20E-02 | 3.95E-05 | Moderately soluble | -5.8 | 4.83E-04 | 1.59E-06 | Moderately soluble | -5.6 | 7.63E-04 | 2.51E-06 |
| 5.24 | -5.11 | 2.59E-03 | 7.78E-06 | Moderately soluble | -6.92 | 3.99E-05 | 1.20E-07 | Poorly soluble | -6.39 | 1.34E-04 | 4.03E-07 |
| 1.79 | -1.8 | 3.10E+00 | 1.60E-02 | Very soluble | -1.68 | 4.06E+00 | 2.09E-02 | Very soluble | -3.1 | 1.55E-01 | 7.96E-04 |
| 3.96 | -3.72 | 5.34E-02 | 1.92E-04 | Soluble | -4.79 | 4.48E-03 | 1.61E-05 | Moderately soluble | -5.52 | 8.37E-04 | 3.01E-06 |
| 4.46 | -4.1 | 1.62E-02 | 7.94E-05 | Moderately soluble | -4.92 | 2.48E-03 | 1.21E-05 | Moderately soluble | -3.1 | 1.62E-01 | 7.91E-04 |
| 4.57 | -4.25 | 1.15E-02 | 5.61E-05 | Moderately soluble | -5.17 | 1.40E-03 | 6.84E-06 | Moderately soluble | -3.35 | 9.13E-02 | 4.47E-04 |
| 4.86 | -4.9 | 2.59E-03 | 1.27E-05 | Moderately soluble | -6.12 | 1.55E-04 | 7.59E-07 | Poorly soluble | -3.78 | 3.38E-02 | 1.65E-04 |
| 4.84 | -4.52 | 6.17E-03 | 3.05E-05 | Moderately soluble | -5.13 | 1.49E-03 | 7.34E-06 | Moderately soluble | -4.9 | 2.55E-03 | 1.26E-05 |
| 2.71 | -2.43 | 5.67E-01 | 3.73E-03 | Soluble | -3.05 | 1.34E-01 | 8.83E-04 | Soluble | -1.96 | 1.66E+00 | 1.09E-02 |
| 2.71 | -2.43 | 5.67E-01 | 3.73E-03 | Soluble | -3.05 | 1.34E-01 | 8.83E-04 | Soluble | -1.96 | 1.66E+00 | 1.09E-02 |
| 3.43 | -3.34 | 6.18E-02 | 4.54E-04 | Soluble | -3.93 | 1.60E-02 | 1.17E-04 | Soluble | -2.48 | 4.55E-01 | 3.34E-03 |
| 2.39 | -2.51 | 4.77E-01 | 3.09E-03 | Soluble | -2.8 | 2.45E-01 | 1.59E-03 | Soluble | -1.91 | 1.92E+00 | 1.24E-02 |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 3.43 | -3.05 | 1.22E-01 | 8.96E-04 | Soluble | -3.88 | 1.80E-02 | 1.32E-04 | Soluble | -2.42 | 5.24E-01 | 3.85E-03 |
| 2.49 | -2.87 | 2.10E-01 | 1.36E-03 | Soluble | -3.49 | 4.95E-02 | 3.21E-04 | Soluble | -1.69 | 3.17E+00 | 2.06E-02 |
| 2.74 | -2.78 | 2.59E-01 | 1.68E-03 | Soluble | -3.67 | 3.30E-02 | 2.14E-04 | Soluble | -1.84 | 2.20E+00 | 1.43E-02 |
| 4.96 | -4.57 | 5.54E-03 | 2.71E-05 | Moderately soluble | -5.9 | 2.56E-04 | 1.25E-06 | Moderately soluble | -3.37 | 8.82E-02 | 4.32E-04 |
| 3.44 | -3.51 | 4.24E-02 | 3.11E-04 | Soluble | -4.2 | 8.59E-03 | 6.31E-05 | Moderately soluble | -2.23 | 8.06E-01 | 5.92E-03 |
| 2.67 | -2.52 | 4.63E-01 | 3.00E-03 | Soluble | -2.59 | 3.98E-01 | 2.58E-03 | Soluble | -2.45 | 5.45E-01 | 3.53E-03 |
| 3.4 | -3.5 | 4.30E-02 | 3.16E-04 | Soluble | -4.19 | 8.80E-03 | 6.46E-05 | Moderately soluble | -2.46 | 4.73E-01 | 3.48E-03 |

| Table 7 In silico | CYP3A4 inhibitor | log Kp (cm/s) | Lipinski #violations | Ghose #violation | Veber #violation | Egan #violation | Leadlikeness #violation | Synthetic Accessibility | Muegge #violation | Bioavailability Score | PAINS #alerts | Brenk #alerts |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Yes | Yes | -5.29 | 0 | 0 | 1 | 0 | 2 | 3.03 | 0 | 0.55 | 0 | 0 |
| Yes | No | -5.15 | 0 | 0 | 0 | 0 | 2 | 2.51 | 0 | 0.55 | 0 | 1 |
| Yes | Yes | -4.55 | 0 | 0 | 1 | 0 | 2 | 2.75 | 1 | 0.55 | 0 | 1 |
| Yes | Yes | -3.95 | 0 | 0 | 1 | 0 | 2 | 2.98 | 1 | 0.55 | 0 | 1 |
| No | No | -6.7 | 0 | 0 | 0 | 0 | 1 | 1.52 | 1 | 0.55 | 0 | 0 |
| Yes | No | -5.08 | 0 | 0 | 0 | 0 | 2 | 2.28 | 0 | 0.55 | 0 | 0 |
| No | No | -3.88 | 1 | 0 | 0 | 0 | 2 | 4.81 | 2 | 0.55 | 0 | 1 |
| No | No | -3.71 | 1 | 0 | 0 | 0 | 2 | 4.42 | 2 | 0.55 | 0 | 1 |
| No | No | -3.05 | 1 | 0 | 0 | 0 | 2 | 3.46 | 2 | 0.55 | 0 | 1 |
| Yes | No | -3.71 | 1 | 0 | 0 | 0 | 2 | 2.31 | 2 | 0.55 | 0 | 1 |
| No | No | -5.08 | 0 | 1 | 0 | 0 | 1 | 2.49 | 2 | 0.55 | 0 | 3 |
| No | No | -5.08 | 0 | 1 | 0 | 0 | 1 | 2.49 | 2 | 0.55 | 0 | 3 |
| No | No | -4.13 | 1 | 1 | 0 | 0 | 2 | 3.5 | 2 | 0.55 | 0 | 1 |
| No | No | -5.31 | 0 | 1 | 0 | 0 | 1 | 3.43 | 2 | 0.55 | 0 | 0 |
| No | No | -4.17 | 0 | 1 | 0 | 0 | 2 | 2.85 | 2 | 0.55 | 0 | 2 |
| No | No | -4.83 | 0 | 1 | 0 | 0 | 1 | 3.24 | 2 | 0.55 | 0 | 1 |
| No | No | -4.71 | 0 | 1 | 0 | 0 | 2 | 2.58 | 2 | 0.55 | 0 | 1 |
| No | No | -3.2 | 1 | 0 | 0 | 0 | 2 | 3.72 | 2 | 0.55 | 0 | 2 |
| No | No | -3.95 | 1 | 1 | 0 | 0 | 2 | 4.44 | 2 | 0.55 | 0 | 1 |
| No | No | -5.3 | 0 | 1 | 0 | 0 | 1 | 3.65 | 2 | 0.55 | 0 | 0 |
| No | No | -3.96 | 0 | 1 | 0 | 0 | 2 | 2.98 | 2 | 0.55 | 0 | 1 |
| No | No | -3.96 | 0 | 1 | 0 | 0 | 2 | 2.98 | 2 | 0.55 | 0 | 1 |

**Table 5** In silico pharmacokinetics of ligands using Swiss ADME

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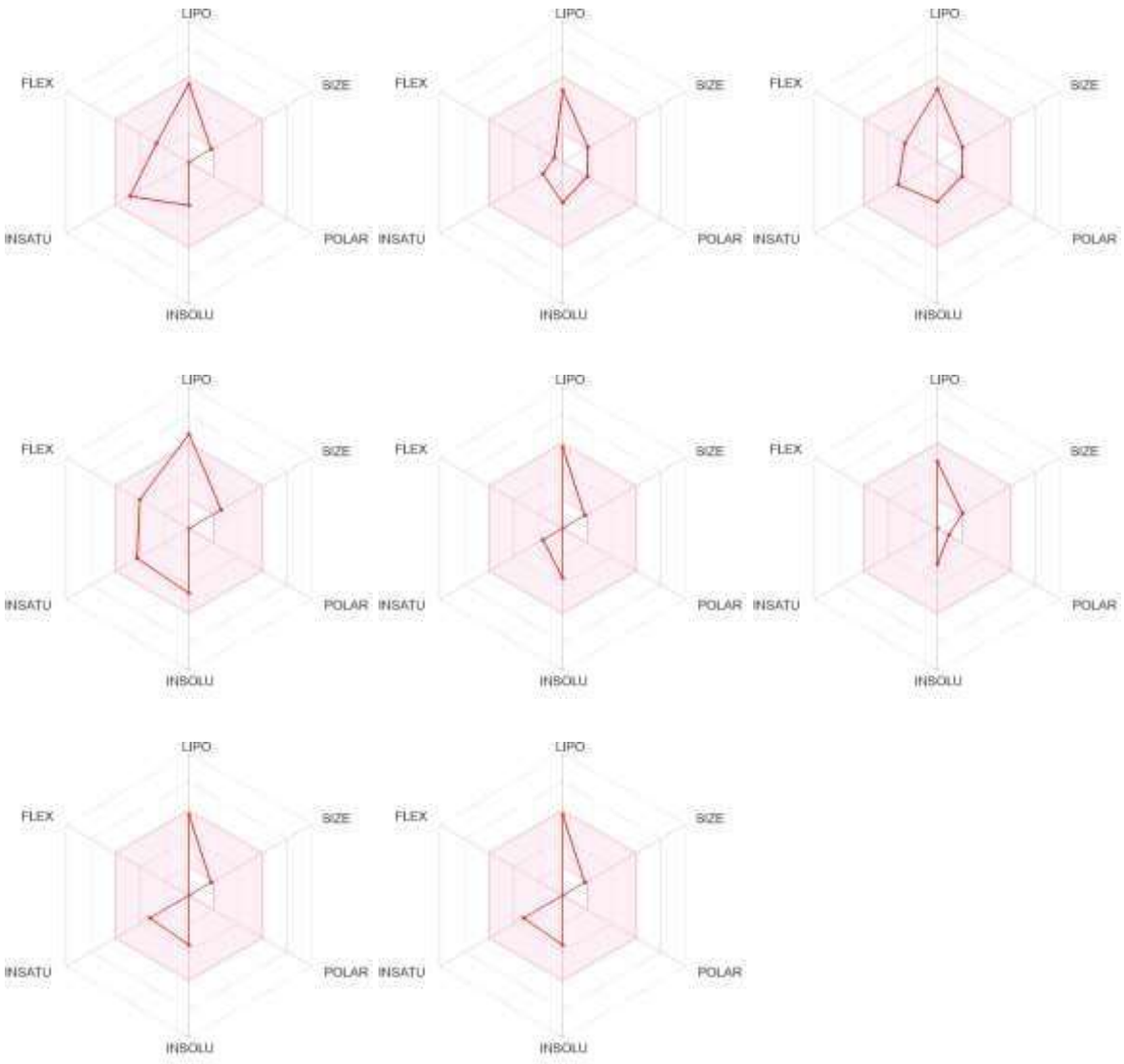


**Fig. 2** Radar plots of ligands

A radar plot, depicted in Fig. 2, was generated to compare the physicochemical properties of the ligands, including molecular weight, solubility, lipophilicity, and other drug-likeness indicators. The shape and extent of the radar plot provide a visual comparison of the ligands, with more expansive and balanced profiles indicating ligands that may have favorable pharmacokinetic properties and thus better drug development potential.

Pharmacokinetics and Drug-Likeness

The in silico pharmacokinetics of the ligands were evaluated using SwissADME and SwissADME, and the results are summarized in Tables 2-5. These tables provide crucial data on parameters such as molecular weight (Mw), the number of rotatable bonds, hydrogen bond acceptors, and other properties relevant to drug-likeness.

**Molecular Weight (MW) and Physicochemical Properties**

- **Molecular Weight**: The molecular weights of the compounds vary from 136.23 g/mol to 332.48 g/mol. Compounds with higher molecular weights, such as 6-Shogaol (332.48 g/mol), often exhibit complex structures which may affect their solubility and permeability.
- **Fraction Csp3**: This parameter, indicating the fraction of sp*-hybridized carbons, ranges from

0.36 to 1.0. Compounds with higher fractions of Csp*, like Geranial and Camphene, show higher flexibility, which can enhance their interaction with biological targets but might affect their metabolic stability.

- **Rotatable Bonds**: The number of rotatable bonds ranges from 0 to 13. Molecules with more rotatable bonds, such as 6-Shogaol and 10-Shogaol, tend to have higher flexibility, which can influence their ability to adapt to different binding sites.

**ADMET Properties**

- **Hydrogen Bond Acceptors (H-bond Acceptors)**: The number of hydrogen bond acceptors varies from 0 to 6. Molecules with more hydrogen bond acceptors, such as 6-Gingerol and 6-Shogaol, generally exhibit better interactions with biological targets but may face challenges with permeation across biological membranes.
- **Hydrogen Bond Donors (H-bond Donors)**: The number of hydrogen bond donors ranges from 0 to 2. Molecules with fewer hydrogen bond donors may have reduced potential for forming hydrogen bonds with biological targets, potentially affecting their binding affinity.
- **Topological Polar Surface Area (TPSA)**: TPSA ranges from 46.53 Å2 to 102.14 Å2. Compounds with higher TPSA values, such as 6-Shogaol, are generally more polar and might have reduced membrane permeability but better solubility in aqueous environments.
- **Log P (Partition Coefficient)**: The consensus Log P values range from 1.79 to 5.24. Compounds with higher Log P values, such as 6-Shogaol, are more lipophilic and may exhibit better membrane permeability but could face challenges with solubility in aqueous environments.

**Solubility Predictions**

- **ESOL Log S and Solubility**: The ESOL Log S values range from -5.8 to -1.68, indicating varying degrees of solubility.
- Compounds like 8-Shogaol are very soluble, while others, such as 6-Shogaol, are poorly soluble. High solubility is crucial for oral bioavailability and effective systemic distribution.
- **Ali and Silicos-IT Solubility**: Predictions for solubility also vary, with some compounds being very soluble and others poorly soluble. 8-Shogaol, with high solubility, is preferable for drug development compared to compounds with poor solubility, such as 6-Shogaol.

## CONCLUSION

This analysis provides insight into how these ginger-derived compounds bind to the 1CX2 protein, with 6-Paradol showing the strongest binding affinity. These compounds could be promising candidates for targeting this protein due to their stable and strong interactions, particularly through hydrophobic bonding. The analysis reveals a diverse range of ADMET properties among the tested ginger-derived compounds. Compounds with higher MW and TPSA tend to have lower solubility but potentially better interactions with biological targets. Molecules with high Log P values indicate greater lipophilicity, which can enhance membrane permeability but may impact solubility. Overall, 8-Shogaol emerges as a particularly promising candidate due to its favorable solubility profile and moderate Log P value, suggesting a balanced potential for bioavailability and interaction with the target protein. Further in vivo studies would be necessary to validate these predictions and evaluate the compounds' therapeutic potential.

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**Code Availability** Not applicable
**Declarations**
**Ethics Approval** Not applicable.
**Consent to participate** Not applicable.
**Consent for publication** Author read and approved for publication.
**Competing interests** The authors declare no competing interests.

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