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Molecular Docking and Physicochemical Profiling of Selected Natural Phenolics for Supporting Color Stability in Goat Meat

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ABSTRACT

Stability of meat color is an important quality trait that impacts consumer acceptance of fresh meat products. The oxidative transformation of myoglobin to metmyoglobin is the major cause of color deterioration throughout storage. Natural phenolic compounds have gained interest as potential antioxidants and can play a role in stabilizing the pigment proteins, consequently prolonging oxidative processes. This study used molecular docking and physicochemical profiling to evaluate the interaction of gallic acid, naringenin, and rosmarinic acid with metmyoglobin (PDB ID: 1YMB). In this study the computational model was used to simulate docking, assess binding affinity and interaction modes at the heme-associated pocket of protein has been done by AutoDock Vina. The observed order of binding energies followed the results as rosmarinic acid (–6.7 kcal/mol) > naringenin (–6.0 kcal/mol) > gallic acid (–4.6 kcal/mol), revealed to a greater interaction potential when comparing larger polyphenolic structures. Analysis of the interaction showed that rotamer rotations of ligands made hydrogen bonding and electrostatic contacts with important residues near to the binding pocket, including Asp109, His113, Ile112, Arg31 and Arg139. SwissADME analysis using for physicochemical properties of the compounds,, also indicated differences between each compound; gallic acid was found to have very polar, high solubility properties, which were confirmed by the naringenin molecule which demonstrated balanced lipophilicity without being too headache inducing and rosmarinic acid displayed having optimal hydrogen bonding capacity and molecular size. These results offer a molecular-level basis for considering the application of natural phenolic compounds as a means to augment pigment stability within meat systems, though experimental confirmation is needed in order to assess practical applicability.
Keywords: Meat color stability; Metmyoglobin; Molecular docking; Phenolic compounds; Natural antioxidants

Introduction

The colour of meat is an important quality factor and the first characteristic that a consumer evaluates, as they primarily purchase meat based on a number of appearance attributes such as the colour of the lean portion. Consumers

can easily perceive differences in the colour of meat and are strongly associated with the purchase intention. Color of meat is an important quality attribute that greatly impacts consumers' perceptions on freshness and acceptability for red meat products (Rizwan et al., 2024, Suman and Joseph, 2013, Carpenter et al., 2001)

The characteristic red color primarily arises from **myoglobin**, a heme-containing protein in muscle whose redox state governs the visible pigment. In the fresh postmortem state, myoglobin exists mainly in its reduced ferrous forms (deoxymyoglobin and oxymyoglobin), which impart desirable red hues to meat. Over time, myoglobin can be oxidized to **metmyoglobin**, a ferric form that causes brown discoloration and is closely associated with color deterioration during storage (Su et al., 2024, Zhu et al., 2024). This oxidation process, which destabilizes the heme environment, contributes significantly to quality loss and reduced consumer appeal in meats such as goat and beef . (Suman and Joseph, 2013, Abdizadeh et al., 2020)

Oxidation reactions in muscle foods are not limited to pigments alone but are interconnected with lipid oxidation processes, which can accelerate myoglobin oxidation and contribute further to quality deterioration, the control and minimization of lipid oxidation in meat and meat products is of great interest to the food industry. (Solva and Lannes, 2018)

Meat scientists have increasingly focused on strategies that mitigate oxidative damage in order to maintain color stability, extend shelf life, and reduce economic loss in the meat industry. (Domínguez et al., 2019) Among these strategies, the incorporation of natural antioxidants has gained attention, driven both by consumer preference for natural additives and by restrictions on synthetic antioxidant use (Luo et al., 2025, Domínguez et al., 2019) Phenolic compounds extracted from plants have demonstrated antioxidant activity through radical scavenging and metal chelation, and have been shown to influence the redox state of myoglobin and related oxidative pathways in meat systems(Zhu et al., 2024, Inai et al., 2014).

Gallic acid (GA) is a polyhydroxyphenolic compound which can be found in various natural products, such as green tea, grapes, strawberries, bananas and many other fruits(Aborehab and Osama, 2019, Firus Khan et al., 2023); Naringenin (citrus) is a powerful bioactive polyphenols(Gungormez, 2026); Rosmarinic acid (RA) is a natural water-soluble polyphenol substance that is extracted from the rosemary plant. Because of its stable properties and ease of procurement, RA plays an important role in dietary and pharmaceutical supplements to improve human health. (Li et al., 2023, Marchev et al., 2021)

However, the molecular basis of interaction between phenolic antioxidants and myoglobin a possible reason how certain compounds preserve pigment proteins and color stability remains less understood than their free-radical scavenging capabilities. Molecular docking is an efficient computational approach based on predicting the binding interactions between natural phenolics and target proteins, where the visualization can be performed at a molecular level. This study, therefore, is focused on the assessment of selected natural phenolic compounds for their probable roles in myoglobin stabilization and color integrity retention in goat meat through molecular docking and various physicochemical profiling.

Materials and Methods

Protein Structure Retrieval and Preparation

The 3D structure of metmyoglobin was obtained from the Protein Data Bank (PDB ID: 1YMB) as presented in figure 1. Selected structure corresponds to ferric (Fe^{3+}) form of myoglobin, enivcely connected with processes of meat discoloration. The protein was prepared using AutoDockTools (ADT, version X.X) Heteroatoms of no interest, including crystallographic waters were removed and the heme prosthetic group (HEM) was retained in structure as it is functional interesting due to its role in pigment chemistry and oxidative mechanisms.

The system was then charged with polar hydrogen atoms, and Gasteiger charges were added to the protein. The resultant prepared structure format was then saved as PDBQT for later docking simulations.

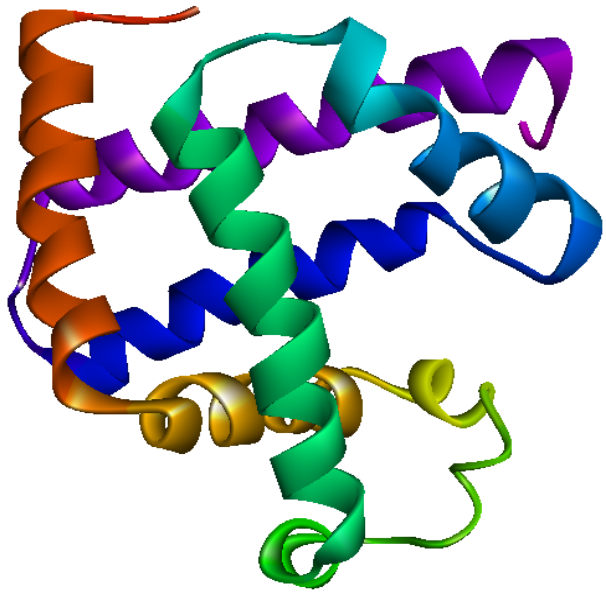

Figure 1: The three-dimensional structure of metmyoglobin (PDB ID: 1YMB)

Ligand Selection and Preparation

Gallic acid, naringenin, and rosmarinic acid were chosen based on their reported antioxidant properties and potential applicability to meat systems (figure 2). The ligands were

obtained from the PubChem database in three-dimensional SDF format.

Ligands were geometry-optimized against the MMFF94 force field to remove steric overlaps and generate energetically favorable conformations. Hydrogen atoms were added and Gasteiger charges were calculated with AutoDockTools. The optimized ligands were formatted to PDBQT for docking.

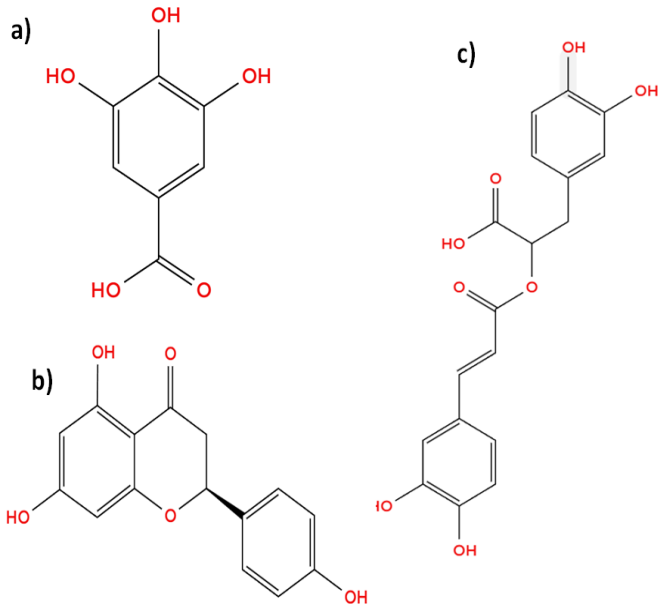

Figure 2: natural compounds a) gallic acid, b) naringenin, and c) rosmarinic acid .

Molecular Docking Protocol

Molecular docking simulations were performed using **AutoDock Vina (version X.X)**. The docking grid box was defined to encompass the heme-binding pocket of metmyoglobin. The grid center was positioned at the coordinates corresponding to the heme iron (Fe) atom to ensure coverage of the functional pigment-binding cavity.

The grid box dimensions were set to adequately cover the distal heme pocket region (e.g., 22 × 22 × 22 Å), allowing sufficient space for ligand flexibility. Docking parameters were maintained consistently across all ligands to ensure comparability: Exhaustiveness: 12; Number of modes: 10; and Energy range: 3 kcal/mol. For each ligand, the best-ranked binding pose based on the lowest binding free energy (kcal/mol) was selected for further interaction analysis. (Jacob et al., 2012)

Interaction Analysis and Visualization

The docked protein–ligand complexes were visualized using PyMOL (version X.X). Hydrogen bonding interactions, hydrophobic contacts, and π–π interactions were analyzed using PLIP and/or Discovery Studio Visualizer. Key amino acid residues involved in ligand binding within the heme pocket region were identified and compared among ligands to evaluate potential stabilization mechanisms.

Physicochemical Profiling (SwissADME)

Physicochemical properties of the selected phenolic compounds were evaluated using the SwissADME web tool. Parameters analyzed included:

- Molecular weight (MW)
- Lipophilicity (LogP)
- Topological polar surface area (TPSA)
- Hydrogen bond donors (HBD)
- Hydrogen bond acceptors (HBA)
- Predicted aqueous solubility

The SwissADME results were interpreted as indicators of formulation feasibility and applicability in meat systems rather than pharmaceutical drug-likeness.

Data Analysis

Docking scores were expressed as binding free energy (kcal/mol). Comparative evaluation among ligands was performed based on binding affinity and interaction patterns within the heme pocket. All simulations were conducted under identical parameters to ensure reproducibility and consistency.

Results and discussion

Physicochemical Profiling of Selected Phenolic Compounds

SwissADME was utilized for the physicochemical profiling of gallic acid, naringenin and rosmarinic acid to discuss their physicochemical or solubility characteristics that would be beneficial in goat meat systems (Table 1). The physicochemical parameters that have been reported to affect compound diffusion, protein interaction behavior and antioxidant properties within food matrices include the molecular weight, lipophilicity (LogP), topological polar surface area (TPSA), hydrogen bonding capacity and aqueous solubility (Domínguez et al., 2019)

The lowest molecular weight (170.12 g/mol) and high polarity (TPSA = 97.99 Å²) was exhibited by gallic acid, while very low lipophilicity (consensus LogP = 0.21). Four hydrogen bond donors and five acceptors show strong potential for hydrogen bonding interactions. Its anticipated high solubility in aqueous conditions may improve distribution into the aqueous muscle matrices, potentially promoting antioxidant availability within lean meat constructs. Nevertheless, polar compounds may have poor penetration into the hydrophobic areas of protein binding sites. (Zhu et al., 2024)

Naringenin exhibited intermediate molecular weight (272.25 g/mol) and moderate lipophilicity (consensus LogP = 1.84), exhibiting a balanced hydrophilic–hydrophobic profile. Naringenin has favorable structural characteristics for both polar and hydrophobic interactions, as indicated by its TPSA (86.99 Å²) and hydrogen bonding capacity (3 donors, 5 acceptors). This well-balanced polarity is generally thought to provide better compatibility with protein binding pockets while offering greater stabilization potential. (Suman and Joseph, 2013)

Rosmarinic acid displayed the highest molecular weight (360.31 g/mol) and greatest polarity (TPSA = 144.52 Å²), along with extensive hydrogen bonding capability (5 donors, 8 acceptors). While its higher polarity may influence diffusion characteristics, the presence of multiple functional groups increases its interaction potential with protein residues. Structural complexity and increased hydrogen bonding sites have been associated with stronger antioxidant–protein interactions in meat systems.(Domínguez et al., 2019) Collectively, the physicochemical profiles reveal a progressive increase in molecular size and interaction capacity from gallic acid to rosmarinic acid. Gallic acid is characterized by high aqueous solubility and strong polarity, naringenin exhibits balanced lipophilicity and polarity, and rosmarinic acid demonstrates enhanced structural complexity and hydrogen bonding potential. These differences are expected to influence their interaction behavior with myoglobin and their functional performance in maintaining color stability in goat meat.

Table 1. Comparative physicochemical properties of gallic acid, naringenin, and rosmarinic acid obtained from SwissADME analysis.

Property	Gallic Acid	Naringenin	Rosmarinic Acid
MW (g/mol)	170.1	272.3	360.3
Consensus LogP	0.21	1.84	1.58
TPSA (Å²)	97.99	86.99	144.52
HBD	4	3	5
HBA	5	5	8
Solubility	Very soluble	Soluble	Soluble/Moderate

Docking-Based Evaluation of Phenolic Binding to Metmyoglobin

Molecular docking analysis demonstrated ligand-dependent binding affinities toward metmyoglobin (PDB ID: 1YMB), indicating differences in predicted stabilization potential within the heme-associated region as shown in figure 3. The best binding energies followed the order: **rosmarinic acid (–6.7 kcal/mol) > naringenin (–6.0 kcal/mol) > gallic acid (–4.6 kcal/mol)**.

Gallic acid exhibited moderate binding affinity (–4.6 kcal/mol), consistent with its small molecular size and high polarity. Phenolic acids with high polarity typically interact through hydrogen bonding with surface-exposed residues rather than deep hydrophobic cavity penetration .(Hussein et al., 2025b, Hussein et al., 2025a) The observed energy distribution (–4.6 to –4.1 kcal/mol) suggests conformational adaptability but relatively weaker stabilization compared with larger polyphenols. Given that myoglobin oxidation is influenced by structural perturbations around the heme group , moderate interaction may contribute indirectly to pigment stabilization.

Naringenin displayed stronger binding affinity (–6.0 kcal/mol), reflecting improved interaction within the defined docking region. Its balanced hydrophilic–hydrophobic profile likely enhances compatibility with both polar and aromatic residues surrounding the heme cavity. Flavonoids are known to engage in hydrogen bonding and π–π stacking interactions, which can improve protein–ligand affinity (Zhu et al., 2024). The relatively narrow energy range (–6.0 to –5.4 kcal/mol) indicates stable conformational accommodation within the binding site.

Rosmarinic acid exhibited the strongest predicted binding (–6.7 kcal/mol). Larger polyphenols containing multiple hydroxyl groups often demonstrate enhanced protein-binding capacity due to increased hydrogen bonding and expanded interaction surfaces (Domínguez et al., 2019). The multiple energetically similar docking modes (–6.1 to –5.7 kcal/mol) further suggest robust interaction stability. Stronger binding near the heme-associated region may influence the microenvironment surrounding the iron center, potentially modulating oxidative processes linked to discoloration .(Suman and Joseph, 2013, Hussein et al., 2025a)

Discoloration in red meat is primarily associated with metmyoglobin formation and oxidative destabilization of the heme environment .(Suman and Joseph, 2013) Natural polyphenols have been widely investigated for their capacity to delay pigment oxidation through both direct protein interaction and radical scavenging mechanisms (Domínguez et al., 2019, Zhu et al., 2024). The docking results suggest a structure-dependent binding trend in which increased molecular size and hydrogen bonding capacity correspond to stronger predicted interaction with metmyoglobin. Thus, rosmarinic acid and naringenin may exhibit greater potential for direct myoglobin stabilization compared with gallic acid, although experimental validation in goat meat systems is required to confirm these predictions.

Distribution of the binding affinity comparison between docking modes is shown in Figure 3. As seen, rosmarinic acid showed lower binding energies against all predicted forms and indicated that it interacts more strongly with metmyoglobin than naringenin and gallic acid. Naringenin displayed moderate binding affinity, and gallic acid was

found to bind more weakly. The progressive energy trend across ligands is the manifestation of a structure dependent interaction pattern that dictates an inversed relationship between the molecular size and the hydrogen bonding potential to binding affinity. The small variation in energy values across all three modes for each ligand also indicates a certain level of stability among conformational behaviors prevalent within the heme-associated binding region.

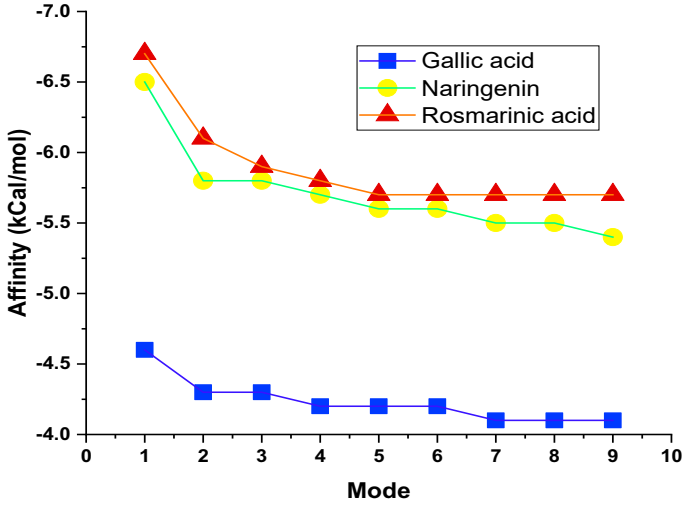

Figure 3. Comparative binding affinity profiles of gallic acid, naringenin and rosmarinic acid toward metmyoglobin (PDB ID: 1YMB) predicted by AutoDock Vina.

Comparative Interaction Analysis of Phenolic Ligands with Metmyoglobin

The molecular docking analysis displayed remarkable variations in binding affinities of metmyoglobin (PDB ID: 1YMB) with the three phenolic compounds, namely gallic acid, naringenin and rosmarinic acid. The predicted binding energies for rosmarinic acid (–6.7 kcal/mol) > naringenin (–6.0 kcal/mol) > gallic acid (–4.6 kcal/mol). Structural visualization of preliminary docking poses showed that all ligands engaged with residues at the surface site close to the heme in metmyoglobin. Gallic acid mainly formed hydrogen bond interactions with polar residues around the binding pocket (Figure 4). Gallic acid shows interaction mainly through surface-oriented contacts instead of penetrating deep into the binding cavity due to its small molecular size and high polarity. Such behavior is typical of phenolic acids, which are often described as water-soluble antioxidants capable to scavenge reactive oxygen species (ROS) within the aqueous milieu found in muscle tissues.(Losetty et al., 2026) Naringenin also showed a higher binding affinity and wider interactions with residues such as Asp109, Ile112, His113, and Arg139 (Figure 5). Naringenin may have strong hydrophobic interactions due to its aromatic flavonoid structure and engage in potential π-related contacts with residues in the binding pocket. It is well established that flavonoids can form stable complexes with proteins through the aromaticity and moderate lipophilicity of their planar structure, which facilitates accommodation in protein cavities Docking results indicate a more efficient interaction between naringenin and hydrophobic regions of the binding pocket than gallic acid.. (Zhu et al., 2024)

Of the compounds analyzed, rosmarinic acid showed the highest predicted binding energy and largest interaction network (Figure 6). The molecule has multiple hydroxyl groups and two aromatic rings, which facilitates the formation of several hydrogen-bonding and electrostatic interactions with residues like Arg31, Asp109, Ile112, His113, Arg139, Gln136. Polifenolic structure with bigger size tend to have stronger protein binding capacity because they increase in interacting surface and passable hydrogen bond with their multiple functional groups (Domínguez et al., 2019). These structural features likely account for the improved binding affinity shown by rosmarinic acid.

The physicochemical profiles from SwissADME analysis also validate the docking trends discussed in this study. Gallic acid had the lowest molecular weight and highest polarity which favors aqueous solubility, although may limit hydrophobic cavity penetration. Naringenin exhibited well-balanced lipophilicity and polarity that facilitated interactions with hydrophilic and hydrophobic residues. Rosmarinic acid had the biggest molecular size and maximum hydrogen Solidity that may lead to protein–ligand interactions in more area than different ligands. Thus, this dependency on structure illustrates that molecular size, polarity, and functional group distribution dictate binding between a ligand to myoglobin.

From a meat science standpoint, stabilization of the myoglobin environment is key to ensuring acceptable color of meat. Oxidation of myoglobin into metmyoglobin results in brown discoloring of meat and low consumer acceptance (Suman and Joseph, 2013). Natural phenolic compounds have been extensively studied for their ability to delay oxidative processes and preserve color stability in meat systems. The docking results here suggest that rosmarinic acid and naringenin could have greater direct interaction potential with myoglobin compared to gallic acid (Domínguez et al., 2019). However, gallic acid could also provide oxidative stability through indirect antioxidant effects like radical scavenging.

Thus overall, the combined docking and physicochemical studies reveal complexity in polyphenolic structure and hydrogen bonding harboring capability to be indispensable properties for ligands which determine their metmyoglobin interaction. The predicted influence of phenolic compounds on protein interactions, provided from computational studies, gives mechanistic clues regarding the biological effects observed in goat meat, but require experimental confirmation in future studies.

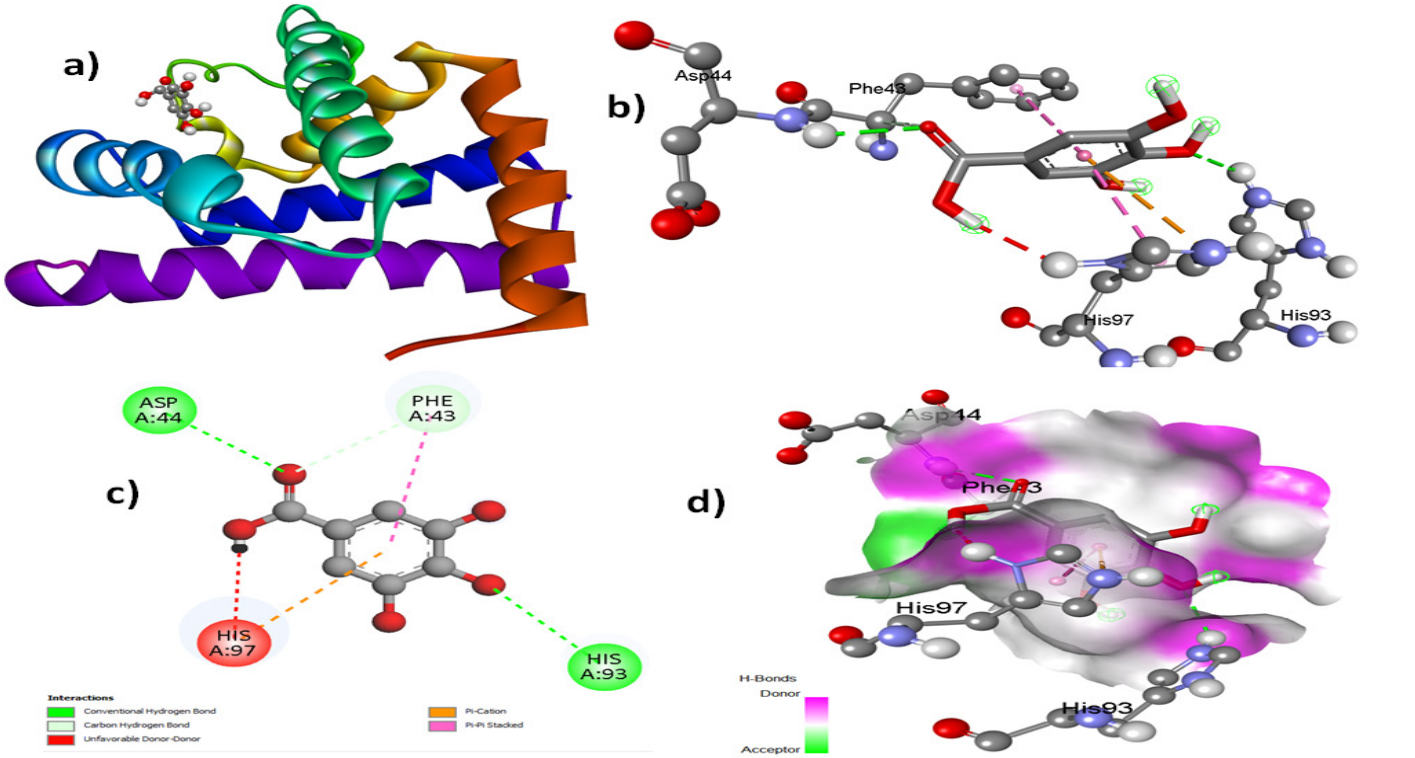

Figure 4. Three-dimensional binding conformation of gallic acid within the metmyoglobin (PDB ID: 1YMB) structure. (a) Overall ribbon representation of metmyoglobin showing the binding location of gallic acid relative to the heme prosthetic group. (b) Detailed view of the protein–ligand interactions highlighting hydrogen bonds and π–π stacking interactions with key residues. (c) Two-dimensional interaction diagram illustrating hydrogen bonding and aromatic contacts between gallic acid and surrounding amino acids. (d) Surface representation of the binding pocket demonstrating ligand accommodation within the heme-associated cavity.

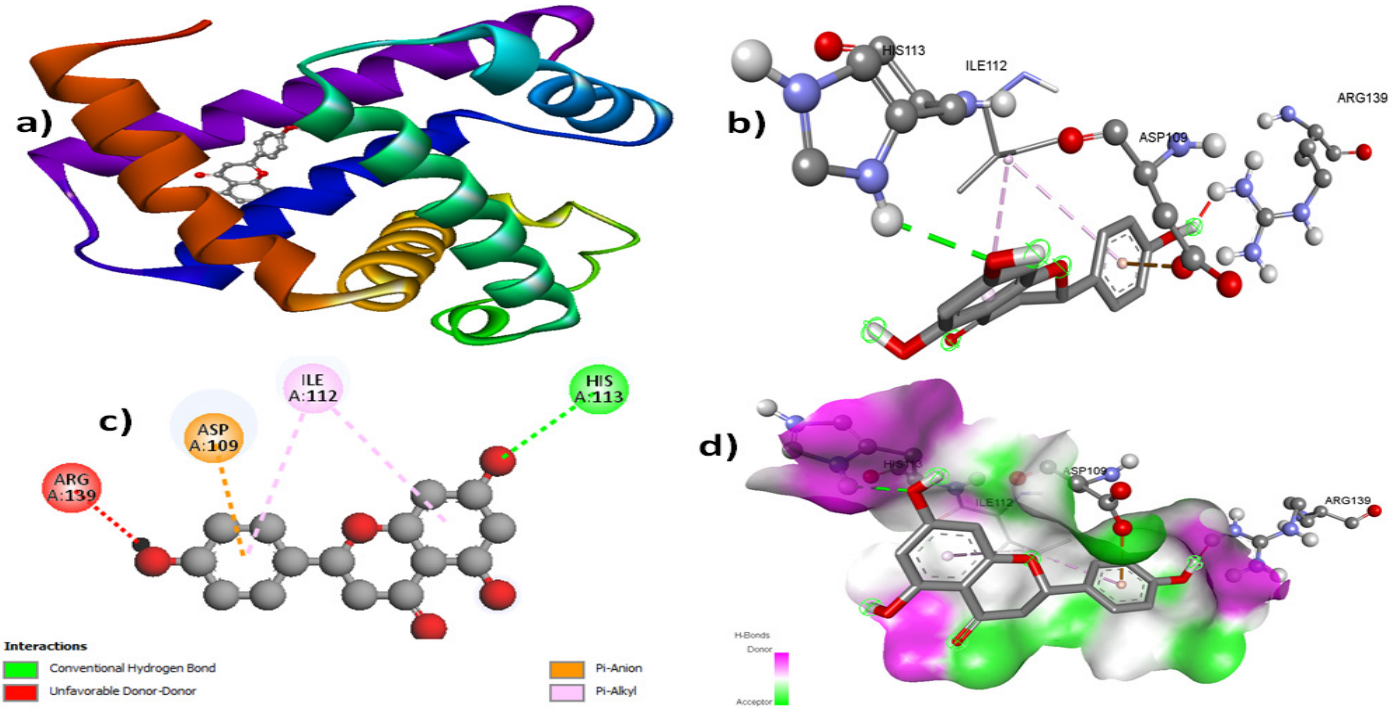

Figure 5. Three-dimensional binding conformation of Naringenin **within the metmyoglobin (PDB ID: 1YMB) structure.** (a) Overall ribbon representation of metmyoglobin showing the binding location of Naringenin relative to the heme prosthetic group. (b) Detailed view of the protein–ligand interactions highlighting hydrogen bonds and π–π stacking interactions with key residues. (c) Two-dimensional interaction diagram illustrating hydrogen bonding and aromatic contacts between Naringenin and surrounding amino acids. (d) Surface representation of the binding pocket demonstrating ligand accommodation within the heme-associated cavity.

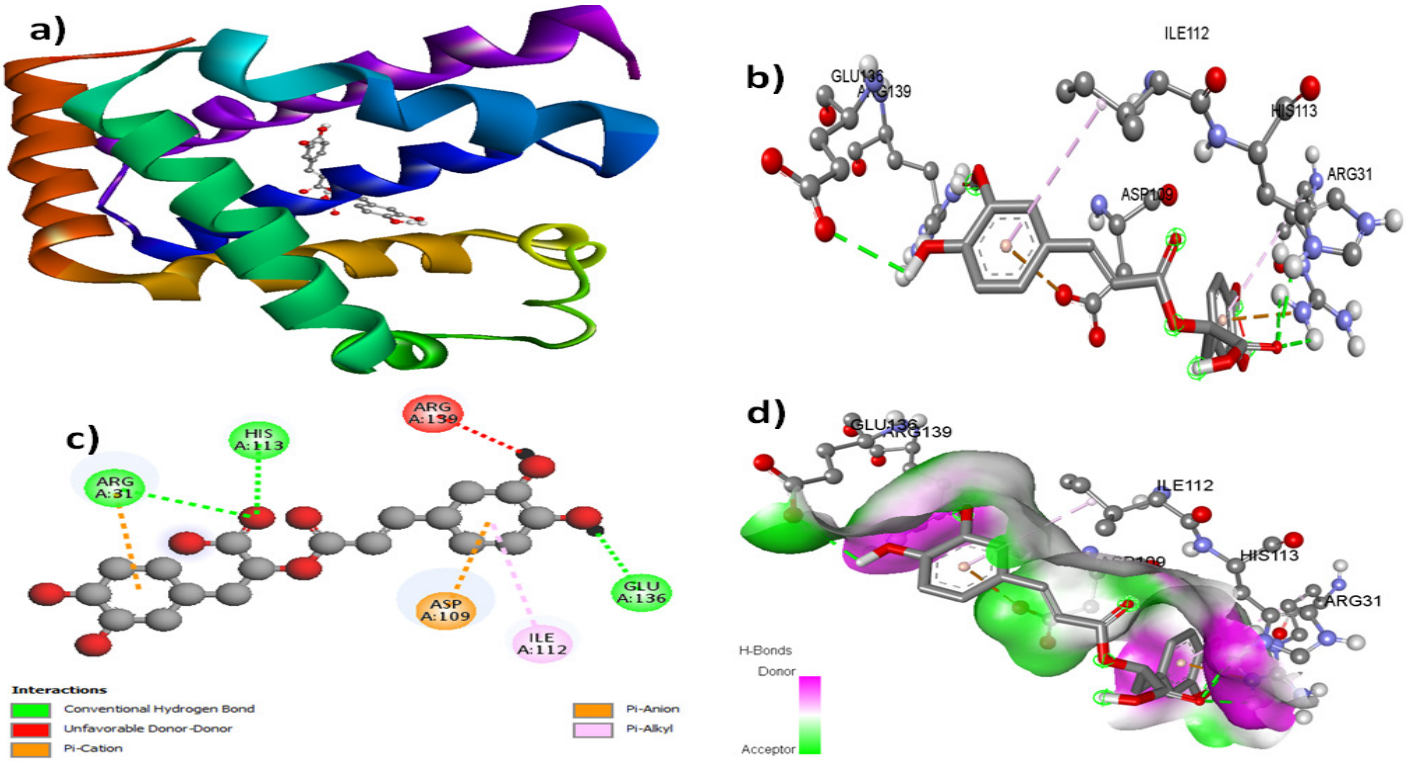

Figure 6. Three-dimensional binding conformation of Rosmarinic acid within the metmyoglobin (PDB ID: 1YMB) structure. (a) Overall ribbon representation of metmyoglobin showing the binding location of Rosmarinic acid relative to the heme prosthetic group. (b) Detailed view of the protein–ligand interactions highlighting hydrogen bonds and π–π stacking interactions with key residues. (c) Two-dimensional interaction diagram illustrating hydrogen bonding and aromatic contacts between Rosmarinic acid and surrounding amino acids. (d) Surface representation of the binding pocket demonstrating ligand accommodation within the heme-associated cavity.

Conclusion

In this study, interaction of food-derived natural phenolic compounds including gallic acid, naringenin and rosmarinic acid with metmyoglobin was investigated using molecular docking and physicochemical profiling strategies. Docking analysis indicated that all three compound bound metmyoglobin′s structure with different affinities, and the predicted binding energy-ranked as following: rosmarinic acid (–6.7 kcal/mol) > naringenin (–6.0 kcal/mol) > gallic acid (–4.6 kcal/mol). Structural studies have shown that these ligands interact with amino acid residues adjacent to the heme-binding pocket in an intermolecular fashion mediated by hydrogen bonds and electrostatic interactions. Expected variations in molecular size, polarity, lipophilicity and hydrogen bonding capacity were also detected by SwissADME physicochemical profiling across the analyzed compounds. Of these, rosmarinic acid with the highest molecular weight and hydrogen bonding potential was demonstrated to exhibit a stronger predict bind free-energy value with metmyoglobin, whereas naringenin exhibited more balanced physicochemical parameters that may support stable protein–ligand interactions. Unlike the others, Gallic acid might contribute to oxidative stability although its binding affinity was lower because of high polarity and water solubility. These findings reveal that ligand recognition of metmyoglobin is not only reliant upon the same mechanisms yet to determine membrane protein binding1280, such as molecular weight 563,147 and aromatic and hydrogen bonding, but also further interestingly appears stable frames for comparable democratic coordination development between. Such mechanistic underpinning derived from the computation may lay the foundation for potential application of natural phenolic compounds as pigment stabilizers in meat systems. However, their real efficacy for improving color stability and shelf-life needs further experimental confirmation in true meat matrices

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