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Klorojenik Asitin Meme Kanserine Karşı Hedeflenen Etkisinin DFT ve Moleküler Yerleştirme Yöntemleri Kullanılarak Araştırılması

Investigation of the Targeted Effect of Chlorogenic Acid Against Breast Cancer Using DFT and Molecular Docking Methods

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ÖZET

Klorojenik asit, antioksidan, antienflamatuvar ve antikanser özellikleriyle dikkat çeken doğal bir polifenolik bileşiktir. Bu çalışmada, klorojenik asidin yapısal, elektronik, doğrusal olmayan optik (NLO) ve biyolojik özellikleri Yoğunluk Fonksiyoneli Teorisi (DFT) hesaplamaları ve moleküler kenetlenme analizleri kullanılarak incelenmiştir. Kuantum kimyasal hesaplamalar Gaussian 09 programında CAM-B3LYP ve PBEPBE fonksiyonelleri ile 6-31G(d,p) temel seti düzeyinde gerçekleştirilmiştir. Optimize edilen moleküler yapı kullanılarak Mulliken atomik yük dağılımları, sınır moleküler orbital (HOMO–LUMO) enerjileri ve küresel reaktivite parametreleri hesaplanmıştır. Ayrıca, Moleküler Elektrostatik Potansiyel (MEP) analizi ile molekülün reaktif bölgeleri belirlenmiş; dipol moment, ortalama polarize edilebilirlik ve birinci dereceden hiperpolarize edilebilirlik değerleri hesaplanarak doğrusal olmayan optik özellikleri değerlendirilmiştir. Klorojenik asidin biyolojik aktivitesini araştırmak amacıyla meme kanseri ile ilişkili hedef proteinler Apoptotik Düzenleyici Bcl-2 (PDB: 6O0K) ve Anti-apoptotik protein Bcl-2 (PDB: 2O21) üzerinde moleküler kenetlenme çalışmaları gerçekleştirilmiş, bağlanma afiniteleri ve ligand–protein etkileşimleri ayrıntılı olarak analiz edilmiştir. Elde edilen bulgular, klorojenik asidin elektronik yapısı, kimyasal reaktivitesi ve biyolojik potansiyeli hakkında önemli bilgiler sunmakta olup, meme kanserine yönelik potansiyel bir terapötik aday olabileceğini göstermektedir.

Anahtar Kelimeler:

Klorojenik asit, Yoğunluk Fonksiyonel Teorisi (DFT), Moleküler kenetlenme, Meme kanseri, HOMO–LUMO

Investigation of the Targeted Effect of Chlorogenic Acid Against Breast Cancer Using DFT and Molecular Docking Methods

ABSTRACT

Chlorogenic acid is a naturally occurring polyphenolic compound with remarkable antioxidant, anti-inflammatory, and anticancer activities. In this study, its structural, electronic, nonlinear optical (NLO), and biological properties were investigated using Density Functional Theory (DFT) calculations and molecular docking analyses. Quantum chemical calculations were performed with the Gaussian 09 software package using the CAM-B3LYP and PBEPBE functionals in combination with the 6-31G(d,p) basis set. The optimized molecular structure was used to determine Mulliken atomic charges, frontier molecular orbital (HOMO–LUMO) energies, and global reactivity descriptors. Molecular Electrostatic Potential (MEP) analysis was carried out to identify the reactive regions of the molecule, while the dipole moment, mean polarizability, and first-order hyperpolarizability were calculated to evaluate its NLO properties. Molecular docking simulations against the breast cancer-related target proteins Apoptosis Regulator Bcl-2 (PDB: 6O0K) and Anti-apoptotic protein Bcl-2 (PDB: 2O21) were performed to investigate the binding affinity and ligand–protein interactions of chlorogenic acid. The obtained results provide valuable insights into the electronic characteristics, chemical reactivity, and biological potential of chlorogenic acid, highlighting its promise as a candidate for breast cancer-related therapeutic applications.

Keywords:

Chlorogenic acid, Density Functional Theory (DFT), Molecular docking, Breast cancer, HOMO–LUMO

Introduction

Chlorogenic acid (CGA) is a naturally occurring polyphenolic compound formed by the esterification of caffeic acid and quinic acid and is one of the major hydroxycinnamic acid derivatives (Naveed et al., 2018). It is widely distributed in coffee beans, tea, fruits, vegetables, and numerous medicinal plants, making it one of the most abundant phenolic compounds in the human diet (Miao & Xiang, 2020). Owing to its multiple hydroxyl groups and conjugated molecular structure, CGA exhibits remarkable antioxidant activity and has attracted increasing scientific interest because of its diverse biological properties, including anti-inflammatory, antimicrobial, antiviral, neuroprotective, cardioprotective, hepatoprotective, and anticancer effects (Liang & Kitts, 2015). Recent experimental studies have demonstrated that CGA regulates oxidative stress, inflammatory signaling pathways, cell proliferation, and apoptosis, suggesting its potential therapeutic value in the prevention and treatment of various diseases, particularly cancer (Nguyen et al., 2024).

Understanding the biological activity of bioactive molecules requires comprehensive knowledge of their structural and electronic characteristics (Gören & Yıldıko, 2024). Density Functional Theory (DFT) has become a reliable computational approach for investigating molecular geometry, electronic structure, frontier molecular orbitals (HOMO and LUMO), global reactivity descriptors, and charge distribution (Bağlan, Gören, et al., 2023b). In addition, Molecular Electrostatic Potential (MEP) analysis provides valuable information regarding electrophilic and nucleophilic reactive regions, whereas nonlinear optical (NLO) calculations enable the evaluation of molecular electronic response through dipole moment, polarizability, and hyperpolarizability parameters (Tahiroğlu, Gören, & Bağlan, 2025). Furthermore, molecular docking has become an effective computational tool for predicting ligand–protein binding modes, binding affinities, and intermolecular interactions at the atomic level, thereby facilitating the identification of potential therapeutic targets (Tahiroğlu, Gören, Kotan, et al., 2025).

In the present study, the structural, electronic, and nonlinear optical (NLO) properties of chlorogenic acid were systematically investigated using DFT calculations at the CAM-B3LYP/6-31G(d,p) and PBEPBE/6-31G(d,p) levels of theory. Mulliken atomic charges, HOMO–LUMO energies, global reactivity descriptors, and Molecular Electrostatic Potential (MEP) maps were analyzed to elucidate the electronic characteristics and reactive behavior of the molecule. In addition, molecular docking simulations were performed against the breast cancer-related target proteins PDB: 6O0K and PDB: 2O21 to evaluate the binding affinity and ligand–protein interactions of chlorogenic acid. The combined theoretical and molecular modeling approaches provide a comprehensive understanding of the electronic behavior and biological potential of chlorogenic acid and support its possible application as a promising natural compound for breast cancer-related therapeutic research.

1. Materials and Methods

The biological potential of chlorogenic acid was comprehensively investigated through quantum chemical calculations and molecular docking. All quantum chemical calculations were performed within the framework of Density Functional Theory (DFT) using the Gaussian 09 software package (Frisch, M.J., 2009). The optimized molecular geometry, electronic properties, and chemical reactivity descriptors of chlorogenic acid were determined employing the CAM-B3LYP and PBEPBE exchange–correlation functionals with the 6-31G(d,p) basis set. Molecular docking simulations were conducted using the crystal structures of the target proteins retrieved from the Protein Data Bank (PDB) (Bank, 2007, 2019). Prior to docking, the protein structures were prepared by removing crystallographic water molecules, adding missing hydrogen atoms, and assigning appropriate protonation states to ensure suitable docking conditions. The binding affinity and binding mode of chlorogenic acid toward the active sites of the target proteins were subsequently evaluated using AutoDock Vina (Eberhardt et al., 2021). The resulting protein–ligand complexes were further analyzed to characterize their binding modes and intermolecular interactions, which were visualized using Discovery Studio Visualizer (BIOVIA, version 2016) (BIOVIA, 2016).

2. Results and Discussion

2.1. Mulliken atomic Charges

Mulliken atomic charge analysis provides important information about the electronic structure and chemical reactivity of a molecule by determining the distribution of electron density among atoms (Bağlan, Gören, et al., 2023a; Gören, Bağlan, & Yıldıko, 2024a). Atoms with a negative Mulliken charge represent electron-rich (nucleophilic) regions, while atoms with a positive charge represent electron-poor (electrophilic) regions (Gören et al., 2022; Gören, Bağlan, & Yıldıko, 2024b). Therefore, Mulliken charges are an important quantum chemical parameter widely used in identifying potential reactive centers within a molecule, explaining charge transfer mechanisms, and evaluating the polarization of chemical bonds (Gören, Bağlan, Tahiroğlu, et al., 2024; Gören, Bağlan, Yıldıko, et al., 2024).

Table 1 presents the Mulliken atomic charges of the chlorogenic acid molecule calculated using the CAM-B3LYP and PBEPBE methods. Both calculation methods yielded very similar results in terms of atomic charge distribution,

indicating that the electronic structure of the molecule is consistent. The highest negative charge values were observed in oxygen atoms. Specifically, atoms O20 (-0.590 and -0.550), O7 (-0.578 and -0.535), O10 (-0.568 and -0.520), O9 (-0.566 and -0.562), and O21 (-0.565 and -0.526) were identified as the most electron-rich regions. This indicates that hydroxyl and carbonyl oxygens possess strong electron-withdrawing characteristics and form potential active centers for nucleophilic interactions. In contrast, the highest positive charges were calculated on carbon atoms. Specifically, atoms C11 (0.628 and 0.581) and C23 (0.601 and 0.569) have the highest positive charge values, suggesting that carbonyl carbons are electron-poor (electrophilic) centers. Furthermore, the positive charge of atoms C16 and C17 reveals that these regions contribute to the intramolecular charge distribution. All hydrogen atoms, as expected, have positive charge values, with higher positive charges calculated particularly on hydrogen atoms attached to hydroxyl groups (H33, H40, H41, H42, and H43). This supports a predisposition to hydrogen bonding. While there are only minor quantitative differences between the CAM-B3LYP and PBEPBE methods in general, both methods similarly described the charge distribution in the chlorogenic acid molecule. The concentration of negative charges on oxygen atoms and positive charges on carbonyl carbons and hydroxyl hydrogens indicates the molecule's potential electrophilic and nucleophilic attack sites, yielding results consistent with electronic properties obtained from MEP and HOMO-LUMO analyses.

Table 1. Mulliken atomic charges of the Chlorogenic acid molecule

ATOMS	CAM-B3LYP	PBEPBE	ATOMS	CAM-B3LYP	PBEPBE
C1	-0.180	-0.200	O21	-0.565	-0.526
C2	0.132	0.121	O22	-0.517	-0.512
C3	0.165	0.092	C23	0.601	0.569
C4	0.170	0.086	O24	-0.461	-0.438
C5	-0.201	-0.204	O25	-0.476	-0.443
C6	0.141	0.092	H27	0.096	0.099
O7	-0.578	-0.535	H28	0.126	0.130
O8	-0.507	-0.457	H29	0.114	0.110
O9	-0.566	-0.562	H30	0.139	0.138
O10	-0.568	-0.520	H31	0.116	0.116
C11	0.628	0.581	H33	0.332	0.318
C12	-0.165	-0.162	H34	0.113	0.119
C13	-0.083	-0.103	H35	0.122	0.127
C14	0.114	0.117	H36	0.106	0.112
C15	-0.140	-0.146	H37	0.089	0.100
C16	0.309	0.291	H38	0.097	0.107
C17	0.290	0.277	H40	0.338	0.334
C18	-0.132	-0.140	H41	0.340	0.330
C19	-0.144	-0.149	H42	0.317	0.314
O20	-0.590	-0.550	H43	0.319	0.342

2.2. HOMO-LUMO Analysis

HOMO–LUMO analysis is a widely used theoretical approach to assessing the electronic structure, chemical stability, and reactivity of a molecule (Bağlan et al., 2022; Gören, Bağlan, & Yıldıko, 2025). HOMO represents the tendency to donate electrons, while LUMO represents the tendency to accept electrons. The energy difference (ΔE) between these two orbitals is a significant indicator of the molecule's stability and chemical reactivity, and together with the spherical reactivity parameters obtained from DFT calculations, it allows for a detailed interpretation of the molecule's electronic behavior (Bağlan, Gören, Tahiroğlu, et al., 2026; Bağlan, Yıldıko, et al., 2023).

The HOMO, HOMO−1, LUMO, and LUMO+1 orbital distributions of chlorogenic acid were calculated using the CAM-B3LYP and PBEPBE/6-31G(d,p) methods, and the results are given in Figure 1, Figure 2, and Table 2. The HOMO–LUMO energy range calculated using the CAM-B3LYP method (9.1622 eV) was found to be higher than that calculated using the PBEPBE method (4.7826 eV). This indicates that the molecule has higher electronic stability and lower chemical reactivity compared to CAM-B3LYP. In contrast, the PBEPBE method reveals that the molecule exhibits higher reactivity and easier electron transition due to its lower energy range. In both methods, the HOMO orbital is predominantly concentrated on the catechol ring and conjugated π-system, while the LUMO orbital is concentrated on the ester bond and conjugated carbon atoms. This distribution suggests that intramolecular charge transfer (ICT) can occur from the phenolic moiety to the ester group during electronic excitation. The CAM-B3LYP method indicates that the molecule is more stable with higher chemical hardness (η=4.5811 eV) and lower chemical softness (s=0.1091), while the PBEPBE method predicts higher chemical reactivity due to lower hardness (η=2.3913 eV) and higher softness (s=0.2091). Furthermore, the higher electrophilicity index (ω=2.6377) calculated using the PBEPBE method shows that the molecule has a greater tendency to accept electrons compared to the CAM-B3LYP method. Overall, both functionals demonstrate that chlorogenic acid possesses an effective charge transfer capacity thanks to its conjugated π-electron system. CAM-B3LYP defines the

molecule as more stable, while the PBEPBE functional predicts higher reactivity and electrophilic character. These differences stem from the fact that the functionals used describe the electronic structure differently.

$$\Delta E = |EHOMO - ELUMO| \quad (1)$$

$$\eta = (I - A)/2 \quad (2)$$

$$s = 1/2\eta \quad (3)$$

$$\mu = \frac{(I+A)}{2} \quad (4)$$

$$\chi = (I + A)/2 \quad (5)$$

$$\omega = \mu^2/2\eta \quad (6)$$

Table 2. The HOMO and LUMO quantum chemical characteristics determined by applying the CAM-B3LYP and PBEPBE techniques for the Chlorogenic acid molecule

	E_{HOMO}	E_{LUMO}	E_{HOMO-1}	E_{LUMO-1}	ΔE	I	*A*	η	*s*	μ	χ	ω
CAM-B3LYP	-7.8516	1.3106	-8.2470	1.6214	9.1622	7.8516	-1.3106	4.5811	0.1091	-3.2705	3.2705	1.1667
PBEPBE	-5.9430	-1.1604	-6.1208	-1.0572	4.7826	5.9430	0.1604	2.3913	0.2091	-3.5517	3.5517	2.6377

ΔE→Energy Gap, I→Ionization Potential($-E_{HOMO}$), *A*→Electron Affinity($-E_{LUMO}$), η→Chemical hardness, *s*→Chemical softness, μ→Chemical Potential, χ→Electronegativity, ω→Electrophilicity in

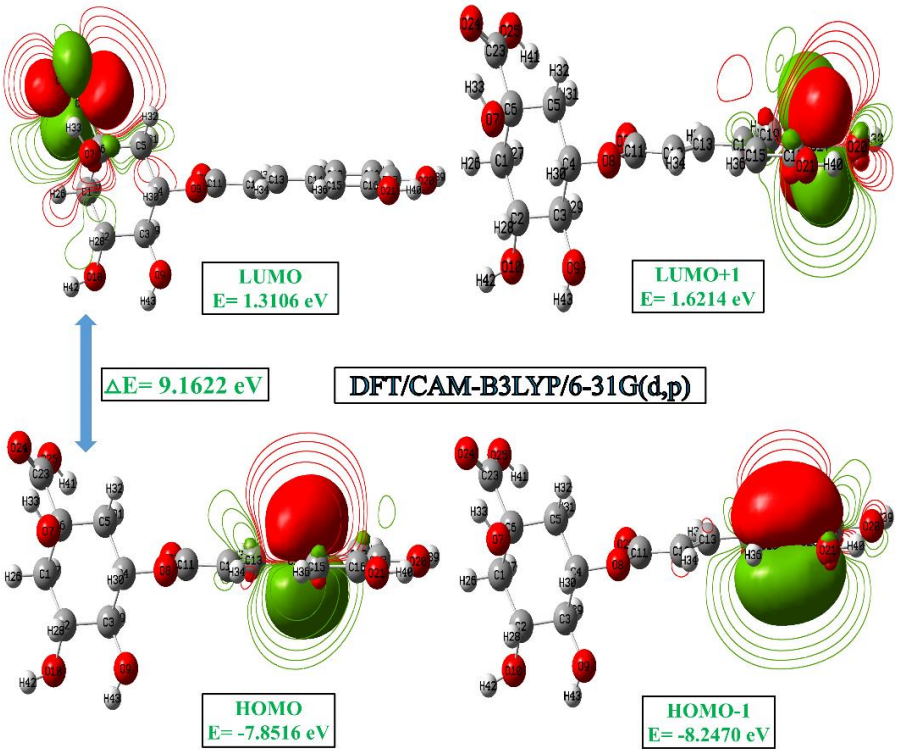

Figure 1. Boundary molecular orbitals of the Chlorogenic acid molecule according to the CAM-B3LYP level

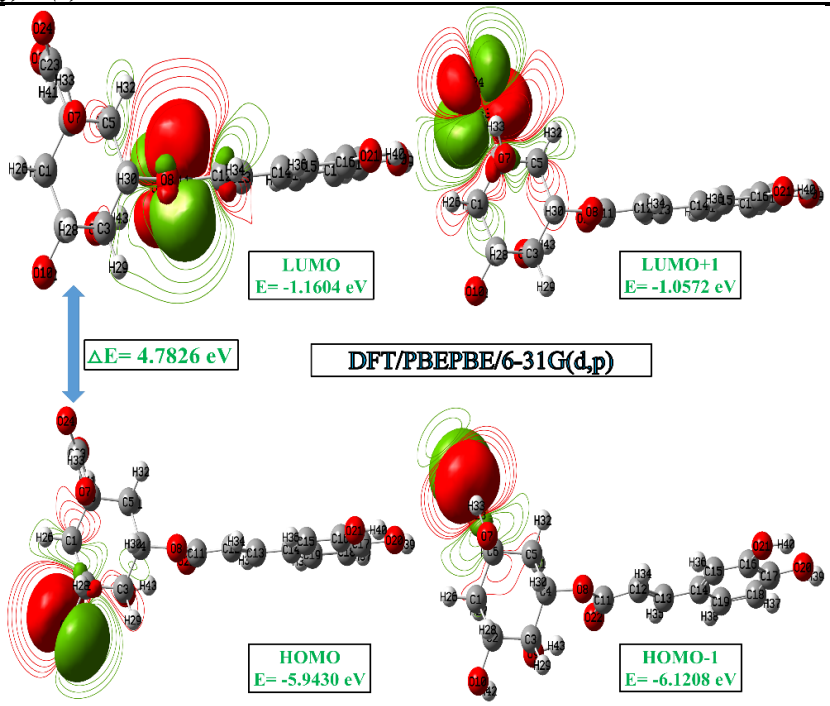

Figure 2. Boundary molecular orbitals of the Chlorogenic acid molecule according to the PBEPBE level

2.3. Molecular electrostatic potential (MEP)

Molecular Electrostatic Potential (MEP) analysis is an effective computational method that provides important information about a molecule's electronic structure and chemical reactivity by visualizing the distribution of electrostatic potential on its surface (Bağlan, Gören, Kotan, et al., 2026; Gören et al., 2026). MEP maps are widely used to identify regions susceptible to electrophilic and nucleophilic attacks on a molecule, as well as to predict weak intermolecular interactions such as hydrogen bonding. On MEP surfaces, red color represents regions with high electron density and negative electrostatic potential, thus representing centers suitable for electrophilic attacks (GÖREN, BAĞLAN, YILDIKO, et al., 2024; Tahiroğlu et al., 2024). In contrast, blue color indicates regions with low electron density and positive electrostatic potential, representing areas more susceptible to nucleophilic attacks. Green color shows neutral regions with approximately zero electrostatic potential (Eberhardt et al., 2021). This distribution of electrostatic potential on the molecular surface allows for the identification of chemically active centers, while also contributing to qualitative assessments of intermolecular interactions, molecular recognition mechanisms, and the overall chemical reactivity of the molecule (Gören, Bağlan, Tahiroğlu, et al., 2025).

Figure 3 presents the Molecular Electrostatic Potential (MEP) surfaces of the chlorogenic acid molecule calculated using the CAM-B3LYP and PBEPBE functionals. Examination of the MEP maps obtained by both methods reveals that the electrostatic potential distribution is quite similar, and the reactive regions of the molecule are consistently determined by both functionals. Electrostatic potential values for the CAM-B3LYP method ranged from −8.097 to +8.097 a.u., while for the PBEPBE method they ranged from −8.812 to +8.812 a.u. The negative electrostatic potential regions shown in red on the MEP maps represent centers with high electron density. These regions are predominantly concentrated around the oxygen atoms in the molecule, indicating that oxygen atoms, particularly those in carboxylic acids, esters, and hydroxyl groups, exhibit an electron-rich character. Therefore, these regions can be considered the most suitable centers for electrophilic attacks and hydrogen bond acceptor interactions. In contrast, the regions of positive electrostatic potential, shown in blue, are observed around hydrogen atoms, particularly those bonded to hydroxyl groups. This indicates that these hydrogen atoms are electron-poor and more prone to interacting as hydrogen bond donors through nucleophilic attacks. The green regions observed over a large portion of the molecular surface represent neutral areas with approximately zero electrostatic potential, suggesting relatively low chemical reactivity. Although there are only minor differences in the magnitude of the electrostatic potential between the CAM-B3LYP and PBEPBE methods, the positions of the negative and positive potential regions largely overlap. This result demonstrates that both DFT functionals reliably characterize the electronic charge distribution of the chlorogenic acid molecule. The obtained MEP maps reveal that the reactive centers of chlorogenic acid are concentrated particularly around oxygen atoms, indicating a high hydrogen bonding capacity of the molecule. These properties can be considered as electronic characteristics that may play an important role in the interactions of chlorogenic acid with biological targets and its antioxidant activity.

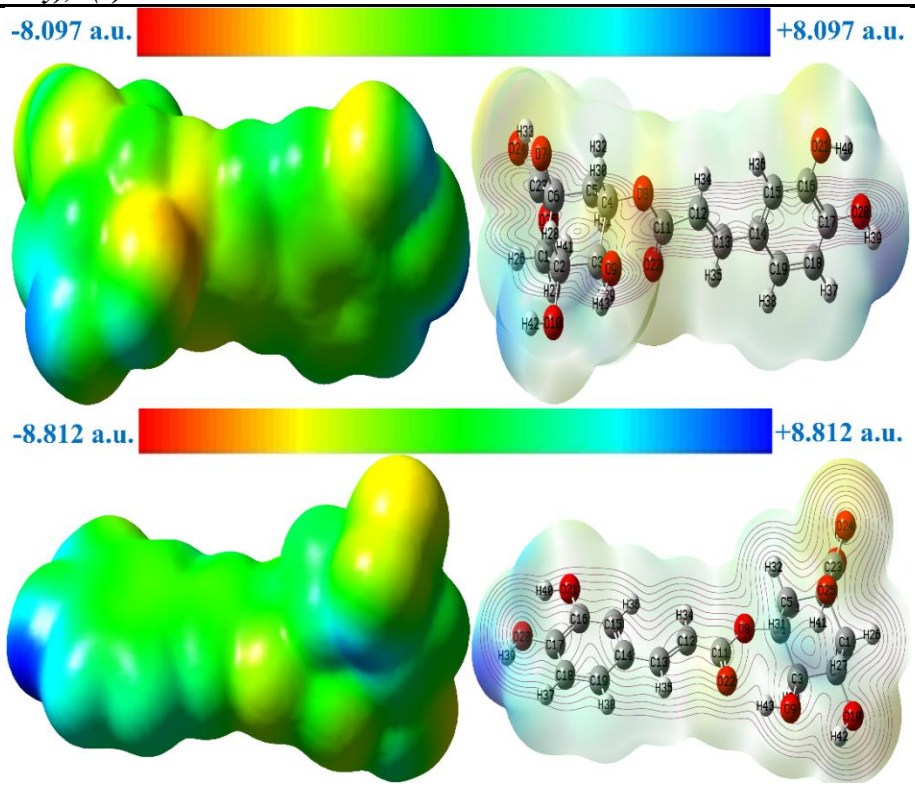

Figure 3. Molecular electrostatic potential surface of the Chlorogenic acid molecule using CAM-B3LYP and PBEPBE methods

2.4. Non-linear optical properties (NLO)

Nonlinear optical (NLO) properties constitute a significant research area in advanced materials applications such as optoelectronics, photonics, and optical data processing technologies (Kartal et al., 2026). The NLO behavior of a molecule is related to its optical response, which arises from the rearrangement of its electronic cloud in the face of an applied electromagnetic field. This response is characterized by changes in the amplitude, phase, and frequency of light and is directly dependent on the electronic structure of the molecule (Shafiq et al., 2024). In the theoretical evaluation of the NLO performance of molecules, fundamental molecular parameters such as dipole moment (μ), mean polarizability (⟨α⟩), polarizability anisotropy (Δα), total first-order hyperpolarizability (βtot), and second-order hyperpolarizability (γ) are used (Asif et al., 2022). These parameters are calculated from the polarizability and hyperpolarizability tensor components obtained from quantum chemical calculations and are considered fundamental indicators in evaluating the nonlinear optical performance of molecules and their potential in optical applications (Sharma & Sekar, 2024).

The nonlinear optical (NLO) properties of chlorogenic acid were investigated using CAM-B3LYP and PBEPBE functionals; the dipole moment (μ), mean polarizability (α), and first-order hyperpolarizability (β) values are given in Table 3. The total dipole moment was calculated as 4.7613 D for the CAM-B3LYP method and 9.6989 D for the PBEPBE method. The higher dipole moment obtained with PBEPBE indicates a more pronounced charge separation within the molecule and a higher polar character. This strengthens the molecule's interaction with external electric fields, providing an advantage for optoelectronic and photonic applications. The mean polarizability (α) values were found to be 130.3949 and 135.7672 a.u. for the CAM-B3LYP and PBEPBE methods, respectively. The higher α value calculated with PBEPBE indicates that the electron cloud can be polarized more easily under the influence of an external electric field, and the optical response of the molecule is enhanced. The first-order total hyperpolarizability (β) values were calculated as 3.85×10^{-30} esu for CAM-B3LYP and 6.21×10^{-30} esu for PBEPBE. The approximately 61% higher β value obtained with PBEPBE shows that this method more effectively describes charge transfer within the molecule. The high β value reveals that chlorogenic acid has significant potential in terms of nonlinear optical applications such as second harmonic generation (SHG), electro-optical modulation, frequency conversion, and optical switching. When the hyperpolarizability tensor components are examined, it is seen that the β_{xxx} component is dominant in both methods. This indicates that the nonlinear optical response is largely due to intramolecular charge transfer in the x-direction. The lower values of the β_{yyy} and β_{zzz} components suggest that the NLO response is concentrated along a specific molecular axis, resulting from electron delocalization between the π-conjugated structure and hydroxyl groups. Overall, both functionals demonstrate that chlorogenic acid possesses high molecular polarity, pronounced polarizability, and strong NLO properties. However, the PBEPBE method yielded systematically higher values for the μ, α, and β parameters. These findings suggest that chlorogenic acid is a promising organic molecule for nonlinear optical materials, photonic devices, and optoelectronic applications.

$$\mu = \left(\mu_x^2 + \mu_y^2 + \mu_z^2\right)^{\frac{1}{2}} \quad (7)$$

$$\alpha(\text{au}) = \frac{1}{3}|(\alpha xx + \alpha yy + \alpha zz)| \quad (8)$$

$$\beta_{Total} = (\beta^2 x + \beta^2 y + \beta^2 z)^{1/2} \quad (9)$$

$$= [(\beta xxx + \beta xyy + \beta xzz)^2 + (\beta yyy + \beta yxx + yzz)^2 + (\beta zzz + \beta zxx + \beta zyy)^2]^{\frac{1}{2}} \quad (10)$$

Table 3. The dipole moments (Debye), polarizability (au), components, and total value of the Chlorogenic acid molecule are computed using CAM-B3LYP and PBEPBE methods

Parameters	CAM-B3LYP	PBEPBE	Parameters	CAM-B3LYP	PBEPBE
β_{XXX}	388.9138	638.9996	**μ_x**	3.6433	9.4356
β_{YYY}	-57.6864	-6.1431	**μ_y**	-0.7170	-0.4985
β_{ZZZ}	-2.8579	-11.6308	**μ_z**	-2.9803	-2.1884
β_{XYY}	-0.1595	53.3344	**$\mu_{(D)}$**	4.7613	9.6989
β_{XXY}	-87.7327	-29.4834	**α_{XX}**	-99.2273	-108.9268
β_{XXZ}	-133.7936	-115.2969	**α_{YY}**	-149.3873	-158.4176
β_{XZZ}	10.2224	15.0685	**α_{ZZ}**	-142.5702	-139.9571
β_{YZZ}	12.4643	-7.4108	**α_{XY}**	25.2242	3.2337
β_{YYZ}	-6.9098	6.4068	**α_{XZ}**	-7.4766	-9.5763
β_{XYZ}	-13.7487	-17.4368	**α_{YZ}**	-1.4089	5.3961
β(esu)	3.85×10^{-30}	6.21×10^{-30}	**α(au)**	130.3949	135.7672

2.5. Molecular docking analysis

Molecular docking is one of the fundamental computational approaches in structure-based drug design and plays a crucial role in modern drug discovery by predicting the binding mode and affinity of small molecules toward biological targets (Gören, Kotan, et al., 2024). This technique enables the identification of the most favorable ligand–protein interactions through three-dimensional simulations, providing valuable insights into the molecular mechanisms underlying biological activity (Agbektas et al., 2026). Compared with conventional experimental screening methods, molecular docking is a rapid, cost-effective, and reliable in silico strategy that significantly reduces both time and resources required during the early stages of drug development (Boy et al., 2026; Kotan et al., 2025). Breast cancer remains one of the most frequently diagnosed malignancies and is a leading cause of cancer-related mortality among women worldwide. Despite considerable advances in diagnosis and treatment, the development of drug resistance, tumor recurrence, and adverse effects associated with current therapeutic agents continue to limit clinical outcomes. Therefore, the identification of novel compounds with high affinity toward breast cancer-associated molecular targets has become an important objective in anticancer drug discovery (Cava & Castiglioni, 2020). In the present study, molecular docking analysis was performed to evaluate the binding interactions of the investigated compounds with selected breast cancer-related protein targets.

The molecular docking scores of chlorogenic acid against the selected breast cancer-related target proteins have been presented in Table 4. The compound exhibited binding affinities of −6.40 kcal/mol toward PDB ID: 6O0K and −7.40 kcal/mol toward PDB ID: 2O21. Since more negative docking scores indicate stronger ligand–protein interactions, chlorogenic acid demonstrated a higher binding affinity for the protein represented by PDB ID: 2O21 than for PDB ID: 6O0K. The docking results suggest that chlorogenic acid can interact favorably with both target proteins through stable ligand–protein complexes. The stronger binding observed for PDB ID: 2O21 indicates that this target may be more susceptible to inhibition by chlorogenic acid. Overall, these findings support the potential biological activity of chlorogenic acid against breast cancer-related molecular targets and provide a theoretical basis for further interaction analysis and experimental validation.

Table 4. Molecular docking interactions scores with PDBID: 6O0K, PDBID: 2O21 enzymes of Chlorogenic acid compound

Compound	Docking Score	
	(PDB: 6O0K)	(PDB: 2O21)
Chlorogenic acid	-6.40	-7.40

Figures 4 and 5 illustrate the three-dimensional (3D) binding conformations and two-dimensional (2D) interaction maps of chlorogenic acid with the breast cancer-related target proteins PDB ID: 6O0K and PDB ID: 2O21, respectively. The 3D representations demonstrate that chlorogenic acid is well accommodated within the active binding pockets of both proteins, indicating favorable geometric complementarity between the ligand and the receptor. The ligand occupies the catalytic cavity without significant steric clashes, supporting the stability of the docked complexes. For PDB ID: 6O0K (Figure 4), chlorogenic acid exhibited a docking score of −6.40 kcal/mol. The 2D interaction diagram reveals that the ligand is stabilized by several conventional hydrogen bonds, particularly with Asp90, Lys53, and Arg45, which contribute significantly to the orientation and stabilization of the ligand inside the binding pocket. In addition, carbon hydrogen bonds and numerous van der Waals interactions with surrounding residues, including Arg29, Ala30, Asp87, and Asn97, further reinforce the ligand–protein complex. The aromatic ring of chlorogenic acid also participates in π–cation and π–sigma interactions, enhancing the overall binding stability through hydrophobic and electrostatic contacts.

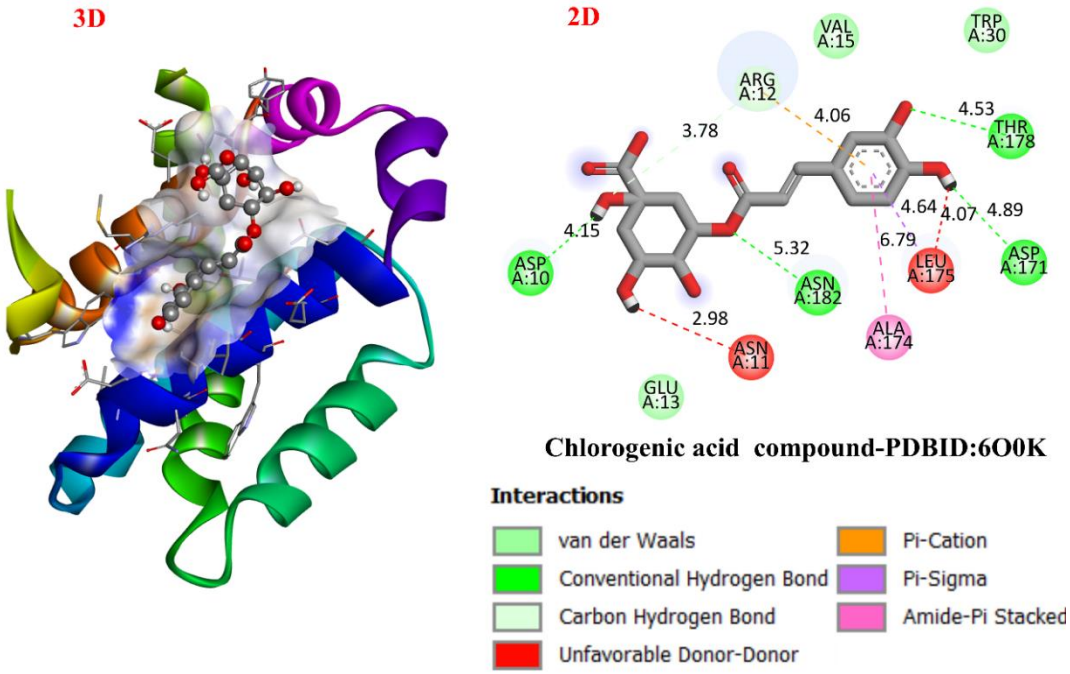

Figure 4. 2D and 3D images of the Chlorogenic acid compound and PDB: 6O0K enzyme

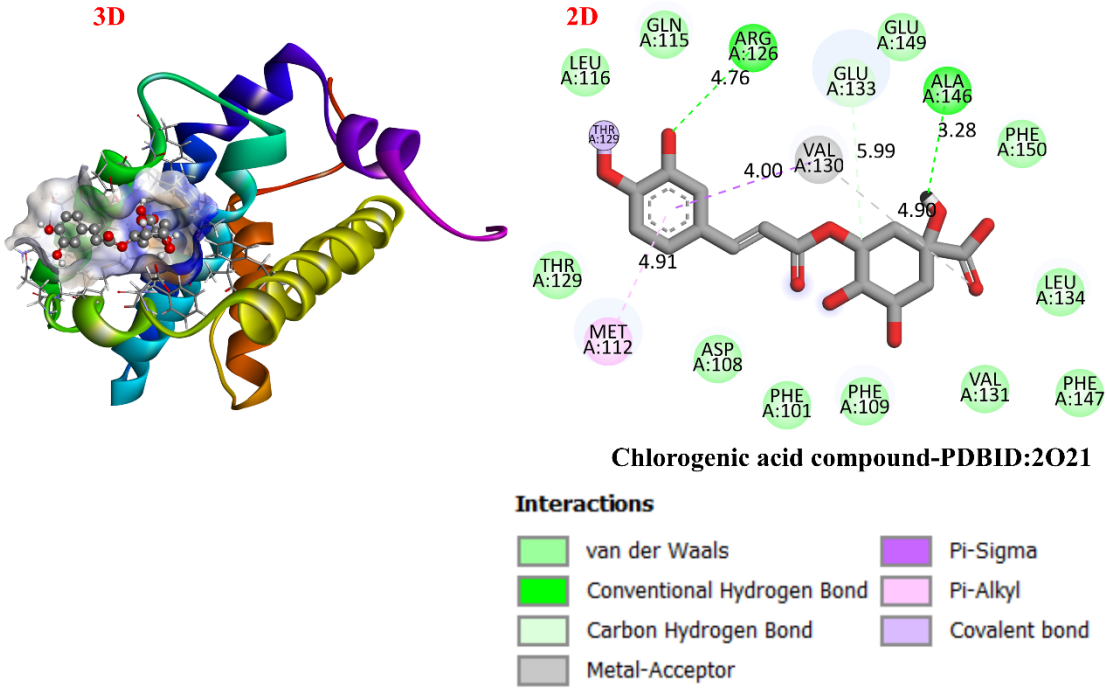

Figure 5. 2D and 3D images of the Chlorogenic acid compound and PDB: 2O21 enzyme

The detailed ligand–protein interaction parameters of chlorogenic acid with PDB IDs 6O0K and 2O21 have been presented in Table 5. The interaction profiles reveal that the stability of both docked complexes is governed by a combination of hydrogen bonding, hydrophobic contacts, electrostatic interactions, and van der Waals forces. For PDB ID: 6O0K, chlorogenic acid established four conventional hydrogen bonds with Asp10, Asn182, Asp171, and Thr178, with bond distances ranging from 4.15 to 5.32 Å. These hydrogen bonds play a significant role in anchoring the ligand within the active site and contribute to the specificity of the ligand–protein interaction. In addition, a carbon hydrogen bond was observed with Arg12 at 3.78 Å, while a π-cation interaction involving the same residue was detected at 4.06 Å, indicating favorable electrostatic attraction between the aromatic ring of chlorogenic acid and the positively charged amino acid side chain. Furthermore, a π-sigma interaction with Leu175 (4.64 Å) and an amide π-stacked interaction with Ala174 (6.79 Å) enhanced the hydrophobic stabilization of the complex. The ligand was also surrounded by several residues, including Val15, Trp30, and Glu13, through van der Waals interactions, which further strengthened the overall binding. Although two unfavorable donor–donor interactions with Asn11 (2.98 Å) and Leu175 (4.07 Å) were identified, their influence appears to be outweighed by the extensive network of favorable intermolecular interactions.

For PDB ID: 2O21, chlorogenic acid exhibited a more compact interaction network that is consistent with its lower docking score (−7.40 kcal/mol). The ligand formed two conventional hydrogen bonds with Arg126 and Ala146, having bond lengths of 4.76 Å and 3.28 Å, respectively. A carbon hydrogen bond with Glu133 (5.99 Å) was also observed.

Hydrophobic stabilization was further supported by a π-sigma interaction with Val130 (4.00 Å) and a π-alkyl interaction with Met112 (4.91 Å). In addition, van der Waals interactions involving Thr129, Asp108, Phe109, Val131, and Leu134 contributed to the stabilization of the ligand within the binding pocket. Interestingly, a metal acceptor interaction involving Thr129 and a covalent interaction with Val130 were also predicted, suggesting additional stabilizing contacts that may enhance ligand retention in the active site. Overall, chlorogenic acid interacted favorably with both breast cancer-related target proteins through multiple non-covalent interactions. The interaction profile of PDB ID: 2O21 indicates a more favorable binding environment, characterized by stronger hydrophobic contacts and additional stabilizing interactions, which is in agreement with its more negative docking score (−7.40 kcal/mol) compared with PDB ID: 6O0K (−6.40 kcal/mol). These findings suggest that chlorogenic acid possesses a higher binding affinity toward the 2O21 target and may therefore exhibit greater inhibitory potential against this breast cancer-associated protein.

Table 5. The interaction parameters between Chlorogenic acid compound and 6O0K, 2O21 enzymes

Type of Bond	Chlorogenic acid PDB: 6O0K	Bond Length (Å)	Chlorogenic acid PDB: 2O21	Bond Length (Å)
Van der Waals Interactions	VAL-15	-	THR-129	-
	TRP-30	-	ASP-108	-
	GLU-13	-	PHE-109	-
	-	-	VAL-131	-
	-	-	LEU-134	-
Conventional Hydrogen Bonds	ASP-10	4.15	ARG-126	4.76
	ASN-182	5.32	ALA-146	3.28
	ASP-171	4.89	-	-
	THR-178	4.53	-	-
Carbon Hydrogen Bond	ARG-12	3.78	GLU-133	5.99
Unfavorable Donor -Donor	ASN-11	2.98	-	-
	LEU-175	4.07	-	-
Pi-Cation	ARG-12	4.06	-	-
Pi-Sigma	LEU-175	4.64	VAL-130	4.00
Amide Pi-Stacked	Ala-174	6.79	-	-
Metal Acceptor	-	-	THR-129	-
Pi-Alkyl	-	-	MET-112	4.91
Covalent Bond	-	-	VAL-130	4.90

Conclusion

In this study, the structural, electronic, nonlinear optical (NLO), and biological properties of chlorogenic acid were comprehensively investigated using Density Functional Theory (DFT) calculations and molecular docking simulations. Mulliken atomic charge and Molecular Electrostatic Potential (MEP) analyses revealed that the molecule's reactive centers are primarily localized on electron-rich oxygen atoms and electron-poor hydroxyl hydrogens, highlighting its strong hydrogen bonding capacity and susceptibility to both electrophilic and nucleophilic interactions. Frontier molecular orbital (HOMO–LUMO) analysis demonstrated effective intramolecular charge transfer, with the PBEPBE functional predicting a narrower energy gap ($\Delta E = 4.7826$ eV) and higher chemical reactivity compared to the CAM-B3LYP functional. Furthermore, NLO calculations indicated that chlorogenic acid possesses a significant dipole moment, mean polarizability, and high first-order hyperpolarizability (β: 6.21×10^{-30} esu via PBEPBE). These strong nonlinear optical responses suggest that the molecule also holds promising potential for future optoelectronic and photonic applications. Molecular docking simulations provided critical insights into the compound's therapeutic potential against breast cancer. Chlorogenic acid successfully accommodated the active sites of both targeted proteins, exhibiting a more favorable binding affinity toward the PDB: 2O21 target (-7.40 kcal/mol) than the PDB: 6O0K target (-6.40 kcal/mol). The stability of the formed ligand–protein complexes is primarily driven by a robust network of conventional hydrogen bonds, reinforced by various hydrophobic contacts, π-interactions, and van der Waals forces. Collectively, these computational and theoretical findings elucidate the distinct electronic behavior and strong binding mechanisms of chlorogenic acid, establishing a solid theoretical foundation for its consideration as a promising therapeutic candidate in breast cancer drug discovery. These predictive results strongly support the need for further *in vitro* and *in vivo* experimental validations.

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