Razooqi and Al-Ani Iraqi Journal of Science, 2022, Vol. 63, No. 6, pp: 2331-2344
DOI: 10.24996/ijs.2022.63.6.2

ISSN: 0067-2904

# Quantum Mechanical Calculations and Electrochemical Study of Vibrational Frequencies, Energies in Some Flavonoids molecules

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Received: 15/7/2021 Accepted: 7/10/2021 Published: 30/6/2022

**Abstract**

Quantum mechanical computations is conducted using DFT (Density Functional Theory) and PM3 (Parameterized Model 3), also, using DFT of (B3LYP) with a 6-311++G (d, p) with G09 application. These molecular three components include structure, electronic charge density and energetic characteristics of chosen phytomedicine compounds. The impact of functional groups on physical characteristics were studied using myricetin, linebacker, and flavone because of their chemical structures. For phytomedicine compounds, we utilized quantum mechanical simulations to estimate bond length, energy, vibration(vib.) modes, charge density and mechanical properties (cruelty, strength, stiffness, for the measurements of the lengths and energy of the bonds). Herzberg convention is used to look for the connections between the frequencies of similar modes which was used. IR absorption of the highest vibration frequencies modes of 3N-6 was measured and assigned for all species. Physical parameters were also calculated these include: heat of production, amount of energy, atomic electronic charge density, dipole moment and (E gap) ($E = E_{LUMO}-E_{HOMO}$). For three phytomedicine molecules, quantum chemical properties were combined. This software also computed and evaluated the electronic charge density distribution on atoms of 3 molecules. The equilibrium geometries of all three molecules were studied.

**Keywords:** Flavonoids, DFT, B3LYP, G09, IR absorption

# حسابات ميكانيك الكم والدراسة الالكتروكيميائية لترددات الاهتزاز والطاقات في بعض جزيئات الفلافونويدات

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**الخلاصة**

تطبيق حسابات ميكانيك الكم لنظرية ( معاملات النموذج 3) PM3 ونظرية الكثافة الوظيفية DFT لـ (B3LYP)6-311++G (p,d) تطبيق Gaussian-09 على جزيئات طب نباتية مختارة، فإن خطوة الدراسة الحسابية هي دعم العناصر الجزيئية التي تؤثر على البنية التركيبية كثافة الشحنات الإلكترونية على الذرات وخصائص الطاقة. تم اختيار myricetin و linebacker و flavone بسبب تركيبتها الكيميائية المميزة، والتي تسمح للباحثين باستكشاف تأثيرات المجموعات الوظيفية على الصفات الفيزيائية. الفحص

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النظري للخصائص الفيزيائية مثل طول الرابطة والطاقة وأنماط الاهتزاز وكثافة الشحن والخواص الميكانيكية لمركبات الطب النباتي باستخدام حسابات ميكانيك الكم. تم قياس وتخصيص امتصاص الأشعة تحت الحمراء لأنماط ترددات الاهتزاز القصوى لـ 3N−6الجميع الأنواع، وتم استخدام طريقة هيرزبرج لإيجاد الارتباطات بين ترددات الأنماط ذات الصلة. تتضمن المعلمات الفيزيائية المحسوبة ، من بين أمور أخرى، حرارة التكوين والطاقة الكلية وكثافة الشحنة الإلكترونية على الذرات والعزم ثنائي القطب وفجوة الطاقة (ΔE = ELUMO−EHOMO). بالنسبة لجزيئات طب النبات الثلاثة، ارتبطت المعلمات الكيميائية وفق ميكانيك الكم. تم استخدام برنامج Gaussian 09 أيضًا لقياس وتقييم توزيع كثافة الشحنة الإلكترونية على ذرات ثلاثة جزيئات؛ تم بحث ووصف الجزيئات الثلاثة في توازنها وهندستها وتناظرها.

## 1. Introduction

Natural flavonoid derivatives are well-known for their biological antibacterial, anti-viral, antioxidant, and anti-inflammatory effects [1-3]. Plants such as Camellia sinensis (popularly known as green tea), fruits such as Euterpe oleracea (açai berry), and plant seeds such as Glycine max have a certain amount of flavonoids (soy). They are composed of a large set of benzopyrone-based polyphenolic chemicals and are reliant on the structure. The chemical character of flavonoids relies on their kind, their degree of hydroxylation and polymerization, other chemical replacements and conjugations [4]. Flavonoids are linked to many biological impacts and health promotion activities[5] among components. Plant-produced flavonoids are polyphenolic chemicals that are known to offer different biological advantages against different human ailments. The role of flavonoids as anti-inflammatory, antibacterial, antifungal, antioxidant, and antiviral agents has been established in several research [6-9]. Density functional theory (DFT) with the B3LYP functional [10] is the theoretical method in this study. Due to considerable interest in its many positive biological properties including antidiabetic, neuroprotective, cardioprotective, and anticancer actions, etc., flavonoids have been widely studied over the past several decades. Flavonoids are typically linked to their antioxidants, that is, they are capable of scavenging free radicals and other reactive species involved in the development of many human disorders [11-15]. Plant pigments are also referred to as flavonoids, which form any place inside plants and in the category of polyphenolic chemicals [16-17]. 4,000 natural flavonoids have been found and this number has been increasing so far [17]. The flavonoids comprise more than 10,000 structures and represent a major group of secondary metabolites. Many lines of evidence reaffirm their idea that higher plants with a wide-ranging of environmental challenges have antioxidant effects [6,18-19]. Flavonoids prevent many biotic and abiotic stressors from occurring and act as unique UV filters [20]. Flavonoids are a promising group of bioactive chemicals with low toxicity. The common secondary metabolites of diverse fruit-vegetable and medicinal plants, natural flavonols, flavanones, and other ingredients of this class [21] are strongly anti-oxidant and anti-inflammatory [22-23]. Dietary polyphenols, such as flavonoids and phenolic acids, which are found in a great number of plant-origin foods, have many positive benefits and play essential roles in chronic and degenerative disease prevention, flavonoids have many properties as, antioxidant, anti-inflammatory and neuroprotective effects, anti-cancer, immunomodulatory, antidiabetic and antiadipogenic [24-25]. Compared to micro- and macronutrients, biological availability of dietary polyphenols is low. But recent research demonstrate that these phytochemicals have prebiotic and anti-pathogenic intestinal Flora characteristics [24]. Flavonoids are a collection of natural compounds that are present in plants with various phenolic structures. A novel compound was extracted from oranges in 1930. It was thought to be a member of a novel class of vitamins at that time and was labeled vitamin P. The fact that this compound was a flavonoid (rutin) has been known later [25] Previous studies have generally shown the SET mechanism as a unique electron transfer from antioxidant to free radical and is subjected to the antioxidant molecule adiabatic ionizing potential (IP)[26]. The chemical hardness (η) has proved to be an effective world index of atoms, molecules, and clusters response based on the density functional theory [27-28] introduced in terms of chemical potential (μ) and hardness (η) the global electrophilicity index (ω) in [29].

$$\omega = \mu^2/2\eta \qquad \text{------------------(1)}$$

For some time, medicinal plants were identified as a potential hub for natural chemicals with antioxidants, especially secondary plant metabolites, i.e. phenolic substances and flavonoids produced in plants to support or encourage growth in adverse conditions(Such as phenolic substances and flavonoids produced in plants to support or encourage growth in adverse conditions). Functional group design, conformation, substitution, and the number of hydroxy groupings have also been altered by flavonoid action, such as radical activity scavenging and/or metal chelation [30]. Generally, hydroxylation positions and numbers are reasonably correlated to flavonoid anti-oxidation. Hydrostatic and electron radicals, which are flavonoid radicals with highly stable, are provided by Ring B hydroxyl groups into hydroxyl, peroxyl, and peroxyacetic radials. Flavonoids, on the other hand, might scavenge the resultant radicals to counteract their previous effect. Based on greatly improved anti-oxidant effects, the requirement for at least two hydroxyl groups in ring B (Figure 1) anti-oxidant capability is recommended [31].

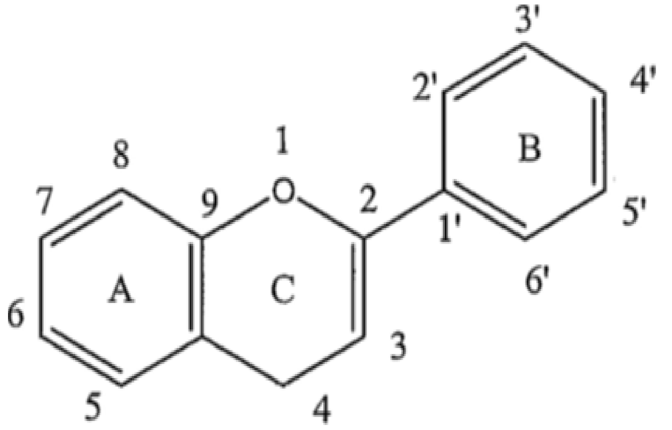


**Figure 1-** Flavonoids have a simple structure.

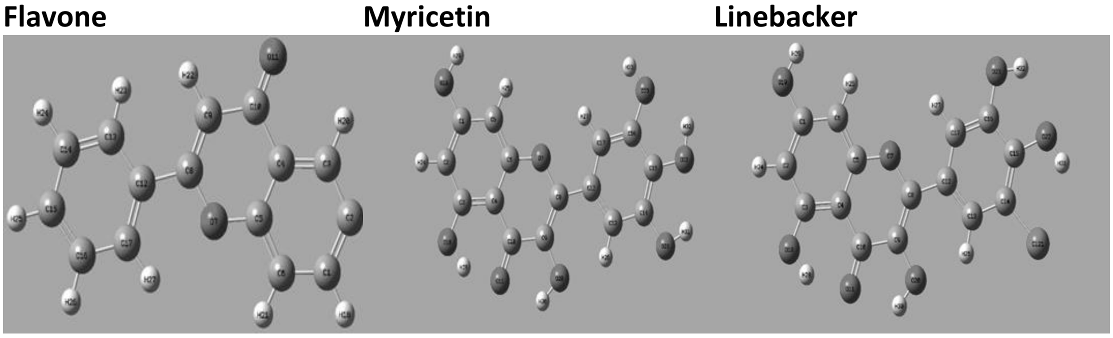
Most of the powerful progress tools in this sector of computational software are virtual chemical methods. This offers incredibly useful low-cost expertise, allowing the impacts of different molecular characteristics. The fundamental objective of this research is to determine how hydroxyls affect the local charges and how they influence geometries and molecular energies[32]. Flavonoid antioxidants counteract reactive oxidation by giving electrons. Despite this, it is widely understood that a little A flavonoid's molecular structure may impact its antioxidant effectiveness.

## 2. Computation Methods

The application of computational chemistry in chemical and medical research has grown in recent years. The Gaussian 09 software was used to do DFT calculations. [33] to calculate the density function theory (DFT) The 6-311++ G basis set was utilized for this project. The possibility for electrostatic attraction [34-37]. Among the physical characteristics that were identified are the optimal equilibrium total energy, dipole moment, partial nuclear charge, and molecular energy orbitals. By utilizing vibrational frequencies, the lack of imaginary values was utilized to demonstrate the presence of a real minimum for the optimized geometries. Atoms in Molecules explores the topological and energy aspects of intramolecular hydrogen bonding as well as molecular characteristics in atoms. For the best constructions, all calculations have been done.

## 3. Discussion and Conclusions

Quantum chemical methods in electrochemistry (the charges on the atoms were calculated, as well as the interpretation of their effect on the molecule in terms of vibrations and energy) are extremely useful because they allow researchers to easily know the structure and function of flavone and 2 closely similar polyphenols. Using quantum chemical computations to determine the physical properties of flavonoids is a routine procedure. The key molecular parameters in Table 2 calculated at the B3LYP/6-311 G++ optimized bond lengths and charges study underscoring the importance of bioactive aromatic groups in antioxidant activities actions for flavone and flavonoid generated from its flavonoids with estimated structures given in (Figure 2) and important molecular characteristics in a Table 2.



Flavone Myricetin Linebacker

**Figure 2-**G09 program is used to calculate the equilibrium bonding and angles of flavone, myricetin, and linebacker compounds.

A high capacity to donate electrons is connected to a high HOMO [36,38] HOMO is the highest in myricetin and the lowest in flavone among the three flavonoid compounds (see Table 1). The following order is in line with HOMO trend:

**myricetin > linebacker > flavone**

The title molecule reactivities are larger because the orbital energy gap on the frontiers is lower and the dipole moment is bigger. The correlation graphs of physical characteristics of flavone, linebacker, and myricetin molecules are shown in Figure 3. E (energy gap) may be thought of as a guess based on chemical data and hence a predictor of compound kinetics. The antioxidant is much more efficient when the E gap is smaller. The low bandgap energy indicates flavonoids are reactive systems. Flavonoid (energy gap) energy different [39].

An examination of border-orbital ( E gap) shows how electron density is distributed across the molecule: **myricetin > linebacker > flavone**

The energy gap of myricetin is bigger than the rest molecules because myricetin contains more groups of OH than the rest of the molecules, this difference appears larger than that of the rest of the molecules because myricetin contains more OH groups than the rest of the molecules at six sites on the molecule while linebacker contains five sites and flavones do not contain an OH group.

It was found, The primary reactive sites are –OH, C-O-C and C=O, this according to the computational techniques. These aggregates are sites for the concentration of charges and also affect the vibration and electro-negative energy.

The electronegative region is mostly above the electrophilic attack site of carbonyl oxygen. The calculated vibratory modes are visible in the comparison of calculated data. The following correlations emerge from comparing the three molecules' measured global hardness (a pertinent metric for assessing charge transfer preventative medicine) (Figure 3)

**Flavone > Linebacker > Myrcetin**

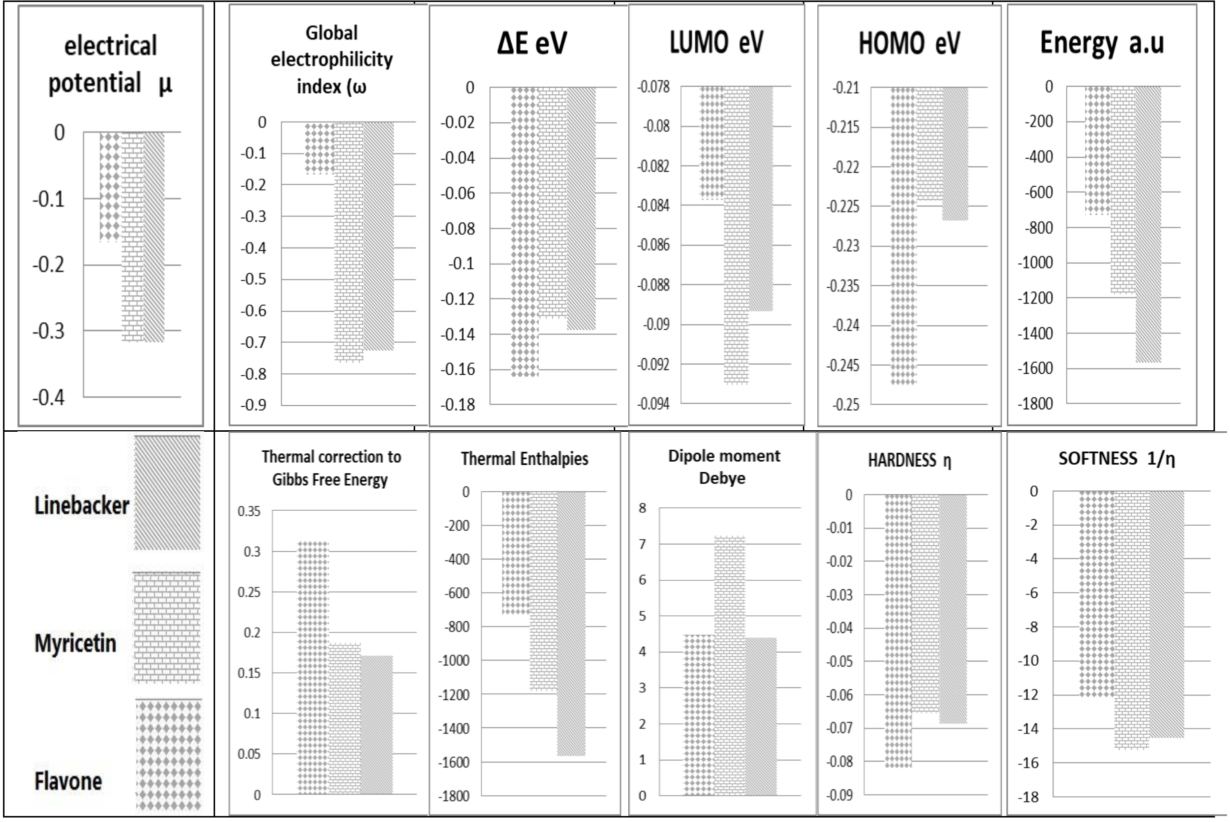


**Figure 3-**G09 software is used to estimate the physical characteristics of flavone, myricetin and linebacker molecules.

In most electronegative regions, oxygen atom of carbonyl, hydroxy and C=O is considered to the electrophilic attacks through the electric charges, this is shown on the molecule in the following:

**Table 1-**Bond lengths of flavone, myricetin, and linebacker geometries which were optimized using DFT at B3LYP/ 6-311++G(d,p).

| Flavone[39] | | Myricetin | | **Linebacker** | |
|---|---|---|---|---|---|
| **Atoms** | **Bond length (Å)** | **Atoms** | **Bond length (Å)** | **Atoms** | **Bond length (Å)** |
| C1-C2 | 1.4031 | C1-C2 | 1.3996 | C1-C2 | 1.4001 |
| C2-C3 | 1.3843 | C2-C3 | 1.3876 | C2-C3 | 1.3850 |
| C3-C4 | 1.4029 | C3-C4 | 1.4264 | C3-C4 | 1.4253 |
| C4-C5 | 1.3977 | C4-C5 | 1.4006 | C4-C5 | 1.4033 |
| C1-C6 | 1.3860 | C5-C6 | 1.3888 | C5-C6 | 1.3901 |
| C5-O7 | 1.3707 | C5-O7 | 1.3828 | C5-O7 | 1.3583 |
| O7-C8 | 1.3623 | O7-C8 | 1.4036 | O7-C8 | 1.3732 |
| C8-C9 | 1.3561 | C8-C9 | 1.3633 | C8-C9 | 1.3663 |
| C9-C10 | 1.4551 | C4-C10 | 1.4225 | C4-C10 | 1.4327 |
| C10-O11 | 1.2270 | C10-O11 | 1.2877 | C10-O11 | 1.2546 |
| C8-C12 | 1.4769 | C8-C12 | 1.4565 | C8-C12 | 1.4656 |
| C12-C13 | 1.4042 | C12-C13 | 1.4084 | C12-C13 | 1.4054 |
| C13-C14 | 1.3892 | C13-C14 | 1.3912 | C13-C14 | 1.3864 |
| C14-C15 | 1.3950 | C14-C15 | 1.3944 | C14-C15 | 1.3920 |

| | | | | | |
|---|---|---|---|---|---|
| C15-C16 | 1.3926 | C15-C16 | 1.3928 | C15-C16 | 1.4031 |
| C16-C17 | 1.3917 | C16-C17 | 1.3836 | C16-C17 | 1.3842 |
| C1-H18 | 1.0839 | C3-O18 | 1.3557 | C3-O18 | 1.3405 |
| C2-H19 | 1.0835 | C1-O19 | 1.3791 | C1-O19 | 1.3594 |
| C3-H20 | 1.0834 | C9-O20 | 1.3754 | C9-O20 | 1.3540 |
| C6-H21 | 1.0830 | C14-O21 | 1.3818 | C14-Cl21 | 1.7622 |
| C9-H22 | 1.0800 | C15-O22 | 1.3888 | C15-O22 | 1.3615 |
| C13-H23 | 1.0822 | C16-O23 | 1.3975 | C16-O23 | 1.3608 |
| C14-H24 | 1.0839 | C2-H24 | 1.0802 | C2-H24 | 1.0815 |
| C15-H25 | 1.0839 | C6-H25 | 1.0801 | C6-H25 | 1.0831 |
| C16-H26 | 1.0840 | C13-H26 | 1.0773 | C13-H26 | 1.0776 |
| C17-H27 | 1.0810 | C17-H27 | 1.0813 | C17-H27 | 1.0799 |
| | | O18-H28 | 1.0294 | O18-H28 | 0.9851 |
| | | O19-H29 | 0.9895 | O19-H29 | 0.9634 |
| | | O20-H30 | 1.0155 | O20-H30 | 0.9772 |
| | | O21-H31 | 0.9972 | O22-H31 | 0.9671 |
| | | O22-H32 | 0.9972 | O23-H32 | 0.9662 |
| | | O23-H33 | 0.9972 | | |

**Table 2-** Electronic charge calculations using G09 software for flavone, myricetin and linebacker molecules.

| **Flavone[39]** | | **myricetin** | | **Linebacker** | |
|---|---|---|---|---|---|
| **Atom** | **Charge** | **Atom** | **Charge** | **Atom** | **Charge** |
| C1 | -0.4455 | C1 | 0.9694 | C 1 | 0.9716 |
| C2 | -0.0949 | C2 | -0.3683 | C2 | 0.3712 |
| C 3 | 0.3117 | C3 | 0.8401 | C3 | 0.8450 |
| C4 | 2.1824 | C4 | -0.5668 | C4 | 0.5680 |
| C5 | -1.7849 | C5 | 0.6311 | C5 | 0.6588 |
| C6 | -0.2937 | C6 | -0.5291 | C6 | -0.5243 |
| O7 | 0.0412 | O7 | -0.6975 | O7 | -0.7266 |
| C8 | 0.6325 | C8 | 0.7482 | C8 | 0.6710 |
| C9 | -0.5558 | C9 | -0.2762 | C9 | -0.2117 |
| C10 | -0.7686 | C10 | 1.3371 | C10 | 1.3334 |
| O11 | -0.2954 | O11 | -1.0378 | O11 | -1.0294 |
| C12 | 1.0963 | C12 | -0.1276 | C12 | -0.0657 |
| C13 | -0.5592 | C13 | -0.1209 | C13 | -0.1556 |
| C14 | -0.5512 | C14 | 0.5376 | C14 | 0.3488 |
| C15 | -0.2950 | C15 | 0.5088 | C15 | 0.4879 |
| C16 | -0.3726 | C16 | 0.4306 | C16 | 0.4822 |
| C17 | 0.0572 | C17 | -0.1319 | C17 | -0.0818 |
| H18 | 0.1790 | O18 | -0.8270 | O18 | -0.8001 |
| H19 | 0.1693 | O19 | -0.8367 | O19 | -0.8461 |
| H20 | 0.1956 | O20 | -0.5955 | O20 | -0.6045 |
| H21 | 0.1665 | O21 | -0.7442 | Cl21 | -0.3311 |

| | | | | | |
|---|---|---|---|---|---|
| H22 | 0.2136 | O22 | -0.9132 | O22 | -0.9004 |
| H23 | 0.0830 | O23 | -0.7225 | O23 | -0.7489 |
| H24 | 0.1898 | H24 | 0.0810 | H24 | 0.0833 |
| H25 | 0.1548 | H25 | 0.0589 | H25 | 0.0637 |
| H26 | 0.1854 | H26 | 0.1301 | H26 | 0.1278 |
| H27 | 0.1583 | H27 | 0.0853 | H27 | 0.1005 |
| | | H28 | 0.4902 | H28 | 0.4384 |
| | | H29 | 0.2939 | H29 | 0.2990 |
| | | H30 | 0.3751 | H30 | 0.3689 |
| | | H31 | 0.3289 | H31 | 0.3507 |
| | | H32 | 0.3513 | H32 | 0.3343 |

## Mulliken Atomic Charges

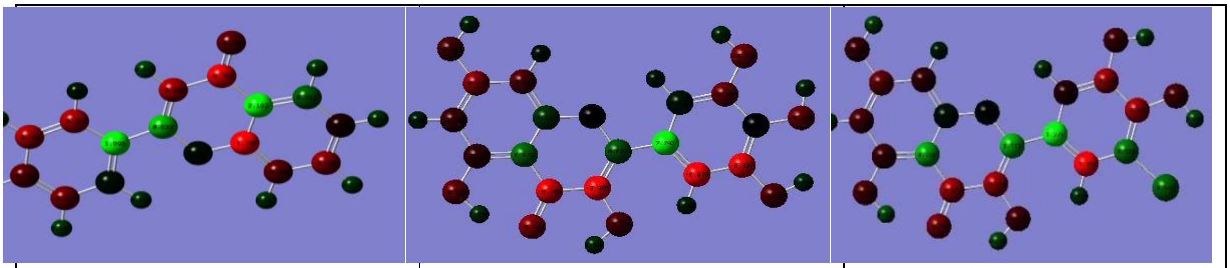
Mulliken charges are a useful tool for interpreting the chemical composition basis of structure. Charge in an atom of the molecule assists to depict the electron density distribution across the molecule in a straightforward way. The chemical under investigation has no net charge. Table 2 shows the Mulliken charge of the title compound calculated using a 6-311++G (d, p) basis set in the gas phase. Some C and H atoms have a higher positive charge, but the oxygen atoms of the three molecules, as well as the Cl atom in a linebacker, have a negative charge. A positive charge exists on all hydrogen atoms. Figure 4 shows a graphical representation of Mulliken charges in the gas phase.

## Electronic Properties

Quantum chemical computations are crucial for deducing information about organic molecules' electrochemical activity. At B3LYP/6-311++G (d, p) level, the title compounds were subjected to a frontier molecular orbital (FMO) study. FMO analysis takes into account the interactions between full and empty molecular orbitals. The primary orbitals involved in the chemical stability of compounds are the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO). The electron donor HOMO and the electron acceptor LUMO work together. The energy gap is the difference between the energies of HOMO and LUMO, which influences a molecule's reactivity and kinetic stability. The energy gap between hard and soft molecules is large for hard molecules and small for soft ones. The following relation describes the HOMO-LUMO energy gap ($\Delta E$) of title compounds and the charge transfer interactions that occur within the molecules in the end:

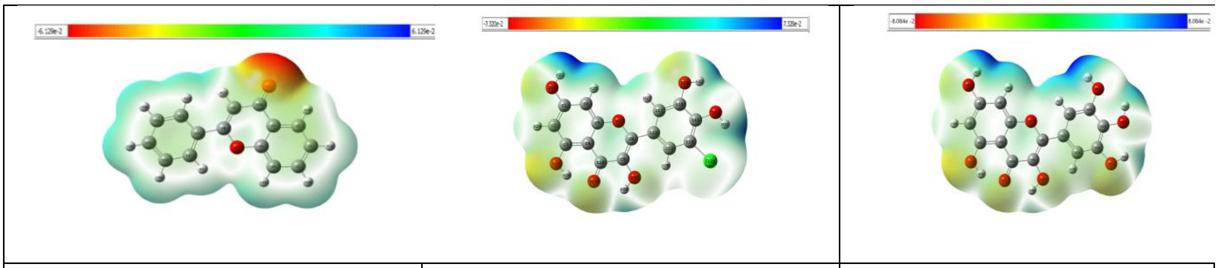
Myricetin > Linebacker > Flavone

The Mulliken atomic charge in the B3LYP level for the three molecules was set at 6-311G++ (d, p) (Table 2). C, O, C = O and OH are the main axis of charge density.



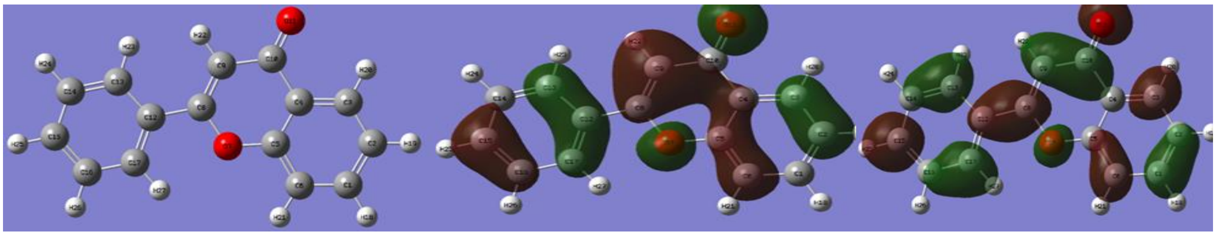
| **Flavone[39]** | **Myricetin** | **Linebacker** |
|---|---|---|

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| 🟥 | -0.788 | 🟩 | 1.317 – 0.853 | 🟧 | -0.245 | ⬛ | 0.033 | 🟩 | 0.217 | **Charge value** |

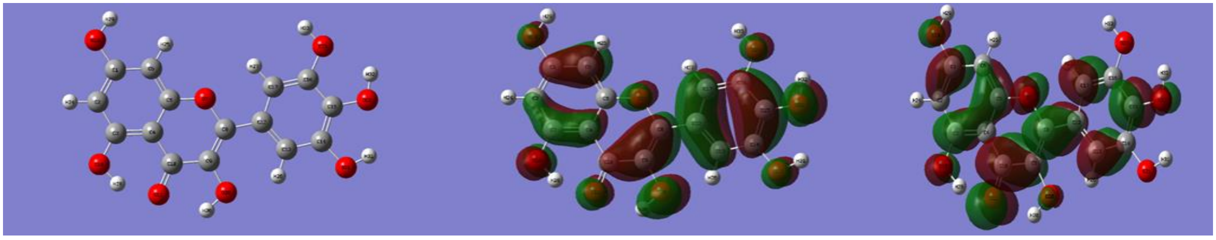


| **Flavone[39]** | **linebacker** | **myricetin** |
|---|---|---|

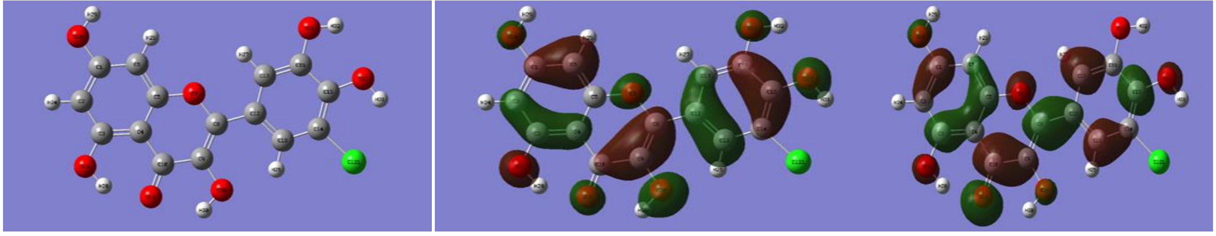
**Figure 4-** Molecular Mulliken charge density of flavone, linebacker, and myricetin molecules using DFT at (B3LYP) 6-311++G (d,p).



flavone [39] Homo = - 0.24746 Lumo = -0.08371



myricetin Homo = - 0.224221 Lumo = - 0.09305



linebacker Homo = - 0.22676 Lumo = -0.08934

**Figure 5-**HOMOs and LUMOs and their energies for flavone, myricetin and linebacker molecules calculated using density functional theory at B3LYP/6-311G++(d,p).

## Vibration frequencies assignment of Flavonoid, Myricetin, and Linebacker molecules.

DFT (B3LYP 6-311++G) calculations were carried out for the estimation of vibration frequencies, and normal coordinates for all flavonoids derivatives, by using the Gaussian-09 program. The results allowed interesting relations between the different vibration modes and could be useful for the discussion of different problems of stability and reactivity of the molecules. For symmetrical stretching of H-O bond due to the O-H group was found to have a values range of (3829.44-3308 cm-1)( DFT (B3LYP 6-311++G(d,p)), For stretching vibration frequency of C-H belonging to the flavone was found 3225.17 $cm^{-1}$, for the myricetin have the value 3260.68 $cm^{-1}$, and for the linebacker have the value of (3400.84 $cm^{-1}$) which was the higher value in linebacker molecule. The highest frequency values correspond to the largest bond force constants. The vibration of a molecule causes deformation in its geometry. Structure deformation is expected to change its physical and chemical properties. While for stretching vibration frequency of (C=O) str. was found to have values range of flavone was the range (502.04 - 117.10 $cm^{-1}$), and for the Applying this comparatively convenient method allowed the valance assignment for the vibration modes of this molecule for the first time, the main subject of this work is to understand how the presence of hydroxyl groups affects and how this is related to geometric structures and molecular parameters and with molecular energy. The vibration of a molecule causes deformation in its geometry, structure deformation is expected to change its physical and chemical properties. The antioxidant properties of polyphenols are related to the nature of their chemical structures. Flavonoids are effective scavengers of hydroxyl, peroxyl, and superoxide anion radicals.

The vibrations that make up the foundation (3N-6) and the effects of the irreducible formulation in subsequent vibration modes are:

**Γvibration = Γtotal - (Γrotation + Γtranslation)**

There are several vibration modes in use (IR). The following are their responsibility:

**CH stretching vibration:**

H atoms are located on the transposition paths. Their mode frequencies vary from to examining the values (Table 3,4), the following relation emerge:

νCHstr.( **Linebacker)** > νCHstr.( **Myricetin**) > νCHstr.( **Flavone)**

**Ring (CCC) stretching vibration:**

Atomic displacement courses reveal that displacement directions are not located at individual C atoms. Their Variations in predicted vibrational modes (Infrared active) show the following relation (Tables 3, and 4):

ν CCC str.( **Linebacker**) > ν CCC str.( **Myricetin**) **>** ν CCC str.( **Flavone**)

**OH stretching vibration**

The estimated Frequency of vibrations (Infrared active) as modes vary between Tables 3and 4, with interesting correlations of:

**ν(OH)str. (Linebacker) > ν(OH)str. ( Myricetin)**

**C=C stretching vibration:**

The Frequency of vibrations (Infrared active) as modes vary between Tables 3and 4, with interesting order of:

**νC=C str.( Linebacker) > ν C=C str.( Flavone**) **>** ν **C=C str.( Myricetin)**

**In-plane CH bending vib. (δCH):**

H atoms are located on the transposition paths. Their mode frequencies vary from to examining the values (Tables 3, and4), the following relation emerge:

**νδCH(Linebacker**) **>νδCH(Flavone) >νδCH(Myricetin)**

**In-plane (ring) bending vibration (δ ring):**

Examining the numbers in Tables 3 and 4 and the estimated vibration frequencies (IR active) reveal the following correlations:

**νδ ring. ( Linebacker) >νδ ring (Flavone)**

**Out of plane CH bending vibration (γCH):**

Frequency of vibrations (Infrared active) as mode varies between Tables 3 and 4 as following.:

**νγ CH(Flavone) >νγ CH(Myricetin) >νγ CH(Linebacker)**

### Out of plane ring bending vibrations (γ ring):

Deformations and pinching vibrations of the ring computed vibrational modes (Infrared active) modes are included. Comparing the estimated frequency modes values molecules to use G09 software reveals the following correlations:

**νγ(CCC)(Linebacker) > νγ(CCC)ring(Flavone)> νγ(CCC)(Myricetin)**

**Table 3-**Vibration. frequencies to calculate modes of flavone, myricetin and linebacker molecule using DFT at B3LYP/ 6-311++G(d,p).

| | Flavone [39] | | myricetin | | linebacker | |
|---|---|---|---|---|---|---|
| **Vib. modes** | **Symmetry and description** | **Frequency** | **Symmetry and description** | **Frequency** | **Symmetry and description** | **Frequency** |
| ν1 | δ ring | 24.74 | ring str ( breathing) | 40.82 | ring str | 15.01 |
| ν2 | δ ring | 57.30 | ring str | 59.54 | ring str | 38.11 |
| ν3 | γ ring | 116.21 | ring str | 98.91 | ring str | 77.30 |
| ν4 | C=O str | 117.10 | C-C str | 101.57 | C-O str | 79.60 |
| ν5 | δCH + δring | 149.80 | C-C str | 123.48 | γ ring | 108.92 |
| ν6 | C=Cstr + C=Ostr | 190.40 | δ C=O | 161.82 | γ OH | 127.79 |
| ν7 | γring | 267.70 | δ C-O | 193.93 | γ ring | 153.85 |
| ν8 | δ CH + δ ring | 281.40 | δ ring | 213.40 | γ Cl | 172.86 |
| ν9 | γ CH + γC=O | 294.07 | δ CH + δ OH | 240.47 | γ CH + γ OH | 219.14 |
| ν10 | γRing + γ C=O | 351.64 | δ OH | 242.36 | δ OH | 228.82 |
| ν11 | δRing | 408.75 | ring str | 260.05 | γ ring | 234.77 |
| ν12 | CH str + ring str | 431.24 | C=C str | 262.58 | γ ring | 245.74 |
| ν13 | CH str + ring str | 467.77 | C-C str | 290.84 | γ Cl + γ OH | 261.70 |
| ν14 | γCH + γ C=O | 502.04 | δ OH | 308.28 | γ ring + γ OH | 281.03 |
| ν15 | γCH + γ ring | 512.97 | γ OH | 336.74 | δ OH | 282.20 |
| ν16 | CH str + C=C str | 533.53 | δ OH | 343.39 | γ OH | 315.47 |
| ν17 | γCH + γ ring | 588.35 | δ OH | 355.27 | γ OH | 315.82 |
| ν18 | γCH | 613.86 | δ ring | 361.04 | δ OH | 338.45 |
| ν19 | γ ring | 634.07 | γ OH | 403.93 | γ OH | 344.99 |
| ν20 | δCH + δ ring | 660.17 | OH str | 409.90 | γ OH | 349.58 |
| ν21 | CH str + C=C str | 679.65 | C-O str + ring str | 417.79 | δ OH + δ C=O | 374.87 |
| ν22 | γ ring | 685.60 | γ C=O | 466.82 | γ OH | 401.96 |
| ν23 | Ring str | 700.50 | γ OH | 518.77 | C-O str | 403.75 |
| ν24 | γCH + γ ring | 755.78 | δ OH + δ CH | 530.14 | γ OH | 411.22 |
| ν25 | CH str + C-C str | 766.63 | γ CH | 531.42 | γ OH + γ ring | 417.70 |
| ν26 | CH str | 781.40 | C=C + C-O | 540.71 | γ OH + γ C=O | 463.55 |
| ν27 | CH str + C=C str | 789.83 | δ OH + δ CH | 572.26 | γ ring | 515.59 |
| ν28 | CH str | 846.07 | γ OH + γ CH | 581.65 | γ CH | 516.79 |
| ν29 | γ CH + γ ring | 860.98 | δ OH | 593.22 | γ CH + γ OH | 529.57 |
| ν30 | CH str | 865.84 | δ OH | 599.78 | γ CH + γ OH | 543.26 |
| ν31 | CH str | 879.85 | δ ring + δ -O- | 625.08 | γ Ring + γ OH | 582.50 |
| ν32 | γCH | 920.01 | δ CH + δ C-O | 629.58 | γ OH | 596.98 |
| ν33 | CH str | 939.76 | γ OH | 640.36 | γ ring + γ OH | 610.29 |
| ν34 | CH str | 977.05 | γ CH | 650.39 | γ ring + γ OH | 616.54 |
| ν35 | CH str | 989.73 | δ ring | 660.41 | γ ring + γ OH | 629.97 |
| ν36 | CH str | 1002.66 | γ OH | 673.96 | γ CH + γ OH | 634.69 |
| ν37 | CH str | 1007.12 | γ OH | 686.13 | γ CH + γ ring | 647.74 |
| ν38 | Ring str | 1015.83 | γ OH | 693.60 | γ CH | 667.30 |
| ν39 | γ CH + γ ring | 1030.93 | γ OH + γ ring | 704.28 | γ ring | 685.57 |
| ν40 | γ CH | 1050.79 | γ CH + γ ring | 722.37 | γ ring + γ CH | 695.15 |
| ν41 | γ CH | 1061.74 | C-C str | 731.25 | γ CH + γ C=C | 725.49 |
| ν42 | γ CH | 1107.57 | δ OH | 748.85 | γ OH + γ C-C | 731.47 |
| ν43 | γ CH | 1111.42 | γ ring | 755.15 | γ ring | 737.68 |
| ν44 | γ CH | 1147.41 | γ CH | 777.45 | γ OH | 769.22 |
| ν45 | γ CH | 1174.36 | γ ring + γ CH | 827.56 | γ CH | 787.36 |
| ν46 | γ CH | 1186.46 | γ CH | 831.41 | δ OH + δ CH | 838.44 |

| | | | | | | |
|---|---|---|---|---|---|---|
| v47 | γ CH | 1211.67 | γ CH | 850.29 | γ CH | 851.57 |
| v48 | γ CH | 1236.34 | γ OH | 876.71 | γ CH | 880.99 |
| v49 | CH str + ring str | 1250.97 | γ OH + γ CH | 884.57 | γ OH | 884.52 |
| v50 | γ CH | 1274.66 | γ OH + γ ring | 936.39 | γ CH | 891.44 |
| v51 | γ CH | 1305.89 | γ CH | 996.99 | γ OH + γ CH | 958.81 |
| v52 | γ CH | 1331.11 | γ OH | 1003.32 | δ CH | 1017.95 |
| v53 | CH str + C=C str | 1356.72 | γ OH + γ CH | 1014.83 | γ CH | 1039.15 |
| v54 | γ CH | 1359.92 | γ CH | 1031.03 | γ ring + γ C-O + γ OH | 1107.60 |
| v55 | γ CH | 1385.41 | γ CH + γ C-O | 1072.04 | γ CH | 1129.09 |
| v56 | CH str + ring str | 1478.34 | γ CH | 1088.68 | γ CH | 1159.84 |
| v57 | γ CH + γ ring | 1492.22 | γ CH | 1136.76 | γ CH | 1172.95 |
| v58 | δ CH | 1500.98 | γ CH | 1151.46 | γ CH | 1195.83 |
| v59 | γ CH | 1526.51 | γ CH + γ OH | 1196.97 | γ OH | 1213.17 |
| v60 | γ ring | 1603.52 | γ CH | 1198.77 | γ OH + γ CH | 1215.06 |
| v61 | CH str+ ring str | 1616.25 | γ CH + γ OH | 1232.75 | γ OH + γ CH | 1249.79 |
| v62 | CH str+ ring str | 1641.27 | δ CH | 1253.24 | γ OH + γ CH | 1263.13 |
| v63 | CH str + ring str | 1643.2 | γ CH + γ OH | 1267.76 | CH str | 1278.35 |
| v64 | Ring str | 1653.58 | γ OH | 1290.06 | OH str | 1300.50 |
| v65 | γ C=O | 1702.84 | γ OH + γ ring | 1309.24 | OH str + CH str | 1342.20 |
| v66 | CH str | 3168.22 | γ OH | 1318.89 | OH str + C=C str | 1353.53 |
| v67 | CH str | 3173.17 | γ OH | 1334.28 | OH str + CH str | 1359.69 |
| v68 | CH str | 3178.14 | γ OH | 1352.95 | OH str | 1368.20 |
| v69 | CH str | 3186.40 | γ OH | 1387.64 | OH str | 1401.51 |
| v70 | CH str | 3189.32 | γ OH | 1397.44 | OH str + C-C str | 1428.68 |
| v71 | CH str | 3197.57 | γ OH + γ CH | 1419.03 | OH str | 1456.67 |
| v72 | CH str | 3199.68 | δ OH | 1438.24 | γ OH + γ ring | 1480.30 |
| v73 | CH str | 3201.61 | OH str | 1460.40 | γ OH + γ ring | 1514.15 |
| v74 | CH str | 3216.85 | OH str + CH str | 1496.22 | γ OH + γ CH | 1519.75 |
| v75 | CH str | 3225.17 | γ CH + γ OH | 1504.88 | δ CH | 1528.32 |
| v76 | | | γ CH + γ OH | 1514.72 | OH str | 1605.93 |
| v77 | | | γ CH + γ OH | 1544.45 | ring str | 1616.31 |
| v78 | | | γ OH | 1566.45 | OH str + ring str | 1627.70 |
| v79 | | | γ OH | 1623.93 | CH + ring str | 1649.04 |
| v80 | | | ring str + OH str | 1641.36 | γ OH + γ ring | 1664.00 |
| v81 | | | OH str | 1648.28 | OH str + ring str | 1686.96 |
| v82 | | | OH str + ring str | 1663.55 | CH str | 3190.83 |
| v83 | | | γ OH | 1685.84 | OH str | 3215.99 |
| v84 | | | γ OH | 2766.53 | CH str | 3233.06 |
| v85 | | | OH str | 3118.46 | CH str | 3256.28 |
| v86 | | | CH str | 3209.08 | CH str | 3400.84 |
| v87 | | | CH str | 3216.22 | OH str | 3600.26 |
| v88 | | | CH str | 3225.93 | OH str | 3767.04 |
| v89 | | | CH str | 3260.68 | OH str | 3791.65 |
| v90 | | | OH str | 3392.23 | OH str | 3829.44 |
| v91 | | | OH str | 3424.03 | | |
| v92 | | | OH str | 3494.92 | | |
| v93 | | | OH str | 3542.07 | | |

**Bending vibrations OH off of plane OH**

Vibration frequencies (IR-active) that have been determined to examine the numbers in Table-3 and Table-4 reveal interactions which were observed between their predicted vibrational modes to use G09 application:

**νγOH (Myricetin)> νγOH (Linebacker )**

**Table 4-**Vibration freq. modes of Flavone, Myricetin, and Linebacker molecule computed using DFT at B3LYP/ 6-311++G. (d,p).

| Vibration modes | Flavone [39] | Myricetin | Linebacker |
|---|---|---|---|
| **CH str** | 3225.17 - 679.65 | 1496.22- 3260.68 | 3260.68 - 3400.84 |
| **ring str** | 1653.58 --1015.83 | 40.82 - 1663.55 | 15.01 - 1686.96 |
| **C=C str** | 679.65 - 190.4 | 262.58 | 1353.53 |
| **C=O str** | 502.04 - 117.10 | --------- | ---------- |
| **C-C str** | 766.63 | 101.57 - 731.25 | --------- |
| **C-O str** | -------------- | 417.79 | 79.6 - 403.75 |
| **OH str** | ------ | 409.9 - 3542.07 | 1300.5 - 3829.44 |
| **δ CH** | 1500.98 | 24047 - 1253.24 | 1017.95 - 1528.32 |
| **δ ring** | 408.75 - 57.30 | 213.4 - 660.41 | --------- |
| **δ OH** | ------ | 240.47 - 1438.24 | 228.82 - 838.44 |
| **γ ring** | 1603.52-116.21 | 755.15 - 1309.24 | 108.92 - 1664 |
| **γ CH** | 3168.22--613.86 | 531.42 - 1544.45 | 219.14 - 1519.75 |
| **γ OH** | ------ | 336.74 - 2766.53 | 127.79 - 1664 |

The highest bond force constant is usually used, whereas the weakest strength constant is used in the relation:

$\nu = 1/2\pi \sqrt{(k/\mu)}$……….(2)

Wheres: (ν) is the frequency in $cm^{-1}$, (k) is the force constant in N/cm, ( μ) is the reduced mass in Kg. The lowest frequency is the lowest bond force constant. There are .no experimental vibrational frequency data for these compounds in the literature to have it compared with our calculations.

## Conclusion

Physical qualities, bond length, energy, modes of vibrations, charge density, and mechanical properties "hardness, softness, and strength" of phytomedicine molecules are all studied using quantum mechanical simulations. A density-function level theory based on B3LYP 6 311++G was used to investigate the compounds Flavone Myricetin and Linebacker (d, p). The presence of C = O, CH3 and the functioning of dihydroxy of the link and promotesis aproved according to the findings. Based on this study, a dihydroxy group within the B ring that provides high radicals stabilization, which may be summarized in two pre-conditions for good antioxidant activity, and the double bond of C2-C3 in connection, at the theoretical level of B3LYP/6-311++G (d, p). In this study, the structural of B3LYP/6-311++G (d, p) technique was used to study three natural polyphenols: flavone, myricetin, and linebacker. The flavonoid also with the lowest energy gap appears when the 3 compounds are examined. These are the three flavonoids that have been linked to the relation:

**myricetin > flavone > linebacker**

The results are in line with theoretical results. At the end of the day, calculated vibrations frequency (Infrared) reveal that carbonyl extending, OH stretching, C=O stretching and OH stretching, C=O stretching vibration frequent values are all present in (C-C-C stretching). Flavone has the highest frequency of vibrations, followed by myricetin and linebacker frequency values, all of which lead to key chemical characteristics.

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