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Therapeutic role of medicinal plants against viral diseases focusing on COVID-19: Application of computational chemistry towards drug design

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Summary

Introduction: The phytocompounds of curcumin, epicatechin-gallate, luteolin-7-glucoside, and zingerol extracted from *Garlic*, *Turmeric/Curcuma*, *Green tea*, *Welsh onion/Leek*, and *Ginger*, respectively, were studied in this paper. Therefore, the purpose of this research is evaluating the effective physicochemical properties of these herbal products to to fight against the SARS-CoV-2 infection. **Materials and Methods:** The properties of these phytocompounds including dipole moment, thermochemistry, chemical shielding tensors, charge density, electrostatic potential and electron donating and electron accepting through frontier orbitals have been computed due to density functional theory (DFT) and m062x/cc-pvdz pseudo=CEP method towards the drug delivery system. **Results and Discussion:** Thermochemical properties have evaluated the combined group contribution and atom connectivity index with uncertainties in the estimated property values. The minimum Gibbs free energy of -1014.602×10^3 and -990.992×10^3 kcal·mol^{-1} for luteolin-7-glucoside and epicatechin-gallate, respectively, has been calculated versus dipole moment, which can indicate the most stability of these structures as natural antiviral medications. In fact, it can be established how phytocompounds of allicin, curcumin, epicatechin-gallate, luteolin-7- glucoside, and zingerol extracted from *Garlic*, *Turmeric/Curcuma*, *Green tea*, *Welsh onion/Leek*, and *Ginger*, respectively, may act as the efficient antiviral of Coronavirus disease receptor. The NMR analysis

has demonstrated the critical points of the principal components of medicinal plants for binding to the active site of TMH (Tyr160-Met-161-Hi162) COVID-19, while each active atom of O or N as the electronegative atoms for binding to the H remarks the maximal shift in all steps in the NMR spectrum. Moreover, UV–VIS spectra reported a positive induction of antioxidant compounds, such as polyphenols and flavonoids. **Conclusions:** Thus, these natural drugs may be either a new or safe treatment or even are employed as antiviral nutraceuticals in elevating immunity and producing endurance to virus infections.

Keywords: COVID-19; TMH protein; medicinal plant; DFT

Resumen

Papel terapéutico de las plantas medicinales contra enfermedades virales centradas en COVID-19: aplicación de la química computacional al diseño de fármacos

Introducción: En este artículo se estudiaron los fitocompuestos de curcumina, galato de epicatequina, luteolina-7-glucósido y zingerol extraídos de ajo, cúrcuma/cúrcuma, té verde, cebolla galesa/puerro y jengibre, respectivamente. Por tanto, el propósito de esta investigación es evaluar las propiedades fisicoquímicas efectivas de estos productos herbales para luchar contra la infección por SARS-CoV-2. **Materiales y métodos:** Las propiedades de estos fitocompuestos, incluido el momento dipolar, la termoquímica, los tensores de protección química, la densidad de carga, el potencial electrostático y los orbitales donadores y receptores de electrones a través de la frontera, se han calculado gracias a la teoría funcional de la densidad (DFT) y el pseudo método m062x/cc-pvdz CEP enfocado en el sistema de administración de fármacos. **Resultados y Discusión:** Las propiedades termoquímicas han evaluado la contribución combinada del grupo y el índice de conectividad atómica con incertidumbres en los valores estimados de las propiedades. La energía libre de Gibbs mínima de $-1014{,}602\times10^{3}$ y $-990{,}992\times10^{3}$ kcal·mol^{-1} para luteolina-7-glucósido y galato de epicatequina, respectivamente, se ha calculado frente al momento dipolar, lo que puede indicar la mayor estabilidad de estas estructuras como Medicamentos antivirales naturales. De hecho, se puede establecer cómo los fitocompuestos de alicina, curcumina, galato de epicatequina, luteolina-7-glucósido y zingerol extraídos de ajo, cúrcuma/cúrcuma, té verde, cebolla galesa/puerro y jengibre, respectivamente, pueden actuar como el eficaz antiviral del receptor de la enfermedad del coronavirus. El análisis de RMN ha demostrado los puntos

críticos de los componentes principales de las plantas medicinales para unirse al sitio activo de TMH (Tyr160-Met-161-Hi162) COVID-19, mientras que cada átomo activo de O o N como átomos electronegativos para unirse a la H señala el cambio máximo en todos los pasos en el espectro de RMN. Además, los espectros UV-VIS informaron una inducción positiva de compuestos antioxidantes, como polifenoles y flavonoides. **Conclusiones:** Por lo tanto, estos medicamentos naturales pueden ser un tratamiento nuevo o seguro o incluso usarse como nutracéuticos antivirales para elevar la inmunidad y producir resistencia a las infecciones virales.

Palabras clave: COVID-19; proteína TMH; planta medicinal; DFT

Resumo

Papel terapêutico das plantas medicinais contra doenças virais com foco no COVID-19: Aplicação da química computacional no design de medicamentos

Introdução: Os fitocompostos de curcumina, epicatequina-galato, luteolina-7-glicosídeo e zingerol extraídos de alho, cúrcuma/cúrcuma, chá verde, cebola galesa/alho-poró e gengibre, respectivamente, foram estudados neste artigo. Portanto, o objetivo desta pesquisa é avaliar as propriedades físico-químicas eficazes desses produtos fitoterápicos no combate à infecção por SARS-CoV-2. **Materiais e Métodos:** As propriedades desses fitocompostos, incluindo momento de dipolo, termoquímica, tensores de proteção química, densidade de carga, potencial eletrostático e doação e aceitação de elétrons através de orbitais de fronteira foram computadas devido à teoria do funcional de densidade (DFT) e pseudo método m062x/cc-pvdz CEP para o sistema de entrega de medicamentos. **Resultados e Discussão:** As propriedades termoquímicas avaliaram a contribuição combinada do grupo e o índice de conectividade atômica com incertezas nos valores estimados das propriedades. A energia livre de Gibbs mínima de $-1014{,}602\times10^{3}$ e $-990{,}992\times10^{3}$ kcal·mol^{-1} para luteolina-7-glicosídeo e epicatequina-galato, respectivamente, foi calculada versus momento dipolar, o que pode indicar a maior estabilidade dessas estruturas como medicamentos antivirais naturais. Na verdade, pode-se estabelecer como os fitocompostos de alicina, curcumina, epicatequina-galato, luteolina-7-glicosídeo e zingerol extraídos do alho, cúrcuma/curcuma, chá verde, cebola galesa/alho-poró e gengibre, respectivamente, podem atuar como o eficiente antiviral do receptor da doença por Coronavírus. A análise de RMN demonstrou os pontos críticos dos principais componentes das plantas medicinais para ligação ao sítio

ativo do TMH (Tyr160-Met-161-Hi162) COVID-19, enquanto cada átomo ativo de O ou N como átomos eletronegativos para ligação ao H observa o deslocamento máximo em todas as etapas do espectro de RMN. Além disso, os espectros UV-VIS relataram uma indução positiva de compostos antioxidantes, como polifenóis e flavonóides. **Conclusões:** Assim, esses medicamentos naturais podem ser um tratamento novo ou seguro ou até mesmo serem empregados como nutracêuticos antivirais para aumentar a imunidade e produzir resistência a infecções virais.

Palavras-chave: COVID-19; proteína TMH; planta medicinal; DFT

Introduction

Notwithstanding vaccine progress, Coronavirus disease therapy still stays dramatically supportive with a prompt demand to recognize impressive anti-coronavirals. A noteworthy method is reusing medications already released for other maladies. In this regard, several investigations have been carried out to inquire whether antimalarial medications could cure Coronavirus disease. Recently, antiviruses have been almost all produced in human cells, transformed animal cells, and these are platforms that require a lot of equipment, which are very long to set up. The arrival of a recent coronavirus, known as the SARS-CoV-2 has initiated a pandemic of Coronavirus disease [1-4].

Natural medications are an important part of common health notwithstanding the progress of the health system. Local treatment in rural zones keeps its importance as the primary procedure in the usual seasonal maladies like colds and flu [5-8]. The most important reason for herbs and medicinal plant treatment is the belief that it will influence healthier. The natural products interrupt the viral life of SARS-CoV-2 [9-14]. Many plant-based antibodies can respond very quickly to the emergence of new variants of Coronavirus disease [15-19].

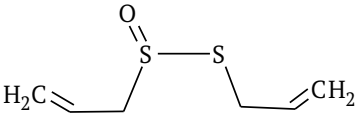
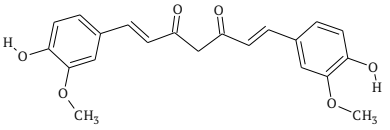
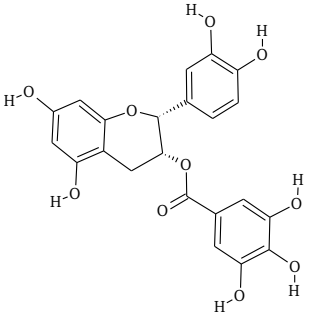
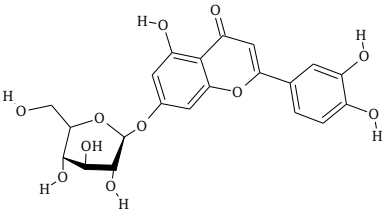
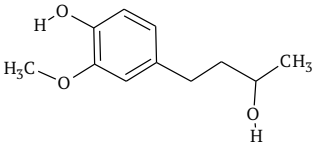
People are reminded to take measures to decrease their risk of COVID-19 consisting of public health and social measures such as wearing masks, hand hygiene, physical distancing, increasing ventilation of inside spaces, preventing crowded spaces, and getting vaccinated [20-22]. It has been announced that the global outbreak of special life-threatening pneumonia resulted about 800 deaths which were world identified as the harsh syndrome CoV (SARS-CoV) [23-27]. In addition, improved researches have exhibited that the source of SARS-CoV based on the phylogenic discussion is most likely from bats which are converted to human aerosols because of intermediate hosts such as infectious palm civets by the virus [28-30]. CoV closely relates to strong breathing syndrome CoV (SARS-CoV), which is an epidemic with a short period of living

time. Moreover, MERS-CoV indicates SARS-like symptoms through human infections, consisting of the signs like influena: high fevers, fatigue, malaise, and rigors, but it has been observed later improvement into typical pneumonia in most samples. Therefore, the animal patience of CoV, through its power of intermediate transition into human, is threatening that has been concluded with a new case of MERS-CoV recommending bats and dromedary camels as the source for this kind of virus sample [31-37].

In some works, it has been explored that a prototype of the Coronaviridae family is an infectious bronchitis virus (IBV) which corresponds to the genetic group III of CoV and produces strong economic problem for the poultry sources in the world society [38-41]. In fact, the researchers have not achieved any vaccine or specific antiviral cures by managing the treatment of symptoms, and collecting the experimental information [42–44]. Environmental elements can greatly affect the secretion of secondary metabolites from tropical plants. Therefore, great attention has been paid to the secondary metabolites conducted by plants in tropical regions that may be developed as medicines [45-47]. Several compounds, such as flavonoids, from medicinal plants, have been reported to have antiviral bioactivities [48-50]. In the present study, it has been investigated the phytochemicals of allicin, curcumin, epicatechin-gallate, luteolin-7- glucoside, and zingerol extracts from *Garlic*, *Turmeric/Curcuma*, *Green tea*, *Welsh onion/Leek*, and *Ginger*, respectively as the probable anti-COVID-19 receptor derived from medicinal plants (Table 1).

The achieving of the present study will provide other researchers with opportunities to identify the right drug to combat COVID-19 by theoretical methodologies to guess the effect of hydrogen bonding in various attachments through seven medicinal plants of allicin, curcumin, epicatechin-gallate, luteolin-7-glucoside, and zingerol extracts from *Garlic*, *Turmeric/Curcuma*, *Green tea*, *Welsh onion/Leek*, and *Ginger*, respectively, bonded to the active site of COVID-19 PDB.

Table 1. Allicin, curcumin, epicatechin-gallate, luteolin-7- glucoside, and zingerol as the probable anti- COVID-19 receptor derived from medicinal plants.

Compound	Molecular structure	Sources
Allicin		*Garlic* 
Curcumin		*Turmeric/Curcuma* 
Epicatechin-gallate		*Green tea* 
Luteolin-7-glucoside		*Welsh onion/ Leek* 
Zingerol		Ginger 

Material and methods

In this article, the properties of thermodynamic parameters of infrared spectroscopy, chemical shielding of nuclear magnetic resonance analysis, charge density, electrostatic potential and electron donating and electron accepting towards a drug design model by GaussView 6.1 [51] and Gaussian 16 revision C.01 program have been done [52]. In addition, the atomic orbitals were affiliated to unravel the gauge subject in the computation of nuclear magnetic resonance for phytocompounds of allicin, curcumin, epicatechin-gallate, luteolin-7- glucoside, and zingerol extracts from *Garlic*, *Turmeric/Curcuma*, *Green tea*, *Welsh onion/Leek*, and *Ginger*, respectively (Table1) [53-55].

First, the attachement of allicin, curcumin, epicatechin-gallate, luteolin-7-glucoside, and zingerol bonded to the active site of COVID-19 protein has been accomplished by forming relatively stable complexes through the hydrogen bonding. Then, one series of quantum force fields including m062x/cc-pvdz pseudo=CEP for complexes of seven inhibitors for COVID-19 has been accomplished though discovering the minimized coordination of the best molecules of natural plant-TMH drug design sample with IR calculations using the Gaussian 16 revision C.01 program [52]. It has been remarked that polarization functions into the employed basis set in the theory always presents us an magnificent achievement on simulation and modeling of theoretical studies [56-60].

Then, normal mode results are the discovery of potential harmonic wells by analytic methodologies that save the movement of all atoms simultaneously in the vibration time range toward a natural discussion of structural vibrations [61-64].

Results and discussion

Geometry optimization

So, the minimized geometry coordination of medicinal ingredients-TMH complexes toward the drug design has been run through the active site of certain O, N, and H atoms in the linkage of bond and torsion angles (Table 2).

For finding a constant molecule of medicinal plant linkage of COVID-19 active site, geometry optimization plus the nuclear magnetic resonance estimation, intensity and harmonic frequency of different normal modes were computed with ab initio methods, and the IR spectral were analyzed. The theoretical computations were run at different levels of calculations to achieve the more accurate equilibrium geometrical consequences and infrared spectral information for each of the certain molecules. It is recommended that polarization functions and an additional diffuse into employed

basis sets in the calculation lead us to the significant improvement on the consequences of theoretical levels. The simulation exhibits the methodologies that produce a common model template at a particular temperature by measuring all physicochemical characteristics through the partition functions. Each part of the model consisting of natural components-TMH, has been minimized by quantum mechanics calculation of DFT level including ECP computations with pseudo=CEP basis sets. Moreover, these systems have been estimated by QM/MM method duty to the ONIOM method.

Table 2. The optimized characteristics of allicin, curcumin, Luteolin-7-glucoside, and zingerol bonded to TMH active site through the drug design method.

Medicinal structures – COVID-19 target	**Bond length**	**(Å)**	**Bond/Torsion angle**	**(°)**
Allicin	C37-O38	1.3600	C37-O38-H39	113.00
	O38-H39	0.9600		
	H39-S4	1.5042	C37-O38- H39- S4	41.81
Curcumin	N95-H96	1.0099	N95-H96-O9	117.25
	H96-O9	0.9706		
	O9-C6	1.3621	N95-H96-O9-C6	78.71
Luteolin-7-glucoside	N100-H101	1.0098	N100- H101-O32	155.14
	H101-O32	0.9362		
	O32-C13	1.3606	N100-H101-O32-C13	-88.90
Zingerol	N78-H79	1.0100	N78-H79-O11	130.22
	H79-O11	0.9966		
	O11-C9	1.4087	N78-H79-O11-C9	148.05

Thermodynamic properties analysis & infrared spectroscopy

Thermodynamic parameters for allicin, curcumin, epicatechin-gallate, luteolin-7-glucoside, and zingerol extracts from *Garlic*, *Turmeric*/*Curcuma*, *Green tea*, *Welsh onion*/*Leek*, and *Ginger*, respectively have been reported in Table 3 and Figure1.

Table 3. Thermodynamic parameters for allicin, curcumin, epicatechin-gallate, and luteolin-7- glucoside, and zingerol using density functional theory method and "m062x/cc-pvdz pseudo=CEP" level.

Phytochemicals	$\Delta E° \times 10^{-3}$ (kcal·mol^{-1})	$\Delta H° \times 10^{-3}$ (kcal·mol^{-1})	$\Delta G° \times 10^{-3}$ (kcal·mol^{-1})	$\Delta S°$ (cal·K^{-1}·mol^{-1})	Dipole moment (Debye)
Allicin	-685.830	-685.829	-685.858	96.825	3.0022
Curcumin	-781.953	-781.953	-781.990	124.909	4.3688
Epicatechin-gallate	-990.953	-990.953	-990.992	133.472	3.7835
Luteolin-7-glucoside	-1014.564	-1014.564	-1014.602	127.737	3.4279
Zingerol	-405.017	-405.017	-405.046	98.991	2.1572

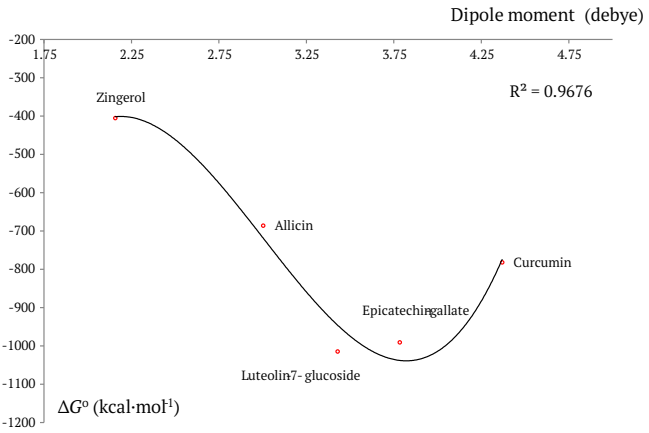


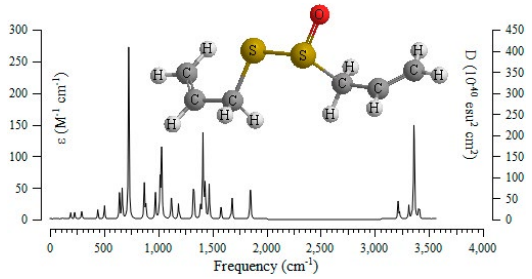
Figure 1. The $\Delta G°$/kcal·mol^{-1} versus dipole moment/ debye for allicin, curcumin, epicatechin-gallate, and luteolin-7-glucoside, and zingerol.

Figure1 has shown the minimum Gibbs free energy consisting of -1014.602×10^3 and -990.992×10^3 kcal·mol^{-1} for luteolin-7-glucoside and epicatechin-gallate, respectively, versus dipole moment which can indicate the most stability of these structures of the antiviral natural medications.

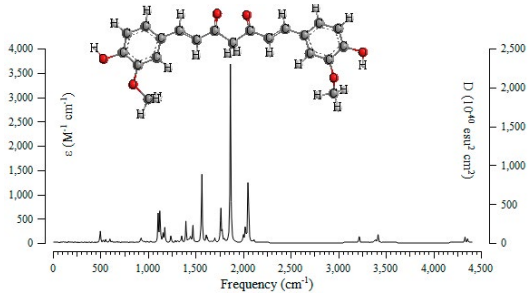
A comparison was made between thermodynamic properties of live matter of the analyzed plants. Moreover, the effectiveness of the process was analyzed through standard enthalpy, entropy, and Gibbs energy of biosynthesis. The pure component properties are estimated for active pharmaceutical ingredients that are related or proposed for the treatment of severe acute respiratory syndrome-CoronaVirus-2. Thermodynamic

properties can estimate the combined group contribution and atom connectivity index with uncertainties in the estimated property values.

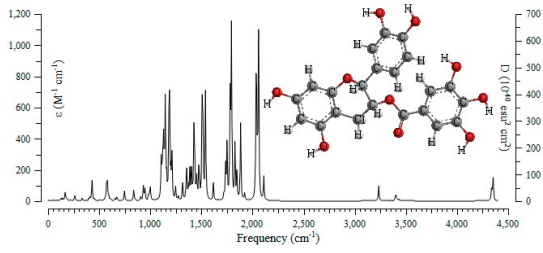
Moreover, the spectroscopy of infrared for major sesquiterpenes of allicin, curcumin, epicatechin-gallate, and luteolin-7-glucoside, and zingerol has been achieved due to density functional theory method and "m062x/cc-pvdz pseudo=CEP " keyword (Figure 2 a-e).



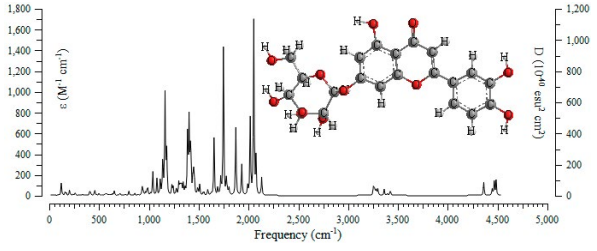
(a)



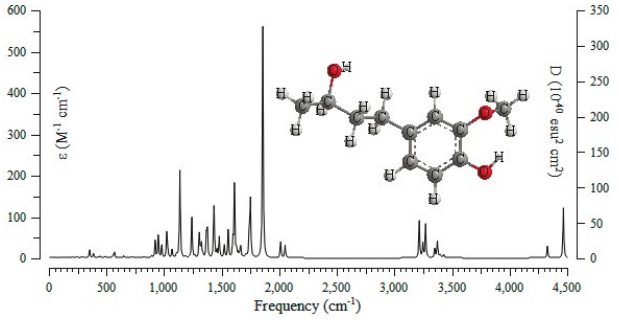
(b)



(c)



(d)



(e)

Figure 2. Infrared spectrums of of a) allicin, b) curcumin, c) epicatechin-gallate, d) luteolin-7-glucoside, and e) zingerol to TMH (Tyr160-Met-161-Hi162) through the drug design method calculated by m062x/cc-pvdz pseudo=CEP.

The most fluctuation of frequency of infrared spectra for allicin, curcumin, epicatechin-gallate, and luteolin-7-glucoside, and zingerol has been approximately seen between 500–2000 cm^{-1} (Figure 2 a-e).

Quality control of plant-based medicine and supplements must be carried out to ensure uniformity in quality and safety in their use, resulting in the need for effective and accurate analytical methods. In this article, IR spectroscopy has analyzed the qualitative and quantitative parameters that is accurate and nondestructive. This approach has been applied for quantitative analysis of compounds in complex matrices such as plant-based medicine and supplements supported by chemometrics techniques.

Chemical shielding insight through nuclear magnetic resonance spectrum

The heterocyclic antiviral phytochemicals of allicin, curcumin, epicatechin-gallate, luteolin-7- glucoside, and zingerol have approximately shown the equal manner from 20 to 200 ppm for different atoms of these phytochemicals (Figure 3 a-e). The nuclear magnetic resonance spectrum displayed the steepest peak in 40 ppm and the fragile peaks of nuclear magnetic resonance have approximately in 100–200 ppm for all three antiviral phytochemicals including allicin, curcumin, epicatechin-gallate, luteolin-7-glucoside, and zingerol, respectively (Figure 3 a-e).

The computation of hydrogen nuclear magnetic resonance on the foundation of amino acids in the beta-sheet conformation Tyrosine-Methionine-Histidine and the five main ingredients of medicinal plants including allicin, curcumin, epicatechin-gallate, luteolin-7-glucoside, and zingerol have been evaluated to explorer the certain atoms

of hydrogen, nitrogen and oxygen in the critical areas of these anti-virus medicines through the generating of H-bonding by identifying the attack point of Tyrosine-Methionine-Histidine (Figure 3 a-e).

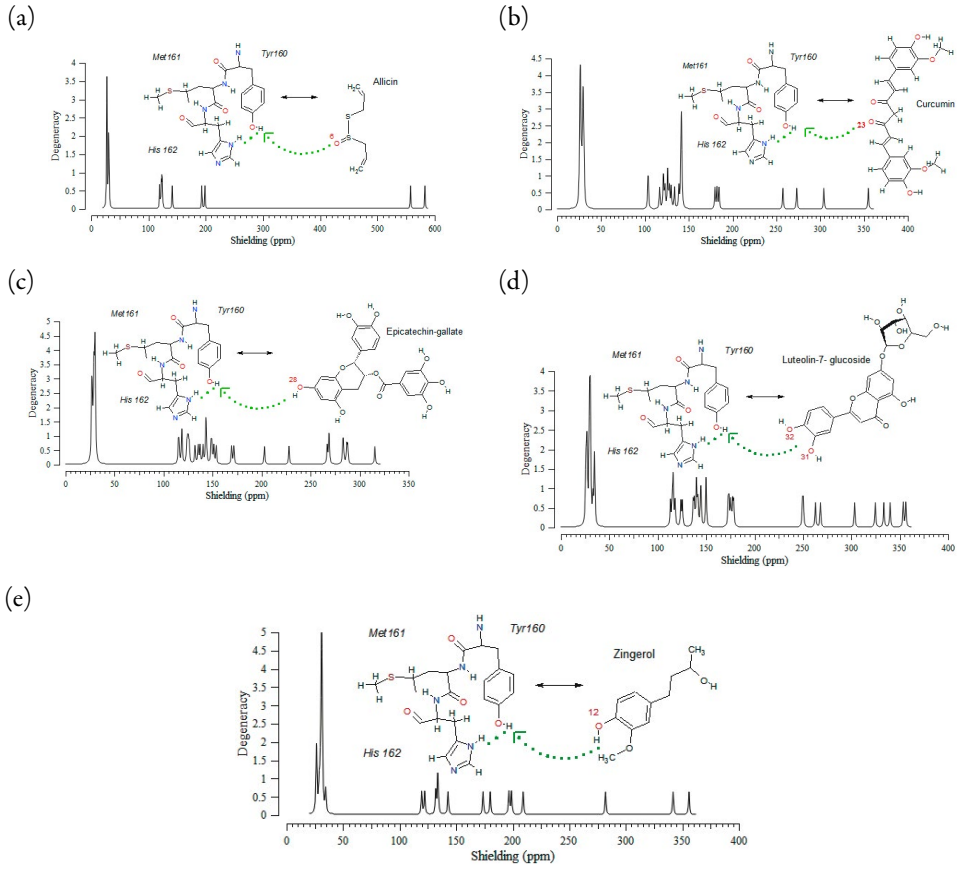


Figure 3. NMR spectra of a) allicin, b) curcumin, c) epicatechin-gallate, d) luteolin-7- glucoside, and e) zingerol bonded to TMH (Tyr160-Met-161-Hi162) COVID-19 active site through the drug design method by showing the active region of TMH in the drug design process.

The nuclear magnetic resonance analysis shows the critical points of the principal components of medicinal plants for binding to the Tyr160-Met161-His162 (TMH) due to producing the anti-virus drugs, while each active atom of O and N as the electronegative atoms for binding to the H remarks the maximal shift in all steps in the NMR spectrum (Figure 3 a-e).

However, NMR method is insensitive and requires a relatively large amount of sample to make a measurement. Furthermore, in herbal medicines analysis, one of the obstacles is the efficiency of the analysis, because the complex components of medicinal plants can complicate the process. In addition, the analysis process can also damage the material.

Frontier orbitals

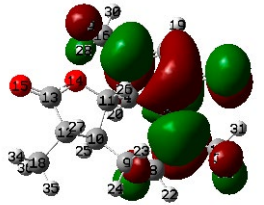
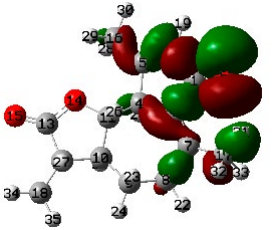
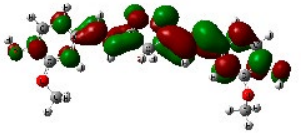
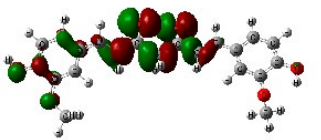
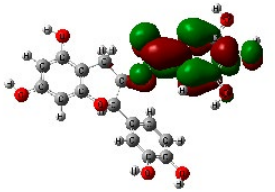
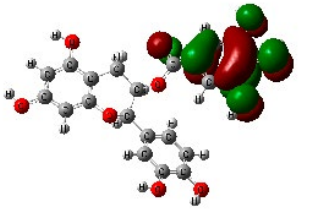
The Frontier orbitals (FMOs) have been estimated for some effective phytochemicals of allicin, curcumin, epicatechin-gallate, luteolin-7-glucoside, and zingerol extracts from *Garlic*, *Turmeric/Curcuma*, *Green tea*, *Welsh onion/Leek*, and *Ginger*, respectively (Table 4).

The highest occupied molecular orbital energy (HOMO/eV), the lowest unoccupied molecular orbital energy (LUMO/eV) and band energy gap "ΔE" (eV) indicated the pictorial description of positive and negative areas that are a crucial agent for recognizing the molecular specifications of antiviral phytochemicals consisting of allicin, curcumin, epicatechin-gallate, luteolin-7-glucoside, and zingerol (Table 4).

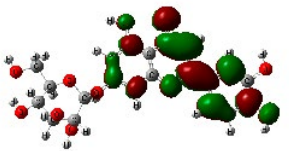
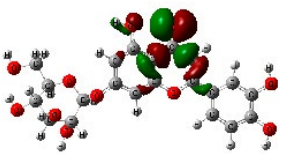
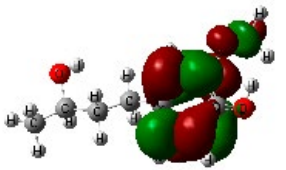
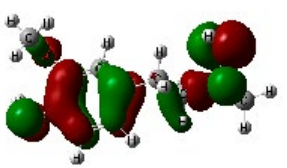
FMOs pinpoint the locality of chemical bonds that are chemically reactive because of the associated orbital energies and thus have achieved great success in describing chemical reactivity, mainly for small systems. Orbitales are localized in both physical and energy spaces and thus contain both orbital locality and energy information.

The applications of allicin, curcumin, epicatechin-gallate, luteolin-7-glucoside, and zingerol in its equilibrium geometry, inter- and intra-molecular charge-transfer systems, and two transition states of a bifurcating reaction demonstrate that FMOs can connect quantum mechanical treatments of chemical systems and chemical reactivities by locating the reactive region of large chemical systems. The role of FMOs can be described for small systems and describe the chemical reactivity of large systems with energy and locality insight, with potentially broad applications.

Table 4. The Frontier orbitals' parameters of antiviral phytochemicals including allicin, curcumin, epicatechin-gallate, luteolin-7- glucoside, and zingerol.

Molecule	E_{LUMO} (eV)		E_{HOMO} (eV)		$\Delta E = E_{LUMO} - E_{HOMO}$ (ev)
Allicin		-0.7246		-8.2145	7.4899
Curcumin		0.9701		-3.3342	4.3043
Epicatechin-gallate		2.2435		-3.2319	5.4754

(Continued)

Molecule	E_{LUMO} (eV)		E_{HOMO} (eV)		$\Delta E = E_{LUMO} - E_{HOMO}$ (ev)
Luteolin-7-glucoside		1.3967		-2.7165	4.1132
Zingerol		3.2506		-3.7105	6.9611
	$\mu = (E_{HOMO} + E_{LUMO})/2$	$\chi = -(E_{HOMO} + E_{LUMO})/2$	$\eta = (E_{LUMO} - E_{HOMO})/2$	$\zeta = 1/(2\eta)$	$\psi = \mu^2/(2\eta)$
Allicin	-4.46955	4.46955	3.74495	0.1335	2.6671
Curcumin	-1.18205	1.18205	2.15215	0.2323	0.3246
Epicatechin-gallate	-0.4942	0.4942	2.7377	0.1826	0.0446
Luteolin-7-glucoside	-0.6599	0.6599	2.0566	0.2431	0.1058
Zingerol	-0.22995	0.22995	3.48055	0.1436	0.0076

Analysis of Ultraviolet-Visible spectroscopy

Generally, organic materials are clear to the large energy radiation which forms the ultraviolet (200–400 nm) and visible (400–700 nm) section of the electromagnetic spectrum.

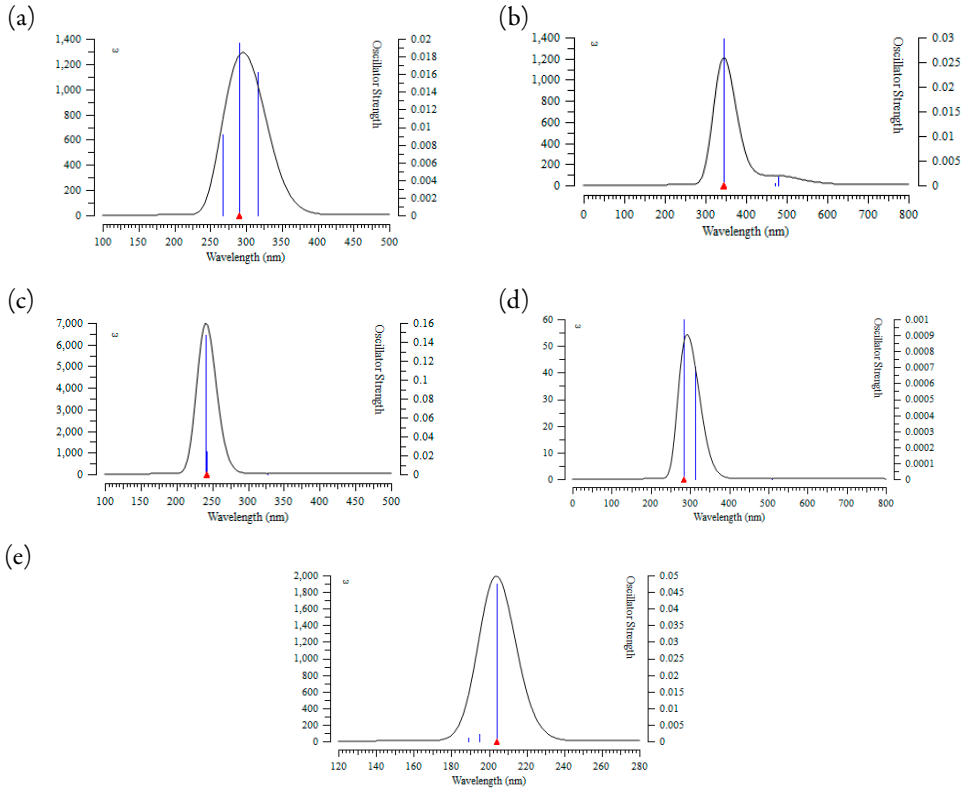


Figure 4. Ultraviolet-Visible spectrums of a) allicin, b) curcumin, c) epicatechin-gallate, d) luteolin-7- glucoside, and e) zingerol.

In the measured amounts of Ultraviolet-Visible spectrums for principal phytocompounds of allicin, curcumin, epicatechin-gallate, luteolin-7-glucoside, and zingerol, there are maximum absorption bands between 250–350 nm for allicin with a sharpest peak in 290 nm (Figure 4a), around 300–400 nm for curcumin with a keen peak in 350 nm (Figure 4b), about 200–250 nm for epicatechin-gallate with a pointed peak in 245 nm (Figure 4c), around 250–350 nm for luteolin-7- glucoside with a strong peak in 290 nm (Figure 4d), and near 180–230 nm for zingerol with a steepest peak in 204 nm (Figure 4e).

The medicinal value of plants depends upon phenolics, antioxidants and volatile yield. Enhanced levels of UV radiation can indeed negatively change plant physiological processes, growth and productivity. However, while studying UV effects on medicinal plants, some interesting phenomena have been discovered. Furthermore, UV radiation seems to be a safe alternative as targeted treatment in medicinal and aromatic plants attributed to concurrent increase in different health-related constituents.

Conclusions

Natural drugs and phytochemical by progressing COVID-19 pandemic have been studied against this viral disease through their biological activities of anti-inflammatory, antibacterial and antioxidant. The results in this article have remarked that natural drugs due to potential active phytocomponents might grow a further effective species in the remedy of the new coronavirus of severe acute respiratory syndrome coronavirus 2 accountable for Coronavirus malady. Some physical and physicochemical attributes from optimized structure of allicin, curcumin, epicatechin-gallate, luteolin-7-glucoside, and zingerol extracts from *Garlic*, *Turmeric*/*Curcuma*, *Green tea*, *Welsh onion*/*Leek*, and *Ginger*, respectively, disclosed to be potent in displaying antiviral activities by interrupting the viral life. Thus, these natural drugs may be either a new or safe treatment or even is employed as antiviral nutraceuticals in elevating immunity and producing endurance to virus infections.

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Conflicts of interest

The authors declare no conflict of interest.

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