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ORIGINAL RESEARCH ARTICLE

Characterizing the structural and physicochemical properties of medicinal plants as a proposal for treating of viral malady

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ABSTRACT

Regarding coronavirus disease (COVID-19) pandemic, this research article wants to study some herbals as the probable therapy for this disease. *Cinnamon leaves*, *curcuma longa* (*turmeric*), *ginger*, *mentha pulegium* (*pennyroyal*), *rosemary*, *salvia divinorum* and *thyme* including some principal chemical compounds of cynnamil, curcumin, gingerol, pulegone, rosmarinic acid, salvinorina A and thymol, respectively, as a probable anti COVID-19 receptor have been selected. The possible roles of these medicinal plants in COVID-19 treatment have been carried out through quantum sensing methods. Formation of hydrogen bonding between principal substances selected in COVID-19 natural drugs bound to Tyrosine-Methionine-Histidine (Tyr-Met-His) or (TMH) (the database amino acids fragment) as the active area of the COVID-19 protein has been evaluated. In fact, it has been exhibited the role of oxygen, nitrogen, and hydrogen atoms in the active sites of these anti-virus medications towards hydrogen bonding in the active site if "TMH" protein. The physical and chemical attributes of nuclear magnetic resonance, vibrational frequency, the highest occupied molecular orbital energy and the lowest unoccupied molecular orbital energy, partial charges and spin density and have been accomplished using density functional theory (DFT) method and 6-311+G (2d,p) basis set by Gaussian 16 revision C.01 program toward the industry of drug design. This research has exhibited that there is a relative agreement among the results that these medicinal plants could be efficient against COVID-19 symptoms.

Keywords: molecular modeling; medicinal plant; COVID-19; Tyr160-Met161-His162

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1. Introduction

Pandemic coronavirus disease (COVID-19) is a serious malady caused by a new coronavirus known as severe acute respiratory syndrome (SARS-CoV-2). There is non-trustworthy remedy or vaccine accessible to fight versus SARS-CoV-2[1–6]. More attempts to probe for antiviral agents against COVID-19 are essential, while phytochemicals can be powerful solution. On top of exhibiting direct antiviral effects, medicinal plants with reported anti-inflammatory activities may have pleiotropic roles in COVID-19 management as the elevation of inflammatory markers[7–11]. Moreover, it has been discovered that a detrimental change in COVID-19 epidemiology should be existed as a (variant of concern) VOC, and the WHO has determined Omicron variant (B.1.1.529 as a VOC).

Local treatment in rural zones keeps its importance as the primary procedure in the usual seasonal maladies like colds and flu. The most important reason for herbs and medicinal plant treatment is the belief that it will influence health. The natural products from medicinal plants are therefore bringing hope to consisting of

phytocompounds which can either kill the SARS-CoV-2 or interferes its replication or make human body immunity strong to fight against.

Recently, antibodies 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. Many plant-based antibodies can respond very quickly to the emergence of new variants of COVID-19. The emergence of a new coronavirus, known as the SARS-CoV-2 has initiated a pandemic of COVID-19. Since its first reported case in Wuhan, China in December 2019, new discovered evidence by both clinicians and researchers globally have helped shed some light on the disease pathogenesis and the nature of the virus itself. The availability of new information subsequently fed policy changes on transmission prevention strategies as well as development of preventative vaccines and therapeutic drug candidates. Enforced physical distancing, hand hygiene, and arguably proper usage of personal protective equipment including wearing a surgical mask remains the most effective way of controlling the spread of the disease, with most countries which adopted such measures reporting some success in curbing the disease spread[12–19].

In the research of phytomedicine, it is common to observe multiple pharmacological properties from a single plant. It is now well understood that a single plant may contain a wide range of phytochemicals, making ethnopharmacology research both full of possibilities yet challenging.

Ćavar Zeljković and his co-workers have indicated that the essential oils from *Mentha aquatica L. cv. Veronica*, *Mentha pulegium L.*, *Mentha microphylla K.Koch*, *Mentha x villosa Huds.*, *Micromeria thymifolia* (*Scop*.) *Fritsch*, and *Ziziphora clinopodioides Lam*., and their monoterpenecomponents, carvone, carvacrol, pelugone, menthofuran, and 1,8-cineole exhibited notable antiviral activity against SARS-CoV-2[20].

New investigations have approved the medicinal advantages of *turmeric* for liver diseases, diabetes, cancer, respiratory diseases, AIDS and Alzheimer's disease. Therefore, the *turmeric* might have the powerful impact against COVID-19. Many therapeutic influences of the natural polyphenol, curcumin, have been exhibited such as potential chemotherapeutic, antioxidant, antiviral, antibacterial, and anti-inflammatory properties[21]. In fact, curcumin can appear a high-affinity for interaction with the S glycoprotein through the establishment of six hydrogen bonds. Moreover, docking results have indicated that curcumin interacted with the active site of the protein, in addition to forming two hydrogen bonds[22].

Thymol (2-isopropyl-5-methylphenol) relates to the phenolic monoterpenes and exists in *thyme* specie which is one of the main compounds of *thyme* essential oil. They have been used in traditional medicine as expectorant, anti-inflammatory, antiviral, antibacterial, and antiseptic agents, in the remedy of the upper respiratory system[23–26].

The pharmacological impacts of *ginger* are related to its terpene and phenolic compounds. The *ginger*-extracted phenolic ingredients consist of gingerols, paradols, shogaols, and zingerone. The major pungent compounds of fresh *ginger* are gingerols. Gingerols have anticancer activity, anti-inflammatory, antioxidant, antiangiogenesis, anti-metastasis, antimicrobial, antifungal, neuroprotective, antiemetic and antihyperlipidemic effects[27,28].

Scientific researches approve that *cinnamon* can be a potent anti-inflammatory, antioxidant functional food and might be fruitful in mitigation of SARS-CoV-2 induced hyper inflammation. During the COVID-19 pandemic, the patients request for consumption of *cinnamon* powder as prophylactic functional food against SARS-CoV-2[29–31].

Herbal of *rosemary* as a natural antioxidant removes reactive oxygen species from tissues, enhances expression on Nrf2 gene and decreases inflammation by inhibiting production of pro-inflammatory cytokines. Furthermore, rosmarinic acid in *rosemary* extract has positive impacts on renin-angiotensin-system. This

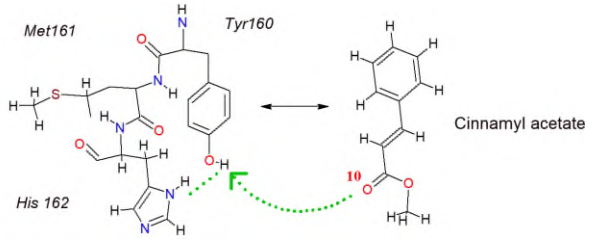
medicinal plant influences respiratory system by decreasing inflammation, oxidative stress, and muscle spasm[32–34].

In the work, it has been studied cynnamil, curcumin, gingerol, pulegone, rosmarinic acid, salvinorina A and thymol as the probable anti-COVID-19 receptor extracts from herbals containing *cinnamon leaves*, *curcuma longa* (*turmeric*), *ginger*, *mentha pulegium* (*pennyroyal*), *rosemary*, *salvia divinorum* and *thyme* (**Table 1**).

Table 1. Cynnamil, curcumin, gingerol, pulegone, rosmarinic acid, salvinorina A and thymol as the anti-COVID-19 receptor extracts from herbals: *cinnamon leaves*, *curcuma longa* (*turmeric*), *ginger*, *mentha pulegium* (*pennyroyal*), *rosemary*, *salvia divinorum* and *thyme*.

Component	**Image**	**Species**	**Symptoms of COVID-19 which can be treated by the medicinal plants[35]**
Cynnamil		*Cinnamon*	Anorexia, skin rash
Curcumin		*Turmeric*	Muscle-joint pain
Gingerol		*Ginger*	Cough
Pulegone		*Mentha*	Nausea-vomiting, headache
Rosmarinic acid		*Rosemary*	Shortness of breath, decreased blood oxygen level, muscle-joint pain
Salvinorina A		*Salvia divinorum*	Sore throat, shortness of breath
Thymol		*Thyme*	Fever

Based on this research, it can been estimated the occasions for discovering the efficient medication against COVID-19 using quantum mechanics computations to measure the effect of hydrogen bonding in the variety of junction with these seven natural drugs' components of cynnamil, curcumin, gingerol, pulegone, rosmarinic acid, salvinorina A and thymol binded to the active area of COVID-19 virus[36–41] (**Figure 1**).



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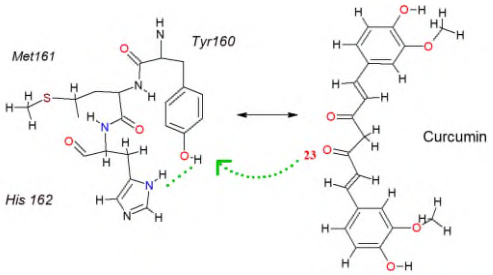

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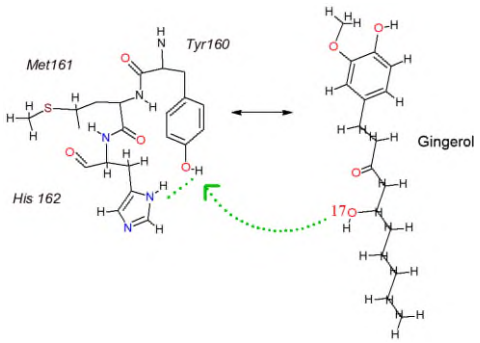

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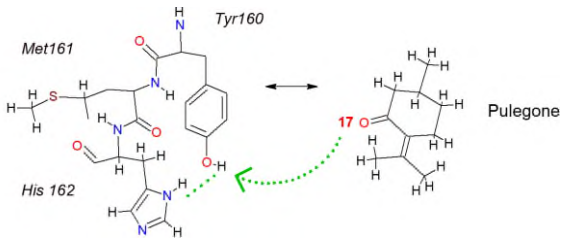

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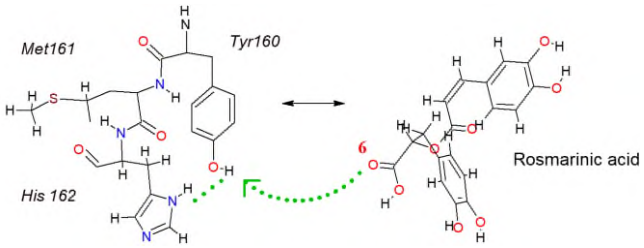

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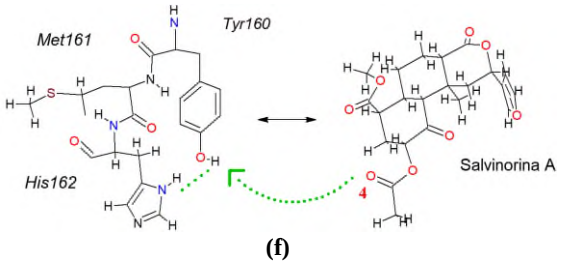

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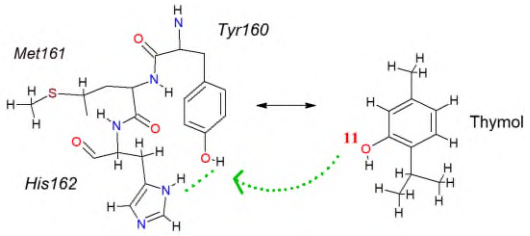


(g)

Figure 1. The junction of **(a)** cynnamil; **(b)** curcumin; **(c)** gingerol; **(d)** pulegone; **(e)** rosmarinic acid; **(f)** salvinorina A; and **(g)** thymol to TMH (Tyr160-Met161-His162) by hydrogen bonding. The sequence of hydrogen bond are as follows: g > e > c > a > f > b > d.

Recently, several traditional medicinal plants including *Glycyrrhiza glabra*, *Nigella sativa*, *Curcuma longa*, *Tinospora cordifolia* and *Withania somnifera* with high potential in modulating the main protease (Mpro) activity and cytokine storm in coronavirus disease infection have indicated remedial impacts on COVID-19 patients[42].

2. Material and method

Cynnamil, curcumin, gingerol, pulegone, rosmarinic acid, salvinorina A and thymol have been attached to the active area of COVID-19 compounds which approves the existence of hydrogen bonds toward resistant complexes. Therefore, quantum mechanics approaches with m062x/cc-pvdz pseudo=CEP function for complexes of seven inhibitors for COVID-19 has been accomplished. The favorable coordination of the optimized substances of phenolic natural drug joint to Tyr160-Met161-His162 with IR spectroscopy using the Gaussian 16 revision C.01 program package[43] has been measured due to the DFT method and m062x/cc-pvdz pseudo=CEP level of theory. The (Perdew-Burke-Ernzerhof) "PBE" functional with high-precision generalized gradient approximation "GGA" has been employed to achieve more authentic results[44].

It has been exhibited that polarization functions into the employed basis set in the calculation always remark us a magnificent prosperity on the simulation and modeling in the drug design industry[45–52]. Frequency achievement is the finding of harmonic potential wells by analytic procedures which keep the activity of all atoms at the same time in the vibration time scale conducting to an inherent illustration of vibrations in molecules[53–57].

Thus, the geometry optimization of coordination in medicinal extracts-TMH agents based on the drug design has been found from the active area of certain atoms of "O", "N" and "H" in the attachment of bond angle and torsion angle values (**Table 2** and **Figure 1a–g**).

For carrying out a firm compound of natural medication attached to COVID-19 active site, chemical shift of nuclear magnetic resonance, vibrational frequency and intensity of the normal modes have been commutated with the "QM" methods, and the original vibrational modes have been analyzed[58–63].

The computational measurements have been carried out in variety of theoretical levels to profit the more precise balance geometrical amounts and infrared spectral information for each of the indicated substances. It is assumed that a further diffuse and polarization functions into the basis set employed in the calculation direct us to the high evolution on the results of methodical approaches[64–67].

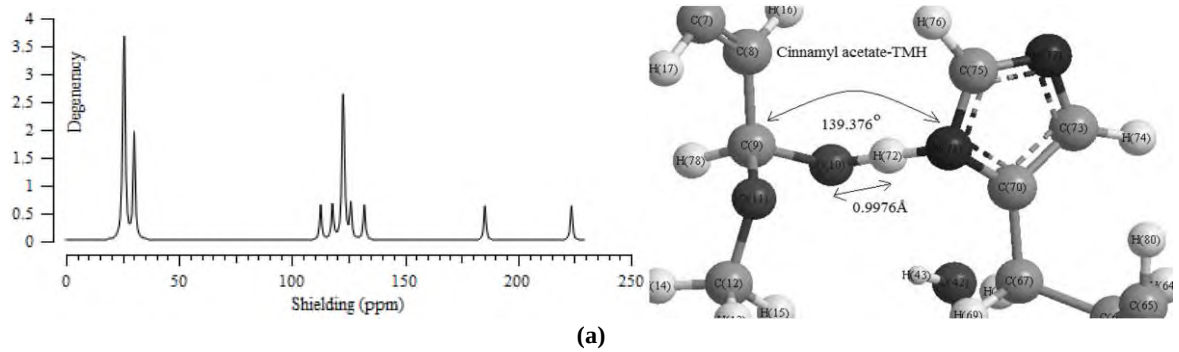
The different approaches in modeling and simulation exhibit the path which can generate a usual model at a particular temperature by evaluating all physical and chemical attributes based on the partition function amounts[68–76].

Table 2. The geometry optimization amounts with m062x/cc-pvdz pseudo=CEP for cynnamil, curcumin, gingerol, pulegone, rosmarinic acid, salvinorina A and thymol binded to active site of COVID-19 protein through the drug design approach.

Medicinal extracts—COVID-19 active area	Bond length	(Å)	Bond/Torsion angle	(°)
Cynnamil acetate	N71–H72	1.03	N71–H72–O10	177.85
	H72–O10	0.99		
	O10–C9	1.42	N71–H72–O10–C9	139.37
Curcumin	N96–H97	1.03	N96–H97–O23	178.49
	H97–O23	0.99		
	O23–C9	1.42	N96–H97–O23–C9	110.09
Gingerol	N95–H96	1.03	N95–H96–O17	178.00
	H96–O17	0.99		
	O17–C11	1.40	N95–H96–O17–C11	−128.61
Pulegone	N49–H50	1.03	N49–H50–O72	176.66
	H50–O72	0.99		
	O72–C57	1.41	N49–H50–O72–C57	172.37
Rosmarinic acid	N91–H92	1.03	N91–H92–O6	174.51
	H92–O6	0.99		
	O6–C5	1.40	N91–H92–O6–C5	−176.79
Salvinorina A	N105–H106	1.03	N105–H106–O4	178.66
	H106–O4	0.99		
	O4–C2	1.41	N105–H106–O4–C2	99.43
Thymol	N73–H 74	1.03	N73–H74–O11	175.09
	H74–O11	0.99		
	O11–C4	1.37	N73–H74–O11–C4	−168.33

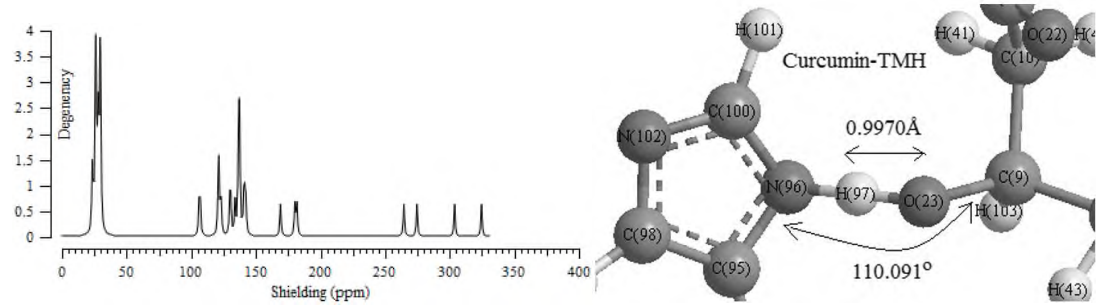
3. Results and discussion

Nuclear magnetic resonance or "NMR" shifts for Tyr160-Met161-His162 through the database of amino acids in beta sheet conformation and four certain extracts of natural medications containing cynnamil, curcumin, gingerol, pulegone, rosmarinic acid, salvinorina A and thymol have been evaluated to discover the exhibited of oxygen, nitrogen, and hydrogen in the active sites of these anti-virus medications through the production of hydrogen bonding by representing the reaction area of "TMH" agent (**Figure 2a–f**).



(a)

Figure 2. (*Continued*).



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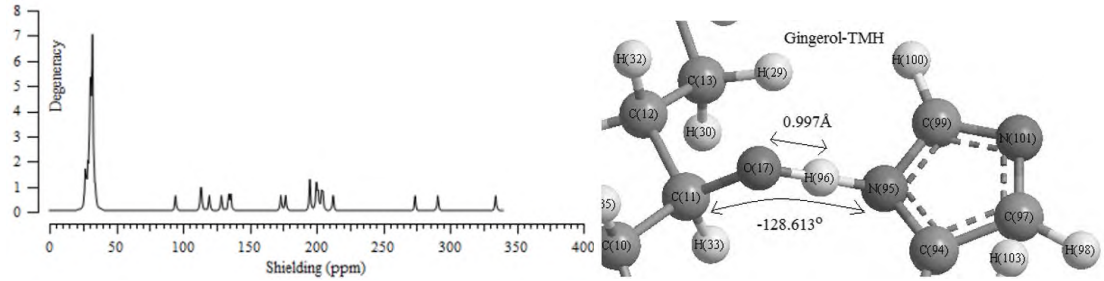

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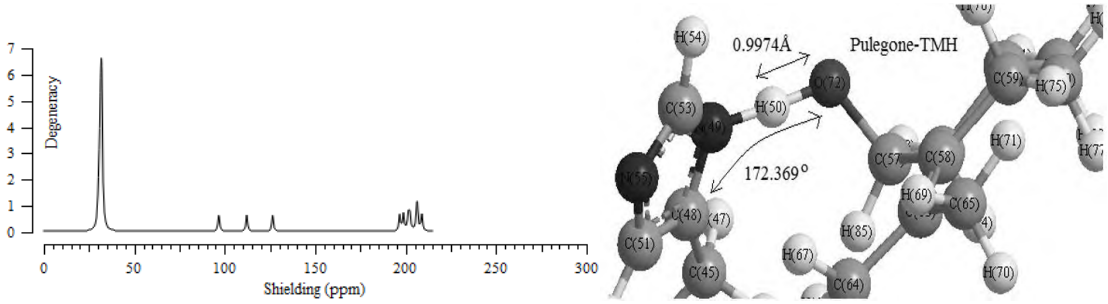

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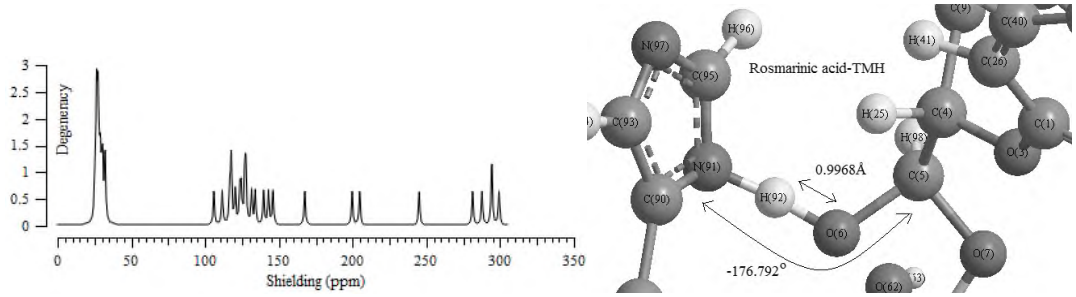

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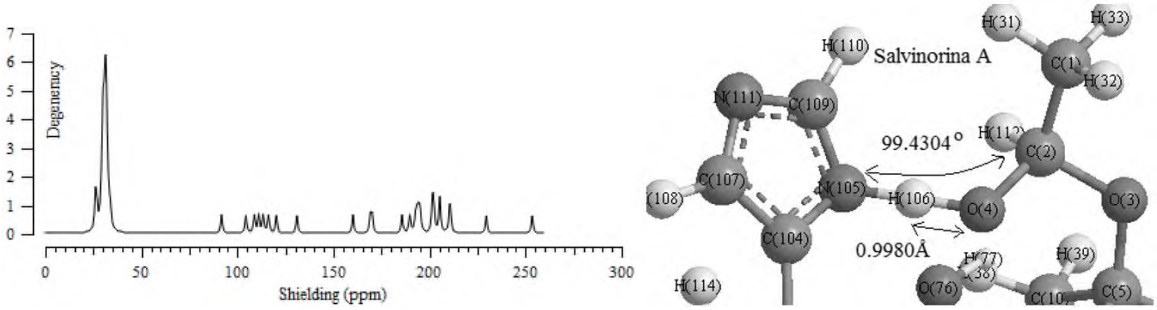

(f)

Figure 2. "NMR" spectroscopy for **(a)** cynnamil acetate; **(b)** curcumin; **(c)** gingerol; **(d)** pulegone; **(e)** rosmarinic acid; **(f)** salvinorina A binded to "TMH" COVID-19 active area through the drug design approach.

NMR properties have denoted the critical points of essential extracts of pharmaceutical kinds for attaching to the Tyr160-Met161-His162 (TMH) in producing the anti-virus medications while each critical atom of "O" and "N" as the electronegative atoms for jointing to the hydrogen has remarked the major changing in the "NMR" graphs (**Figure 2a–f**).

The technique of infrared (IR) for main ingredients of medicinal plants including cynnamil, curcumin, gingerol, pulegone, rosmarinic acid, salvinorina A and thymol have been calculated for fixing the intersection of Tyr160-Met161-His162 as the COVID-19 medication through the drug design approach applying "IR" spectroscopy using Gaussian 16 revision C.01 program to obtain the best amounts for geometrical coordination and thermochemical parameters. Then, thermodynamic properties have distinguished the resistant anti-COVID-19 agent complexes of principal extracts of pharmaceutical kinds of "TMH" through the hydrogen bonding constitution employing the drug design framework (**Table 3**).

Table 3. Physical and thermochemical properties of cynnamil, curcumin, gingerol, pulegone, rosmarinic acid, salvinorina A and thymol jointed to COVID-19 active site (TMH) complexes at 300 K.

Component-COVID-19 active site	**$E_{electronic} \times 10^{-4}$ (kcal.mol^{-1})**	**$E_{core\text{-}core} \times 10^{-4}$ (kcal.mol^{-1})**	**$\Delta G \times 10^{-4}$ (kcal.mol^{-1})**	**ΔS (kcal.K^{-1}. mol^{-1})**	**$T\Delta S \times 10^{-4}$ (kcal/K^{-1}. mol^{-1})**
Cynnamil acetate	−167.07	151.18	−15.88	529.81	15.89
Curcumin	−267.14	245.21	−21.93	731.67	21.95
Gingerol	−244.84	225.18	−19.66	655.03	19.65
Pulegone	−175.39	159.96	−15.43	514.44	15.43
Rosmarinic acid	−268.87	246.53	−22.34	744.48	22.33
Salvinorina A	−330.98	307.19	−23.79	792.74	23.78
Thymol	−166.91	151.62	−15.28	509.72	15.29

In cynnamil, curcumin, gingerol, pulegone, rosmarinic acid, salvinorina A and thymol attached to Tyr160-Met161-His162 through its database of amino acids in beta sheet conformation, as the critical point of COVID-19 protein compound in the procedure of drug design steps, the thermodynamic properties of pharmaceutical extracts-TMH complexes have been discovered to be significantly distinct through the resistance of hydrogen bonding organized between critical point of COVID-19 agent and pharmaceutical extracts which establishes the anti-COVID-19 medication (**Table 3** and **Figure 3**).

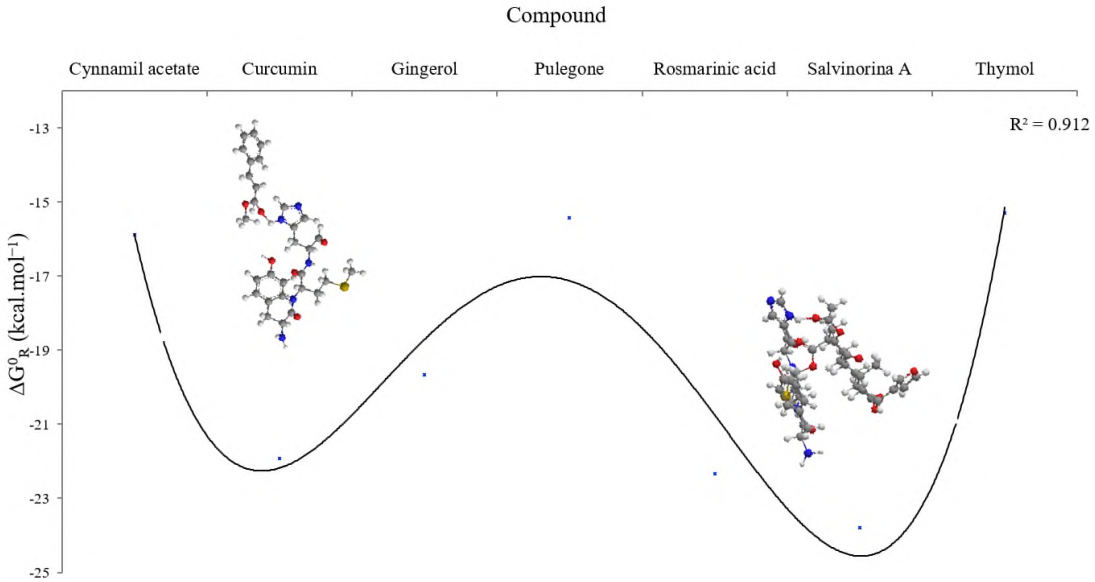

Figure 3. (*Continued*).

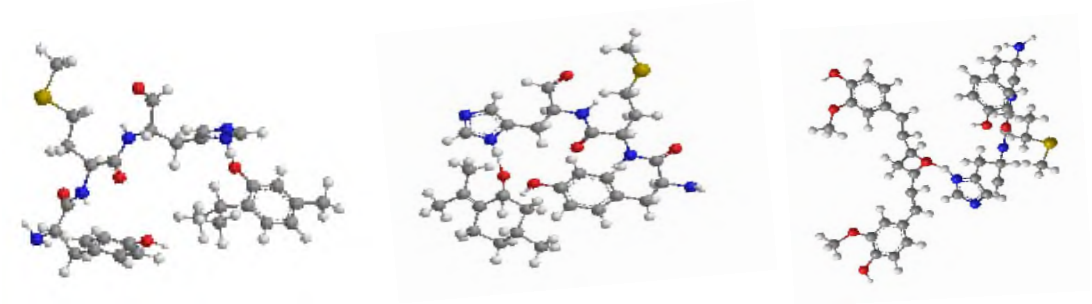

Figure 3. $\Delta G°_R$ for the stable anti-COVID-19 complexes of cynnamil, curcumin, gingerol, pulegone, rosmarinic acid, salvinorina A and thymol jointed to TMH through the H-bonding formation using the drug design method.

Moreover, the heat formation ($\Delta H°_f$) for cynnamil, curcumin, gingerol, pulegone, rosmarinic acid, salvinorina A and thymol jointed to COVID-19 has been discussed the H-bonding due to the database of amino acids in beta sheet conformation; Tyr160-Met161-His162 ($\Delta H°_{TMH}$ = 25.8242 × 10^{+4} kcal.mol^{-1}) as the active site of the COVID-19 variant B.1.1.529 molecule. Finally, the reaction heat formation $\Delta H°_R$ have been calculated as follows (**Table 4**, **Figure 4**):

$$\Delta H°_R = \Delta H°_{f(X\text{-}TMH)} - (\Delta H°_{f,TMH} + \Delta H°_{f,X}),$$

where X is cynnamil acetate, curcumin, gingerol, pulegone, rosmarinic acid, salvinorina A, thymol.

Table 4. The heat of formation, $\Delta H°_f$ (kcal.mol^{-1}), $\Delta H°_R$(kcal.mol^{-1}) among cynnamil, curcumin, gingerol, pulegone, rosmarinic acid, salvinorina A and thymol jointed to COVID-19 active site (TMH) complexes at 300 K.

$\Delta H°_f \times 10^{-4}$	$\Delta H°_f \times 10^{-4}$	$\Delta H°_R \times 10^{-4}$
Cynnamil acetate −29.6736	Cynnamil acetate-TMH 66.9460	−25.8146
Curcumin 115.3026	Curcumin-TMH 192.8237	−25.8165
Gingerol −145.3195	Gingerol-TMH −70.9553	−25.8168
Pulegone −48.9909	Pulegone-TMH 21.7634	−25.8172
Rosmarinic acid 355.7935	Rosmarinic acid-TMH −107.7616	−25.8706
Salvinorina A −218.2009	Salvinorina A-TMH −134.8384	−25.8159
Thymol −28.9166	Thymol-TMH 53.7594	−25.8160

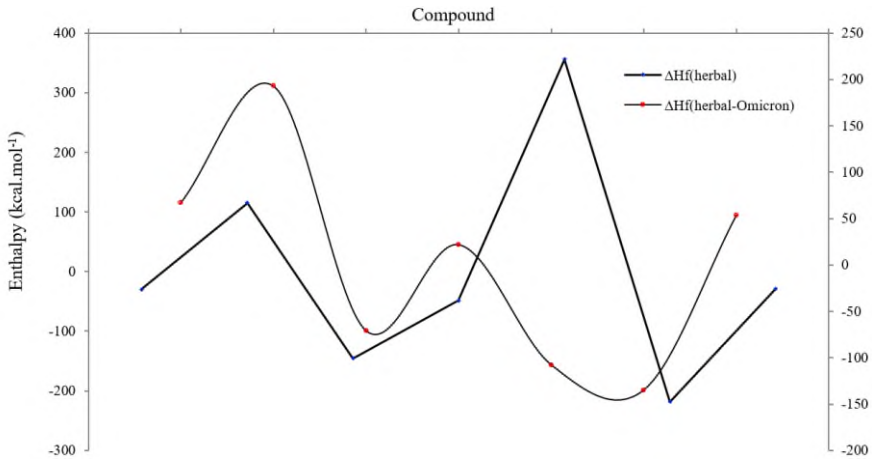

Figure 4. The difference of ΔH_F among cynnamil, curcumin, gingerol, pulegone, rosmarinic acid, salvinorina A and thymol jointed to COVID-19 active site (TMH) complexes at 300 K.

In cynnamil acetate, gingerol, pulegone, and thymol linked to the database of amino acids in beta sheet conformation, as the active site of COVID-19 protein (Tyr160-Met161-His162) in the process of drug design, the frequency and intensity of different infrared (IR) normal modes of medicinal components-TMH complexes have been discovered to be significantly distinct through the stability of H–bonding formed between active site of COVID-19 variant B.1.1.529 and medicinal ingredients which prove the anti-COVID-19 variant (**Table 5** and **Figure 5**).

Table 5. Cynnamil acetate, gingerol, pulegone and thymol as anti-COVID-19 drugs in distinct normal modes of infrared spectrums.

Inhibitor	Normal mode	Frequency (cm^{-1})	Intensity ($km.mol^{-1}$)	Dipole (Debyes)
Cynnamil acetate	234	3680.71	115.4354	5.034
Gingerol	109	1943.71	67.268	4.291
Pulegone	248	3424.38	829.8741	5.439
Thymol	236	3275.85	4169.9663	8.826

In **Table 5**, it has been shown that intermolecular force of a hydrogen bond forms a special type of dipole-dipole attraction when the hydrogen atom in the active site if "TMH" protein bonded to a strongly electronegative atom becomes in the vicinity of another electronegative atom with a lone pair of electrons in gingerol, cynnamil acetate, pulegone and thymol with dipole mement of 4.291, 5.034, 5.439 and 8.826 debye, respectively.

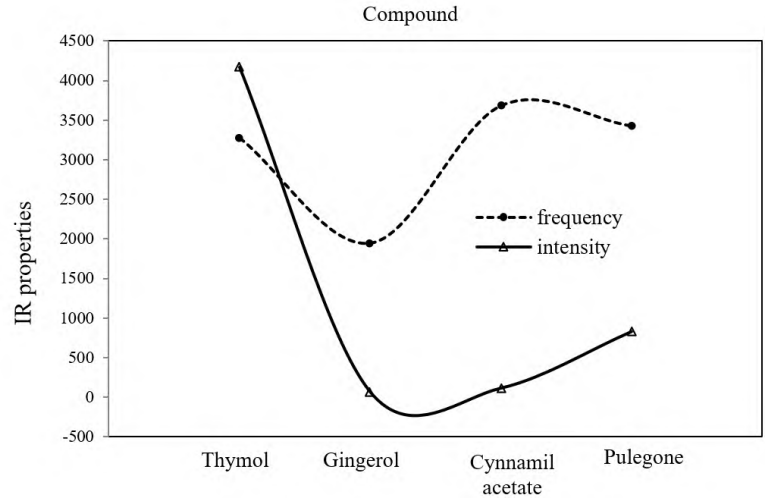

Figure 5. "IR" properties for the phytochemicals of cynnamil acetate, gingerol, pulegone and thymol anti-COVID-19 drugs.

In this part, the atomic charge of certain atoms of "O" attachment of cynnamil, curcumin, gingerol, pulegone, rosmarinic acid, salvinorina A and thymol with Tyr160-Met161-His162 agent has been measured in the critical point of hydrogen bonding existence (**Table 6**).

In **Table 6**, it has been sketched the alterations of "Q" of indicated "O" atoms for optimized molecules of cynnamil, curcumin, gingerol, pulegone, rosmarinic acid, salvinorina A and thymol attached to Tyr160-Met161-His162 agent due to existence of hydrogen bonding. Thus, the consequences of **Table 6** in a polar area have notified the consistency of COVID-19 medications which have been accomplished considering the oxygen as the electronegative atoms in growth of the hydrogen bonding using the drug design insight which has proposed the modeling of anti-COVID-19 drug. In fact, hydrogen bonding is a weak force present in polar compounds when the H atom attached to the more electronegative atom having a lone pair of electron. This leaves a partial positive charge on H atom and a partial negative charge on electronegative atom. So, it is observed that the electronegativity of an atom is related to its ability to pull the electron towards itself in covalent bond and this power to pull electrons depends on the size of atom. The results in this article have

manifested that medicinal plants and phytocompounds can have a considerable function due to their substantial antiviral activity against COVID-19 and other coronaviruses. Cynnamil, curcumin, gingerol, pulegone, rosmarinic acid, salvinorina A and thymol extracted from *cinnamon leaves*, *curcuma longa* (*turmeric*), *ginger*, *mentha pulegium* (*pennyroyal*), *rosemary*, *salvia divinorum* and *thyme*, respectively, were identified through in-silico molecular modeling by using DFT screening. Identified natural phytocompounds revealed to be potential in exhibiting antiviral activities by disrupting the viral life cycle including viral entrance, replication, assembly, and discharge, as well as virus specific host targets. Thus, this prompt increasing of pharmaceutical industry focused on phytochemical extracts from medicinal plants, and aromatic herbs in the hopes of discovering lead compounds, with purposeful to antiviral medications.

Table 6. The amounts of atomic charge (Q) for indicated "O" atoms in the linkage of cynnamil, curcumin, gingerol, pulegone, rosmarinic acid, salvinorina A and thymol to Tyr160-Met161-His162.

Cynnamil acetate	**Q (e)**	**Curcumin**	**Q (e)**	**Rosmarinic acid**	**Q (e)**
O10	−0.39	O20	−0.19	O2	0.14
O11	−0.24	O21	−0.24	O3	−0.20
		O22	−0.3473	O6	−0.37
		O23	−0.3482	O7	−0.28
		O24	−0.2328	O16	−0.23
		O25	−0.2122	O17	−0.24
				O33	−0.22
				O34	−0.22
Thymol	**Q (e)**	**Gingerol**	**Q (e)**	**Salvinorina A**	**Q (e)**
O11	−0.26	O17	−0.31	O3	−0.20
		O18	−0.30	O4	−0.38
		O19	−0.17	O12	−0.23
		O20	−0.23	O13	−0.36
Pulegone	**Q (e)**			O20	−0.29
O17	−0.34			O22	−0.24
				O25	−0.33
				O28	−0.04

Moreover, a research has compared the total phenolic (TPC), flavonoid (TFC), radical scavenging and cytotoxic activities in the aqueous methanolic extracts of *Angelica sinensis*, *Dioscorea polystachya*, *Ginkgo biloba*, *Glycyrrhiza uralensis* and *Lycium barbarum* with two dietary plants of *Brassica oleracea* and *Zingiber officinale* that all of them were considered inactive and safe for consumption[77]. For instance, the effect of *Peperomia pellucida* (*L.*) *Kunth* as the medicinal plant on the inflammatory illnesses such as conjunctivitis, and gastrointestinal and respiratory tract disorders in tropical and subtropical regions[78].

Moreover, it has been evaluated the bioactive compounds in *Peperomia pellucida* (*L.*) *Kunth* with liquid-liquid partitioning method and compare their anti-glycaemic, anti-inflammatory, antioxidant, and anti-glycation potential in different solvent fractions[79].

Another investigation has approved the pharmacological activities of anti-inflammatory, anti-diabetic, antioxidant and anti-glycation potential for the phenolic compounds, flavonoid, tannin, saponin, alkaloid in the plant fractions[80]. They have shown that ethyl acetate fraction exhibited relatively high anti-inflammatory, anti-diabetic, antioxidant and anti-glycation potential while the non-toxic methanolic and aqueous fractions exhibited high hyaluronidase and lipoxygenase inhibitory activities, respectively[80].

4. Conclusion

Medicinal plants of *cinnamon leaves*, *curcuma longa* (*turmeric*), *ginger*, *mentha pulegium* (*pennyroyal*), *rosemary*, *salvia divinorum* and *thyme* are puissant to adhere the database amino acids segment of Tyr160-Met161-His162 agent as the appointive area of the COVID-19 through exhibiting the alteration in their frequency and intensity spectrums after approximation by "NMR" approach which are influenced by the atomic configuration of the anti-virus macromolecule. The resistance of hydrogen bonding between several pharmaceutical extracts of cynnamil, curcumin, gingerol, pulegone, rosmarinic acid, salvinorina A, thymol and COVID-19 through the constitution of anti-COVID-19 through two possibilities of [N⋯H] and [O⋯H] with distinct atomic charges have been inquired using "IR" approaches. Therefore, the thermodynamic attributes of Gibbs free energy, enthalpy of formation, electronic energy, core-core interaction can authorize the consistency of anti-COVID-19 due to hydrogen bonding foundation using the drug design framework. Here, we used the network pharmacology, metabolite analysis, and molecular simulation to comprehend the biochemical basis of the health-boosting impact of medicinal plants. The present study investigates the drug ability, metabolites and potential interaction of the title tea with genes associated with COVID-19-induced pathogenesis. Altogether, the evidence presented in this work supports the notion that medicinal plants have promising therapeutic potential, especially in the case of herb products against viral infections.

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Conflict of interest

The author declares no conflict of interest.

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