

Original Research Article

Computational study of the effectiveness of natural herbal derivatives on COVID-19 virus

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ABSTRACT

In the present paper, an attempt has been made to study the COVID-19 virus that caused hundreds of thousands of deaths and instigated widespread fear, threatening the world's most advanced health security. In 2020, natural herbal derivatives are among the drugs tested against the coronavirus pandemic and showed an apparent efficacy. In the present work, We report a systematic study of e-learning by chemical computing the natural herbs have been proposed as a potential antiviral for the treatment of COVID-19 diseases combining DFT and molecular docking calculations Molecular geometries, electronic properties, and molecular electrostatic potential were investigated by using software Hyperchem 08, where the internal energy of seasonal influenza virus and COVID-19 respectively, (-1678.045 kcal/mol) and (-3020 kcal/mol) to find that the difference in energy is twice for seasonal influenza, which makes the kinetic energy high for COVID-19 Which is attributable to the high temperature and headache for people with it, so that internal energy of the plants used as a temporary treatment (Thyme, Anise, Cinnamon, and Eugenol) respectively (4.056 kcal/mol, -47.40 kcal/mol, -53.83 kcal/mol, -218.84 kcal/mol) which is anise closest in internal energy of the virus COVID-19 so, remains incomplete, will be as a temporary protector as a reliever in case of infection.

Research highlights

- Were able to identify the internal energy of Covid 19 and seasonal influenza and compared them.
- Were collected a range of natural herbal formulas and also compared them.
- Were calculated the internal energy of natural herbs and were able to identify which herbs were closer to the inner energy, which is anise.
- For future study, any researcher is asked to collect herbs in a single computational overlap and to note the internal energy is closer to the energy of Covid 19, because this needs special specifications from large computers with large RAM in order to accommodate as many complexes and organic compositions as possible.

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INTRODUCTION

Computing is the cause of overlap between pc science and chemistry to supply rapid and pressing options to some of the problems that stand in the way of chemistry [1]. As in other chemistry humans the usage of laptop chemistry equipment apprehend interactions and chemical approaches, this department makes use of laptop simulation to create high-quality mathematical apnea and strengthen algorithms and software programs to calculate the houses of molecules such as molecules. Total energy, bipolar torque, quadruple torque, seismic and reactive spectroscopic frequencies, transverse sections of particle collision with different molecules at atomic and subatomic stages as used in many calculations. At present, the research of any compound or interplay has ended up one of the most essential lookup techniques to find out about all its components and recognize opportunities of its software and get the first-rate effects from these studies [2]. To learn about the electricity of seasonal viruses and corona, we want complete thinking that coronaviruses are a huge vary of viruses that purpose a vary of stress in humans, ranging from an ordinary bloodless to acute respiratory syndrome, and viruses from this crew reason a number of animal diseases [3, 4]. This precise pressure of coronavirus has by no means been recognized in humans. The records accessible is very confined on the transmission, injury, and medical effect of the virus, and it is acknowledged that a number of coronaviruses in people reason respiratory infections ranging from frequent colds to extra extreme illnesses such as Middle East Respiratory Syndrome (MERS) and Acute Respiratory Syndrome (SARS). The lately determined virus is Covone-19. (COVID-19) [5, 6].

Definition and symptoms

COVID-19 is a giant species of COVID-19 that can motive ailment to animals and humans. COVID-

19 belongs to the straight COVID-19 inside the COVID-19 household inside the order of the nighttime viruses. [7][8] COVID-19 are viruses encapsulated with a single-chain repose DNA genome and have a comparable helical venom. The COVID-19 genome is about 26 to 32 kilo base, the biggest of RNA viruses. (RNA virus). They are positive-tape RNA viruses, and they are unified into the Corona virginal subfamily inside the Coronaviridae family. [9][10] Along with three different households (Arteriviridae, Roniviridae, and Mesoniviridae), Corona Miridae is the first rating [11] in accordance to the present day classification, the Coronaviridae household involves 4 races referred to as Alpha-Beta-Gamma-and Delta COVID-19. In some cases, these races had been divided into different breeds.

Coronary viruses infect an extensive variety of mammals and birds and consist of pathogens of vital medical, veterinary and monetary importance. [9][10] Extreme acute respiratory syndrome (SARS-CoV), Middle East Respiratory Syndrome (MERS), and Coronaviruses (MERS-CoV) furnish two wonderful examples of animal coronary viruses that motive acute respiratory illnesses in human beings [12-16]. Ribonucleic Acid, recognized utilizing RNA, the RNA converts the genetic facts discovered in the DNA to the place it builds proteins and then transfers these proteins to what is recognized as reposed protein plants, RNA consists of a cue (thread) of nucleotides. Messenger RNA: It copies sections of the genetic code and transfers it to ribosomes (ribosomes are mobile phone factories that produce proteins from the genetic code). Ribosomal RNA: It is one of the most necessary factors of the plant ribosome so it is very vital for the manufacturing of protein. Transfer RNA: Is accountable for the switch of amino acids and quintessential proteins to the protein manufacturing plant life in the cell [17].

Regarding the herbs utilized in this study, first of all, thyme. Thyme is autochthonous to the Mediterranean region [18] *Thymus serpyllum* grows within the Levant, wherever it would be 1st cultivated. Ancient Egyptians used thyme for embalming [19].

Oil of thyme, the volatile oil of thyme (*Thymus vulgaris*), contains 20–54% phenol [20]. Thyme volatile oil additionally contains a spread of further compounds, like p-cymene, myrcene, borneol, and volatile oil [21]. phenol, associate antiseptic, is a lively ingredient in varied commercially made mouthwashes like Listerine [22]. Before the appearance of contemporary antibiotics, oil of thyme was accustomed to medicating bandages [23]. As for the anise herb additionally referred to as seasoning or seldom Unix, [24] could be a spermatophyte within the family Umbelliferae native to the jap Mediterranean region and Southwest Asia. The distinctive smell would provide a warning just in case of warming [25]. The most use of anise in ancient European flavoring medication was for its carminative result (reducing flatulence), [24] whereas cinnamon herb contains a long history of use in ancient medication as a biological process aide, however, modern studies are unable to seek out proof of any important meditative or therapeutic result [26]. and at last Eugenol herp is employed in perfumes, flavorings, and essential oils. it's additionally used as a neighborhood antiseptic and anesthetic [27, 28]. Eugenol is combined with flowers of zinc to create flowers of zinc eugenol that have restorative and dentistry applications in odontology.

The idea of the study included calculating the internal energies of the COVID-19, seasonal flu, and all these medicinal herbs, so that the least in internal energy, that is, the most stable and stable, is the possibility of removing this virus by staying with it as long as possible.

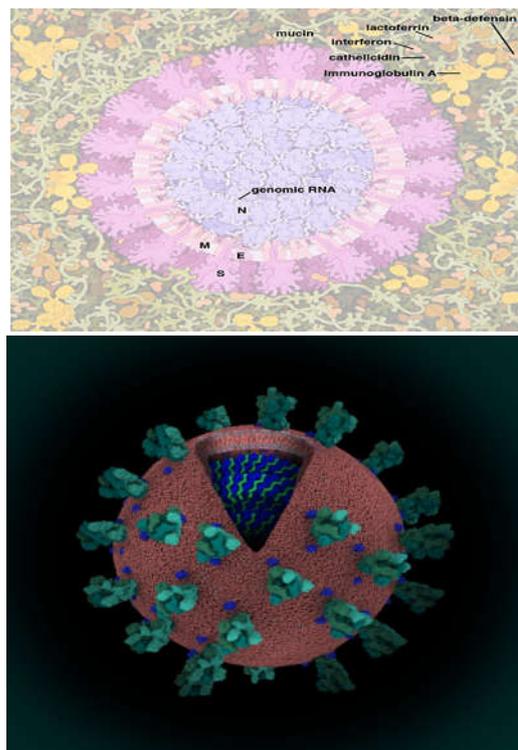


Fig 1. An external and internal cross-section to illustrate RNA for the Covid-19 virus [29].

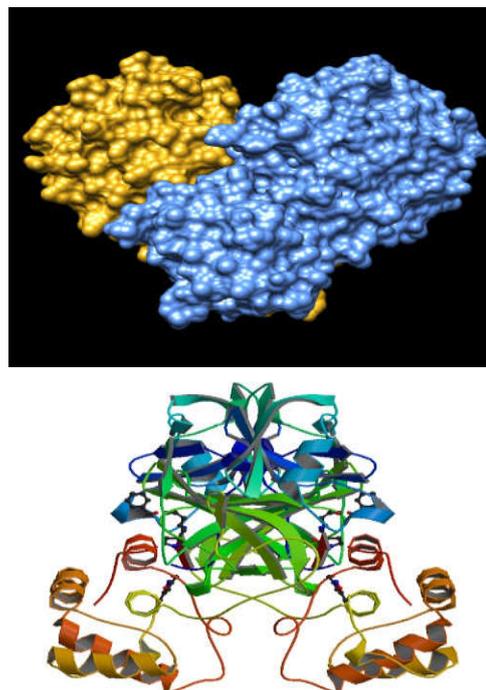


Fig 2. Molecular modeling by chemical computing of the internal composition of the Covid-19 virus. [30].

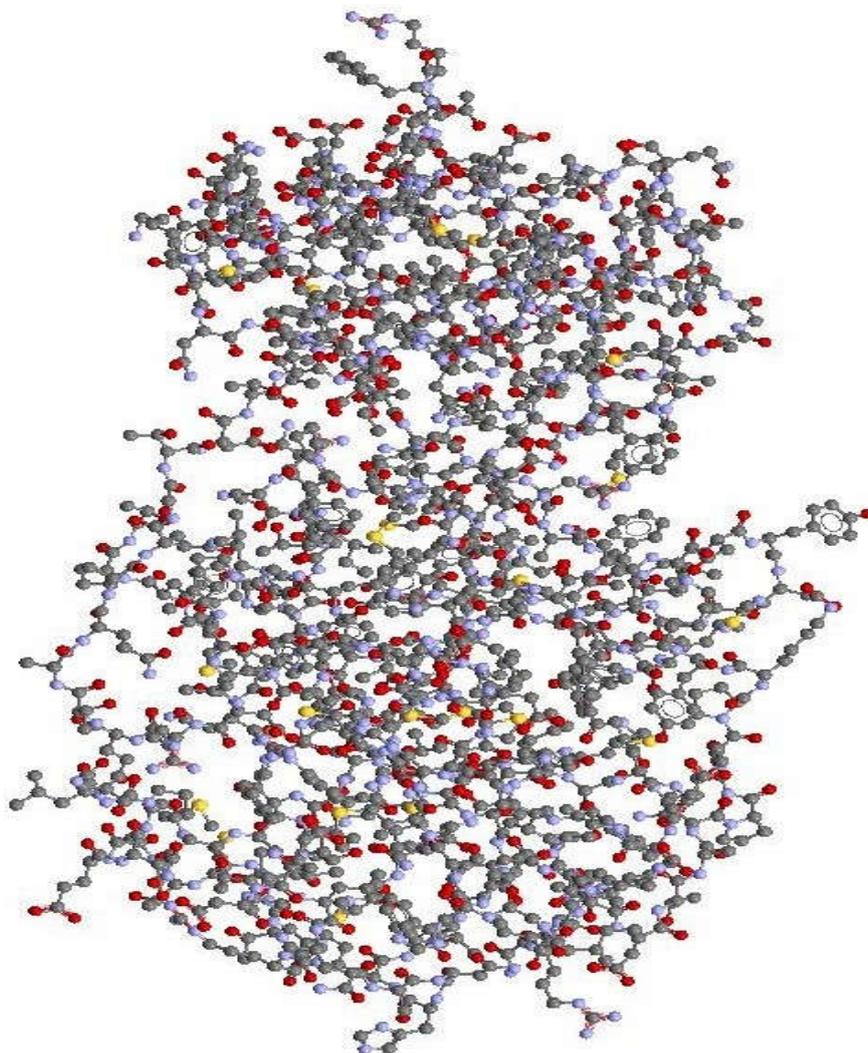


Fig 3. Molecular modeling by chemical computing of the internal composition of the Covid-19 virus [30].

Computational method

The preliminary geometric alcove buildings had been constructed, based totally on buildings created from crystalline parameters supplied by way of Cambridge Structural, and multiplied one after the other with the use of the Geometry optimization calculations method [31].

Start-up engineers had been constructed for compact complexes with the use of HyperChem (Version 8.0, Hypercube, and Gainesville, FL, USA). By DFT method * # b3lyp/6-31g geom=connectivity*

$$E_{DFT} [\rho] = T_{[\rho]} + E_{ne} [\rho] + J_{[\rho]} + Exc_{[\rho]}$$

Where E is the energy, T is the kinetic energy of the electrons, E_{ne} is the nuclear-electron attraction (Columbic) energy, J is the electron-electron repulsive (Columbic) energy, and Exec is the electron-electron exchange-correlation energy. Notice that each of these terms is a function of the function ρ, the electron density, which is itself a function of the three positional coordinates (x, y, and z). As such, each of the terms above – T, E_{ne}, J, and Exec is functional. The challenge now becomes to determine the value of each of these four functional.

This method was applied to compare the internal energy of natural herpes in this study

and the results were as presented in the results and discussion.

Results and discussion

The results and discussion showed us how much difference in the internal total energy of Covid-19 is from the seasonal influenza virus, The internal energy of seasonal influenza virus and

COVID-19 respectively, (-1678.045 kcal/mol) and (-3020 kcal/mol) to find that the difference in energy is twice for seasonal influenza, which makes the kinetic energy high for COVID-19 Which is attributable to the high temperature and headache for people with it.

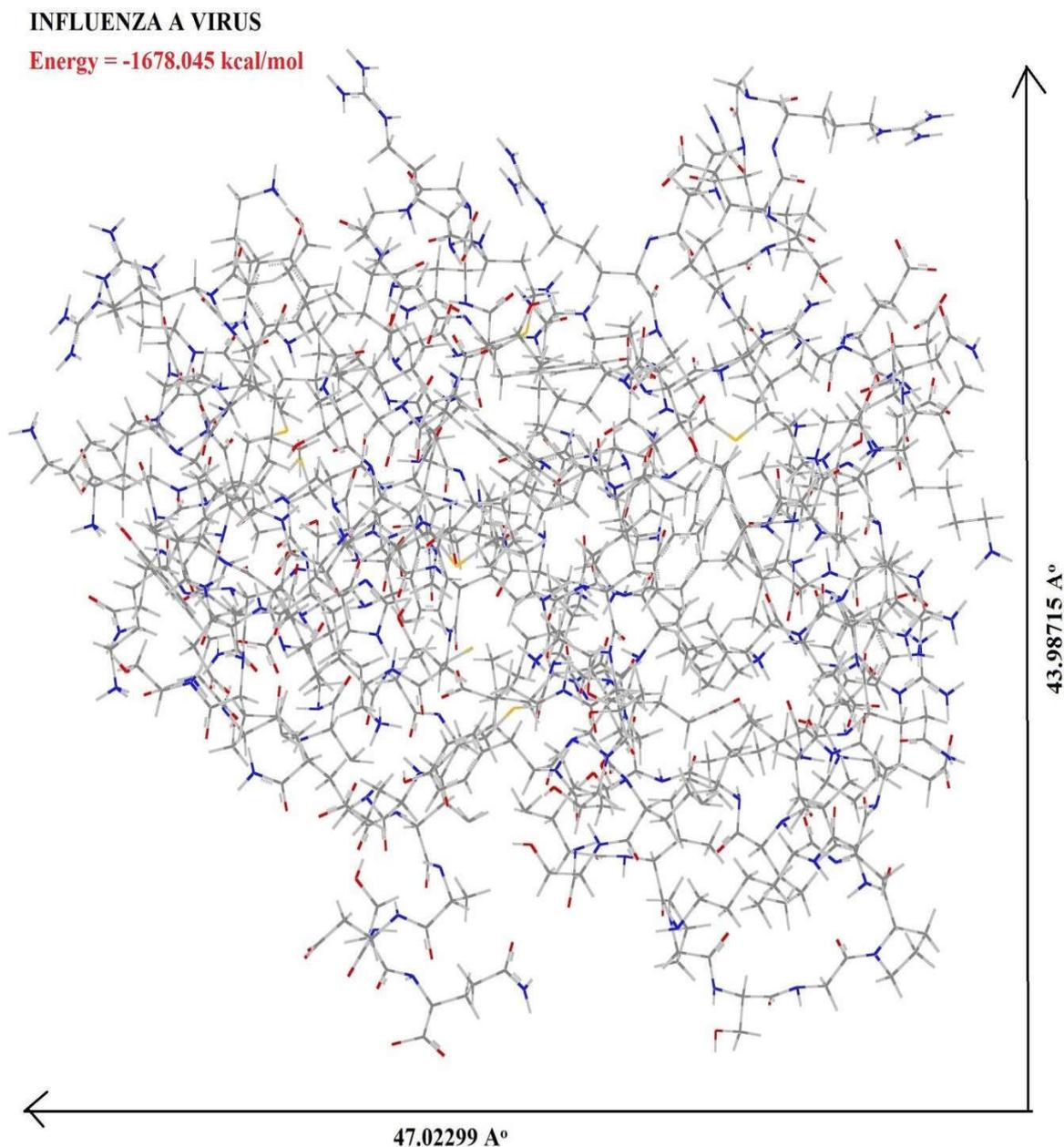


Fig 4. The binding energy for seasonal influenza and quantum parameters.

CORONAVIRUS-19

Energy = -3020 kcal/mol

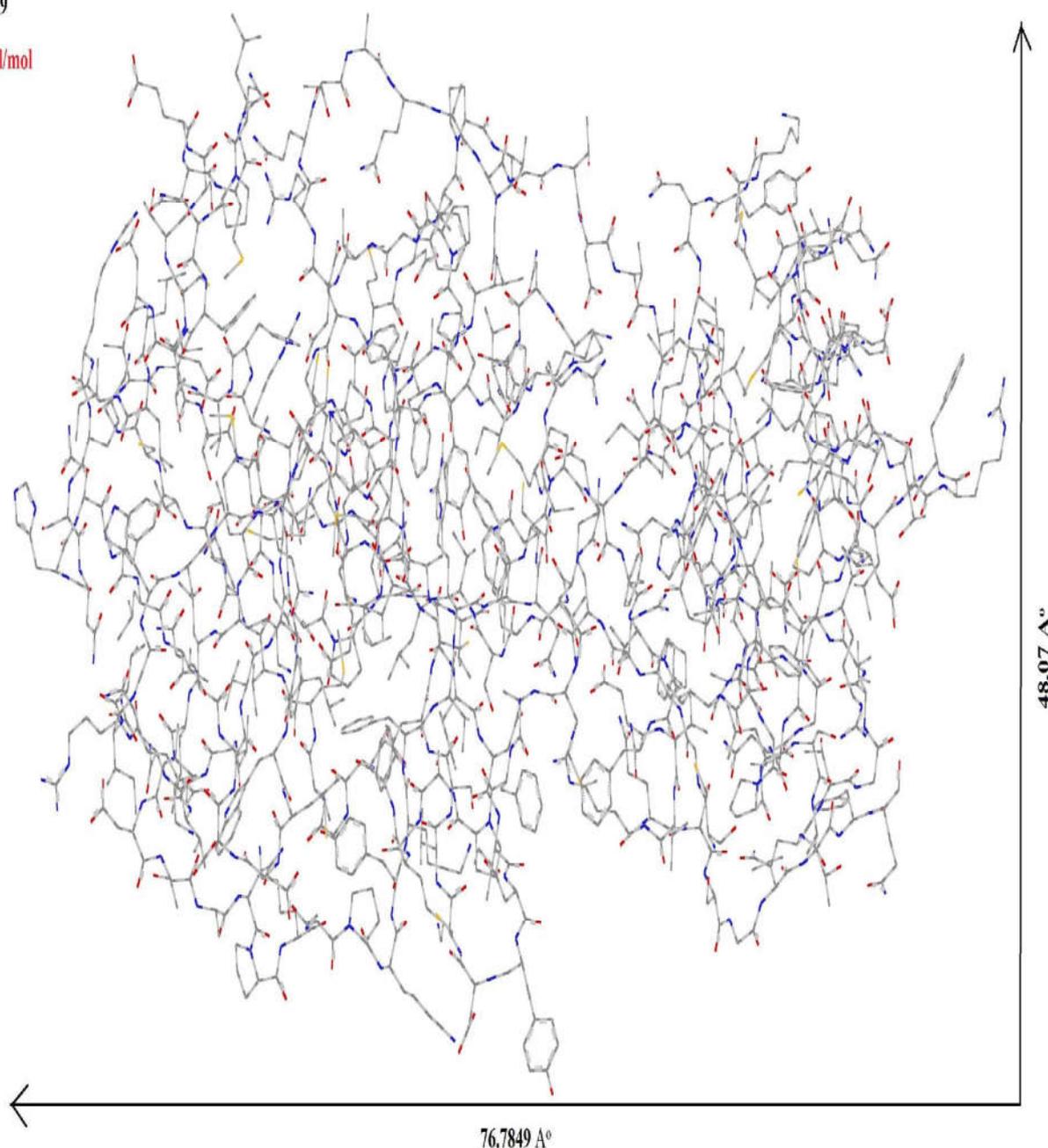


Fig 5. The binding energy for COVID-19 and quantum parameters.

Which confirms the high stability of the CORONA-19 virus from normal influenza, and the results of natural herbs were converging in energies but far from approaching the internal energy of the CORONA-19 virus, which makes

the composition of each natural herb not enough to definitively eliminate the treatment of this virus, only anise herb, which was the best internal energies among all the herbs used in this study as included in Table 1.

Table 1. Total binding energy.

Spices	Binding Energy (kcal/mol)
COVID-19	-3020
Seasonal Influenza	-1678.045
Anise	-218.84
Eugenol	-53.83
Thyme	-47.50
Cinnamon	4.056

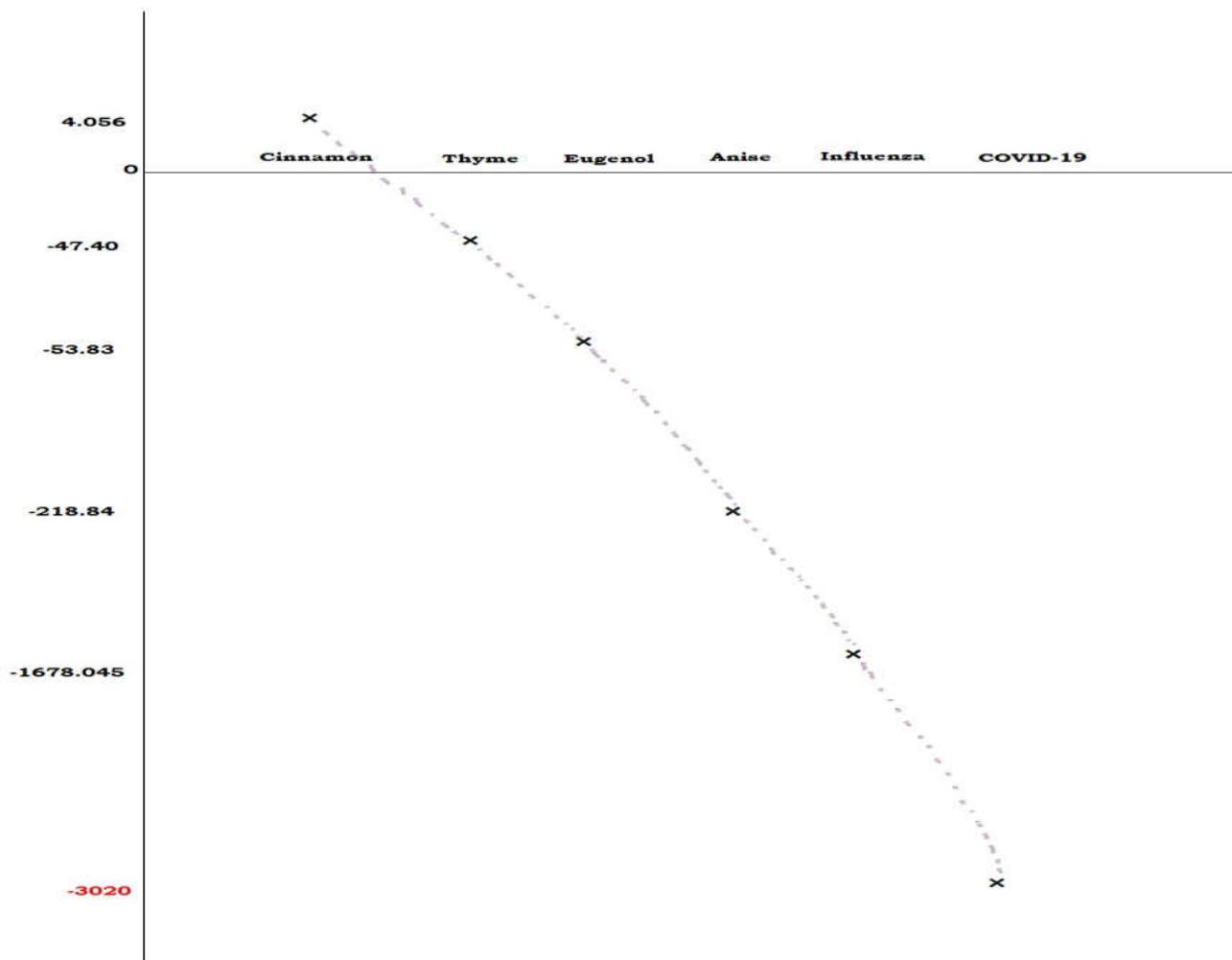


Fig 6. Comparison of binding energy curve for COVID-19, influenza, Thyme, Anise, Cinnamon, and Eugenol.

We conclude from the energy values of COVID-19 and seasonal influenza that they cannot be treated at all using all these natural herbs, only that may reduce their activity within the human body, but the best standard result among these herbs used in this study was herb

anise. And specifically at hydrogen atom number 18, which shows the best stable interaction point among all the other atoms. The details of its internal measurements are in Table 2.

Table 2. Input Orientation for Anise.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	C	-0.187100	0.492300	-0.098900
2	6	C	0.778200	0.495400	0.927400
3	6	C	1.408200	1.694100	1.302500
4	6	C	1.091900	2.904000	0.650400
5	6	C	0.119000	2.910700	-0.370200
6	6	C	-0.508300	1.702000	-0.742600
7	1	H	1.055500	-0.414200	1.437400
8	1	H	2.130600	1.673000	2.105100
9	1	H	-1.249000	1.688200	-1.528300
10	8	O	-0.172200	4.097200	-0.973500
11	8	O	1.670100	4.087700	0.999500
12	6	C	-0.874200	-0.730900	-0.540000
13	1	H	-1.441500	-0.690800	-1.424000
14	6	C	-0.874900	-1.931200	0.191000
15	1	H	-0.419900	-1.992400	1.134300
16	6	C	-1.653900	-3.120800	-0.324500
17	1	H	-1.367700	-3.326500	-1.356000
18	1	H	-1.438600	-3.994700	0.290500
19	1	H	-2.721200	-2.902300	-0.281500
20	6	C	-1.150000	4.293600	-1.977700
21	1	H	-2.133600	4.027700	-1.590000
22	1	H	-1.153600	5.342400	-2.274100
23	1	H	-0.918300	3.677000	-2.846600
24	6	C	2.929300	4.293600	1.379300
25	6	C	3.250900	5.764600	1.669300
26	1	H	2.322500	6.273800	1.933400
27	6	C	3.822700	6.451500	0.421900
28	1	H	3.106500	6.375100	-0.397100
29	1	H	4.008000	7.505900	0.630500
30	1	H	4.757400	5.974100	0.124900
31	6	C	4.213400	5.916000	2.856200
32	1	H	3.784400	5.440600	3.738800
33	1	H	5.172800	5.450000	2.628400
34	1	H	4.372800	6.973700	3.068900
35	8	O	3.840000	3.465700	1.316200

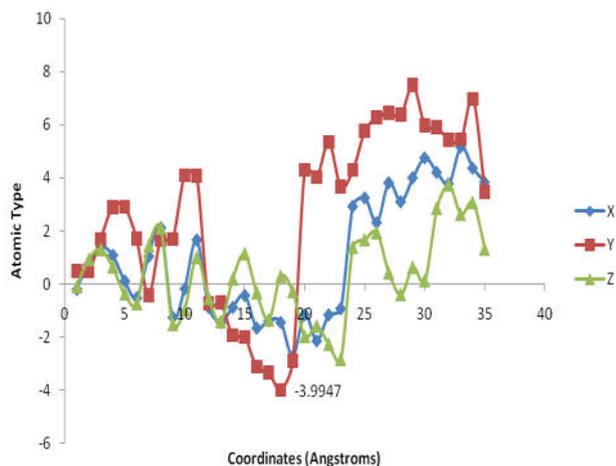


Fig 7. Coordinates of anise atoms.

Fig. 7 shows the distribution of internal energy patterns of anise complex atoms, and also demonstrates the best low and stable energy pattern at the 18th-ranked hydrogen atom in the anise compound. This would be the best correlation or overlap between anise compound and COVID-19 starting from the hydrogen atom referred to in Fig. 8.

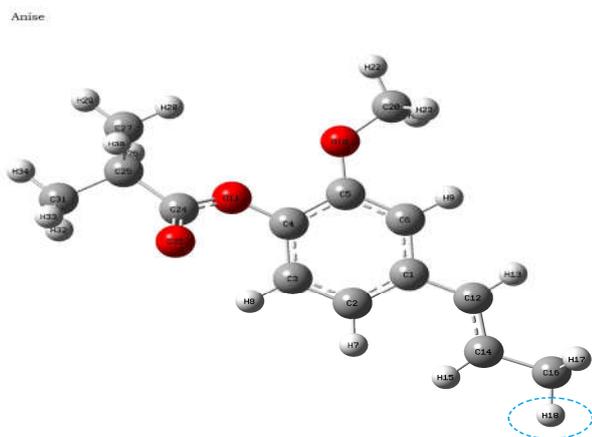


Fig 8. Final modeling of the anise herb at the best stable internal energy.

Conclusion

Energy specifications those are completely different from the seasonal influenza virus. So, the best herb used in the study is ANISE herb, but only reducing it does not treat the virus definitively based on the internal energy of the

herb significantly greater than the internal capacity of covid-19.

Recommendation

Using chemical computing as a field of research to ascertain the possibility of interactions to save time, effort, and cost, and the speed of the formation of a drug with an internal capacity equal to or less than the internal energy of COVID-19, and we emphasize the need to diverge and use medical muzzles that protect each user, we also recommend transferring the results of this study to direct application so that many cares about the need to protect themselves until the arrival of the installation of drugs eliminates this virus.

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