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Research Article

Long COVID-19: Electronic Characterization of the SARS-CoV-2 Envelope Protein Using DFT as a Basis for Therapeutic Hypothesis

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Abstract

Long COVID, or post-COVID-19, is emerging as a prevalent and complex syndrome affecting a significant percentage of patients who have recovered from the acute phase of SARS-CoV-2 infection. The viral envelope protein (E), a 75 amino acid ion channel, is a crucial structural component involved in viral pathogenesis. This study employs density functional theory (DFT) principles to calculate global reactivity descriptors of the short hydrophilic N-terminal domain of the E protein. The results indicate an ionization potential (*IP*) of 6.47eV, an electron affinity (*EA*) of 4.39eV, and a molecular hardness (η) of 1.04eV, suggesting moderate to high chemical reactivity. An electrophilicity (ω) value of 14.17eV reveals a marked tendency to accept electrons. These electronic descriptors, along with the described biological functions of the E protein, such as its role in viral assembly, budding, and modulation of the host inflammatory response, position it as a promising therapeutic target. We also report on the reactivity sites (*HOMO-LUMO*) present in the short hydrophilic N-terminal domain. Inhibition of the E protein could alter key viral processes and attenuate the immune dysregulation underlying persistent COVID-19, opening new avenues for rational drug design.

Keywords

SARS-CoV-2, E Protein, Long COVID-19, DFT, *HOMO-LUMO*, Global Reactivity Descriptors, Therapeutic Target, Drug Design

1. Introduction

Severe acute respiratory syndrome coronavirus 2 (SARS-Cov-2), the causative agent of COVID-19, has had an unprecedented global impact due to its high transmissibility and ability toeVade the immune response [1]. The

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SARS-Cov-2 envelope (E) protein is a key structural component that plays multiple roles in the viral cycle, including virion assembly and release, and modulation of the host immune response [2, 3]. This transmembrane protein exhibits a specific topology in eukaryotic membranes, facilitating its interaction with other viral and cellular proteins [4]. Furthermore, structural and biophysical research has identified functional regions within the E protein, such as the PDZ-binding motif at its C-terminus, whose accessibility to the cytoplasm regulates processes associated with pathogenicity and represents a potential target for the development of therapies [5, 6]. In this context, theoretical approaches based on density functional theory (DFT) have proven to be valuable tools for studying molecular reactivity and predicting physicochemical properties to rational drug design [7, 8].

In this research work, we focus on the structural and functional analysis of the short hydrophilic N-terminal domain (NTD) of the E protein. Our goal is to provideeVidence that contributes to the identification of possible therapeutic target, and to a better understanding of the correlation that exists between its global reactivity descriptors (GRDs) at the quantum level and its biological functions, mainly its role in viral pathogenesis.

2. Materials and Methods

We constructed the structure of the short hydrophilic N-terminal domain of protein E following the amino acid (AAs) sequences deposited in the databases: https://www.uniprot.org/uniprotkb/ and https://www.ncbi.nlm.nih.gov/protein6. The short N-terminal luminal domain is composed of the AAs: MYSFVSEETGTLI. We optimized the ground-state geometry using density functional theory (DFT) without symmetry constraints, which allowed for relaxation of intramolecular hydrogen bonds. The convergence criteria for geometric optimization were set at 1.0×10^{-5} Ha for energy, 0.002 Ha/Å for force, and 0.005 Å for atomic displacement. We confirmed the optimized structure as a true minimum on the potential energy surface using vibrational frequency analysis, which revealed no imaginary frequencies. We described the exchange-correlation effects using the generalized gradient approximation (GGA) with the Becke-Lee-Yang Parr (BLYP) functional. This method, which has the favorable "accuracy/cost" ratio, belongs to the DFT family and allows for viable DFT calculations for a relatively large system [9]. All geometric optimization calculations and reactivity descriptors were performed using the DMol3 tool in Material Studio 2020. To account for non-bonding interactions, particularly Van der Waals force, DFT-D3 scattering correction was included using the TS (Tkatchenko-Scheffler) scheme, applying a numerical basis set of double zeta atomic orbitals with polarization functions (DND). We used a spin-restricted method and assumed a closed-shell system. This approach was adopted because the molecular species studied are in their natural singlet ground state, without the presence of free radicals or paramagnetic metal centers at the reactive sites. Solvation effects of the aqueous biological environment were simulates using a conductor-like screening model (COSMO) with the dielectric constant of water (ε = 78.36). After optimizing the geometry, the calculation directly yields the energies of the frontier molecular orbitals: the highest occupied molecular orbital (*HOMO*) and the lowest unoccupied molecular orbital (*LUMO*). The *LUMO-HOMO* energy gap (ΔE) results from subtracting these energies. The total energies of the system in its neutral (N), anionic (N+1), and cation (N-1) states, denoted as $E(N)$, $E(N+1)$, and $E(N-1)$, respectively, provide the basis for deriving overall reactivity descriptors [7-13]. Using absolute energy values within the DFT conceptual framework, the following equation calculate key parameters:

$$\text{Ionization potential } (IP): IP = E(N-1) - E(N) \quad (1)$$

$$\text{Electron affinity } (EA): EA = E(N) - E(N+1) \quad (2)$$

$$\text{Chemical potential } (\mu): \mu = -(IP+EA)/2 \quad (3)$$

$$\text{Chemical hardness } (\eta): \eta = (IP-EA)/2 \quad (4)$$

$$\text{Electronegativity } (\chi): \chi = (IP+EA)/2 \quad (5)$$

$$\text{Electrophilicity index } (\omega): \omega = \mu^2/(2\eta) \quad (6)$$

$$\text{Softness}(S): S = 1/(2\eta) \quad (7)$$

3. Results and Discussion

We constructed, modeled, and optimized the most stable structure of the short hydrophilic N-terminal domain (NTD) of the E protein of the SARS-CoV-2 virus. This domain consists of the 13 amino acids (AAs) arranged from 1 to 13 in the following order: MYSFVSEETGTLI, which corresponds to 1: methionine, 2: tyrosine, 3: serine, 4: phenylalanine, 5: valine, 6: serine, 7: glutamic acids, 8: glutamic acids, 9: threonine, 10: glycine, 11: threonine, 12: leucine, and 13: isoleucine. It is worth noting that the NTD is exposed to the outside of the virus, it is made up of 204 atoms with an electron density of 788 electrons, as shown in Figure 1. Table 1 shows the global reactivity descriptors of the NTD of the E protein. Figure 2 presents the *HOMO-LUMO* frontier molecular orbitals. These frontier orbitals delineate the regions of the molecules most susceptible to electronic interaction, fundamentally governing its propensity to done or accept electrons. As such, the *HOMO-LUMO* analysis provides essential insight into the electronic structure, polarisability, and chemical reactivity, proving to be crucial for quantum mechanical characterization according to Fukui ś principles [13].

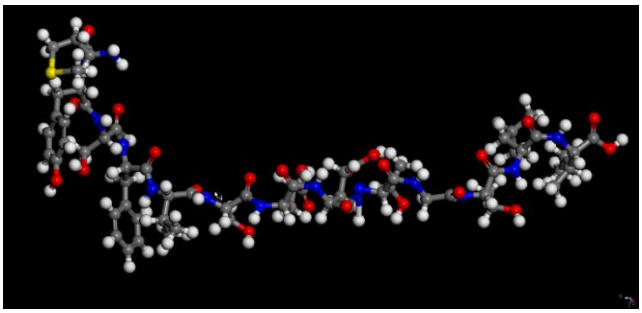

Figure 1. *Optimized molecular structure of the N-terminal domain (NTD) of the SARS-CoV-2 virus E protein, obtained using density functional theory (DFT) calculations. Color scheme of atoms: sulfur (yellow), oxygen (red), carbon (grey), nitrogen (blue), hydrogen (white).*

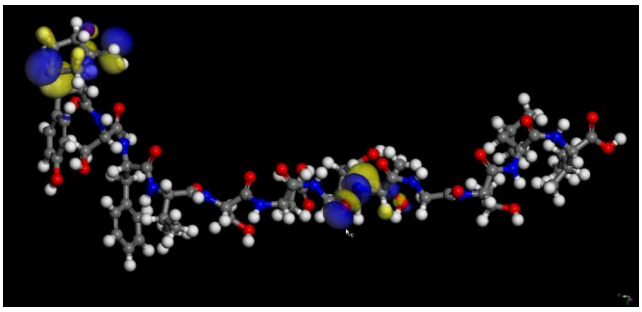

Figure 2. *Electron density surfaces of the NTD frontier molecular orbitals of the E protein of the SARS-CoV-2 virus. The highest occupied molecular orbital (HOMO, left, -4.56eV) locates the regions most susceptible to nucleophilic attack, while the lowest unoccupied molecular orbital (LUMO, right, -1.61eV) indicates the areas prone to electrophilic attack. The orbitals are visualized at an isosurface value of 0.02 a.u.*

Table 1. *Global reactivity descriptors of the NTD domain of the SARS-CoV-2 E protein.*

Descriptor	Symbol	EnergyeV	Interpretation
Ionization Potential	*IP*	6.47	Moderate-high stability
Electronic Affinity	*EA*	4.39	Significant ability to accept electrons
Molecular Hardness	η	1.04	Moderate-high reactivity
Electronegativity	χ	5.43	Medium-high electronegativity
Chemical potential	μ	-5.43	Electrophile, strong electron acceptor
Electrophilicity	ω	14.17	Marked electrophilic character
Softness*	*S*	0.48	Moderately reactive and able to interact
Highest Occupied Molecular Orbital	*HOMO*	-4.56	Ability of the molecule to donate an electron
Lowest Unoccupied Molecular Orbital	*LUMO*	-1.61	Ability to accept electrons
Gap *HOMO-LUMO*	ΔE	2.95	Moderate kinetic stability.

*Since softness (*S*) is the inverse of hardness (η), its units are the inverse of the units of energy, i.e., eV^{-1}

The hydrophilic NTD of the E protein of the SARS-CoV-2 virus has a *HOMO-LUMO* gap of 2.95eV, meaning that it a molecule that requires at least of 2.95eV energy for an electron to transition from the highest occupied molecular orbital (*HOMO*) to the lowest unoccupied molecular orbital (*LUMO*). This energy is related to the optical properties and molecular stability of the NTD [12]. Furthermore, we report that the NTD can donate electrons (*HOMO*) or receive electrons (*LUMO*) at AAs 1: methionine, 2: tyrosine, 9: threonine, and 10: glycine (Figure 2).

The overall electronic GRDs (Table 1) indicate low molecular hardness and high electrophilicity, positioning the NTD of the SARS-CoV-2 envelope (E) protein as key reactive site. The moderate softness (inverse of η) suggest conformational flexibility that facilitates interactions with ligands or proteins [3], while the marked electrophilic character implies a tendency to act as an electron acceptor in contact with cellular nucleophilic species [4]. The calculated electronic reactivity is consistent with the key biological function of the E protein reported previously [2-4]. In viral assembly and budding, the E protein promotes the formation of virion-containing vesicles in the endoplasmic reticulum-Golgi intermediate compartment (ERGIC). Its conformational flexibility, derived from its low stiffness, facilitates interactions with the M protein and the retention of the S protein, essential for assembly [2, 4, 14]. As a viroporin, protein E forms ion channels that disrupt H^+ homeostasis in compartments such as the Golgi, promoting inflammation and contributing to the cytokine storm in severe and persistent COVID-19 [1, 3, 6]. Its electrophilic character could mediate

ion transport, according to structures in PDB (7K3G) showing a dehydrated pore sensitive to pH and drugs such as hexamethylene amiloride [15]. In interactions with host protein, the PDZ-binding motif (PBM) at the C-terminus binds to human PDZ domains, disrupting cellular signaling [5]. NTD reactivity could modulate the accessibility of this motif, as indicated by protein-RNA interactions in infected cells [6]. Furthermore, the E protein is reported to induce necroptosis and regulate immune tolerance via TLR2, linking its reactivity to pathogenesis [5, 16]. Persistent immune dysregulation represent a central hypothesis in the pathophysiology of persistent COVID-19 [1]. The E protein drives this chronic inflammation through its viroporin activity, eVen without active viral replication, disrupting barriers such as the blood-brain barrier [3]. Specifically inhibiting the E protein could offer a dual therapeutic benefit [17]. The implications for Long COVID-19 and the drug design strategy should be oriented towards a direct antiviral effect, disrupting viral assembly and release, reducing viral load [2, 3]. Also promote and indirect immunomodulatory effect, blocking the ion channel, attenuating inflammasome activation and the release of proinflammatory cytokines (IL-6, IL-1β), mitigating persistent symptoms [1, 3]. The computed profile of GRDs (Table 1) informs the rational design of targeted NTD inhibitors. Based on this electronic profile, nucleophilic compounds are predicted to exhibit favourable interaction with the electrophilic domains of the protein [7-13]. Proposed design strategies include: (I) the development of competitive peptide mimetics for the PBM site [5], and (II) the identification of small molecules that bind within the viroporins hydrophobic pore, thereby blocking ion conduction in manner similar amiloride and derivatives, as demonstrated for other viroporins [3]. It is important to note that our results provide theoretical guidance rather than direct experimentaleVidence; however, they correlate with experimental reports published over the last five years.

We acknowledge that our study is limited to the NTD domain of the SARS-CoV-2 E protein, composed of 13 AAs. While this domain is crucial due to its exposure in the exterior of the virus, making it a potential target, including the rest of the complete protein could influence the overall electronic properties or long-term folding dynamics. However, it is advantageous that the NTD domain of the E protein does not exhibit a high mutation rate in its constituent AAs, compared to the S (spike) protein. We believe it is suitable for studying the calculated GRDs and establishes a solid quantitative basis for research in the rational design of inhibitor molecules or drugs against SARS-CoV-2.

4. Conclusions

Quantum mechanical analysis of the N-terminal domain of the SARS-CoV-2 E protein, performed using density functional theory reveals a distinctive electronic profile characterized by high reactivity and marked electrophilic nature. These electronic properties are consistent with the protein ś critical role in the viral life cycle and pathogenesis. Furthermore, emergingeVidence suggests that the E protein could be key factor in the immune dysregulation observed in persistent COVID-19 syndrome. In conclusion, inhibition of this protein represents a promising therapeutic strategy, not only for the acute phase of COVID-19 but also for managing its long-term sequelae. The global reactivity descriptors calculated in this study establish a solid quantitative foundation for future research, including *in silico* molecular docking studies and the rational design of drugs against SARS-CoV-2.

Abbreviations

SARS-CoV-2	Severe Acute Respiratory Syndrome CoV-2
COVID-19	Coronavirus Disease 2019
PBM	*PDZ-Binding Motif*
PDZ	Protein Interaction Modules
DFT	Density Functional Theory
GRDs	Global Reactivity Descriptors
AAs	Amino Acid
Å	Angstrom
GGA	Gradient Approximation
BLYP	Becke-Lee-Yang Parr functional
DFT-D3	Van Der Waals Dispersion Correction
TS	Tkatchenko-Scheffler, Correction Dispersion
COSMO	Conductor-like Screening Model
HOMO	Highest Occupied Frontier Molecular Orbital
LUMO	Lowest Unoccupied Molecular Orbital
ΔE	Gap LUMO-HOMO Energy Difference
NTD	N-Terminal Domain
eV	Electronvolt, Unit of Energy
IP	Ionization Potential
EA	Electron Affinity
η	Chemical Hardness
χ	Electronegativity
μ	Chemical Potential
ω	Electrophilicity Index
S	Softness
ERGIC	Endoplasmic reticulum-Golgi Inter-compartment
H^+	Protons
PDB	Protein Data Bank
RNA	Ribonucleic Acid
TLR2	Toll-Like Receiver 2
IL-6	Interleukin 6
IL-1β	Interleukin 1β

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Author Contributions

Juan Carlos Santiago-Jiménez: Conceptualization, data curation, formal analysis, methodology, project management, resources, software, supervision, validation, visualization, Writing – original draft, Writing – review & editing

Gabriel Ramirez-Damaso: Conceptualization, data curation, formal analysis, methodology, project management, resources, software, supervision, validation, visualization, Writing – original draft, Writing – review & editing

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Fray de Landa Castillo-Alvarado: Conceptualization, data curation, formal analysis, methodology, project management, resources, software, supervision, validation, visualization, Writing – original draft, Writing – review & editing

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Data Availability Statement

The data supporting the outcome of this research work has been reported in this manuscript.

Conflicts of Interest

The authors declare no conflicts of interest.

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Biography

Juan Carlos Santiago-Jiménez is a professor in the Department of Experimental Sciences at INGIA SC (CONAHCYT-RENIECYT-1801688) and has been a professor at UACM since 2015. He holds a PhD in Physics from ESFM-IPN and another in Genomic Sciences from UACM. He also holds a Master's degree in Experimental Biology from UMSNH and another in Inclusion and Special Educational Needs from CESUVER. He has a Bachelor's degree in Animal Production from UAM-I, as well as a degree in Pedagogy from CESUVER. He participates in various research projects at UACM and UMSNH. He is a member of the AcademiceValuation Committees for Higher Education for the National Higher Education Admission Examination at CENEVAL, Mexico. He is a member of the Mexican Materials Society (SMMater) and the Mexican Hydrogen Society (SMH). He is a reviewer for the Journal of Molecular Modelling and the Journal of Electronic Structure.

Gabriel Ramirez-Damaso is a professor of Physics Department at High School of Physics and Matematics (ESFM) of Instituto Politecnico Nacional (IPN) in Mexico City. Professor Ramirez completed his Ph. D. in Physics of Materials in ESFM-IPN (2011) and his Master Degree in ESFM-IPN (2003). He has been professor of Mathematics and Physics since 1993; he has directed more than eight research projects at IPN and has directed six master's degree thesis. Professor Ramirez has been Reviewer of research projects at IPN and SECIHTI-Mexico, and a Reviewer of articles published in International Journal of Hydrogen Energy, Applied Surface Science, Silicon and Revista Mexicana de Física.

Alberto Garcia-Quiroz is a senior professor and researcher at the Mexico City Autonomous University, in the Technology and Sciences Section (UACM-CCyT) since 2006 until today. He is a researcher on the thermodynamics and energy fields mainly. He made his master degree in the Advanced Studies and Investigation Center of National Polytechnic Institute (CINVESTAV). in the Physics Department finishing 1997 and made his PhD in Campinas State University, in the Wleb Gatahing Physics Institute (IFGW-UNICAMP) obtaining his Ph-Degree graduating at 2002 year. He has worked in several other fields such as molecular simulation applied to medicine, chemistry, energy and others. Like some other, he is actually Researchers National System, SNI, of the CONAHCYT of Mexico recognized as SNI 1.

Francisco-Caballero is a professor at Superior Studies Faculty (FES) Zaragoza campus, Chemical Engineering Department. He completed his PhD in Chemical Sciences from National Autonomous University of Mexico (UNAM) 2005, and his Master of Chemical Engineering in Drying process from UAM Iztapalapa Campus. Dr. Caballero has been honored with PRODEP Desirable Profile for Faculty Members. In addition, he holds a SNI 1 certification in accordance with CONAHCYT Mexico. He has participated in multiple national research collaboration projects collectively with UNAM and Advanced Studies and Investigation Center of National Polytechnic Institute (CINVESTAV).

Fray de Landa Castillo-Alvarado is a retired professor from the Escuela Superior de Fisica y Matematicas (ESFM) of the Instituto Politecnico Nacional (IPN), since May 2023. After 53 years of service at that institution, Professor Castillo-Alvarado earned his doctorate from ESFM-IPN (1984) and his master's degree from the University of Chicago, USA (1975). He has supervised 13 doctoral dissertations, 27 master's theses, and 10 undergraduate theses. He has received awards from international, national, and institutional universities. Professor Castillo-Alvarado is a National Researcher Emeritus of CONAHCYT, Mexico.

Research Field

Juan Carlos Santiago-Jiménez: Molecular Modeling and Simulation, Biomolecules, Biomedicine, Chemistry, Physics, Veterinary Medicine, Genomics, Emerging and Re-emerging Diseases, Energy.

Gabriel Ramirez-Damaso: Molecular Modelling and Simulation, Magnetism in Solids, Hydrogen Storage, Semiconductor Modelling, Modelling of Solar Cells.

Alberto Garcia-Quiroz: Molecular Modeling and Simulation, Biomolecules, Chemistry, Physics, Energy.

Francisco-Caballero: Modelling and simulation, Drying process, Reactors Engineering, Chemical physics phenomena, Process control and observers.

Fray de Landa Castillo-Alvarado: Molecular Modelling and Simulation, Biomolecules, Chemistry, Physics, Energy.