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Sites and Zones of Maximum Reactivity of the most Stable Structure of the Receptor-binding Domain of Wild-type SARS-CoV-2 Spike Protein: A Quantum Density Functional Theory Study

Today, it is well known that Severe Acute Respiratory Syndrome Coronavirus 2 (SARS-CoV-2) has four types of proteins within its structure, between them the spike protein (S). The infection mechanism is carried out by the entry of the virus into the human host cell through the S protein, which strongly interacts with the human cell receptor angiotensin-converting enzyme 2 (ACE2). In this work, we propose an atomic model of the Receptor Binding Domain (RBD) of the S spike protein of the wild-type SARS-CoV-2 virus. The molecular structure of the model was composed of 50 amino acids that were chemically bonded, starting with Leucine and ending with one amino acid Tyrosine. The novelty of our work lies in the importance of knowing the sites and zones of maximum reactivity of the RBD from the fundamental levels of quantum mechanics considering the atomic structure of matter. For this, the local and global reactivity indices of the RBD were calculated, such as frontier orbitals, Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO), Fukui indices, chemical potential, chemical hardness, electrophilicity index; with this, it will be possible to know what type of molecules are more likely to interact with the RBD structure, and in this way, new knowledge will be generated at the quantum, atomic and molecular level to inhibit the virulent effects of wild-type SARS-CoV-2. Finally, in order to identify the functional groups within the most stable structure and thereby verify the future reactions that can be carried out between the RBD structure and biomolecules, the Infrared (IR) absorption spectrum was calculated. For this work, we used Material Studio v6.0 which uses the density functional theory (DFT) implemented in its DMol3 computational code. The IR spectrum was obtained using the Spartan ‘94 computer code. One novelty would be that we found nine amino acids more that could make the RBD and ACE2 binding further the already known. Thus, the Mulliken charge distribution indicates that the highest concentrations of positive and negative charge are found in the zones 477S, 478T, 484E, and 501N amino acids letting ionic or Van der Waals possible interactions with other structures.

Opinion **Published Date:-2024-03-07 16:28:12**

Why is Pain not Characteristic of Inflammation of the Lung Tissue?

The article presents materials that make it possible to understand the reason for the absence of one of the classic signs of inflammatory processes in patients with acute pneumonia. The peculiarities of the functional significance of the lungs for the body are the reason that in the case of inflammation in the tissues of the organ, nature has provided for the presence of a more important adaptive mechanism instead of pain as a signal sign. Understanding the causes of the absence of pain in pneumonia in the initial period, which is most responsible for timely and effective care for these patients, allows us to look at the pathogenesis of the disease from a new point of view, which is of fundamental importance for the correction and selection of pathogenetic means of care.

Retrospective Study **Published Date:-2024-01-19 15:25:31**

Tracheotomy in Severe Head Trauma: Early vs. Late

Introduction: The evolution of a patient with severe traumatic brain injury may require the use of a tracheostomy as part of respiratory weaning. The central question revolves around the optimal timing to replace intubation with tracheostomy. The aim of this study is to evaluate the hypothesis that early tracheostomy reduces the incidence of ventilator-associated pneumonia (VAP), the duration of mechanical ventilation (MV), and the length of stay in the intensive care unit (ICU).
Materials and methods: This was a retrospective study including all patients admitted to the department over a period of 08 months. Various historical, demographic, clinical, biological, and progression-related covariates were collected upon admission.
Results: Among the 69 patients included in the study who underwent surgical tracheostomy,
two groups were formed: those who underwent early tracheostomy (within the first 8 days of mechanical ventilation) and those with late tracheostomy (after 8 days). The early group showed a significant reduction in the duration of mechanical ventilation (16 ± 3 days) and length of stay in the intensive care unit (17 ± 3 days) compared to the late group (23 ± 6 days and 30 ± 11 days, respectively). No significant differences were observed regarding the incidence of ventilator-associated pneumonia (VAP) and mortality between the two groups.
Conclusion: This study strengthens the existing literature by demonstrating that early tracheostomy is associated with a reduction in the duration of MV and length of stay in the ICU.