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Computational Analysis of the Antioxidant Potential of Organic Compounds Using the Density Functional Theory Method

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INTRODUCTION & AIM

Antioxidant potential refers to the ability to neutralize free radicals and reduce oxidative stress caused by external factors such as pollution, smoking, and radiation (TANG et al., 2022; SHOHAG et al., 2022). These radicals can damage DNA, RNA, and proteins, contributing to diseases and aging. Their antioxidant potential is not only based on their ability to directly interact with free radicals, but also on their capacity to modulate complex biological mechanisms, such as redox signaling pathways and endogenous defense enzymatic systems. Antioxidants, including vitamins and polyphenols, whether natural or synthetic, help combat this stress. Experimental and computational methods are employed to assess and predict antioxidant activity, analyzing their mechanisms at the molecular level.

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METHOD

The methodology of this study will use molecular modeling tools and computational simulations to investigate organic compounds with antioxidant potential, such as flavonoids and phenols, known for functional groups like hydroxyl (-OH), carbonyl (C=O), and amino (-NH2) (TOHMA et al., 2017). Quantum chemistry methods, such as DFT with the B3LYP functional and the 6-311++G(d,p) basis set, implemented in the Gaussian 09 software, will be employed to perform the calculations (Frisch,M.J,2016) . The simulations will focus on determining key molecular properties, such as the total electronic energy, HOMO-LUMO gap, and bond dissociation energies, which are critical to understanding the antioxidant mechanism. Additionally, the study will explore the stability and reactivity of these compounds in various environments by evaluating their interaction with reactive oxygen species (ROS).

- **Density Functional Theory (DFT)**

Density Functional Theory (DFT) is a quantum computational method used to study electronic structure, theoretically exact in principle. Its primary objective is to model electronic interactions, as it describes the behavior of strongly bound electrons in the presence of the electrostatic field of ions. This is one of the most widely used methods in quantum calculations, both in condensed matter physics and quantum chemistry (DREIZLER, 1990).

Thus, DFT has enabled the development of a way to study the world around us, where computers are used to help us understand and predict the properties of atoms, molecules, and solids. DFT is also used to optimize the geometry of molecular systems and their interaction energies. As a result, all properties of the system are expressed as functionals of the electronic density (ATKINS, JONES; LAVERMAN, 2016).

One of the advantages of DFT is its ability to study systems of moderate to large size with good chemical accuracy, often at a computational cost significantly lower than that of traditional correlated methods. This makes DFT an efficient computational tool for exploring the properties and behaviors of complex molecular systems (ATKINS; FRIEDMAN, 2011).

RESULTS & DISCUSSION

The results of this study allow for the rapid identification of promising compounds for experimental testing, revealing their mechanisms of action. Our research highlights the importance of antioxidants, such as vitamins (C and E) and polyphenols, in reducing oxidative stress and preventing chronic diseases. A diet rich in antioxidants is crucial for preserving cellular health, slowing down aging, and promoting a healthy life, provided the compounds are well absorbed and metabolized.

Furthermore, it is important to consider that the effectiveness of antioxidants is not limited to their presence in the diet but also depends on their bioavailability and ability to reach target tissues in the body. Therefore, the use of computational methods, such as Density Functional Theory (DFT), becomes a powerful tool for studying the antioxidant properties of these compounds, allowing for the modeling of their molecular interactions and optimizing their biological activity. The results also contribute to improving our understanding of the role of antioxidants in human health and demonstrate new therapeutic approaches for the treatment of diseases related to oxidative stress, such as cardiovascular diseases, neurodegenerative disorders, and even certain types of cancer.

CONCLUSION

This study demonstrates that computational analysis has been crucial in evaluating the antioxidant potential of organic compounds, highlighting the effectiveness of natural and phenolic compounds in neutralizing free radicals. The application of Density Functional Theory (DFT) has accelerated the discovery of new antioxidants, contributing to the development of more effective treatments against oxidative stress. Moreover, the combination of computational and experimental techniques has enabled a more comprehensive and precise evaluation of the biological potential of these compounds. The results emphasize the importance of computational methods in antioxidant research, opening up new possibilities for therapeutic strategies in the fight against diseases related to oxidative stress.

FUTURE WORK / REFERENCES

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