Predicting Antioxidant Synergism via Artificial Intelligence (2023-046)

Artificial intelligence model based on deep learning architecture to both predict the type of interaction of known mixtures, as well as unveil new antioxidant combinations.

Market Overview

Lipid oxidation is a major issue affecting products containing unsaturated fatty acids as ingredients or components. In specific, the formation of low molecular-weight species with diverse functional groups has the potential to impart off-odors and off-flavors. This process, also known as rancidity, and can not only impart an unpleasant taste, but also diminish the nutritional value, shelf-life, and the overall quality of products, which ultimately impacts all segments of the supply chain. The impacted products include, for instance, cosmetics, vegetable oils, seafood, processed meat, animal feed, and other food samples. While current approaches to controlling this process through the addition of antioxidants minimizes the potential organoleptic and toxic effects of these compounds, empirically predicting how these mixtures of antioxidants will behave has traditionally been one of the most challenging tasks, often leading to simple additive (or even antagonistic) instead of the desired synergistic effects. To address this current gap in knowledge, a novel artificial intelligence model was developed based on deep learning architecture to both predict the type of interaction (synergistic, additive, and antagonistic) of known mixtures as well as to unveil new antioxidant combinations.

Technical Summary

This invention is the first example of using Artificial Intelligence based on deep learning architecture to predict antioxidant interactions. The algorithm was trained using the SMILES notation for the antioxidants and a combination index to account for the interaction. This AI algorithm pulls from a propriety database of approximately 1100 entries and has been enhanced with abundant experimental data in order to provide suitable predictions with statistical relevance. The proposed augmentation approach leads to a more representative chemical space during the model training, which addresses common overfitting problems due to the use of relatively small datasets. As this novel strategy enables a broader and more rational predictions related to the antioxidant mixtures behavior, it could be used as an auxiliary tool in benchmark analysis routines.

Application

Impacts on consumer health and economic supply chain for products including cosmetics, vegetable oils, seafood, processed meat, animal feed, and other food samples

Development Stage

TRL 4

Advantages

- First AI model to predict how mixtures of antioxidants will behave and potential additive, antagonistic, or synergistic effects
- Accounts for the complexity and multifaceted nature of antioxidant response
- Broader and more rational predictions compared to the traditional, empirically driven approaches

About the Inventors

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Dr. Carlos D. Garcia received his Ph.D. in Chemistry from the National University of Cordoba (Argentina) in 2001 and joined Clemson University in 2015. His group is focused on the study of interactions of proteins with nanostructured surfaces and their use in analytical chemistry. His research has received support from the National Institutes of Health, National Science Foundation, National Agency for Space and Aeronautics, and the Office of Naval Research.

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Dr. Daniel Whitehead received his Ph.D. in Organic Chemistry from Michigan State University in 2009 and has been a faculty member at Clemson University since 2011. His bio-organic chemistry lab focuses on the development of new organic chemistry reactions, the discovery of new drugs for chronic diseases driven parasites and bacteria, and functional nanomaterials for environmental and biomedical applications.

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Lucas de Brito Ayres earned his Bachelor's in Pharmacy-Biochemistry from the University of Sao Paulo (Brazil). He is currently pursuing his PhD in Chemistry and is interested in continuing working with low-cost sensors, instrumentation, and automation.

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