United States Department of Agriculture
Project Initiation

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Project Title

DSFAS: Harnessing the Power of Artificial Intelligence and Deep Eutectic Solvents to Boost Antioxidant Synergism

Project Details

Sponsoring Institution National Institute of Food and Agriculture	**Project Status** ACTIVE
Funding Source NIFA Non Formula	**Grant Year** 2024
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Program Code [A1541] Food and Agriculture Cyberinformatics and Tools	

Project Director

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Performing Department

Chemistry

Non Technical Summary

Despite more than 150 years of research, lipid oxidation remains a major challenge for the food industry due to the complexity of the products and the multiple elements that influence oxidation. Besides the economic losses, rancid food can also affect the health of consumers. To control this process, antioxidants are commonly added to foods, often in combinations of two or more compounds. This approach can effectively increase the total antioxidant capacity of the mixture and allows one to decrease the total amount of antioxidant used and/or extend the shelf-life of foods. One issue with this strategy is that predicting the intricate interplay of variables involved in these interactions remains a significant scientific challenge. Thus, our group seeks to leverage the power of artificial intelligence and data science to streamline the development of novel antioxidant formulations. We aim to develop a robust AI model that can significantly accelerate the discovery and vetting of new antioxidant combinations that will enhance food safety and ensure the stability of fats and oils that are critical to the food supply chain.

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Animal Health Component

Animal Health Component: 0%

Research Effort Categories

Basic	30%
Applied	40%
Developmental	30%

Classification

Knowledge Area (KA)	Subject of Investigation (SOI)	Field of Science (FOS)	Percent
501	5010	2000	100%

Knowledge Area

[501] New and Improved Food Processing Technologies

Subject Of Investigation

[5010] Food (not readily associated with specific plant and animal products)

Field Of Science

[2000] Chemistry

Keywords

antioxidants, synergism, Artificial intelligence, deep eutectic solvents

Goals / Objectives

Our group seeks to leverage the power of artificial intelligence and data science to streamline the development of novel antioxidant formulations, efforts that are directly tied to NIFA-AFRI Priority Area 3: to promote "food safety, nutrition, and health". We aim to develop a robust AI model that can significantly accelerate the discovery and vetting of new antioxidant combinations that will enhance food safety and ensure the stability of fats and oils that are critical to the food supply chain, thus advancing both agricultural sciences and data science/AI.Specifically, we propose to:Task #1: Develop and implement advanced AI models based on molecular fingerprints to predict synergistic mixtures of antioxidants.Task #2: Leverage and expand our existing deep eutectic solvent (DES) AI model to develop the first series of functional DES, integrating synergistic mixtures of antioxidants in their structure.Task #3: Experimentally verify the predictions of our models using real samples of fats (lard, tallow, chicken) and oils (soybean, rapeseed, olive).

Project Methods

Task #1: As a starting point, we will start the activities using the existing language-based algorithm, pre-trained using general unlabeled chemical data. This algorithm will be fine-tuned as a regressor using an existing database of antioxidant mixtures. This transformer-based neural network model is trained to recognize the patterns in SMILES strings of a sequence of mixtures in a database and predict the corresponding CI values, from which the antioxidant

mixtures can be classified as synergistic, additive, or antagonistic. As we tackle the proposed activities, outcomes from this approach will be used to train the students and generate the controls required to benchmark the advantages of the advanced model over the existing one.Task #2:We will first apply an existing complementary algorithm, pre-trained using general unlabeled chemical data and fined-tuned as a binary classifier using an existing DES database. This transformer-based neural network model is trained to recognize the patterns in strings that lead to the formation of either stable NADES or simple mixtures of compounds not leading to the formation of stable DES (binary classification). This is accomplished by implementing a SoftMax function on the raw output of the last layer from the deep neural network model. All the predicted DES with their respective stability scores will be then postprocessed and in a compound finder module, that allows filtering and ranking the output according to their probability to form a stable DES.Task #3: We will test the validity of our hypotheses by determining the antioxidant power of the synergistic mixtures identified in Task #1 and Task #2. For these experiments, we propose to use real samples of fats (lard, tallow, chicken) and oils (soybean, rapeseed, olive). In this way, we will obtain specific data and kinetics related to the oxidation process. These results will not only allow us to understand the effect of the sample type but also compare the oxidation process for bare samples with that of samples mixed with each of the selected antioxidants, their synergistic mixtures, and the DES-forms of the synergistic mixtures. Besides the controls, we propose to challenge the algorithm by experimentally measuring the antioxidant power of the 20 most synergistic mixtures, at 3 concentration levels, and specifically addressing the kinetics of the process (data collected at least at 5 different times). For these experiments, we will evaluate the extent of lipid oxidation by the thiobarbituric acid reactive substances (TBARS) assay, a common marker for lipid oxidation