

Antioxidant capacity of chemicals

Successfully predicted with high accuracy

#Organic #Chemical #Material Science #Material Informatics #Deep learning with minimal data # High-precision predictions

The antioxidant capacity of chemicals in food is considered an important factor for health. Here, we focused on the measurement of reactive oxygen species (ROS) scavenging activity of fat-soluble components by the singlet oxygen absorption capacity (SOAC) method. And developed an AI model to predict the antioxidant capacity of chemical substances in food.

Challenge

Experimental determination of SOAC values for new or untested antioxidants is time-consuming and resource intensive. The relationship between molecular structure, solvent parameters, and SOAC values is often non-linear and complex.

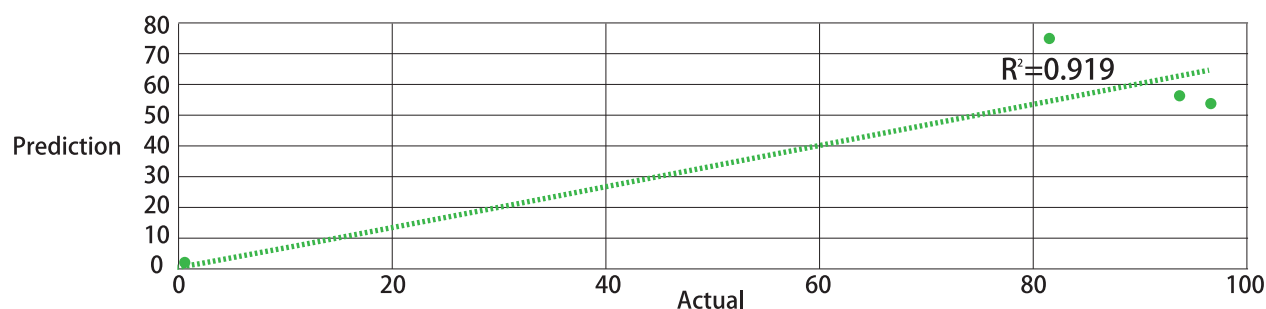
Solution

An AI model was developed to predict the SOAC values of antioxidants with their respective molecular fingerprints as input parameters, which were generated from their respective SMILES (Simplified Molecular Input Line Entry System) notation. Polyphenol and carotenoid antioxidants were categorized based on the magnitude of their SOAC values. Solvent parameters were acquired and incorporated into the SOAC value calculations to enhance prediction accuracy. The model was trained with a dataset comprising 153 known SOAC values of antioxidants and 42 values for validation.

Result

Created a highly accurate AI model: For SOAC values 10 or higher, RMSE was 0.094. For SOAC values less than 10, RMSE was 0.071.

Predictive performance: Coefficient of determination (R^2) of predicted versus actual was 0.919, indicating highly accurate predictions of antioxidant capacity of various antioxidants.



Conducted in collaboration with Shinichi Nagaoka (Affinity Science Corp.)

Reference

Ouchi A., Aizawa K., Iwasaki Y., Inakuma T., Terao J., Nagaoka S., Mukai K. Kinetic study of the quenching reaction of singlet oxygen by carotenoids and food extracts in solution. Development of a singlet oxygen absorption capacity (SOAC) assay method. *J. Agric. Food Chem.* 2010;58:9967–9978.

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