

Chapter 18

Artificial Neural Network (ANN) Modeling of Odor Threshold Property of Diverse Chemical Constituents of Black Tea and Coffee

Jillella Gopala Krishna

NIPER Kolkata, Kolkata, India

Probir Kumar Ojha

 <https://orcid.org/0000-0003-4796-3915>

Jadavpur University, Kolkata, India

ABSTRACT

The authors have developed an artificial neural network model using odor threshold (OT) property data for diverse odorant components present in black tea (76 components) and coffee (46 components). The models were validated in terms of both internal and external validation criteria signifying acceptable results. The authors found the significant features controlling the OT property using Mean Absolute Error (MAE)-based criteria in a backward elimination of descriptors, one in each turn. The present results well-corroborated the previously published PLS-regression based chemometric model results.

1. INTRODUCTION

Tea is the most commonly consumed nonalcoholic beverage after water. The consumption of tea is a very ancient habit. In 1978, an Archeological research reported by Jelinek suggested that the infusion of leaves from the tea tree was probably practiced more than 500 000 years ago (Gutman, & Ryu, 1996). Black tea is originated from the two varieties such as *Camellia assamica* and *Camellia sinensis*. Black tea and green tea are produced from the same plant *Camellia sinensis* but the name varies due to how the

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plant's leaves are processed (Hara, Luo, Wickremashinghe, & Yamanishi, 1995). Black tea is grown and processed all over the world in varying geographies and climates. Though, China is the largest producer of tea, but India, Sri Lanka and Africa are the top three producers of black tea today (Mary, & Robert, 2011). Among the different varieties of tea, black tea is most widely used worldwide due to its flavour. In case of black tea preparation, before the heat processing and drying, the leaves are allowed to oxidize fully which turn the leaves from the rich dark brown to black colour for which black tea leaves are famous for. The change of colour occurs due to the interactions between the tea plant cell walls and oxygen. This oxidation process alters the flavor profile of black tea. The enzyme, catechol oxidase, acts as a catalyst in the oxidation process leading to the formation of theaflavins and thearubigins from flavanols which are responsible for the characteristic colour and flavor of fermented tea (Robertson, 1992; Borse, Rao, Nagalakshmi, & Krishnamurthy, 2002; Bhattacharyya et al., 2008). Thus, the characteristics flavour is the key element for identification or evaluation of tea. Flavour of black tea is due to the presence of taste and aroma active components. Volatile components (around 600 volatile compounds have been reported in tea leaves) like aldehydes, alcohols, ketones, furans, and aromatic compounds control the aroma of black tea while the non-volatile components like organic acids, polyphenols, sugars, caffeine, catechin, theaflavins, thearubigins and free amino acids, among others are responsible for taste of black tea (Wang et al., 2011; Rawat et al., 2007; Bondarovich et al., 1967). Though, the volatile components are present in minute amount, but these have high impact to regulate the flavour of the black tea due to their low threshold values (Rawat et al., 2007).

Like tea, coffee, though young, is also an important beverage used worldwide due to its flavour as well as its potential health benefit (Balentine, Wiseman, & Bouwens, 1997; Halder et al., 2005). Coffee is prepared from roasted coffee beans, the seeds of berries from certain *Coffea* species. This is one of the major sources of income for many countries like Brazil, Vietnam, Colombia, Indonesia, Ethiopia, India, Honduras, Uganda, Mexico, Guatemala, Peru, etc. As of 2018, Brazil is producing one-third of the world total coffee (Coffee Annual Brazil - USDA GAIN reports, 2018). The worldwide popularity of this beverage is due to some factors, among which, flavour is the main reason. Thus, distinctive characteristics of smell can help in the identification of different food and beverages. This is also very helpful in case of perfume and beverage industries for masking the obnoxious odor of chemicals used in different food, pharmaceuticals and cosmetic products. An odor is the impression in the brain obtained by the recognition of a volatile compound at a very low concentration by odorant receptors (ORs) which is perceived by the sense of olfaction of human or other animals.

1.1. Odor Threshold and Evaluation

The odor threshold (OT) is the minimum concentration at which all panelists have been able to recognize the odor sensitivity (Leonardos, Kendall, & Barnard, 1969). A trained Panel of four staff members of the Food and Flavor Section of Arthur D. Little, Inc. was used for determining the odor threshold of each chemical. The Panel members were selected from a pool of approximately fifteen observers with more than one year of analytical odor work. Only one chemical was observed per day by the panel. Before the observations of a chemical, the Panel examined the odor at diverse dilutions to familiarize with the odor type. Each chemical was examined with the five different concentrations. The first odor observation of the day was the background level of test room. A concentration range was selected for inclusion of the odor threshold. The Panel members were not informed of the concentration of the chemical in the test room. The results obtained from each panelist were examined separately. Each Panel member was

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