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Short Communication

Challenges and Impact of the Increase of Data and Information on Bioactive Polyphenols in Food

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Introduction

The prevention of chronic diseases is a challenge of the food sciences, along with other biomedical sciences. Diseases as cancer, cardiovascular, diabetes mellitus, neurodegenerative, among others, are high prevalent around the world. Different sciences can contribute to improve global health. A multidisciplinary effort, which includes biomedicine, chemistry, mathematics, physics, in conjunction with computer science, is the ideal approach. It would be interesting to contribute to solve this global problem from the characterization of bioactive compounds present in food and understand the challenges we face with the increase of data compiled in food databases.

In this sense, the bioactive components of food have been studied. Among them polyphenolic compounds have been studied in recent decades. They are chemical substances that isolated or in the food matrix can provide benefits to this health problem. There is epidemiological evidence linking the beneficial effects of dietary polyphenols to the prevention of such diseases [1-3]. Diets rich in fruits and vegetables, for example, have been linked to lower mortality rates associated with cardiovascular diseases and some types of cancer [4-6].

There are numerous studies that have focused on the beneficial role of polyphenols when they act as antioxidants by different mechanisms. This interest is mainly due to the discovery of its antioxidant effects in vitro and its proposed beneficial role in several chronic diseases [7-10]. However, these results become controversial, especially when some of those substances have also been associated with contrary activities, for example pro-oxidant activity.

Polyphenols on diet are present in fruits, vegetables, cereals, some seeds and drinks such as wine, tea or beer, among others [6]. Other matrices carrying these phytochemicals are functional foods (FFs), fortified foods, nutraceuticals and dietary supplements [11]. Many of these are also investigated for their potential as drugs, due to the multiple activities they may present [12].

There are controversial aspects that require a deep benefit/safety study of this type of bioactive compounds. One aspect discussed is the benefit of polyphenols when they act as antioxidants, since current studies are inconclusive, and in some cases contradictory [10]. In this sense, Bouayed (2010) stated that some of these benefits have been overestimated as "double-edged edge" in the redox cell state [13]. Some determining factors that impact on the balance between the beneficial or harmful effects of these natural compounds are the chemical structure of the antioxidant polyphenols, the dose and the matrix that supports them [13].

Other paradoxical aspects are based on the fact that some antioxidants can act as pro-oxidants under certain conditions [4,13]. Pro-oxidants can be beneficial, increasing the levels of endogenous antioxidant defenses [14-17]. They have also been investigated for their potential as anticancer agents [12]. But because of the pro-oxidant mechanisms, polyphenols can also become genotoxic, and by clastogenic processes damage DNA [18].

Due to the increased interest in polyphenols, both academic and industrial, the information on the amount and type of them in food has recently increased [19]. This is one of the novel aspects in food science we want to highlight for future challenges. New food composition databases (FCDb) have been developed. They are different from the traditional ones, being focused on the amount and

type of polyphenols present in different dietary matrices. These FCDbs contain information on hundreds of foods. Examples of this are those published by the USDA (United States Department of Agriculture), such as: Database for the Flavonoid Content of Selected Foods, Database for the Isoflavone Content of Selected Foods, Phenol-Exlorer and EuroFIR-BASIS [20-23]. The proper management of this data through different predictive methodologies offer the possibility of generating new information and exploring the complex interactions between diet and the human organism [5,24]. This is an emerging challenge for food science and public health. Collaborative work between computer scientists, and the use of artificial intelligence techniques, can contribute to generate new knowledge, so far not provided. The complexity of the food must be taken into account. In this sense, Fardet (2015) has proposed to analyze the health benefits of bioactives from a holistic and non-reductionist perspective [25]. To achieve such challenges, the use of chemoinformatics could be of interest [24], a tool that has been poorly explored in the characterization of the bioactivity of phenolic compounds in foods. The FAO (Food and Agriculture Organization) uses it in the search for safe additives, using software that is sometimes not affordable [26].

The evidence described above suggests the interest of future work on the safety of such compounds [27]. Although polyphenols and their derivatives are supposedly safe at physiological doses as part of the diet, the modifications of the dosage and the matrix that supports them (as is the case of nutritional supplementation) have not reached the expected results [10]. The relationship that could exist between the chemical structure of an antioxidant/pro-oxidant and the prediction of possible oxidative damage to DNA, either isolated or analyzed in the context of a food matrix, are also unknown. All these aspects become more important in view of the different design strategies of FFs or enriched ones, in nutritional supplements and even drugs.

It is interesting to note that the use of complex classification and regression models in biomedical sciences is increasing [28]. The development of chemoinformatics is an example. Chemoinformatics aims to produce useful models that can predict the chemical and biological properties of compounds [29]. Its main application has been focused on the area of knowledge of pharmaceutical sciences. The background of its use in the food sciences is more limited and focused mainly on the development of food additives [30]. The models obtained by these multivariate techniques have good predictive quality and have been carried out for example in beverages and infusions: fruit juices [31], Moscatel wine [32,22], red wine and green tea [34].

Highlighting important ideas and evidences

Dietary polyphenols are present in various dietary matrices, either forming a natural part in foods belonging to different food groups or forming part as a bioactive component of FFs.

FFs have recently been defined by Functional Food Center as: "natural or processed foods containing known or unknown biologically active compounds; which in defined quantities provide clinically proven health benefits for the prevention, management and treatment of chronic diseases" [35].

Polyphenols can also be part of other dietary matrices such as dietary supplements that are designed according to different pharmaceutical forms. For example, ellagic acid is a phenolic acid that has been marketed as a nutraceutical, functional food and dietary supplement [11].

New paradigms related to the food-health binomial emphasize on the positive aspects of the diet. The available data on the amount and type of polyphenols in food are increasing every day [7-8]. Several polyphenols have been described in foods and beverages [36], which are known by a variety of physicochemical properties, bioavailability, biological properties and effects on health [37]. These aspects are essential for a detailed and complete information on the nature and amounts of polyphenols found in main foods consumed by humans.

The number of polyphenols in food is an important information for researchers in the food sciences and nutrition, food producers, regulatory authorities, dieticians or consumers. It gives the possibility to generate new knowledge such as: compare the polyphenols content between foods, calculate the intake of polyphenols by populations, study the association with health and diseases and/or to evaluate the relative contribution of these products to the intake of a particular polyphenol, compared to other food sources.

The access to these FCDb allows to verify the existence of a high amount of data/information that had been dispersed and to explore it in search of new information and knowledge. However, there are still few applications derived from the use of these databases [38,39].

It can be interesting to process information from the data offered by the FCDb of phytochemicals, through artificial intelligence techniques, because they are considered complex systems.

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