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Phenolcalc: facilitating the calculation of polyphenols in foods

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ABSTRACT

Introduction: Due to the proven beneficial activities, interest in polyphenols has increased and consequently, interest in determining the distribution and quantity of these compounds in foods has also increased.

Objective: To develop a tool to facilitate the estimation of polyphenols in food-specific portions using data from the online database Phenol-Explorer 3.6 (2016).

Methods: Microsoft Excel® software (version 2013) was used to develop the study and data collected on the Phenol-Explorer 3.6 online platform (version 2016). Data from various foods and their corresponding phenolic compounds were entered into the Excel spreadsheet. By applying the required formulas to each data point, it is possible to obtain the final value of the amount of phenolic compound for a specific food.

Results: The generated material was composed of two workbooks: "Phenol-Explorer - 2016", which included the restructured data from the online database showing the content of phenolic compounds in various foods and "Estimation of polyphenols", intended for users who want to quantitatively estimate the amount of phenolic compounds present in food, organized into six meals a day.

Discussion: Many software applications are currently designed to speed up the tedious daily activities of its users. Although these programs contribute to nutritional planning, they do not have the functionality to calculate the amounts of polyphenols that have been consumed and / or will be offered at meals.

Conclusions: "PhenolCalc" allows fast and simplified estimation of polyphenols in foods and meals. Such a tool would contribute to the popularization of the analysis of these compounds at the food planning level. This is important due to the scientifically established relationship between polyphenol intake and health promotion.

KEYWORDS

Food composition, nutritional planning, database, polyphenols, bioactive compounds.

ABBREVIATIONS

BC: bioactive compounds.

NCCD: non-communicable chronic diseases.

HPLC: High-Performance Liquid Chromatography.

CSIC: Spanish Council for Scientific Research.

BTFC: Brazilian Table of Food Composition.

INTRODUCTION

Phenolic compounds, also known as polyphenols, are substances derived from secondary plant metabolism and are commonly divided into four chemical classes: flavonoids, phenolic acids, stilbenes, and lignans. The main food sources of polyphenols are fruits, vegetables, and greens[1]. The literature reports suggest that in addition to its antioxidant activity, these bioactive compounds (BC) also act as anti-inflammatory agents, antiallergics, antibiotics, anticancer agents, and cardioprotectors[2,3,4]. Owing to these beneficial factors, studies show that the regular intake of polyphenol-containing food and drinks is associated with a reduced risk of some chronic, non-communicable diseases (NCCD). These include obesity[5], diabetes[6,7], cardiovascular disease[8,9], and cancer[10,11].

Because of these proven beneficial activities, interest in polyphenols has increased, particularly among health profes-

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sionals, researchers, industrialists, educators, and consumers. Consequently, interest in determining the distribution and quantity of these compounds in foods has also increased. Faced with this demand, various tools have been developed that can be applied to the estimation of polyphenol food content. One such tool is the online database, Phenol-Explorer 3.6 (www.phenol-explorer.eu)[12], which contains 502 polyphenols associated with 452 foods[13]. The database is useful for the estimation of polyphenols because of the large variety of foods in its library, but the lack of an available field for the calculation of BC for portions other than 100 grams, makes the search for specific information regarding consumption and supply of polyphenols somewhat tedious. To fill this gap, the present study aims to develop a tool for the facile estimation of polyphenols in specific portions of food, from the data present in the online database Phenol-Explorer 3.6[12].

METHODS

The software used for the development of the study was Microsoft Excel® (version 2013) and the data was collected from the online platform Phenol-Explorer 3.6 (www.phenol-explorer.eu) (version 2016)[12].

Initially, a file was downloaded in .xlsx format, containing the complete data of the bank (composition-data), available from the above-mentioned website. The worksheet was divided into foods (group, subgroup, and food), experimental method, and phenolic compounds (group, subgroup, and compound).

Each food was selected along with the experimental method used and all foods were organized into groups and then into subgroups. If a given food had more than one value for the compound in the subgroup, they were added together.

Thereafter, the feeds were placed in rows and the corresponding phenolic compound entered into the columns. If a compound was not in the database, it was assigned the value of "zero" to complete its respective row. Subsequently, formulas were applied to each cell in the spreadsheet, whereby the phenolic compound value was multiplied by the unit in the online database (mg/100 g fresh weight for solid foods and oils, and mg/100 mL for beverages and other liquid foods) and divided by 100, thus affording the final value of the phenolic compound for the food.

RESULTS

The material developed consists of two workbooks: "Phenol-Explorer - 2016" and "Estimation of polyphenols," as shown in Figures 1 and 2, respectively.

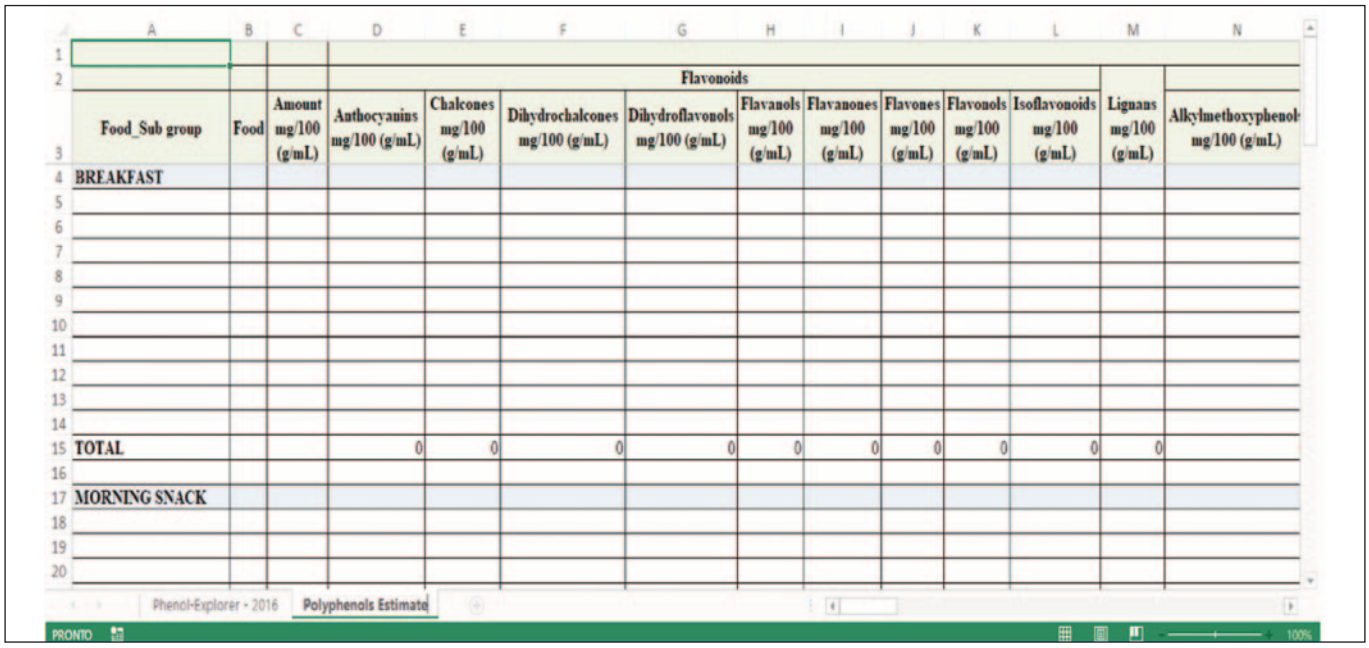
The worksheet, Phenol-Explorer - 2016, contains the restructured data from the online database. Here, the foods were distributed in groups including alcoholic beverages, cereals and cereal products, coffee and cocoa, fruits and fruit products, non-alcoholic beverages, oils, seasonings, seeds, and vegetables.

The polyphenol content of the foods in the database was determined by the following experimental methods: chromatography, which is a commonly used technique for estimating phenolic compounds in foods where polyphenol glycosides, phenolic acid esters, aglycones, and free phenolic acids are simultaneously quantified; chromatography after hydrolysis (acidic or alkaline), for glycosylated or esterified polyphenols; Folin assay, which is used to simultaneously determine all phenolic compounds, thereby providing a crude estimate of total antioxidant concentration; normal-phase high-performance liquid chromatography (HPLC), which enables the estimation of proanthocyanidin oligomers according

Figure 1. "Phenol-Explorer-2016" Workbook on the "PhenolCalc" Worksheet, 2019.

	A	B	C	D	E	F	G	H	I	J	
1											
2				Flavonoids							
3	Food_Sub group	Food	Amount mg/100 (g/mL)	Anthocyanins mg/100 (g/mL)	Chalcones mg/100 (g/mL)	Dihydrochalcones mg/100 (g/mL)	Dihydroflavonols mg/100 (g/mL)	Flavanols mg/100 (g/mL)	Flavanones mg/100 (g/mL)	Flavones mg/100 (g/mL)	Fla mg (g
4	Alcoholic beverages										
5	Beers	Beer [Alcohol free]	100	0	0,0003	0	0	0,10856	0,011	0	
6	Beers	Beer [Ale]	100	0	0,015	0	0	0,38715	0,23467	0	
7	Beers	Beer [Dark]	100	0	0,03017	0	0	0,03	0,15566	0	
8	Beers	Beer [Regular]	100	0	0,00141	0	0	0,59569	0,04824	0,00417	
9	Ciders	Cider	100	0	0	0	0	0,03	0	0	
10	Liquors - Nut liquors	Walnut, liquor	100	0	0	0	0	1,5525	0	0	
11	Spirits - Brandy	Cognac	100	0	0	0	0	0	0	0	
12	Spirits - Rum	Rum	100	0	0	0	0	0	0	0	
13	Spirits - Whisky	Scotch whisky	100	0	0	0	0	0	0	0	
14	Wines - Berry wines	Black crowberry, wine	100	0	0	0	0	0	0	0	
15	Wines - Berry wines	Blackcurrant, wine	100	0	0	0	0	0	0	0	
16	Wines - Berry wines	Fox grape, red wine	100	0	0	0	0	0	0	0	
17	Wines - Berry wines	Fox grape, white wine	100	0	0	0	0	0	0	0	

Figure 2. "Polyphenols Estimate" Workbook on the "PhenolCalc" Worksheet, 2019.



Food_Sub group	Food	Amount mg/100 (g/mL)	Flavonoids: Anthocyanins mg/100 (g/mL)	Chalcones mg/100 (g/mL)	Dihydrochalcones mg/100 (g/mL)	Dihydroflavonols mg/100 (g/mL)	Flavanols mg/100 (g/mL)	Flavanones mg/100 (g/mL)	Flavones mg/100 (g/mL)	Flavonols mg/100 (g/mL)	Isoflavonoids mg/100 (g/mL)	Lignans mg/100 (g/mL)	Alkylmethoxyphenol mg/100 (g/mL)
BREAKFAST													
TOTAL			0	0	0	0	0	0	0	0	0	0	
MORNING SNACK													

to their degree of polymerization that cannot be easily separated by reverse-phase HPLC; pH differential method, which is commonly used method to determine the total content of anthocyanins. Other methods were not included in the database as they were used by a limited number of authors, or because of their unreliability[12,13].

The phenolic compounds present in the spreadsheet represent flavonoids, lignans, phenolic acids, stilbenes, other polyphenols, and total polyphenols. Each of these has a subgroup, which corresponds to the variability of each group.

The "Polyphenols Estimate" tab (Figure 2) is intended for users who wish to quantitatively estimate the compounds present in foods, organized in six meals a day (breakfast, morning snack, lunch, afternoon snack, dinner, and supper) by inserting the data from the "Phenol-Explorer - 2016" spreadsheet. When all the foods that make up each meal are inserted, content values are automatically calculated, allowing one to know how much was offered/consumed at each meal and at the end of the day. Additionally, the weight of each food can be changed, and the calculation is be performed automatically.

By using Microsoft Excel Software® for "PheenolCalc", one has access to all the features within Excel and can be used on any computer which has the installed program.

DISCUSSION

Based on the Phenol-Explorer 3.6 online database, the "PhenolCalc" worksheet is intended to assist academicians, researchers, and health professionals in the estimation of the polyphenol content present in any given amount of food.

"PhenolCalc" is a spreadsheet developed using Microsoft Excel (2013), is easy to use, and is compatible with all computers which have the software installed. After a systematic analysis of 638 publications[13], the online database Phenol-Explorer 3.6[12] was selected because it offered an extensive compilation of composition data for 502 polyphenols present in 452 foods.

Currently, several software applications have been developed to expedite daily, tedious activities of its users. In the field of nutrition science, a number of programs stand out. One example is "NUTRISOL"—a free access program that combines the Food Composition Tables of the Spanish Council for Scientific Research (CSIC), common household measures in the country, and diets and anthropometry data, resulting in three modules: nutritional epidemiology, analysis of diets and recipes, and application of different diets for diseases, all of which can be modified and adapted, rendering data that can be exported to statistical programs[14].

To evaluate the nutritional status of patients, assist in the training of health professionals, carry out epidemiological studies, and for educational purposes, the "UNyDIET" computer program was developed in Spain and is customizable and updatable[15]. Another example is the NutPlan software, offering individual and group nutritional planning functions, recipe calculation, food labeling, diet planning, and nutrient intake assessment. NutPlan was developed to serve the countries of the Balkan Peninsula; as it is updatable, food from other countries can be added, as well as other complete databases[16].

Regarding the use of Excel® spreadsheets for organizing and making food composition data, Black et al. from Ireland,

grouped 938 foods and tabulated macro and micronutrient values, totaling 41 components. Tabulated data originated from national food consumption surveys between 1997 and 2006. This spreadsheet is available online in Excel format, making it easy to access the tool[17].

In Brazil, the free access CalcNut Platform, has two spreadsheets that can be utilized in the estimation of Total Energy Spend, portions and diet fractionation, and the calculation of diets. The platform uses secondary data from the Brazilian Table of Food Composition (BTFC, versions 2006 and 2011) and from the Table of Nutritional Composition of Foods Consumed in Brazil -2008/2009[18]. Another Brazilian database is the Brazilian Mineral Database (BMD), which contains the data for 22 minerals found in 860 different foods, grouped according to the guidelines proposed by the International Network of Food Data Systems. According to the authors, the values found were relevant in comparison to the BTFC data for most of the mineral data[19].

In addition, there are several paid software platforms in use by nutritionists that offer different functionalities, such as DietSmart[20] which allows the user to perform a meal plan, anamnesis, body composition, and nutritional guidelines for their patients. The Nutrisoft Brazil[21], which has a nutritional platform encompassing nutritional profiles, history, nutrient analysis, dietary recall, and anthropometric and laboratory evaluation. Dietbox[22], allows for the calculation of food plans, anamnesis, anthropometry, energy expenditure calculations and laboratory evaluations; it also generates shopping lists and recipes from the alimentary plans, thus providing an application for the patient, facilitating the work of the professional, and helping to maintain it.

Although these programs contribute to nutritional planning, they do not have the functionality to calculate the amounts of phenolic compounds that have been consumed and/or will be offered in the meals of their patients. Therefore, the "PhenolCalc" with this additional information can be a differential in food care and planning, particularly with regard to nutritional care in the NCCD.

One of the advantages of "PhenolCalc" in relation to Phenol-Explorer 3.6, is that in the online platform there is no specific field to estimate the polyphenol content as a function of food portions other than 100 g. The worksheet developed here, facilitates this operation, thus optimizing time use in the elaboration of projects, activities in health education, and in professional practice. In addition, the tool is free and can be used offline. One limitation of the present study is that although the online database Phenol-Explorer 3.6 contains data for a wide variety of foods, it does not include information on some foods commonly consumed and/or native to Brazil and other countries in the Southern Hemisphere. As such, using this method may lead to an underestimation of polyphenol content in Brazilian diets.

CONCLUSION

"PhenolCalc" is a worksheet that contributes to the rapid and simplified estimation of polyphenols in foods and meals, contributing to the popularization of the analysis of these compounds at the level of food planning, whether for individuals or groups. This is of significance due to the scientifically established relationship between the ingestion of polyphenols and the promotion of health.

The FenolCalc spreadsheet is currently made available by the authors, upon request via the email: fenolcalc@gmail.com. In the near future, interested persons will be able to download it from a website by completing an electronic form.

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REFERENCES

1. Pérez-Jiménez, J., Neveu, V., Vos, F., Scalbert, A. Identification of the 100 richest dietary sources of polyphenols - An application of the Phenol-Explorer database. European Journal of Clinical Nutrition. 2010; 64, 112-120.

2. Mlcek, J., Jurikova, T., Skrovankova, S., Sochor, J. Quercetin and Its Anti-Allergic Immune Response. Molecules. 2016; 21, 2-15.

3. Mojzer, EB, Hrnˇciˇc, MK, Škerget, M., Knez, Z., Bren, U. Polyphenols: Extraction Methods, Antioxidative Action, Bioavailability and Anticarcinogenic Effects. Molecules. 2016; 21, 2-38.

4. Li, AN, Li, S., Zhang, YJ, Xu, XR, Chen, YM, Li, HB. Resources and Biological Activities of Natural Polyphenols. Nutrients. 2014; 6, 6020-6047.

5. Corrêa, TAF, Rogero, MM. Polyphenols regulating microRNAs and inflammation biomarkers in obesity. Nutrition. 2019; 59, 150-157.

6. Aryaeian, N., Sedehi, SK, Arablou, A. Polyphenols and their effects on diabetes management: A review. Medical Journal of the Islamic Republic of Iran. 2017; 31, 1-14.

7. Wedick, NM, Pan, A., Cassidy, A., Rimm, EB, Sampson, L., Rosner, B., Willett, W., Hu, FB, Sun, Q., Dam, R.M. Dietary flavonoid intakes and risk of type 2 diabetes in US men and women. The American Journal of Clinical Nutrition. 2012; 95, 925–933.

8. Mendonça, R., Carvalho, N., Martin-Moreno, J., Pimenta, A., Lopes, A., Gea, A., Martinez-Gonzalez, M., Bes-Rastrollo, M. Total polyphenol intake, polyphenol subtypes and incidence of cardiovascular disease: The SUN cohort study. Nutrition, Metabolism and Cardiovascular Diseases. 2019; 29, 69-78.

9. Quiñones, M., Miguel, M., Aleixandre, A. Beneficial effects of polyphenols on cardiovascular disease. Pharmacological Research. 2013; 68, 125–131.

10. Sur, S., Panda, CK. Molecular aspects of cancer chemopreventive and therapeutic efficacies of tea and tea polyphenols, Nutrition. 2017; 43, 8-15.

11. Siddiqui, IA, Sanna, V., Ahmad, N., Sechi, M., Mukhtar, H. Resveratrol nanoformulation for cancer preventionand therapy. The New York Academy of Science. 2015; 1348, 20-31.

12. PHENOL-EXPLORER. Database on polyphenol content in foods [Internet]. 2019 [cited June 04, 2019]. Available from: http://phenol-explorer.eu/

13. Pérez-Jiménez, J., Neveu, V., Vos, F., Scalbert, A. Systematic analysis of the content of 502 polyphenols in 452 foods and beverages: an application of the phenol-explorer database. Journal of agricultural and food chemistry. 2010; 58, 4959-4969.

14. Gutierrez-Bedmar, M., Gómez-Aracena, J., Mariscal, A., García-Rodríguez, A., Gómez-Gracia, E., Carnero-Varo, M., Villalobos, JL, Fernández-Crehuet, J. NUTRISOL: a computer programme for communitary and hospital nutritional evaluation of free access. Nutrición Hospitalaria. 2008; 23, 20-26.

15. García de Diego, L., Cuervo, M., Martínez, JA. Programa informático para la realización de una valoración nutricional fenotípica y genotípica integral. Nutrición Hospitalaria. 2013; 28, 1622-1632.

16. Gurinovic, M., Kadvan, A., Bucchini, L., Matthys, C., Torres, D., Novakovic, R., Smith, R., Glibetic, M. EURRECA nutritional planning and dietary assessment software tool: NutPlan. European Journal of Clinical Nutrition. 2010; 64, 38–42.

17. Black, LJ, Ireland, J., Møller, A., Roe, M., Walton, J., Flynn, A., Finglas, PM., Kiely, M. Development of an on-line Irish food composition database for nutrientes. Journal of Food Composition and Analysis. 2011; 24, 1017–1023.

18. Da Costa, THM (org.). CalcNut: plataforma para cálculo de dieta [Internet]. 2019 [cited April 12, 2019]. Available from: https://fs.unb.br/nutricao/calcnut/

19. Lopes, TVC, Giuntini, EP, Lajolo, FM, Dan, MCT, Menezes, EW (2015). Compilation of mineral data: Feasibility of updating the food composition database. Journal of Food Composition and Analysis. 2015; 39, 87–93.

20. DIETSMART. Software de atendimento nutricional [Internet]. 2019 [cited June 04, 2019]. Available from: https://www.dietsmartsystem.com/DietSmart/#home

21. NUTRISOFT BRAZIL. Software de avaliação nutricional [Internet]. 2019 [cited June 04, 2019]. Available from: https://nutrisoft.com.br/software-de-nutricao/

22. DIETBOX. Software de avaliação nutricional [Internet]. 2019 [cited June 04, 2019]. Available from: https://dietbox.me/pt-BR