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Abstract

Molecular Design of Functional Ingredients Starting from Natural Bioactive Compounds †

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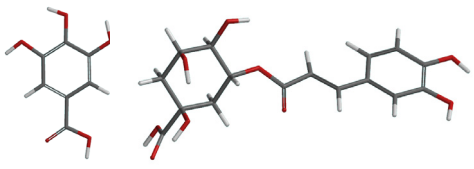
In the last few years, a new concept of functional foods has been developed, leading to the diversification of food production. Thus, not only basic nutrients are provided, but also products for good health and longevity. Phenolic acid derivatives are major bioactive compounds widely found in the vegetal world. Attempts to give them an added-value as functional food ingredients with beneficial health applications are recently discussed in literature data [1,2]. Thus, studies on gallic acid (3,4,5-trihydroxybenzoic acid) found in rice, corn, or wheat [3] indicate its possible effects in reduced obesity and ameliorated related complications [4]. In this research, an extensively computational approach using dedicated software tools for predicting bioactivity and pharmaceutical properties are conducted on phenolic acids derivatives, such as gallic and chlorogenic acids, aiming to highlight their potential use as functional ingredients in yoghurt type dietary products. The geometry of investigated structures was optimized in a multi-step procedure by molecular mechanics force fields, resulting in the lower energy conformers, as shown in Figure 1a,b. Properties are calculated using ωB97X-D level of theory [5]. Bioactivity scores towards protein-coupled receptor (GPCR) ligand, ion channel modulators, kinase inhibitors, nuclear receptor ligands, protease inhibitors, and other enzyme targets are predicted using Molinspiration online platform. Molecular properties and features of studied phytocompounds are obtained: area, volume, polar surface area, ovality, polarizability, dipole moment, water–octanol partition coefficient, energies of frontier molecular orbitals, descriptors related with the flexibility and electrophilic/nucleophilic sites.



(**a**) (**b**)

Figure 1. (**a**) gallic acid 3D optimized structure; (**b**) chlorogenic acid 3D optimized structure.

In conclusion, the evaluation of relevant physical and chemical descriptors for hydrophilic–lipophilic balance concerning the investigated structures, suggests preliminary data to design furthermore functional ingredients with nutraceutical value.

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