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DESIGN, SYNTHESIS AND EVALUATION OF FUNCTIONAL MONOMERS FOR DETECTION OF CHLOROGENIC ACIDS IN COFFEE

Ângelo Monteiro,[a] Anggy Gutièrrez,[b] Federico Berti,[b] Cristina Forzato,[b] Luciano Navarini,[c] Marina Resmini[a]

[a]*School of Biological and Chemical Sciences, Queen Mary University of London, Mile End Road, London E1 4NS, United Kingdom*

[b]*Dipartimento di Scienze Chimiche e Farmaceutiche, Università degli Studi di Trieste, via L. Giorgieri 1, 34127 Trieste*

[c]*illycaffè S.p.A., via Flavia 143, 34100, Trieste*

Coffee is one of the most popular beverages worldwide, and its production actually represents a giant global industry. It is one of the major sources of chlorogenic acid (CGA) in the human diet, known for its beneficial antioxidants characteristics, but it is also an important indicator of coffee quality. Its content, greatly dependent on the roasting process, is responsible for the flavour and aroma of coffee which determine the commercial value of coffee. Therefore, the development of reliable, rapid and simple methods having good sensitivity and selectivity for CGA is a relevant aspect of the quality control in coffee and, considering its beneficial health character, could be of great importance for food safety and industry.

The main objective of this project is to obtain imprinted polymers for CGA. The characteristic of high-selectivity, easy preparation, chemical and thermal stability of MIPs can be exploited in the development of a device capable to detect CGA in a simple, rapid and reliable way. A series of the functional monomers to interact non-covalently with CGA was identified based on the interaction of chlorogenic acid (or related compounds) with amino acids residues present in biologic systems. These interactions were studied using a computational protocol, based on the density functional theory (DFT) method to select the most appropriate monomers. Data obtained from the computational work is presented together with the evaluation of the interactions of the functional monomers with CGA by spectroscopic techniques, such as UV-Vis and NMR spectroscopies.

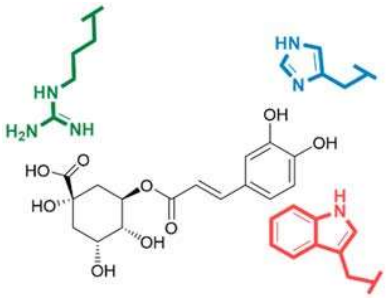

Figure. 1. Interactions made between CGA and potential functional monomers.

References

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