POSTER /

A combined experimental and theoretical study on the structure of genipin in solution

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ABSTRACT : Today the design of new low-impact materials mimicking structures and/or functions of natural systems is a challenge in research. So in the field of food, fabric and hair coloring, large efforts have been made in such a goal. For instance, starting from naturally colored molecules, new technologies have been developed to obtain natural, not toxic and effective final products.

Among the natural sources of colorants, the fruit of *Gardenia jasminoides* provides a series of yellow blue and red colorants already used in food industry [1]. Blue and red pigments can be obtained from one of primary actives of gardenia fruits, the iridoid glycoside geniposide [1, 2]. In particular, the product of the enzymatic hydrolysis of geniposide is the aglycone genipin, well known to easy react with primary amines [3, 4] yielding blue pigments [5, 6]. Despite the applicative and industrial interests of genipin, its experimental characterization is still far to be complete.

In such a scientific context characterized by a lack of information and contrasting mechanistic hypotheses, theoretical modeling can be a powerful tool to support experimental data in unambiguously identifying molecular structures and better understanding of their stability in solution. With this aim at scope, a combined experimental and theoretical work is here presented with regard to the analysis of the tridimensional structure of genipin in solution through ^{1}H-NMR spectroscopy and modeling. Starting from these results, the equilibrium between the different genipin forms in solution has been then investigated at theoretical level, by also taking into account also the possible role of the solvent (ethanol and/or water).

References

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