NMR and molecular fluorescence spectroscopic study of the structure and thermodynamic parameters of EGCG/?-cyclodextrin inclusion complexes with potential antioxidant activity

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The present study is focused on the characterization of the interaction between (-)-epigallocatechingallate (EGCG) and cyclodextrins like ?-cyclodextrin (?CD), heptakis(2,6 di-O-methyl)-?-cyclodextrin (DM?CD), and hydroxypropyl-?-cyclodextrin (HP?CD) in aqueous solution. These inclusion complexes previously demonstrated improvements in the antioxidant activity respect to free EGCG. The structural evidence obtained by 2D-ROESY and selective 1D-ROESY experiments was rationalized by autodock studies and indicates that all the complexes have similar inclusion geometries, but the difference resides on the exposition degree of the antioxidant rings of EGCG, such as pyrogallol and galloyl groups. The thermodynamic study allowed estimating that the inclusion process is entalpically driven for the derivatized cyclodextrins complexes and entropically driven for ?CD complexes due to the predominance of hydrophobic interactions with EGCG.