Supplementary information to "Simple approach to enhance green tea epigallocatechin gallate stability in aqueous solutions and bioavailability: experimental and theoretical characterizations"

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Structural elucidation of gallic acid

Regarding the mainly detected degradation product (Figure 7, retention time = about 4.5 min), its accurate mass in LC-HRMS (Figure S1 (a); accurate mass = 169.0145) corresponded to the molecular formula $C_7H_5O_5^-$ (mass error=4.98 ppm) which could be assigned to gallic acid whose structure is reported in Figure S1 (a). This hypothesis was confirmed by the base peak (Figure S1 (b); accurate mass=125.02478) obtained when submitting m/z = 169 to collision induced dissociation (LC-HRMS^2). Indeed, its accurate mass corresponds to the loss of the carboxylic acid moiety (mass error= 7.21 ppm). As far as the other detected compounds, they have been identified as (+)-catechin, (+)-Epicatechin-3-O-gallate and GCG based upon their respective accurate masses.

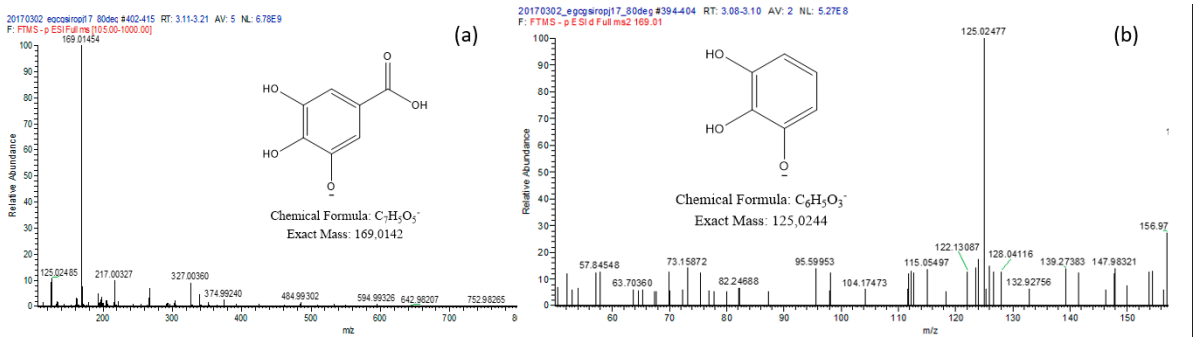


Figure S1. (a) : LC-HRMS spectrum obtained at the retention time of the main degradation product ; (b): LC-HRMS^2 spectrum of the main product ion detected in the LC-HRMS spectrum (m/z=169)