Quantitative studies on the formation of phenol/2-furfurylthiol conjugates in coffee beverages toward the understanding of the molecular mechanisms of coffee aroma staling

Abstract:
To gain a more comprehensive knowledge of the contribution of recently identified phenol/thiol conjugates to the storage-induced degradation of odorous thiols, the concentrations of the sulfury-roasty smelling key odorant 2-furfurylthiol and the concentrations of the putative thiol-receptive di- and trihydroxybenzenes pyrogallol (1), hydroxyhydroquinone (2), catechol (3), 4-ethylcatechol (4), 4-methylcatechol (5), and 3-methylcatechol (6), as well as of the phenol/thiol conjugates 3-[(2-furylmethyl)sulfanyl]catechol (7), 3-[(2-furylmethyl)sulfanyl]-5-ethylcatechol (8), 4-[(2-furylmethyl)sulfanyl]hydroxyhydroquinone (9), and 3,4-bis[(2-furylmethyl)sulfanyl]hydroxyhydroquinone (10) were quantitatively determined in fresh and stored coffee beverages by means of stable isotope dilution analyses (SIDA). Although 2 was found to be the quantitatively predominant trihydroxybenzene in freshly prepared coffee brew, this compound exhibited a very high reactivity and decreased rapidly during coffee storage to generate the conjugates 9 and 10. After only 10 min, about 60(%) of the initial amount of 2-furfurylthiol in a coffee beverage reacted with 2 to give 9 and 10. In contrast, conjugate 7 was found to be exclusively formed during coffee roasting because its initial concentration as well as the amount of its putative precursor, phenol 3, was not affected by
storage. It is interesting to note that the concentration of 8 was increased with increasing incubation time, but its putative precursor 4 was not affected, thus indicating another formation pathway most likely via the chlorogenic acid degradation product 4-vinylcatechol. This study demonstrates for the first time that the loss of 2-furfurylthiol during coffee storage is mainly due to the oxidative coupling of the odorant to hydroxyhydroquinone (2), giving rise to the conjugates 9 and 10.