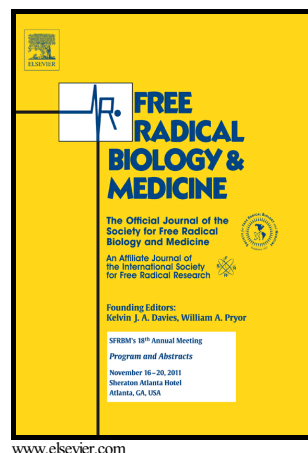


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The chemical reactivity of (-)-epicatechin quinone mainly resides in its B-ring

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Abstract

As one of the important dietary antioxidants, (-)-epicatechin is a potent reactive oxygen species (ROS) scavenger involved in the redox modulation of the cell. When scavenging ROS, (-)-epicatechin will donate two electrons and become (-)-epicatechin quinone, and thus take over part of the oxidative potential of the ROS. The aim of the study is to determine where this chemical reactivity resides in (-)-epicatechin quinone. When this reactivity is spread out over the entire molecule, i.e. over the AC-ring and B-ring, this will lead to partial epimerization of (-)-epicatechin quinone to (-)-catechin quinone. In our experiments, (-)-epicatechin quinone was generated with tyrosinase. The formation of (-)-epicatechin quinone was confirmed by trapping with GSH, and identification of (-)-epicatechin-GSH adducts. Moreover, (-)-epicatechin quinone could be detected using Q-TOF/MS despite its short half-life. To detect the epimerization, the ability of ascorbate to reduce the unstable flavonoid quinones into the corresponding stable flavonoids was used. The results showed that the reduction of the formed (-)-epicatechin quinone by ascorbate did not result in the formation of an appreciable amount of (-)-catechin. Therefore it can be concluded that the chemical reactivity of (-)-epicatechin quinone mainly resides in its B-ring. This could be corroborated by quantum chemical calculations. Understanding the

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