New evidence that caffeine is a healthful antioxidant in coffee

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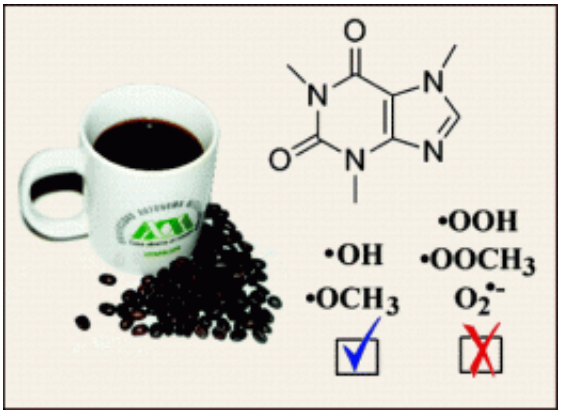

Scientists are reporting an in-depth analysis of how the caffeine in coffee, tea, and other foods seems to protect against conditions such as Alzheimer's disease and heart disease on the most fundamental levels. The report, which describes the chemistry behind caffeine's antioxidant effects, appears in ACS' *Journal of Physical Chemistry B*.

Annia Galano and Jorge Rafael León-Carmona describe evidence suggesting that coffee is one of the richest sources of healthful antioxidants in the average person's diet. Some of the newest research points to caffeine (also present in tea, cocoa, and other foods) as the source of powerful antioxidant effects that may help protect people from Alzheimer's and other diseases. However, scientists know little about

exactly how caffeine works in scavenging the so-called free radicals that have damaging effects in the body. And those few studies sometimes have reached contradictory conclusions.

In an effort to bolster scientific knowledge about caffeine, they present detailed theoretical calculations on caffeine's interactions with free radicals. Their theoretical conclusions show "excellent" consistency with the results that other scientists have report from animal and other experiments, bolstering the likelihood that caffeine is, indeed, a source of healthful antioxidant activity in coffee.

More information: "Is Caffeine a Good Scavenger of Oxygenated Free Radicals?" *Journal of Physical Chemistry B*. DOI: 10.1021/jp201383y

Abstract
The reactions of caffeine (CAF) with different reactive oxygen species (ROS) have been studied using density functional theory. Five mechanisms of reaction have been considered, namely, radical adduct formation (RAF), hydrogen atom transfer (HAT), single electron transfer (SET), sequential electron proton transfer (SEPT), and proton coupled electron transfer (PCET). The SET, SEPT, and PCET mechanisms have been ruled out for the reactions of CAF with •OH, O2•−, ROO•, and RO• radicals. It was found that caffeine is inefficient for directly scavenging O2•− and •OOCH3 radicals and most likely other alkyl peroxyl radicals. The overall reactivity of CAF toward •OH was found to be diffusion-controlled, regardless of the polarity of the environment, supporting the excellent •OH scavenging activity of CAF. On the other hand, it is predicted to be a modest scavenger of •OCH3, and probably of other alkoxyl radicals, and a poor scavenger of HOO•. RAF has been identified as the main mechanism involved in the direct ROS scavenging activity of CAF. The excellent agreement with the available experimental data supports the reliability of the present

calculations.

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