

A neural network analysis of theobromine vs. fluoride on the enamel surface of human teeth.

A neural network analysis of theobromine vs. fluoride on the enamel surface of human teeth: An experimental case study with strong implications for the production of a new line of revolutionary and natural non-fluoride based dentifrices.

Sadeghpour, Arman

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Dental caries are, to this day, the most preventable disease still plaguing humankind. Since the mid 1900's, there has been little to no innovation in commercial fluoride dentifrices, in that, the active agent as a caries preventative is 0.24% sodium fluoride (0.15% fluoride ion), or 0.76% sodium monofluorophosphate. The purpose of the current work is to examine the effects of theobromine versus fluoride on the enamel surface of human teeth by use of an artificial neural network. Theobromine (3,7 dimethylxanthine) is a white crystalline powder and differs by only one methyl group to its sister molecule, caffeine (1,3,7 dimethylxanthine). The dissertation focuses on a brief introduction to theobromine and the previous literature, the experimental materials, method, and design, and finally to the analysis of enamel surface microhardness data by the artificial neural network model. A subsequent *in vivo* acid dissolution also leads us to believe that theobromine might be a particularly effective agent in helping the enamel surface of human teeth resist the effects of bacterial acid demineralization. The implications of the current work are that theobromine, which occurs naturally in chocolates, teas, and cocoa products worldwide, is a natural, nontoxic, more efficacious, and viable alternative to fluoride additives in commercial dentifrices.

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Chocolate Constituent Bests Fluoride

By Janet Raloff

"Chocolate Toothpaste? Extract of Tasty Treat Could Fight Tooth Decay."

That's how Tulane University's news office provocatively titled a press release it issued last week. Sound sweet? Unfortunately, it's anything but. The extract, theobromine, is a bitter constituent of a number of plants, including the beans used to make chocolate. A chemical cousin to caffeine, this compound is also a stimulant—and doesn't taste the least bit chocolaty.

That said, theobromine does show promise in fighting cavities. In preliminary tests, Tulane scientists have shown that this chemical—which chocolate-lovers regularly consume—strengthens teeth better than fluoride.

Theobromine's affect on the crystalline structure of teeth offers an additional benefit. For protecting our choppers from erosion by acids, it outperforms an equal concentration of the sodium fluoride found in most toothpastes. That suggests the new extract could limit the ravages of the acid-producing bacteria responsible for most tooth decay.

Since tooth decay is "the most preventable disease still plaguing humankind," the findings are potentially quite important, maintains engineer Arman Sadeghpour, who led the research. Moreover, he notes, the last half-century has witnessed "little to no innovation" in cavity-fighting additives for toothpastes.

So why not just eat chocolate? Because its sugars feed the bacteria that foster tooth decay. The fats in chocolate, which impart the food's delicious creaminess, also risk swelling the waistlines of a population that already collectively weighs far more than is healthy.

Caffeine's kin

For his doctoral research, Sadeghpour evaluated the tooth-protecting prowess of theobromine, also known as 3,7-dimethylxanthine. Caffeine is 1,3,7-trimethylxanthine; that means it's basically the same compound, except that it has one additional methyl group—a carbon atom bound to three hydrogens—dangling from its double-ring-shaped structure.

But the subtle structural distinctions between these two xanthines account for their profound physiological differences, Sadeghpour notes. Whereas caffeine may harm bones and teeth, theobromine appears to bolster both structural materials.

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Teeth and bones are continually dissolving, on a microscopic scale, and then reforming, or remineralizing. Six years ago, researchers in the lab where Sadeghpour works obtained a patent to use theobromine to foster the remineralization of our pearly whites.

In his new work, Sadeghpour evaluated how theobromine treatment affects the integrity of teeth. In one set of experiments, he took leftover human molars from 13 individuals and cut each into pieces. Then he treated some pieces with fluoride at varying doses and exposed other pieces to varying doses of theobromine.

He then put all molar slices into a machine fitted with a diamond bit. For 5 seconds, the bit pressed into each piece of tooth, creating an indentation. The depth of that depression offers a gauge of the tooth enamel's hardness. In these tests, theobromine outperformed fluoride.

In another set of tests, Sadeghpour covered all but a tiny portion of each piece of tooth and subjected the exposed area overnight to solutions containing either fluoride or theobromine. The next day, he exposed the treated tooth surface for 10 minutes to strong acid. When he later analyzed the acid to measure how much calcium had leached into it, he found that theobromine-treated teeth had lost 8 percent less calcium than fluoride-treated teeth.

Of course, these are fairly unnatural tests. Sadeghpour's group now wants to evaluate whether theobromine treatment helps teeth survive a real-world acid test—exposure to the cavity-producing bacteria found in our mouths. His group is also looking to team up with a manufacturer to evaluate whether a toothpaste fortified with theobromine can yield cavity-fighting benefits.

In the mean time, Sadeghpour has whipped up a prototype toothpaste in the lab. He stores it in bottles, not squeezable tubes. And to mask theobromine's bitterness, he's flavored the concoction with—you guessed it—mint.

Chocolate Toothpaste Better than Fluoride, Researcher Says Michael Strecker Phone: (504) 865-5210 mstreck@tulane.edu

For a healthy smile brush between meals, floss regularly and eat plenty of chocolate? According to Tulane University doctoral candidate Arman Sadeghpour an extract of cocoa powder that occurs naturally in chocolates, teas, and other products might be an effective natural alternative to fluoride in toothpaste. In fact, his research revealed that the cocoa extract was even more effective than fluoride in fighting cavities.

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The extract, a white crystalline powder whose chemical makeup is similar to caffeine, helps harden teeth enamel, making users less susceptible to tooth decay. The cocoa extract could offer the first major innovation to commercial toothpaste since manufacturers began adding fluoride to toothpaste in 1914.

The extract has been proven effective in the animal model, but it will probably be another two to four years before the product is approved for human use and available for sale, Sadeghpour says. But he has already created a prototype of peppermint flavored toothpaste with the cavity-fighting cocoa extract added, and his doctoral thesis research compared the extract side by side to fluoride on the enamel surface of human teeth.

Sadeghpour's research group included scientists from Tulane, the University of New Orleans, and Louisiana State University's School of Dentistry.

Sadeghpour will earn his PhD from Tulane University on May 19.