Quantum chemistry-based verification of antioxidative action of iodide in mitochondria

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Abstract

Background: In view of the well-known health-care qualities of aqueous potassium iodide (KI), quantum chemistry-based molecular modeling, i.e., density functional theory-based molecular modeling (DFT/MM) is undertaken to understand how iodide ion (I-) show antioxidative ptoperties on aqueous phosphorylation process in mitochondria (mt) of alive cells.

Materials and methods: We perform DFT/MM equivalent to the quantum mechanics/molecular mechanics (QM/MM) method, by using the B3LYP exchange-correlation function and the 6–31G(d) basis set with Spartan’18 (Wavefunction, Inc. Irvine, CA).

Results: Iodide ion (I-) is in equilibrium with hydrogen iodide (HI), being oxidized to hypoiodous acid (HOI) by ground state oxygen (3O2) or by hydrogen peroxide (HOOH) in aqueous systems. DFT/MM also verifies that van der Waals force (vdW) induces van der Waal (vdW) aggregation of hypoiodous acid (HOI) with phenylalanine, resulting in giving tyrosine, and that vdW works strongly on aggregation of tyrosine with HOI, leading to formation of 2,6-diiodotyrosine via 2-iodotyrosine. 2,6-Diiodotyrosine as homolog of thyroid hormones T4 is validated to show antioxidative action to evil active oxygen in mt, i.e., HOOH and hydroxyl radical.

ヨウ素が腫瘍を抑制するという論文の紹介

Differential action of iodine on mitochondria from human tumoral- and extra-tumoral tissue in inducing the release of apoptogenic proteins.

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Abstract

Iodide is actively concentrated in the thyroid gland for thyroid hormone biosynthesis. Excess iodine has been observed to induce apoptosis in thyrocytes and mammary cells. The mechanism of iodine induced apoptosis is poorly understood. Among various cell organelles, mitochondria is known to provide conducive environment for the organification of iodine, i.e. iodination of different proteins. Mitochondria also play a central role in execution of apoptosis. To study the role of mitochondria in iodine induced apoptosis, we investigated the direct interaction of iodine and human breast mitochondria vis-a-vis its role in the initiation of apoptosis in vitro. We observed that mitochondria isolated from the tumor (TT) and extra-tumoral tissue (ET) of human breast display significant uptake of iodine. Mitochondrial proteins were observed to be predominantly iodinated in ET but not in TT mitochondria. Treatment with iodine showed an increase in mitochondrial permeability transition of TT and decrease in ET. Iodine induced released factor(s) other than cytochrome c from tumor mitochondria initiate(s) apoptosis in vitro, while those from ET mitochondria were non-apoptogenic in nature. To our knowledge, this is first report demonstrating that iodine acts differentially on mitochondria of tumor and extratumoral origin to release apoptogenic proteins from TT and has a protective effect on ET.

**文献；Iodine and Cancer**

ヨウ素投与の様々ながんに関する影響の論文です。
URLを下記に表記しますので、関心のある方は、
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Iodine and Cancer
A summary of the evidence to date
By Tina Kaczor, ND, FABNO

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