

# Deamination features of 5-hydroxymethylcytosine, a radical and enzymatic DNA oxidation product

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The 5-methylcytosine derivative 5-hydroxymethylcytosine (5hmCyt), which is generated via enzymatic oxidation, is sometimes referred to as the sixth nucleobase due to its widespread presence in the DNA of brain and embryonic stem cells. In this study, we used density functional based methods and reactivity indices from conceptual DFT to explore the mechanism and key features of the hydrolytic deamination of 5hmCyt. The data obtained are used to compare and contrast this deamination reaction with those of other cytosine derivatives. The deamination process for 5hmCyt is similar to the corresponding processes for other unsaturated derivatives in that the amino form is the reactive one and water addition is the rate-limiting step. However, several differences due to the rotameric asymmetry of the current system are also noted. © Springer-Verlag 2014.

5-Hydroxymethylcytosine

Deamination

Enzymatic dna oxidation

Mutation

Radical oxidation

5 hydroxymethylcytosine

cytosine derivative

DNA

nucleic acid base

5-hydroxymethylcytosine

cytosine

DNA

water

article

deamination

density functional theory

hydrolysis

oxidation

priority journal

reaction analysis

analogs and derivatives

chemical model

chemical structure

chemistry

computer simulation

deamination

energy transfer

metabolism

oxidation reduction reaction

quantum theory

structure activity relation

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Deamination

DNA

Energy Transfer

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Models, Chemical

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Molecular Structure

Oxidation-Reduction

Quantum Theory

Structure-Activity Relationship

Water