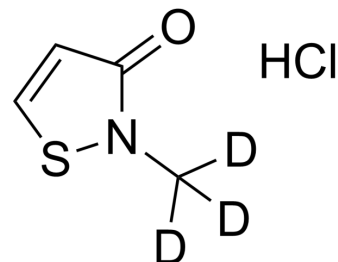


## Methylisothiazolinone-d<sub>3</sub> hydrochloride

<b>Cat. No.:</b>	HY-W010243S
<b>CAS No.:</b>	1329509-49-0
<b>Molecular Formula:</b>	C <sub>4</sub> H <sub>3</sub> D <sub>3</sub> ClNOS
<b>Molecular Weight:</b>	154.63
<b>Target:</b>	Bacterial; Isotope-Labeled Compounds
<b>Pathway:</b>	Anti-infection; Others
<b>Storage:</b>	Please store the product under the recommended conditions in the Certificate of Analysis.



### BIOLOGICAL ACTIVITY

<b>Description</b>	<p>Methylisothiazolinone-d<sub>3</sub> (hydrochloride) is the deuterium labeled Methylisothiazolinone (hydrochloride). Methylisothiazolinone hydrochloride is the constituent of the biocide Kathon CG. Methylisothiazolinone hydrochloride is an isothiazolone derivative widely used as a preservative. Methylisothiazolinone hydrochloride is also a moderate sensitizer and reacts with GSH.</p>
<b>In Vitro</b>	<p>Stable heavy isotopes of hydrogen, carbon, and other elements have been incorporated into drug molecules, largely as tracers for quantitation during the drug development process. Deuteration has gained attention because of its potential to affect the pharmacokinetic and metabolic profiles of drugs<sup>[1]</sup>. MCE has not independently confirmed the accuracy of these methods. They are for reference only.</p>

### REFERENCES

- [1]. Aynur O Aptula, et al. From Experiment to Theory: Molecular Orbital Parameters to Interpret the Skin Sensitization Potential of 5-chloro-2-methylisothiazol-3-one and 2-methylisothiazol-3-one. *Chem Res Toxicol.* 2005 Feb;18(2):324-9.
- [2]. Rubén Alvarez-Sánchez, et al. Covalent Binding of the <sup>13</sup>C-labeled Skin Sensitizers 5-chloro-2-methylisothiazol-3-one (MCI) and 2-methylisothiazol-3-one (MI) to a Model Peptide and Glutathione. *Bioorg Med Chem Lett.* 2004 Jan 19;14(2):365-8.
- [3]. Russak EM, et al. Impact of Deuterium Substitution on the Pharmacokinetics of Pharmaceuticals. *Ann Pharmacother.* 2019 Feb;53(2):211-216.

**Caution: Product has not been fully validated for medical applications. For research use only.**

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