

Certificate of Analysis

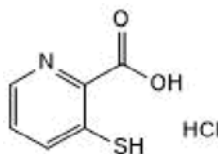
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Product Name: 3-Mercaptopyridinic acid hydrochloride
CAS Number: 320386-54-7
IUPAC Name: 3-Mercapto-2-pyridinecarboxylic acid hydrochloride

Catalog No.: 7577 **Batch No.:** 1

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₆H₅NO₂S.HCl.¾H₂O
Batch Molecular Weight: 205.14
Physical Appearance: Beige solid
Solubility: DMSO to 20 mM
 water to 10 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen	Chlorine
Theoretical	35.13	3.69	6.83	17.28
Found	34.67	3.82	6.5	16.82

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

Product Name: 3-Mercaptopicolinic acid hydrochloride

Catalog No.: 7577

1

CAS Number: 320386-54-7

IUPAC Name: 3-Mercapto-2-pyridinecarboxylic acid hydrochloride

Description:

3-Mercaptopicolinic acid hydrochloride is a phosphoenolpyruvate carboxykinase (PEPCK) inhibitor ($IC_{50} = 7.5 \mu\text{M}$ at hPEPCK). Inhibits glucose synthesis. In vitro, 3-Mercaptopicolinic acid reduces proliferation of T_{reg} cells, induces myogenic differentiation of C2C12 cells, and reduces colony growth formation of MCF7 cells. Also sensitizes melanoma cells to Vemurafenib (Cat. No. 7309) via inhibition of cytoplasmic PEPCK.

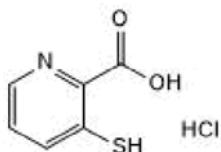
Physical and Chemical Properties:

Batch Molecular Formula: $C_6H_5NO_2S.HCl.\frac{3}{4}H_2O$

Batch Molecular Weight: 205.14

Physical Appearance: Beige solid

Batch Molecular Structure:



References:

Ren et al (2022) Overcoming chemoresistance to b-raf inhibitor in melanoma via targeted inhibition of phosphoenolpyruvate carboxykinase1 using 3-mercaptopropionic acid. *Bioengineered* **13** 13571.

Watson et al (2021) Metabolic support of tumour-infiltrating regulatory T cells by lactic acid. *Nature* **591** 645. PMID: 33589820.

Aragó et al (2020) Pharmacology and preclinical validation of a novel anticancer compound targeting PEPCK-M. *Biomed.Pharmacother.* **121** 109601. PMID: 31739159.

Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 20 mM

water to 10 mM

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a $45-60^{\circ}\text{C}$ water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

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