

Product Name: TH 5427 hydrochloride

Catalog No.: 6534

Batch No.: 1

IUPAC Name: 7-[[[5-(3,4-Dichlorophenyl)-1,3,4-oxadiazol-2-yl]methyl]-1,3-dimethyl-8-(piperazine-1-yl)-1*H*-purine-2,6-dione hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₀H₂₀Cl₂N₈O₃.HCl.1¼H₂O

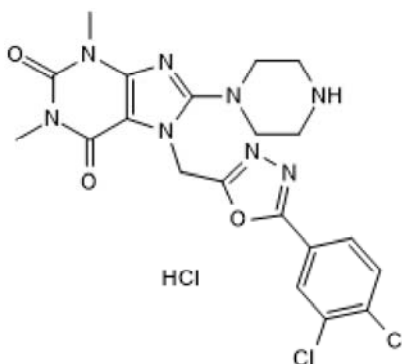
Batch Molecular Weight: 550.31

Physical Appearance: White solid

Solubility: water to 100 mM
DMSO to 100 mM

Storage: Desiccate at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.7% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	43.65	4.3	20.36
Found	43.32	4.39	20.68

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Description:

Potent nudix hydrolase 5 (NUDT5) inhibitor (IC_{50} = 29 nM). Displays >650-fold selectivity for NUDT5 over MTH1. Inhibits ATP synthesis, chromatin remodeling, gene expression and proliferation in progestin-treated breast cancer cells in vitro.

Physical and Chemical Properties:

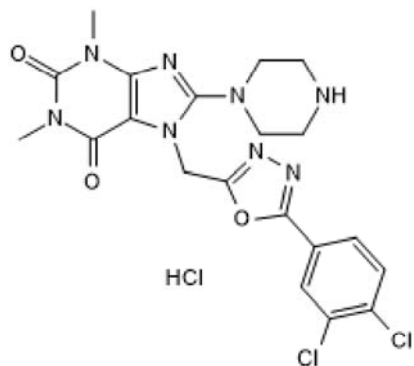
Batch Molecular Formula: $C_{20}H_{20}Cl_2N_8O_3 \cdot HCl \cdot 1\frac{1}{4}H_2O$

Batch Molecular Weight: 550.31

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Desiccate at RT

Solubility & Usage Info:

water to 100 mM

DMSO to 100 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°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.

Licensing Information:

Sold under license from Thomas Helleday's Foundation for Medical Research and Oxcia AB.

References:

Page *et al* (2018) Targeted NUDT5 inhibitors block hormone signaling in breast cancer cells. *Nat. Commun.* **9** 250. PMID: 29343827.

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bio-techne.com

info@bio-techne.com

techsupport@bio-techne.com

North America

Tel: (800) 343 7475

China

info.cn@bio-techne.com

Tel: +86 (21) 52380373

Europe Middle East Africa

Tel: +44 (0)1235 529449

Rest of World

www.tocris.com/distributors

Tel: +1 612 379 2956