

Certificate of Analysis

www.tocris.com

Product Name: TH 1217

Catalog No.: 6522

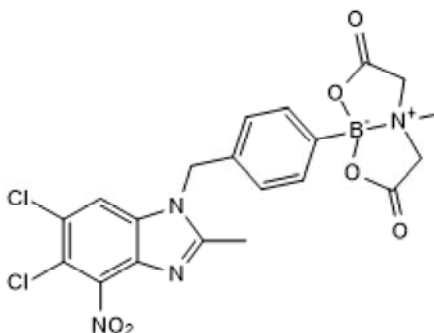
Batch No.: 1

CAS Number: 1862212-48-3

IUPAC Name: 2-[4-[[5,6-Dichloro-2-methyl-4-nitro-1*H*-benzo[d]-imidazol-1-yl)methyl]phenyl]-6-methyl-1,3,6,2-dioxazaborocane-4,8-dione

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₀H₁₇BCl₂N₄O₆
Batch Molecular Weight: 491.09
Physical Appearance: Off White solid
Solubility: DMSO to 100 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.2 (Ethyl acetate)
HPLC: Shows 97.3% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	48.91	3.49	11.41
Found	49.01	3.51	11.26

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

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

Product Information

www.tocris.com

Product Name: TH 1217

Catalog No.: 6522

Batch No.: 1

CAS Number: 1862212-48-3

IUPAC Name: 2-[4-[[5,6-Dichloro-2-methyl-4-nitro-1*H*-benzo[d]-imidazol-1-yl]methyl]phenyl]-6-methyl-1,3,6,2-dioxazaborocane-4,8-dione

Description:

TH 1217 is a potent dCTPase pyrophosphatase 1 inhibitor (IC_{50} = 47 nM). TH 1217 is not stable in aqueous solution. It is recommended that fresh samples are prepared and used immediately.

Physical and Chemical Properties:

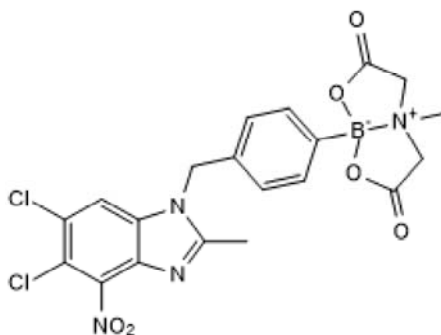
Batch Molecular Formula: $C_{20}H_{17}BCl_2N_4O_6$

Batch Molecular Weight: 491.09

Physical Appearance: Off White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM

Not stable in aqueous solution. Prepare fresh samples and use immediately.

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:

Llona-Minguez *et al* (2016) Discovery of the first potent and selective inhibitors of human dCTP pyrophosphatase 1. *J.Med.Chem.* **59** 1140. PMID: 26771665.

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

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