

Certificate of Analysis

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Product Name: KD 5170

Catalog No.: 4001

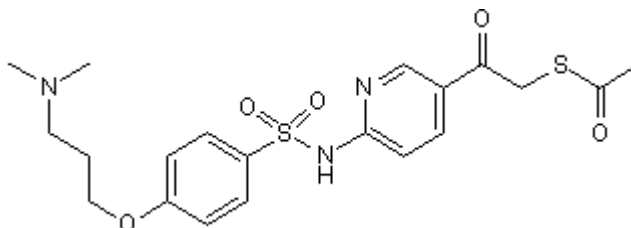
Batch No.: 1

CAS Number: 940943-37-3

IUPAC Name: S-[2-[6-[[[4-[3-(Dimethylamino)propoxy]phenyl]sulfonyl]amino]-3-pyridinyl]-2-oxoethyl]ethanethioc acid ester

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{20}H_{25}N_3O_5S_2$
Batch Molecular Weight: 451.56
Physical Appearance: White solid
Solubility: 1eq. HCl to 100 mM
DMSO to 100 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: $R_f = 0.52$ (Dichloromethane:Methanol [4:1])
HPLC: Shows 95.7% purity
 1H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

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

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Description:

Class I and II histone deacetylase (HDAC) inhibitor (IC_{50} = 0.045 μ M; EC_{50} = 0.025 μ M in HeLa screening and HeLa cell-based assays, respectively). Exhibits broad spectrum inhibition of HDAC classes I and II in assays using purified recombinant human isoforms. Displays less potent inhibition of HDAC2 (IC_{50} values are 0.014, 0.020, 0.026, 0.075 and 2.0 μ M for HDAC6, HDAC1, HDAC4, HDAC3 and HDAC2 respectively). Displays cytotoxicity against numerous cell lines derived from human tumors. Orally available.

Physical and Chemical Properties:

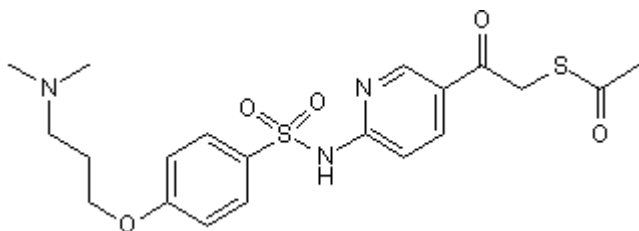
Batch Molecular Formula: $C_{20}H_{25}N_3O_5S_2$

Batch Molecular Weight: 451.56

Physical Appearance: White solid

Minimum Purity: >95%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

1eq. HCl 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.

References:

Feng *et al* (2008) KD5170, a novel mercaptoketone-based histone deacetylase inhibitor, exerts antimyeloma effects by DNA damage and mitochondrial signaling. *Mol.Cancer Ther.* **7** 1494. PMID: 18566220.

Hassig *et al* (2008) KD5170, a novel mercaptoketone-based histone deacetylase inhibitor that exhibits broad-spectrum antitumor activity *in vitro* and *in vivo*. *Mol.Cancer Ther.* **7** 1054. PMID: 18483295.

Payne *et al* (2008) Identification of KD5170: a novel mercaptoketone-based histone deacetylase inhibitor. *Bioorg.Med.Chem.Lett.* **18** 6093. PMID: 18954983.

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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