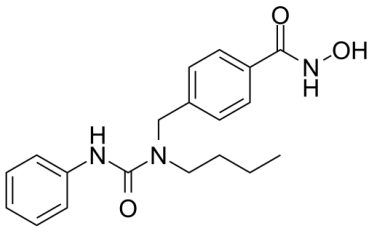
Data Sheet

Product Name:	Nexturastat A
Cat. No.:	CS-3268
CAS No.:	1403783-31-2
Molecular Formula:	$C_{19}H_{23}N_3O_3$
Molecular Weight:	341.40
Target:	HDAC
Pathway:	Cell Cycle/DNA Damage; Epigenetics
Solubility:	DMSO : ≥ 56 mg/mL (164.03 mM)



BIOLOGICAL ACTIVITY:

Nexturastat A is a potent **HDAC6** inhibitor with an **IC_{50}** of 5 nM[1]. Nexturastat A also inhibits **HDAC10** and **metallo-β-lactamase domain-containing protein 2 (MBLAC2)**[2][3]. **In Vitro:** Nexturastat A displays low micromolar activity compared to the low nanomolar activity against HDAC6. Moreover, it also demonstrates high levels of selective inhibition against members of the related Class 2 HDAC isozymes reaching >1000-fold selective in some cases. Compared to the pan-selective HDACI LBH589, Nexturastat A is approximately 100-fold less potent in inducing murine B16 melanoma cell death[1].

PROTOCOL (Extracted from published papers and Only for reference)

Cell assay [1] B16 murine melanoma cells were plated at 5×103/well in 96 well flat bottom plates. The following day, media was changed to that containing various concentrations of HDACi or matched DMSO vehicle concentrations diluted in complete medium done in triplicate. Cells were incubated for 48 hours at 37°C and 5% CO2. Density of viable, metabolically active cells was quantified using a standard MTS assay (CellTiter 96?AQueous One, Promega, Madison, WI) as per manufacturer's instructions. Briefly, 20μL of reagent were added per well and incubated at 37°C for 3 hours. Absorbances at 490nM were measured spectrophotometrically with background subtraction at 690 nM. All values were then normalized and expressed as a percentage of medium control (100%).

References:

[1]. Bergman JA, et al. Selective histone deacetylase 6 inhibitors bearing substituted urea linkers inhibit melanoma cell growth. J Med Chem. 2012 Nov 26;55(22):9891-9.

[2]. Magalie Géraldy,, et al. Selective Inhibition of Histone Deacetylase 10: Hydrogen Bonding to the Gatekeeper Residue is Implicated. J Med Chem. 2019 May 9;62(9):4426-4443.

[3]. everin Lechner, et al. Target deconvolution of HDAC pharmacopoeia reveals MBLAC2 as common off-target. Nat Chem Biol. 2022 Apr 28.

CAIndexNames:

Benzamide, 4-[[butyl[(phenylamino)carbonyl]amino]methyl]-N-hydroxy-

SMILES:

O=C(NO)C1=CC=C(CN(CCCC)C(NC2=CC=CC=C2)=O)C=C1

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

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