

Product Name: A 485

Catalog No.: 6387

Batch No.: 1

CAS Number: 1889279-16-6

IUPAC Name: (1*R*)-*N*-[(4-Fluorophenyl)methyl]-2,3-dihydro-5-[[[(methylamino)carbonyl]amino]-2',4'-dioxo-*N*-[(1*S*)-2,2,2-trifluoro-1-methylethyl]spiro[1*H*-indene-1,5'-oxazolidine]-3'-acetamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₅H₂₄F₄N₄O₅ · ½H₂O

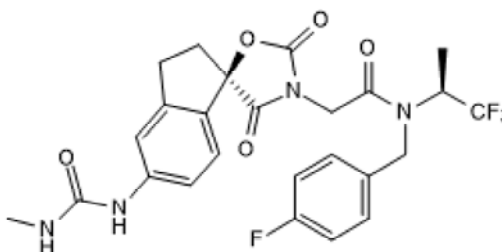
Batch Molecular Weight: 545.49

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.57 (Dichloromethane:Methanol [9:1])

HPLC: Shows 99.9% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: [α]_D = +43.6 (Concentration = 0.74, Solvent = Methanol)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	55.05	4.62	10.27
Found	55	4.66	10.22

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

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Description:

Potent and selective p300/CREB-binding protein (CBP) HAT domain inhibitor (IC₅₀ values are 2.6 and 9.8 nM for the CBP-bromodomain HAT-C/H3 (BHC) and p300-BHC domains, respectively). Displays > 1000-fold selectivity over closely related HATs. Suppresses proliferation in several hematological malignancies and AR⁺ prostate cancer cell lines in vitro. Inhibits tumor growth in a castration-resistant prostate cancer xenograft model. Orally bioavailable. To request the negative control for A 485, please fill out the A 486 request form on the SGC website. Please see product datasheet on www.tocris.com for full description.

Physical and Chemical Properties:

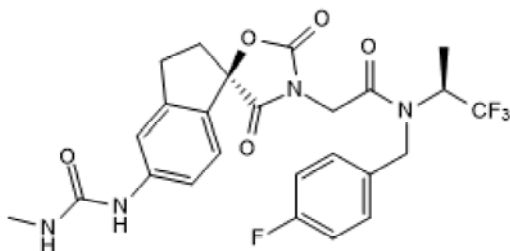
Batch Molecular Formula: C₂₅H₂₄F₄N₄O₅·½H₂O

Batch Molecular Weight: 545.49

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



References:

Kodadek et al (2018) Another one (of the "undruggable" targets) bites the dust: discovery of a potent and selective inhibitor of the histone acetyl transferase p300/CBP. *Biochemistry* **57** 899. PMID: 29244478.

Weinert et al (2018) Time-Resolved Analysis Reveals Rapid Dynamics and Broad Scope of the CBP/p300 Acetylome. *Cell.* PMID: 29804834 .

Lasko et al (2017) Discovery of a selective catalytic p300/CBP inhibitor that targets lineage-specific tumours. *Nature* **550** 128. PMID: 28953875.

Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol 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:

This probe is supplied in conjunction with the Structural Genomics Consortium. For further characterization details, please visit the A-485 probe summary on the SGC website.

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