

Product Name: A 485

Catalog No.: 6387

Batch No.: 2

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 · ¼H₂O

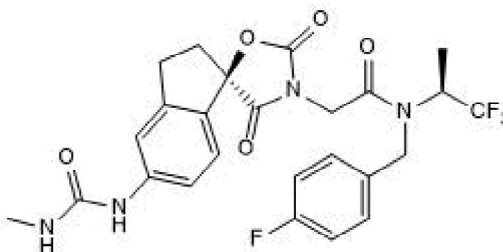
Batch Molecular Weight: 540.98

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 100% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: [α]_D = +53.4 (Concentration = 0.74, Solvent = Methanol)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	55.51	4.56	10.36
Found	55.4	4.65	10.33

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Description:

A 485 is a 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), which displays > 1000-fold selectivity over closely related HATs. A 485 suppresses proliferation in several hematological malignancies and AR⁺ prostate cancer cell lines in vitro, and also inhibits tumor growth in a castration-resistant prostate cancer xenograft model. A 485 is 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 specific page on www.tocris.com for full description.

Physical and Chemical Properties:

Batch Molecular Formula: C₂₅H₂₄F₄N₄O₅·1/4H₂O

Batch Molecular Weight: 540.98

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



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. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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.

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.

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