

Product Name: I-CBP 112

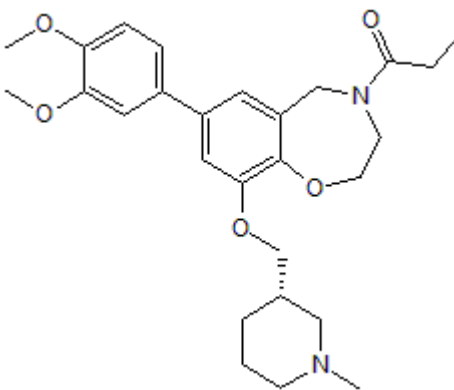
Catalog No.: 4891

Batch No.: 1

IUPAC Name: 1-[7-(3,4-Dimethoxyphenyl)-9-[[[(3S)-1-methylpiperidin-3-yl]methoxy]-2,3,4,5-tetrahydro-1,4-benzoxazepin-4-yl]propan-1-one

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₇H₃₆N₂O₅·H₂O
Batch Molecular Weight: 486.61
Physical Appearance: White Brittle Foam
Solubility: DMSO to 100 mM
 1eq. HCl to 100 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.15 (Dichloromethane:Methanol [9:1])
HPLC: Shows 98.7% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Optical Rotation: [α]_D = -9.2 (Concentration = 1, Solvent = CHCl₃)
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	66.65	7.87	5.76
Found	66.77	7.53	5.53

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

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Description:

CBP/p300 bromodomain inhibitor (IC₅₀ values are 0.142-0.17 and 0.625 μM for CBP and p300 respectively). Selective for CBP and p300 over ATAD2, BAZ2B, BRD2(2), BRD4(1), PB1 (5), PCAF, PHIP(2) and TIF1α bromodomains in a BLI assay. Accelerates FRAP recovery in cells at a concentration of 1 μM.

Physical and Chemical Properties:

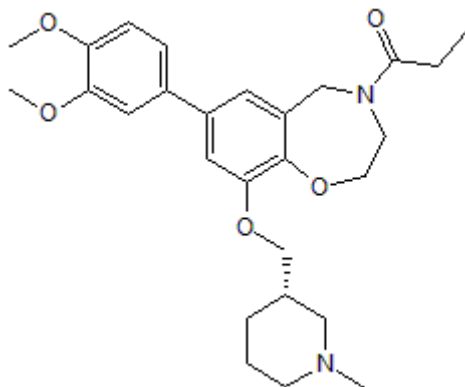
Batch Molecular Formula: C₂₇H₃₆N₂O₅.H₂O

Batch Molecular Weight: 486.61

Physical Appearance: White Brittle Foam

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM

1eq. HCl 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:

Gallenkamp et al (2014) Bromodomains and their pharmacological inhibitors. *ChemMedChem* **9** 438. PMID: 24497428.

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