

**Product Name:** I-CBP 112

**Catalog No.:** 4891

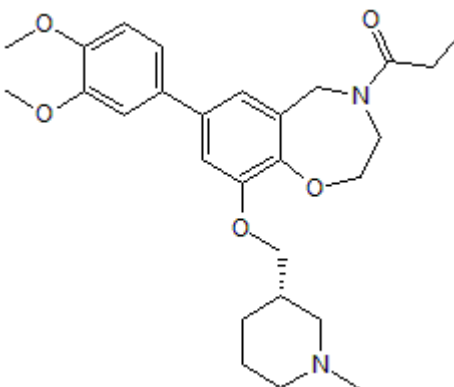
**Batch No.:** 1

CAS Number: 1640282-31-0

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:** C<sub>27</sub>H<sub>36</sub>N<sub>2</sub>O<sub>5</sub>·H<sub>2</sub>O  
**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<sub>f</sub> = 0.15 (Dichloromethane:Methanol [9:1])  
**HPLC:** Shows 98.7% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure  
**Optical Rotation:** [α]<sub>D</sub> = -9.2 (Concentration = 1, Solvent = CHCl<sub>3</sub>)  
**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	66.65	7.87	5.76
Found	66.77	7.53	5.53

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**Description:**

CBP/p300 bromodomain inhibitor (IC<sub>50</sub> 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:**

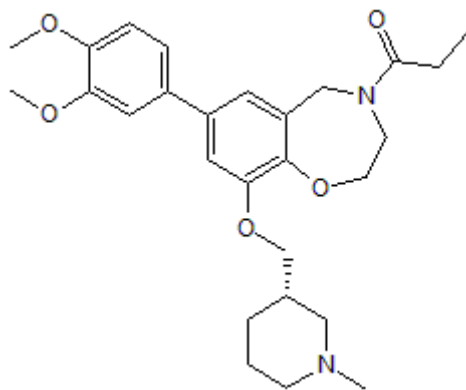
Batch Molecular Formula: C<sub>27</sub>H<sub>36</sub>N<sub>2</sub>O<sub>5</sub>.H<sub>2</sub>O

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.

**Licensing Information:**

This probe is supplied in conjunction with the Structural Genomics Consortium. For further characterization details, please visit the I-CBP 112 probe summary on the SGC website.

**References:**

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

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