Product Name: **SGC-CBP30** **Catalog No.: 4889** **Batch No.: 2**

IUPAC Name: 2-[2-(3-Chloro-4-methoxyphenyl)ethyl]-5-(dimethyl-1,2-oxazol-4-yl)-1-[(2*S*)-2-(morpholin-4-yl)propyl]-1*H*-1,3-benzodiazole

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{28}H_{33}ClN_4O_3.¾H_2O$

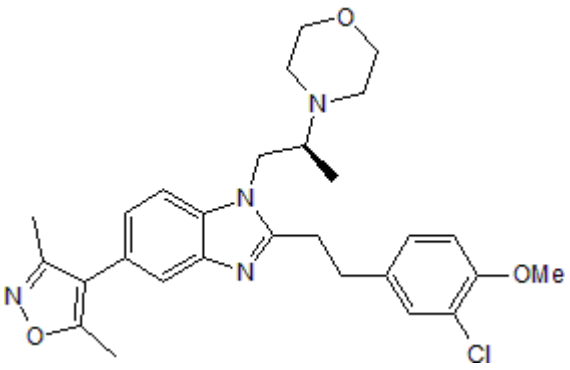
Batch Molecular Weight: 522.55

Physical Appearance: Off-white solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.58 (Ethyl acetate:Methanol [9:1])

HPLC: Shows 98.2% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: $[\alpha]_D$ = +17.4 (Concentration = 1, Solvent = Ethanol)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	64.36	6.65	10.72
Found	64.28	6.4	10.67

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Description:

Potent CBP/p300 bromodomain (BRD) inhibitor (K_d values are 21 and 32 nM for CBP and p300 BRDs respectively). Exhibits 40-fold and 250-fold selectivity for CBP over the first BRD of BRD4 (BRD4(1)) and BRD4(2) respectively. Accelerates FRAP recovery in cells at a concentration of 1 µM.

Physical and Chemical Properties:

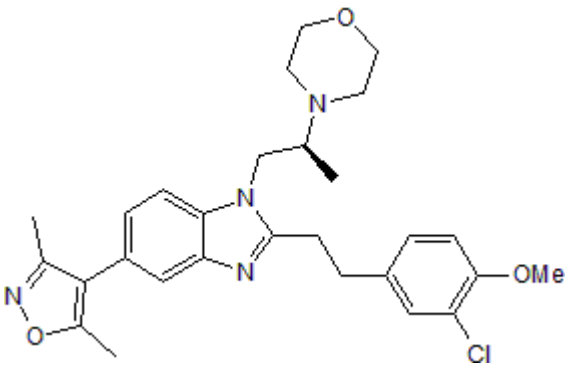
Batch Molecular Formula: $C_{28}H_{33}ClN_4O_3.¾H_2O$

Batch Molecular Weight: 522.55

Physical Appearance: Off-white solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°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.

References:

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

Hay *et al* (2014) Discovery and optimization of small-molecule ligands for the CBP/p300 bromodomains. J.Am.Chem.Soc. ***136*** 9308. PMID: 24946055.