bio-techne
TOCRIS

Print Date: Nov 7th 2024

Certificate of Analysis

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Product Name: **NICE 01** **Catalog No.: 8088** **Batch No.: 1**

CAS Number: 2982819-94-1

IUPAC Name: (*R*)-1-(3-((14-((*S*)-4-(4-Chlorophenyl)-2,3,9-trimethyl-6*H*-thieno[3,2-*f*][1,2,4]triazolo[4,3-*a*][1,4]diazepin-6-yl)-2,13-dioxo-6,9-dioxa-3,12-diazatetradecyl)oxy)phenyl)-3-(3,4-dimethoxyphenyl)propyl (*S*)-1-((*S*)-2-(3,4,5-trimethoxyphenyl)butanoyl)piperidine-2-carboxylate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{63}H_{76}ClN_7O_{13}S.H_2O$

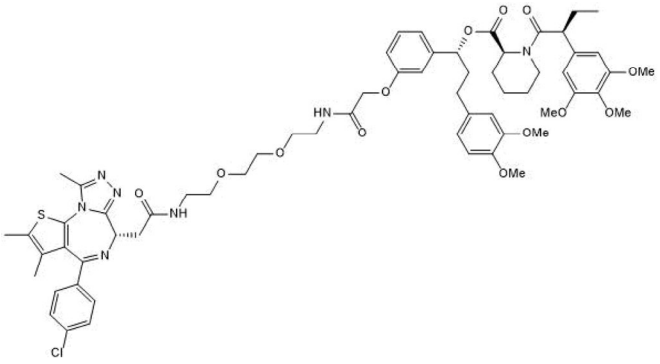
Batch Molecular Weight: 1224.87

Physical Appearance: White solid

Solubility: DMSO to 50 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.8% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	61.78	6.42	8
Found	60.76	6.25	7.76

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Description:

NICE 01 is a bifunctional molecule consisting of (+)-JQ1 (Cat. No. 4499) and AP 1867 (Cat. No. 6207), with a PEG2-diamine linker. It has a high affinity (K_d = 94 pM) for $FKBP^{F36V}$ tagged proteins. It can induce nuclear localization of cytosolic proteins and target transcriptional regulation. It can be used to calculate the kinetic constant and passive diffusion across the nuclear pore.

Physical and Chemical Properties:

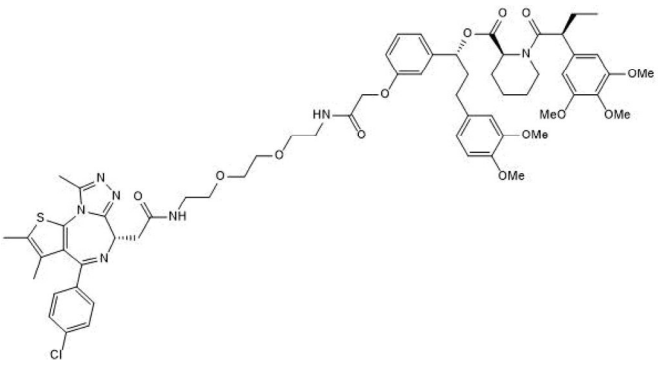
Batch Molecular Formula: $C_{63}H_{76}ClN_7O_{13}S.H_2O$

Batch Molecular Weight: 1224.87

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 50 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.

References:

Gibson *et al* (2023) Bifunctional small molecules that induce nuclear localization and targeted transcriptional regulation. J.Am.Chem.Soc. ***145*** 26028. PMID: 37461636.

Lu *et al* (2022) Bioorthogonal chemical epigenetic modifiers enable dose-dependent CRISPR targeted gene activation in mammalian cells. A.C.S.Synth.Biol. ***11*** 1397. PMID: 35302756.