bio-techne
TOCRIS

Print Date: May 15th 2023

Certificate of Analysis

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Product Name: **LL-K9-3** **Catalog No.: 7813** **Batch No.: 1**

CAS Number: 2809353-52-2

IUPAC Name: *N*-[5-[[[5-(1,1-Dimethylethyl)-2-oxazolyl]methyl]thio]-2-thiazolyl]-1-[[2-[[2-[[(1*R*,2*S*,5*R*)-5-methyl-2-(1-methylethyl) cyclohexyl]oxy]acetyl]amino]ethyl]sulfonyl]-4-piperidinecarboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{31}H_{49}N_5O_6S_3$

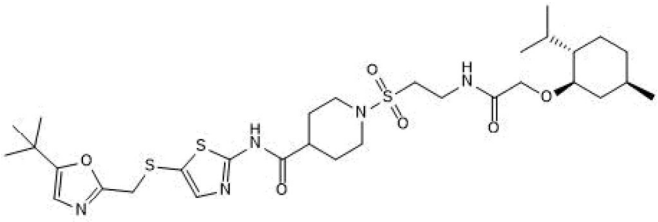
Batch Molecular Weight: 683.94

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 5 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.2% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	54.44	7.22	10.24
Found	53.89	7.15	9.9

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Description:

LL-K9-3 is a selective hydrophobic tagging technologies (HyT) -based Degrader of the CDK9-cyclin T1 complex (DC_{50} values are 589 and 662 nM for cyclin T1 and CDK9, respectively). It comprises a CDK9 inhibitor, SNS 032 (Cat. No. 4075), joined by a glycol linker to hydrophobic tag. LL-K9-3 exhibits no degradation of other CDKs (CDK1, 2, 4, 5, 6, and 7). In 22RV1 cells. LL-K9-3 reduces expression of androgen receptor (AR) and cMyc by inducing selective and synchronous degradation of CDK9 and cyclin T1.

Physical and Chemical Properties:

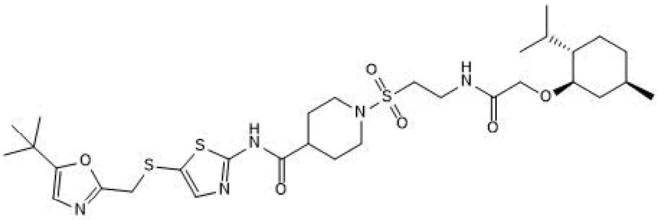
Batch Molecular Formula: $C_{31}H_{49}N_5O_6S_3$

Batch Molecular Weight: 683.94

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol to 5 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:

Li *et al* (2022) Discovery of small-molecule degraders of the CDK9-cyclin T1 complex for targeting transcriptional addiction in prostate cancer. J.Med.Chem. ***65*** 11034. PMID: 35925880.