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TOCRIS

Print Date: Feb 22nd 2024

Certificate of Analysis

www.tocris.com

Product Name: **TBK1 PROTAC® 3i** **Catalog No.: 7259** **Batch No.: 1**

CAS Number: 2052306-13-3

IUPAC Name: (2 ,4)-1-(( )-18-(4-((5-Bromo-4-((3-(*N*-methylcyclobutanecarboxamido)propyl)amino)pyrimidin-2-yl)amino) phenoxy)-2-(*tert*-butyl)-4-oxo-6,10,15-trioxa-3-azaoctadecanoyl)-4-hydroxy-*N*-(4-(4-methylthiazol-5-yl)benzyl) pyrrolidine-2-carboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{53}H_{74}BrN_9O_9S.\ H_2O$

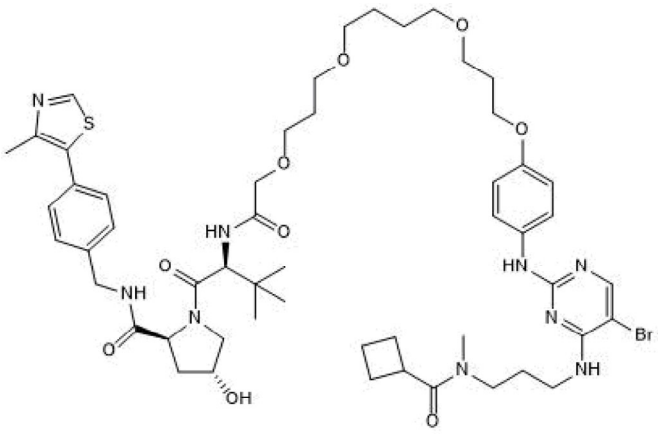
Batch Molecular Weight: 1106.7

Physical Appearance: White solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.2% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	57.52	6.88	11.39
Found	57.15	6.86	11.24

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

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Description:

TBK1 PROTAC® 3i is a potent TANK-binding kinase 1 (TBK1) PROTAC® Degrader (DC_{50} = 12 nM, D_{max} = 96%). Exhibits 50-fold selectivity for TBK1 over the closely related IKK . Comprises a ligand for von-Hippel Lindau (VHL) protein joined by a linker to a TBK1-targeting moiety. Brings about near complete degradation of TBK1 in mutant K-Ras and wild-type cancer cell lines with no significant effect of proliferation. Negative control TBK1 control PROTAC® 4 (Cat. No. 7260) and TBK1 antibodies validated for Simple Western™ (automated Western Blot) instruments and Western Blot also available: Catalog # AF9934 and NB100-... Please see product specific page on www.tocris.com for full description.

Physical and Chemical Properties:

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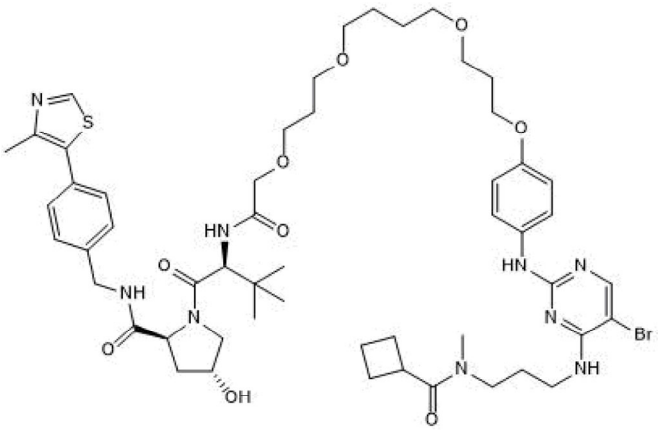
Batch Molecular Weight: 1106.7

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO 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. *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:

Crew *et al* (2018) Identification and characterization of Von Hippel-Lindau-recruiting proteolysis targeting chimeras (PROTACs) of TANK-binding kinase 1. J.Med.Chem. ***61*** 583. PMID: 28692295.