bio-techne
TOCRIS

Print Date: Apr 16th 2024

Certificate of Analysis

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Product Name: **JNJ 1013** **Catalog No.: 8029** **Batch No.: 1**

CAS Number: 2597343-08-1

IUPAC Name: *N*-(4-(4-(2-(((*S*)-1-((2*S*,4*R*)-4-Hydroxy-2-(((*S*)-1-(4-(4-methylthiazol-5-yl)phenyl)ethyl)carbamoyl)pyrrolidin-1-yl)-3,3-dimethyl-1-oxobutan-2-yl)amino)-2-oxoethoxy)piperidin-1-yl)-2-methoxyphenyl)-6-(1*H*-pyrazol-5-yl)picolinamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{46}H_{55}N_9O_7S.½H_2O$

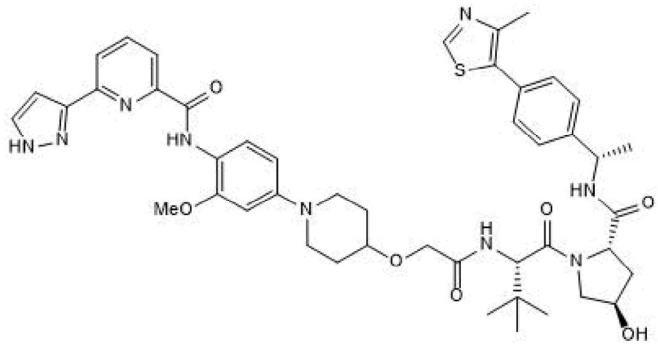
Batch Molecular Weight: 887.07

Physical Appearance: Yellow solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.3% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	62.28	6.36	14.21
Found	61.5	6.38	14

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Description:

JNJ 1013 is a potent interleukin 1 receptor associated kinase 1 (IRAK1) Degrader (PROTAC®; DC_{50} = 3 nM; D_{max} = 96%). In ABC DLBCL cell lines with MyD88 L265P mutation, JNJ 1013 potently inhibits IRAK1 downstream signaling pathways, induces apoptosis, and shows strong anti-proliferative effects. PROTAC® is a registered trademark of Arvinas Operations, Inc., and is used under license.

Physical and Chemical Properties:

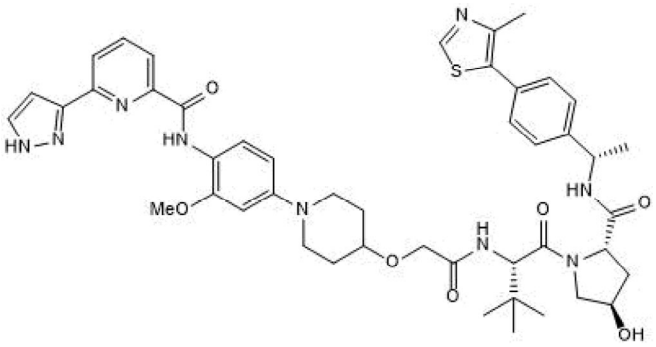
Batch Molecular Formula: $C_{46}H_{55}N_9O_7S.½H_2O$

Batch Molecular Weight: 887.07

Physical Appearance: Yellow solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

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:

Fu *et al* (2021) Discovery of highly potent and selective IRAK1 Degraders to probe scaffolding functions of IRAK1 in ABC DLBCL. J.Med.Chem. ***64*** 10878. PMID: 34279092.