Certificate of Analysis

Product Name: **A 1331852** **Catalog No.: 7661** **Batch No.: 1**

CAS Number: 1430844-80-6

IUPAC Name: 6-[8-[(2-Benzothiazolylamino)carbonyl]-3,4-dihydro-2(1*H*)-isoquinolinyl]-3-[5-methyl-1-(tricyclo[3.3.1.1^{3,7}]dec-1-ylmethyl)-1*H*-pyrazol-4-yl]-2-pyridinecarboxylic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{38}H_{38}N_6O_3S.¾H_2O$

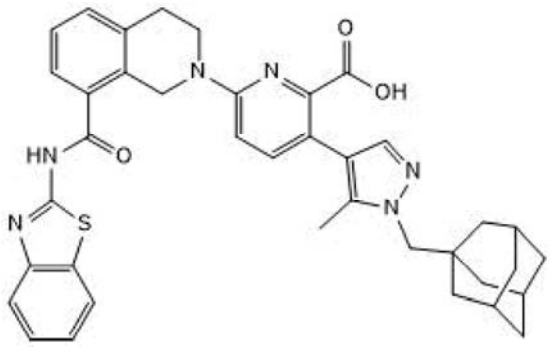
Batch Molecular Weight: 672.32

Physical Appearance: White solid

Solubility: DMSO to 20 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.6% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	67.88	5.92	12.5
Found	67.67	5.65	12.36

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Description:

A 1331852 is a high affinity and selective Bcl-xL inhibitor (K_i <0.01 nM), also inhibits Bcl-W, Bcl-2, and Mcl-1 (K_i values are 4, 6 and 142 nM, respectively). A 1331852 inhibits Bcl-xL-dependent Molt 4 acute lymphoblastic leukemia cell growth in vitro (EC_{50} = 6 nM). It enhances antitumor effects of Docetaxel (Cat. No. 4056) and Venetoclax (Cat. No. 6960) in xenograft models of breast and lung cancer. A 1331852 also induces apoptosis in and clears senescent biliary epithelial cells (BECs), and induces apoptosis in xenograft models of EBV-associated T- and natural killer cell lymphoma. Please see product specific page on www.tocris.com for full description.

Physical and Chemical Properties:

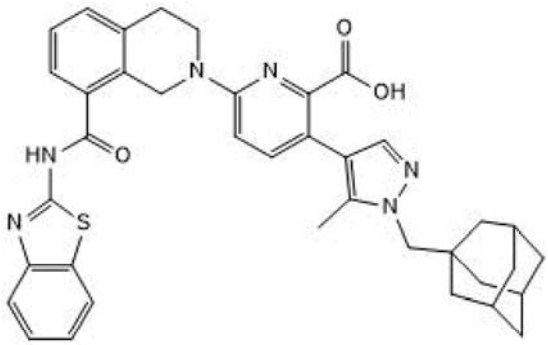
Batch Molecular Formula: $C_{38}H_{38}N_6O_3S.¾H_2O$

Batch Molecular Weight: 672.32

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 20 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:

Bierbrauer *et al* (2020) A direct comparison of selective BH3-mimetics reveals BCL-X_L, BCL-2 and MCL-1 as promising therapeutic targets in neuroblastoma. Br.J.Cancer ***122*** 1544. PMID: 32203216.

Moujalled *et al* (2020) Cotargeting BCL-2 and MCL-1 in high-risk B-ALL. Blood Adv. ***4*** 2762. PMID: 32569380.

Sasaki *et al* (2020) Increased p16^{INK4a}-expressing senescent bile ductular cells are associated with inadequate response to ursodeoxycholic acid in primary biliary cholangitis. J.Autoimmun. ***107*** 102377. PMID: 31812332.

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