

Product Name: ABT 199

Catalog No.: 6960

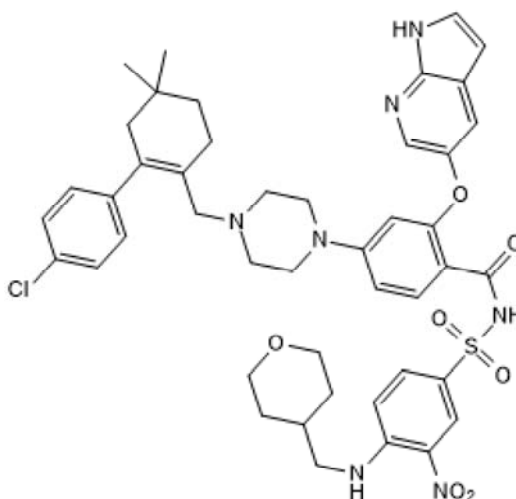
Batch No.: 2

CAS Number: 1257044-40-8

IUPAC Name: 4-[4-[[2-(4-Chlorophenyl)-4,4-dimethyl-1-cyclohexen-1-yl]methyl]-1-piperazinyl]-N-[[[3-nitro-4-[[[(tetrahydro-2H-pyran-4-yl)methyl]amino]phenyl]sulfonyl]-2-(1H-pyrrolo[2,3-b]pyridin-5-yloxy)benzamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:	C ₄₅ H ₅₀ ClN ₇ O ₇ S
Batch Molecular Weight:	868.45
Physical Appearance:	Yellow solid
Solubility:	DMSO to 100 mM
Storage:	Store at -20°C
Batch Molecular Structure:	



2. ANALYTICAL DATA

HPLC:	Shows 99.6% purity
¹H NMR:	Consistent with structure
Mass Spectrum:	Consistent with structure
Microanalysis:	

	Carbon	Hydrogen	Nitrogen
Theoretical	62.24	5.8	11.29
Found	61.84	5.75	11.11

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

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Description:

ABT 199 is a selective, high affinity Bcl-2 inhibitor ($K_i < 0.010$ nM). Exhibits >4800-fold selectivity for Bcl-2 over Bcl-xL and Bcl-w, and displays no measurable activity at Mcl-1 ($K_i > 444$ nM). Potently induces apoptosis in FL5.12-BCL-2 cells ($EC_{50} = 261$ nM) and reduces tumor burden in chronic lymphocytic leukemia (CLL) primary samples ($EC_{50} = 3$ nM). Shows reduced toxicity to platelets compared to similar compounds. Enhances efficacy of clinically relevant chemotherapy and immunotherapy drugs. Orally bioavailable. Exhibits binding to SARS-CoV-2 3C-like protease (3CL^{pro}) active site in a virtual screen. ABT 199 reverses oxidat... Please see product specific page on www.tocris.com for full description.

Physical and Chemical Properties:

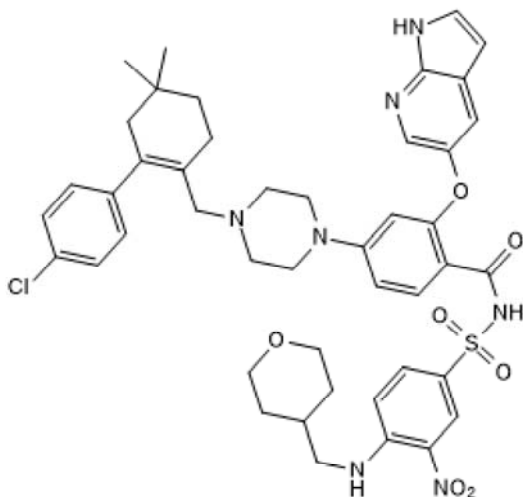
Batch Molecular Formula: C₄₅H₅₀ClN₇O₇S.

Batch Molecular Weight: 868.45

Physical Appearance: Yellow 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. 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:

Bosc et al (2021) Mitochondrial inhibitors circumvent adaptive resistance to venetoclax and cytarabine combination therapy in acute myeloid leukemia. *Nat.cancer* **2** 1204. PMID: 35122057.

Liu et al (2019) Balancing apoptosis and autophagy for Parkinson's disease therapy: targeting BCL-2. *ACS Chem.Neurosci.* **10** 792. PMID: 30400738.

Soderquist et al (2018) Systematic mapping of BCL-2 gene dependencies in cancer reveals molecular determinants of BH3 mimetic sensitivity. *Nat.Commun.* **9** 3513. PMID: 30158527.

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