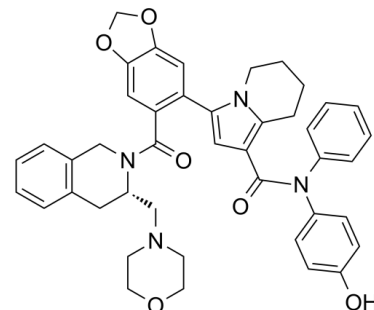


Data Sheet

Product Name:	S55746
Cat. No.:	CS-0065115
CAS No.:	1448584-12-0
Molecular Formula:	C43H42N4O6
Molecular Weight:	710.82
Target:	Bcl-2 Family
Pathway:	Apoptosis
Solubility:	H2O : < 0.1 mg/mL (insoluble); DMSO : 50 mg/mL (70.34 mM); Need ultrasonic)



BIOLOGICAL ACTIVITY:

S55746 (BLC201) is a potent, orally active and selective BCL-2 inhibitor, with a K_i of 1.3 nM and a K_d of 3.9 nM. S55746 (BLC201) has antitumor activity with low toxicity^[1]. IC50 & Target: K_i : 1.3 nM (BCL-2)^[1]. **In Vitro:** S55746 (0-1 μ M) potently and selectively induces cell death^[1].

S55746 selectively induces apoptosis through BCL-2 inhibition in a BAX/BAK-dependent manner^[1]. **In Vivo:** S55746 is a highly efficacious and well-tolerated (even at doses up to 300 mg/kg) orally active BCL-2 inhibitor^[1].

S55746 (20-100 mg/kg, p.o.) inhibits xenograft growth in RS4;11 and Toledo models time- and dose-dependently^[1].

PROTOCOL (Extracted from published papers and Only for reference)

Cell Assay: ^[1]Cells are seeded into 96-well plates and treated at 8 points with 1:2 serial dilution of S55746. Cell viability is assessed and assayed for viability using CellTiter-Glo reagent. Plates are read using luminescence plate reader. Results are normalized to the viability of cells without S55746 (control wells). The IC₅₀ values are calculated using nonlinear regression algorithms in XCell software^[1].

Animal Administration: ^[1]Mice^[1]

Experiments are performed in SCID/beige female mice. RS4;11 Acute Lymphoblastic Leukemia cell lines and human cell lines are used. For each experiment, female SCID/beige mice are implanted subcutaneously with 3×10^6 Toledo or RS4;11. Body weights are recorded and tumors are measured with digital calipers twice to three times a week. When tumors reached approximately 200 mm³ for efficacy studies or 300 mm³ for pharmacodynamics studies, mice are randomized. S55746 is formulated in PEG300/EtOH/water (40/10/50). Mice are treated via oral gavage at 10 mL/kg with different doses (e.g., S55746: 20, 50, 100 mg/kg)^[1].

References:

[1]. Casara P, et al. S55746 is a novel orally active BCL-2 selective and potent inhibitor that impairs hematological tumor growth. *Oncotarget*. 2018 Apr 13;9(28):20075-20088.

CAIndexNames:

1-Indolizinecarboxamide, 3-[6-[[[(3S)-3,4-dihydro-3-(4-morpholinylmethyl)-2(1H)-isoquinolinyl]carbonyl]-1,3-benzodioxol-5-yl]-5,6,7,8-tetrahydro-N-(4-hydroxyphenyl)-N-phenyl-

SMILES:

O=C(C1=C2CCCCN2C(C3=C(C(N4CC5=C(C=CC=C5)C[C@H]4CN6CCOCC6)=O)C=C(OCO7)C7=C3)=C1)N(C8=CC=C(O)C=C8)C9=CC=CC=C9

Caution: Product has not been fully validated for medical applications. For research use only.

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