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Product Data Sheet

PU-WS13

Cat. No.: HY-18680

CAS No.: 1454619-14-7

Molecular Formula: $C_{17}H_{20}Cl_2N_6S$

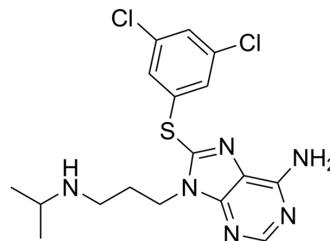
Molecular Weight: 411.35

Target: HSP

Pathway: Cell Cycle/DNA Damage; Metabolic Enzyme/Protease

Storage:

Powder	-20°C	3 years
	4°C	2 years
In solvent	-80°C	6 months
	-20°C	1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : ≥ 40 mg/mL (97.24 mM)

* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions

Concentration \ Solvent \ Mass	1 mg	5 mg	10 mg
1 mM	2.4310 mL	12.1551 mL	24.3102 mL
5 mM	0.4862 mL	2.4310 mL	4.8620 mL
10 mM	0.2431 mL	1.2155 mL	2.4310 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.5 mg/mL (6.08 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (6.08 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (6.08 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

PU-WS13 is a selective Grp94 inhibitor, with an EC_{50} of 0.22 µM.

IC_{50} & Target

GRP94	HSP90α	HSP90β	TRAP-1
0.22 µM (EC50)	27.3 µM (EC50)	41.8 µM (EC50)	7.3 µM (EC50)

In Vitro

PU-WS13 is a Grp94 inhibitor, with an EC_{50} of 0.22 µM. PU-WS13 also slightly suppresses Hsp90α, Hsp90β and Trap-1, with EC

$_{50}$s of 27.3, 41.8 and 7.3 μM, respectively. PU-WS13 (2.5-20 μM) shows no toxicity on two nonmalignant cell lines. PU-WS13 (15 μM) disrupts the circular architecture of HER2 at the plasma membrane of SKBr3 cells mediated through Grp94. PU-WS13 inhibits Grp94, and the inhibition induces apoptosis in and reduce the viability of HER2 overexpressing breast cancer cells[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

PROTOCOL

Kinase Assay [1]

The Hsp90 FP competition assays are carried out in black 96-well micro-plates in a total volume of 100 μL in each well. A stock of 10 μM cy3B-GM and PU-FITC3 is prepared in DMSO and diluted with Felts buffer (20 mM Hepes (K), pH 7.3, 50 mM KCl, 2 mM DTT, 5 mM $MgCl_2$, 20 mM Na_2MoO_4 and 0.01% NP40 with 0.1 mg/mL BGG). To each well is added the fluorescent dye-labeled Hsp90 ligand (6 nM cy3B-GM for Hsp90α, Hsp90β and Grp94 and 3 nM PU-FITC3 for Trap-1), protein (10 nM Hsp90α, 10 nM Hsp90β, 10 nM Grp94, 30 nM Trap-1) and tested inhibitor (including PU-WS13, initial stock in DMSO) in a final volume of 100 μL Felts buffer. Compounds are added in duplicate or triplicate wells. For each assay, background wells (buffer only), tracer controls (free, fluorescent dye-labeled Hsp90 ligand only) and bound controls (fluorescent dye-labeled Hsp90 ligand in the presence of protein) are included on each assay plate. The assay plate is incubated on a shaker at 4°C for 24 h, and the FP values (in mP) are measured. The fraction of fluorescent dye-labeled Hsp90 ligand bound to Hsp90 is correlated to the mP value and plotted against values of competitor concentrations. The inhibitor concentration at which 50% of bound fluorescent dye-labeled Hsp90 ligand is displaced is obtained by fitting the data. For cy3B-GM, an excitation filter at 530 nm and an emission filter at 580 nm are used with a dichroic mirror of 561 nm. For PU-FITC3, an excitation filter at 485 nm and an emission filter at 530 nm are used with a dichroic mirror of 505 nm. All of the experimental data are analyzed, and binding affinity values are given as relative binding affinity values (EC_{50}, concentration at which 50% of fluorescent ligand is competed off by compound)[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Cell Assay [1]

Cells are treated for 72 h with inhibitors (including PU-WS13) or transfected with Grp94 siRNA or control siRNA, and their viability is assessed using CellTiter-Glo luminescent Cell Viability Assay. The method determines the number of viable cells in culture based on quantification of the ATP present, which signals the presence of metabolically active cells[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

CUSTOMER VALIDATION

- Theranostics. 2019 Jan 1;9(2):554-572.
- Research Square Preprint. 2021 Sep.

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REFERENCES

[1]. Patel PD, et al. Paralog-selective Hsp90 inhibitors define tumor-specific regulation of HER2. Nat Chem Biol. 2013 Nov;9(11):677-684.

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

Tel: 609-228-6898 Fax: 609-228-5909 E-mail: tech@MedChemExpress.com

Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA