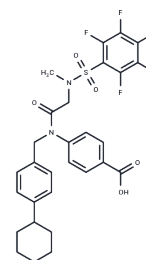


SH-4-54

Chemical Properties

CAS No. : 1456632-40-8
 Formula: C₂₉H₂₇F₅N₂O₅
 Molecular Weight: 610.59
 Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year
 Actual storage temperature shall be subject to the COA.



Biological Description

| | |
|---------------|--|
| Description | SH-4-54 is a most potent, small molecule, nonphosphorylated STAT3 inhibitor. |
| Targets(IC50) | STAT |
| In vitro | SH-4-54 effectively inhibits the phosphorylation of STAT3 and its downstream transcription targets. Additionally, SH-4-54 demonstrates unparalleled cytotoxicity against human malignant gliomas and liver cancer cells while showing no toxicity toward human embryonic astrocytes. |
| In vivo | Intraperitoneal injection of 10 mg/kg SH-4-54 into mice with orthotopic xenografts of BT73 effectively inhibited the growth of glioma and suppressed pSTAT3 activation. |
| Kinase Assay | Surface Plasmon Resonance (SPR) studies: The binding experiments are carried out on a ProteOn XPR36 biosensor at 25°C using the HTE sensor chip. The flow cells of the sensor chip are loaded with a nickel solution at 30 µL/min for 120 s to saturate the Tris-NTA surface with Ni(II) ions. Purified His-tagged STAT3 and STAT5 in PBST buffer (PBS with 0.005% (v/v) Tween-20 and 0.001% DMSO pH 7.4) is injected in the first and second channels of the chip respectively in the vertical direction at a flow rate of 25 µg/µL for 300 s, which attained, on average, ~8000 resonance unit (RU). After a wash with PBST buffer, inhibitors binding to the immobilized proteins is monitored by injecting a range of concentrations along with a blank at a flow rate of 100 µL/min for 200 s for each of these small molecules. When the injection of the small molecule inhibitor is completed, running buffer is allowed to flow over the immobilized substrates for the non-specifically bound inhibitors to dissociate for 600 s. Following dissociation of the inhibitors, the chip surface is regenerated with an injection of 1 M NaCl at a flow rate of 100 µL/ml for 18 s. Interspot channel reference is used for non-specific binding corrections and the blank channel used with each analyte injection served as a double reference to correct for possible baseline drift. Data are analyzed using ProteOn Manager Software version 3.1. The Langmuir 1:1 binding model was used to determine the KD values. |
| Cell Research | BTSC spheres are dissociated to single cells with the enzyme Accumax, seeded at 1500 cells/ 96-well and treated with drug or vehicle (DMSO) one day after plating. Cytotoxicity studies are repeated independently using BTSC lines 25M, 67EF, 73EF, 84EF and 127EF. BTSC spheres are dissociated to single cells as above and plated in 96 well plates in triplicate at 3000 cells/ 96-well. In both sets of experiments drugs are used as serial |

A DRUG SCREENING EXPERT

| | |
|---------------|--|
| Cell Research | dilutions within the range of 5 μ M to 100 nM in the first set and 25 μ M to 10 nM. Cell viability following drug treatment is assessed three days later using the alamarBlue assay according to the manufacturer's instructions. All culture experiments are performed in triplicate with a minimum of three wells per condition.(Only for Reference) |
|---------------|--|

Solubility Information

| | |
|---------------------|---|
| Solubility | DMSO: 250 mg/mL (409.44 mM),Sonication is recommended. H2O: < 1 mg/mL (insoluble or slightly soluble), Ethanol: 47 mg/mL (76.97 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble) |
| In vivo Formulation | 10% DMSO+40% PEG300+5% Tween 80+45% Saline: 3.3 mg/mL (5.4 mM),Sonication is recommended. <i>Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.</i> |

Preparing Stock Solutions

| | 1mg | 5mg | 10mg |
|-------|-----------|-----------|------------|
| 1 mM | 1.6378 mL | 8.1888 mL | 16.3776 mL |
| 5 mM | 0.3276 mL | 1.6378 mL | 3.2755 mL |
| 10 mM | 0.1638 mL | 0.8189 mL | 1.6378 mL |
| 50 mM | 0.0328 mL | 0.1638 mL | 0.3276 mL |

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

Haftchenary S, et al. ACS Med Chem Lett. 2013, 4(11), 1102-1107.

Inhibitor · Natural Compounds · Compound Libraries · Recombinant Proteins

This product is for Research Use Only · Not for Human or Veterinary or Therapeutic Use

Tel:781-999-4286 E_mail:info@targetmol.com Address:34 Washington Street,Wellesley Hills,MA 02481