Screening Libraries

Product Data Sheet

JAB-3068 hydrochloride

Cat. No.: HY-131132A CAS No.: 2169223-49-6 Molecular Formula: $C_{22}H_{27}ClF_{2}N_{6}O_{2}S$

Molecular Weight: 513

Target: Phosphatase; SHP2

Pathway: Metabolic Enzyme/Protease; Protein Tyrosine Kinase/RTK

Storage: -20°C, sealed storage, away from moisture and light

* In solvent: -80°C, 6 months; -20°C, 1 month (sealed storage, away from moisture

and light)

SOLVENT & SOLUBILITY

In Vitro

DMSO: 115 mg/mL (224.17 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent Mass Concentration	1 mg	5 mg	10 mg
	1 mM	1.9493 mL	9.7466 mL	19.4932 mL
	5 mM	0.3899 mL	1.9493 mL	3.8986 mL
	10 mM	0.1949 mL	0.9747 mL	1.9493 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: ≥ 5.75 mg/mL (11.21 mM); Clear solution
- 2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline) Solubility: ≥ 5.75 mg/mL (11.21 mM); Clear solution

BIOLOGICAL ACTIVITY

Description	JAB-3068 (SHP2-IN-6) hydrochloride is a potent SHP2 inhibitor with an IC $_{50}$ of 25.8 nM. JAB-3068 hydrochloride is extracted from patent WO2017211303A1, compound $7^{[1]}$.
In Vitro	JAB-3068 hydrochloride inhibits the proliferation of KYSE-520 cells with an IC $_{50}$ of 2.17 μ M $^{[1]}$. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Cunbo Ma, et al. Novel heterocyclic derivatives useful as shp2 inhibitors. WO2017211303A1.

 $\label{lem:caution:Product} \textbf{Caution: Product has not been fully validated for medical applications. For research use only.}$

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