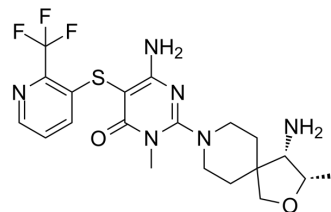


## SHP394

|                           |  |
|---------------------------|--|
| <b>Cat. No.:</b>          | HY-114397  |
| <b>CAS No.:</b>           | 2055757-40-7   |
| <b>Molecular Formula:</b> | C <sub>20</sub> H <sub>25</sub> F <sub>3</sub> N <sub>6</sub> O <sub>2</sub> S |
| <b>Molecular Weight:</b>  | 470.51   |
| <b>Target:</b>            | Phosphatase  |
| <b>Pathway:</b>           | Metabolic Enzyme/Protease  |
| <b>Storage:</b>           | 4°C, stored under nitrogen   |
|                           | * In solvent : -80°C, 6 months; -20°C, 1 month (stored under nitrogen)         |



### SOLVENT & SOLUBILITY

|   |  |                          |              |            |            |
|---|--|--------------------------|--------------|------------|------------|
| <b>In Vitro</b>   | DMSO : 24 mg/mL (51.01 mM; Need ultrasonic)  |                          |              |            |            |
|   |  | Solvent<br>Concentration | Mass<br>1 mg | 5 mg       | 10 mg      |
|   | <b>Preparing Stock Solutions</b>   | 1 mM                     | 2.1254 mL    | 10.6268 mL | 21.2535 mL |
|   |  | 5 mM                     | 0.4251 mL    | 2.1254 mL  | 4.2507 mL  |
|   |  | 10 mM                    | 0.2125 mL    | 1.0627 mL  | 2.1254 mL  |
| Please refer to the solubility information to select the appropriate solvent. |  |                          |              |            |            |
| <b>In Vivo</b>  | <ol style="list-style-type: none"> <li>Add each solvent one by one: 10% DMSO &gt;&gt; 40% PEG300 &gt;&gt; 5% Tween-80 &gt;&gt; 45% saline<br/>Solubility: ≥ 6.25 mg/mL (13.28 mM); Clear solution</li> <li>Add each solvent one by one: 10% DMSO &gt;&gt; 90% (20% SBE-β-CD in saline)<br/>Solubility: ≥ 6.25 mg/mL (13.28 mM); Clear solution</li> <li>Add each solvent one by one: 10% DMSO &gt;&gt; 90% corn oil<br/>Solubility: ≥ 6.25 mg/mL (13.28 mM); Clear solution</li> </ol> |                          |              |            |            |

### BIOLOGICAL ACTIVITY

|                                     |  |
|-------------------------------------|--|
| <b>Description</b>                  | SHP394 is an orally active, selective and allosteric inhibitor of SHP2, with an IC <sub>50</sub> of 23 nM <sup>[1]</sup> .   |
| <b>IC<sub>50</sub> &amp; Target</b> | IC <sub>50</sub> : 23 nM (SHP2) <sup>[1]</sup>   |
| <b>In Vitro</b>                     | <p>SHP394 inhibits Caco-2 cells proliferation with the IC<sub>50</sub> of 297 nM<sup>[1]</sup>.</p> <p>SHP394 exhibits antiproliferation activity against the Detroit-562 pharyngeal carcinoma cell line in vitro (IC<sub>50</sub>= 1.38 μM)<sup>[1]</sup>.</p> <p>SHP394 decreases p-ERK with an IC<sub>50</sub> of 18 nM KYSE520 cells<sup>[1]</sup>.</p> <p>MCE has not independently confirmed the accuracy of these methods. They are for reference only.</p> |

**In Vivo**

SHP394 (20-80 mg/kg; oral gavage; twice daily) dose-dependent reduces tumor volume<sup>[1]</sup>.  
SHP394 (80 mg/kg; oral gavage; twice daily) causes tumor 34% regression and reduces mouse host bodyweight after dosing for 14 days<sup>[1]</sup>.

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

|                 |  |
|-----------------|--|
| Animal Model:   | Six-week old female athymic NU/NU mice were inoculated subcutaneously with Detroit-562 pharyngeal carcinoma cells <sup>[1]</sup> . |
| Dosage:         | 20, 40, and 80 mg/kg   |
| Administration: | Oral gavage; twice daily   |
| Result:         | Demonstrated a clear dose-dependent reduction in tumor volume.   |

**REFERENCES**

[1]. Sarver P, et al. 6-Amino-3-methylpyrimidinones as Potent, Selective, and Orally Efficacious SHP2 Inhibitors. J Med Chem. 2019 Feb 28;62(4):1793-1802.

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

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