Proteins



## ASK1-IN-1

Cat. No.: HY-133554 CAS No.: 2411382-24-4 Molecular Formula:  $C_{19}H_{19}N_{9}O_{2}$ Molecular Weight: 405.41 Target: p38 MAPK

Pathway: MAPK/ERK Pathway

Storage: Powder -20°C 3 years

4°C 2 years

In solvent -80°C 2 years

> -20°C 1 year

**Product** Data Sheet

## **SOLVENT & SOLUBILITY**

In Vitro DMF: 4 mg/mL (9.87 mM; Need ultrasonic)

> DMSO: < 1 mg/mL (insoluble or slightly soluble) Ethanol: < 1 mg/mL (ultrasonic) (insoluble)

| Preparing<br>Stock Solutions | Solvent Mass<br>Concentration | 1 mg      | 5 mg       | 10 mg      |
|------------------------------|-------------------------------|-----------|------------|------------|
|                              | 1 mM                          | 2.4666 mL | 12.3332 mL | 24.6664 mL |
|                              | 5 mM                          | 0.4933 mL | 2.4666 mL  | 4.9333 mL  |
|                              | 10 mM                         |           |            |            |

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

## **BIOLOGICAL ACTIVITY**

| Description               | ASK1-IN-1 is a CNS-penetrant ASK1 (apoptosis signal-regulating kinase 1) inhibitor, with good potency (cell IC $_{50}$ =138 nM; Biochemical IC $_{50}$ =21 nM) $^{[1]}$ .  |
|---------------------------|--|
| IC <sub>50</sub> & Target | IC50: 138/21 nM (ASK1 in cell and Biochemical assays, respectively) <sup>[1]</sup>   |
| In Vitro                  | ASK1-IN-1 (compound 21) has superior CYP inhibition profile and it is also inactive in a hERG assay. ASK1-IN-1 is selected for a kinase selectivity profile against a panel of 468 kinases and it is found to be moderately selective <sup>[1]</sup> .  MCE has not independently confirmed the accuracy of these methods. They are for reference only.                  |
| In Vivo                   | ASK1-IN-1 (10 mg/kg; p.o.) covers the cellular $IC_{50}/IC_{70}/IC_{90}$ at trough in the brain for 12 hours of 50/115/435 mg/kg respectively. ASK1-IN-1 has good biochemical and cellular potency, low clearance and good brain penetration in rodents <sup>[1]</sup> . MCE has not independently confirmed the accuracy of these methods. They are for reference only. |

| REFERENCES                          |                                 |  |  |                                       |     |
|-------------------------------------|---------------------------------|--|--|---------------------------------------|-----|
| [1]. Xin Z, et al. Discovery of CNS | -Penetrant Apoptosis Signa      | al-Regulating Kinase 1 (ASK1) Inh                  | nibitors. ACS Med Chem Lett. 2020                | );11(4):485-490. Published 2020 Feb 1 | 12. |
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|                                     |                                 |  | edical applications. For resea                   |                                       |     |
|                                     | Tel: 609-228-6898<br>Address: 1 | Fax: 609-228-5909<br>L Deer Park Dr, Suite Q, Monm | E-mail: tech@MedChemouth Junction, NJ 08852, USA |                                       |     |
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