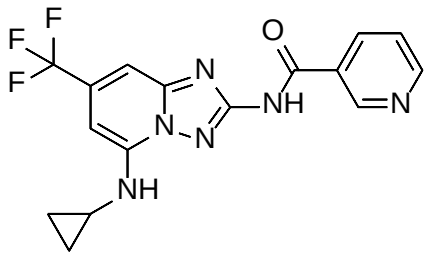
Product data sheet

MedKoo Cat#: 523124 Name: MSC 2032964A CAS: 1124381-43-6 Chemical Formula: $C_{16}H_{13}F_3N_6O$ Exact Mass: 362.1103 Molecular Weight: 362.3162	
Product supplied as:	Powder
Purity (by HPLC):	≥ 98%
Shipping conditions	Ambient temperature
Storage conditions:	Powder: -20°C 3 years; 4°C 2 years.
	In solvent: -80°C 3 months; -20°C 2 weeks.

1. Product description:
MSC 2032964A is a potent and selective ASK1 inhibitor (IC_{50} = 93 nM). It blocks LPS-induced ASK1 and p38 phosphorylation in cultured mouse astrocytes and suppresses neuroinflammation in a mouse EAE model. MSC 2032964A is orally bioavailable and brain penetrant.

2. CoA, QC data, SDS, and handling instruction
SDS and handling instruction, CoA with copies of QC data (NMR, HPLC and MS analytical spectra) can be downloaded from the product web page under "QC And Documents" section. Note: copies of analytical spectra may not be available if the product is being supplied by MedKoo partners. Whether the product was made by MedKoo or provided by its partners, the quality is 100% guaranteed.

3. Solubility data

Solvent	Max Conc. mg/mL	Max Conc. mM
DMSO	7.25	20.0

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	2.76 mL	13.80 mL	26.60 mL
5 mM	1.38 mL	6.90 mL	13.80 mL
10 mM	0.28 mL	1.38 mL	2.76 mL
50 mM	0.14 mL	0.28 mL	1.38 mL

5. Molarity Calculator, Reconstitution Calculator, Dilution Calculator
Please refer the product web page under section of "Calculator"

6. Recommended literature which reported protocols for in vitro and in vivo study
In vitro study

Guo X, Harada C, Namekata K, Matsuzawa A, Camps M, Ji H, Swinnen D, Jorand-Lebrun C, Muzerelle M, Vitte PA, Rückle T, Kimura A, Kohyama K, Matsumoto Y, Ichijo H, Harada T. Regulation of the severity of neuroinflammation and demyelination by TLR-ASK1-p38 pathway. EMBO Mol Med. 2010 Dec;2(12):504-15. doi: 10.1002/emmm.201000103. PMID: 21064192; PMCID: PMC3377347.

In vivo study

Guo X, Harada C, Namekata K, Matsuzawa A, Camps M, Ji H, Swinnen D, Jorand-Lebrun C, Muzerelle M, Vitte PA, Rückle T, Kimura A, Kohyama K, Matsumoto Y, Ichijo H, Harada T. Regulation of the severity of neuroinflammation and demyelination by TLR-ASK1-p38 pathway. EMBO Mol Med. 2010 Dec;2(12):504-15. doi: 10.1002/emmm.201000103. PMID: 21064192; PMCID: PMC3377347.

7. Bioactivity
Biological target:

MSC 2032964A is a potent and selective ASK1 inhibitor (IC_{50} = 93 nM).

In vitro activity

Product data sheet

To this aim, this study performed a high-throughput screening with purified ASK1 and have identified one small molecule inhibitor Hit Series. The most potent compound from the Series, MSC1946002A, showed a moderate inhibition of the enzymatic activity of ASK1 (IC_{50} of 3000 ± 320 nM). The profiling of MSC2032964A revealed an excellent overall in vitro ADME profile.

Reference: EMBO Mol Med. 2010 Dec;2(12):504-15. https://pubmed.ncbi.nlm.nih.gov/21064192/

In vivo activity

This study tested MSC2032964A in in vivo inflammation models and found that it blocked LPS-induced ASK1 and p38 phosphorylation in cultured mouse astrocytes (Fig 7A). The disease incidence of EAE was not different between vehicle- and 30 mg/kg MSC2032964A-treated groups, but MSC2032964A induced a significantly attenuated disease course after d18, nearly reproducing the phenotype observed in $ASK1^{-/-}$ mice (Fig 7B).

Reference: EMBO Mol Med. 2010 Dec;2(12):504-15. https://pubmed.ncbi.nlm.nih.gov/21064192/