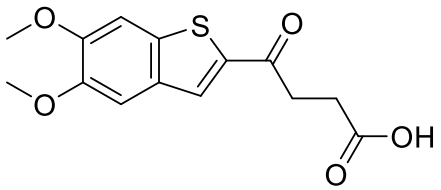
Product data sheet

MedKoo Cat#: 463682 Name: MSA-2 CAS#: 129425-81-6 Chemical Formula: $C_{14}H_{14}O_5S$ Exact Mass: 294.0562 Molecular Weight: 294.321	
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:
MSA 2 is a non-nucleotide STING agonist. It exhibits antitumor activity and stimulates interferon-β secretion in tumors. MSA 2 induces tumor regression with durable antitumor immunity, and synergizes with anti-PD-1 in syngeneic mouse tumor models. It is also orally bioavailable.

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	50	169.88

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	3.40 mL	16.99 mL	33.98 mL
5 mM	0.68 mL	3.40 mL	6.80 mL
10 mM	0.34 mL	1.70 mL	3.40 mL
50 mM	0.07 mL	0.34 mL	0.68 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

1. Pan BS, Perera SA, Piesvaux JA, Presland JP, Schroeder GK, Cumming JN, Trotter BW, Altman MD, Buevich AV, Cash B, Cemerski S, Chang W, Chen Y, Dandliker PJ, Feng G, Haidle A, Henderson T, Jewell J, Kariv I, Knemeyer I, Kopinja J, Lacey BM, Laskey J, Lesburg CA, Liang R, Long BJ, Lu M, Ma Y, Minnihan EC, O'Donnell G, Otte R, Price L, Rakhilina L, Sauvagnat B, Sharma S, Tyagarajan S, Woo H, Wyss DF, Xu S, Bennett DJ, Addona GH. An orally available non-nucleotide STING agonist with antitumor activity. Science. 2020 Aug 21;369(6506):eaba6098. doi: 10.1126/science.aba6098. PMID: 32820094.

In vivo study

1. Pan BS, Perera SA, Piesvaux JA, Presland JP, Schroeder GK, Cumming JN, Trotter BW, Altman MD, Buevich AV, Cash B, Cemerski S, Chang W, Chen Y, Dandliker PJ, Feng G, Haidle A, Henderson T, Jewell J, Kariv I, Knemeyer I, Kopinja J, Lacey BM, Laskey J, Lesburg CA, Liang R, Long BJ, Lu M, Ma Y, Minnihan EC, O'Donnell G, Otte R, Price L, Rakhilina L, Sauvagnat B, Sharma S, Tyagarajan S, Woo H, Wyss DF, Xu S, Bennett DJ, Addona GH. An orally available non-nucleotide STING agonist with antitumor activity. Science. 2020 Aug 21;369(6506):eaba6098. doi: 10.1126/science.aba6098. PMID: 32820094.

7. Bioactivity
Biological target:

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MSA-2, a potent and orally available non-nucleotide STING agonist, is bound to STING as a noncovalent dimer with nanomolar affinity. MSA-2 shows EC50s of 8.3 and 24 μM for human STING isoforms WT and HAQ, respectively.

In vitro activity

MSA-2 in solution exists as monomers and noncovalent dimers in an equilibrium that strongly favors monomers; MSA-2 monomers cannot bind STING, whereas the noncovalent MSA-2 dimers bind STING with nanomolar affinity. MSA-2 exhibits substantially higher cellular potency in an acidified tumor microenvironment than normal tissue, owing to increased cellular entry and retention combined with the inherently steep MSA-2 concentration dependence of STING occupancy.

Reference: Science. 2020 Aug 21;369(6506):eaba6098. https://www.sciencemag.org/cgi/pmidlookup?view=long&pmid=32820094

In vivo activity

MSA-2 is orally available, manifesting similar oral and subcutaneous exposure in mice. In tumor-bearing mice, MSA-2 induced elevations of interferon-b in plasma and tumors by both routes of administration. Well-tolerated regimens of MSA-2 induced tumor regressions in mice bearing MC38 syngeneic tumors. In tumor models that are moderately or poorly responsive to PD-1 blockade, combinations of MSA-2 and anti-PD-1 antibody are superior in inhibiting tumor growth and prolonging survival over monotherapy.

Reference: Science. 2020 Aug 21;369(6506):eaba6098. https://www.sciencemag.org/cgi/pmidlookup?view=long&pmid=32820094

Note: The information listed here was extracted from literature. MedKoo has not independently retested and confirmed the accuracy of these methods. Customer should use it just for a reference only.