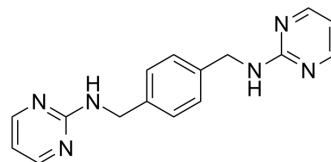


## MSX-122

Cat. No.:	HY-13696		
CAS No.:	897657-95-3		
Molecular Formula:	C <sub>16</sub> H <sub>16</sub> N <sub>6</sub>		
Molecular Weight:	292.34		
Target:	CXCR		
Pathway:	GPCR/G Protein; Immunology/Inflammation		
Storage:	Powder	-20°C	3 years
		4°C	2 years
	In solvent	-80°C	2 years
		-20°C	1 year



## SOLVENT & SOLUBILITY

### In Vitro

DMSO : 4 mg/mL (13.68 mM; Need ultrasonic)

Concentration	Solvent	Mass		
		1 mg	5 mg	10 mg
Preparing Stock Solutions	1 mM	3.4207 mL	17.1034 mL	34.2067 mL
	5 mM	0.6841 mL	3.4207 mL	6.8413 mL
	10 mM	0.3421 mL	1.7103 mL	3.4207 mL

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

### In Vivo

- Add each solvent one by one: 0.5% CMC-Na/saline water  
Solubility: 10 mg/mL (34.21 mM); Suspended solution; Need ultrasonic
- Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline  
Solubility: ≥ 0.4 mg/mL (1.37 mM); Clear solution
- Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)  
Solubility: ≥ 0.4 mg/mL (1.37 mM); Clear solution
- Add each solvent one by one: 10% DMSO >> 90% corn oil  
Solubility: ≥ 0.4 mg/mL (1.37 mM); Clear solution

## BIOLOGICAL ACTIVITY

### Description

MSX-122 is an orally active partial antagonist of CXCR4, inhibiting CXCR4/CXCL12 actions, with an IC<sub>50</sub> of ~10 nM. MSX-122 has anti-inflammatory and anti-metastatic activity.

### IC<sub>50</sub> & Target

CXCR4/CXCL12  
~10 nM (IC<sub>50</sub>)

<b>In Vitro</b>	<p>MSX-122 is a partial antagonist of CXCR4, inhibiting CXCR4/CXCL12 actions, with an IC<sub>50</sub> of -10 nM. MSX-122 shows no inhibition on cAMP reduction mediated by their corresponding ligands CCR3/CCL5 and CCR5/CCL5. MSX-122 (100 nM) potently blocks invasion of 78% MDA-MB-231 cells. However, MSX-122 does not suppress T-tropic HIV infection and is inactive in calcium flux assay<sup>[1]</sup>.</p> <p>MCE has not independently confirmed the accuracy of these methods. They are for reference only.</p>
<b>In Vivo</b>	<p>MSX-122 (10 mg/kg, i.p.) blocks inflammation induced by carrageenan and lung fibrosis induced by bleomycin in mice. MSX-122 (4 mg/kg, i.p., daily) blocks metastasis in an experimental animal model of breast cancer metastasis. Furthermore, MSX-122 (10 mg/kg i.p., daily) significantly decreases the numbers of hepatic micrometastases<sup>[1]</sup>.</p> <p>MCE has not independently confirmed the accuracy of these methods. They are for reference only.</p>

## PROTOCOL

### Animal Administration <sup>[1]</sup>

Mice<sup>[1]</sup>

Six- to eight-week-old female nude mice are given injections of  $1.5 \times 10^6$  MDA-MB-231 breast cancer cells mixed with the compound (1  $\mu$ M, less than 5 min preincubation) through the tail vein (10/group). From the following day, mice in the treated group are given 4 mg/kg MSX-122ms (salt form) daily by i.p. injection. The animals are sacrificed 35 days after the tumor cell injection. Whole lung tissues are harvested and sectioned for real-time RT-PCR for human CXCR4 and H&E histostaining to evaluate the metastatic tumor area in five fields per section microscopically. These experiments are repeated once more to confirm the results. For the head and neck cancer animal model, metastatic subclones of 686LN-Ms cells are injected in the same way as MDA-MB-231 cells. [<sup>18</sup>F]FDG-PET is performed. For the uveal melanoma micrometastasis mouse model, on day 0, each mouse is inoculated with  $1 \times 10^6$  wild-type OMM2.3 cells expressing HGF/TGF- $\beta$ /CXCR4/MMP2 into the posterior chamber of right eye. On day 3, mice are treated with 10 mg/kg MSX-122 in 0.1 mL volume of 45% CD daily by i.p. injection, whereas the control mice are injected with 0.1 mL 45% CD only. On day 7, eyes with tumor are enucleated. The growth of tumor is checked by histological methods. On day 28, hepatic tissues are collected and fixed in 10% formalin, processed, H&E stained, and the number of hepatic micrometastases is counted under microscope. Six sections through the center of the liver are microscopically examined for the presence of micrometastases (<100  $\mu$ m diameter) and the average number of micrometastases per section is determined. Ten mice per group are used. A table summarizing animal experiments for three metastasis models can be found in the Data S3<sup>[1]</sup>.

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

## CUSTOMER VALIDATION

- Br J Haematol. 2022 Dec 19.

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## REFERENCES

[1]. Liang Z, et al. Development of a unique small molecule modulator of CXCR4. PLoS One. 2012;7(4):e34038.

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

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