Product Data Sheet

NUCC-390 dihydrochloride

Cat. No.: HY-111793A CAS No.: 2749281-71-6 Molecular Formula: $C_{23}H_{35}Cl_{2}N_{5}O$ Molecular Weight: 468.46

CXCR Target:

Pathway: GPCR/G Protein; Immunology/Inflammation

Storage: 4°C, stored under nitrogen

* In solvent: -80°C, 6 months; -20°C, 1 month (stored under nitrogen)

SOLVENT & SOLUBILITY

In Vitro

DMSO: 100 mg/mL (213.47 mM; Need ultrasonic) H₂O: 25 mg/mL (53.37 mM; Need ultrasonic)

| | Solvent Mass Concentration | 1 mg | 5 mg | 10 mg |
|------------------------------|-------------------------------|-----------|------------|------------|
| Preparing Stock Solutions | 1 mM | 2.1347 mL | 10.6733 mL | 21.3465 mL |
| | 5 mM | 0.4269 mL | 2.1347 mL | 4.2693 mL |
| | 10 mM | 0.2135 mL | 1.0673 mL | 2.1347 mL |

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

In Vivo

- 1. Add each solvent one by one: PBS Solubility: 20 mg/mL (42.69 mM); Clear solution; Need ultrasonic and warming and heat to 60°C
- 2. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline Solubility: ≥ 2.5 mg/mL (5.34 mM); Clear solution
- 3. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline) Solubility: ≥ 2.5 mg/mL (5.34 mM); Clear solution
- 4. Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: ≥ 2.5 mg/mL (5.34 mM); Clear solution

BIOLOGICAL ACTIVITY

| Description | NUCC-390 dihydrochloride is a novel and selective small-molecule CXCR4 receptor agonist. NUCC-390 dihydrochloride induces internalization of CXCR4 receptors and acts in an opposite way of AMD3100 (HY-10046) ^[1] . NUCC-390 dihydrochloride promotes nerve recovery of function after neurodegeneration in vivo ^[2] . |
|---------------------------|---|
| IC ₅₀ & Target | CXCR4 |

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In Vitro

NUCC-390 dihydrochloride (10 μ M) produces strong (Ca)i response, but this effect can be blocked by the known potent and selective CXCR4 antagonist AMD3100^[1].

NUCC-390 dihydrochloride (10 μ M; pre-treatment 30 mins) leads to increased levels of pERK, it has the capability of stimulating signaling activity downstream of CXCR4 receptors^[1].

NUCC-390 dihydrochloride (10 μ M; 2 hours) can induce CXCR4 receptor internalization, and non-treated cells exhibit some diffuse expression of CXCR4-YFP throughout the cytosol and clear expression in the cell membrane in HEK cells^[1]. NUCC-390 dihydrochloride (0-1.25 μ M; 24 hours) boosts axonal growth in cultured cerebellar granule neurons (CGNs) via CXCR4^[2].

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

Western Blot Analysis $^{[1]}$

| Cell Line: | C8161 cells |
|------------------|------------------------------|
| Concentration: | 10 μΜ |
| Incubation Time: | Pre-treated 30 mins |
| Result: | Increased the level of pERK. |

Cell Proliferation Assay^[2]

| Cell Line: | Cerebellar granule neurons (CGNs) | |
|------------------|-------------------------------------|--|
| Concentration: | 0 μΜ; 0.0625 μΜ; 0.25 μΜ; 1.25 μΜ | |
| Incubation Time: | 24 hours | |
| Result: | Stimulated axonal growth via CXCR4. | |

In Vivo

NUCC-390 dihydrochloride (hind limb injection; 3.2 mg/kg; twice daily; 3 days) contributes to the functional and anatomical recovery of the neuromuscular junction (NMJ) following an acute nerve terminal damage by α -LTx in CD-1 mice^[2]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

| Animal Model: | Six to eight-week-old CD1 mice ^[2] | |
|-----------------|---|--|
| Dosage: | 3.2 mg/kg | |
| Administration: | Hind limb injection; twice daily; 3 days | |
| Result: | Promoted functional and anatomical recovery of the NMJ. | |

CUSTOMER VALIDATION

• Neurosci Res. 2022 Dec 30;S0168-0102(22)00323-6.

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REFERENCES

[1]. Mishra RK, et al. Discovery and characterization of novel small-molecule CXCR4 receptor agonists and antagonists. Sci Rep. 2016 Jul 26;6:30155.

 $\label{lem:caution:Product} \textbf{Caution: Product has not been fully validated for medical applications. For research use only.}$

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