

Product Name: CMPI hydrochloride

Catalog No.: 5963

Batch No.: 1

CAS Number: 2250025-94-4

IUPAC Name: 3-(2-Chlorophenyl)-5-(5-methyl-1-(piperidin-4-yl)-1H-pyrazol-4-yl)isoxazole hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₈H₁₉ClN₄O.HCl

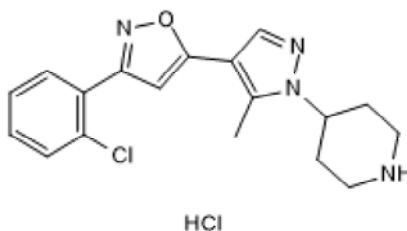
Batch Molecular Weight: 379.28

Physical Appearance: Off White solid

Solubility: water to 50 mM
DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	57	5.31	14.76
Found	57.15	5.3	14.74

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Description:

CMPI hydrochloride is a potent positive allosteric modulator of $\alpha 4\beta 2$ nAChRs (EC_{50} values are 20 and 18 nM for rat and human, respectively). Selective for $\alpha 4\beta 2$ over $\alpha 3\beta 2$, $\alpha 3\beta 4$ and $\alpha 7$. Inhibits $(\alpha 4)_2(\beta 2)_3$, muscle-type and Torpedo nAChRs (IC_{50} values are 0.5, 0.7 and 0.2 μ M, respectively), but not $(\alpha 4)_3(\beta 2)_2$ receptors. Exhibits ability to photoincorporate into aliphatic and nucleophilic amino acid side chains.

Physical and Chemical Properties:

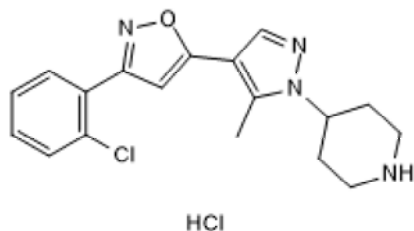
Batch Molecular Formula: $C_{18}H_{19}ClN_4O \cdot HCl$

Batch Molecular Weight: 379.28

Physical Appearance: Off White solid

Minimum Purity: $\geq 98\%$

Batch Molecular Structure:



References:

Wang et al (2017) Unraveling amino acid residues critical for allosteric potentiation of $(\alpha 4)_3(\beta 2)_2$ -type nicotinic acetylcholine receptor responses. *J.Biol.Chem.* **292** 9988. PMID: 28446611.

Hamouda (2016) Photolabeling a nicotinic acetylcholine receptor (nAChR) with an $(\alpha 4)_3(\beta 2)_2$ nAChR-selective positive allosteric modulator. *Mol.Pharmacol.* **89** 575. PMID: 26976945.

Albrecht et al (2008) Discovery and optimization of substituted piperidines as potent, selective, CNS-penetrant $\alpha 4\beta 2$ nicotinic acetylcholine receptor potentiators. *Bioorg.Med.Chem.Lett.* **18** 5209. PMID: 18789861.

Storage: Store at $-20^{\circ}C$

Solubility & Usage Info:

water to 50 mM

DMSO to 100 mM

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a $45-60^{\circ}C$ water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at $-20^{\circ}C$ or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

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