

Product Name: LEI 101 hydrochloride

Catalog No.: 5826

Batch No.: 1

CAS Number: 2250025-91-1

IUPAC Name: 3-Cyclopropyl-1-[[4-[6-[(1,1-dioxido-4-thiomorpholinyl)methyl]-5-fluoro-2-pyridinyl]phenyl]methyl]-2,4-imidazolidinedione hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₃H₂₅FN₄O₄S.HCl

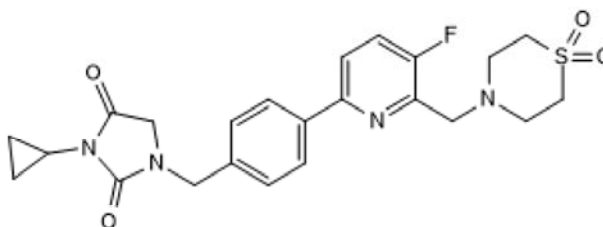
Batch Molecular Weight: 508.99

Physical Appearance: White solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



HCl

2. ANALYTICAL DATA

HPLC: Shows 100% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen	Chlorine
Theoretical	54.27	5.15	11.01	6.97
Found	54.34	5.11	10.88	6.76

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Description:

Potent and selective CB₂ partial agonist (pEC₅₀ = 8.0). Exhibits >100-fold selectivity for CB₂ over CB₁ and no significant interaction with hFAAH, MAGL, DAGL or NAPE-PLD. Displays antinociceptive activity in a rat neuropathic pain model and attenuates renal inflammation in a mouse kidney damage model. Orally bioavailable with low brain penetration.

Physical and Chemical Properties:

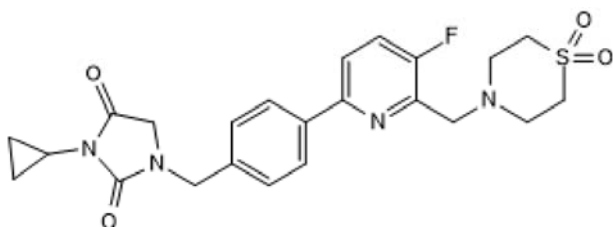
Batch Molecular Formula: C₂₃H₂₅FN₄O₄S.HCl

Batch Molecular Weight: 508.99

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



HCl

Storage: Store at -20°C

Solubility & Usage Info:

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°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°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

References:

Mukhopadhyay et al (2016) The novel, orally available and peripherally restricted selective cannabinoid CB₂ receptor agonist LEI-101 prevents cisplatin-induced nephrotoxicity. *Br.J.Pharmacol.* **173** 446. PMID: 26398481 .

van der Stelt M et al (2011) Discovery and optimization of 1-(4-(pyridin-2-yl)benzyl)imidazolidine-2,4-dione derivatives as a novel class of selective cannabinoid CB₂ receptor agonists. *J.Med.Chem.* **54** 7350. PMID: 21923175.

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