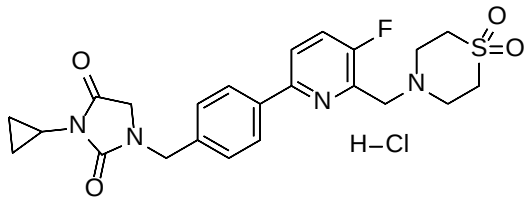
Product data sheet

MedKoo Cat#: 462210 Name: LEI 101 hydrochloride CAS: 2250025-91-1 Chemical Formula: $C_{23}H_{26}ClFN_4O_4S$ Exact Mass: 508.1347 Molecular Weight: 508.9934	
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:
LEI 101 hydrochloride is potent and selective CB2 partial agonist.

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	50.9	100.0

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	1.96 mL	9.82 mL	19.65 mL
5 mM	0.39 mL	1.96 mL	3.93 mL
10 mM	0.20 mL	0.98 mL	1.96 mL
50 mM	0.04 mL	0.20 mL	0.39 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. Mukhopadhyay P, Baggelaar M, Erdelyi K, Cao Z, Cinar R, Fezza F, Ignatowska-Janlowska B, Wilkerson J, van Gils N, Hansen T, Ruben M, Soethoudt M, Heitman L, Kunos G, Maccarrone M, Lichtman A, Pacher P, Van der Stelt M. The novel, orally available and peripherally restricted selective cannabinoid CB2 receptor agonist LEI-101 prevents cisplatin-induced nephrotoxicity. Br J Pharmacol. 2016 Feb;173(3):446-58. doi: 10.1111/bph.13338. Epub 2016 Jan 15. PMID: 26398481; PMCID: PMC4728411.
2. van der Stelt M, Cals J, Broeders-Josten S, Cottney J, van der Doelen AA, Hermkens M, de Kimpe V, King A, Klomp J, Oosterom J, Pols-de Rooij I, de Roos J, van Tilborg M, Boyce S, Baker J. 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. 2011 Oct 27;54(20):7350-62. doi: 10.1021/jm200916p. Epub 2011 Sep 29. PMID: 21923175.

In vivo study

1. Mukhopadhyay P, Baggelaar M, Erdelyi K, Cao Z, Cinar R, Fezza F, Ignatowska-Janlowska B, Wilkerson J, van Gils N, Hansen T, Ruben M, Soethoudt M, Heitman L, Kunos G, Maccarrone M, Lichtman A, Pacher P, Van der Stelt M. The novel, orally available and peripherally restricted selective cannabinoid CB2 receptor agonist LEI-101 prevents cisplatin-induced nephrotoxicity. Br J Pharmacol. 2016 Feb;173(3):446-58. doi: 10.1111/bph.13338. Epub 2016 Jan 15. PMID: 26398481; PMCID: PMC4728411.
2. van der Stelt M, Cals J, Broeders-Josten S, Cottney J, van der Doelen AA, Hermkens M, de Kimpe V, King A, Klomp J, Oosterom J, Pols-de Rooij I, de Roos J, van Tilborg M, Boyce S, Baker J. 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. 2011 Oct 27;54(20):7350-62. doi: 10.1021/jm200916p. Epub 2011 Sep 29. PMID: 21923175.

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7. Bioactivity

Biological target:

LEI-101 is a potent, selective, and orally bioavailable cannabinoid CB2 receptor agonist, with a pEC_{50} of 8 for hCB2, and a pK_i of less than 4 for hERG.

In vitro activity

LEI-101 behaved as a partial agonist at CB2 receptors using β-arrestin and GTPγS assays and was ~100-fold selective in CB2 /CB1 receptor-binding assays.

Reference: Br J Pharmacol. 2016 Feb;173(3):446-58. https://pubmed.ncbi.nlm.nih.gov/21923175/

In vivo activity

Systematic modification of physicochemical properties, such as lipophilicity and basicity, was used to optimize the pharmacokinetic profile and hERG affinity of this novel class of cannabinoid CB2 receptor agonists. This led to the identification of 44 (LEI 101) as a potent, selective, and orally bioavailable cannabinoid CB2 receptor agonist (hCB2 pEC(50) = 8.0; hERG pK(i) < 4; F(po) = 100%), which was active in a rat spinal nerve ligation model of neuropathic pain.

Reference: J Med Chem. 2011 Oct 27;54(20):7350-62. https://pubmed.ncbi.nlm.nih.gov/21923175/

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.