

## Catalog # 10-3880 JNJ-63533054

CAS# 1802326-66-4

(S)-3-Chloro-N-(2-oxo-2-((1-phenylethyl)amino)ethyl) benzamide Lot # X109531

Potent and selective brain-penetrant GPR139 agonist (EC<sub>50</sub>=16 nM) an orphan G-protein-coupled receptor expressed in the CNS.<sup>1</sup> Tritium-labeled JNJ-63533054 binds to cell membranes expressing GPR139 and can be displaced by putative endogenous ligands.<sup>2</sup> Decreases compulsive-like alcohol drinking and hyperalgesia in alcohol-dependent rodents.<sup>3</sup> Suppresses morphine intake in a mouse self-administration model.<sup>4</sup>

- 1) Dvorak et al. (2015), Identification and SAR of Glycine Benzamides as Potent Agonists for the GPR139 Receptor; ACS Med. Chem. Lett., **6** 1015
- 2) Liu et al. (2015), GPR139, an Orphan Receptor Highly Enriched in the Habenula and Septum, Is Activated by the Essential Amino Acids L-Tryptophan and L-Phenylalanine; Mol. Pharmacol., 88 911
- 3) Kononoff et al. (2018), Systemic and Intra-Habenular Activation of the Orphan G Protein-Coupled Receptor GPR139 Decreases Compulsive-Like Alcohol Drinking and Hyperalgesia in Alcohol-Dependent Rats; eNeuro, 5 ENEURO 0153-18 2018
- 4) Wang et al. (2019), Genetic behavioral screen identifies an orphan anti-opioid system; Science, 365 1267

## PHYSICAL DATA

Molecular Weight: 316.78

Molecular Formula: C<sub>17</sub>H<sub>17</sub>ClN<sub>2</sub>O<sub>2</sub>
Purity: 98% by HPLC

NMR: (Conforms)

Solubility: DMSO (up to 35 mg/ml)

Physical Description: White solid

Storage and Stability: Store as supplied desiccated at -20°C for up to 2 years from the date of purchase. Solutions in

DMSO may be stored at -20°C for up to 2 months.

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