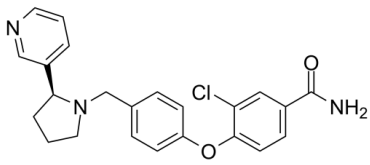
Data Sheet

Product Name:	LY2795050
Cat. No.:	CS-1519
CAS No.:	1346133-08-1
Molecular Formula:	C23H22ClN3O2
Molecular Weight:	407.89
Target:	Opioid Receptor
Pathway:	GPCR/G Protein; Neuronal Signaling
Solubility:	DMSO : 50 mg/mL (122.58 mM; Need ultrasonic)



BIOLOGICAL ACTIVITY:

LY2795050 is a novel selective κ-opioid Receptor (KOR) antagonist (IC50=0.72 nM) and has the potential as a PET tracer to image KOR in vivo. IC50 Value: 0.72 nM (κ-opioid Receptor); 25.8 nM (κ-opioid) [1] Target: κ-opioid Receptor in vitro: LY2795050 displays full antagonist activity and high binding affinity and selectivity for KOR with a ki value of 0.72 nM [1]. in vivo: In the brain, (11)C-LY2795050 displayed fast uptake kinetics (regional activity peak times of <20 min) and an uptake pattern consistent with the distribution of KOR in primates [1]. The LY2795050 ED50 at MOR was 119 μg/kg based on a 1-site model for 11C-carfentanil. The 1-site binding model was also deemed sufficient to describe the specific binding of 11C-LY2795050 at KOR. The ED50 at KOR estimated from the 1-site model was 15.6 μg/kg. Thus, the ED50 ratio for MOR:KOR was 7.6 [2].

References:

[1]. Mitch, Charles H.; Quimby, Steven J.; Diaz, Nuria; et al. Discovery of Aminobenzyloxyarylamides as κ Opioid Receptor Selective Antagonists: Application to Preclinical Development of a κ Opioid Receptor Antagonist Receptor Occupancy Tracer. Journal of Medicinal Chemistry (2011), 54(23), 8000-8012.

[2]. Zheng MQ, Nabulsi N, Kim SJ, Synthesis and evaluation of 11C-LY2795050 as a κ-opioid receptor antagonist radiotracer for PET imaging. J Nucl Med. 2013 Mar;54(3):455-63.

[3]. Kim SJ, Zheng MQ, Nabulsi N, Determination of the In Vivo Selectivity of a New κ-Opioid Receptor Antagonist PET Tracer 11C-LY2795050 in the Rhesus Monkey. J Nucl Med. 2013 Aug 5.

CAIndexNames:

Benzamide, 3-chloro-4-[4-[[(2S)-2-(3-pyridinyl)-1-pyrrolidinyl]methyl]phenoxy]-

SMILES:

O=C(N)C1=CC=C(OC2=CC=C(CN3[C@H](C4=CC=CN=C4)CCC3)C=C2)C(Cl)=C1

Caution: Product has not been fully validated for medical applications. For research use only.

Tel: 732-484-9848 Fax: 888-484-5008 E-mail: sales@ChemScene.com

Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA