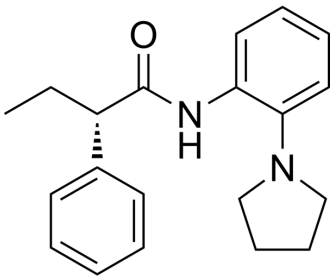
ML252

Cat. No.:	HY-18063
CAS No.:	1392494-64-2
Molecular Formula:	$C_{20}H_{24}N_2O$
Molecular Weight:	308.42
Target:	Potassium Channel; Cytochrome P450
Pathway:	Membrane Transporter/Ion Channel; Metabolic Enzyme/Protease
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description	ML252 is a selective inhibitor of potassium channel, targeting to KCNQ2 channel (Kv7.2) (IC_{50}=69 nM). ML252 also inhibits Cytochrome P450 with IC_{50}s of 6.1 nM (CYP1A2), 18.9 nM (CYP2C9), 3.9 nM (CYP3A4), 19.9 nM (CYP2D6), respectively[1][2].

IC_{50} & Target	CYP1A2	CYP2C9	CYP2D6	CYP3A4
	6.1 μM (IC_{50})	18.9 μM (IC_{50})	19.9 μM (IC_{50})	3.9 μM (IC_{50})

In Vitro	ML252 targets to KCNQ1, KCNQ1/E1, KCNQ2/3, and KCNQ4 with IC50s of 2.92 μM, 8.12 μM, 0.12 μM, 0.20 μM, respectively[1]. ML252 (1 μM; 0-48 h) shows an intrinsic clearance and subsequent predicted hepativ clearance of 1720 mL/min/kd and 67.3 mL/min/kg, respectively, in rat hepatic microsomes[1]. ML252 (0.1-10 μM) inhibits the current of KCNQ2 at 0.3 μM, and completely inhibits the current at 1 μM in CHO-KCNQ2 cell line[1]. ML252 (30 μM; 48 h) has no acute toxicity to CHO cells[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	ML252 has the metabolic stability unsuitable for oral administration[2]. ML252 (10 mg/kg, 3 mg/mL; ip; single dose; measured at 1 hr after) shows a highly brain penetrant with a B:P ratio of 1.9 and absolute brain levels of 672 nM in rat model[1].ML252 □□ KCNQ1□KCNQ1/E1□KCNQ2/3 □ KCNQ4□IC_{50} □□□ 2.92 μM□8.12 μM□0.12 μM □ 0.20 μM[1]□ MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Yu H, et al. Identification of a novel, small molecule inhibitor of KCNQ2 channels. 2011 Oct 28 [updated 2013 Feb 25]. In: Probe Reports from the NIH Molecular Libraries Program [Internet]. Bethesda (MD): National Center for Biotechnology Information (US); 2010–.

[2]. Cheung YY, et al. Discovery of a series of 2-phenyl-N-(2-(pyrrolidin-1-yl)phenyl)acetamides as novel molecular switches that modulate modes of K(v)7.2 (KCNQ2) channel pharmacology: identification of (S)-2-phenyl-N-(2-(pyrrolidin-1-yl)phenyl)butanamide (ML252) as a potent, brain penetrant K(v)7.2 channel inhibitor. J Med Chem. 2012 Aug 9;55(15):6975-9.

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

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