Product Name: Nepicastat (SYN-117) HCl

Revision Date: 6/30/2018

Product Data Sheet

Chemical Properties

Product Name: Nepicastat (SYN-117) HCl
Cas No.: 170151-24-3
M.Wt: 331.81
Formula: C14H15F2N3S.HCl

Chemical Name: 4-(aminomethyl)-3-[(2S)-5,7-difluoro-1,2,3,4-tetrahydronaphthalen-2-yl]-1H-imidazole-2-thione;hydrochloride

Canonical SMILES: C1CC2=C(C=C(C2CC1N3C(=C(CN)C3=S)CN)F)F.Cl

Solubility: \( \geq 16.6 \text{mg/mL} \) in DMSO

Storage: Store at -20°C

General tips: For obtaining a higher solubility, please warm the tube at 37°C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C for several months.

Shopping Condition: Evaluation sample solution: ship with blue ice
All other available size: ship with RT, or blue ice upon request

Biological Activity

Targets: Metabolism
Pathways: Dopamine β-hydroxylase

Description:
Nepicastat (SYN-117) HCl is a potent and selective inhibitor of dopamine-β-hydroxylase with IC\textsubscript{50} values of 8.5 and 9.0 nM in bovine and human, respectively [1]. Dopamine-β-hydroxylase is an enzyme involved in the synthesis of small-molecule membrane-bound neurotransmitters. Dopamine-β-hydroxylase catalyses the synthesis of noradrenaline [1].

Nepicastat (SYN-117) HCl is a potent and selective dopamine-β-hydroxylase inhibitor. (R)-Nepicastat exhibited 2-3 fold less potent than nepicastat [1].
In beagle dogs and spontaneously hypertensive rats, nepicastat reduced noradrenaline in a dose-dependent way and increased dopamine and dopamine/noradrenaline ratio in cerebral cortex, left ventricle and the artery. In beagle dogs, nepicastat (2 mg/kg) significantly reduced noradrenaline by 52% and increased dopamine by 646% and dopamine/noradrenaline ratio in plasma [1]. In pithed spontaneously hypertensive rats, nepicastat inhibited the pressor and positive chronotropic due to preganglionic sympathetic nerve stimulation. In spontaneously hypertensive rats, nepicastat (3 mg/kg) exhibited antihypertensive effects and reduced renin vascular resistance by 38% [2]. In rats, nepicastat significantly increased extracellular dopamine accumulation induced by cocaine and amphetamine in the medial prefrontal cortex [3].

Reference: