Print Date: Mar 16th 2022

Certificate of Analysis

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Product Name: **PPTN hydrochloride** **Catalog No.: 4862** **Batch No.: 1**

CAS Number: 1992047-65-0

IUPAC Name: 4-[4-(4-Piperidinyl)phenyl]-7-[4-(trifluoromethyl)phenyl]-2-naphthalenecarboxylic acid hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{29}H_{24}F_3NO_2.HCl.¼H_2O$

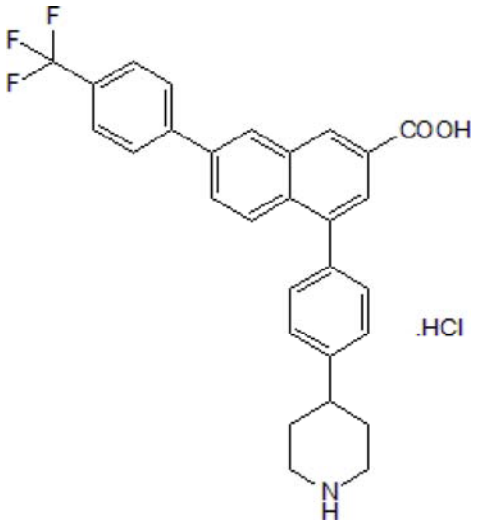
Batch Molecular Weight: 516.46

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 20 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.2 (Chloroform:Methanol [1:4])

HPLC: Shows 99.9% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	67.44	4.98	2.71
Found	67.07	4.83	2.66

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Product Information

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CAS Number: 1992047-65-0

IUPAC Name: 4-[4-(4-Piperidinyl)phenyl]-7-[4-(trifluoromethyl)phenyl]-2-naphthalenecarboxylic acid hydrochloride

Description:

PPTN hydrochloride is a high affinity and selective $P2Y_{14}$ antagonist (K_B = 434 pM), which exhibits >10,000-fold selectivity for $P2Y_{14}$ over other P2Y receptors. PPTN inhibits UDP-glucose and MRS 2690-induced porcine pancreatic artery contraction ex vivo, and also blocks UDP-glucose-induced chemotaxis of HL-60 leukemia cells in vitro.

Physical and Chemical Properties:

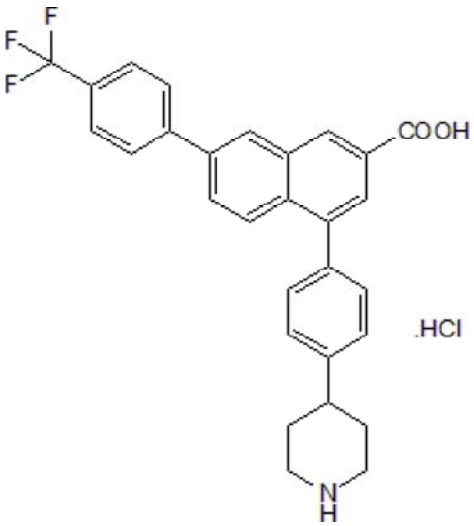
Batch Molecular Formula: $C_{29}H_{24}F_3NO_2.HCl.¼H_2O$

Batch Molecular Weight: 516.46

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol to 20 mM

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

References:

Alsaqati *et al* (2014) Novel vasocontractile role of the $P2Y_{14}$ receptor: characterization of its signalling in porcine isolated pancreatic arteries. Br.J.Pharmacol. ***171*** 701. PMID: 24138077.

Barrett *et al* (2013) A selective high-affinity antagonist of the $P2Y_{14}$ receptor inhibits UDP-glucose-stimulated chemotaxis of human neutrophils. Mol.Pharmacol. ***84*** 41. PMID: 23592514 .

Gao *et al* (2013) The role of $P2Y_{14}$ and other P2Y receptors in degranulation of human LAD2 mast cells. Purinergic Signal. ***9*** 31. PMID: 22825617.