TOCRIS
a bio-techne brand

Print Date: Feb 4th 2020

Certificate of Analysis

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Product Name: **A 317491 sodium salt** **Catalog No.: 6493** **Batch No.: 1**

IUPAC Name: 5-[[[(3-Phenoxyphenyl)methyl][(1*S*)-1,2,3,4-tetrahydro-1-naphthalenyl]amino]carbonyl]-1,2,4-benzenetricarboxylic acid disodium salt

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{33}H_{25}NO_8Na_2.2¾H_2O$

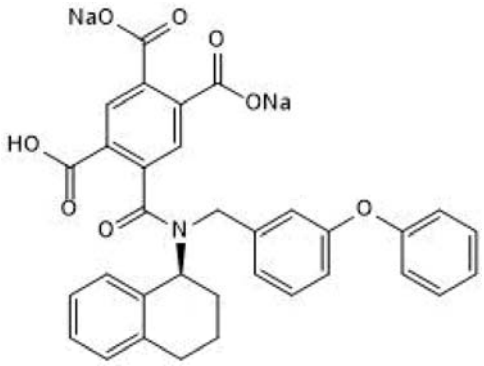
Batch Molecular Weight: 659.08

Physical Appearance: White solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.6% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	60.14	4.66	2.13
Found	59.73	4.56	1.95

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Product Information

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Description:

Selective, high affinity non-nucleotide $P2X_3$ and $P2X_{2/3}$ receptor antagonist (K_i values are 9, 22, 22 and 92 nM at human $P2X_{2/3}$, rat $P2X_3$, human $P2X_3$ and rat $P2X_{2/3}$, respectively); blocks recombinant human and rat $P2X_3$ and $P2X_{2/3}$ receptor-mediated calcium flux (K_i = 22 - 92 nM). Exhibits selectivity over other P2 receptors and other neurotransmitter receptors, ion channels, and enzymes (IC_{50} > 5 µM). Reduces mechanical allodynia and thermal hyperalgesia in the CCI in vivo models. Antinociceptive.

Physical and Chemical Properties:

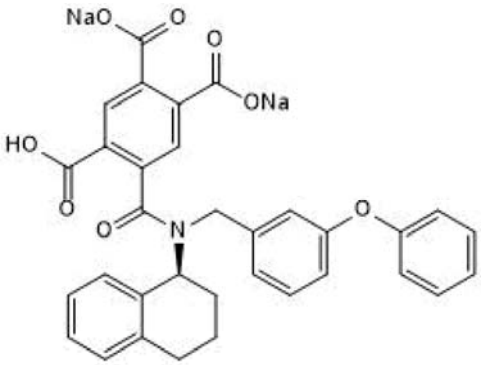
Batch Molecular Formula: $C_{33}H_{25}NO_8Na_2.2¾H_2O$

Batch Molecular Weight: 659.08

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 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:

Mansoor *et al* (2016) X-ray structures define human $P2X_3$ receptor gating cycle and antagonist action. Nature ***538*** 66. PMID: 27626375.

McGaraughty *et al* (2005) Endogenous opioid mechanisms partially mediate P2X3/P2X2/3-related antinociception in rat models of inflammatory and chemogenic pain but not neuropathic pain. Br.J.Pharmacol. ***146*** 180. PMID: 16041397.

McGaraughty *et al* (2003) Effects of A-317491, a novel and selective $P2X_3$/$P2X_{2/3}$ receptor antagonist, on neuropathic, inflammatory and chemogenic nociception following intrathecal and intraplantar administration. Br.J.Pharmacol. ***140*** 1381. PMID: 14623769.

Neelands *et al* (2003) 2', 3'-O-(2,4,6,trinitrophenyl)-ATP and A-317491 are competitive antagonists at a slowly desensitizing chimeric human $P2X_3$ receptor. Br.J.Pharmacol. ***140*** 202. PMID: 12967950.

Jarvis *et al* (2002) A-317491, a novel potent and selective non-nucleotide antagonist of $P2X_3$ and $P2X_{2/3}$ receptors, reduces chronic inflammatory and neuropathic pain in the rat. Proc.Nat.Acad.Sci.USA ***99*** 17179. PMID: 12482951 .

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