Print Date: Nov 18th 2021

Certificate of Analysis

www.tocris.com

Product Name: **TAK 779** **Catalog No.: 4340** **Batch No.: 1**

CAS Number: 229005-80-5

IUPAC Name: *N*-[[4-[[[6,7-Dihydro-2-(4-methylphenyl)-5*H*-benzocyclohepten-8-yl]carbonyl]amino]phenyl]methyl] tetrahydro-*N*,*N*-dimethyl-2*H*-pyran-4-aminium chloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{33}H_{39}N_2O_2.Cl.3½H_2O$

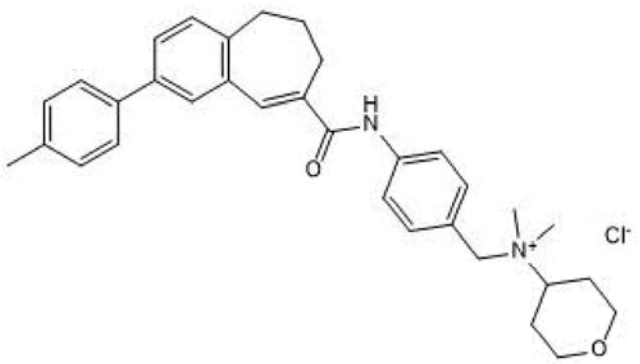
Batch Molecular Weight: 594.18

Physical Appearance: Cream solid

Solubility: water to 10 mM
DMSO to 5 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.8% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	66.71	7.8	4.71
Found	66.35	7.57	4.69

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Product Information

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Description:

TAK 779 is a potent and selective CCR5 and CCR2 chemokine receptor antagonist (IC_{50} values = 1 nM and 27 nM, respectively). TAK 779 blocks the binding of macrophage inflammatory protein 1α and 1β to CHO cells (IC_{50} = 1 nM) and inhibits replication of R5 HIV-1 at 1.6-3.7 nM. In animal models, TAK 779 protects against ischemic brain injury and prevents development of asthma features.

Physical and Chemical Properties:

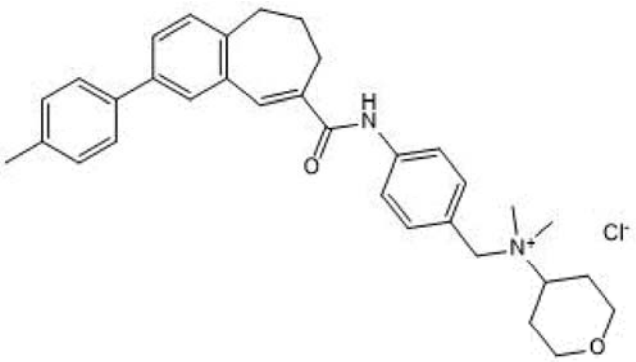
Batch Molecular Formula: $C_{33}H_{39}N_2O_2.Cl.3½H_2O$

Batch Molecular Weight: 594.18

Physical Appearance: Cream solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

water to 10 mM
DMSO to 5 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:

Suzaki *et al* (2008) A small-molecule compound targetinCCR5 and CXCR3 prevents airway hyperresponsiveness and inflammation. Eur.Respir.J. ***31*** 783. PMID: 18094012.

Takami *et al* (2002) TAK-779, a nonpeptide CC chemokine receptor antagonist, protects the brain against focal cerebral ischemia in mice. J.Cereb.Blood Flow Metab. ***22*** 780. PMID: 12142563.

Baba *et al* (1999) A small-molecule, nonpeptide CCR5 antagonist with highly potent and selective anti-HIV-1 activity. Proc.Natl.Acad.Sci.U.S.A. ***96*** 5698. PMID: 10318947.