TOCRIS
a bio-techne brand

Print Date: Jan 15th 2016

Certificate of Analysis

www.tocris.com

Product Name: **BX 513 hydrochloride** **Catalog No.: 2769** **Batch No.: 1**

CAS Number: 1216540-18-9

IUPAC Name: 4-(4-Chlorophenyl)-4-hydroxy-α,α-diphenyl-1-piperidinepentanenitrile hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{28}H_{29}ClN_2O.HCl$

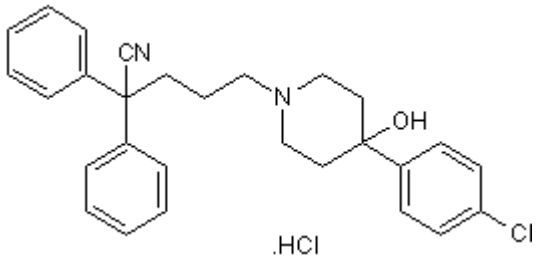
Batch Molecular Weight: 481.46

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 50 mM

Storage: Desiccate at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.3 (Chloroform:Methanol [95:5])

HPLC: Shows >99.2% purity

^{1}H NMR: Consistent with structure

^{13}C NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	69.85	6.28	5.82
Found	69.52	6.32	5.84

bio-techne.com
info@bio-techne.com
techsupport@bio-techne.com

North America
Tel: (800) 343 7475

China
info.cn@bio-techne.com
Tel: +86 (21) 52380373

Europe Middle East Africa
Tel: +44 (0)1235 529449

Rest of World
www.tocris.com/distributors
Tel:+1 612 379 2956

Product Information

Product Name: **BX 513 hydrochloride** **Catalog No.: 2769** **Batch No.: 1**

CAS Number: 1216540-18-9

IUPAC Name: 4-(4-Chlorophenyl)-4-hydroxy-α,α-diphenyl-1-piperidinepentanenitrile hydrochloride

Description:

Selective CCR1 receptor antagonist (K_i values are 0.04, > 10, > 10 and > 10 nM for CCR1, CCR5, CXCR2 and CXCR4 receptors respectively). Inhibits MIP-1α-induced intracellular calcium mobilization (IC_{50} = 2.5 μM). Also a full inverse agonist at US28, a HCMV-encoded chemokine receptor.

Physical and Chemical Properties:

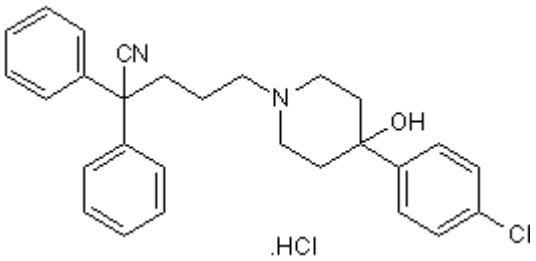
Batch Molecular Formula: $C_{28}H_{29}ClN_2O.HCl$

Batch Molecular Weight: 481.46

Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Desiccate at +4°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol to 50 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:

Hesselgesser *et al* (1998) Identification and characterisation of small molecule functional antagonists of the CCR1 chemokine receptor. J.Biol.Chem. ***273*** 15687. PMID: 9624164.

Ng *et al* (1999) Discovery of a novel non-peptide CCR1 receptor antagonists. J.Med.Chem. ***42*** 4680. PMID: 10579830.

Casarosa *et al* (2003) Identification of the first nonpeptidergic inverse agonist for a constitutively active viral-encoded G-protein-coupled receptor. J.Biol.Chem. ***278*** 5172. PMID: 12456673.

bio-techne.com
info@bio-techne.com
techsupport@bio-techne.com

North America
Tel: (800) 343 7475

China
info.cn@bio-techne.com
Tel: +86 (21) 52380373

Europe Middle East Africa
Tel: +44 (0)1235 529449

Rest of World
www.tocris.com/distributors
Tel:+1 612 379 2956