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Print Date: Jan 8th 2016

Certificate of Analysis

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Product Name: **L-745,870 trihydrochloride** **Catalog No.: 1002** **Batch No.: 7**

CAS Number: 866021-03-6

IUPAC Name: 3-(4-[4-Chlorophenyl]piperazin-1-yl)-methyl-1*H*-pyrrolo[2,3-*b*]pyridine trihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{18}H_{19}N_4Cl.3HCl.½H_2O$

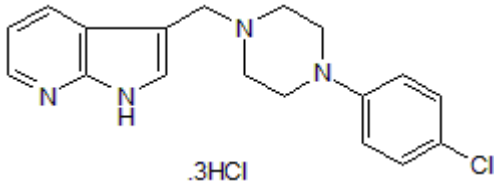
Batch Molecular Weight: 445.22

Physical Appearance: White solid

Solubility: water to 100 mM
physiological saline to 50 mM with gentle warming

Storage: Desiccate at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.48 (Chloroform:Methanol:Ammonia soln. [90:9:1])

HPLC: Shows >99.5% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	48.56	5.21	12.58
Found	48.51	5.15	12.4

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

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Description:

A highly potent and selective D_4 dopamine receptor antagonist; L-745,870 has K_i values of 0.51, 2300 and 960 nM for D_4, D_3 and D_2 subtypes respectively and > 1000-fold selectivity over 5-HT_2, D_1 and D_5 receptors.

Physical and Chemical Properties:

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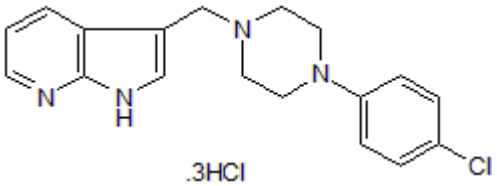
Batch Molecular Weight: 445.22

Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Desiccate at +4°C

Solubility & Usage Info:

water to 100 mM
physiological saline to 50 mM with gentle warming

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:

Kulagowski *et al* (1996) 3-[[4-(4-Chlorophenyl)piperazin-1-yl]methyl-1*H*-pyrrolo[2,3-b]pyridine: an antagonist with high affinity and selectivity for the human D_4 receptor. J.Med.Chem. ***39*** 1941. PMID: 8642550.

Patel *et al* (1997) Biological profile of L-745,870, a selective antagonist with high affinity for the dopamine D_4 receptor. J.Pharmacol.Exp.Ther. ***283*** 636. PMID: 9353380.

Bristow *et al* (1997) Schizophrenia and L-745, 870 a novel dopamine D_4 receptor antagonist. TiPS ***18*** 186. PMID: 9226994.

Pillai *et al* (1998) Human D_2 and D_4 dopamine receptors couple through βγ G-protein subunits to inwardly rectifying K^+ channels (GIRK1) in a *Xenopus* oocyte expression system: selective antagonism by L-741,626 and L-745,870 respectively. Neuropharmacology ***37*** 983. PMID: 9833627.