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Print Date: Sep 16th 2016

Certificate of Analysis

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Product Name: **PG 01037 dihydrochloride** **Catalog No.: 3887** **Batch No.: 2**

CAS Number: 675599-62-9

IUPAC Name: *N*-[(2*E*)-4-[4-(2,3-Dichlorophenyl)-1-piperazinyl]-2-buten-1-yl]-4-(2-pyridyl)-benzamide dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{26}H_{26}Cl_2N_4O.2HCl.1¼H_2O$

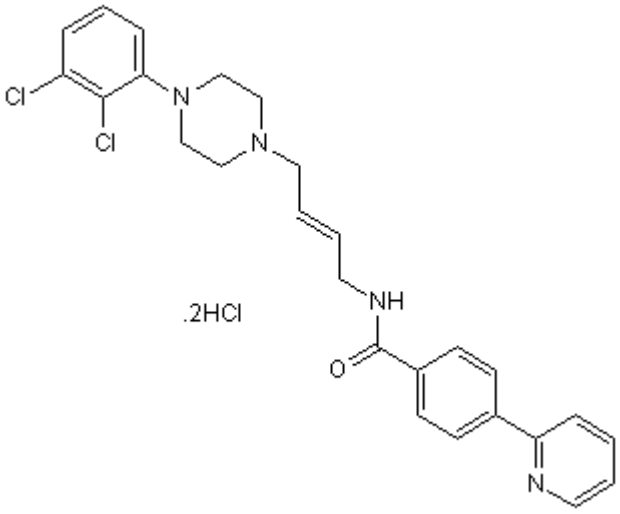
Batch Molecular Weight: 576.86

Physical Appearance: White solid

Solubility: water to 20 mM with gentle warming
DMSO to 100 mM

Storage: Desiccate at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.3 (10% MeOH/CHCl3 (+NH4OH))

HPLC: Shows >98.9% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	54.14	5.33	9.71
Found	53.83	5.22	9.61

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Description:

Dopamine D_3 receptor antagonist; 133-fold selective for D_3 over D_2 receptors in vitro (K_i values are 0.70, 93.3 and 375 nM for D_3, D_2 and D_4 receptors respectively). Attenuates abnormal involuntary movements associated with L-DOPA (Cat. No. 3788) in rat models of Parkinson's disease. Inhibits the effects of methamphetamine; attenuates drug-induced behaviors in vivo.

Physical and Chemical Properties:

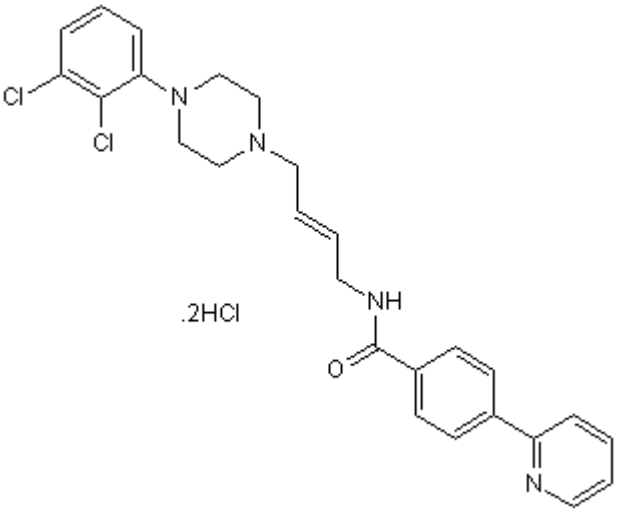
Batch Molecular Formula: $C_{26}H_{26}Cl_2N_4O.2HCl.1¼H_2O$

Batch Molecular Weight: 576.86

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Desiccate at +4°C

Solubility & Usage Info:

water to 20 mM with gentle warming
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:

Mason *et al* (2010) Characterization of the transport, metabolism, and pharmacokinetics of the dopamine D3 receptor-delective fluorenyl-and 2-pyridylphenyl amides developed for treatment of psychostimulant abuse. J.Pharm.Exp.Ther. ***333*** 854.

Kumar *et al* (2009) Evaluation of the D3 dopamine receptor selective antagonist PG01037 on L-dopa-dependent abnormal involuntary movements in rats. Neuropharmacology ***56*** 944. PMID: 19371585.

Grundt *et al* (2007) Heterocyclic analogues of *N*-(4-(4-(2,3-dichlorophenyl)piperazin-1-butyl)arylcarboxamides with functionalized linking chains as novel dopamine D3 receptor ligands: potential substance abuse therapeutic agents. J.Med.Chem. ***50*** 4135. PMID: 17672446.

Grundt *et al* (2005) Novel heterocyclic trans olefin analogues of *N*-{4-[4-(2,3-dichlorophenyl)piperazin-1-yl]butyl}arylcarboxamides as selective probes with high affinity for the dopamine D3 receptor. J.Med.Chem. ***48*** 839. PMID: 15689168.

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