

Certificate of Analysis

Product Name: JHW 007 hydrochloride

Catalog No.: 4351

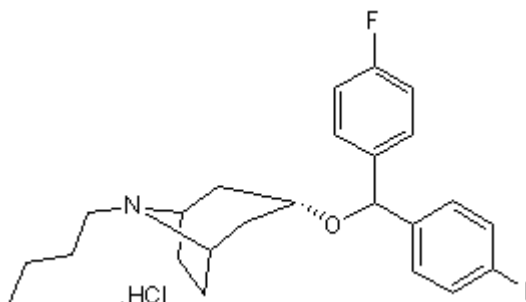
Batch No.: 1

CAS Number: 202645-74-7

IUPAC Name: (3-endo)-3-[Bis(4-fluorophenyl)methoxy]-8-butyl-8-azabicyclo[3.2.1]octane hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:	C ₂₄ H ₂₉ F ₂ NO.HCl
Batch Molecular Weight:	421.95
Physical Appearance:	White solid
Solubility:	DMSO to 100 mM ethanol to 100 mM
Storage:	Store at -20°C
Batch Molecular Structure:	



2. ANALYTICAL DATA

TLC:	R _f = 0.7 (Dichloromethane:Methanol:Ammonia soln. [9:1:0.05])
HPLC:	Shows 100% purity
¹H NMR:	Consistent with structure
Mass Spectrum:	Consistent with structure
Microanalysis:	

	Carbon	Hydrogen	Nitrogen
Theoretical	68.32	7.17	3.32
Found	68.46	7.22	3.33

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

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Description:

Dopamine uptake inhibitor; displays high affinity for the dopamine transporter (DAT) ($K_i = 25$ nM compared to 1330 and 1730 for NET and SERT respectively). Suppresses the effects of cocaine administration in a dose-dependent manner and decreases cocaine and methamphetamine self-administration in rats.

Physical and Chemical Properties:

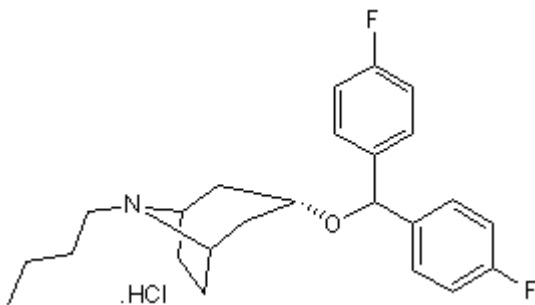
Batch Molecular Formula: $C_{24}H_{29}F_2NO.HCl$

Batch Molecular Weight: 421.95

Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol 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:

Kopajtic et al (2010) Dopamine transporter-dependent and -independent striatal binding of the benztrapine analog JHW 007, a cocaine antagonist with low abuse liability. *J.Pharmacol.Exp.Ther.* **335** 703. PMID: 20855444.

Velaquez-Sanchez et al (2010) The high affinity dopamine uptake inhibitor, JHW 007, blocks cocaine-induced reward, locomotor stimulation and sensitization. *Eur.Neuropsychopharmacol.* **20** 501. PMID: 20413276.

Kristensen et al (2011) SLC6 neurotransmitter transporters: structure, function, and regulation. *Pharm.Rev.* **63** (3) 585.

Hiranita et al (2014) Preclinical efficacy of N-substituted benztrapine analogs as antagonists of methamphetamine self-administration in rats. *J.Pharmacol.Exp.Ther.* **348** 174. PMID: 24194527.

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