bio-techne
TOCRIS

Print Date: Aug 10th 2023

Certificate of Analysis

www.tocris.com

Product Name: **L-368,899 hydrochloride** **Catalog No.: 2641** **Batch No.: 4**

IUPAC Name: (2*S*)-2-Amino-*N*-[(1*S*,2*S*,4*R*)-7,7-dimethyl-1-[[[4-(2-methylphenyl)-1-piperazinyl]sulfonyl]methyl]bicyclo[2.2.1]hept-2-yl]-4-(methylsulfonyl)butanamide dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{26}H_{42}N_4O_5S_2.2HCl$.

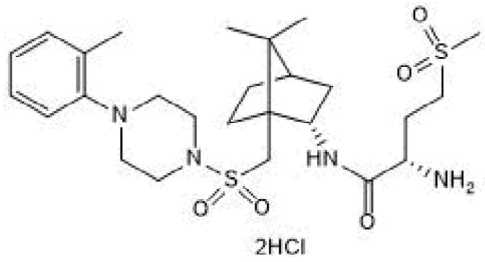
Batch Molecular Weight: 627.7

Physical Appearance: Off-white solid

Solubility: water to 100 mM
DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.5% purity

Chiral HPLC: Shows 100.0% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: $[\alpha]_D$ = +20 (Concentration = 1, Solvent = Methanol)

Microanalysis:

	Carbon	Hydrogen	Nitrogen	Chlorine
Theoretical	49.75	7.07	8.93	11.3
Found	49.03	7.42	8.78	9.6

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 Name: **L-368,899 hydrochloride** **Catalog No.: 2641** **4**

IUPAC Name: (2*S*)-2-Amino-*N*-[(1*S*,2*S*,4*R*)-7,7-dimethyl-1-[[[4-(2-methylphenyl)-1-piperazinyl]sulfonyl]methyl]bicyclo[2.2.1]hept-2-yl]-4-(methylsulfonyl)butanamide dihydrochloride

Description:

L-368,899 hydrochloride is a potent, non-peptide and orally active oxytocin receptor antagonist (IC_{50} = 8.9 nM) that displays > 40-fold selectivity over vasopressin V_{1a} and V_2 receptors (IC_{50} values are 370 and 570 nM respectively). Antagonizes oxytocin-induced uterine contractions in vitro and in vivo.

Physical and Chemical Properties:

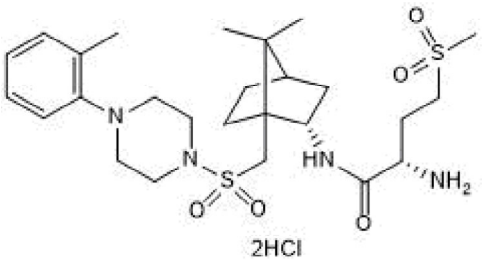
Batch Molecular Formula: $C_{26}H_{42}N_4O_5S_2.2HCl$.

Batch Molecular Weight: 627.7

Physical Appearance: Off-white solid

Minimum Purity: ≥97%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

water to 100 mM
DMSO to 100 mM

When purchased as a 1mg unit, this product is supplied as a lyophilized solid and may be very hard to visualize. Solutions should be made by adding solvent directly to the vial. The vial should then be vortexed vigorously to ensure the product has completely dissolved.

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. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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:

Borthwick (2010) Oral oxyt. antagonists. J.Med.Chem. ***53*** 6525. PMID: 20550119.

Quattropani *et al* (2005) Discovery and development of a new class of potent, selective, orally active oxyt. receptor antagonist. J.Med.Chem. ***48*** 7882. PMID: 16302826.

Mann *et al* (2003) Attenuation of $PGE_{2\alpha}$ release in ewes infused with the oxyt. antagonist L-368,899. Domest.Anim.Endocrinol. ***25*** 255. PMID: 14550509.