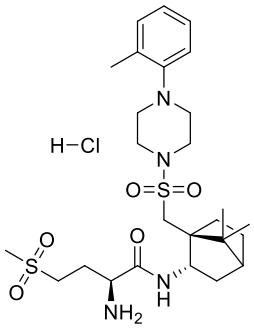
Product data sheet

MedKoo Cat#: 532058 Name: L-368899 HCl CAS: 160312-62-9 (HCl) Chemical Formula: $C_{26}H_{43}ClN_4O_5S_2$ Exact Mass: 590.2363 Molecular Weight: 591.223	
Product supplied as:	Powder
Purity (by HPLC):	≥ 98%
Shipping conditions	Ambient temperature
Storage conditions:	Powder: -20°C 3 years; 4°C 2 years.
	In solvent: -80°C 3 months; -20°C 2 weeks.

1. Product description:
L-368899 is a non-peptide and orally active oxytocin receptor antagonist that displays > 40-fold selectivity over vasopressin V1a and V2 receptors. L-368,899 HCl antagonizes oxytocin-induced uterine contractions in vitro and in vivo.

2. CoA, QC data, SDS, and handling instruction
SDS and handling instruction, CoA with copies of QC data (NMR, HPLC and MS analytical spectra) can be downloaded from the product web page under "QC And Documents" section. Note: copies of analytical spectra may not be available if the product is being supplied by MedKoo partners. Whether the product was made by MedKoo or provided by its partners, the quality is 100% guaranteed.

3. Solubility data

Solvent	Max Conc. mg/mL	Max Conc. mM
DMSO	94.56	159.94
Water	54.56	92.28

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	1.69 mL	8.46 mL	16.91 mL
5 mM	0.34 mL	1.69 mL	3.38 mL
10 mM	0.17 mL	0.85 mL	1.69 mL
50 mM	0.03 mL	0.17 mL	0.34 mL

5. Molarity Calculator, Reconstitution Calculator, Dilution Calculator
Please refer the product web page under section of "Calculator"

6. Recommended literature which reported protocols for in vitro and in vivo study
In vitro study

1. Williams PD, Anderson PS, Ball RG, Bock MG, Carroll L, Chiu SH, Clineschmidt BV, Culberson JC, Erb JM, Evans BE, et al. 1-((7,7-Dimethyl-2(S)-(2(S)-amino-4-(methylsulfonyl)butyramido)bicyclo [2.2.1]-heptan-1(S)-yl)methyl)sulfonyl)-4-(2-methylphenyl)piperaz ine (L-368,899): an orally bioavailable, non-peptide oxytocin antagonist with potential utility for managing preterm labor. J Med Chem. 1994 Mar 4;37(5):565-71. doi: 10.1021/jm00031a004. PMID: 8126695.

In vivo study

1. Williams PD, Anderson PS, Ball RG, Bock MG, Carroll L, Chiu SH, Clineschmidt BV, Culberson JC, Erb JM, Evans BE, et al. 1-((7,7-Dimethyl-2(S)-(2(S)-amino-4-(methylsulfonyl)butyramido)bicyclo [2.2.1]-heptan-1(S)-yl)methyl)sulfonyl)-4-(2-methylphenyl)piperaz ine (L-368,899): an orally bioavailable, non-peptide oxytocin antagonist with potential utility for managing preterm labor. J Med Chem. 1994 Mar 4;37(5):565-71. doi: 10.1021/jm00031a004. PMID: 8126695.

7. Bioactivity
Biological target:

L-368,899 hydrochloride is a potent, selective, orally bioavailable, non-peptide Oxytocin Receptor antagonist, with IC_{50}s of 8.9 nM and 26 nM for rat uterus and human uterus oxytocin receptor, respectively.

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In vitro activity

Compound 7 (L-368,899) exhibited the best overall profile of OT receptor affinity (IC50 = 8.9 nM, rat uterus; 26 nM, human uterus), potency for inhibition of OT-stimulated contractions of the isolated rat uterus (pA2 = 8.9) and in situ rat uterus (AD50 = 0.35 mg/kg after intravenous (i.v.) administration and 7.0 mg/kg after intraduodenal administration), aqueous solubility (3.7 mg/mL at pH 5.0), and oral bioavailability in several species (35% (rat), 25% (dog), and 21% (chimpanzee) as estimated from radioreceptor determination of drug levels in plasma after oral and i.v. dosing).

Reference: J Med Chem. 1994 Mar 4;37(5):565-71. https://pubmed.ncbi.nlm.nih.gov/8126695/

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