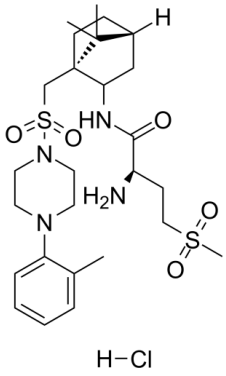
Data Sheet

Product Name:	L-368,899 hydrochloride
Cat. No.:	CS-0029461
CAS No.:	160312-62-9
Molecular Formula:	C26H43ClN4O5S2
Molecular Weight:	591.23
Target:	Oxytocin Receptor
Pathway:	GPCR/G Protein
Solubility:	DMSO : 130 mg/mL (219.88 mM; Need ultrasonic)



BIOLOGICAL ACTIVITY:

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, used as a tocolytic agent. IC50 & Target: IC50: 8.9 nM (rat uterus oxytocin receptor), 26 nM (human uterus oxytocin receptor)[1] **In Vitro:** L-368,899 hydrochloride is a potent, 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. L-368,899 is less active on vasopressin receptor in human liver and kidney, rat liver and kidney (IC_{50}, 510 nM, 960 nM, 890 nM, 2400 nM, respectively)[1].

References:

[1]. Williams PD, 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.

CAIndexNames:

Butanamide, 2-amino-N-[7,7-dimethyl-1-[[[4-(2-methylphenyl)-1-piperazinyl]sulfonyl]methyl]bicyclo[2.2.1]hept-2-yl]-4-(methylsulfonyl)-, monohydrochloride, [1S-[1α,2α(R*),4β]]-

SMILES:

O=C(NC1[C@@](C2(C)C)(CS(=O)(N3CCN(C4=CC=CC=C4C)CC3)=O)CC[C@]2([H])C1)[C@H](N)CCS(=O)(C)=O.[H]Cl

Caution: Product has not been fully validated for medical applications. For research use only.

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