

**Product Name:** TC OT 39

**Catalog No.:** 4625

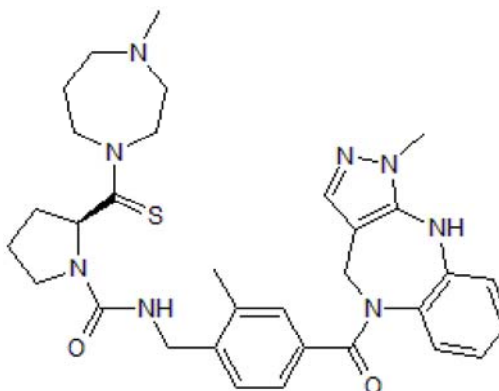
**Batch No.:** 1

CAS Number: 479232-57-0

IUPAC Name: (2S)-N-[[4-[(4,10-Dihydro-1-methylpyrazolo[3,4-b][1,5]benzodiazepin-5(1H)-yl)carbonyl]-2-methylphenyl]methyl]-2-[(hexahydro-4-methyl-1H-1,4-diazepin-1-yl)thioxomethyl]-1-pyrrolidinecarboxamide

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>32</sub>H<sub>40</sub>N<sub>8</sub>O<sub>2</sub>S.H<sub>2</sub>O  
**Batch Molecular Weight:** 618.8  
**Physical Appearance:** Off White solid  
**Solubility:** 1eq. HCl to 100 mM  
DMSO to 100 mM  
**Storage:** Store at -20°C  
**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**TLC:** R<sub>f</sub> = 0.26 (Dichloromethane:Methanol [85:15])  
**HPLC:** Shows 97.7% purity  
**Chiral HPLC:** Shows 98.3% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure  
**Optical Rotation:** [α]<sub>D</sub> = -18.1 (Concentration = 1, Solvent = Methanol)  
**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	62.11	6.84	18.11
Found	61.95	6.58	18.02

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

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**Description:**

Potent non-peptide oxytocin receptor partial agonist (EC<sub>50</sub> values are 33 nM and 850 nM for the oxytocin receptor and V<sub>2</sub> vasopressin receptor respectively). Also a V<sub>1a</sub> vasopressin receptor antagonist (K<sub>i</sub> = 330 nM). Active in vivo in a rat model of uterine response.

**Physical and Chemical Properties:**

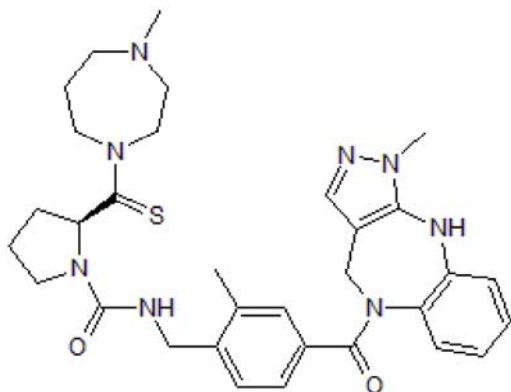
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Batch Molecular Weight: 618.8

Physical Appearance: Off White solid

**Minimum Purity:** >97%

**Batch Molecular Structure:**



**Storage:** Store at -20°C

**Solubility & Usage Info:**

1eq. HCl to 100 mM

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:**

**Frantz et al** (2010) Subtlety of the structure-affinity and structure-efficacy relationships around a nonpeptide oxyt. receptor agonist. *J.Med.Chem.* **53** 1546. PMID: 20104850.

**Pitt et al** (2004) Non-peptide oxyt. agonists. *Bioorg.Med.Chem.Lett.* **14** 4585. PMID: 15357997.

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