

Product Name: YNT 185

Catalog No.: 6739

Batch No.: 1

CAS Number: 1804978-82-2

IUPAC Name: 3'-[[[3-[[2-[[2-(Dimethylamino)benzoyl]amino]ethyl]amino]phenyl]amino]sulfonyl]-4'-methoxy-*N,N*-dimethyl-[1,1'-biphenyl]-3-carboxamide dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₃₃H₃₇N₅O₅S.2HCl.2H₂O

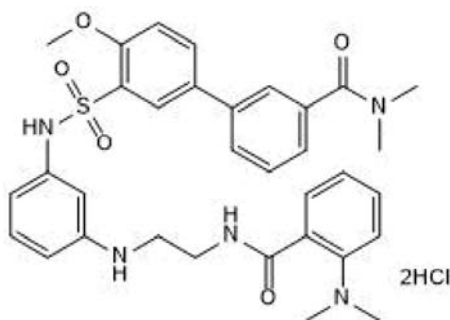
Batch Molecular Weight: 724.69

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 98.1% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

| | Carbon | Hydrogen | Nitrogen | Chlorine |
|-------------|--------|----------|----------|----------|
| Theoretical | 54.69 | 5.98 | 9.66 | 9.78 |
| Found | 55.19 | 5.72 | 9.48 | 8.97 |

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

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Description:

Potent and selective orexin OX₂ receptor agonist (EC₅₀ = 28 nM at human OX₂ expressed in CHO cells). Displays approximately 100-fold selectivity for OX₂ over OX₁ (EC₅₀ = 2.75 μM at human OX₁ expressed in CHO cells). Depolarizes OX₂-expressing histaminergic neurons in mouse brain slices. Increases wake time in wild type mice. Suppresses cataplexy-like symptoms in OX knockout mice.

Physical and Chemical Properties:

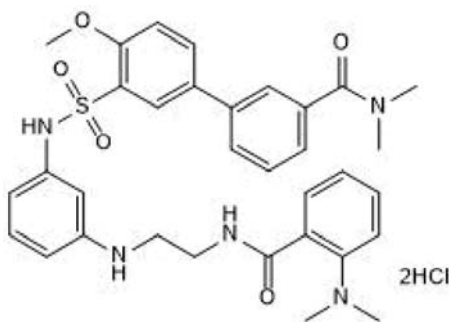
Batch Molecular Formula: C₃₃H₃₇N₅O₅S.2HCl.2H₂O

Batch Molecular Weight: 724.69

Physical Appearance: Off-white solid

Minimum Purity: ≥98%

Batch Molecular Structure:



References:

Irukayama-Tomobe et al (2017) Nonpeptide orexin type-2 receptor agonist ameliorates narcolepsy-cataplexy symptoms in mouse models. *Proc.Natl.Acad.Sci.USA.* **144** 5731. PMID: 28507129.

Nagahara et al (2015) Design and synthesis of non-peptide, selective orexin receptor 2 agonists. *J.Med.Chem.* **58** 7931. PMID: 26267383.

Storage: Store at -20°C

Solubility & Usage Info:

water 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.

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