

**Product Name:** ACT 335827

**Catalog No.:** 4983

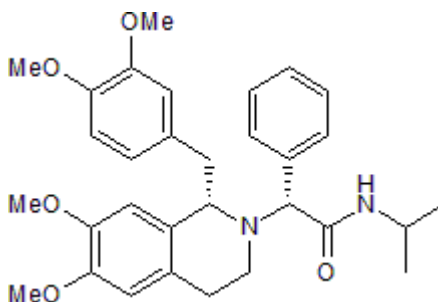
**Batch No.:** 2

CAS Number: 1354039-86-3

IUPAC Name: (aR,1S)-1-[(3,4-Dimethoxyphenyl)methyl]-3,4-dihydro-6,7-dimethoxy-N-(1-methylethyl)-a-phenyl-2(1H)-isoquinolineacetamide

## 1. PHYSICAL AND CHEMICAL PROPERTIES

<b>Batch Molecular Formula:</b>	C <sub>31</sub> H <sub>38</sub> N <sub>2</sub> O <sub>5</sub> ·½H <sub>2</sub> O
<b>Batch Molecular Weight:</b>	523.14
<b>Physical Appearance:</b>	Off-white solid
<b>Solubility:</b>	DMSO to 100 mM ethanol to 100 mM
<b>Storage:</b>	Store at -20°C
<b>Batch Molecular Structure:</b>	



## 2. ANALYTICAL DATA

<b>TLC:</b>	R <sub>f</sub> = 0.4 (Ethyl acetate:Petroleum ether [2:1])
<b>HPLC:</b>	Shows >98.7% purity
<b>Chiral HPLC:</b>	Shows 100% purity
<b><sup>1</sup>H NMR:</b>	Consistent with structure
<b>Mass Spectrum:</b>	Consistent with structure
<b>Optical Rotation:</b>	[α] <sub>D</sub> = -9.8 (Concentration = 1, Solvent = Chloroform)
<b>Microanalysis:</b>	

	Carbon	Hydrogen	Nitrogen
Theoretical	71.17	7.42	5.35
Found	71	7.39	5.38

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

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**Description:**

Potent and selective orexin OX<sub>1</sub> receptor antagonist (K<sub>b</sub> values are 41 and 560 nM for OX<sub>1</sub> and OX<sub>2</sub> receptors respectively). Elicits anxiolytic effects in vivo. Brain penetrant and orally available.

**Physical and Chemical Properties:**

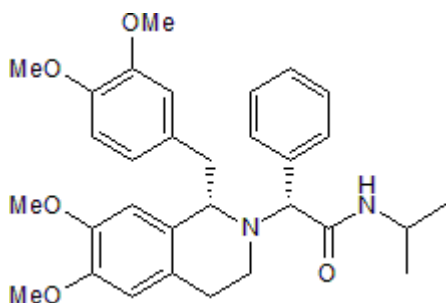
Batch Molecular Formula: C<sub>31</sub>H<sub>38</sub>N<sub>2</sub>O<sub>5</sub> · ¼H<sub>2</sub>O

Batch Molecular Weight: 523.14

Physical Appearance: Off-white solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**References:**

**Steiner et al** (2013) Discovery and characterization of ACT-335827, an orally available, brain penetrant orexin receptor type 1 selective antagonist. *ChemMedChem* **8** 898. PMID: 23589487.

**Storage:** Store at -20°C

**Solubility & Usage Info:**

DMSO to 100 mM  
ethanol 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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