

**Product Name:** ACT 335827

**Catalog No.:** 4983

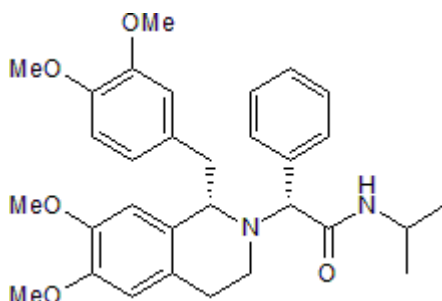
**Batch No.:** 1

**CAS Number:** 1354039-86-3

**IUPAC Name:** ( $\alpha R, 1 S$ )-1-[(3,4-Dimethoxyphenyl)methyl]-3,4-dihydro-6,7-dimethoxy-*N*-(1-methylethyl)- $\alpha$ -phenyl-2(1*H*)-isoquinolineacetamide

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>31</sub>H<sub>38</sub>N<sub>2</sub>O<sub>5</sub>  
**Batch Molecular Weight:** 518.64  
**Physical Appearance:** Off-white solid  
**Solubility:** DMSO to 100 mM  
 ethanol to 100 mM  
**Storage:** Store at -20°C  
**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**TLC:** R<sub>f</sub> = 0.4 (Ethyl acetate:Petroleum ether [2:1])  
**HPLC:** Shows 99.1% purity  
**Chiral HPLC:** Shows 100% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure  
**Optical Rotation:** [α]<sub>D</sub> = -18.7 (Concentration = 1, Solvent = Chloroform)  
**Microanalysis:**

	Carbon Hydrogen Nitrogen		
Theoretical	71.79	7.38	5.4
Found	71.45	7.44	5.36

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:**

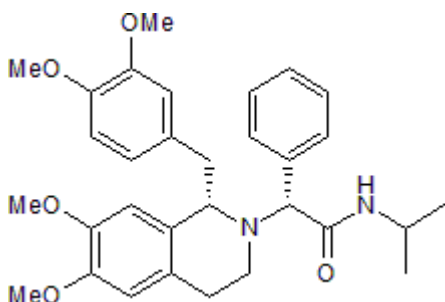
Batch Molecular Formula: C<sub>31</sub>H<sub>38</sub>N<sub>2</sub>O<sub>5</sub>.

Batch Molecular Weight: 518.64

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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