# TOCRIS a biotechne brand

## Print Date: Apr 26th 2021

# **Certificate of Analysis**

## www.tocris.com

Batch No.: 3

Catalog No.: 3351

## Product Name: Selexipag

CAS Number: 475086-01-2

IUPAC Name:

2-[4-[(5,6-Diphenyl-2-pyrazinyl)(1-methylethyl)amino]butoxy]-N-(methylsulfonyl)acetamide

## 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility: Storage: Batch Molecular Structure: C<sub>26</sub>H<sub>32</sub>N<sub>4</sub>O<sub>4</sub>S 496.62 Off-white solid DMSO to 100 mM Store at -20°C

# 2. ANALYTICAL DATA

HPLC: <sup>1</sup>H NMR: Mass Spectrum: Microanalysis: Shows 99.9% purity Consistent with structure Consistent with structure

	Carbon Hydrogen Nitrogen			
Theoretical	62.88	6.49	11.28	
Found	62.87	6.54	11.38	

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

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## **Description:**

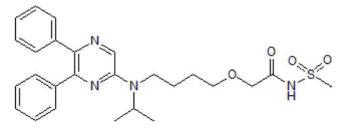
Selective prostacyclin IP<sub>1</sub> receptor agonist (K<sub>i</sub> values are 260 and 2100 nM and for human and rat IP receptors, and >10  $\mu$ M for EP<sub>1-4</sub>, DP, FP, and TP receptors). Prodrug for the active form of MRE 269. Ameliorates vascular endothelial dysfunction and increases femoral skin blood flow in rats. Orally available.

### **Physical and Chemical Properties:**

Batch Molecular Formula: C<sub>26</sub>H<sub>32</sub>N<sub>4</sub>O<sub>4</sub>S Batch Molecular Weight: 496.62 Physical Appearance: Off-white solid

### Minimum Purity: ≥98%

### **Batch Molecular Structure:**



### Storage: Store at -20°C

Solubility & Usage Info: 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).

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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.

## Licensing Information:

Sold with the permission of Nippon Shinyaku Co.

## **References:**

**Morrison** *et al* (2010) Selexipag: a selective prostacyclin receptor agonist that does not affect rat gastric function. J.Pharmacol.Exp.Ther. **335** 249. PMID: 20660124.

**Kuwano** *et al* (2008) A long-acting and highly selective prostacyclin receptor agonist prodrug, 2-{4-[(5,6-diphenylpyrazin-2-yl)(isopropyl) amino]butoxy}-N-(methylsulfonyl)acetamide (NS-304), ameliorates rat pulmonary hypertension with unique relaxant responses of its active fo J.Pharmacol.Exp.Ther. **326** 691. PMID: 18552131.

**Kuwano** *et al* (2007) 2-[4-[(5,6-diphenylpyrazin-2-yl)(isopropyl)amino]butoxy]-N-(methylsulfonyl)acetamide (NS-304), an orally available and long-acting prostacyclin receptor agonist prodrug. J.Pharmacol.Exp.Ther. **322** 1181. PMID: 17545310.

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