

Product Name: GSK 1562590 hydrochloride

Catalog No.: 5110

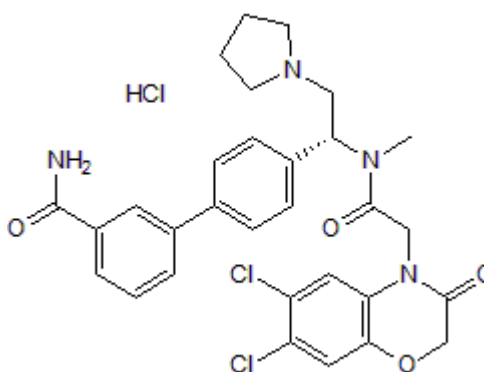
Batch No.: 1

CAS Number: 1003878-07-6

IUPAC Name: *N*-[(1*R*)-1-[3'-(Aminocarbonyl)[1,1'-biphenyl]-4-yl]-2-(1-pyrrolidinyl)ethyl]-6,7-dichloro-2,3-dihydro-*N*-methyl-3-oxo-4*H*-1,4-benzoxazine-4-acetamide hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{30}H_{30}Cl_2N_4O_4 \cdot HCl \cdot \frac{1}{2}H_2O$
Batch Molecular Weight: 626.96
Physical Appearance: Off-white Solid
Solubility: DMSO to 100 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: $R_f = 0.42$ (Chloroform:Methanol:Ammonia soln. [90:9:1])
HPLC: Shows >99.9% purity
Chiral HPLC: Shows >99.9% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Optical Rotation: $[\alpha]_D = -195.4$ (Concentration = 1, Solvent = DMF)
Microanalysis:

	Carbon Hydrogen Nitrogen		
Theoretical	57.47	5.14	8.94
Found	57.5	5.08	8.85

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

Tocris Bioscience is an R&D Systems company
 USA & CANADA Tel: (800) 343-7475 EUROPE Tel: +44 (0)1235 529449 CHINA Tel: +86 (21) 52380373
 www.RnDSystems.com

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Description:

High affinity and selective urotensin II (UT) receptor antagonist (pK_i values are 9.14, 9.28, 9.34, 9.64 and 9.66 at monkey, human, mouse, cat and rat recombinant receptors respectively). Exhibits selectivity for UT receptors over a range of GPCRs, ion channels, enzymes and neurotransmitter transporters. Suppresses human urotensin-II (hU-II)-induced contraction of isolated rat aorta in vitro and ex vivo. Inhibits the hU-II-induced increase in mean blood pressure in vivo. Orally active.

Physical and Chemical Properties:

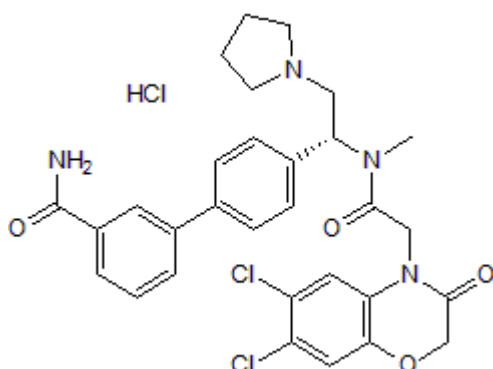
Batch Molecular Formula: C₃₀H₃₀Cl₂N₄O₄.HCl.½H₂O

Batch Molecular Weight: 626.96

Physical Appearance: Off-white Solid

Minimum Purity: >98%

Batch Molecular Structure:



References:

Behm et al (2010) GSK1562590, a slowly dissociating urotensin-II receptor antagonist, exhibits prolonged pharmacodynamic activity ex vivo. *Br.J.Pharmacol.* **161** 207. PMID: 20718751.

Storage: Store at +4°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).

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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