

Certificate of Analysis

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Product Name: BMS 191011

Catalog No.: 2665

Batch No.: 2

CAS Number: 202821-81-6

IUPAC Name: 3-[(5-Chloro-2-hydroxyphenyl)methyl]-5-[4-(trifluoromethyl)phenyl]-1,3,4-oxadiazol-2(3H)-one

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₆H₁₀ClF₃N₂O₃

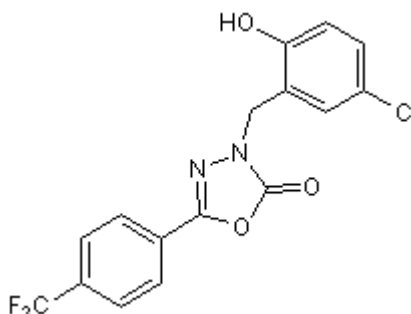
Batch Molecular Weight: 370.71

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 15 mM

Storage: Store at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.22 (Ethyl acetate:Petroleum ether [1:4])

HPLC: Shows 99.1% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	51.84	2.72	7.56
Found	51.86	2.64	7.61

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

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Description:

Potent BK_{Ca} channel opener (large-conductance Ca²⁺-activated potassium channel, K_{Ca}1.1). Neuroprotectant in two distinct animal models of stroke (MCAO in the SHR rat and a normotensive model of focal stroke).

Physical and Chemical Properties:

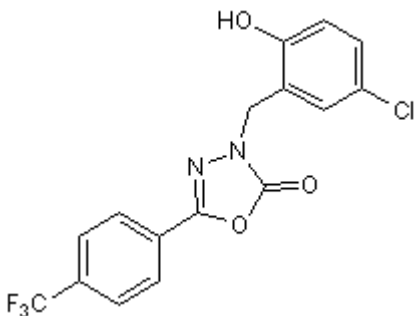
Batch Molecular Formula: C₁₆H₁₀ClF₃N₂O₃

Batch Molecular Weight: 370.71

Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:



References:

Hewawasam et al (2003) Synthesis of water-soluble prodrugs of BMS-191011: a Maxi-K channel opener targeted for post-stroke neuroprotection. *Bioorg.Med.Chem.Letts.* **13** 1695.

Romine et al (2007) 3-[(5-chloro-2-hydroxyphenyl)methyl]-5-[4-(trifluoromethyl)phenyl]-1,3,4-oxadiazol-2(3H)-one, BMS-191011: opener of large-conductance Ca²⁺-activated potassium (Maki-K) channels, identification, solubility, and SAR. *J.Med.Chem.* **50** 528. PMID: 17266205.

Storage: Store at RT

Solubility & Usage Info:

DMSO to 100 mM

ethanol to 15 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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