

Certificate of Analysis

Print Date: Jan 13th 2016 **WWW.tocris.com**

Product Name: CI 1020 Catalog No.: 2942 Batch No.: 2

CAS Number: 162256-50-0

IUPAC Name: 3-(1,3-Benzodioxol-5-yl)-5-hydroxy-5-(4-methoxyphenyl)-4-[(3,4,5-trimethoxyphenyl)methyl]-2(5H)-furanone

1. PHYSICAL AND CHEMICAL PROPERTIES

 $\begin{array}{lll} \textbf{Batch Molecular Formula:} & \textbf{C_{28}H}_{26}$O_9 \\ \textbf{Batch Molecular Weight:} & 506.5 \\ \textbf{Physical Appearance:} & \text{White solid} \\ \textbf{Solubility:} & \text{DMSO to 50 mM} \\ \textbf{Storage:} & \text{Store at -20°C} \\ \end{array}$

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.26$ (Ethyl acetate:Petroleum ether [1:1])

HPLC: Shows 98.0% purity

¹H NMR: Consistent with structure Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 66.4 5.17 Found 66.28 5.14



Product Information

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Description:

Highly selective, orally active, non-peptide endothelin-A receptor (ET_A) antagonist $(IC_{50}$ values are 0.3 and 480 nM for ET_A and ET_B receptors respectively). Antihypertensive; blocks ET-1-induced pressor responses following oral administration.

Physical and Chemical Properties:

Batch Molecular Formula: C₂₈H₂₆O₉ Batch Molecular Weight: 506.5 Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 50 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.

References:

Doherty *et al* (1995) Discovery of a novel series of orally active non-peptide endothelin-A (ET_A) receptor-selective antagonists. J.Med.Chem. *38* 1259. PMID: 7731010.

Jones *et al* (1999) The effect of the endothelin ET_A receptor antagonist CI-1020 on hypoxic pulmonary vasoconstriction. Eur.J.Pharmacol. **374** 367. PMID: 10422781.

Coe et al (2002) The endothelin A receptor antagonists PD 156707 (CI-1020) and PD 180988 (CI-1034) reverse the hypoxic pulmonary vasoconstriction in ther perinatal lamb. J.Pharmacol.Exp.Ther. 302 672. PMID: 12130731.