

Certificate of Analysis

Print Date: Jan 15th 2016

www.tocris.com

Product Name: PD 198306 Catalog No.: 2605 Batch No.: 1

CAS Number: 212631-61-3

IUPAC Name: N-(Cyclopropylmethoxy)-3,4,5-trifluoro-2-[(4-iodo-2-methylphenyl)amino]-benzamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{18}H_{16}F_3IN_2O_2$

Batch Molecular Weight: 476.23 **Physical Appearance:** White solid

Solubility: DMSO to 100 mM

ethanol to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.43$ (Ethyl acetate:Petroleum ether [1:3])

Melting Point:Between 140 - 141°CHPLC:Shows >98.8% purity¹H NMR:Consistent with structureMass Spectrum:Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 45.4 3.39 5.88 Found 45.37 3.29 5.8



Product Information

Print Date: Jan 15th 2016

www.tocris.com

Product Name: PD 198306 Catalog No.: 2605 Batch No.: 1

CAS Number: 212631-61-3

IUPAC Name: N-(Cyclopropylmethoxy)-3,4,5-trifluoro-2-[(4-iodo-2-methylphenyl)amino]-benzamide

Description:

Potent inhibitor of MEK1/2. Inhibits isolated enzyme at a concentration of 8 nM and inhibits MEK activity in synovial fibroblasts at concentrations of 30 - 100 nM. Highly selective for MEK; IC $_{50}$ values are > 1, > 4, > 4 and > 10 μ M for ERK, c-Src, cdks and PI 3-kinase γ respectively. Antihyperalgesic; blocks static allodynia in the streptozocin model of neuropathic pain following i.t. administration.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₈H₁₆F₃IN₂O₂ Batch Molecular Weight: 476.23 Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Store at +4°C

CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

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.

References:

Ciruela et al (2003) Identification of MEK1 as a novel target for the treatment of neuropathic pain. Br.J.Pharmacol. 138 751. PMID: 12642375.

Pelletier *et al* (2003) In vivo selective inhibition of mitogen-activated protein kinase kinase 1/2 in rabbit experimental osteoarthritis is associated with a reduction in the development of structural changes. Arthrit.Rheumat. *48* 1582.