

Product Name: TCS ERK 11e

Catalog No.: 4465

Batch No.: 2

CAS Number: 896720-20-0

IUPAC Name: 4-[2-[(2-Chloro-4-fluorophenyl)amino]-5-methyl-4-pyrimidinyl]-*N*-[(1*S*)-1-(3-chlorophenyl)-2-hydroxyethyl]-1*H*-pyrrole-2-carboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₄H₂₀Cl₂FN₅O₂·¼H₂O

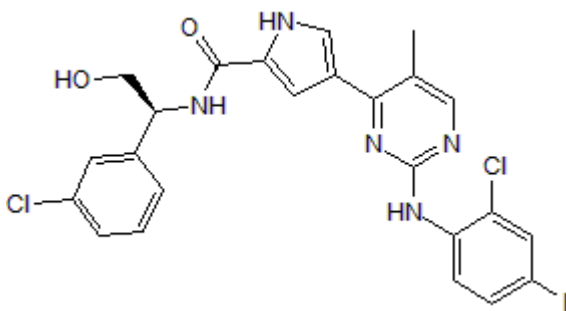
Batch Molecular Weight: 504.85

Physical Appearance: Off White solid

Solubility: DMSO to 100 mM
ethanol to 25 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.7% purity

Chiral HPLC: Shows 99.4% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: [α]_D = -180.6 (Concentration = 0.33, Solvent = Ethanol)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	57.1	4.09	13.87
Found	57.03	4.04	13.61

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

Product Name: TCS ERK 11e

Catalog No.: 4465

Batch No.: 2

CAS Number: 896720-20-0

IUPAC Name: 4-[2-[(2-Chloro-4-fluorophenyl)amino]-5-methyl-4-pyrimidinyl]-N-[(1S)-1-(3-chlorophenyl)-2-hydroxyethyl]-1H-pyrrole-2-carboxamide

Description:

Potent and selective extracellular signal-related kinase 2 (ERK2) inhibitor (K_i values are <2, 395, 540 and 852 nM for ERK2, GSK-3, Aurora Kinase A and Cdk2 respectively). Potently blocks proliferation of HT29 cells (IC_{50} = 48 nM). Orally bioavailable.

Physical and Chemical Properties:

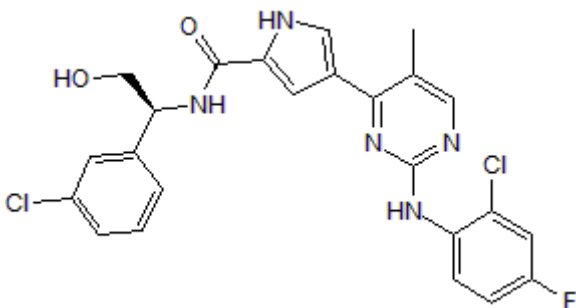
Batch Molecular Formula: $C_{24}H_{20}Cl_2FN_5O_2 \cdot \frac{1}{4}H_2O$

Batch Molecular Weight: 504.85

Physical Appearance: Off White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol to 25 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:

Aronov et al (2009) Structure-guided design of potent and selective pyrimidylpyrrole inhibitors of extracellular signal-related kinase (ERK) using conformational control. *J.Med.Chem.* **52** 6362. PMID: 19827834.

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

bio-techne.com

info@bio-techne.com

techsupport@bio-techne.com

North America

Tel: (800) 343 7475

China

info.cn@bio-techne.com

Tel: +86 (21) 52380373

Europe Middle East Africa

Tel: +44 (0)1235 529449

Rest of World

www.tocris.com/distributors

Tel: +1 612 379 2956