

**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

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>24</sub>H<sub>20</sub>Cl<sub>2</sub>FN<sub>5</sub>O<sub>2</sub>·¼H<sub>2</sub>O

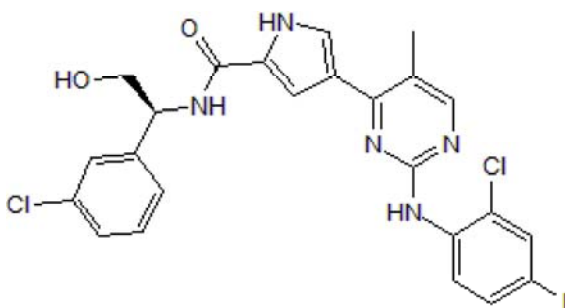
**Batch Molecular Weight:** 504.85

**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 98.9% purity

**Chiral HPLC:** Shows 99.4% purity

**<sup>1</sup>H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Optical Rotation:** [α]<sub>D</sub> = -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

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**Description:**

TCS ERK 11e is a 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:**

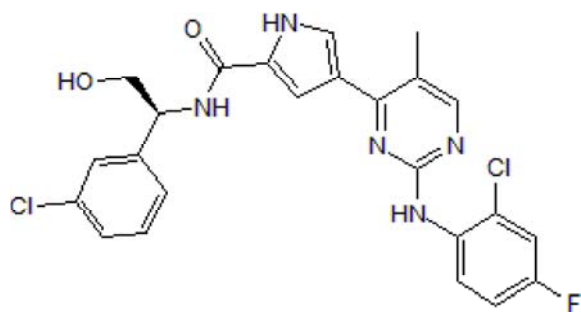
Batch Molecular Formula:  $C_{24}H_{20}Cl_2FN_5O_2 \cdot \frac{1}{4}H_2O$

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.

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