

**Product Name:** TCS 21311

**Catalog No.:** 4221

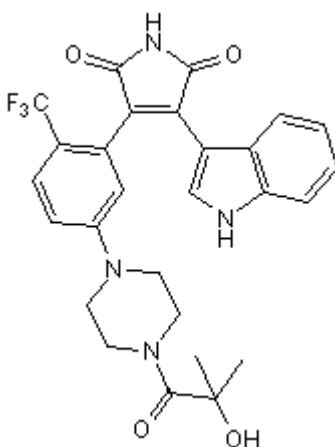
**Batch No.:** 1

CAS Number: 1260181-14-3

IUPAC Name: 3-[5-[4-(2-Hydroxy-2-methyl-1-oxopropyl)-1-piperazinyl]-2-(trifluoromethyl)phenyl]-4-(1*H*-indol-3-yl)-1*H*-pyrrole-2,5-dione

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>27</sub>H<sub>25</sub>F<sub>3</sub>N<sub>4</sub>O<sub>4</sub>·1½H<sub>2</sub>O  
**Batch Molecular Weight:** 553.53  
**Physical Appearance:** Yellow solid  
**Solubility:** DMSO to 100 mM  
**Storage:** Desiccate at RT  
**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**TLC:** R<sub>f</sub> = 0.18 (Chloroform:Methanol:Ammonia soln. [9:1:3drops])  
**HPLC:** Shows 98.4% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure  
**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	58.6	5.1	10.12
Found	58.56	4.72	9.9

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**Description:**

Potent JAK3 inhibitor (IC<sub>50</sub> = 8 nM). Selective for JAK3 over JAK1, JAK2 and TYK2 (IC<sub>50</sub> values are 1017, 2550 and 8055 nM respectively). Also inhibits GSK-3β, PKCα and PKCθ (IC<sub>50</sub> values are 3, 13 and 68 nM respectively).

**Physical and Chemical Properties:**

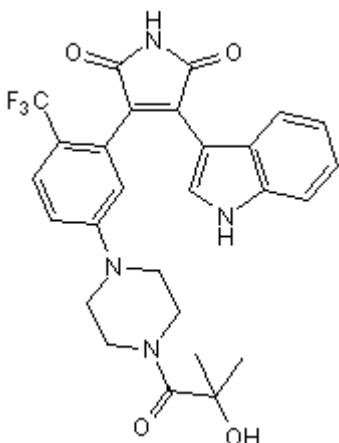
Batch Molecular Formula: C<sub>27</sub>H<sub>25</sub>F<sub>3</sub>N<sub>4</sub>O<sub>4</sub> · 1½H<sub>2</sub>O

Batch Molecular Weight: 553.53

Physical Appearance: Yellow solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**References:**

Thoma *et al* (2010) Identification of a potent Janus kinase 3 inhibitor with high selectivity within the Janus kinase family. *J.Med.Chem.* **54** 284.

**Storage:** Desiccate at RT

**Solubility & Usage Info:**

DMSO 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.

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