TOCRIS
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Print Date: Sep 29th 2016

# Certificate of Analysis

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**Product Name:** **GSK 2606414** **Catalog No.: 5107** **Batch No.: 2**

CAS Number: 1337531-36-8

IUPAC Name: 1-[5-(4-Amino-7-methyl-7*H*-pyrrolo[2,3-*d*]pyrimidin-5-yl]-2,3-dihydro-1*H*-indol-1-yl]-2-[3-(trifluoromethyl)phenyl] ethanone

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** $C_{24}H_{20}F_3N_5O.½H_2O$

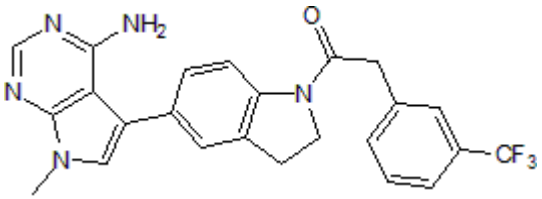
**Batch Molecular Weight:** 460.45

**Physical Appearance:** Off White solid

**Solubility:** DMSO to 100 mM

**Storage:** Store at -20°C

**Batch Molecular Structure:**




## 2. ANALYTICAL DATA

**HPLC:** Shows 99% purity

**$^1$H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

| | Carbon | Hydrogen | Nitrogen |
|---|---|---|---|
| Theoretical | 62.6 | 4.6 | 15.21 |
| Found | 62.35 | 4.6 | 15.18 |



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**Description:**

Potent and selective protein kinase R-like ER kinase (PERK) inhibitor ($IC_{50}$ = 0.4 nM). Exhibits >1000-fold selectivity for PERK over HR1 and PKR. Inhibits thapsigargin-induced PERK phosphorylation in lung carcinoma A549 cells. Attenuates subcutaneous pancreatic human tumor xenograft growth in mice. Orally bioavailable.

**Physical and Chemical Properties:**

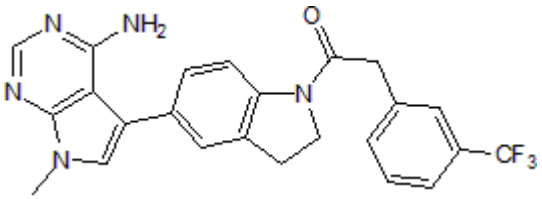
Batch Molecular Formula: $C_{24}H_{20}F_3N_5O.½H_2O$

Batch Molecular Weight: 460.45

Physical Appearance: Off White solid

**Minimum Purity:** >99%

**Batch Molecular Structure:**




**Storage:** Store at -20°C

**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.

**Licensing Information:**

Sold for research purposes only under agreement from GlaxoSmithKline

**References:**

**Axten** *et al* (2012) Discovery of 7-methyl-5-(1-{[3-(trifluoromethyl)phenyl]acetyl}-2,3-dihydro-1H-indol-5-yl)-7H-pyrrolo[2,3-d]pyrimidin-4-amine (GSK2606414), a potent and selective first-in-class inhibitor of protein kinase R (PKR)-like endoplasmic reticulum kinase (PERK). J.Med.Chem. ***55*** 7193. PMID: 22827572.

**Harding** *et al* (2012) Uncoupling proteostasis and development in vitro with a small molecule inhibitor of the pancreatic endoplasmic reticulum kinase, PERK. J.Biol.Chem. ***287*** 44338. PMID: 23148209.