

Product Name: GSK 2606414

Catalog No.: 5107

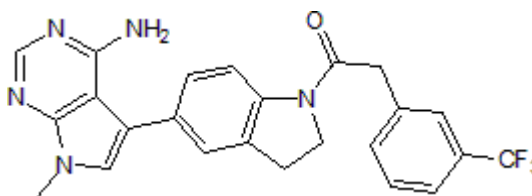
Batch No.: 1

CAS Number: 1337531-36-8

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

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₄H₂₀F₃N₅O
Batch Molecular Weight: 451.44
Physical Appearance: White solid
Solubility: DMSO to 100 mM
 1eq. HCl to 20 mM with gentle warming
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.5 (Ethyl acetate:Methanol [19:1])
HPLC: Shows >99.8% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	63.85	4.47	15.51
Found	63.83	4.43	15.6

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

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Description:

Potent and selective protein kinase R-like ER kinase (PERK) inhibitor (IC₅₀ = 0.4 nM). 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:

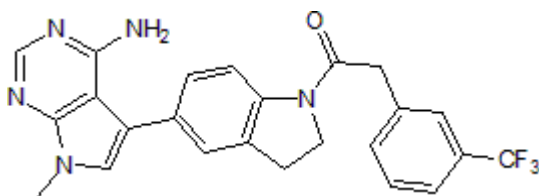
Batch Molecular Formula: C₂₄H₂₀F₃N₅O

Batch Molecular Weight: 451.44

Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM

1eq. HCl to 20 mM with gentle warming

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:

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.

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