

Product Name: GSK 1838705

Catalog No.: 5111

Batch No.: 1

CAS Number: 1116235-97-2

IUPAC Name: 2-[[2-[[1-[(Dimethylamino)ethanoyl]-5-(methoxy)-2,3-dihydro-1H-indol-6-yl]amino]-7H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-6-fluoro-N-methylbenzamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₇H₂₉FN₈O₃ · 1½H₂O

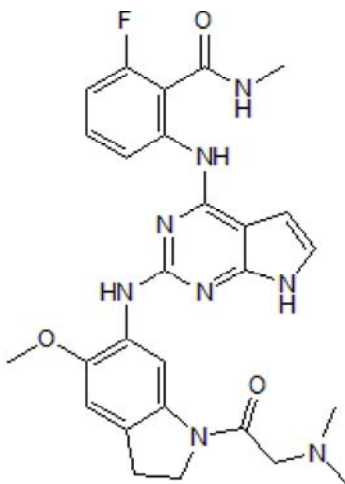
Batch Molecular Weight: 559.59

Physical Appearance: Beige solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 97.9% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	57.95	5.76	20.02
Found	57.8	5.63	19.94

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

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Description:

Potent insulin receptor (IR) and insulin-like growth factor-1 receptor (IGF1R) inhibitor (IC₅₀ values are 1.6 and 2 nM, respectively). Also inhibits anaplastic lymphoma kinase (ALK) (IC₅₀ = 0.5 nM). Displays > 800-fold selectivity for IR, IGFR1 and ALK over a panel of 44 kinases including JNK. Blocks proliferation of cancer cell lines in vitro, and causes complete regression of ALK-dependent tumors in vivo. Orally bioavailable.

Physical and Chemical Properties:

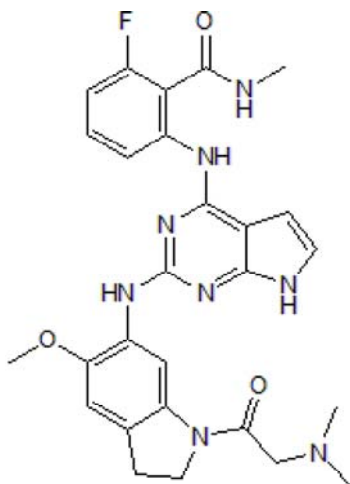
Batch Molecular Formula: C₂₇H₂₉FN₈O₃·1½H₂O

Batch Molecular Weight: 559.59

Physical Appearance: Beige solid

Minimum Purity: >98%

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 under agreement from GlaxoSmithKline.

References:

Gao et al (2014) Site-specific activation of AKT protects cells from death induced by glucose deprivation. *Oncogene* **33** 745. PMID: 23396361.

Chamberlain et al (2009) Optimization of 4,6-bis-anilino-1H-pyrrolo[2,3-d]pyrimidine IGF-1R tyrosine kinase inhibitors towards JNK selectivity. *Bioorg.Med.Chem.Lett.* **19** 360. PMID: 19071018.

Sabbatini et al (2009) GSK1838705A inhibits the Ins-like growth factor-1 receptor and anaplastic lymphoma kinase and shows antitumor activity in experimental models of human cancers. *Mol.Cancer.Ther.* **8** 2811. PMID: 19825801.

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