

Product Name: G 5555

Catalog No.: 6051

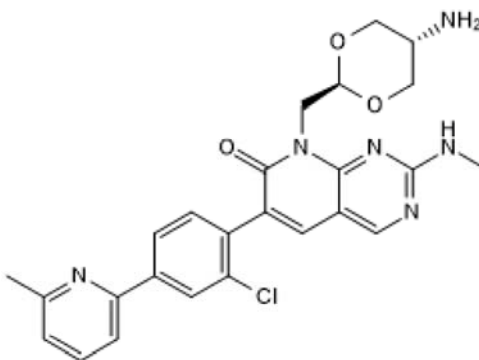
Batch No.: 1

CAS Number: 1648863-90-4

IUPAC Name: 8-[(*trans*-5-Amino-1,3-dioxan-2-yl)methyl]-6-[2-chloro-4-(6-methyl-2-pyridinyl)phenyl]-2-(methylamino)-pyrido[2,3-d]pyrimidin-7(8*H*)-one

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:	C ₂₅ H ₂₅ ClN ₆ O ₃ · ½H ₂ O
Batch Molecular Weight:	501.97
Physical Appearance:	White solid
Solubility:	1eq. HCl to 100 mM DMSO to 20 mM with gentle warming
Storage:	Store at -20°C
Batch Molecular Structure:	



2. ANALYTICAL DATA

TLC:	R _f = 0.21 (Dichloromethane:Methanol [95:5])
HPLC:	Shows 99.3% purity
¹H NMR:	Consistent with structure
Mass Spectrum:	Consistent with structure

Microanalysis:	Carbon	Hydrogen	Nitrogen
Theoretical	59.82	5.22	16.74
Found	59.98	5.12	16.78

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

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Description:

High affinity group 1 PAK (pan-PAK1, 2 and 3) inhibitor ($K_i = 3.7$ nM; pMEK $IC_{50} = 69$ nM). Of 235 kinases tested, other than PAK1, eight (PAK2, PAK3, KHS1, Lck, MST3, MST4, SIK2, and YSK1) were inhibited >70%. Exhibits low hERG channel activity (<50% inhibition at 10 μ M). Orally bioavailable.

Physical and Chemical Properties:

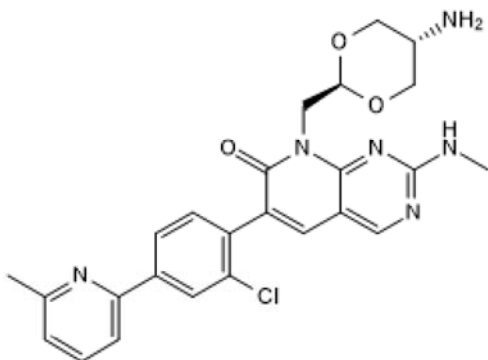
Batch Molecular Formula: $C_{25}H_{25}ClN_6O_3 \cdot \frac{1}{2}H_2O$

Batch Molecular Weight: 501.97

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



References:

Ndubaku *et al* (2015) Design of selective PAK1 inhibitor G-5555: improving properties by employing an unorthodox low-pK a polar moiety. *ACS Med.Chem.Lett.* **6** 1241. PMID: 26713112.

Storage: Store at -20°C

Solubility & Usage Info:

1eq. HCl to 100 mM

DMSO 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.

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