

Product Name: TCS 2312

Catalog No.: 3038

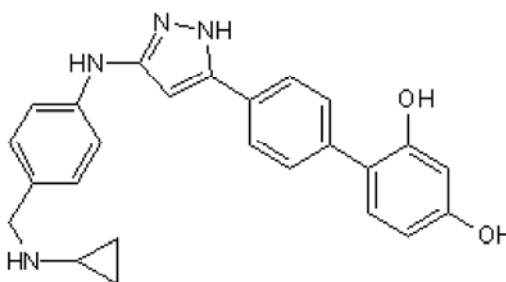
Batch No.: 5

CAS Number: 838823-31-7

IUPAC Name: 4'-[5-[[3-[(Cyclopropylamino)methyl]phenyl]amino]-1H-pyrazol-3-yl]-[1,1'-biphenyl]-2,4-diol

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₅H₂₄N₄O₂
Batch Molecular Weight: 412.48
Physical Appearance: Pale yellow solid
Solubility: DMSO to 20 mM
Storage: Store at -80°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.4 (9/1, DCM/1M NH₃ in MeOH)
HPLC: Shows >98.3% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

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

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Description:

Potent and selective checkpoint kinase 1 (chk1) inhibitor (K_i = 0.38 nM, EC_{50} = 60 nM). Enhances the cell killing activity of Gemcitabine (Cat. No. 3259) in breast and prostate cancer cell lines and displays antiproliferative effects in vitro.

Physical and Chemical Properties:

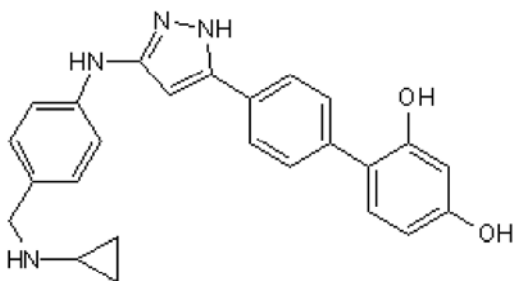
Batch Molecular Formula: $C_{25}H_{24}N_4O_2$

Batch Molecular Weight: 412.48

Physical Appearance: Pale yellow solid

Minimum Purity: >97%

Batch Molecular Structure:



Storage: Store at -80°C

CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

Solubility & Usage Info:

DMSO to 20 mM

This product is supplied as a lyophilized solid and may be very hard to visualize. Solutions should be made by adding solvent directly to the vial. The vial should then be vortexed vigorously to ensure the product has completely dissolved.

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:

Teng *et al* (2007) Structure-based design of (5-arylamino-2H-pyrazol-3-yl)-biphenyl-2',4'-diols as novel and potent human CHK1 inhibitors. *J.Med.Chem.* **50** 5253. PMID: 17887663.

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