

Product Name: TCS 2312

Catalog No.: 3038

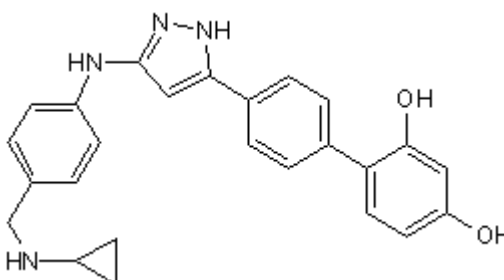
Batch No.: 3

CAS Number: 838823-31-7

IUPAC Name: 4'-[5-[[3-[(Cyclopropylamino)methyl]phenyl]amino]-1*H*-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: Yellow solid
Solubility: DMSO to 20 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.42 (Dichloromethane:Methanol:Ammonia soln. [90:10:0.1])
HPLC: Shows >98.5% 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:

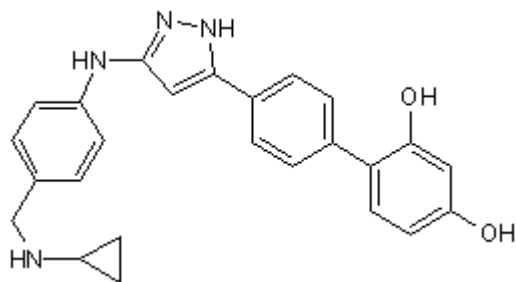
Batch Molecular Formula: $C_{25}H_{24}N_4O_2$

Batch Molecular Weight: 412.48

Physical Appearance: Yellow solid

Minimum Purity: >97%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 20 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.

References:

Teng et al (2007) Structure-based design of (5-aryl-amino-2*H*-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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