

Product Name: CGK 733

Catalog No.: 2639

Batch No.: 2

CAS Number: 905973-89-9

IUPAC Name: α -Phenyl-N-[2,2,2-trichloro-1-[[[(4-fluoro-3-nitrophenyl)amino]thioxomethyl]amino]ethyl]benzeneacetamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₃H₁₈Cl₃FN₄O₃S

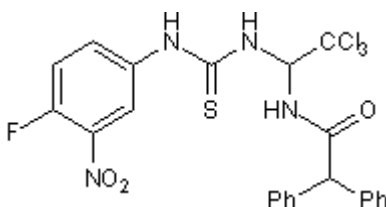
Batch Molecular Weight: 555.84

Physical Appearance: Pale yellow solid

Solubility: DMSO to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.3 (Ethyl acetate:Petroleum ether [1:1])

Melting Point: Between 185 - 186°C(dec)

HPLC: Shows >99.31% purity

¹H NMR: Consistent with structure

¹³C NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	49.7	3.26	10.08
Found	49.7	3.13	9.98

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

Tocris Bioscience is an R&D Systems company
 USA & CANADA Tel: (800) 343-7475 EUROPE Tel: +44 (0)1235 529449 CHINA Tel: +86 (21) 52380373
 www.RnDSystems.com

R&D
SYSTEMS®

Product Name: CGK 733

Catalog No.: 2639

Batch No.: 2

CAS Number: 905973-89-9

IUPAC Name: α -Phenyl-N-[2,2,2-trichloro-1-[[[(4-fluoro-3-nitrophenyl)amino]thioxomethyl]amino]ethyl]benzeneacetamide

Description:

Originally defined as a selective inhibitor of ATR and ATM kinases. Induces cell death in prematurely senescent breast cancer cells. Decreases p21^{CIP1} levels in premature senescent MCF-7 and HCT-116 cells; also exhibits antiproliferative activity in a range of cancer cell lines. Blocks camptothecin-induced p53 phosphorylation and protects cells from camptothecin-induced apoptosis.

Physical and Chemical Properties:

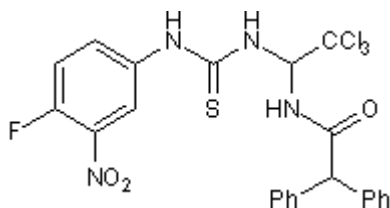
Batch Molecular Formula: C₂₃H₁₈Cl₃FN₄O₃S

Batch Molecular Weight: 555.84

Physical Appearance: Pale yellow solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°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.

References:

Goldstein et al (2008) Apoptotic death induced by the cyclophosphamide analogue mafosfamide in human lymphoblastoid cells: Contribution of DNA replication, transcription inhibition and Chk/p53 signaling. *Toxicol.Appl.Pharmacol.* **229** 20. PMID: 18289623.

Crescenzi et al (2008) Ataxia telangiectasia mutated and p21CIP1 modulate cell survival of drug-induced senescent tumor cells: Implications for chemotherapy. *Clin.Cancer Res.* **14** 1877. PMID: 18347191.

Cruet-Hennequart et al (2008) Enhanced DNA-PK-mediated RPA2 hyperphosphorylation in DNA polymerase η -deficient human cells treated with cisplatin and oxaliplatin. *DNA Repair* **7** 582. PMID: 18289945.

Won et al (2008) Retraction: small molecule-based reversible reprogramming of cellular lifespan. *Nat.Chem.Biol.* **4** 431. PMID: 18560433.

Bhattacharya et al (2009) Role of polyamines in p53-dependent apoptosis of intestinal epithelial cells. *Cell Signal.* **21** 509. PMID: 19136059.

Alao and Sunnerhagen (2009) The ATM and ATR inhibitors CGK733 and caffeine suppress cyclin D1 levels and inhibit cell proliferation. *Radiat.Oncol.* **10** 4. PMID: 19903334.

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

Tocris Bioscience is an R&D Systems company
USA & CANADA Tel: (800) 343-7475 EUROPE Tel: +44 (0)1235 529449 CHINA Tel: +86 (21) 52380373
www.RnDSystems.com

R&D
SYSTEMS®