

Product Name: SCH 529074

Catalog No.: 4240

Batch No.: 2

CAS Number: 922150-11-6

IUPAC Name: N³-[2-[[4-[Bis(4-chlorophenyl)methyl]-1-piperazinyl]methyl]-4-quinazoliny]-N¹,N¹-dimethyl-1,3-propanediamine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₃₁H₃₆Cl₂N₆·½H₂O

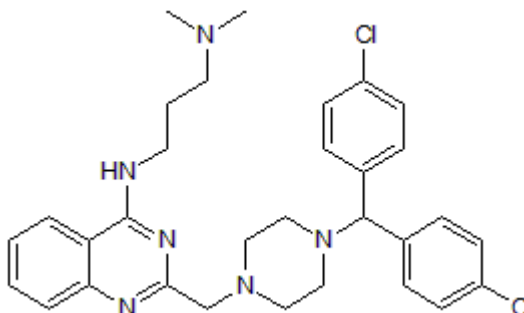
Batch Molecular Weight: 572.57

Physical Appearance: Cream solid

Solubility: ethanol to 100 mM
DMSO to 10 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.33 (Dichloromethane:Methanol:Ammonia soln. [95:5:1])

HPLC: Shows 99.1% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	65.03	6.51	14.68
Found	65.13	6.5	14.75

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

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Description:

Restores mutant p53 activity. Binds p53 DNA binding domain ($K_d = 1-2 \mu\text{M}$) and restores wild-type function to many oncogenic mutants by acting as a chaperone. Inhibits ubiquitination of p53 by HDM2. Triggers apoptosis in tumor cell lines and reduces tumor growth in a xenograft model.

Physical and Chemical Properties:

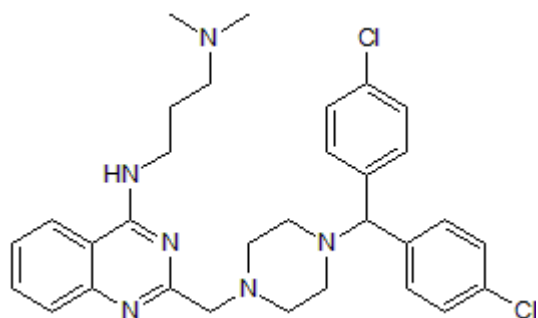
Batch Molecular Formula: C₃₁H₃₆Cl₂N₆·½H₂O

Batch Molecular Weight: 572.57

Physical Appearance: Cream solid

Minimum Purity: >98%

Batch Molecular Structure:



References:

Demma et al (2010) SCH529074, a small molecule activator of mutant p53, which binds p53 DNA binding domain (DBD), restores growth-suppressive function to mutant p53 and interrupts HDM2-mediated ubiquitination of wild type p53. *J.Biol.Chem.* **285** 10198. PMID: 20124408.

Essmann & Schulze-Osthoff (2012) Translational approaches targeting the p53 pathway for anti-cancer therapy. *Br.J.Pharmacol.* **165** 328. PMID: 21718309.

Storage: Store at -20°C

Solubility & Usage Info:

ethanol to 100 mM

DMSO to 10 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.

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