

Product Name: TNP

Catalog No.: 3946

Batch No.: 1

CAS Number: 519178-28-0

IUPAC Name: N⁶-[[4-nitrophenyl)methyl]-N²-[[3-(trifluoromethyl)phenyl)methyl]-9H-Purine-2,6-diamine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₀H₁₆F₃N₇O₂·H₂O

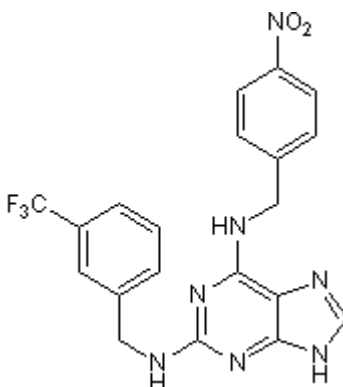
Batch Molecular Weight: 461.4

Physical Appearance: Yellow solid

Solubility: DMSO to 100 mM
ethanol to 25 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.05 (Dichloromethane:Methanol [9:1])

HPLC: Shows 97.40% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	52.06	3.93	21.25
Found	51.82	3.83	21.14

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

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Description:

Reversible inositol hexakisphosphate kinase (IP6K) inhibitor (IC₅₀ = 0.47 μM for inhibition of InsP₇ formation). Also inhibits inositol 1,4,5-trisphosphate 3-kinase (IP3K) (IC₅₀ = 10.2 μM). Binds to the ATP binding site of IP3K (K_i = 4.3 μM).

Physical and Chemical Properties:

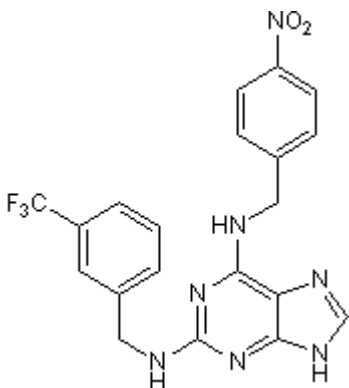
Batch Molecular Formula: C₂₀H₁₆F₃N₇O₂·H₂O

Batch Molecular Weight: 461.4

Physical Appearance: Yellow solid

Minimum Purity: >97%

Batch Molecular Structure:



Storage: Store at +4°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 100 mM

ethanol to 25 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:

Padmanabhan et al (2009) Characterization of a selective inhibitor of inositol hexakisphosphate kinases. Use in defining biological roles and metabolic relationships of inositol pyrophosphates. *J.Biol.Chem.* **284** 10571. PMID: 19208622.

Chang et al (2002) Purine-based inhibitors of inositol-1,4,5-trisphosphate-3-kinase. *Chembiochem* **3** 897. PMID: 12210991.

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