

Product Name: PF 04479745

Catalog No.: 5755

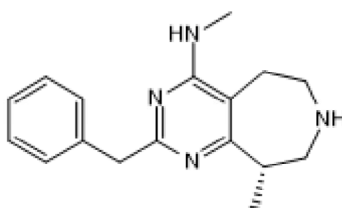
Batch No.: 1

CAS Number: 1065110-43-1

IUPAC Name: (9S)-6,7,8,9-Tetrahydro-*N*,9-dimethyl-2-(phenylmethyl)-5*H*-pyrimido[4,5-*d*]azepin-4-amine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₇H₂₂N₄·¼H₂O
Batch Molecular Weight: 286.89
Physical Appearance: Pale yellow solid
Solubility: DMSO to 100 mM
 ethanol to 100 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.4% purity
Chiral HPLC: Shows 99.2% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	71.17	7.9	19.53
Found	70.83	7.95	19.48

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

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IUPAC Name: (9S)-6,7,8,9-Tetrahydro-N,9-dimethyl-2-(phenylmethyl)-5H-pyrimido[4,5-d]azepin-4-amine

Description:

PF 04479745 is a potent and selective 5-HT_{2C} agonist (EC₅₀ = 10 nM). Exhibits > 100-fold selectivity over a panel of 90 receptors, enzymes and ion channels, except for 5-HT_{2A} (IC₅₀ = 360 nM antagonist), 5-HT_{2B} (EC₅₀ = 67 nM antagonist), 5-HT_{1A} and 5-HT₆ (functional activity not tested).

Physical and Chemical Properties:

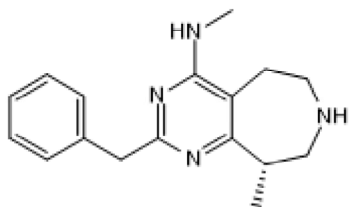
Batch Molecular Formula: C₁₇H₂₂N₄·¼H₂O

Batch Molecular Weight: 286.89

Physical Appearance: Pale yellow solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM

ethanol to 100 mM

This product is supplied in lyophilized form. It may appear as a solid, gel or film and 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. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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.

Licensing Information:

Sold for research purposes under agreement from Pfizer Inc.

References:

Storer et al (2014) Multiparameter optimization in CNS drug discovery: Design of pyrimido[4,5-d]azepines as potent 5-hydroxytryptamine 2C (5-HT_{2C}) receptor agonists with exquisite functional selectivity over 5-HT_{2A} and 5-HT_{2B} receptors. *J.Med.Chem.* **57** 5258. PMID: 24878222.

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