

Product Name: PHP 501 trifluoroacetate

Catalog No.: 4466

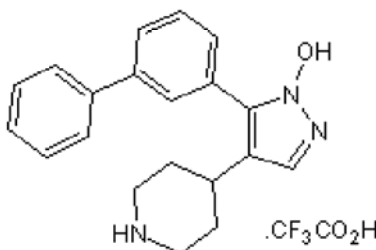
Batch No.: 1

CAS Number: 1781880-44-1

IUPAC Name: 4-(5-[1,1'-Biphenyl]-3-yl-1-hydroxy-1H-pyrazol-4-yl)piperidine trifluoroacetate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₀H₂₁N₃O.CF₃CO₂H.½H₂O
Batch Molecular Weight: 442.43
Physical Appearance: Off-white solid
Solubility: DMSO to 100 mM
ethanol to 10 mM with gentle warming
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.2% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	59.73	5.24	9.5
Found	59.66	5.51	9.95

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Description:

Potent GABA_A antagonist ($K_i = 0.0028 \mu\text{M}$ at rat GABA_A receptors; $IC_{50} = 0.024 \mu\text{M}$ at human $\alpha_1\beta_2\gamma_2$ GABA_A-expressing tsA201 cells). Displays no inhibitory activity at hGAT-1, hGAT-2, hGAT-3 or hBGT-1 GABA transporters.

Physical and Chemical Properties:

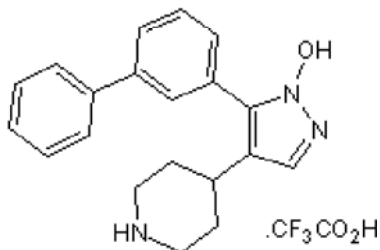
Batch Molecular Formula: $\text{C}_{20}\text{H}_{21}\text{N}_3\text{O} \cdot \text{CF}_3\text{CO}_2\text{H} \cdot \frac{1}{2}\text{H}_2\text{O}$

Batch Molecular Weight: 442.43

Physical Appearance: Off-white solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM

ethanol to 10 mM with gentle warming

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a $45\text{-}60^\circ\text{C}$ 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:

Møller *et al* (2010) Novel 4-(piperidin-4-yl)-1-hydroxypyrazoles as gamma-aminobutyric acid(A) receptor ligands: synthesis, pharmacology, and structure-activity relationships. *J.Med.Chem.* **53** 3417. PMID: 20355712.

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