

Product Name: PD 144418 oxalate

Catalog No.: 2606

Batch No.: 2

CAS Number: 1794760-28-3

IUPAC Name: 1,2,3,6-Tetrahydro-5-[3-(4-methylphenyl)-5-isoxazolyl]-1-propylpyridine oxalate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₈H₂₂N₂O.C₂H₂O₄.½H₂O

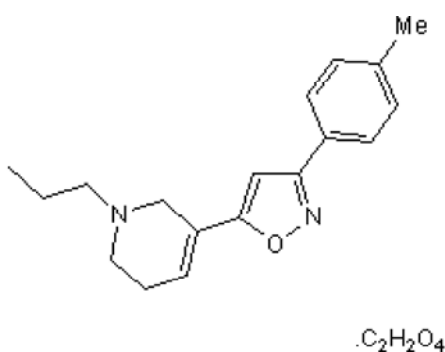
Batch Molecular Weight: 381.43

Physical Appearance: Off-white solid

Solubility: DMSO to 50 mM

Storage: Desiccate at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.5% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	62.98	6.61	7.34
Found	65.12	6.57	7.47

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

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Description:

High affinity, selective σ_1 ligand (K_i values are 0.08 and 1377 nM for σ_1 and σ_2 respectively). Displays no significant activity at a wide range of other receptors, ion channels and enzymes. Antagonizes mescaline-induced scratching in mice following i.p. administration. Also attenuates cocaine-induced hyperactivity in mice.

Physical and Chemical Properties:

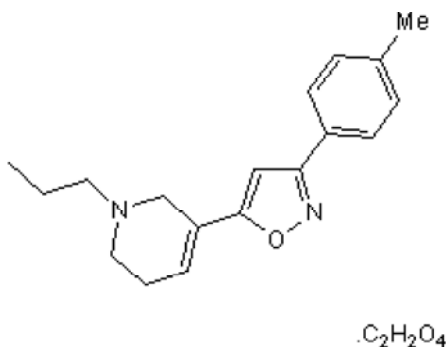
Batch Molecular Formula: $C_{18}H_{22}N_2O \cdot C_2H_2O_4 \cdot \frac{1}{2}H_2O$

Batch Molecular Weight: 381.43

Physical Appearance: Off-white solid

Minimum Purity: $\geq 98\%$

Batch Molecular Structure:



References:

Lever et al (2014) Relationship between cerebral sigma-1 receptor occupancy and attenuation of cocaine's motor stimulatory effects in mice by PD144418. *J.Pharmacol.Exp.Ther.* **351** 153. PMID: 25100754.

Akunne et al (1997) The pharmacology of the novel and selective sigma ligand, PD 144418. *Neuropharmacology* **36** 51. PMID: 9144641.

Storage: Desiccate at RT

Solubility & Usage Info:

DMSO to 50 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.

Licensing Information:

Sold for research purposes under agreement from Pfizer Inc.

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