

Product Data Sheet

Product Name: PF-4981517

Cat. No.: GC12280

Chemical Properties

Cas. No. 1390637-82-7

Chemical Name 1-methyl-3-[1-methyl-5-(4-methylphenyl)pyrazol-4-yl]-4-[(3S)-3-piperidin-1-ylpyrrolidin-1-yl]pyrazolo[3,4-d]pyrimidine

SMILES CC1=CC=C(C=C1)C2=C(C=NN2C)C3=NN(C4=C3C(=NC=N4)N5CCC(C5)N6CCCCC6)C

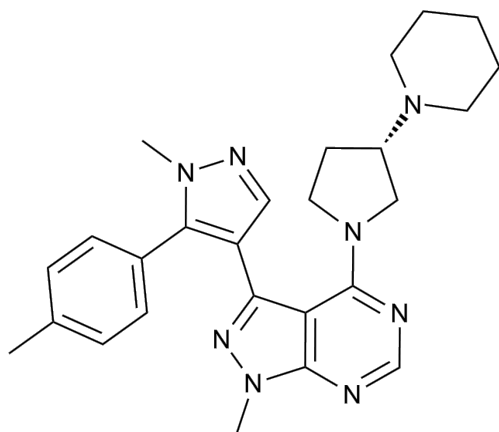
Formula $C_{26}H_{32}N_8$ M.Wt 456.59

Solubility DMF: 30 mg/ml, DMF:PBS(pH 7.2) (1:1): 0.5 mg/ml, DMSO: 20 mg/ml, Ethanol: 2 mg/ml Storage Store at -20°C

General tips For obtaining a higher solubility, please warm the tube at 37 °C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C for several months.

Shipping Condition Evaluation sample solution: ship with blue ice All other available size: ship with RT, or blue ice upon request.

Structure



Background

PF-4981517, also named CYP3cide, is a potent, efficient, and specific time-dependent inactivator of human CYP3A4. PF-4981517 is a very useful tool for understanding the relative roles of CYP3A4 versus CYP3A5 and the impact of CYP3A5 genetic polymorphism on a compound's

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pharmacokinetics. PF-4981517 is a lipophilic compound with a pKa which will render it cationic at physiological pH. Thus, it is possible that if incubate with high concentrations of microsomes, it can nonspecifically partition into microsomal phospholipid, and its apparent potency will be reduced. PF-4981517 should be useful to investigators seeking to delineate the relative contribution of CYP3A4 versus CYP3A5 in the metabolism of compounds cleared by CYP3A.

Reference

[1].Robert L. Walsky, R. Scott Obach, Ruth Hyland, Ping Kang, Sue Zhou, Michael West, Kieran F. Geoghegan, Christopher J. Helal, Gregory S. Walker, Theunis C. Goosen and Michael A. Zientek. *Selective Mechanism-Based Inactivation of CYP3A4 by CYP3cide (PF-04981517) and Its Utility as an In Vitro Tool for Delineating the Relative Roles of CYP3A4 versus CYP3A5 in the Metabolism of Drugs*. DMD September 2012 vol. 40 no. 9 1686-1697.

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