

Product Data Sheet

Product Name: PhiKan 083

Cat. No.: GC12658

Chemical Properties

Cas. No. 880813-36-5

Chemical Name 1-(9-ethyl-9H-carbazol-3-yl)-N-methylmethanamine hydrochloride

SMILES CNCC1=CC2=C(C=C1)N(CC)C3=C2C=CC=C3.Cl

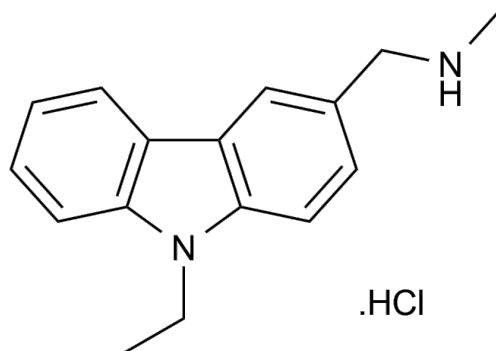
Formula $C_{16}H_{18}N_2.HCl$ M.Wt 274.79

Solubility <13.74mg/ml in Water; <27.48mg/ml in DMSO Storage Store at 4°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

Ki: ≈ 150 M

PhiKan 083 is a critical p53 stabilizing agent by bonding its mutation Y220C

The mutation Y220C of p53 exists a surface cavity that destabilizes the protein by 4 kcal/mol, at a site that is not functional. A p53 stabilizing agent binding it is able to slow rate of thermal denaturation [1].

Caution: Product has not been fully validated for medical applications. For research use only.

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In vitro: Isothermal titration of PhiKan083 with T-p53C-Y220C exhibited 1:1 stoichiometry and a K_d of 125 ± 10 M. PhiKan083 stabilized T-p53C-Y220C in a concentration-dependent manner. In a simple binding model for PhiKan083 (T-p53C-Y220C at 310 K (37°C)), in the absence of ligand, the protein gave a half-life of 3.8 min, while it increased to 15.7 min at saturating concentrations of PhiKan083. This is a proposed anticancer drug that could be developed for the Y220C mutant using p53 stabilizing agent. The site of mutation in the oncogenic Y220C mutant PhiKan083 binds with reasonable affinity is a druggable target. Interestingly, the site of mutation does not exist in a region of the protein that is functionally important, it will be an excellent target for drug stabilization therapy. This suggests the crystal structure of the complex will be a fresh start for further rounds of drug design and refinement [1].

In vivo: So far, no study in vivo has been conducted.

Clinical trial: So far, no clinical study has been conducted.

Reference:

[1] Boeckler FM, Joerger AC, Jaggi G, Rutherford TJ, Veprintsev DB, Fersht AR. Targeted rescue of a destabilized mutant of p53 by an in silico screened drug. Proc Natl Acad Sci U S A. 2008 Jul 29; 105(30):10360-5.

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