

## Product Data Sheet

Product Name: LY2940680

Cat. No.: GC15683

### Chemical Properties

Cas. No. 1258861-20-9

Chemical Name 4-fluoro-N-methyl-N-[1-[4-(2-methylpyrazol-3-yl)phthalazin-1-yl]piperidin-4-yl]-2-(trifluoromethyl)benzamide

SMILES CN1C(=CC=N1)C2=NN=C(C3=CC=CC=C32)N4CCC(CC4)N(C)C(=O)C5=C(C=C(C=C5)F)C(F)(F)F

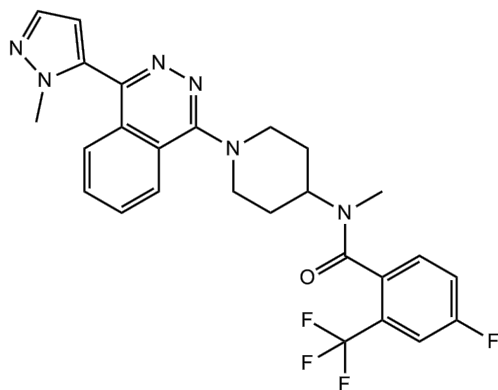
Formula  $C_{26}H_{24}F_4N_6O$  M.Wt 512.5

Solubility  $\geq 51.3\text{mg/mL}$  in DMSO with ultrasonic and warming Storage Store at  $-20^{\circ}\text{C}$

General tips For obtaining a higher solubility, please warm the tube at  $37^{\circ}\text{C}$  and shake it in the ultrasonic bath for a while. Stock solution can be stored below  $-20^{\circ}\text{C}$  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

LY2940680 is a selective inhibitor of Smo receptor and thus inhibits Hh signaling pathway [1].

Smoothed(Smo) receptor is a member of class F G protein-coupled receptors, which plays an important role in the main transducer of the Hedgehog (Hh) signaling pathway that implicated in a wide range of developmental and adult processes [2].

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

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LY2940680 is a potent Smo receptor inhibitor that binds mostly to extracellular loops and has a different functioning site with the reported Smo receptor inhibitor SANT-1 which binds to 7TM [2]. When tested with cell lines containing a mutation in the gene encoding Smoothed that researchers had previously observed in patient with cancer who developed resistance to vismodegib, LY2940680 inhibited cell proliferation [3].

Many studies have shown that Hh signaling pathway plays a pivotal role in CSCs and Hh inhibition caused many aspects of transformation attributed to CSCs. In patients with basal cell carcinoma and medulloblastoma, LY2940680 showed good efficacy as a monotherapy [1].

### References:

- [1]. Justilien, V. and A.P. Fields, Molecular pathways: novel approaches for improved therapeutic targeting of Hedgehog signaling in cancer stem cells. Clin Cancer Res, 2015. 21(3): p. 505-13.
- [2]. Hoch, L., et al., MRT-92 inhibits Hedgehog signaling by blocking overlapping binding sites in the transmembrane domain of the Smoothed receptor. Faseb j, 2015. 29(5): p. 1817-29.
- [3]. Redmond, E.M., et al., Investigational Notch and Hedgehog inhibitors--therapies for cardiovascular disease. Expert Opin Investig Drugs, 2011. 20(12): p. 1649-64.

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