
Product Data Sheet

Product Name: 3F8
Cat. No.: GC14306

Chemical Properties

Cas. No. 159109-11-2

Chemical Name 5-ethyl-1-hydroxy-7,8-dimethoxy-3H-pyrrolo[3,4-c]isoquinolin-3-one

SMILES CCC1=NC2=C(C(O)=NC2=O)C3=CC(OC)=C(OC)C=C31

Formula $C_{15}H_{14}N_2O_4$ M.Wt 286.28

Solubility Soluble in DMSO Storage Store at $-20^{\circ}C$

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

IC50: 34 and 304 nM in the presence of 10 and 100 μM ATP, respectively.

3F8 is a potent and selective GSK-3 β (Glycogen Synthase Kinase 3) inhibitor

GSK3 was identified as a serine/threonine protein kinase for the first time in the late 1970s and is highly conserved in all animals examined. GSK3 can regulate cell differentiation and apoptosis, and is an important component of the canonical Wnt pathway as well as the hedgehog pathway

In vitro: 3F8 specifically abolishes eye and forebrain formation in zebrafish embryos with the similar as a typical Wnt overexpression phenotype. Cell reporter assays, chemical informatics analysis and in vitro kinase experiments exhibited that 3F8 is a selective GSK3 inhibitor with more potent than SB216763 (a commonly used GSK3 inhibitor). Together, 3F8 and its derivatives could be useful as new agents and potential therapeutic candidates for GSK3 related diseases [1].

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

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The interaction of 3F8 with its binding site were studied. To this end, first computational analysis conducted, and the results suggested that maleimide moiety of 3F8 might interact with the ATP binding site of GSK-3 β , and the N-4 and C-5 positions were solvent-exposed, indicating the less key role of this region to the binding affinity. [2].

In vivo: The lowest ratio (CE/IC₅₀ = 221) of 3F8 implied that 3F8 was more efficient in vivo, likely according to better absorption and/or stability [1]. By injection of a sub-lethal amount of morpholino antisense oligonucleotides, individual knockdown of gsk3a and gsk3b translations in zebrafish caused cardiac defect [1].

Clinical trial: Clinical study has been conducted.

References:

[1]. Zhong H, Zou H, Semenov MV, Moshinsky D, He X, Huang H, Li S, Quan J, Yang Z, Lin S. Characterization and development of novel small-molecules inhibiting GSK3 and activating Wnt signaling. *Mol Biosyst.* 2009 Nov;5(11):1356-60.

[2]. Zou H, Zhou L, Li Y, Cui Y, Zhong H, Pan Z, Yang Z, Quan J. Benzo[e]isoindole-1,3-diones as potential inhibitors of glycogen synthase kinase-3 (GSK-3). Synthesis, kinase inhibitory activity, zebrafish phenotype, and modeling of binding mode. *J Med Chem.* 2010 Feb 11;53(3):994-1003.

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