

Product Data Sheet

Product Name: I-BRD9
Cat. No.: GC12588

Chemical Properties

Cas. No. 1714146-59-4

Chemical Name N-(1,1-dioxidotetrahydro-2H-thiopyran-4-yl)-5-ethyl-4-oxo-7-(3-(trifluoromethyl)phenyl)-4,5-dihydrothieno[3,2-c]pyridine-2-carboximidamide

SMILES N=C(C(S1)=CC2=C1C(C3=CC=CC(C(F)(F)F)=C3)=CN(CC)C2=O)NC(CC4)CCS4(=O)=O

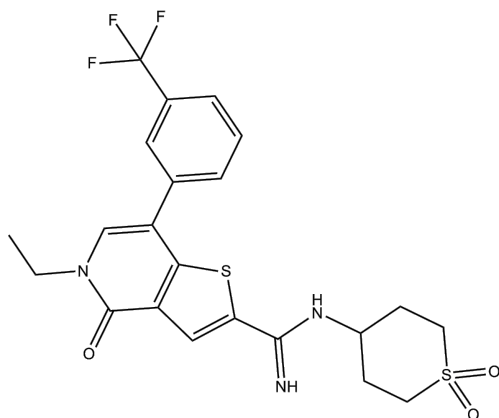
Formula $C_{22}H_{22}F_3N_3O_3S_2$ M.Wt 497.55

Solubility DMF: 30 mg/mL, DMF:PBS(pH 7.2) (1:1): 0.5 mg/mL, DMSO: 25 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

pIC50: 7.3

I-BRD9 is a BRD9 inhibitor.

BRD9 is identified as a bromodomain containing protein forming a small sub-branch of the

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bromodomain family tree. Human BRD9 has a single bromodomain and contains five isoforms which are produced by alternative splicing.

In vitro: In previous study, the I-BRD9 development was driven by iterative medicinal chemistry, using structure based design to result in nanomolar potency at BRD9, over 700-fold selectivity against the BET family as well as more than 70-fold to a panel of 34 bromodomains. In Kasumi-1 cells, I-BRD9 could downregulate DUSP6, CLEC1, SAMS1 and FES genes. Moreover, I-BRD9 was used to explore genes regulated by BRD9 in Kasumi-1 cells involved in immune response and oncology pathways. In addition, when BRD4 was used as a representative member of the BET family for initial selectivity screening, I-BRD9 was found to have a pIC₅₀ of 5.3 against this protein. I-BRD9 thus represented the first available selective tool compound to investigate the cellular phenotype of the inhibition of BRD9 bromodomain [1].

In vivo: So far, there is no animal in vivo data reported for I-BRD9.

Clinical trial: Up to now, I-BRD9 is still in the preclinical development stage.

Reference:

[1] Theodoulou NH et al. Discovery of I-BRD9, a Selective Cell Active Chemical Probe for Bromodomain Containing Protein 9 Inhibition. J Med Chem. 2016 Feb 25;59(4):1425-39.

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