

PRODUCT INFORMATION

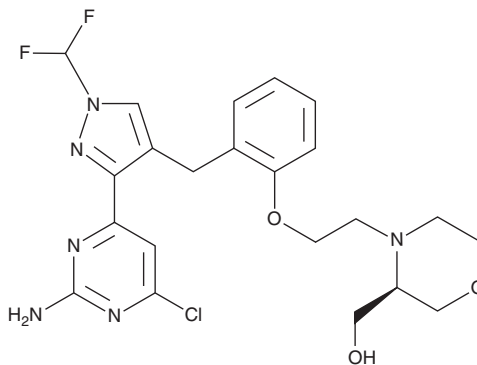


TDI-11861

Item No. 39922

CAS Registry No.: 2857049-72-8
Formal Name: (3R)-4-[2-[2-[[3-(2-amino-6-chloro-4-pyrimidinyl)-1-(difluoromethyl)-1H-pyrazol-4-yl]methyl]phenoxy]ethyl]-3-morpholinemethanol

MF: C₂₂H₂₅ClF₂N₆O₃
FW: 494.9
Purity: ≥95%
Supplied as: A solid
Storage: -20°C
Stability: ≥4 years



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

Laboratory Procedures

TDI-11861 is supplied as a solid. A stock solution may be made by dissolving the TDI-11861 in the solvent of choice, which should be purged with an inert gas. TDI-11861 is soluble in the organic solvent DMSO.

Description

TDI-11861 is an inhibitor of soluble adenylyl cyclase (sAC; IC₅₀ = 3.3 nM), a bicarbonate-regulated cytosolic enzyme also known as AC10.¹ It is selective for sAC over the transmembrane ACs (tmACs) AC1, AC2, AC5, AC8, and AC9 at 100 nM, a panel of 322 kinases (IC₅₀s = >1,000 nM for all), and 46 other targets, including G protein-coupled receptors (GPCRs), nuclear receptors, and ion channels, with 50% response concentration values (RC₅₀s) of greater than 9 μM. TDI-11861 has an increased residence time when binding to sAC in a surface plasmon resonance (SPR) assay and a slower dissociation rate in a jump dilution recovery assay compared with the sAC inhibitor TDI-10229 (Item No. 37674), indicating a lower risk of post-copulation female genital tract dilution. It inhibits capacitation-induced cAMP accumulation in isolated mouse and human sperm when used at a concentration of 5 μM and reduces sodium bicarbonate-induced increases in mouse and human sperm beat frequency.² Oral administration of a single dose of TDI-11861 (50 mg/kg) induces temporary infertility in male mice without affecting mating behavior.

References

1. Miller, M., Rossetti, T., Ferreira, J., *et al.* Design, synthesis, and pharmacological evaluation of second-generation soluble adenylyl cyclase (sAC, ADCY10) inhibitors with slow dissociation rates. *J. Med. Chem.* **65**(22), 15208-15226 (2022).
2. Balbach, M., Rossetti, T., Ferreira, J., *et al.* On-demand male contraception via acute inhibition of soluble adenylyl cyclase. *Nat. Commun.* **14**(1), 637 (2023).

WARNING

THIS PRODUCT IS FOR RESEARCH ONLY - NOT FOR HUMAN OR VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

SAFETY DATA

This material should be considered hazardous until further information becomes available. Do not ingest, inhale, get in eyes, on skin, or on clothing. Wash thoroughly after handling. Before use, the user must review the complete Safety Data Sheet, which has been sent via email to your institution.

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