

Product Name: TDI 11861

Catalog No.: 8036

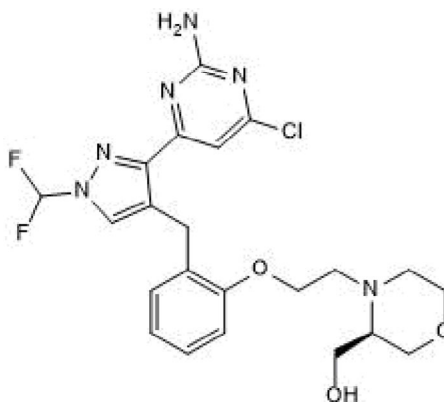
Batch No.: 1

CAS Number: 2857049-72-8

IUPAC Name: (3*R*)-4-[2-[2-[[3-(2-Amino-6-chloro-4-pyrimidinyl)-1-(difluoromethyl)-1*H*-pyrazol-4-yl]methyl]phenoxy]ethyl]-3-morpholinemethanol

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₂H₂₅ClF₂N₆O₃.
Batch Molecular Weight: 494.93
Physical Appearance: White solid
Solubility: DMSO to 100 mM
 ethanol to 100 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.3% purity
Chiral HPLC: Shows 100.0% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	53.39	5.09	16.98
Found	53.55	4.91	16.91

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Description:

TDI 11861 is a potent and selective soluble adenylyl cyclase (sAC) inhibitor (IC₅₀ values are 3.3 nM and 5.5 nM in biochemical and cellular assays, respectively; K_d = 1.4 nM). Inhibits cellular sAC-specific cAMP accumulation (IC₅₀ = 7 nM) and blocks sperm capacitation in vitro. Cell permeable, not cytotoxic and suitable for both in vivo and in vitro use.

Physical and Chemical Properties:

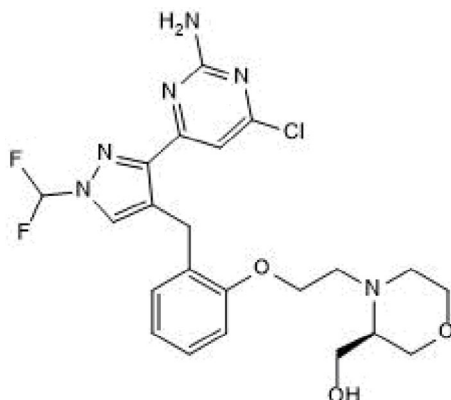
Batch Molecular Formula: C₂₂H₂₅ClF₂N₆O₃.

Batch Molecular Weight: 494.93

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol to 100 mM

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

Licensing Information:

Sold under license from Cornell University

References:

Balbach et al (2023) On-demand male contraception via acute inhibition of soluble adenylyl cyclase. Nat.Commun. **14** 637. PMID: 36788210.

Miller et al (2022) Design, synthesis, and pharmacological evaluation of second-generation soluble adenylyl cyclase (sAC, ADCY10) inhibitors with slow dissociation rates. J.Med.Chem. **65** 15208. PMID: 36346696.

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