

Product Name: DX3-213B

Catalog No.: 8070

Batch No.: 1

CAS Number: 2749555-66-4

IUPAC Name: (4,4-Difluoro-1-piperidiny)[(3*R*)-1-[4-[(1-methylethyl)sulfonyl]phenyl]sulfonyl]-3-piperidiny]methanone

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₀H₂₈F₂N₂O₅S₂

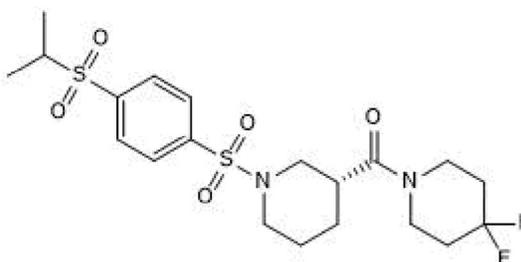
Batch Molecular Weight: 478.57

Physical Appearance: White solid

Solubility: DMSO to 50 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 97.0% purity

Chiral HPLC: Shows 100.0% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	50.19	5.9	5.85
Found	50.26	5.95	5.71

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Description:

DX3-213B is a potent oxidative phosphorylation (OXPHOS) complex I (also known as NDUFS7) antagonist (IC₅₀ = 3.6 nM). DX3-213B impairs ATP generation (IC₅₀ = 11 nM) and inhibits the proliferation of MIA PaCa-2 cells (IC₅₀ = 9 nM) in galactose-containing media. In vivo, DX3-213B significantly delays tumor growth in a syngeneic mouse model of pancreatic cancer. DX3-213B is orally bioavailable.

Physical and Chemical Properties:

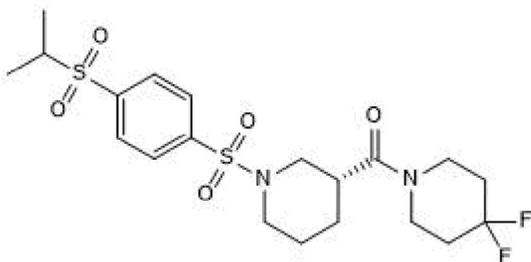
Batch Molecular Formula: C₂₀H₂₈F₂N₂O₅S₂

Batch Molecular Weight: 478.57

Physical Appearance: White solid

Minimum Purity: ≥97%

Batch Molecular Structure:



References:

Xu et al (2023) First-in-class NADH/Ubiquinone oxidoreductase core subunit S7 (NDUFS7) antagonist for the treatment of pancreatic cancer. *ACS Pharmacol. Transl. Sci.* **6** 1164. PMID: 37588763.

Xue et al (2022) Multiparameter optimization of oxidative phosphorylation inhibitors for the treatment of pancreatic cancer. *J. Med. Chem.* **65** 3404. PMID: 35167303.

Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 50 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 the University of Michigan

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