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Certificate of Analysis

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Product Name: SJPYT 310

Catalog No.: 8839 Batch No.: 1

CAS Number: 2883814-84-2 IUPAC Name: *N*-I5-(1.1-Dime

N-[5-(1,1-Dimethylethyl)-2-[(1S)-1-methylbutoxy]phenyl]-1-(2-methoxy-5-methylphenyl)-5-methyl-1*H*-1,2,3-triazole-4-carboxamide

0

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility: $C_{27}H_{36}N_4O_3$. 464.61 Pale pink solid DMSO to 100 mM ethanol to 100 mM

Store at -20°C

Storage:

2. ANALYTICAL DATA

Mass Spectrum:

Microanalysis:

Chiral HPLC:

HPLC:

¹H NMR:

Batch Molecular Structure:

Shows 99.9% purity Shows 97.8% purity Consistent with structure

Consistent with structure

	Carbon Hydrogen Nitrog			
Theoretical	69.8	7.81	12.06	
Found	69.22	7.85	11.98	

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

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Print Date: May 9th 2025

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Description:

SJPYT 310 is a potent and selective PXR antagonist (IC_{50} values are 4 and 9 nM for biding and cellular activity, respectively). SJPYT 310 displays selectivity for hPXR without affecting the activity of mPXR, hCAR, hFXR, hLXR α , or hVDR. SJPYT 310 shows no toxicity.

Physical and Chemical Properties:

Batch Molecular Formula: C₂₇H₃₆N₄O₃. Batch Molecular Weight: 464.61 Physical Appearance: Pale pink 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).

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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 St. Jude Children's Research Hospital

References:

Garcia-Maldonado et al (2024) Chemical manipulation of an activation/inhibition switch in the nuclear receptor PXR. Nat.Commun. 15 4054. PMID: 38744881.

Li (2022) Design and optimization of 1 H-1,2,3-Triazole-4-carboxamides as novel, potent, and selective inverse agonists and antagonists of PXR. J.Med.Chem. 65 16829. PMID: 36480704.

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