

Product Name: SJPYT 328

Catalog No.: 8840

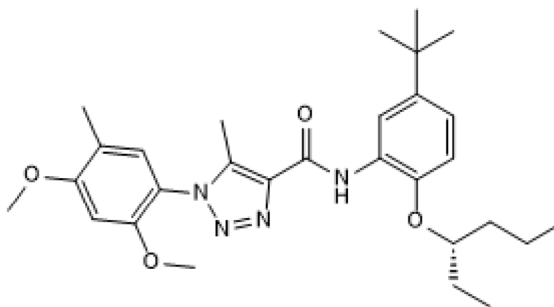
Batch No.: 1

CAS Number: 2998548-72-2

IUPAC Name: 1-(2,4-Dimethoxy-5-methylphenyl)-N-[5-(1,1-dimethylethyl)-2-[(1S)-1-ethylbutoxy]phenyl]-5-methyl-1*H*-1,2,3-triazole-4-carboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₉H₄₀N₄O₄.
Batch Molecular Weight: 508.66
Physical Appearance: White solid
Solubility: DMSO to 10 mM
 ethanol to 10 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.3% purity
Chiral HPLC: Shows 98.3% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	68.48	7.93	11.01
Found	68.66	8.05	11.05

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

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Description:

SJPYT 328 is a potent and selective PXR1 agonist ($IC_{50} = 7$ nM). SJPYT 328 displays selectivity for hPXR without affecting the activity of mPXR, hCAR, hFXR, hLXR α , or hVDR. SJPYT 328 and SJPYT (PXR1 antagonist) are a useful pair of compounds for referencing "full agonist" and "full antagonist" when screening for new drugs in cellular models. SJPYT 328 shows no toxicity.

Physical and Chemical Properties:

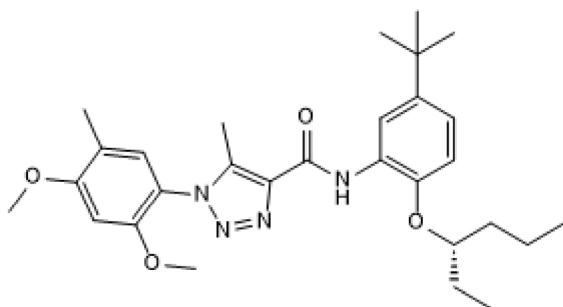
Batch Molecular Formula: $C_{29}H_{40}N_4O_4$.

Batch Molecular Weight: 508.66

Physical Appearance: White solid

Minimum Purity: $\geq 98\%$

Batch Molecular Structure:



Storage: Store at $-20^{\circ}C$

Solubility & Usage Info:

DMSO to 10 mM

ethanol to 10 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 $45-60^{\circ}C$ 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 $-20^{\circ}C$ 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.Comms.* **15** 4054. PMID: 38744881.

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bio-techne.com

info@bio-techne.com

techsupport@bio-techne.com

North America

Tel: (800) 343 7475

China

info.cn@bio-techne.com

Tel: +86 (21) 52380373

Europe Middle East Africa

Tel: +44 (0)1235 529449

Rest of World

www.tocris.com/distributors

Tel:+1 612 379 2956