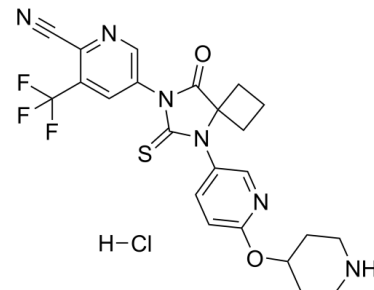


Data Sheet

Product Name:	JNJ-63576253
Cat. No.:	CS-0149492
CAS No.:	2110428-64-1
Molecular Formula:	C ₂₃ H ₂₂ ClF ₃ N ₆ O ₂ S
Molecular Weight:	538.97
Target:	Androgen Receptor
Pathway:	Others
Solubility:	DMSO : 250 mg/mL (463.85 mM; Need ultrasonic)



BIOLOGICAL ACTIVITY:

JNJ-63576253 (TRC-253) is a potent and orally active full antagonist of **androgen receptor (AR)**, with IC₅₀s of 37 and 54 nM for F877L mutant AR and wild-type AR in LNCaP cells. JNJ-63576253 can be used for the research of castration-resistant prostate cancer (CRPC)^[1]. IC₅₀ & Target: IC₅₀: 37 nM (F877L mutant AR in LNCaP cells); 54 nM (wild-type AR in LNCaP cells)^[1] **In Vitro**: JNJ-63576253 (0.0003-100 μM; 5 d) inhibits the growth of VCaP cells, with an IC₅₀ of 265 nM^[1]. JNJ-63576253 is stable in human liver microsomes, with an T_{1/2} of >180 min^[1]. **In Vivo**: JNJ-63576253 (30 mg/kg; p.o. once daily for 72 days) significantly inhibits the growth of prostate LNCaP SRα F877L tumor in mice^[1]. JNJ-63576253 (30 mg/kg; p.o. once daily for 10 days) inhibits the five androgen sensitive organs (ASOs) under stimulation by testosterone propionate (TP) in mice^[1]. JNJ-63576253 (10 mg/kg; p.o.) exhibits moderate oral bioavailability (45%), C_{max} (0.66 μM) and AUC_{last} (4.9 μg•h/mL) in mice^[1]. JNJ-63576253 (2 mg/kg; i.v.) exhibits reasonable half-life (5.99 h), CL (15.0 mL/min/kg) and Vdss (6.11 L/kg) in mice^[1].

References:

[1]. Zhang Z, et, al. Discovery of JNJ-63576253: A Clinical Stage Androgen Receptor Antagonist for F877L Mutant and Wild-Type Castration-Resistant Prostate Cancer (mCRPC). J Med Chem. 2021 Jan 28;64(2):909-924.

CAIndexNames:

2-Pyridinecarbonitrile, 5-[8-oxo-5-[6-(4-piperidinyloxy)-3-pyridinyl]-6-thioxo-5,7-diazaspiro[3.4]oct-7-yl]-3-(trifluoromethyl)-, hydrochloride (1:1)

SMILES:

[H]Cl.O=C(N(C(N1C2=CC=C(N=C2)OC3CCNCC3)=S)C(C=C4C(F)(F)F)=CN=C4#N)C51CCC5

Caution: Product has not been fully validated for medical applications. For research use only.

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