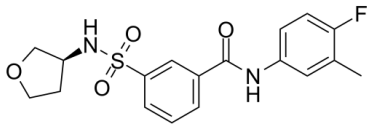
Data Sheet

Product Name:	JNJ-632
Cat. No.:	CS-0046637
CAS No.:	1572510-42-9
Molecular Formula:	$C_{18}H_{19}FN_2O_4S$
Molecular Weight:	378.42
Target:	HBV
Pathway:	Anti-infection
Solubility:	DMSO : 125 mg/mL (330.32 mM; Need ultrasonic)



BIOLOGICAL ACTIVITY:

JNJ-632 is a hepatitis B virus (**HBV**) capsid assembly modulator (**CAM**). IC50 & Target: HBV[1] **In Vitro:** JNJ-632 is a capsid assembly modulator inhibiting hepatitis B virus (HBV). JNJ-632 inhibits HBV DNA HepG2.2.15 and HBV DNA HepG2.117 with EC_{50}s of 0.12 and 0.43 μM, respectively. In the high-content multiparameter cytotoxicity (HepG2), JNJ-632 shows EC_{20}s in the 10-30 μM range (considered weakly cytotoxic)[1]. **In Vivo:** The single dose PK profile of JNJ-632 is evaluated in C57BL/6 mice following intravenous (iv) and oral (po) administration. JNJ-632 has a moderate plasma clearance of 34 mL/min/kg and a moderate volume of distribution of 1.3 L/kg. The oral bioavailability is 40% following oral administration of 10 mg/kg and 66% following oral administration of 50 mg/kg. JNJ-632 has moderate terminal elimination half-life with $t_{1/2}$s of 0.42±0.06 h, 1.1±0.67 h, 2.4±2.3 h, and 5.3±0.1 h for 2.5 mg/kg (iv), 10 mg/kg (po), 50 mg/kg (po), and 50 mg/kg (sc).To circumvent the first pass metabolism, JNJ-632 is also dosed subcutaneously at 50 mg/kg in C57BL/6 mice and this results in a concentration in plasma after 24 h of dosing of 102 ng/mL and concentration in liver after 24 h of dosing of 1297 ng/g[1].

PROTOCOL (Extracted from published papers and Only for reference)

Animal Administration: JNJ-632 is formulated as a 0.5 mg/mL solution in PEG400/water (70/30) (i.v.)[1].
JNJ-632 is formulated as 0.5 and 2.5 mg/mL suspension in methocel 0.5% w/v (p.o.)[1].[1]Mice[1]
The pharmacokinetic profile is evaluated in fed **male C57BL/6 mice** (n=3/group). Mice are **i.v.** injected with **JNJ-632** at **2.5 mg/kg**, formulated as a 0.5 mg/mL solution in PEG400/water (70/30), and blood samples are collected from the saphenous vein at 0.05, 0.17, 0.5, 1, 2, 4, 7, and 24 hours into EDTA-containing microcentrifuge tubes. **JNJ-632** is administered **p.o. at 10 and 50 mg/kg**, formulated as 0.5 and 2.5 mg/mL suspension in methocel 0.5% w/v, and blood samples are collected from the saphenous vein at 0.5, 1, 2, 4, 7, 9 and 24 hours into EDTA-containing microcentrifuge tubes. **JNJ-632** is administered **s.c. at 50 mg/kg**, and blood samples are collected. The blood samples are immediately centrifuged at 4°C and the plasma was stored at -20°C[1].

References:

[1]. Vandyck K, et al. Synthesis and Evaluation of N-Phenyl-3-sulfamoyl-benzamide Derivatives as Capsid Assembly Modulators Inhibiting Hepatitis B Virus (HBV). J Med Chem. 2018 Jul 26;61(14):6247-6260.

CAIndexNames:

Benzamide, N-(4-fluoro-3-methylphenyl)-3-[[[(3S)-tetrahydro-3-furanyl]amino]sulfonyl]-

SMILES:

O=C(NC1=CC=C(F)C(C)=C1)C2=CC=CC(S(=O)(N[C@@H]3COCC3)=O)=C2

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

Tel: 610-426-3128 Fax: 888-484-5008 E-mail: sales@ChemScene.com

Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA