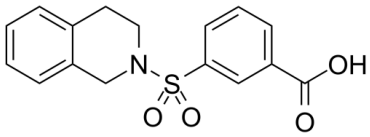
Data Sheet

Product Name:	AKR1C3-IN-1
Cat. No.:	CS-7878
CAS No.:	327092-81-9
Molecular Formula:	C16H15NO4S
Molecular Weight:	317.36
Target:	Others
Pathway:	Others
Solubility:	DMSO : ≥ 100 mg/mL (315.10 mM)



BIOLOGICAL ACTIVITY:

AKR1C3-IN-1 is a potent, highly selective inhibitor of **AKR1C3**, with an **IC_{50}** of 13 nM. IC50 & Target: IC50: 13 nM (AKR1C3)[1] **In Vitro:** AKR1C3-IN-1 shows less potent activities with 20.3±3.8 μM against AKR1C1 and >30 μM against AKR1C2 and AKR1C4. AKR1C3-IN-1 inhibits AKR1C3 activity (inhibiting PR-104H formation) with an IC_{50} of 0.027±0.002 μM[1].

PROTOCOL (Extracted from published papers and Only for reference)

Kinase Assay: [1]A competitive fluorescence assay is used to measure AKR1C enzyme activity, where a nonfluorescent ketone probe (probe 5) selective for the AKR1C enzyme isoforms is reduced to a fluorescent alcohol in the presence of AKR1C enzyme and NADPH. Briefly, purified protein (2 μg/mL AKR1C1, 1 μg/mL AKR1C2, 2 μg/mL AKR1C3, and 5 μg/mL AKR1C4) are incubated with 40 μM probe 5, AKR1C3-IN-1, and 50 μM NADPH in an assay buffer of 10 mM MOPS (pH=7.2), 130 mM NaCl, 1 mM DTT, and 0.01% Triton-X-100 for 1 h at 37°C. The reaction is stopped by addition of 35 mM NaOH, and fluorescence is read in a SpectraMax M2 microplate reader at excitation/emission wavelengths of 420/510 nM. The compounds and known AKR1C3 inhibitors (flufenamic acid, indomethacin, naproxen, meclofenamic acid, S(+)-ibuprofen and flurbiprofen) are tested at multiple concentrations between 0.1 nM and 100 μM in 2% DMSO to generate AKR1C enzyme inhibition data. Compound IC_{50} values are calculated by fitting the inhibition data to a four-parameter logistic sigmoidal dose-response curve using Prism 5.02.

References:

[1]. Jamieson SM, et al. 3-(3,4-Dihydroisoquinolin-2(1H)-ylsulfonyl)benzoic Acids: highly potent and selective inhibitors of the type 5 17-β-hydroxysteroid dehydrogenase AKR1C3. J Med Chem. 2012 Sep 13;55(17):7746-58.

CAIndexNames:

Benzoic acid, 3-[(3,4-dihydro-2(1H)-isoquinolinyl)sulfonyl]-

SMILES:

O=S(N1CC2=CC=CC=C2CC1)(C3=CC(C(O)=O)=CC=C3)=O

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

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