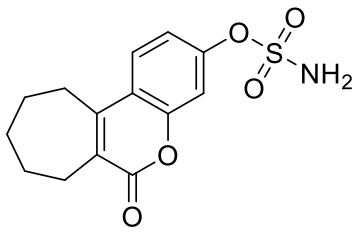
Product data sheet

MedKoo Cat#: 200550 Name: Irosustat CAS: 288628-05-7 Chemical Formula: $C_{14}H_{15}NO_5S$ Exact Mass: 309.0671 Molecular Weight: 309.3376	
Product supplied as:	Powder
Purity (by HPLC):	≥ 98%
Shipping conditions	Ambient temperature
Storage conditions:	Powder: -20°C 3 years; 4°C 2 years.
	In solvent: -80°C 3 months; -20°C 2 weeks.

1. Product description:

Irosustat, also known as STX64, BN83495 and 667 coumate, is a potent, irreversible inhibitor of steroid sulfatase. Inhibition of steroid sulfatase (STS), the enzyme responsible for the hydrolysis of steroid sulfates, represents a potential novel treatment for postmenopausal women with hormone-dependent breast cancer. Estrone and DHEA are formed by this sulfatase pathway and can be converted to steroids (estradiol and androstenediol, respectively), which have potent estrogenic properties. STX64 (667 coumate) is a potent tricylic coumarin-based sulfamate that irreversibly inhibits STS activity (IC50 = 8 nM in a placental microsomal assay system). Estrone sulfamate (EMATE) is also a potent STS inhibitor, but has estrogenic activity.

2. CoA, QC data, SDS, and handling instruction

SDS and handling instruction, CoA with copies of QC data (NMR, HPLC and MS analytical spectra) can be downloaded from the product web page under "QC And Documents" section. Note: copies of analytical spectra may not be available if the product is being supplied by MedKoo partners. Whether the product was made by MedKoo or provided by its partners, the quality is 100% guaranteed.

3. Solubility data

Solvent	Max Conc. mg/mL	Max Conc. mM
DMF	30.0	96.98
DMSO	53.23	175.09
Ethanol	9.05	29.24

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	3.23 mL	16.16 mL	32.33 mL
5 mM	0.65 mL	3.23 mL	6.47 mL
10 mM	0.32 mL	1.62 mL	3.23 mL
50 mM	0.07 mL	0.32 mL	0.65 mL

5. Molarity Calculator, Reconstitution Calculator, Dilution Calculator

Please refer the product web page under section of "Calculator"

6. Recommended literature which reported protocols for in vitro and in vivo study

In vitro study

1. Biernacki K, Ciupak O, Daśko M, Rachon J, Kozak W, Rak J, Kubiński K, Masłyk M, Martyna A, Śliwka-Kaszyńska M, Wietrzyk J, Świtalska M, Nocentini A, Supuran CT, Demkowicz S. Development of Sulfamoylated 4-(1-Phenyl-1H-1,2,3-triazol-4-yl)phenol Derivatives as Potent Steroid Sulfatase Inhibitors for Efficient Treatment of Breast Cancer. J Med Chem. 2022 Mar 24;65(6):5044-5056. doi: 10.1021/acs.jmedchem.1c02220. Epub 2022 Mar 2. PMID: 35235747; PMCID: PMC8958511.
2. Woo LW, Ganeshapillai D, Thomas MP, Sutcliffe OB, Malini B, Mahon MF, Purohit A, Potter BV. Structure-activity relationship for the first-in-class clinical steroid sulfatase inhibitor Irosustat (STX64, BN83495). ChemMedChem. 2011 Nov 4;6(11):2019-34. doi: 10.1002/cmdc.201100288. Epub 2011 Aug 25. PMID: 21990014; PMCID: PMC3262147.

In vivo study

1. Purohit A, Chander SK, Woo LW, Parsons MF, Jhalli R, Potter BV, Reed MJ. Inhibition of steroid sulphatase activity via the percutaneous route: a new option for breast cancer therapy. Anticancer Res. 2008 May-Jun;28(3A):1517-23. PMID: 18630506.

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2. Foster PA, Woo LW, Potter BV, Reed MJ, Purohit A. The use of steroid sulfatase inhibitors as a novel therapeutic strategy against hormone-dependent endometrial cancer. Endocrinology. 2008 Aug;149(8):4035-42. doi: 10.1210/en.2008-0223. Epub 2008 May 1. PMID: 18450955; PMCID: PMC2488239.

7. Bioactivity

Biological target:

Irosustat is a potent steroid sulfatase inhibitor, with an IC_{50} of 8 nM, and exhibits anti-breast cancer activity.

In vitro activity

In comparison, 10 nM concentration Irosustat led to a 12.9% residual enzymatic action. The experiment at a 1 nM inhibitor concentration showed a notable STS residual activity of 13.6% after incubation with 5l, even lower than the 16.8% produced by reference Irosustat. Relevantly, 4a, 4b, 5e, 5g, and 5l demonstrated STS inhibitory potency comparable to or greater than that of Irosustat. In fact, 4a, 4b, 5e, and 5g showed IC_{50} values of 1.90, 1.71, 2.95, and 1.69 nM, respectively, that are comparable to that of 1.06 nM detected for *Irosustat*.

Reference: J Med Chem. 2022 Mar 24;65(6):5044-5056. https://pubmed.ncbi.nlm.nih.gov/35235747/

In vivo activity

In this study the ability of the STS inhibitor STX64 (BN83495) and its N,N-dimethyl analogue (STX289) to inhibit liver and skin STS when applied orally or topically to nude mice was examined. It is concluded that both STX64 and STX289 are not only effective inhibitors of skin STS, but also liver STS when applied topically.

Reference: Anticancer Res. 2008 May-Jun;28(3A):1517-23. https://pubmed.ncbi.nlm.nih.gov/18630506/

Note: The information listed here was extracted from literature. MedKoo has not independently retested and confirmed the accuracy of these methods. Customer should use it just for a reference only.