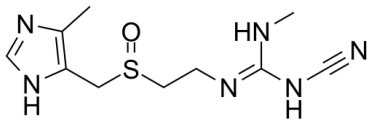
Data Sheet

Product Name:	Cimetidine sulfoxide
Cat. No.:	CS-0128291
CAS No.:	54237-72-8
Molecular Formula:	$C_{10}H_{16}N_6OS$
Molecular Weight:	268.34
Target:	Histamine Receptor
Pathway:	GPCR/G Protein; Immunology/Inflammation; Neuronal Signaling
Solubility:	DMSO : 83.33 mg/mL (310.54 mM; ultrasonic and warming and heat to 60°C)



BIOLOGICAL ACTIVITY:

Cimetidine sulfoxide (Cimetidine sulphoxide) is a sulfoxide metabolite of Cimetidine. Cimetidine is a **histamine H_2-receptor** antagonist. Cimetidine has the potential for peptic ulcer disease and upper gastrointestinal haemorrhage treatment[1]. IC50 & Target: Histamine H_2-receptor[1] **In Vitro:** Active transport of Cimetidine across the rat small intestine is observable at lower substrate concentrations (40 and 200 μM), but is masked by passive transfer at higher concentrations (400 μM). Cimetidine sulfoxide is detected after some incubations[2]. **In Vivo:** The enantiomeric composition of Cimetidine sulfoxide is also determined in rat urine (24 h) following the administration of Cimetidine (30 mg/kg; po) to male Wistar rats. The enantiomeric ratio in this case is found to be (+/−) 57:43[3].

References:

[1]. Larsson R, et al. The pharmacokinetics of cimetidine and its sulphoxide metabolite in patients with normal and impaired renal function. Br J Clin Pharmacol. 1982;13(2):163-170.

[2]. HE Barber, et al. The Transport of Cimetidine Across the Rat Small Intestine in Vitro. B r J Pharmacol. 1979 Jul;66(3):496P-497P.

[3]. Ryta A. Kuzel, et al. Investigations into the chirality of the metabolic sulfoxidation of cimetidine. Chirality (1994), 6(8), 607-14.

CAIndexNames:

Guanidine, N-cyano-N′-methyl-N″-[2-[[(4-methyl-1H-imidazol-5-yl)methyl]sulfinyl]ethyl]-

SMILES:

O=S(CC/N=C(NC)/NC#N)CC1=C(C)N=CN1

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

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