Product Data Sheet

Product Name: Omeprazole sulfone
Cat. No.: GC11155

Chemical Properties

Cas. No.	88546-55-8		
Chemical Name	6-methoxy-2-[[(4-methoxy-3,5-dimethyl-2-pyridinyl)methyl]sulfonyl]-1H-benzimidazole		
SMILES	COC1=CC=C2C(N=C(S(CC3=C(C)C(OC)=C(C)C=N3)(=O)=O)N2)=C1		
Formula	$C_{17}H_{19}N_3O_4S$	M.Wt	361.4
Solubility	≤5mg/ml in ethanol;30mg/ml in DMSO;30mg/ml in dimethyl formamide	Storage	Store at -20°C
General tips	For obtaining a higher solubility , please warm the tube at 37 ℃ and shake it in the ultrasonic bath for a while.Stock solution can be stored below -20℃ for several months.		
Shipping Condition	Evaluation sample solution : ship with blue ice All other available size: ship with RT , or blue ice upon request.		
Structure	Omeprazole sulfone		

Background

Omeprazole sulfone is the major metabolite of the gastric proton pump inhibitor, omeprazole [1]. The Proton Pump Inhibitor, Omeprazole, is a metabolism-dependent inhibitor of CYP2C19 with a relatively low incidence of adverse events and pharmacokinetic drug-drug interactions (DDIs) [1]. Omeprazole sulfone is produced by cytochrome P450 (CYP)3A4 sulfoxidation of esomeprazole and has been found in plasma [2]. Cytochrome P450 was once believed to be mainly a hepatic drug detoxication system, but is now understood to include a myriad of enzymic reactions implicated in important life processes. Mutations in many CYP genes cause inborn errors of metabolism and lead to many clinically relevant diseases [3].

In vitro: Omeprazole sulfone has been shown to act as a reversible direct-acting and metabolism-dependent inhibitor of CYP2C19 in pooled human liver microsomes with an IC50 of 18 μM [1].

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In vivo: Three hours after intake of 20 mg omeprazole only, the geometric mean plasma concentration of omeprazole sulfone were 106 nmol/l in 22 samples from subjects known to be extensive CYP2C19 metabolizers (EM) and 672 nmol/l in the five subjects known to be poor CYP2C19 metabolizers (PM). The mean log10(omeprazole/omeprazole sulfone) ratio was 0.18 [4].

References:

[1] Nebert D W, Russell D W. Clinical importance of the cytochromes P450[J]. The Lancet, 2002, 360(9340): 1155-1162.
[2] bel A, Andersson T B, Antonsson M, et al. Stereoselective metabolism of omeprazole by human cytochrome P450 enzymes[J]. Drug Metabolism and Disposition, 2000, 28(8): 966-972.
[3] Nebert D W, Russell D W. Clinical importance of the cytochromes P450[J]. The Lancet, 2002, 360(9340): 1155-1162.
[4] Bttiger Y. Use of omeprazole sulfone in a single plasma sample as a probe for CYP3A4[J]. European journal of clinical pharmacology, 2006, 62(8): 621-625.

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