Product Data Sheet

Product Name: Benzenesulfonamide
Cat. No.: GC17003

Chemical Properties

Cas. No.	98-10-2		
Chemical Name	benzenesulfonamide		
SMILES	NS(C1=CC=CC=C1)(=O)=O		
Formula	$C_6H_7NO_2S$	M.Wt	157.19
Solubility	DMSO : 31mg/mL	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	Benzenesulfonamide		

Background

Benzenesulfonamide, the amide of benzenesulfonic acid, has been used to produce various derivatives, especially those used as intermediates in the synthesis of photochemicals, dyes, disinfectants, as well as pharmaceuticals.

In vitro: In a previous study, a series of N-aryl-β-alanine- and diazo-derivatives of benzenesulfonamide were designed, synthesized, and their binding affinities to carbonic anhydrases (CA) I, II, VI, VII, XII, and XIII was investigated by the use of isothermal titration calorimetry and fluorescent thermal shift assay. The results indicated that 4-substituted diazobenzenesulfonamides were found to be most potent CA binders among the synthesized derivatives. In addition, the majority of the N-aryl-β-alanine derivatives had better affinity for CA II while diazobenzenesulfonamides showed nanomolar affinities towards CA I isozyme. Moreover, the X-ray crystallographic data showed the binding modes of both derivative groups [1].

In vivo: In the rat CPE model, the most potnet benzenesulfonamide indole derivative at

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10 mg/kg in the MC/TW formulation displayed oral efficacy. Moreover, this compound, when administered in another preferred, minimal formulation in the same in vivo model, demonstrated superior oral efficacy to the lead phenylmethane sulfonamide WAY-196025 orally administered in a lipid-based formulation. In addition, this benzenesulfonamide indole derivative was also orally efficacious at 1 mg/kg by attenuating both LAR and the associated AHR to aerosolized carbachol in naturally sensitized sheep, which had been challenged through the airways with A. suum antigen [2].

Clinical trial: Up to now, benzenesulfonamide is still in the preclinical development stage.

References:
[1] Rutkauskas K et al. 4-amino-substituted benzenesulfonamides as inhibitors of human carbonic anhydrases. Molecules. 2014 Oct 28;19(11):17356-80.
[2] Lee KL et al. Benzenesulfonamide indole inhibitors of cytosolic phospholipase A2α: Optimization of in vitro potency and rat pharmacokinetics for oral efficacy. Bioorganic and Medicinal Chemistry. 2008 16(3), 1345-1358.