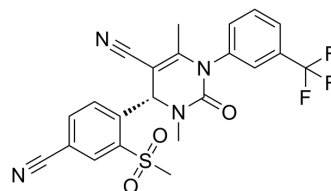


BAY-85-8501

Cat. No.:	HY-19908		
CAS No.:	1161921-82-9		
Molecular Formula:	C ₂₂ H ₁₇ F ₃ N ₄ O ₃ S		
Molecular Weight:	474.46		
Target:	Elastase		
Pathway:	Metabolic Enzyme/Protease		
Storage:	Powder	-20°C	3 years
		4°C	2 years
	In solvent	-80°C	2 years
		-20°C	1 year



SOLVENT & SOLUBILITY

In Vitro	DMSO : 200 mg/mL (421.53 mM; Need ultrasonic)				
		Solvent Concentration	Mass 1 mg	5 mg	10 mg
	Preparing Stock Solutions	1 mM	2.1077 mL	10.5383 mL	21.0766 mL
		5 mM	0.4215 mL	2.1077 mL	4.2153 mL
10 mM		0.2108 mL	1.0538 mL	2.1077 mL	
Please refer to the solubility information to select the appropriate solvent.					
In Vivo	<ol style="list-style-type: none"> Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline Solubility: ≥ 5 mg/mL (10.54 mM); Clear solution Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: ≥ 5 mg/mL (10.54 mM); Clear solution Add each solvent one by one: 5% DMSO >> 40% PEG300 >> 5% Tween-80 >> 50% saline Solubility: 2.5 mg/mL (5.27 mM); Suspended solution; Need ultrasonic 				

BIOLOGICAL ACTIVITY

Description	BAY-85-8501 is a selective, reversible and potent inhibitor of Human Neutrophil Elastase (HNE), with an IC ₅₀ of 65 pM.
IC₅₀ & Target	IC ₅₀ : 65 pM (HNE) ^[1] .
In Vivo	In this model the exogenous HNE noxa is the primary cause of injury and lung hemorrhage. Based on picomolar potency against HNE as well as single digit potency versus MNE, BAY-85-8501 (29) completely prevents the development of lung injury and subsequent inflammation when administered 1 h prior to the HNE noxa. In the 0.01 mg/kg dose group,

hemoglobin concentration is already significantly decreased. At a dose of 0.1 mg/kg, a significant effect on neutrophil count is observed. In this setup, efficacy is predominantly driven by potency against HNE ($K_i=0.08$ nM). As the highly HNE-selective inhibitor BAY 85-8501 has no effect on PPE, BAY-85-8501 could not prevent the primary lung injury in this setup. Nevertheless, BAY-85-8501 could inhibit MNE, the endogenous driver of inflammation and secondary injury, although with decreased potency. Consequently, the effects of BAY-85-8501 on inflammation and secondary injury are weaker at this point, and only observed at 30-fold higher doses. Efficacy is predominantly driven by potency against MNE ($K_i=6$ nM) in this second setup^[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

PROTOCOL

Animal Administration ^[1]

Mice^[1]

Elastase-induced lung failure in mice, rats or hamsters is a widely used animal model of acute lung failure. The animals are treated 1 hour prior to orotracheal instillation of human neutrophil elastase (HNE) or porcine pancreatic elastase (PPE). In this study, each mouse receives BAY-85-8501 with different concentrations (0.003, 0.01, 0.03, 0.1, 0.3, 3, 10, 30 mg/kg) by P.O. ^[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

CUSTOMER VALIDATION

- bioRxiv. 2023 Nov 13.
- Patent. US20230058557A1.
- Chinese Academy of Sciences. 2019 Aug.

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REFERENCES

[1]. Von Nussbaum F, et al. Freezing the Bioactive Conformation to Boost Potency: The Identification of BAY 85-8501, a Selective and Potent Inhibitor of Human Neutrophil Elastase for Pulmonary Diseases. ChemMedChem. 2015 Jul;10(7):1163-73.

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

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