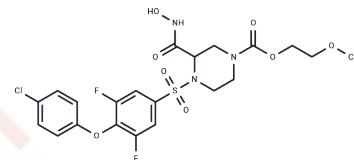


XL-784 free base

Chemical Properties

CAS No. :	1356992-21-6
Formula:	C ₂₁ H ₂₂ ClF ₂ N ₃ O ₈ S
Molecular Weight:	549.93
Storage:	Powder: -20°C for 3 years In solvent: -80°C for 1 year Actual storage temperature shall be subject to the COA.



Biological Description

Description	XL-784 free base is a selective inhibitor of matrix metalloproteinases (MMP) with IC ₅₀ values of ~1900, 0.81, 120, 10.8, 18, and 0.56 nM for MMP-1, MMP-2, MMP-3, MMP-8, MMP-9, and MMP-13, respectively.
Targets(IC ₅₀)	MMP,Others
In vitro	XL-784 is a low-molecular-weight (1,122 g/mol) MMPs inhibitor. XL-784 potently inhibits MMP-2, MMP-13, and ADAM10 [TNF- α -converting enzyme (TACE)] activity in vitro (IC ₅₀ values in the range of 1-2 nM). XL-784 also inhibits MMP-9 (IC ₅₀ ~20 nM) activity and ADAM17 (IC ₅₀ ~70 nM) also known as TACE. However, XL-784 exhibits low potency for inhibition of MMP-1 (IC ₅₀ ~2,000 nM)[1].
In vivo	Treatment with all doses of XL-784 and doxycycline are effective in inhibiting aortic dilatation. There is a clear dose-response relationship between XL-784 and reductions in aortic dilatation at harvest (50 mg/kg 140.4% \pm 3.2%; 125 mg/kg 129.3% \pm 5.1%; 250 mg/kg 119.2% \pm 3.5%; all Ps < 0.01 compared to control). This continues with the higher doses (375 mg/kg 88.6% \pm 4.4%; 500 mg/kg 76.0% \pm 3.5%). The two doses of the highest dose of XL-784 tested were more effective than doxycycline in inhibiting the maximum expansion of the aorta after elastase infusion (112.2% \pm 2.0%, P < 0.05) [2].

Solubility Information

Solubility	DMSO: 250 mg/mL (454.6 mM), Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween-80+45% Saline: 3.3 mg/mL (6 mM), Sonication is recommended. <i>Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.</i>

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	1.8184 mL	9.0921 mL	18.1841 mL
5 mM	0.3637 mL	1.8184 mL	3.6368 mL
10 mM	0.1818 mL	0.9092 mL	1.8184 mL
50 mM	0.0364 mL	0.1818 mL	0.3637 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

- Williams JM, et al. Evaluation of metalloprotease inhibitors on hypertension and diabetic nephropathy. *Am J Physiol Renal Physiol.* 2011 Apr;300(4):F983-98.
- Ennis T, et al. Effect of novel limited-spectrum MMP inhibitor XL784 in abdominal aortic aneurysms. *J Cardiovasc Pharmacol Ther.* 2012 Dec;17(4):417-26.

Inhibitor · Natural Compounds · Compound Libraries · Recombinant Proteins

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