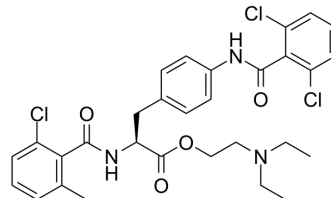


Valategrast

Cat. No.:	HY-14190
CAS No.:	220847-86-9
Molecular Formula:	C ₃₀ H ₃₂ Cl ₃ N ₃ O ₄
Molecular Weight:	604.95
Target:	Integrin
Pathway:	Cytoskeleton
Storage:	-80°C, stored under nitrogen



SOLVENT & SOLUBILITY

In Vitro	DMSO : 170 mg/mL (281.01 mM; Need ultrasonic)				
		Solvent Concentration	Mass		
	Preparing Stock Solutions		1 mg	5 mg	10 mg
		1 mM	1.6530 mL	8.2651 mL	16.5303 mL
		5 mM	0.3306 mL	1.6530 mL	3.3061 mL
	10 mM	0.1653 mL	0.8265 mL	1.6530 mL	
Please refer to the solubility information to select the appropriate solvent.					
In Vivo	1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline Solubility: ≥ 4.25 mg/mL (7.03 mM); Clear solution				
	2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline) Solubility: ≥ 4.25 mg/mL (7.03 mM); Clear solution				
	3. Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: ≥ 4.25 mg/mL (7.03 mM); Clear solution				

BIOLOGICAL ACTIVITY

Description	Valategrast (R-411 free base) is a potent and orally active integrin α4β1 (VLA-4) and α4β7 dual antagonist. Valategrast has the potential for Chronic obstructive pulmonary disease (COPD) and asthma treatment ^{[1][2]} .
IC ₅₀ & Target	Integrin α4β1; Integrin α4β7 ^[2]
In Vitro	Valategrast contains a common l-phenylalanine-N-royl motif where the carboxylic acid is responsible for binding to the metal ion in the metal-ion-dependent adhesion site (MIDAS) ^[2] . MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

- [1]. Woodside DG, et al. Cell adhesion antagonists: therapeutic potential in asthma and chronic obstructive pulmonary disease. *BioDrugs*. 2008;22(2):85-100.
- [2]. Halland N, et al. Small Macrocycles As Highly Active Integrin $\alpha2\beta1$ Antagonists. *ACS Med Chem Lett*. 2014 Jan 10;5(2):193-8.
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Caution: Product has not been fully validated for medical applications. For research use only.

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