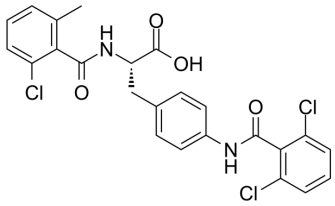
RO0270608

Cat. No.:	HY-138542
CAS No.:	220846-33-3
Molecular Formula:	$C_{24}H_{19}Cl_3N_2O_4$
Molecular Weight:	505.78
Target:	Integrin
Pathway:	Cytoskeleton
Storage:	Powder -20°C 3 years 4°C 2 years In solvent -80°C 6 months -20°C 1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 12.5 mg/mL (24.71 mM; ultrasonic and warming and heat to 60°C)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	1.9771 mL	9.8857 mL	19.7714 mL
	5 mM	0.3954 mL	1.9771 mL	3.9543 mL
	10 mM	0.1977 mL	0.9886 mL	1.9771 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: ≥ 1.25 mg/mL (2.47 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 1.25 mg/mL (2.47 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 1.25 mg/mL (2.47 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

RO0270608, the active metabolite of R411, is a dual alpha4beta1-alpha4beta7 (α4β1/α4β7) integrin antagonist. Antiinflammatory activity[1][2].

IC_{50} & Target	α4β1	α4β7

In Vitro

RO0270608 inhibits α4/β7 mediated cell adhesion with an IC50 of 33 nM. In a human T-cell VCAM/anti CD3 costimulation assay RO0270608 causes a pronounced inhibition of T-cell proliferation (IC_{50}=30 nM)[2].

	MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	In a murine OVA-model of airway inflammation, RO0270608 i.n. abolishes allergen-induced inflammatory cell accumulation [2] MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Hijazi Y, et al. Pharmacokinetics, safety, and tolerability of R411, a dual alpha4beta1-alpha4beta7 integrin antagonist after oral administration at single and multiple once-daily ascending doses in healthy volunteers. J Clin Pharmacol. 2004;44(12):1368-1378.

[2]. M. Renzetti, et al. Dual α4/β1–α4/β7 vs α4/β1 selective antagonism is required for attenuation of allergic inflammatory responses. Journal of Allergy and Clinical Immunology. Volume 113, Issue 2, Supplement, February 2004, Page S221.

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