

## Building Blocks, Pharmaceutical Intermediates, Chemical Reagents, Catalysts & Ligands www.ChemScene.com

# **Data Sheet**

Product Name:	Icanbelimod
Cat. No.:	CS-6254
CAS No.:	1514888-56-2
Molecular Formula:	C <sub>23</sub> H <sub>24</sub> FN <sub>3</sub> O <sub>3</sub>
Molecular Weight:	409.45
Target:	LPL Receptor
Pathway:	GPCR/G Protein
Solubility:	DMSO : 6.8 mg/mL (ultrasonic;warming)

## **BIOLOGICAL ACTIVITY:**

S1p receptor agonist 1 is a potent and orally active **S1P receptor** agonist, exhibits an activity of inducing S1P1 internalization (**EC**<sub>50</sub> =9.83 nM). S1p receptor agonist 1 has the potential for the study of arthritis and EAE (experimental autoimmune encephalitis). S1p receptor agonist 1 is extracted from patent WO2015039587A1, Compound  $2^{[1]}$ . IC50 & Target:EC50: 9.83 nM (S1P1 internalization) <sup>[1]</sup> *In Vivo:* S1p receptor agonist 1 (oral administration; 0.01 mg/kg-1 mg/kg) at all dose is active, and only a dose of 0.01 mg/kg is required to observe a decrease in the number of peripheral blood lymphocytes by more than 50% and a decrease in the 1 mg/kg dose. Besides, this compound is lymphocyte-specific, which dose not significantly alter the number of peripheral monocytes and other white blood cells in SD rats<sup>[1]</sup>.

S1p receptor agonist 1 (oral administration; 3 mg/kg; 12 days) is has been proved to block lymphocyte efflux. In the development of type II collagen-induced arthritis in rat model, compound 2 is effective in inhibiting the development of joint swelling in arthritis and joint structure destruction<sup>[1]</sup>.

S1p receptor agonist 1 (oral administration; 0.3-1mg/kg; 30 days; once daily) inhibits the development of experimental autoimmune encephalitis (EAE) as a dose-dependent manner in mice model<sup>[1]</sup>.

### **References:**

[1]. Zhenwei, et al. Immune adjustment compound, use thereof and pharmaceutical composition comprising same. Patent WO2015039587A1

#### **CAIndexNames:**

3-Azetidinecarboxylic acid, 1-[[2-fluoro-4-[5-[4-(2-methylpropyl)phenyl]-1,2,4-oxadiazol-3-yl]phenyl]methyl]-

### SMILES:

O=C(C1CN(CC2=CC=C(C3=NOC(C4=CC=C(CC(C)C)C=C4)=N3)C=C2F)C1)O

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

Tel: 610-426-3128

Fax: 888-484-5008

Address: 1 Deer Park Dr, Suite F, Monmouth Junction, NJ 08852, USA

E-mail: sales@ChemScene.com