Product Data Sheet

Chemical Properties

**Product Name:** Firategrast  
**Cas No.:** 402567-16-2  
**M.Wt:** 499.5  
**Formula:** C27H27F2NO6  
**Synonyms:** SB683699;SB-683699

**Chemical Name:** (2S)-2-[(2,6-difluorobenzoyl)amino]-3-[4-[(ethoxymethyl)-2,6-dimethoxyphenyl]phenyl]propanoic acid

**Canonical SMILES:** CCOC1=CC(=C(=C1)OC)C2=CC=C(C=C2)CC(C(=O)O)NC(=O)C3=C(C=C3F)F)OC

**Solubility:** >50mg/ml in DMSO

**Storage:** Store at -20°C

**General tips:** For obtaining a higher solubility, please warm the tube at 37°C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C for several months.

**Shopping Condition:** Evaluation sample solution: ship with blue ice  
All other available size: ship with RT, or blue ice upon request

Biological Activity

**Targets:** Angiogenesis

**Pathways:** Integrin

**Description:** Firategrast is a bioavailable small-molecule antagonist of α4β1 and α4β7 integrins [1]. The integrins are a sort of transmembrane receptors that modulate the signal transduction from ECM to the cell. They are associated with a lot of diseases such as cancer, inflammation and thrombotic diseases. Since part of the integrin is exposed to the cell outside and is easy to
combine with the drug, integrins are thought to be attracted targets. There are many drugs target the integrins have been designed and generated, such as abciximab, tirofiban, lamifiban and natalizumab. Among these, firategrast is a drug for the treatment of multiple sclerosis (MS) which is found to be caused by the migration of leucocytes (such as monocytes, T cells, B cells and dendritic cells) into CNS. And the integrin α4β1 is found to take participate in the migration through activating the leucocytes [1, 2].

Firategrast has a much shorter half-life than natalizumab with about 2.5 hours to 4.5 hours. It is found to inhibit the binding of the integrins to the associated ligands, including vascular cell adhesion protein 1 and mucosal addressin cell adhesion molecule 1. In CNS, firategrast treatment caused moderate decreases of total lymphocyte count, lymphocyte subset count and the ratio of CD4 to CD8. In peripheral blood, firategrast treatment resulted in the increases of total lymphocyte count, all lymphocyte subset count as well as the peripheral CD34+ early haematopoietic progenitor cell count [1, 3].

Firategrast was well tolerated at the maximum doses of 1200 mg for men and 900 mg for women. Firategrast showed no side effects, such as PML or JC-virus reactivation, at these doses. In Phase I clinical trials, the administration of firategrast significantly reduced the cumulative number of new gadolinium-enhancing lesions in patients with relapsing remitting MS [1, 3].

Reference:

Caution

FOR RESEARCH PURPOSES ONLY.

NOT FOR HUMAN, VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

Specific storage and handling information for each product is indicated on the product datasheet. Most ApexBio products are stable under the recommended conditions. Products are sometimes shipped at a temperature that differs from the recommended storage temperature. Shortterm storage of many products are stable in the short-term at temperatures that differ from that required for long-term storage. We ensure that the product is shipped under conditions that will maintain the quality of the reagents. Upon receipt of the product, follow the storage recommendations on the product data sheet.