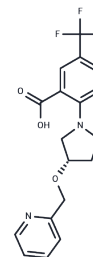


XEN445

## Chemical Properties

CAS No. : 1515856-92-4  
 Formula: C<sub>18</sub>H<sub>17</sub>F<sub>3</sub>N<sub>2</sub>O<sub>3</sub>  
 Molecular Weight: 366.33  
 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                | XEN445, a potent and selective endothelial lipase(EL) inhibitor (IC <sub>50</sub> =0.237 μM), exhibits good ADME and PK properties.  |
| Targets(IC <sub>50</sub> ) | Others,Lipase  |
| In vitro                   | XEN445 exhibits good specificity over LPL and HL, and great inhibition activity against EL.  |
| Kinase Assay               | In vitro PI3K lipid kinase assay: (1) For PI3Kγ: human PI3Kγ (100 ng) is incubated at RT with kinase buffer (10 mM MgCl <sub>2</sub> , 1 mM β-glycerophosphate, 1 mM DTT, 0.1 mM Na <sub>3</sub> VO <sub>4</sub> , 0.1% Na Cholate and 15 μM ATP/100 nCi γ[ <sup>33</sup> P]ATP, final concentrations) and lipid vesicles containing 18 μM PtdIns and 250 μM of PtdSer (final concentrations), in the presence of AS-605240 or DMSO. Kinase reaction is stopped by adding 250 μg of Neomycin-coated Scintillation Proximity Assay (SPA) beads. (2) For PI3Kα, β, and δ: varying amounts of ATP are incubated with the different purified PI3K isoforms and saturating concentrations of PtdIns. Consequently, IC <sub>50</sub> determinations with PI3Kα, β, and δ, to evaluate inhibitor selectivity are performed as follows: 60 ng of PI3Kα are incubated at RT with kinase buffer, as described for PI3Kγ (but containing 89 μM ATP/300 nCi γ[ <sup>33</sup> P]ATP and no Na Cholate, instead) and lipid vesicles containing 212 μM PtdIns and 58 μM of PtdSer. 100 ng of PI3Kβ are incubated at RT with kinase buffer (containing 70 μM ATP/300 nCi γ[ <sup>33</sup> P]ATP, 4 mM MgCl <sub>2</sub> and no Na Cholate) and lipid vesicles containing 225 μM PtdIns and 45 μM of PtdSer. 90 ng of PI3Kδ are incubated with kinase buffer (containing 65 μM ATP/300 nCi γ[ <sup>33</sup> P]ATP, 1 mM MgCl <sub>2</sub> , and no Na Cholate) and lipid vesicles containing 100 μM PtdIns and 170 μM of PtdSer. The reactions are stopped after 2 hours. |

## Solubility Information

|            |   |
|------------|---|
| Solubility | Ethanol: 36.6 mg/mL (99.91 mM),Sonication is recommended.<br>DMSO: 60 mg/mL (163.79 mM),Sonication is recommended.<br>(< 1 mg/ml refers to the product slightly soluble or insoluble) |
|------------|---|

### Preparing Stock Solutions

---

|       | 1mg       | 5mg        | 10mg       |
|-------|-----------|------------|------------|
| 1 mM  | 2.7298 mL | 13.6489 mL | 27.2978 mL |
| 5 mM  | 0.546 mL  | 2.7298 mL  | 5.4596 mL  |
| 10 mM | 0.273 mL  | 1.3649 mL  | 2.7298 mL  |
| 50 mM | 0.0546 mL | 0.273 mL   | 0.546 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

Sun S, et al. Bioorg Med Chem. 2013, 21(24), 7724-7734.

**Inhibitor · Natural Compounds · Compound Libraries · Recombinant Proteins**

This product is for Research Use Only · Not for Human or Veterinary or Therapeutic Use

Tel:781-999-4286 E\_mail:info@targetmol.com Address:34 Washington Street,Wellesley Hills,MA 02481