Product Data Sheet

Chemical Properties

Product Name: ML-211
Cas No.: 
M.Wt: 418.5
Formula: C25H30N4O2

Chemical Name: (4-(tert-butyl)piperidin-1-yl)(4-(hydroxydiphenylmethyl)-2H-1,2,3-triazol-2-yl)methanone
Canonical SMILES: CC(C)(C1CCN(C(N2N=C(C(C3=CC=CC=C3)(O)C4=CC=CC=C4)C=N2)=O)CC1

Solubility: \( \leq 10 \text{mg/ml in ethanol; 30mg/ml in DMSO; 30mg/ml in dimethyl formamide} \)

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: Metabolism
Pathways: Hydrolase

Description:
IC50: LYPLA1 (17 nM) and the related LYPLA2 (30 nM)

ML-211 is a dual inhibitor of LYPLA1 and the related LYPLA2.
Lysophospholipase 1 (LYPLA1), a protein palmitoyl thioesterase, is responsible for depalmitoylation of the oncogene HRas. Palmitoylation of such oncogenes is considered to be required for trafficking and malignant transformation, making LYPLA1 a promising target for downregulating oncogenic signaling.

In vitro: ML-211 was identified as a carbamate-based dual inhibitor of LYPLA1 and the related LYPLA2. ML-211 could inhibit the serine hydrolase ABHD11 with an IC50 value of 10 nM but was over 50-fold selective for LYPLA in a panel of 20 additional serine hydrolases. Given the high structural homology between LYPLA1 and LYPLA2, it was anticipated that ML211 modified LYPLA2 in an analogous manner. In addition, out of more than 20 serine hydrolases (SHs), ML211 was observed to have one anti-target, alpha/beta hydrolase domain-containing protein 11 (ABHD11). ML211 and the anti-probe ML226 were evaluated for cell toxicity using both serum-free and serum-supplemented media, and the results showed that both compounds had a CC50 greater than 6 μM, which was 200-fold greater than the concentration necessary for complete inhibition of their respective target enzyme(s) [1].

In situ: It was found that both ML211 and ML226 were shown to be highly active in situ against their targets, completely inhibiting their target enzymes in serum-containing media after two hours at 30 nM concentration [1].

Clinical trial: So far, no clinical study has been conducted.

**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. Short-term 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.