Product Data Sheet

Product Name: ML-211
Cat. No.: GC12150

Chemical Properties

Cas. No.	2205032-89-7		
Chemical Name	(4-(tert-butyl)piperidin-1-yl)(4-(hydroxydiphenylmethyl)-2H-1,2,3-triazol-2-yl)methanone		
SMILES	CC(C)(C)C1CCN(C(N2N=C(C(C3=CC=CC=C3)(O)C4=CC=CC=C4)C=N2)=O)CC1		
Formula	$C_{25}H_{30}N_4O_2$	M.Wt	418.5
Solubility	≤10mg/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 ℃ and shake it in the ultrasonic bath for a while.Stock solution can be stored below -20℃ for several months.		
Shipping Condition	Evaluation sample solution : ship with blue ice All other available size: ship with RT , or blue ice upon request.		
Structure	ML-211		

Background

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

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anticipated that ML211 modified LYPLA2 in an analogous manner. In additioin, 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:
[1] Adibekian, A. ,Martin, B.R.,Speers, A.E., et al. Optimization and characterization of a triazole urea dual inhibitor for lysophospholipase 1 (LYPLA1) and lysophospholipase 2 (LYPLA2). 1 R01 CA132630, 1-42 (2013).