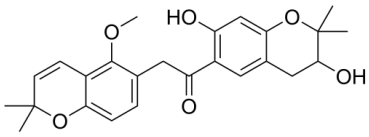
Data Sheet

Product Name:	Dihydromunduletone
Cat. No.:	CS-0021520
CAS No.:	674786-20-0
Molecular Formula:	$C_{25}H_{28}O_6$
Molecular Weight:	424.49
Target:	Drug Derivative
Pathway:	GPCR/G Protein; Others
Solubility:	DMSO : 250 mg/mL (ultrasonic)



BIOLOGICAL ACTIVITY:

Dihydromunduletone (DHM) is a rotenoid derivative and a selective, potent **adhesion G protein-coupled receptor (aGPCR)** (**GPR56 and GPR114/ADGRG5**) antagonist with an **IC $_{50}$** of 20.9 μM for **GPR56**, but not inhibit GPR110 or class A GPCRs[1]. IC50 & Target:IC50: 20.9 μM (GPR56)[1]; GPR114[1] ***In Vitro:***Assays are initiated by the addition of [^{35}S]GTPγS, and the rates of aGPCR-stimulated G protein activation ([^{35}S]GTPγS binding to Gα) are measured with or without the influence of added compounds. Dihydromunduletone (DHM) inhibits the kinetics of GPR56 7TM-stimulated G13 GTPγS binding to varying degrees. Dihydromunduletone is the best inhibitory compound and reduced the rate at which GPR56 7TM activated G13 >75% (from 0.18 to 0.04 minute ^{1})[1].

At a concentration of Dihydromunduletone (DHM) that maximally inhibits GPR56 (50 μM), the rate of GPR114 7TM-stimulated Gs activity is also inhibited dramatically. When Dihydromunduletone (50 μM) is applied to the GPR110 7TM, it fails to inhibit GPR110 stimulation of Gq GTPγS binding[1].

Cells transfected with GPR56 A386M 7TM are incubated with increasing concentrations of Dihydromunduletone. P7 peptide agonist is added, and SRE-luciferase activity is measured. Dihydromunduletone inhibits the P7 peptide-induced luciferase activity in a concentration-dependent manner. Cells are also treated with a fixed concentration of 3 μM Dihydromunduletone and then stimulated with an increasing concentration of P7 peptide agonist. Dihydromunduletone treatment blunts P7 peptide activation at each concentration. In conclusion, Dihydromunduletone antagonizes synthetic-peptide agonist and tethered-peptide agonist-mediated aGPCR activation in isolated membranes and HEK293T cell-based assays, but it does not inhibit basal receptor signaling[1].

References:

[1]. Hannah M. Stoveken, et al. Dihydromunduletone Is a Small-Molecule Selective Adhesion G Protein–Coupled Receptor Antagonist. Mol Pharmacol. 2016 Sep; 90(3): 214–224.

CAIndexNames:

Ethanone, 1-(3,4-dihydro-3,7-dihydroxy-2,2-dimethyl-2H-1-benzopyran-6-yl)-2-(5-methoxy-2,2-dimethyl-2H-1-benzopyran-6-yl)-

SMILES:

CC1(C)C=CC2=C(OC)C(CC(C3=C(O)C=C4C(CC(O)C(C)(C)O4)=C3)=O)=CC=C2O1

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

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