

Data Sheet

 Product Name:
 PGD2-IN-1

 Cat. No.:
 CS-6338

 CAS No.:
 885066-67-1

 Molecular Formula:
 C23H23Cl2N3O3

Molecular Weight: 460.35
Target: Others
Pathway: Others

Solubility: DMSO : \geq 25 mg/mL (54.31 mM)

BIOLOGICAL ACTIVITY:

PGD2-IN-1 is an antagonist of **DP** extracted from patent WO 2006044732 A2, example 15 (d); has an IC_{50} of 0.3 nM. IC50 & Target: IC50: 0.3 nM^[1] In Vitro: Prostaglandin D2 (PGD2) is a major inflammatory mediator implicated in asthma and allergic rhinitis. It is largely produced as the major cyclooxygenase metabolite upon allergen-provoked degranulation from mast cells. Blockage of PGD2 using DP antagonists has been shown to be effective at alleviating the symptoms of allergic rhinitis in multiple species and more specifically has been shown to inhibit the antigen-induced nasal congestion^[2].

References:

- [1]. Lim, Sungtaek, et al. 2, 6-SUBSTITUTED-4-MONOSUBSTITUTEDAMINO-PYRIMIDINE AS PROSTAGLANDIN D2 RECEPTOR ANTAGONISTS. WO2006044732A2.
- [2]. Mu L, et al. Understanding DP receptor antagonism using a CoMSIA approach. Bioorg Med Chem Lett. 2011 Jan 1;21(1):66-75.

CAIndexNames:

 $Benzene acetic\ acid,\ 3-[6-[[2-(2,4-dichlorophenyl)ethyl]amino]-2-methoxy-4-pyrimidinyl]-\alpha, \alpha-dimethyl-method acid,\ 3-[6-[[2-(2,4-dichlorophenyl)ethyl]amino]-2-methoxy-4-pyrimidinyl]-\alpha, \alpha-dimethoxy-4-pyrimidinylamino]-2-me$

SMILES:

O = C(O)C(C)(C)C1 = CC = CC(C2 = NC(OC) = NC(NCCC3 = CC = C(CI)C = C3CI) = C2) = C1

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

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