# Data Sheet

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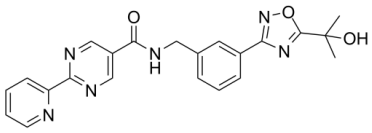
| **Product Name:** | hPGDS-IN-1 |
| **Cat. No.:** | CS-5139 |
| **CAS No.:** | 1234708-04-3 |
| **Molecular Formula:** | C22H20N6O3 |
| **Molecular Weight:** | 416.43 |
| **Target:** | PGE synthase |
| **Pathway:** | Immunology/Inflammation |
| **Solubility:** | DMSO : ≥ 30 mg/mL (72.04 mM) |



## BIOLOGICAL ACTIVITY:

hPGDS-IN-1 is a hPGDS inhibitor ,with IC50 of 12 nM in the Fluorescence Polarization Assay or the EIA assay. IC50 value: 12 nM Target: hPGDS The detailed information please refer to WO2011044307A1 and WO2010080563A2

## PROTOCOL (Extracted from published papers and Only for reference)

Enzyme assay [1] Add 60 μL of enzyme solution to compound well and positive control (without hPGDS-IN-1) in U-bottom polypropylene plate on ice. Add 60 μL of reaction buffer and 6.6 μL of 5% DMSO in reaction buffer into negative control wells in the plate. Add 6.6 μL of diluted hPGDS-IN-1 in reaction buffer to the compound wells and mix. Add 6.6 μL of 5% DMSO in reaction buffer to the positive control well. Incubate the plate in ice for at least 30 min. Add 20 μL of substrate (PGH2) solution to compound, negative and positive control wells in the U-bottom 96 well plate on ice. Dry the plate in cold room for about 25-28 min. Pipette 45 μL of enzyme solution in to 96 well with dried PGH2 and mix 3 times. Incubate on the ice for 1 min. Add 45 μL of FeCl2 solution into each wells and mix. Add 90 μL of MOX solution and mix. Incubate for 30 min at 60℃. Dilute the samples 2500X with EIA buffer. Animal administration [2] Fifty male Brown Norway rats(4-7 weeks old, 50-124 g each) were dosed via twice daily oral gavage at 5 ml/kg, starting immediately prior to lasting and continuing for 14 days. hPGDS-IN-1 were formulated in vehicle twice weekly during the study. Vehicle consisted of 0.5% methylcellulose, 0.2% Tween 20 in sterile water for injection, and was formulated once weekly.

## References:

[1]. Vandeusen, Christopher L, et al. Phenyloxadiazole derivatives as PGD inhibitors and their preparation, pharmaceutical compositions and use in the treatment of allergic and inflammatory disorders. From PCT Int. Appl. (2011), WO 2011044307 A1 20110414.

[2]. Hahn Chang S. Method for treating macular degeneration using syk multikinase inhibitor, an hPGDS inhibitor and a DP antagonist. From PCT Int. Appl. (2010), WO 2010080563 A2 20100715.

[3]. Weiberth Franz J, et al. Demonstration on Pilot-Plant Scale of the Utility of 1,5,7-Triazabicyclo[4.4.0]dec-5-ene (TBD) as a Catalyst in the Efficient Amidation of an Unactivated Methyl Ester. From Organic Process Research & Development (2012), 16(12), 1967-1969.

## CAIndexNames:

5-Pyrimidinecarboxamide, N-[[3-[5-(1-hydroxy-1-methylethyl)-1,2,4-oxadiazol-3-yl]phenyl]methyl]-2-(2-pyridinyl)-

## SMILES:

OC(C)(C)C1=NC(C2=CC(CNC(C(C=N3)=CN=C3C4=CC=CC=N4)=O)=CC=C2)=NO1



Tel: 732-484-9848 Fax: 888-484-5008 E-mail: sales@ChemScene.com

Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA