Product Information



CID-2745687

Item No. 12046

CAS Registry No.: 264233-05-8

Formal Name: 1-(2,4-difluorophenyl)-5-[[2-[[(1,

1-dimethylethyl)amino]thioxomethyl] hydrazinylidene]methyl]-1H-pyrazole-

4-carboxylic acid, methyl ester

Synonym: ML-194

MF: $C_{17}H_{19}F_2N_5O_2S$

395.4 FW: ≥95% **Purity:**

≥2 years at -20°C Stability: Supplied as: A crystalline solid UV/Vis.: λ_{max} : 242, 338 nm

Laboratory Procedures

For long term storage, we suggest that CID-2745687 be stored as supplied at -20°C. It should be stable for at least two

CID-2745687 is supplied as a crystalline solid. A stock solution may be made by dissolving the CID-2745687 in the solvent of choice. CID-2745687 is soluble in DMSO at a concentration of approximately 10 mg/ml.

GPR35 is a G protein-coupled receptor that is activated by kynurenic acid and 2-acyl lysophosphatidic acids (e.g., 2-oleoyl lysophosphatidic acid). 1-3 It is expressed predominantly on immune cells, the brain, and in the gastrointestinal tract.^{2,4} GPR35 is overexpressed in gastric cancer cells.⁵ CID-2745687 is a reversible, competitive antagonist of GPR35, blocking activation by the synthetic agonist pamoic acid with a K_i value of 12.8 nM.⁶ It less potently blocks activation of GPR35 by zaprinast (Item No. 10010421) (IC₅₀ = 160 nM). It shows ~57-fold selectivity for GPR35 over the related receptor GPR55 (IC₅₀ = $9.08 \mu M$).⁷

References

- 1. Oka, S., Ota, R., Shima, M., et al. GPR35 is a novel lysophosphatidic acid receptor. Biochem. Biophys. Res. Commun. **395(2)**, 232-237 (2010).
- Wang, J., Simonavicius, N., Wu, X., et al. Kynurenic acid as a ligand for orphan G protein-coupled receptor GPR35. J. Biol. Chem. 281(31), 22021-22028 (2006).
- 3. MacKenzie, A.E., Lappin, J.E., Taylor, D.L., et al. GPR35 as a novel therapeutic target. Front. Endocrinol. (Lausanne) 2, 68 (2011).
- 4. O'Dowd, B.F., Nguyen, T., Marchese, A., et al. Discovery of three novel G-protein-coupled receptor genes. Genomics 47, 310-313 (1998).
- 5. Okumura, S., Baba, H., Kumada, T., et al. Cloning of a G-protein-coupled receptor that shows an activity to transform NIH3T3 cells and is expressed in gastric cancer cells. Cancer Sci. 95(2), 131-135 (2004).
- Zhao, P., Sharir, H., Kapur, A., et al. Targeting of the orphan receptor GPR35 by pamoic acid: A potent activator of extracellular signal-regulated kinase and β-arrestin2 with antinociceptive activity. Mol. Pharmacol. 78(4), 560-568
- Heynen-Genel, S., Dahl, R., Shi, S., et al. Selective GPR35 antagonists: Antagonists for the orphan receptor GPR35, in Probe Reports from the NIH Molecular Libraries Program, Probe 3, 1 (2011).

Related Products

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WARNING: This product is for laboratory research only: not for administration to humans. Not for human or veterinary DIAGNOSTIC OR THERAPEUTIC USE.

This material should be considered hazardous until information to the contrary becomes available. Do not ingest, swallow, or inhale. Do not get in eyes, on skin, or on clothing. Wash thoroughly after handling. This information contains some, but not all, of the information required for the safe and proper use of this material. Before use, the user must review the complete Safety Data Sheet, which has been sent via email to your institution.

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