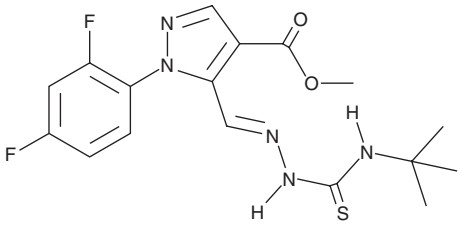
PRODUCT INFORMATION

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:	$C_{17}H_{19}F_2N_5O_2S$
FW:	395.4
Purity:	≥95%
UV/Vis.:	λ_{max}: 242, 338 nm
Supplied as:	A crystalline solid
Storage:	-20°C
Stability:	≥4 years



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

Laboratory Procedures

CID-2745687 is supplied as a crystalline solid. A stock solution may be made by dissolving the CID-2745687 in the solvent of choice, which should be purged with an inert gas. CID-2745687 is soluble in the organic solvent DMSO at a concentration of approximately 10 mg/ml.

Description

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) (IC_{50} = 160 nM).[7] It shows ~57-fold selectivity for GPR35 over the related receptor GPR55 (IC_{50} = 9.08 µM).[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).
2. 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).
6. 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 b-arrestin2 with antinociceptive activity. *Mol. Pharmacol.* **78(4)**, 560-568 (2010).
7. 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).

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