

# PRODUCT INFORMATION

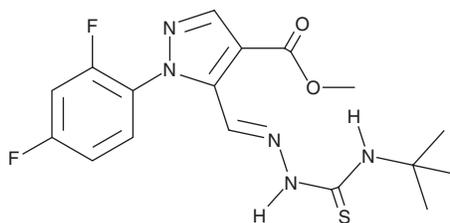


**CID-2745687**

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<sub>17</sub>H<sub>19</sub>F<sub>2</sub>N<sub>5</sub>O<sub>2</sub>S  
**FW:** 395.4  
**Purity:** ≥95%  
**UV/Vis.:** λ<sub>max</sub>: 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).<sup>1-3</sup> It is expressed predominantly on immune cells, the brain, and in the gastrointestinal tract.<sup>2,4</sup> GPR35 is overexpressed in gastric cancer cells.<sup>5</sup> CID-2745687 is a reversible, competitive antagonist of GPR35, blocking activation by the synthetic agonist pamoic acid with a K<sub>i</sub> value of 12.8 nM.<sup>6</sup> It less potently blocks activation of GPR35 by zaprinast (Item No. 10010421) (IC<sub>50</sub> = 160 nM).<sup>7</sup> It shows ~57-fold selectivity for GPR35 over the related receptor GPR55 (IC<sub>50</sub> = 9.08 μM).<sup>7</sup>

## 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).

### WARNING

THIS PRODUCT IS FOR RESEARCH ONLY - NOT FOR HUMAN OR VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

### SAFETY DATA

This material should be considered hazardous until further information becomes available. Do not ingest, inhale, get in eyes, on skin, or on clothing. Wash thoroughly after handling. Before use, the user must review the complete Safety Data Sheet, which has been sent via email to your institution.

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