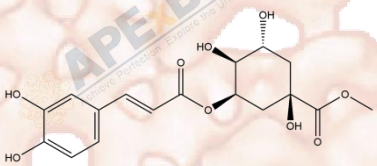
Product Data Sheet

5-O-Caffeoylquinic acid methyl ester

Cat. No.: C8658
CAS No.: 123410-65-1
Formula: C17H20O9
M.Wt:
Synonyms: Neochlorogenic acid methyl ester
Target: HBV
Pathway: Protease
Storage: Store at 4° C



Solvent & Solubility

In Vitro

Preparing Stock Solutions

Mass / Solvent / Concentration	1mg	5mg	10mg
1 mM	1.#INF mL	1.#INF mL	1.#INF mL
5 mM	1.#INF mL	1.#INF mL	1.#INF mL
10 mM	1.#INF mL	1.#INF mL	1.#INF mL

Please refer to the solubility information to select the appropriate solvent.

Biological Activity

Shortsummary

5-O-Methyl caffeoylquinic acid (methyl neochlorogenic acid, CAS No.: 123410-65-1) is a caffeoylquinic acid derivative derived from Lonicera japonica (honeysuckle). When used alone, it shows no significant toxicity to liver cancer cells (such as HepG2). However, when combined with glycolysis inhibitors such as 2-deoxy-D-glucose (2-DG) and 3-bromopyruvate (3-BP), it can enhance the inhibitory effect on liver cancer cell proliferation by 1.5 – 3 times (more pronounced under low-glucose conditions). This is achieved by inhibiting HKII to block glucose phosphorylation and inhibiting PKM2 to reduce pyruvate production, thereby weakening the Warburg effect (aerobic glycolysis) in liver cancer cells, reducing ATP and ROS production. At the same time, the combination can block the activation of the ROS-GLUT1/3 signaling axis induced by these inhibitors, effectively delaying the development of drug resistance in liver cancer cells[1]. Due to methyl

esterification, 5-O-methyl caffeoylquinic acid loses its free carboxyl group, resulting in the loss of in vitro anti-HBV activity[2]. References： [1] Hunan Agricultural University, Wenzhou Medical University. A pharmaceutical composition for reducing drug resistance in liver cancer cells and its application: CN202111179728.1[P]. 2022-05-13. [2] Ge L, Wan H, Tang S, Chen H, Li J, Zhang K, Zhou B, Fei J, Wu S, Zeng X. Novel caffeoylquinic acid derivatives from Lonicera japonica Thunb. flower buds exert pronounced anti-HBV activities. RSC Adv. 2018 Oct 15;8(62):35374-35385. doi: 10.1039/c8ra07549b. PMID: 35547940; PMCID: PMC9088017.</p>

IC_{50} & Target	

In Vitro

Cell Viability Assay

Cell Line:	HepG 2.2.15 cells
Preparation method:	HepG 2.2.15 cells were seeded in 24-well culture plates at a density of 5*10^5 cells/mL. After 2 days, culture medium was replaced with fresh medium supplemented with (or without) the tested samples; this was repeated every other day for an additional 5 days. The real-time PCR assay was used to detect the HBV DNA.
Reacting conditions:	5-375 μg/mL, 5 days
Applications:	Neochlorogenic acid methyl ester showed dramatically decreased anti-HBV activity in comparation with neochlorogenic acid, indicating that the substituted carboxyl group of neochlorogenic acid is closely associated to the anti-HBV activity.

In Vivo

Animal experiment

Applications:	
Other notes:	The technical data provided above is for reference only.

Product Citations

See more customer validations on www.apexbt.com.

References

1. Zhao Y, Geng CA, Ma YB, Huang XY, Chen H, Cao TW, He K, Wang H, Zhang XM, Chen JJ. UFLC/MS-IT-TOF guided isolation of anti-HBV active chlorogenic acid analogues from Artemisia capillaris as a traditional Chinese herb for the treatment of hepatitis. J Ethnopharmacol. 2014 Oct 28;156:147-54. doi: 10.1016/j.jep.2014.08.043. Epub 2014 Sep 8. PMID: 25219603.

Caution

FOR RESEARCH PURPOSES ONLY.

NOT FOR HUMAN, VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

Specific storage and handling information for each product is indicated on the product datasheet. Most APExBIO products are stable under the recommended conditions. Products are sometimes shipped at a temperature that differs from the recommended storage temperature. Shortterm storage of many products are stable in the short-term at temperatures that differ from that required for long-term storage. We ensure that the product is shipped under conditions that will maintain the quality of the reagents. Upon receipt of the product, follow the storage recommendations on the product data sheet.

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