

Product Data Sheet

1-Caffeoylquinic acid

Cat. No.: HY-N0460

CAS No.: 1241-87-8

Molecular Formula: $C_{16}H_{18}O_9$ Molecular Weight: 354.31

Target: NF- κ B

Pathway: NF- κ B

Storage: 4°C, protect from light

* In solvent: -80°C, 6 months; -20°C, 1 month (protect from light)

SOLVENT & SOLUBILITY

In Vitro

DMSO: 250 mg/mL (705.60 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent Mass Concentration	1 mg	5 mg	10 mg
	1 mM	2.8224 mL	14.1119 mL	28.2239 mL
	5 mM	0.5645 mL	2.8224 mL	5.6448 mL
	10 mM	0.2822 mL	1.4112 mL	2.8224 mL

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

BIOLOGICAL ACTIVITY

Description 1-Caffeoylquinic acid is an effective NF-κB inhibitor, shows significant binding affinity to the RH domain of p105 with K_i of

 $0.002~\mu\text{M}$ and binding energy of $1.50~\text{Kcal/mol}^{[1]}$. 1-Caffeoylquinic acid has anti-oxidative stress ability $^{[2]}$. 1-Caffeoylquinic

acid inhibits PD-1/PD-L1 interact $^{[3]}$.

IC₅₀ & Target Ki: 0.002 μM (1-Caffeoylquinic acid)^[1]

REFERENCES

[1]. Khan MK, et al. Dietary phytochemicals as potent chemotherapeutic agents against breast cancer: Inhibition of NF-кВ pathway via molecular interactions in rel homology domain of its precursor protein p105. Pharmacogn Mag. 2013 Jan;9(33):51-7.

[2]. Jiang Y, et al. Caffeoylquinic acid derivatives rich extract from Gnaphalium pensylvanicum willd. Ameliorates hyperuricemia and acute gouty arthritis in animal model. BMC Complement Altern Med. 2017 Jun 17;17(1):320.

[3]. Han Y, et al. PD-1/PD-L1 inhibitor screening of caffeoylquinic acid compounds using surface plasmon resonance spectroscopy. Anal Biochem. 2018 Apr 15;547:52-56.

 $\label{lem:caution:Product} \textbf{Caution: Product has not been fully validated for medical applications. For research use only.}$

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