(1R,3S)-THCCA-Asn

Cat. No.: HY-151146

CAS No.: 1349084-71-4

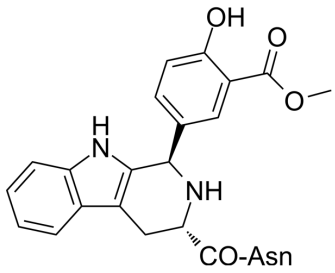
Molecular Formula: $C_{24}H_{24}N_4O_6$

Molecular Weight: 464.47

Target: Thrombin

Pathway: Metabolic Enzyme/Protease

Storage: Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description

(1R,3S)-THCCA-Asn (4j) is a selective thrombin inhibitor with the IC_{50} value in the range of 0.07 to 0.14 μM. ((1R,3S)-THCCA-Asn has antithrombotic activity[1].

In Vitro

(1R,3S)-THCCA-Asn (4j) (0.001-500 μM) has anti-platelet aggregation activity with the IC_{50} value ranged from 0.07 μM to 0.14 μM, and inhibits ADP-induced platelet aggregation by less than 20% as well as AA-induced platelet aggregation by less than 10%[1].

(1R,3S)-THCCA-Asn (4j) (0.001-1000 μM, 48 h) has less toxic to mammalian cells such as liver cell, colon mucosa cell and human dermal fibroblasts in vitro[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Cell Proliferation Assay[1]

Cell Line:	Liver cell (L02), colon mucosa cell (NCM460) and human dermal fibroblasts cell (NHDF)
Concentration:	0.001-1000 μM
Incubation Time:	48 hours
Result:	Showed that the IC_{50} values for cell viability were all higher than 125 μM.

In Vivo

(1R,3S)-THCCA-Asn (4j) (p.o., 0.001-1 nM/kg) can act against thrombosis of rats in a dose-dependent manner with no toxic side effects[1].

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Animal Model:	Male SD (Sprague Dawley) rats weighing 250-300 g[1]
Dosage:	0.001, 0.01, 1 nM/kg
Administration:	p.o.
Result:	Resulted in a reduction in thrombus weight of 19.19 mg at the dose of 1 nM/kg compared to the untreated thrombus weight of about 30 mg.

REFERENCES

[1]. Xiaoyi Zhang, et al. (1R,3S)-THCCA-Asn: To show the discovery of selective inhibitor of thrombin by successfully combining virtual screening and biological assay,European Journal of Medicinal Chemistry,Volume 242,2022,114681.

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