Dimethylfraxetin

Cat. No.: HY-N0085

CAS No.: 6035-49-0

Molecular Formula: $C_{12}H_{12}O_5$

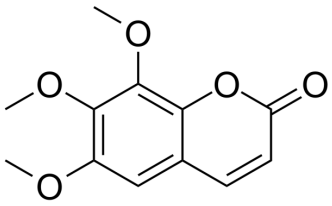
Molecular Weight: 236.22

Target: Carbonic Anhydrase

Pathway: Metabolic Enzyme/Protease

Storage:

Powder	-20°C	3 years
	4°C	2 years
In solvent	-80°C	6 months
	-20°C	1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 125 mg/mL (529.17 mM; Need ultrasonic and warming)

Preparing Stock Solutions

Concentration \ Solvent \ Mass	1 mg	5 mg	10 mg
1 mM	4.2333 mL	21.1667 mL	42.3334 mL
5 mM	0.8467 mL	4.2333 mL	8.4667 mL
10 mM	0.4233 mL	2.1167 mL	4.2333 mL

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

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.08 mg/mL (8.81 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.08 mg/mL (8.81 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.08 mg/mL (8.81 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

Dimethylfraxetin is a Carbonic anhydrase inhibitor, with a K_i value of 0.0097 μM.

IC_{50} & Target

Ki: 0.0097 μM (Carbonic anhydrase)[1]

In Vitro

At CA I there is one stand out compound being Dimethylfraxetin (compound 17), a nanomolar CA I inhibitor. This trimethoxy coumarin is the most potent of any of the NP coumarins across the six CA isozymes of the present study[1].

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

PROTOCOL

Kinase Assay [1]

Inhibitor (including Dimethylfraxetin) and enzyme solutions are preincubated together for 6 h at room temperature prior to assay, in order to allow for the formation of the enzyme-inhibitor complex[1].

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

REFERENCES

[1]. Davis RA, et al. Natural product coumarins that inhibit human carbonic anhydrases. Bioorg Med Chem. 2013 Mar 15;21(6):1539-43.

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