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# **Data Sheet**

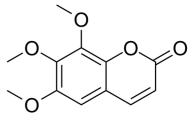
Product Name: Dimethylfraxetin

Cat. No.: CS-7783
CAS No.: 6035-49-0
Molecular Formula: C12H12O5
Molecular Weight: 236.22

Target: Carbonic Anhydrase

Pathway: Metabolic Enzyme/Protease

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



#### **BIOLOGICAL ACTIVITY:**

Dimethylfraxetin is a **Carbonic anhydrase** inhibitor, with a  $K_i$  value of 0.0097  $\mu$ M. IC50 & Target: Ki: 0.0097  $\mu$ M (Carbonic anhydrase)<sup>[1]</sup> **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<sup>[1]</sup>.

### PROTOCOL (Extracted from published papers and Only for reference)

**Kinase Assay:** <sup>[1]</sup>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<sup>[1]</sup>.

#### References:

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

## **CAIndexNames:**

2H-1-Benzopyran-2-one, 6,7,8-trimethoxy-

# **SMILES:**

O=C1C=CC2=CC(OC)=C(OC)C(OC)=C2O1

Caution: Product has not been fully validated for medical applications. For research use only.

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