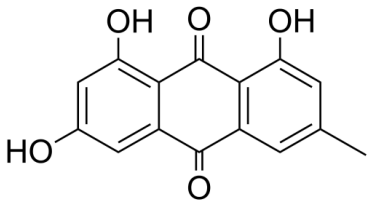
Data Sheet

Product Name:	Emodin
Cat. No.:	CS-1412
CAS No.:	518-82-1
Molecular Formula:	$C_{15}H_{10}O_5$
Molecular Weight:	270.24
Target:	11β-HSD; Autophagy; Casein Kinase; SARS-CoV
Pathway:	Anti-infection; Autophagy; Cell Cycle/DNA Damage; Metabolic Enzyme/Protease; Stem Cell/Wnt
Solubility:	Acetone : 10.87 mg/mL (ultrasonic);Ethanol : < 1 mg/mL (ultrasonic);DMSO : 5.41 mg/mL (ultrasonic)



BIOLOGICAL ACTIVITY:

Emodin (Frangula emodin), an anthraquinone derivative, is an anti-**SARS-CoV** compound. Emodin blocks the SARS coronavirus spike protein and angiotensin-converting enzyme 2 (ACE2) interaction[1]. Emodin inhibits **casein kinase-2** (**CK2**). Anti-inflammatory and anticancer effects[2]. Emodin is a potent selective **11β-HSD1** inhibitor with the **IC_{50}** of 186 and 86 nM for human and mouse 11β-HSD1, respectively. Emodin ameliorates metabolic disorder in diet-induced obese mice[3]. IC50 & Target:IC50: 2 μM (CKII)[1] ***In Vitro:*** Emodin (10-400 μM) blocks the binding of S protein to ACE2 in a dose-dependent manner with the IC_{50} value of 200 μM[1].

Emodin (5-50 μM) inhibits the S protein-pseudotyped retrovirus infectivity in a dose-dependent manner. Emodin blocks the SARS-CoV S protein binding to Vero E6 cells[1].

Emodin inhibits casein kinase-2 (CK2) with IC_{50}s of 5.9, 30.0, and 7.1 μM for CK2α Wild-type, Ile174Ala mutant, and His160Ala mutant at ATP concentration is 50 μM, respectively. The IC_{50}s are 1.40 and 38.00 μM for CK2α Wild-type, and Val66Ala mutant at ATP concentration is 10 μM[2].

Emodin exhibits low inhibitory activity against mouse and human 11β-hydroxysteroid dehydrogenase type 2 (11β-HSD2), with an IC_{50} higher than 1 mM, indicating that Emodin is more than 5000-fold selective for the human and mouse 11β-HSD1 enzymes over the type 2 isoenzyme[3]. ***In Vivo:***Emodin (single oral administration of 100 or 200 mg/kg) inhibits 11β-HSD1 activity in normal C57BL/6J male mice[3].

Emodin (100 mg/kg; oral administration; b.i.d.) improves insulin sensitivity and lipid metabolism, and lowers blood glucose and hepatic PEPCK, and glucose-6-phosphatase mRNA in diet-induced obese (DIO) mice[3].

PROTOCOL (Extracted from published papers and Only for reference)

Cell Assay:[4]The T24 human bladder cancer cells, the HCV-29 normal bladder epithelial cells and J82 human bladder cancer cells are are cultured in RPMI 1640 medium supplemented with 10 % fetal bovine serum at 37°C in a humidified atmosphere containing 5 % CO_2. Cells are seeded in 96-well plates with 2×10^4 cells per well. The cells are incubated with Emodin for 24 h at different concentrations (0, 5, 10, 20, 30, 40, 50, 60, 70 μM) and chose the critical concentration (20 μM) treated with cells for 0, 6, 12, 24, 48, 72, 96 h. The cells are incubated with cisplatin for 24 h at different concentrations (0, 0.5, 1.0, 1.5, 2.0, 2.5, 3.0 μg/mL). MTT assay is used to analyze the cell viability. Cells are treated with drugs for 24 h and apoptotic rates are assessed with flow cytometry using AnnexinV-fluorescein isothiocyanate (AnnexinV-FITC)/propidium iodide (PI) kit. Samples are prepared according to the manufacturer's instruction and analyzed by a flow cytometry (FCM) Calibur[4]. **Animal Administration:**Emodin is prepared in 0.5% carboxymethylcellulose (CMC)[3].[4]Mice[4]

3×10^6 T24 cells are harvested, washed, and resuspended in serum-free optimum medium and then injected subcutaneously into 6-week old BALB/c-nu/nu mice (n=8 mice per group). Three days after inoculation, the mice are intraperitoneally administered with

PBS, Emodin (50 mg/kg), Cisplatin (1 mg/kg), or Emodin/cisplatin every two days. On day 18, every mouse is sacrificed. After body weight measurement, tumors are isolated, weighted and fixed in 4 % paraformaldehyde (PFA). Hearts, livers and kidneys are stained with Hematoxylin & Eosin to determine the systemic toxicity. Terminal deoxynucleotidyl transferase(TdT)-mediated dUTP nick end label (TUNEL) assay is performed on paraformaldehyde-fixed and paraffin-embedded tumor sections.

References:

[1]. Tin-Yun Ho, et al. Emodin blocks the SARS coronavirus spike protein and angiotensin-converting enzyme 2 interaction. Antiviral Res. 2007 May;74(2):92-101.

[2]. Ying Feng, et al. Emodin, a natural product, selectively inhibits 11beta-hydroxysteroid dehydrogenase type 1 and ameliorates metabolic disorder in diet-induced obese mice. Br J Pharmacol. 2010 Sep;161(1):113-26.

[3]. Stefania Sarno, et al. Toward the rational design of protein kinase casein kinase-2 inhibitors. Pharmacol Ther. Feb-Mar 2002;93(2-3):159-68.

CAIndexNames:

9,10-Anthracenedione, 1,3,8-trihydroxy-6-methyl-

SMILES:

O=C1C2=C(C=C(C)C=C2O)C(C3=CC(O)=CC(O)=C31)=O

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