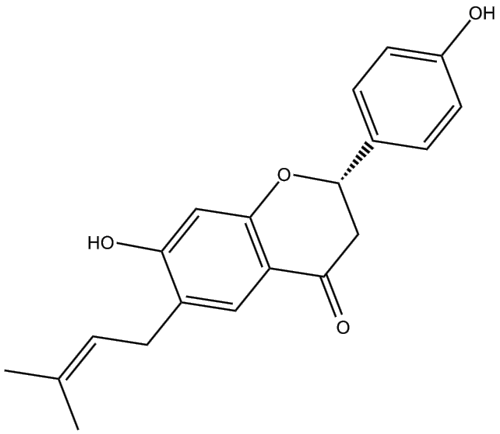
Product Data Sheet

Product Name: Bavachin
Cat. No.: GC17588

Chemical Properties

Cas. No.	19879-32-4		
Chemical Name	(2S)-2,3-dihydro-7-hydroxy-2-(4-hydroxyphenyl)-6-(3-methyl-2-butenyl)-4H-1-benzopyran-4-one		
SMILES	OC1=CC(O[C@H](C2=CC=C(O)C=C2)CC3=O)=C3C=C1C/C=C(C)/C		
Formula	$C_{20}H_{20}O_4$	M.Wt	324.4
Solubility	≤20mg/ml in ethanol;30mg/ml in DMSO;50mg/ml in dimethyl formamide	Storage	Store at -20°C,protect from light
General tips	For obtaining a higher solubility , please warm the tube at 37 °C and shake it in the ultrasonic bath for a while.Stock solution can be stored below -20°C for several months.		
Shipping Condition	Evaluation sample solution : ship with blue ice All other available size: ship with RT , or blue ice upon request.		

Structure



Protocol

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Kinase experiment: The chemiluminescent assay is used to confirm PCSEE MAO-A and MAO-B inhibitory effects and to test BNN and BVN hMAO-A and hMAO-B inhibition using MAO-Glo kit. Each enzyme's Arbitrary Light Unit (ALU) is measured in the presence of PCSEE, BNN, BVN, and standard DEP as an MAO-BI positive control. Briefly, hMAO-A and hMAO-B isozymes are diluted to 2× with reaction buffer (pH 7.4) and preincubated with 4× PCSEE, BNN, BVN, or DEP working solutions at RT for 30 min in white opaque 96-well plates. For determining activity inhibition, final 8.5 μg/mL concentrations of PCSEE, BNN, BVN, and DEP are used. For IC50 determination, 8× PCSEE and BNN working solutions are serially diluted using reaction buffers (pH 7.4) to make a 4× concentration. Ten points' range of PCSEE (1.0 to 250.0 μg/mL) and BNN (up to 400 μM (135.4 μg/mL)) final concentrations is used. Controls used are with and without ethanol. Ethanol solvent in controls is kept to a maximum final (volume) of ≤2%. Each isozyme is substituted with the reaction buffer for the blank. Based on our preliminary optimizations and Valley's method, the reaction is initiated by adding 4× luciferin derivative substrate (LDS) for a final (concentration) of 40 and 4 μM for hMAO-A and hMAO-B reactions, respectively. The final volume per well of each reaction is 50 μL. The reaction is optimized for the amount of A and B enzyme used to be incubated for less than 3.5 h at RT. To stop the reaction and produce the luminescence signal RLDR is added to all wells, 50 μL to each well, and incubated for a further 30 min.

Cell experiment: MTT solution (20 μL) is added to each well of the 96-well plates, the cells are cultured for 4 h, the solution is discarded, and the purple crystal is dissolved in the wells with 150 μL DMSO solution, agitated in a 37°C incubator shaker for 10 min, and the optical density (OD) is measured at 490 nm by the microplate reader.

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

[1]. Wang JH, et al. Effects of bavachin and its regulation of melanin synthesis in A375 cells. Biomed Rep. 2016 Jul;5(1):87-92. Epub 2016 May 20.
[2]. Lee H, et al. Bavachin from Psoralea corylifolia Improves Insulin-Dependent Glucose Uptake through Insulin Signaling and AMPK Activation in 3T3-L1 Adipocytes. Int J Mol Sci. 2016 Apr 8;17(4):527.
[3]. Zarmouh NO, et al. Evaluation of the Inhibitory Effects of Bavachinin and Bavachin on Human Monoamine Oxidases A and B. Evid Based Complement Alternat Med. 2015;2015:852194.
[4]. Park J, et al. Activation of Estrogen Receptor by Bavachin from Psoralea corylifolia. Biomol Ther (Seoul). 2012 Mar;20(2):183-8.

Background

Bavachin is an acyl-coenzyme A: cholesterol acyltransferase inhibitor [1].

Acyl-coenzyme A: cholesterol acyl transferase (ACAT) is an enzyme responsible for the intracellular esterification of free cholesterol with fatty acids and plays dominant roles in intestinal absorption of cholesterol, hepatic production of lipoproteins and accumulation of cholesteryl ester within macrophages and smooth muscle cells. [1].

Bavachin showed a significant inhibition of ACAT enzyme. The IC50 value of bavachin was 86.0 μM in the ACAT assay system using rat liver microsome [1]. Bavachin is a flavonoid first isolated from Psoralea corylifolia that has been used as a traditional medicine in Asia. In CV-1 cells transfected with plasmids ERα or ERβ, bavachin showed ER ligand binding activity with an EC50 of 320 nM and 680 nM, respectively. Bavachin increased the mRNA levels of estrogen-responsive genes such as pS2 and PR, and decreased the protein level of ERα by proteasomal pathway [2]. Bavachin activated gene expression of proliferator-activated receptorγ (PPARγ), adipogenic transcriptional factors, and CCAAT/enhancer binding protein-α (C/EBPα). Bavachin increased adiponectin expression and secretion in adipocytes. Bavachin increased insulin-induced glucose uptake by differentiated adipocytes and myoblasts. In differentiated adipocytes, bavachin enhanced glucose uptake [3].

References:

[1] Choi J H, Rho M C, Lee S W, et al. Bavachin and isobavachalcone, acyl-coenzyme A: cholesterol acyltransferase inhibitors from Psoralea corylifolia[J]. Archives of pharmacal research, 2008, 31(11):

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[2] Park J, Kim D H, Ahn H N, et al. Activation of estrogen receptor by bavachin from Psoralea corylifolia[J]. Biomolecules & therapeutics, 2012, 20(2): 183-188.
[3] Lee H, Li H, Noh M, et al. Bavachin from Psoralea corylifolia improves insulin-dependent glucose uptake through insulin signaling and AMPK activation in 3T3-L1 adipocytes[J]. International journal of molecular sciences, 2016, 17(4): 527.