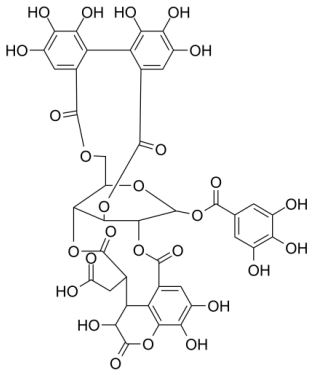
Data Sheet

Product Name:	Chebulagic acid
Cat. No.:	CS-5820
CAS No.:	23094-71-5
Molecular Formula:	$C_{41}H_{30}O_{27}$
Molecular Weight:	954.66
Target:	COX; Influenza Virus; Lipoxygenase; SARS-CoV
Pathway:	Anti-infection; Immunology/Inflammation; Metabolic Enzyme/Protease
Solubility:	DMSO : 100 mg/mL (104.75 mM; Need ultrasonic)



BIOLOGICAL ACTIVITY:

Chebulagic acid is a **COX-LOX** dual inhibitor isolated from the fruits of Terminalia chebula Retz, on angiogenesis. Chebulagic acid is a **M2 serine to asparagine 31 mutation (S31N)** inhibitor and influenza antiviral. Chebulagic acid also against **SARS-CoV-2** viral replication with an **EC_{50}** of 9.76 μM. **In Vitro:** Chebulagic acid can enhance the autophagy. Chebulagic acid exert anti-inflammatory and anti-infective effects. Chebulagic acid also shows a protective effect against 1-methyl-4-phenylpyridinium (MPP+)-induce cytotoxicity which mimics the pathological symptom of Parkinson's disease. Chebulagic acid inhibits the LPS-induced upregulation of TNF-α and IL-1β in a dose- and time-dependent manner. Furthermore, LPS-activated MAPK signaling is inhibited by Chebulagic acid treatment in the EA.hy926 cells.

References:

[1]. Kim HJ et al. Neuroprotective Effect of Chebulagic Acid via Autophagy Induction in SH-SY5Y Cells. Biomol Ther (Seoul). 2014 Jul;22(4):275-81.

[2]. Liu Y et al. Chebulagic acid inhibits the LPS-induced expression of TNF-α and IL-1β in endothelial cells by suppressing MAPK activation. Exp Ther Med. 2015 Jul;10(1):263-268.

[3]. Athira AP et al. Inhibition of Angiogenesis In Vitro by Chebulagic Acid: A COX-LOX Dual Inhibitor. Int J Vasc Med. 2013;2013:843897.

[4]. Maggie C. Duncan, et al. Virtual Screening Identifies Chebulagic Acid as an Inhibitor of the M2(S31N) Viral Ion Channel and Influenza A Virus. Molecules 2020, 25, 2903.

[5]. RuikunDu, et al. Discovery of Chebulagic Acid and Punicalagin as Novel Allosteric Inhibitors of SARS-CoV-2 3CLpro. Antivir Res. 2021, 105075.

CAIndexNames:

β-D-Glucopyranose, cyclic 3,6-[(1R)-4,4',5,5',6,6'-hexahydroxy[1,1'-biphenyl]-2,2'-dicarboxylate] 1-(3,4,5-trihydroxybenzoate), cyclic 2→2:4→1-ester with (2S)-2-[(3S,4S)-5-carboxy-3,4-dihydro-3,7,8-trihydroxy-2-oxo-2H-1-benzopyran-4-yl]butanedioic acid

SMILES:

OC(CC(C(O[C@H]([C@@H](COC(C1=CC(O)=C2O)=O)O[C@@H]3OC(C4=CC(O)=C(O)C(O)=C4)=O)[C@H](OC(C5=CC(O)=C(O)C(O)=C5C1=C2O)=O)[C@H]3OC6=O)=O)C(C7O)C(C6=CC(O)=C8O)=C8OC7=O)=O

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

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