



Andrographolide

Cat. No.:	OB0225WX-2475
Appearance:	Solid
Purity:	≥99%
Identity:	Confirmed by NMR, and HPLC.
Size:	20 mg; 50 mg; 200 mg; 1 g

This product is for research use only and is not intended for diagnostic use.

Product Overview

Description	Andrographolide is a labdane diterpenoid lactone that serves as the primary bioactive secondary metabolite derived from the medicinal herb <i>Andrographis paniculata</i> .
Synonym	5508-58-7; Andrographolide; (S,E)-4-Hydroxy-3-(2-((1R,4a S,5R,6R,8aS)-6-hydroxy-5-(hydroxymethyl)-5,8a-dimethyl-2-methylenedecahydronaphthalen-1-yl)ethylidene)dihydrofuran-2(3H)-one; 3α,14,15,18-tetrahydroxy-5b,9bH,10a-labda-8(20),12-dien-16-oic acid gamma-Lactone; (3 E,4S)-3-[2-[(1R,4aS,5R,6R,8aS)-6-hydroxy-5-(hydroxymethyl)-5,8a-dimethyl-2-methylidene-3,4,4a,6,7,8-hexahydro-1H-naphthalen-1-yl]ethylidene]-4-hydroxyoxolan-2-one; 3-(2-(Decahydro-6-hydroxy-5-(hydroxymethyl)-5,8a-dimethyl-2-methylenenaphthyl)ethylidene)dihydro-4-hydroxyfuran-2(3H)-one; (1R-(1-α(E(S)),4β,5α,6α,8α))-3-(2-(decahydro-6-hydroxy-5-(hydroxymethyl)-5,8a-dimethyl-2-methylene-1-naphthalenyl)ethylidene)dihydro-4-hydroxy-2(3H)-furanone
CAS No.	5508-58-7
Compound CID	5318517
Formula	C ₂₀ H ₃₀ O ₅
Formula Weight	350.45

Specification



IUPAC Name	(3 <i>E</i> ,4 <i>S</i>)-3-[2-[(1 <i>R</i> ,4 <i>aS</i> ,5 <i>R</i> ,6 <i>R</i> ,8 <i>aS</i>)-6-Hydroxy-5-(hydroxymethyl)-5,8 <i>a</i> -dimethyl-2-methylidene-3,4,4 <i>a</i> ,6,7,8-hexahydro -1 <i>H</i> -naphthalen-1-yl]ethylidene]-4-hydroxyoxolan-2-one
InChI	InChI=1S/C20H30O5/c1-12-4-7-16-19(2,9-8-17(23)20(16,3)11-21)14(12)6-5-13-15(22)10-25-18(13)24/h5,14-17,21-23H,1,4,6-11H2,2-3H3/b13-5+/t14-,15-,16+,17-,19+,20+/m1/s1
InChI Key	BOJKULTULYSRAS-OTESTREVSA-N
SMILES string	<chem>C[C@@]12CC[C@H]([C@@]([C@H]1CCC(=C)[C@H]2C/C=C/3\[C@@H](COC3=O)O)(C)CO)O</chem>
Stability	3 years in powder form.
Storage	Storage at -20°C.
Applications	Andrographolide is utilized in phytochemical and immunological research to examine the inhibition of NF-kappaB signaling and its role in modulating pro-inflammatory cytokine production.

Library Information

Target	NF-κB
Receptor	NF-κB
Pathways	NF-κB
Plate Number	L6700-03
Empty Location	a1-h1; a12-h12
Container	96-well plate
Formulation	10mM DMSO
DMSO Max Solubility	70 mg/mL; 199.74 mM
ALogP	2.056
HBA_Count	2
HBD_Count	3
Rotatable Bond	3