



Product Information

Rotundic acid

Cat. No.: X23-04-XQ282

Size: 20 mg; 50 mg; 100 mg; 200 mg

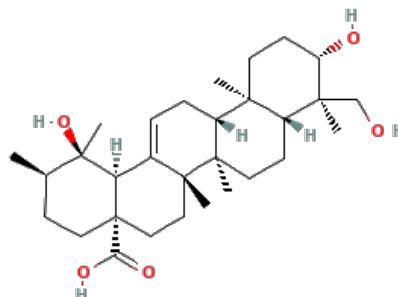
MDL: MFCD13186912

CAS Number: 20137-37-5

Compound CID: 12315075

Synonym: 20137-37-5; Rotundic acid; Rutundic acid; 22-Deoxyilexolic acid A

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



Product Information

Description	Rotundic acid is a triterpenoid exhibit cytotoxic activities toward human hepatocellular carcinoma (HepG2), malignant melanoma (A375), SCLC (NCI-H446), breast cancer (MCF-7), and colon cancer (HT-29) cell lines.
Molecular Weight	488.709
Molecular Formula	C ₃₀ H ₄₈ O ₅
IUPAC Name	(1R,2R,4aS,6aR,6aS,6bR,8aR,9R,10S,12aR,14bS)-1,10-Dihydroxy-9-(hydroxymethyl)-1,2,6a,6b,9,12a-hexamethyl-2,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydronicene-4a-carboxylic acid
InChI	InChI=1S/C30H48O5/c1-18-9-14-30(24(33)34)16-15-27(4)19(23(30)29(18,6)35)7-8-21-25(2)12-11-22(32)26(3,17-31)20(25)10-13-28(21,27)5/h7,18,20-23,31-32,35H,8-17H2,1-6H3,(H,33,34)/t18-,20-,21-,22+,23-,25+,26+,27-,28-,29-,30+/m1/s1
InChI Key	YLHQFGOOMKJFLP-LTFXOGOQSA-N
Canonical SMILES	CC1CCC2(CCC3(C(=CCC4C3(CCC5C4(CCC(C5(C)CO)O)C)C)C2C1(C)O)C)C(=O)O
Isomeric SMILES	C[C@@H]1CC[C@@]2(CC[C@@]3(C(=CC[C@H]4[C@]3(CC[C@@H]5[C@@]4(CC[C@@H]([C@]5(C)CO)O)C)C)[C@@H]2[C@]1(C)O)C)C(=O)O
Source	<i>Clethra barbinerv</i> and the seeds of <i>Llex rotunda</i>
Purity	>98%, determined by HPLC.
Identity	Confirmed by NMR and MS.
Stability	The product is stable for two years when stored at the recommended temperature.
Applications	Rotundic acid can be used for cytotoxic activity experiments, etc.
Storage	Store at 4°C. Protect from light.



Safety Information

Personal Protective Equipment	Gloves, eyeshields, N95 mask
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