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Reference Substances
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Certificate of analysis

Article: 80435 α,β -Elemolic acid
Certificate # / Lot Number: 301815
Material batch: 13229
Sample-ID: 266949
End of analysis: 06/2025
Expiry date: 10/2026

Test	Unit	Specified value	Testresult
Appearance, SOP 100005		powder	conform
Color, SOP 100006		white	conform
Identification (UV spectrum from HPLC-DAD analysis) according to specification, SOP 204311		conform	conform
Identification (1H-NMR-spectroscopy), (outsourced), SOP 206010		conform	conform
Identification (13C-NMR-spectroscopy), (outsourced), SOP 206020		conform	conform
Identification (HPLC-HR/MS), SOP 204125		conform	conform
Identification (IR-spectroscopy, Ph.Eur. 10.3, 2.2.24 / USP43 NF37 <197>), SOP 206000		conform	conform
alpha,beta-Elemolic acid (HPLC), method 1 (% AU), SOP 440473	%	≥ 75.00	81.67
Peakpurity, (HPLC), SOP 401367		conform	conform

Certificate of analysis

Article: 80435 α,β -Elemolic acid
Material batch: 13229

Test	Unit	Specified value	Testresult
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The reference substance alpha,beta-elemolic acid is a mixture of alpha-elemolic acid (CAS #28282-27-1) and beta-elemolic acid (CAS # 28282-54-4).

Vestenbergsreuth, 09/Oct/2025

Laura Schnell

QC Reference Substances

This is a computer print and valid without signature. A signed certificate of analysis can be taken on request.

Certificate of analysis

Article: 80435 α,β -Elemolic acid
Material batch: 13229

Further information:

Shelf life/stability: The stated expiry date applies when the reference substance is stored in the original unopened container within the specified temperature range. PhytoLab does not guarantee the stability of the reference substance once the vial has been opened.

Long-term storage and handling: The reference standard should be stored in the original unopened vial, protected against light and humidity in an airtight container, within the temperature range given on the label and accompanying data sheet. If stored below room temperature, the vial should be warmed up to room temperature in a desiccator before it is opened in order to avoid condensation of humidity. The user assumes responsibility for deciding how previously opened reference standard vials should be used and the user must ensure that the contents of opened vials are still suitable for their intended use.

Exact weight: the exact weight of each vial is given on the label of the inner vial to two decimal places. This information may be used to produce stock solutions of a known concentration without having to weigh in the reference substance again. If used for this purpose, the content of the vial must be quantitatively transferred to a volumetric flask and filled up to the required level. Please note that PhytoLab is unable to guarantee the stability of the reference standard in solution.

Intended use: this reference standard is solely intended for laboratory analytical purposes, research & development, and scientific teaching and training purposes. It may not be used for any other purpose and particularly not for use in, or the production of, food, animal feed, human or veterinary drugs, cosmetics, medicinal products or diagnostic agents, including in-vitro diagnostic agents. PhytoLab is unable to guarantee the suitability of this reference standard for any particular application other than its qualitative and quantitative use in chromatography and identification testing.

Further information about this reference standard can be found on the accompanying data sheet or in our webshop. Spectral and chromatographic data, and a description of the applied chromatographic method, are provided in the attachments to this COA. A detailed explanation of all data given on the COA can be found in the guide that is available from the download area in our webshop, where you can also download all of the safety data sheets.

Product Data Sheet

alpha,beta-Elemolic acid

Product #: 80435

Physicochemical Data

CAS #:

Molecular formula: C₃₀H₄₈O₃

Molecular weight [g/mol]: 456.71

Synonyms: α,β -Elemadienolic acid; α,β -Elemic acid; 3 α,β -Hydroxytirucallic acid

Substance class: Isoprenoids

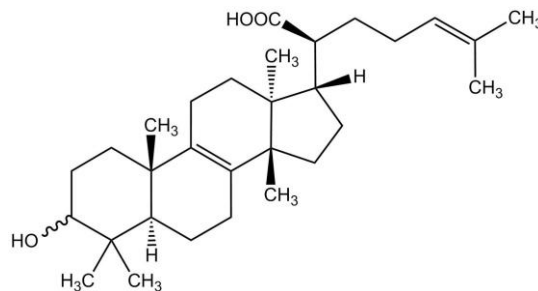
Subgroup 1: Terpenoid-type

Subgroup 2: Triterpenes

Subgroup 3: Triterpene sapogenins

Solubility: soluble in ethanol and methanol

Please note that this solubility information is based on in-house experience or taken from published data. It is not meant to guarantee solubility up to a specific concentration, nor does it guarantee stability of the reference substance in solution.



Additional Information

Please note: The reference substance alpha,beta-elemolic acid is a mixture of alpha-Elemolic acid (CAS # 28282-27-1) and beta-Elemolic acid (CAS # 28282-54-4).

Source: botanical origin

Long-term storage conditions: < -15 °C

Manufacturer: Phytolab GmbH & Co.KG
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Shop: <https://phyproof.phytolab.com>



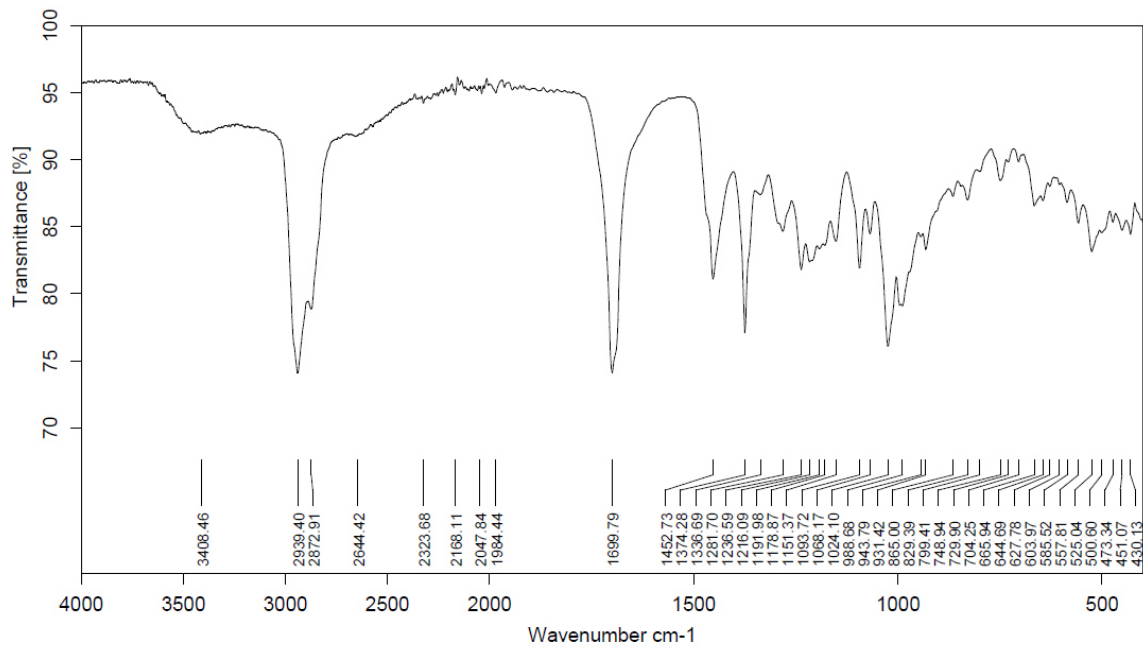
Supplements

alpha,beta-Elemolic acid
Product # 80435

Batch # 13229

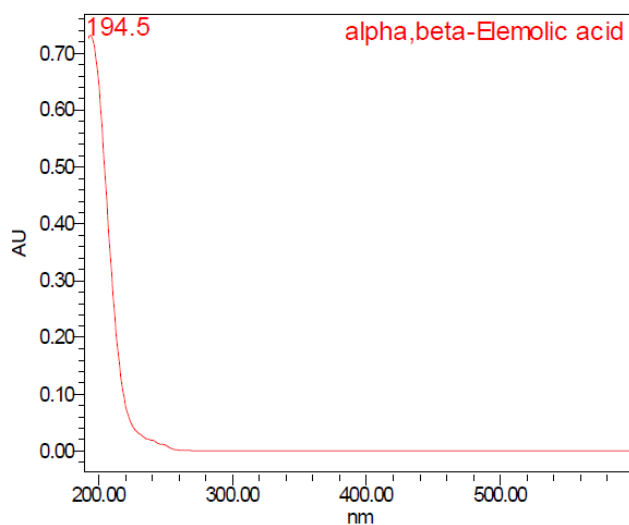
Identity tests:

IR spectrum



C:\Bruker\DATA\80435_alpha,beta-Elemolsäure_13229_0.0

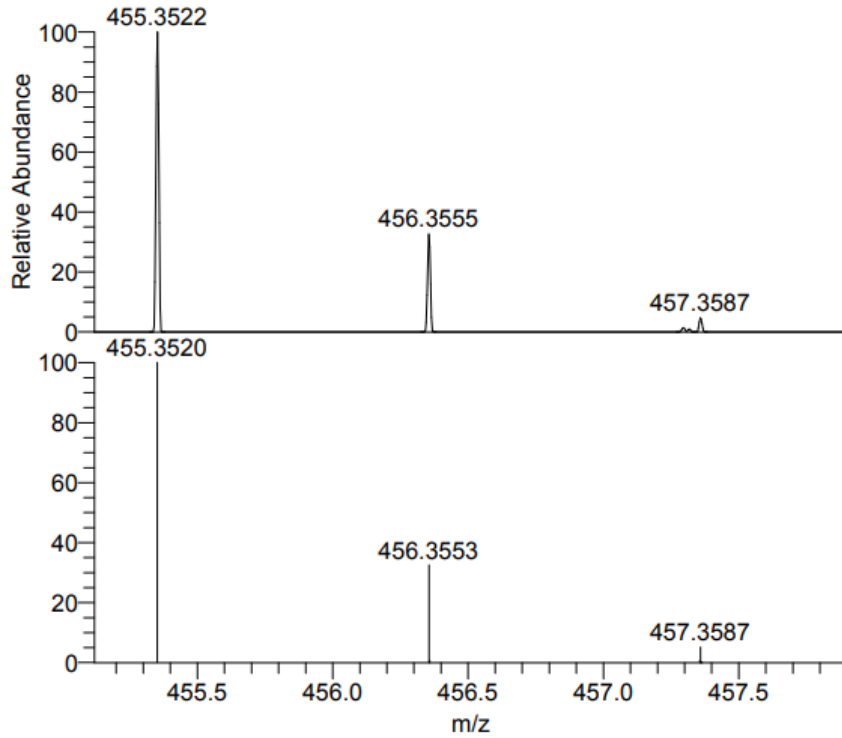
UV spectrum (derived from HPLC/PDA)





MS spectrum (ESI)

Detection: negative mode (compared with predicted spectrum)



NL:
3.05E4
230809_005#1551 RT: 17.68
AV: 1 SB: 159 7.72-8.47 ,
10.12-11.16 T: FTMS {1,1} - p
ESI Full ms [100.00-1500.00]

NL:
7.15E5
C₃₀ H₄₇ O₃:
C₃₀ H₄₇ O₃
pa Chrg 1

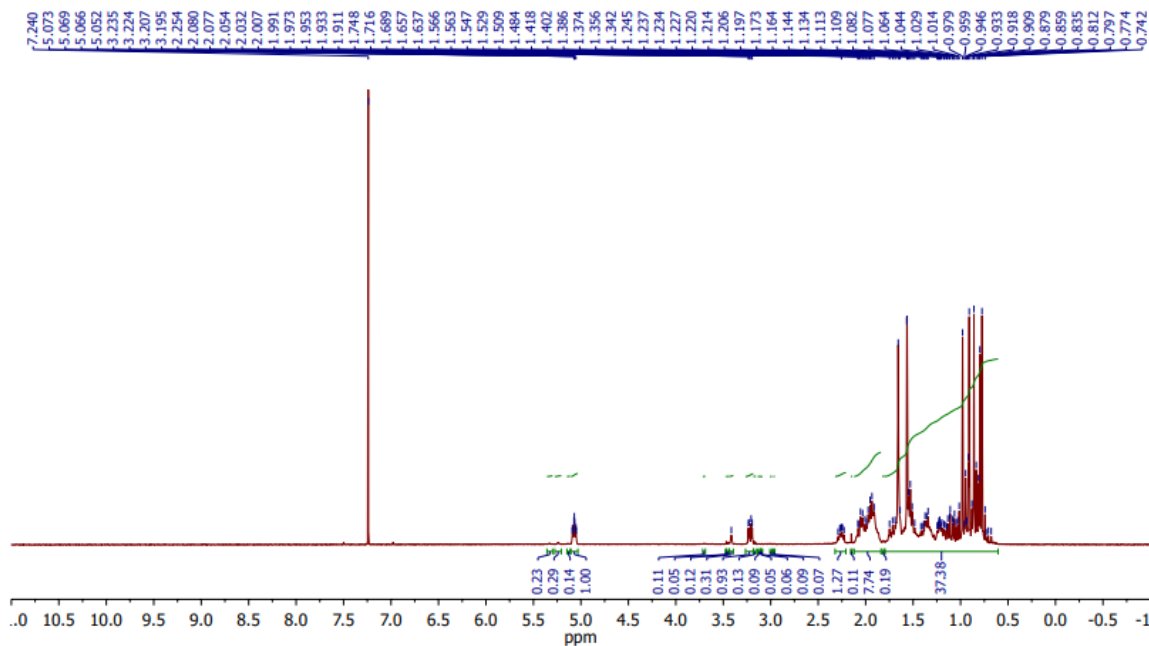


NMR spectra

¹H-NMR

PhytoLab GmbH & Co. KG
α,β-Elemolsäure, Charge: 13229
10.2 mg ad 0.7 ml CDCl₃

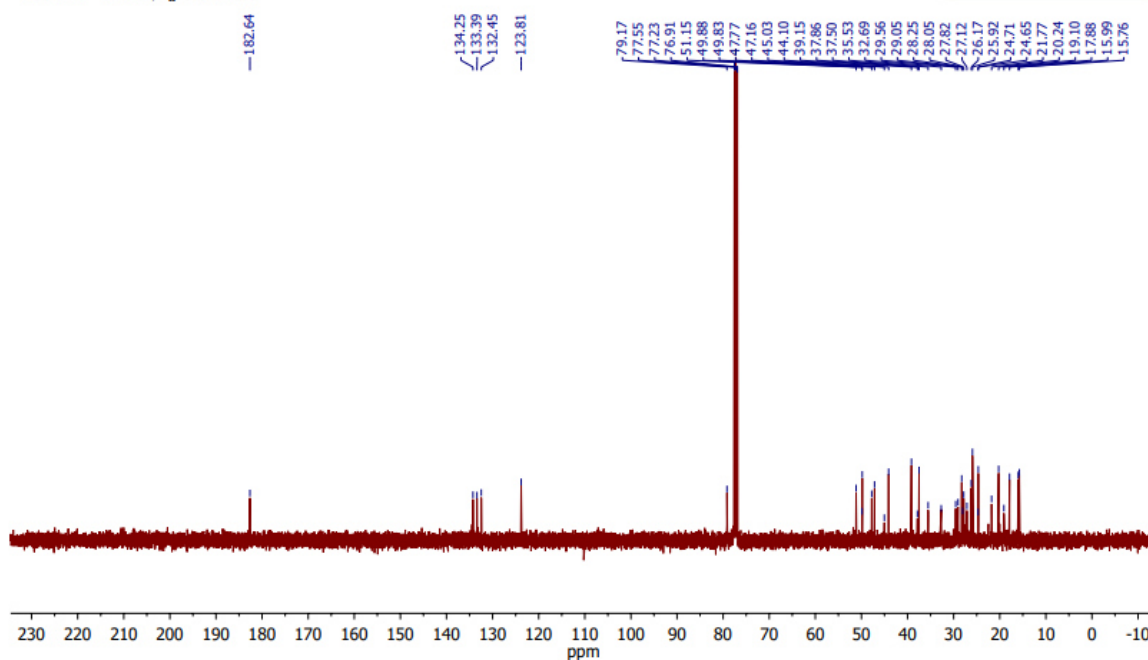
400 MHz ¹H-NMR, Agilent MR400



¹³C-NMR

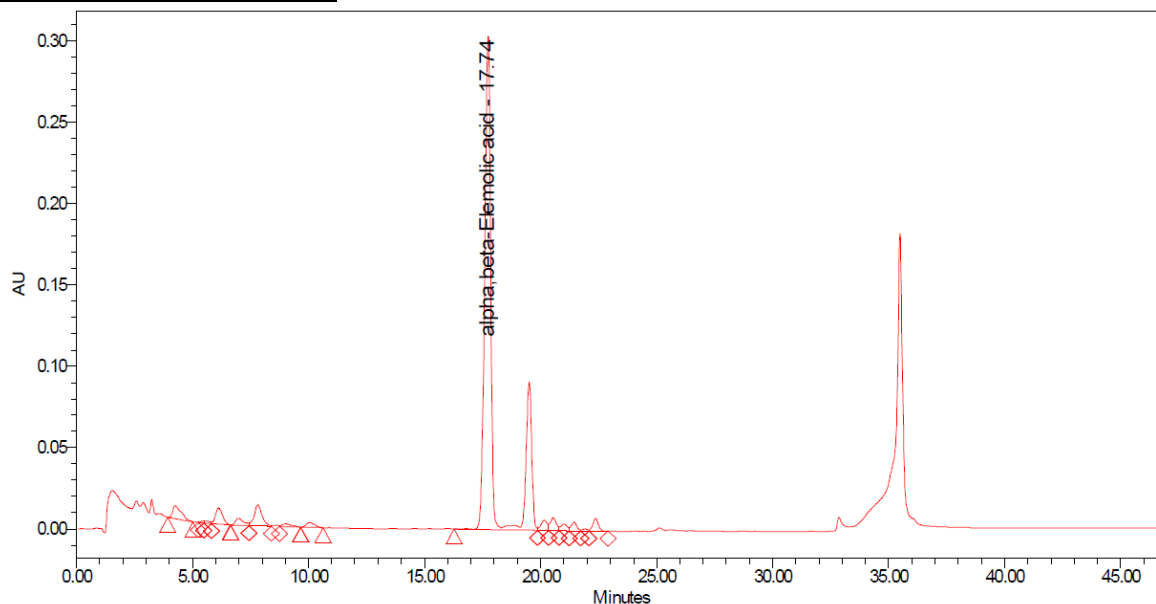
PhytoLab GmbH & Co. KG
α,β-Elemolsäure, Charge: 13229
10.2 mg ad 0.7 ml CDCl₃

100 MHz ¹³C-NMR, Agilent MR400





Chromatographic purity:



Peak Results

Name	RT	Area	Height	Chromatographic_Purity	Amount	Units
1	4.257	207548	7992	2.43		
2	5.458	10134	1127	0.12		
3	5.619	22884	1360	0.27		
4	6.125	208010	9892	2.43		
5	6.978	105197	4220	1.23		
6	7.818	301849	12791	3.53		
7	9.042	52380	1822	0.61		
8	10.058	74736	2971	0.87		
9	alpha.beta-Elemolic acid	17.740	6967257	303515	81.70	23.600 mg/100mL
10	20.161	120230	6260	1.41		
11	20.549	143318	7979	1.68		
12	21.014	78901	4087	0.92		
13	21.446	88973	5253	1.04		
14	21.922	19204	1237	0.22		
15	22.371	131621	7798	1.54		

Analytical conditions

Column: Luna C18, 250 x 4.6mm, 5µm
 Mobile Phase: eluent A: H₂O pH 2.0 (H₃PO₄)
 eluent B: CH₃CN
 Mode: gradient

Time [min]	Eluent A [%]	Eluent B [%]
0	30	70
30	0	100
32	30	70
47	30	70

Flow: 0.8 ml/min
 Injection Volume: 60 µl
 Column Temperature: 23 °C
 Sample concentration: approx. 23.6 mg/100 ml
 Sample preparation: dissolved in CH₃CN
 Detection: UV, 210 nm
 Special note: -

Please note: Values on the certificate of analysis may vary as these are average values of at least six injections while above chromatogram and report is only one example. Non-integrated peaks originate from the blank injection.