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Reference Substances  
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<https://phyproof.phytolab.com>

## Certificate of analysis

|                             |                                     |
|-----------------------------|-------------------------------------|
| Article:                    | 80435 $\alpha,\beta$ -Elemolic acid |
| Certificate # / Lot Number: | 266852                              |
| Material batch:             | 13229                               |
| Sample-ID:                  | 266949                              |
| End of analysis:            | 06/2025                             |
| Expiry date:                | 06/2026                             |

| 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                          | %    | $\geq 75.00$    | 81.67      |
| Peakpurity, (HPLC), SOP 401367                                                             |      | conform         | conform    |

## Certificate of analysis

Article: 80435  $\alpha,\beta$ -Elemolic acid  
Material batch: 13229

| Test | Unit | Specified value | Testresult |
|------|------|-----------------|------------|
|------|------|-----------------|------------|

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, 30/Jun/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  $\alpha,\beta$ -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: C<sub>30</sub>H<sub>48</sub>O<sub>3</sub>

Molecular weight [g/mol]: 456.71

Synonyms:  $\alpha,\beta$ -Elemadienolic acid;  $\alpha,\beta$ -Elemic acid; 3 $\alpha,\beta$ -Hydroxytirucallic acid

Substance class: Isoprenoids

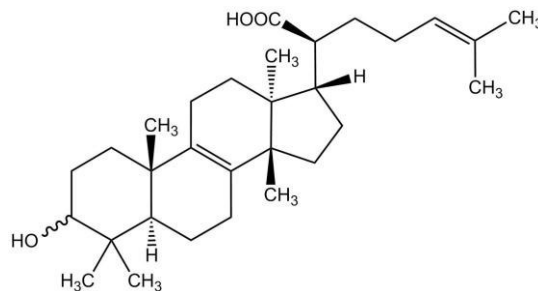
Subgroup 1: Terpenoid-type

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  
Dutendorfer Straße 5-7  
91487 Vestenbergsgreuth  
Germany

Tel.: +49 9163 88-395  
Fax: +49 9163 88-456  
Mail: [ref-substances@phytolab.de](mailto:ref-substances@phytolab.de)  
Shop: <https://phyproof.phytolab.com>



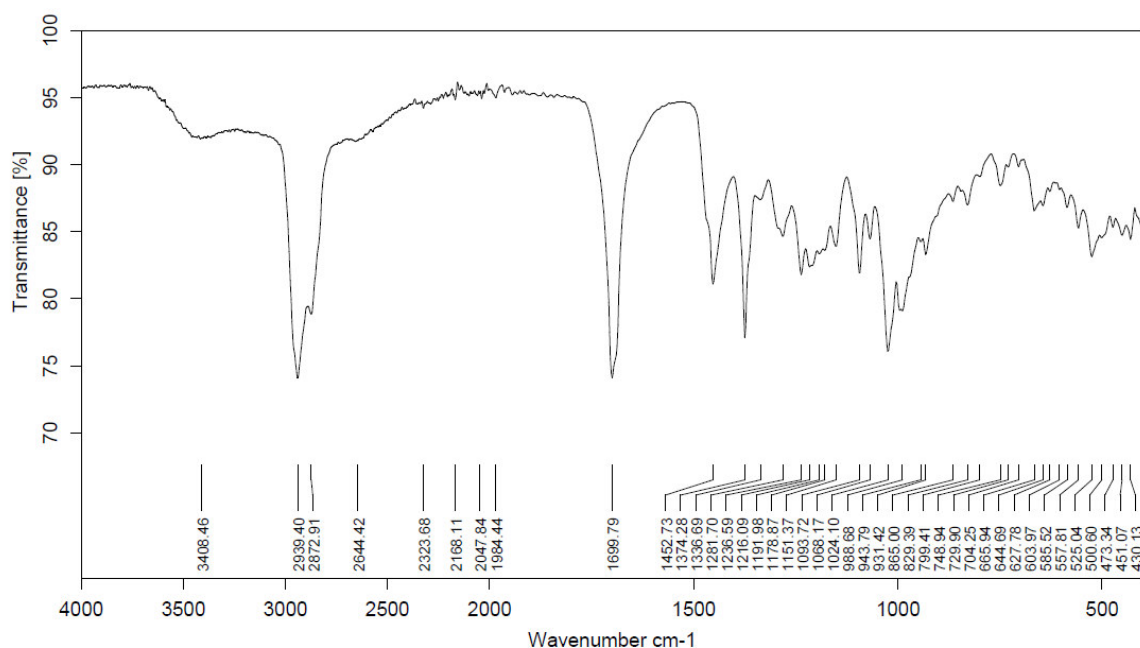
## Supplements

**alpha,beta-Elemolic acid**  
**Product # 80435**

**Batch # 13229**

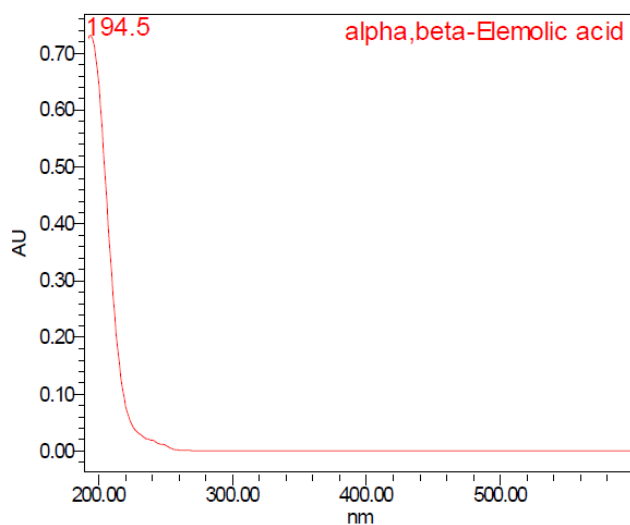
Identity tests:

### IR spectrum



C:\Bruker\DATA\80435\_alpha,beta-Elemolsäure\_13229\_0.0

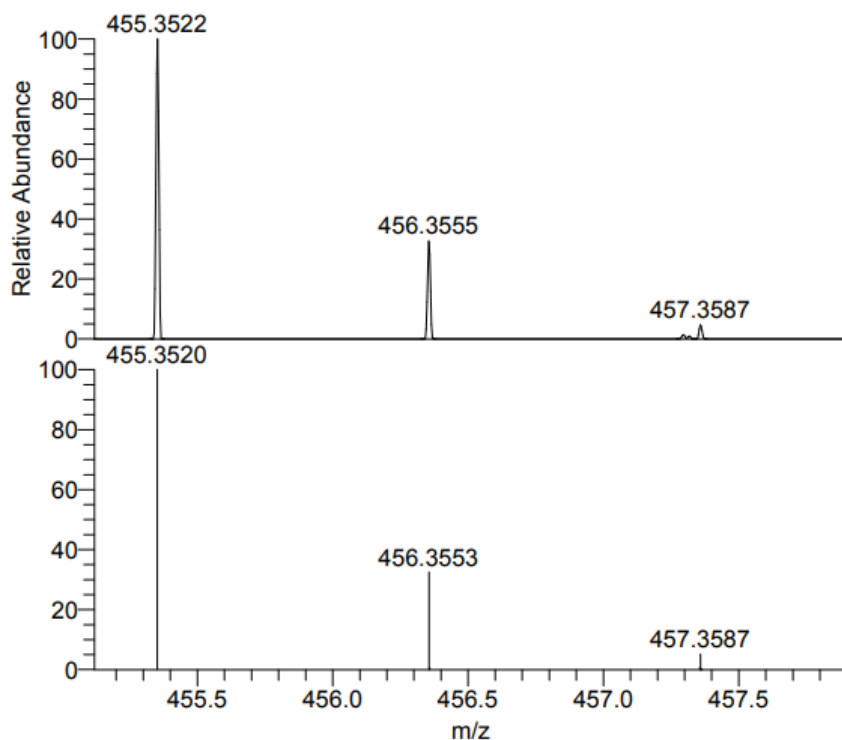
### UV spectrum (derived from HPLC/PDA)





## 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  
C<sub>30</sub> H<sub>47</sub> O<sub>3</sub>:  
C<sub>30</sub> H<sub>47</sub> O<sub>3</sub>  
pa Chrg 1



**PhytoLab**

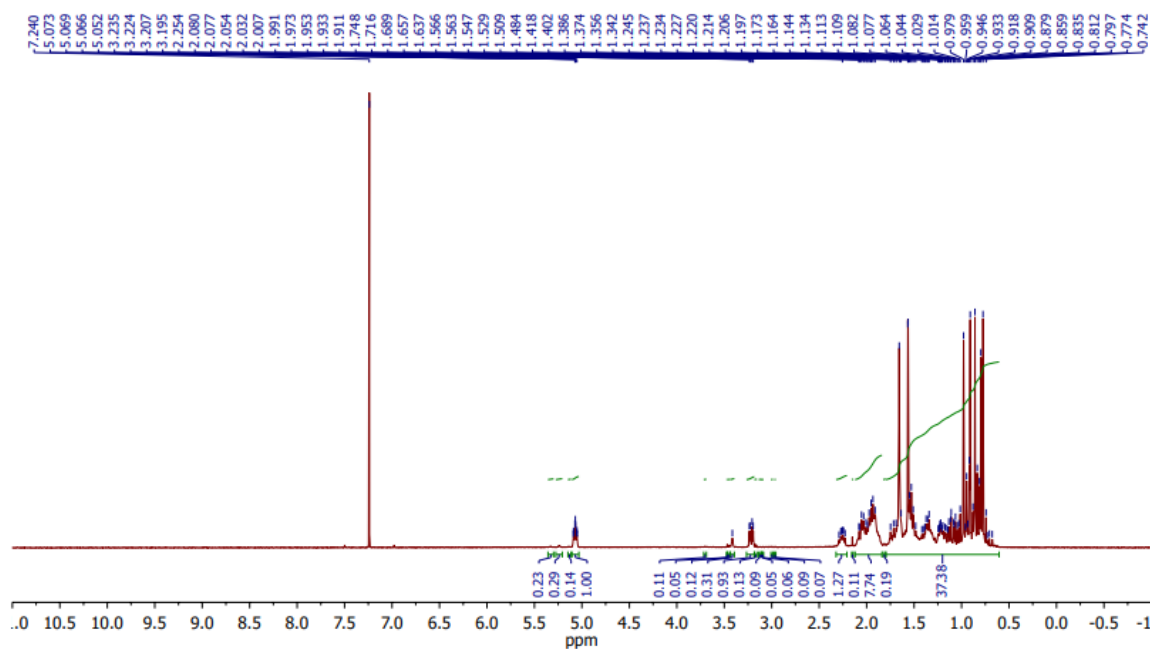
SAFEGUARDING BOTANICAL QUALITY.

## NMR spectra

### $^1\text{H}$ -NMR

PhytoLab GmbH & Co. KG  
 $\alpha,\beta$ -Elemolsäure, Charge: 13229  
10.2 mg ad 0.7 ml  $\text{CDCl}_3$

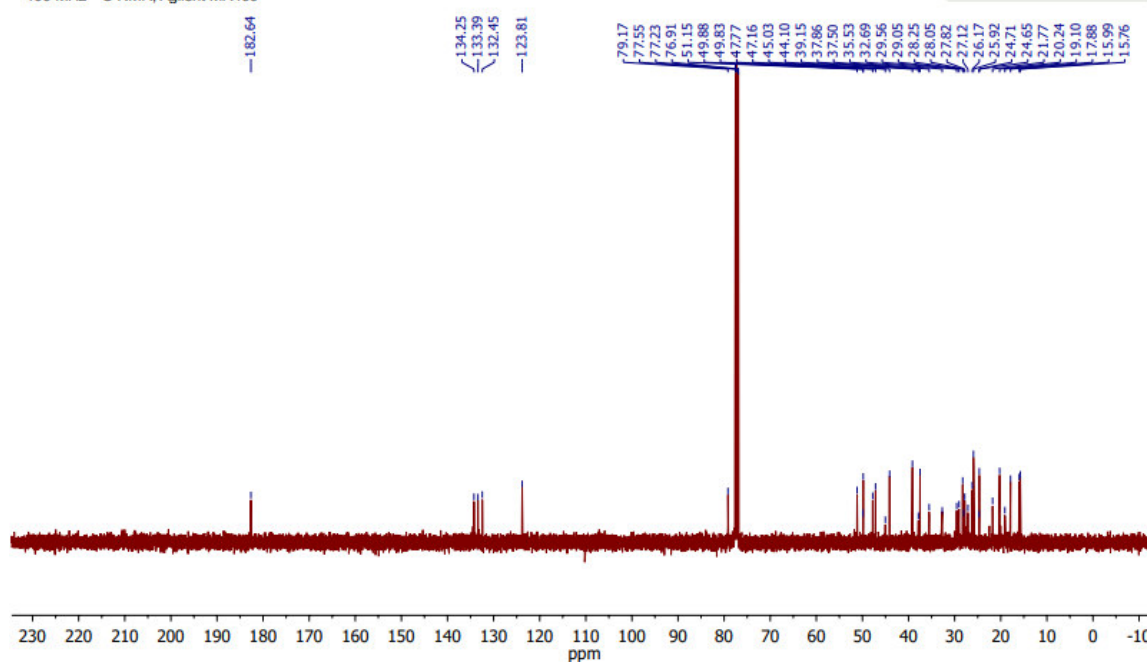
400 MHz  $^1\text{H}$ -NMR, Agilent MR400

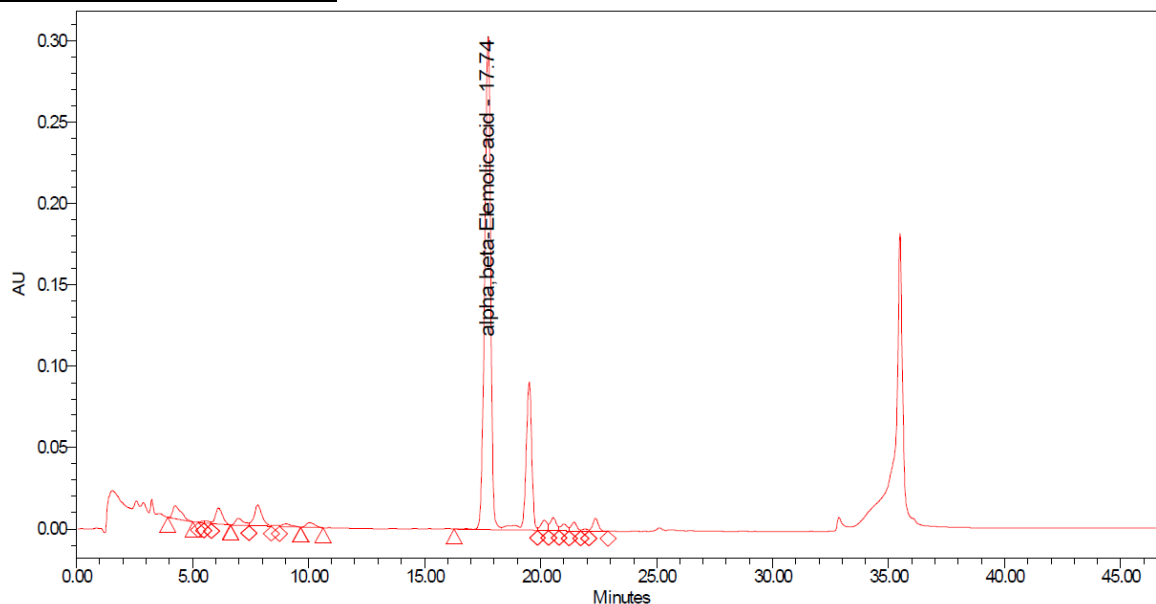


### $^{13}\text{C}$ -NMR

PhytoLab GmbH & Co. KG  
 $\alpha,\beta$ -Elemolsäure, Charge: 13229  
10.2 mg ad 0.7 ml  $\text{CDCl}_3$

100 MHz  $^{13}\text{C}$ -NMR, Agilent MR400



**Chromatographic purity:**

| Peak Results |      |       |        |        |                        |        |       |    |                          |        |         |        |       |
|--------------|------|-------|--------|--------|------------------------|--------|-------|----|--------------------------|--------|---------|--------|-------|
|              | Name | RT    | Area   | Height | Chromatographic_Purity | Amount | Units |    |                          |        |         |        |       |
| 1            |      | 4.257 | 207548 | 7992   | 2.43                   |        |       | 8  |                          | 10.058 | 74736   | 2971   | 0.87  |
| 2            |      | 5.468 | 10134  | 1127   | 0.12                   |        |       | 9  | alpha,beta-Elemolic acid | 17.740 | 6687257 | 303515 | 81.70 |
| 3            |      | 5.619 | 22884  | 1360   | 0.27                   |        |       | 10 |                          | 20.161 | 120230  | 6260   | 1.41  |
| 4            |      | 6.125 | 208010 | 9892   | 2.43                   |        |       | 11 |                          | 20.549 | 143318  | 7979   | 1.68  |
| 5            |      | 6.978 | 105197 | 4220   | 1.23                   |        |       | 12 |                          | 21.014 | 78931   | 4087   | 0.92  |
| 6            |      | 7.818 | 301849 | 12791  | 3.53                   |        |       | 13 |                          | 21.446 | 88973   | 5253   | 1.04  |
| 7            |      | 9.042 | 52380  | 1822   | 0.61                   |        |       | 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: H<sub>2</sub>O pH 2.0 (H<sub>3</sub>PO<sub>4</sub>)  
eluent B: CH<sub>3</sub>CN  
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 CH<sub>3</sub>CN  
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.