

Your contact at PhytoLab:
Reference Substances
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ref-substances@phytolab.de
<https://phyproof.phytolab.com>

Certificate of analysis

Article:	89177 Chicoric acid
Certificate # / Lot Number:	251543
Material batch:	1000438
Sample-ID:	90635
End of analysis:	11/2023
Expiry date:	05/2030

Test	Unit	Specified value	Testresult
Appearance, SOP 100005		powder	conform
Color, SOP 100006		white	conform
Identity test (UV spectrum from HPLC-DAD analysis) according to specification, SOP 204311		conform	conform
Identity test (1H-NMR-spectroscopy), (outsourced), SOP 206010		conform	conform
Identity test (13C-NMR-spectroscopy), (outsourced), SOP 206020		conform	conform
Identity test (HPLC-HR/MS), SOP 204125		conform	conform
Identity test (IR-spectroscopy), Ph. Eur. 2.2.24, Absorption Spectrophotometry, Infrared (01/2021:20224) and USP chapter 197, Spectroscopic Identification Tests (Official as of 01-Sep-2021), SOP 206000		conform	conform
Determination of water (coulometric titration), Ph. Eur. 2.5.32, Water: micro determination (07/2019:20532), SOP 304291, Vers. 2018-01 (double	%		0.4

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Test	Unit	Specified value	Testresult
analysis) Mean value			
Specific optical rotation, Ph. Eur. 2.2.7, Optical rotation (07/2018:20207), SOP 305501 (c = 0.25; MeOH)			-398.11
Chichoric acid (HPLC), method 1 (% AU), SOP 440419	%	≥ 95.00	98.52
Peakpurity, (HPLC), SOP 401367		conform	conform
Inorganic impurities, (ICP-MS), for reference substances, SOP 811701: Calcium	%		<0.1
Potassium	%		<0.1
Magnesium	%		<0.1
Sulfur	%		<1.0
Sodium	%		<0.1
Phosphorus	%		<0.1
Aluminium	%		<0.1
Residual solvents, (headspace-GC), SOP 805765:	%		
Residual solvents (LOQ: 0.050)			<LOQ
Content, SOP 890000, calculated in (%): (100 - water - residual solvents - inorganic impurities) x chromatographic purity / 100	%		98

This PhytoLab phyproof© reference standard is by definition a primary reference standard and does not need to be qualified against any other reference standard. The identity of the reference standard has been substantiated by at least two independent analytical methods such as IR, NMR, UV or MS analysis. A mass balance approach, which takes chromatographic

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purity into account, as well as the contents of water, residual solvents, inorganic impurities, and the counter ion (if the reference standard is present as a salt) is applied in the calculation of the absolute purity as given in this COA (see description of SOP 8900XX).

The absolute purity value (and not just the chromatographic purity result obtained by means of HPLC or GC) must be used in all quantitative calculations as the chromatographic techniques do not yet account for water, residual solvents and inorganic impurities.

Vestenbergsreuth, 02/May/2025

Nicole Fuchs

QC Reference Substances

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

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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.

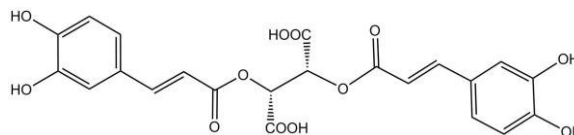
Further information about this reference standard can be found on the accompanying data sheet or in our webshop. Spectral and chromatographic data, and a description of the applied chromatographic method, are provided in the attachments to this COA. A detailed explanation of all data given on the COA 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

Chicoric acid

Product #: 89177

Physicochemical Data



CAS #:	70831-56-0
Molecular formula:	C ₂₂ H ₁₈ O ₁₂
Molecular weight [g/mol]:	474.38
Synonyms	Caffeoyltartaric acid; Cichoric acid; Dicafeoyltartaric acid
Substance class:	Phenylpropanes
Subgroup 1:	Cinnamic acid derivatives
Subgroup 2:	Caffeic acid esters
Solubility:	soluble in methanol and water 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

Source:	botanical origin	
Long-term storage conditions:	2-8 °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 Shop: https://phyproof.phytolab.com



Supplements

Chicoric acid
Product # 89177

Batch # 1000438

Identity tests:

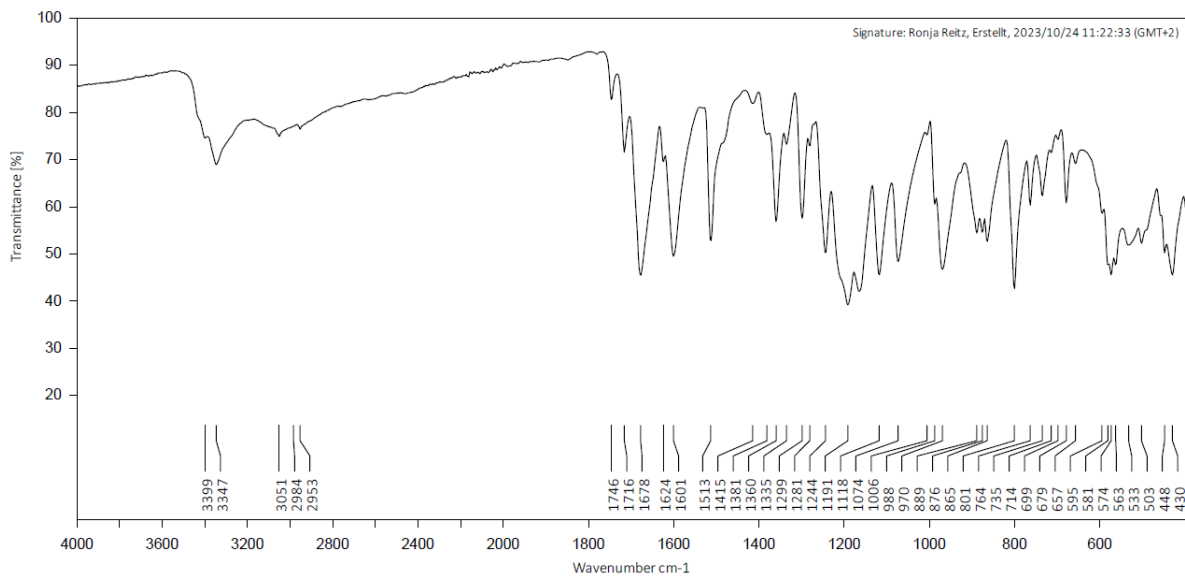
IR spectrum



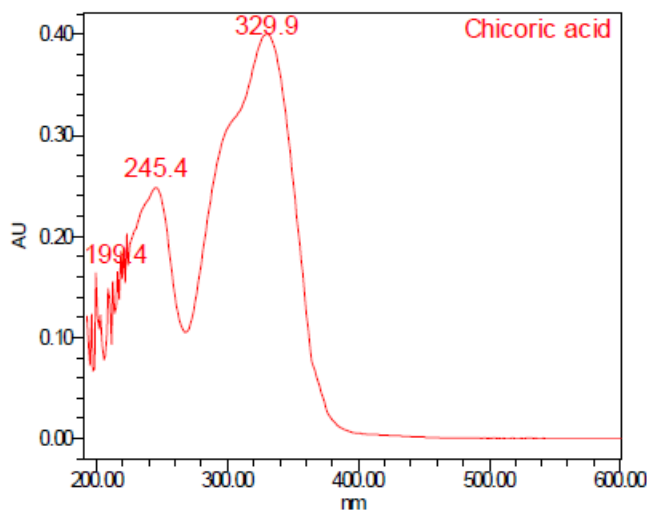
PhytoLab

SAFEGUARDING BOTANICAL QUALITY.

89177_Chicoric acid_1000438



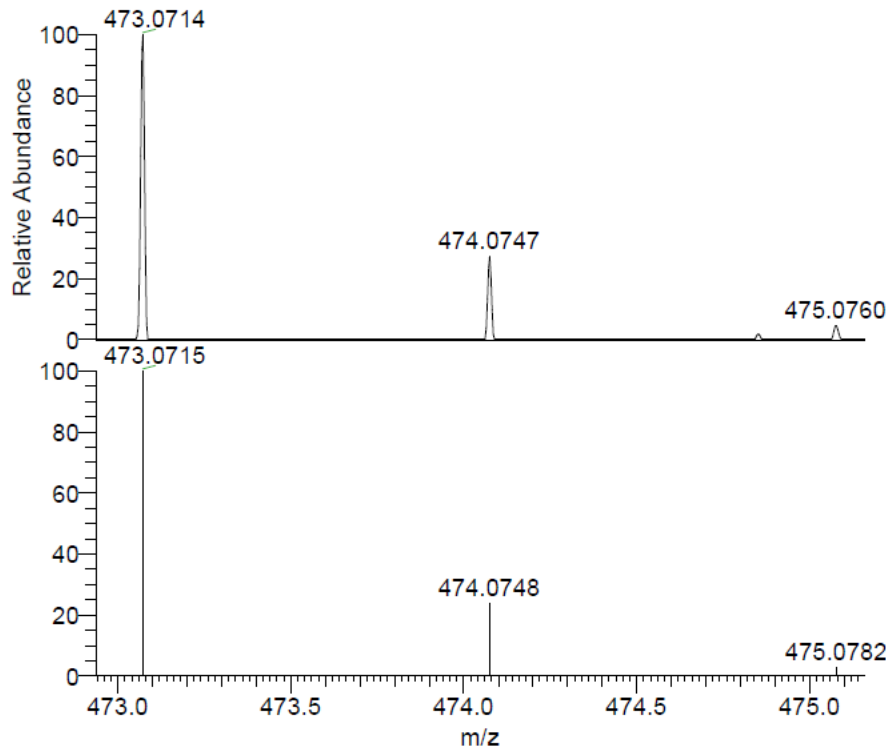
UV spectrum (derived from HPLC/PDA)





MS spectrum (ESI)

Detection: negative mode (compared with predicted spectrum)



NL:
7.37E3
231110_006#909 RT: 10.36
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:
7.65E5
C₂₂ H₁₇ O₁₂:
C₂₂ H₁₇ O₁₂
pa Chrg 1

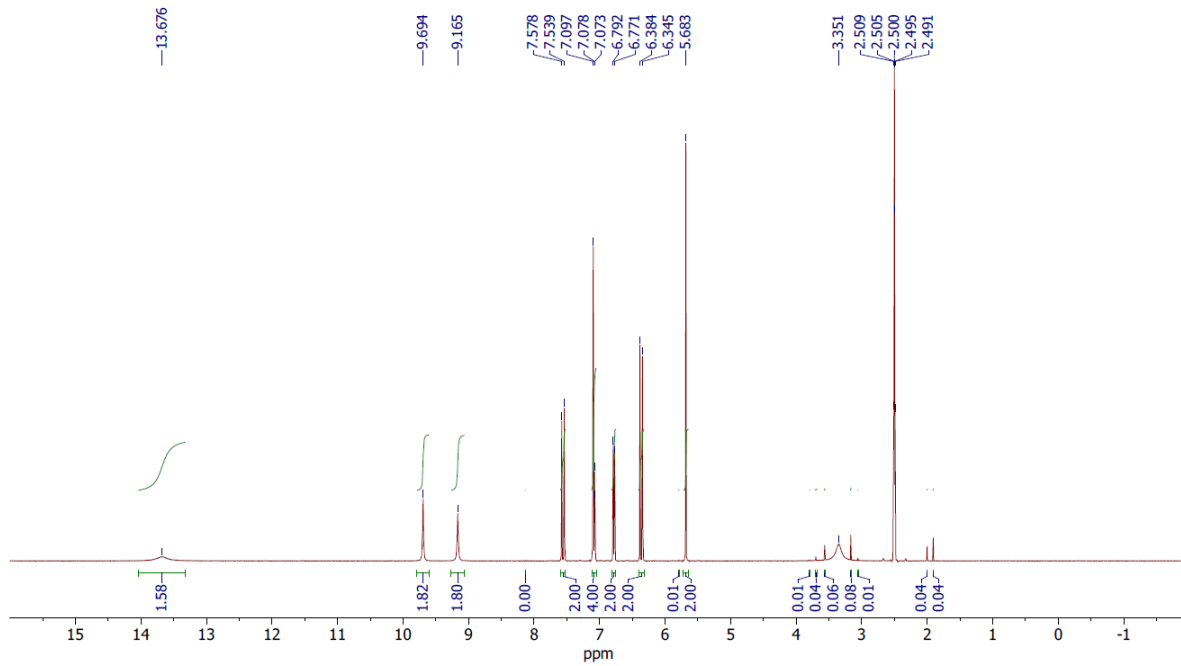


NMR spectra

¹H-NMR

PhytoLab GmbH & Co. KG
Cichoriensäure, Charge: 1000438
10.9 mg ad 0.7 ml DMSO-d₆

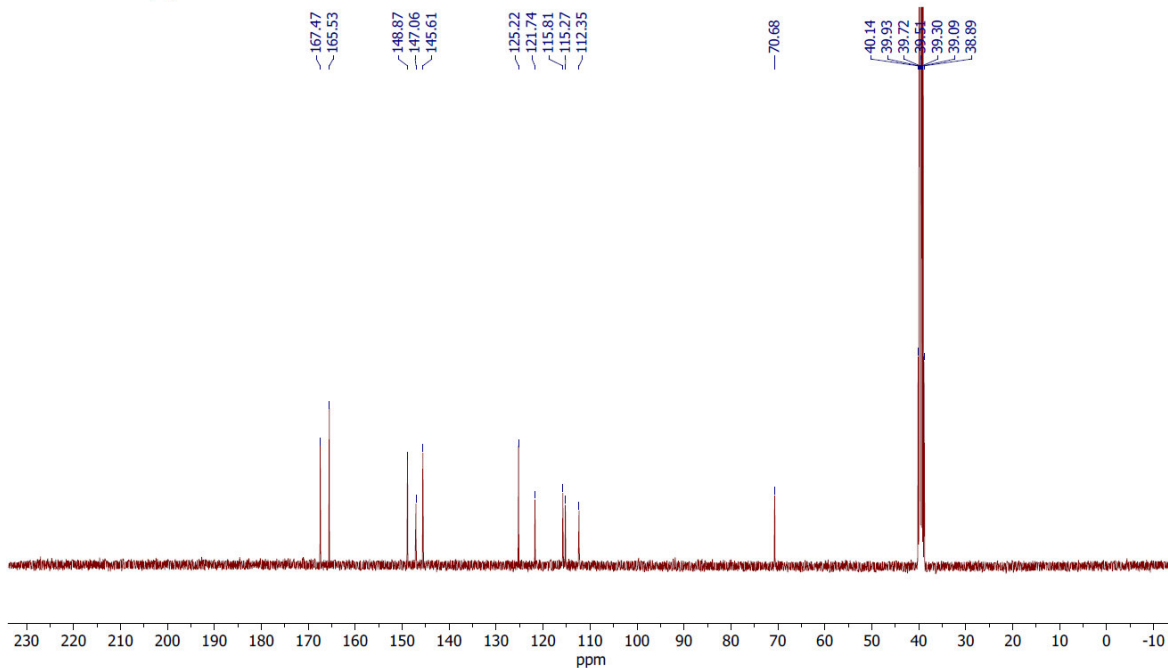
400 MHz ¹H-NMR, Agilent MR400



¹³C-NMR

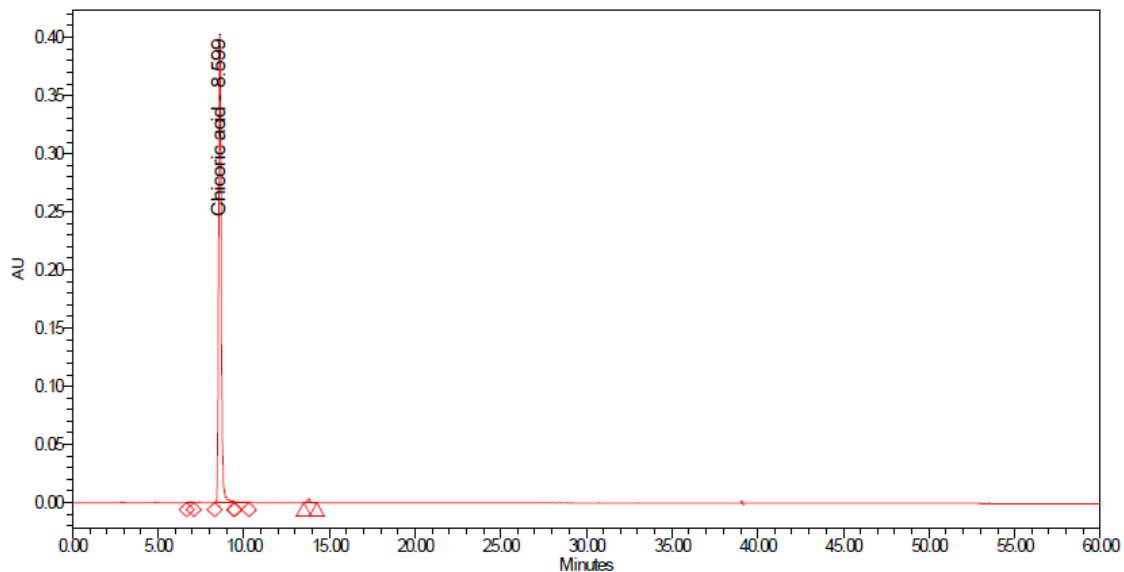
PhytoLab GmbH & Co. KG
Cichoriensäure, Charge: 1000438
10.9 mg ad 0.7 ml DMSO-d₆

100 MHz ¹³C-NMR, Agilent MR400





Chromatographic purity:



Peak Results

	Name	RT	Area	Height	Chromatographic_Purity	Amount	Units
1		6.909	6154	622	0.14		
2	Chicoric acid	8.599	4209608	402246	98.58	1.006	mg/100mL
3		9.497	20432	837	0.48		
4		13.779	33964	3454	0.80		

Analytical conditions

Column: Luna C8, 250 x 4.6 mm, 5 µm
Mobile Phase: eluent A: 2% Acetic Acid
eluent B: CH₃OH
Mode: gradient

Time [min]	Eluent A [%]	Eluent B [%]
0	70	30
30	0	100
35	0	100
40	70	30
60	70	30

Flow: 1.0 ml/min
Injection Volume: 20 µl
Column Temperature: 30 °C
Sample concentration: approx. 5.1 mg/100 ml
Sample preparation: dissolved in 20% CH₃OH
Detection: UV, 292 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.