

PhytoLab GmbH & Co. KG Dutendorfer Straße 5-7 91487 Vestenbergsgreuth

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

Certificate of analysis

Article: 83252 Apocynin
 Certificate # / Lot Number: 109505

Material batch: 10023
 Sample-ID: 50374
 End of analysis: 11/2020
 Expiry date: 12/2028

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	
Purity test (TLC), SOP 300324	conform	conform	
Water content, (micro determination, coulometric titration), Ph.Eur. 10.0., 2.5.32, SOP 304291 Vers. 2018-01: Mean value	%	<0.1	

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Test	Unit	Specified value	Testresult
Apocynin (HPLC), method 1 (%AU), SOP 441334	%	≥ 95.00	100.00
Peakpurity, (HPLC), SOP 401367		conform	conform
Inorganic impurities, (ICP-MS), for reference substances, SOP 811701: Calcium	%	<0.1	
Potassium	%	<0.1	
Magnesium	%	<0.1	
Sodium	%	<0.1	
Phosphorus	%	<0.1	
Aluminium	%	<0.1	
Residual solvents, (headspace-GC), SOP 805765:	%		
Residual solvents (LOQ: 0.050)		<0.050	
Content, SOP 890000, calculated in (%): (100 - water - residual solvents - inorganic impurities) x chromatographic purity / 100	%	100	

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 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

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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.

Vestenbergsgreuth, 15/Dec/2023

Katharina Kleiber

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.

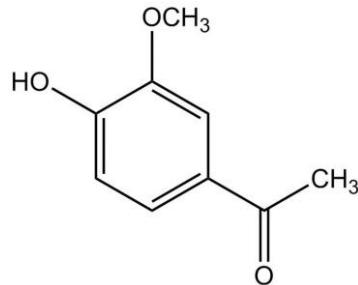
Further information about this reference standard can be found on the accompanying data sheet or in our webshop. Spectral and chromatographic data, and a description of the applied chromatographic method, are provided in the attachments to this COA. A detailed explanation of all data given on the COA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

Apocynin

Product #: 83252

Physicochemical Data



CAS #: 498-02-2

Molecular formula: C9H10O3

Molecular weight [g/mol]: 166.18

Synonyms Acetovanillone; 4-Acetylguaiacol; 4'-Hydroxy 3'-methoxyacetophenone; 2-Methoxy 4-acetylphenol

Substance class: Aldehydes & Ketones

Subgroup 1: Ketones

Solubility: soluble in 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

Source: synthetic

Long-term storage conditions: 15-25 °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
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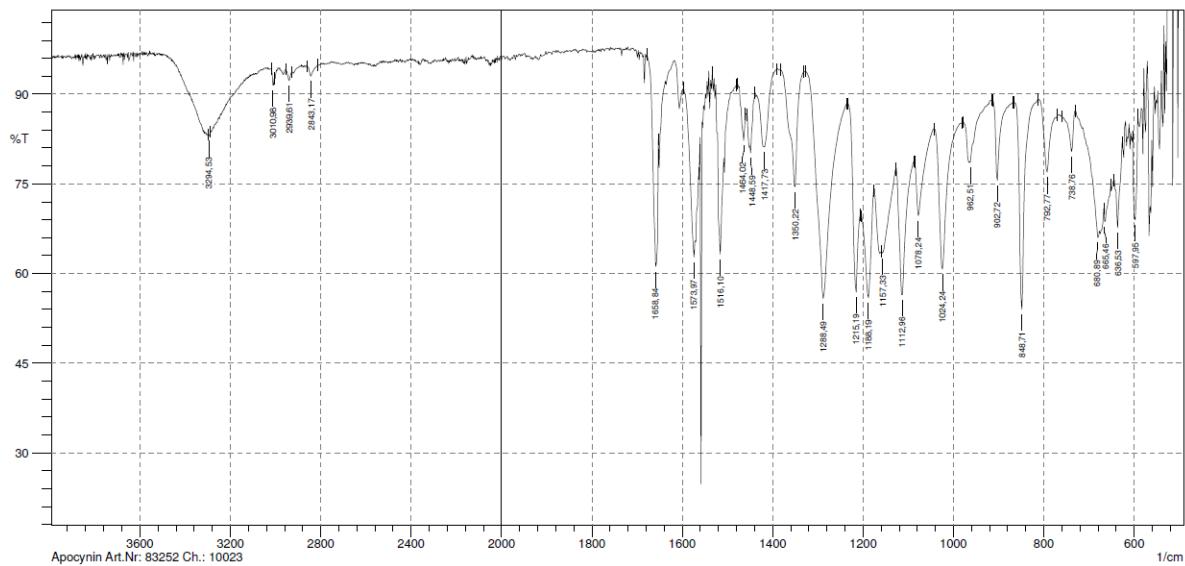
Supplements

Apocynin
Product # 83252

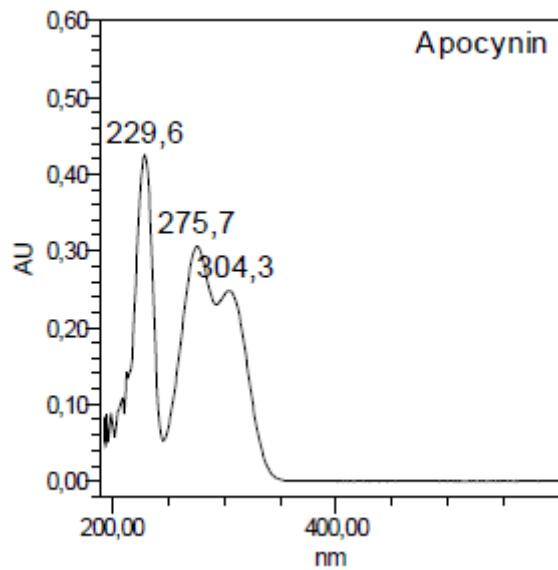
Batch # 10023

Identity tests:

IR spectrum

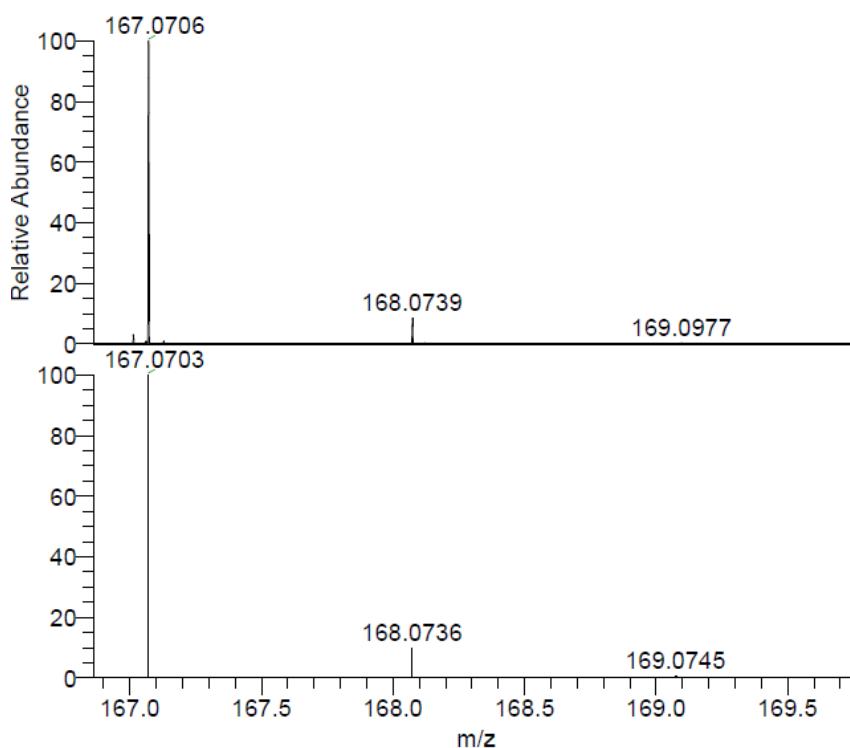


UV spectrum (derived from HPLC/PDA)



**MS spectrum (ESI)**

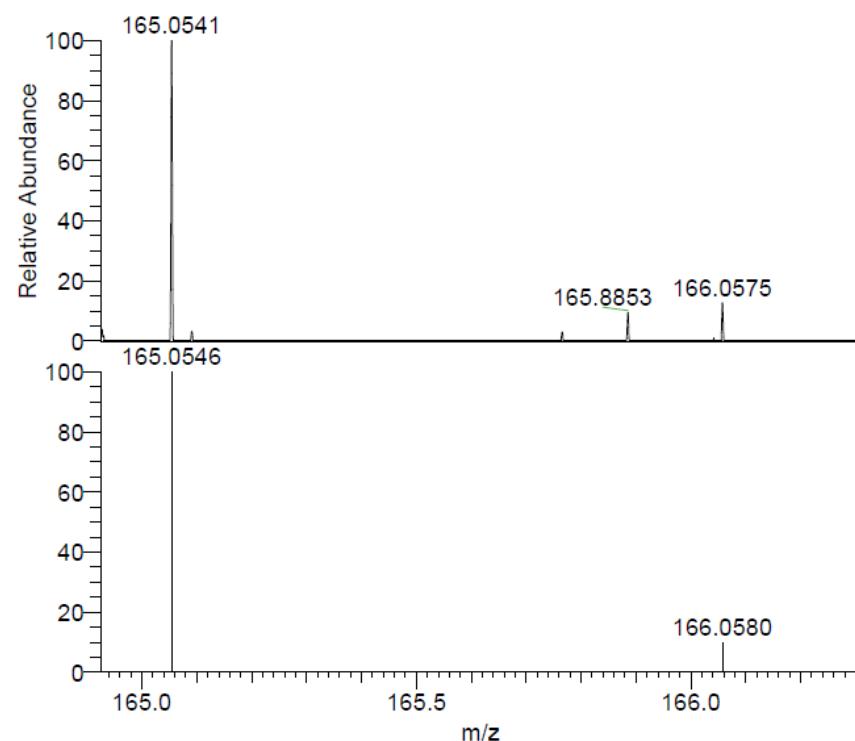
Detection: positive mode (compared with predicted spectrum)



NL:
9.33E4
201119_006#930 RT: 9.69
AV: 1 SB: 171 7.72-8.47 ,
10.12-11.16 T: FTMS {1,1} +
p ESI Full ms
[100.00-1500.00]

NL:
9.00E5
 $C_9 H_{11} O_3$:
 $C_9 H_{11} O_3$
pa Chrg 1

Detection: negative mode (compared with predicted spectrum)



NL:
3.08E3
201119_007#858 RT: 9.78
AV: 1 SB: 158 7.72-8.46 ,
10.12-11.16 T: FTMS {1,1} -
p ESI Full ms
[100.00-1500.00]

NL:
9.00E5
 $C_9 H_9 O_3$:
 $C_9 H_9 O_3$
pa Chrg 1



NMR spectra

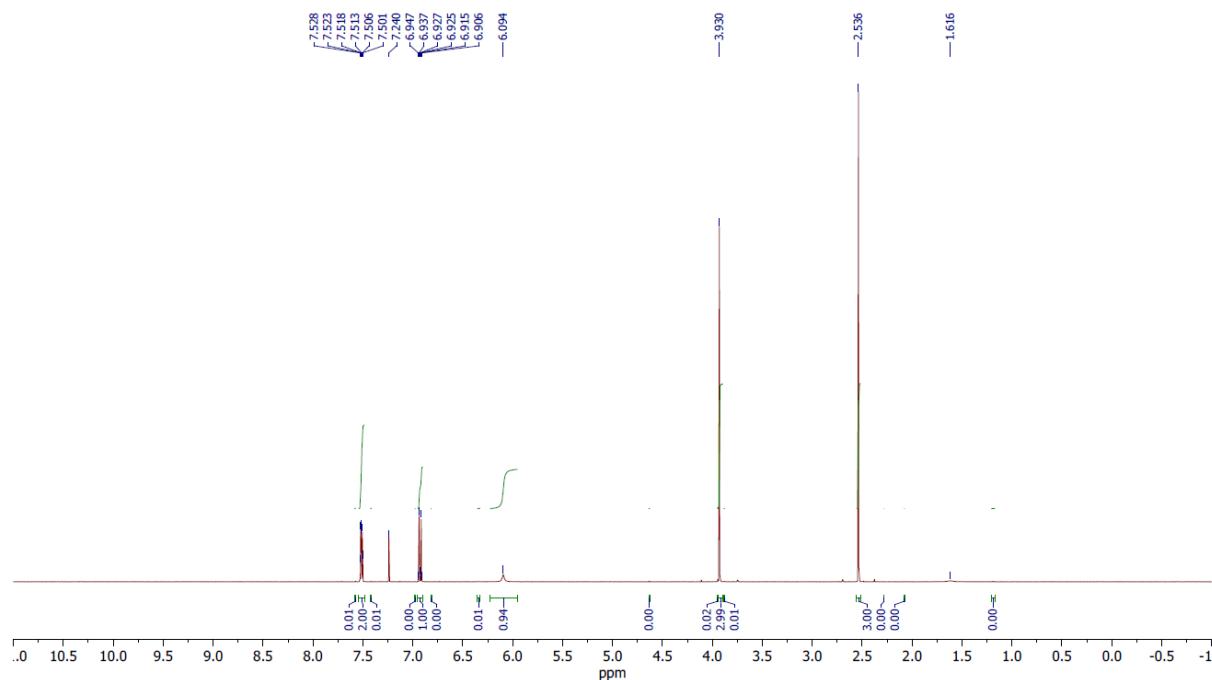
¹H-NMR

PhytoLab GmbH & Co. KG
Apocynin, Charge: 10023
10.3 mg ad 0.7 ml CDCl₃

400 MHz ¹H-NMR, Agilent MR400



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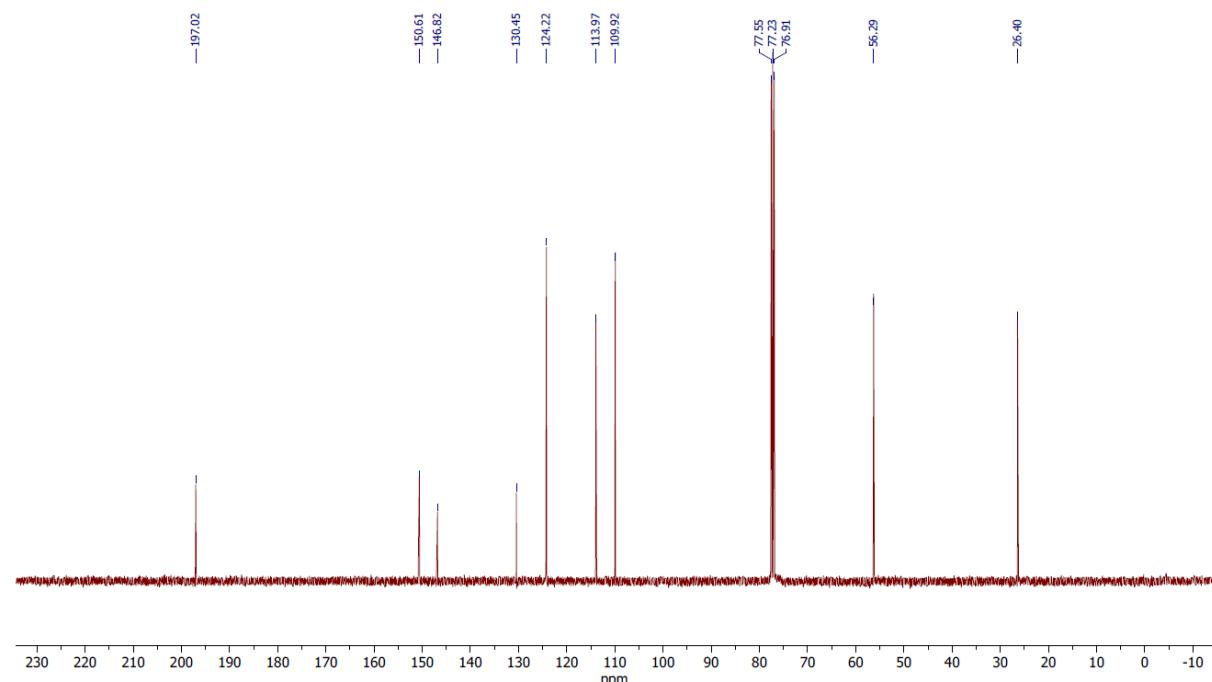
¹³C-NMR

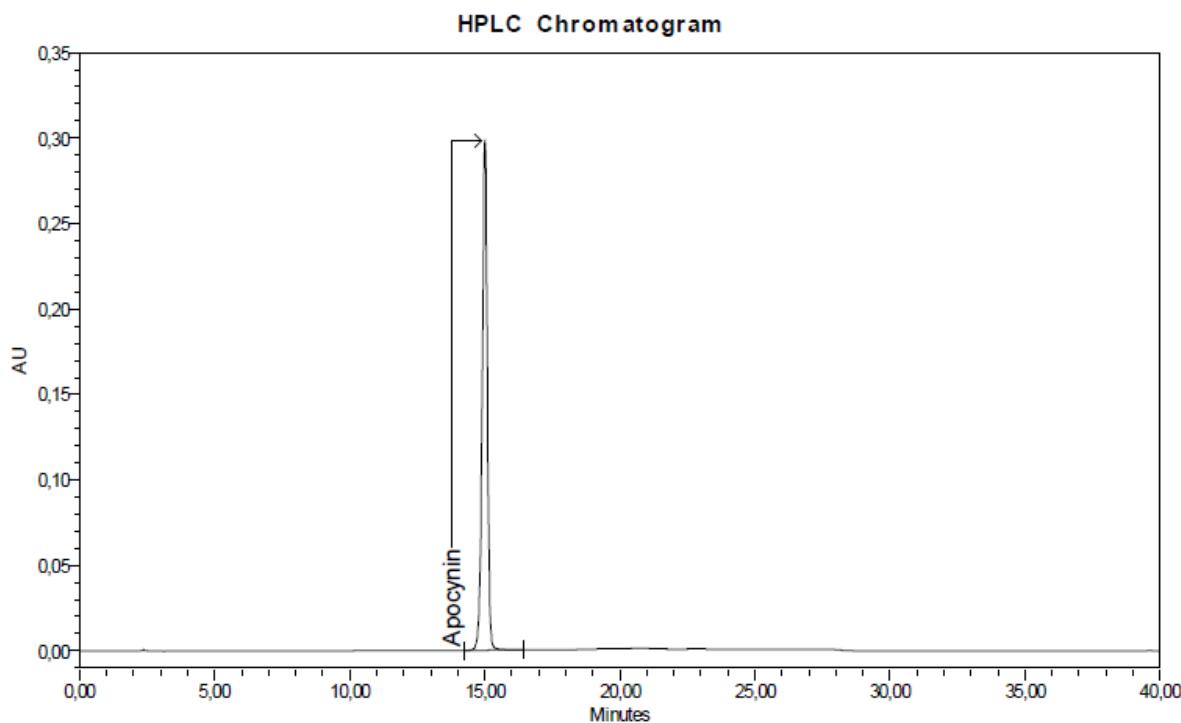
PhytoLab GmbH & Co. KG
Apocynin, Charge: 10023
10.3 mg ad 0.7 ml CDCl₃

100 MHz ¹³C-NMR, Agilent MR400



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Chromatographic purity:**Peak Results**

	Name	RT	Area	% Area
1	Apocynin	15,003	3918040	100,00
Sum				100,00

Analytical conditions

Column: LiChrospher 100 RP-18, 250 x 4.0 mm, 5 µm

Mobile Phase: eluent A: 1% Acetic acid

eluent B: CH₃OH

Mode: gradient

Time [min]	Eluent A [%]	Eluent B [%]
0	85	15
20	40	60
25	40	60
27	85	15
40	85	15

Flow: 1.0 ml/min

Injection Volume: 20 µl

Column Temperature: 25 °C

Sample concentration: approx. 5.3 mg/100 ml

Sample preparation: dissolved in 80% CH₃OH

Detection: UV, 276 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.