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Certificate of analysis

Article:	89626 Delphinidin 3,5-diglucoside chloride
Certificate # / Lot Number:	104581
Material batch:	14877
Sample-ID:	41724
End of analysis:	02/2023
Expiry date:	12/2028

Test	Unit	Specified value	Testresult
Appearance, SOP 100005		powder	conform
Color, SOP 100006		dark red - black	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
Water content, (micro determination, coulometric titration), Ph.Eur. 10.0., 2.5.32, SOP 304291 Vers. 2018-01: Mean value	%		5.9
Anthocyanidins (HPLC), multi-method, SOP 442160: Delphinidin 3,5-diglucoside chloride	%	≥ 95.00	98.85

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Test	Unit	Specified value	Testresult
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)			<0.050
Chloride (argentometric titration), No. 400897 (double analysis, outsourced) Mean value	%		0.58
Content, SOP 890002, calculated in (%): (100 - water - residual solvents - inorganic impurities - counterion) x chromatographic purity / 100. For detailed information refer to attached data sheet!	%		92

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 calcula-

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tion 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.

Vestenbergsgreuth, 04/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.

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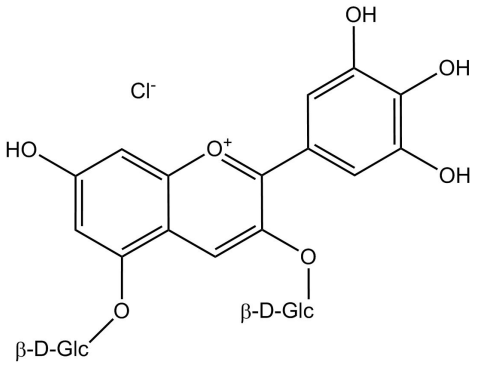
Product Data Sheet

Delphinidin 3,5-diglucoside chloride



Product #: 89626

Physicochemical Data

CAS #:	17670-06-3
Molecular formula:	C27H31O17Cl
Molecular weight [g/mol]:	662.99
Synonyms:	Awobanin A chloride, Delphin chloride
Substance class:	Flavonoids
Subgroup 1:	Anthocyanidins
Subgroup 2:	Anthocyans
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

Please note:	The counterion is determined quantitatively and treated as an impurity in the calculation of the absolute purity of this reference substance. The assigned absolute purity on the certificate of analysis of this reference standard, therefore, refers to the pure delphinidin 3,5-diglucoside.
Handling instructions:	Dissolve preferably in methanol acidified with 0.01% HCl and warm up. In the case of a low chloride content, the solubility decreases accordingly.
Source:	botanical origin
Long-term storage conditions:	< -15 °C

Manufacturer:
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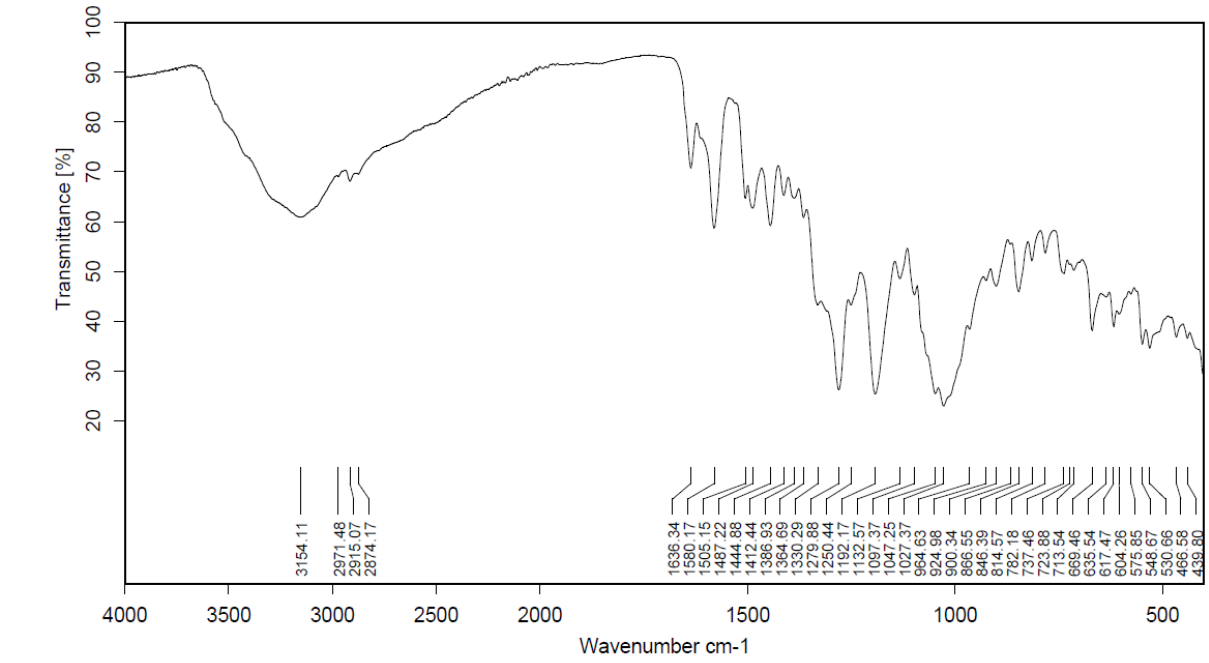
Supplements

Delphinidin 3,5-diglucoside chloride **Batch # 14877**
Product # 89626

Identity tests:

IR spectrum



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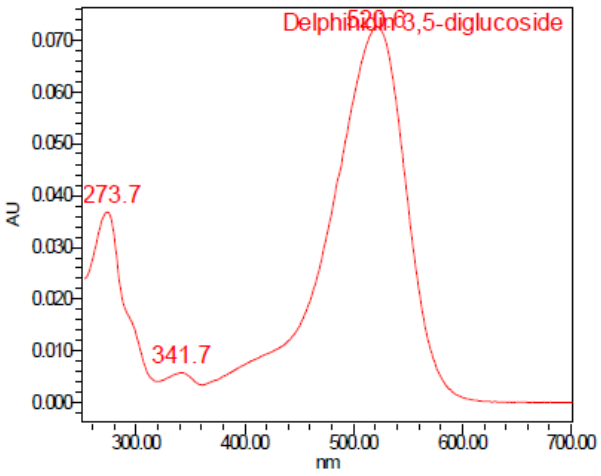
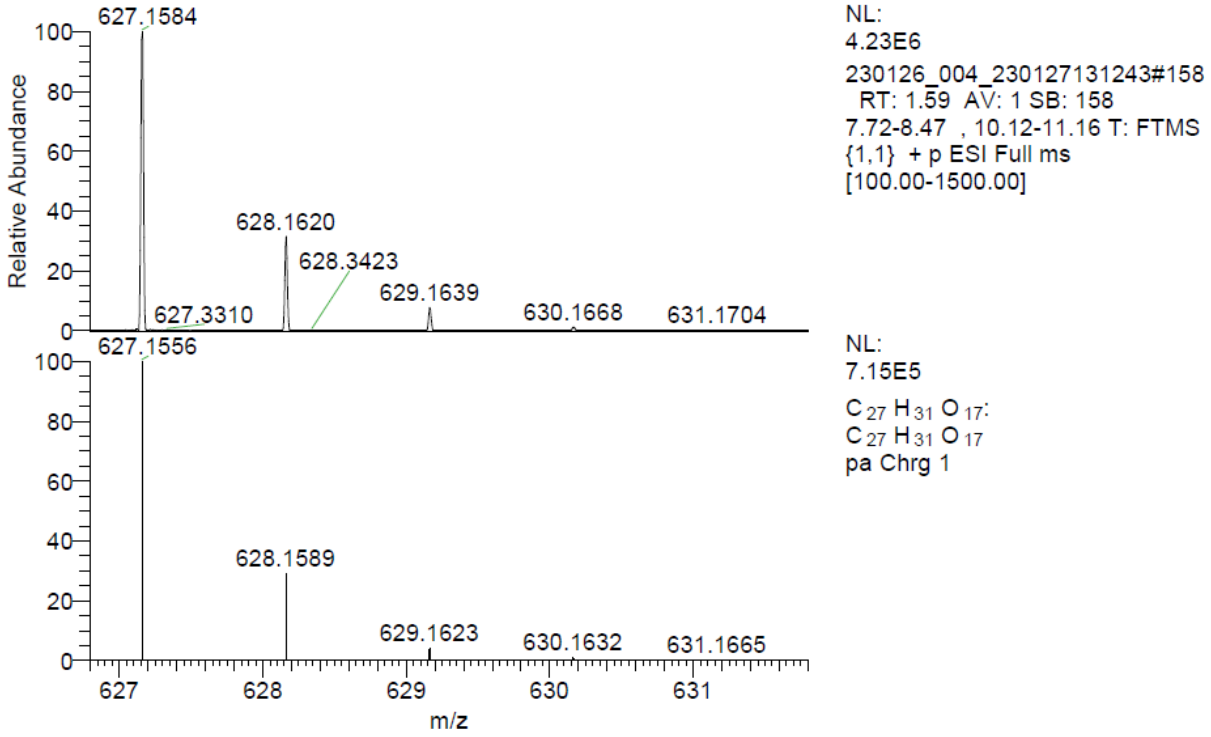
UV spectrum (derived from HPLC/PDA)



MS spectrum (ESI)

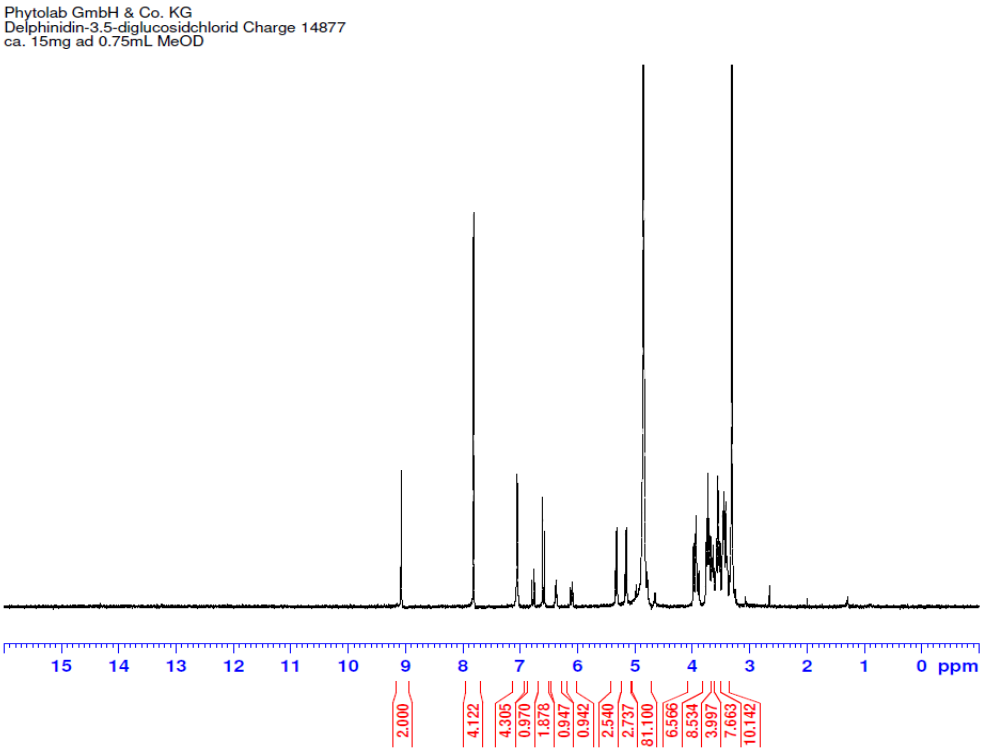
Detection: positive mode (compared with predicted spectrum)



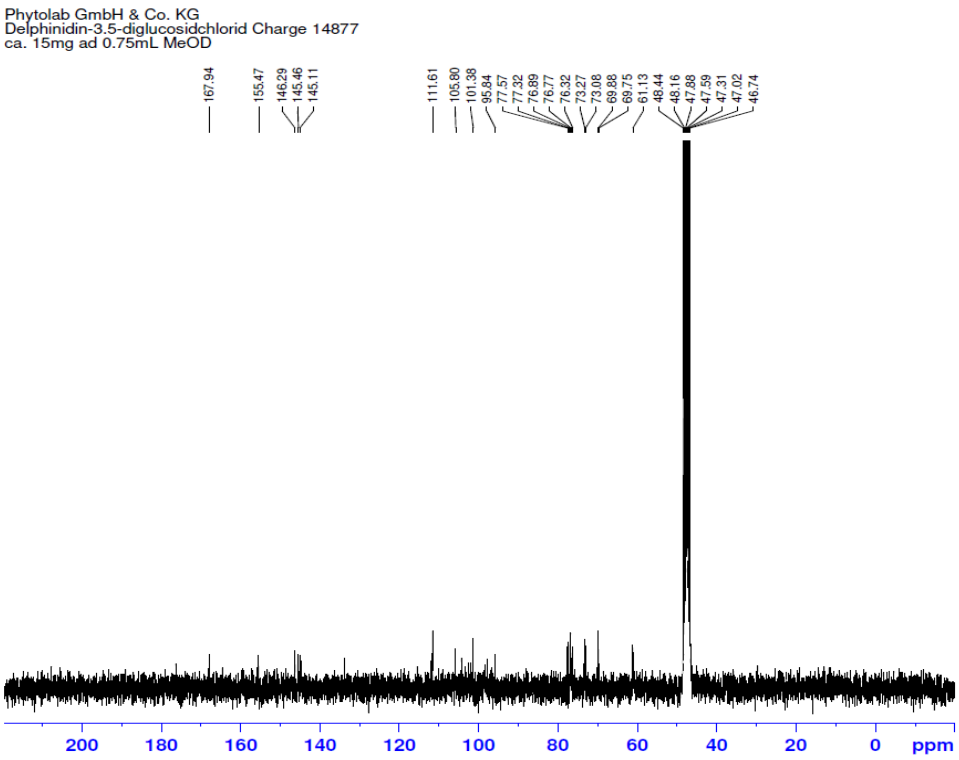
Detection: negative mode (compared with predicted spectrum)

NMR spectra

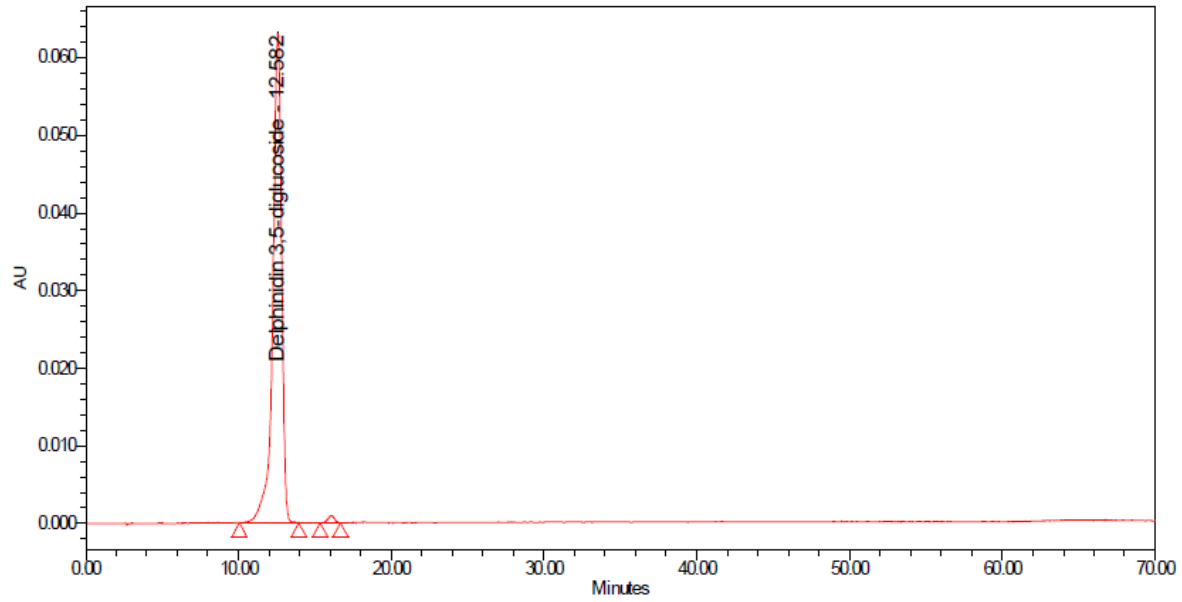
^{1}H-NMR



^{13}C-NMR



Chromatographic purity:



Peak Results

	Name	RT	Area	Height	Chromatographic_Purity	Amount	Units
1	Delphinidin 3,5-diglucoside	12.582	2521278	63186	98.88	5.100	mg/100mL
2		16.090	28648	907	1.12		

Analytical conditions

Column: Xterra MS C18, 250 x 4.6 mm, 5 µm
Mobile Phase: eluent A: H_2O/ HCOOH (90/10 V/V)
eluent B: CH_3OH/ CH_3CN/ H_2O/ HCOOH (22.5/22.5/40/10 V/V/V/V)
Mode: gradient

Time [min]	Eluent A [%]	Eluent B [%]
0	93	7
35	73	27
45	35	65
46	0	100
50	0	100
53	93	7
70	93	7

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 CH_3OH/HCl (98/2 V/V) and diluted aqua.H_3PO_4
Detection: UV, 513 nm
Special note: aqua. H_3PO_4: 13.45 ml H_3PO_4 + 177 ml H_2O

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.