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

Certificate of analysis

Article: 83881 Oleacein
Certificate # / Lot Number: 248823

Material batch: 1001379
Sample-ID: 166826
End of analysis: 08/2024
Expiry date: 04/2027

Test	Unit	Specified value	Testresult
Appearance, SOP 100005		viscous	conform
Color, SOP 100006		light yellow - brown	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
Oleacein (HPLC), method 2 (%AU), SOP 441668	%	≥ 90.00	98.28

Certificate of analysis

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Test	Unit	Specified value	Testresult
Peakpurity, (HPLC), SOP 401367		conform	conform

Vestenbergsgreuth, 22/Apr/2025

Sibylle Friess

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

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Material batch: 1001379

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.

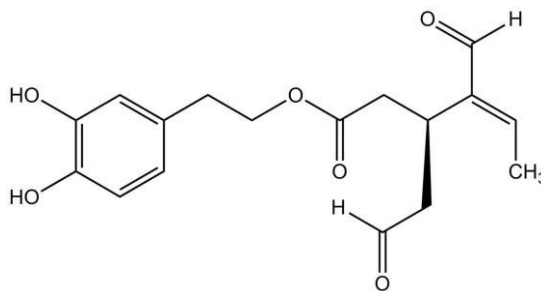
Product Data Sheet

Oleacein

Product #: 83881

Physicochemical Data

CAS #:	149183-75-5
Molecular formula:	C ₁₇ H ₂₀ O ₆
Molecular weight [g/mol]:	320.34
Substance class:	Aldehydes & Ketones
Subgroup 1:	Aldehydes
Solubility:	soluble in chloroform and ethanol 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:	Packed under nitrogen. Recommended to be stored under inert atmosphere. Avoid exposure to oxygen.
Handling instructions:	Recommended to be used for qualitative purposes due to its instability. The compound is an oily liquid and not very stable in aqueous or methanolic solutions. For HPLC a derivatization method with 2,4-DNPH was used. LC/MS investigations proved the integrated substance peaks to be E/Z isomers. The exact weight is given on the label of the vial. In order to produce a stock solution of known concentration please transfer the contents of the vial quantitatively into a volumetric flask by repeated rinsing with excess solvent and fill to the mark.
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 Shop: https://phyproof.phytolab.com



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Supplements

Oleacein
Product # 83881

Batch # 1001379

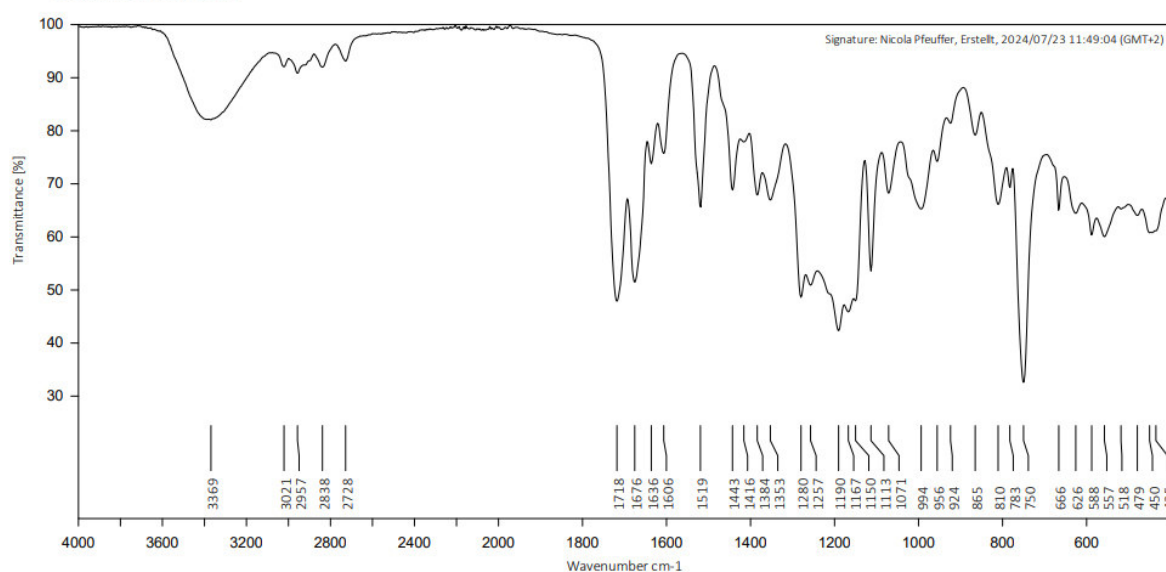
Identity tests:

IR spectrum

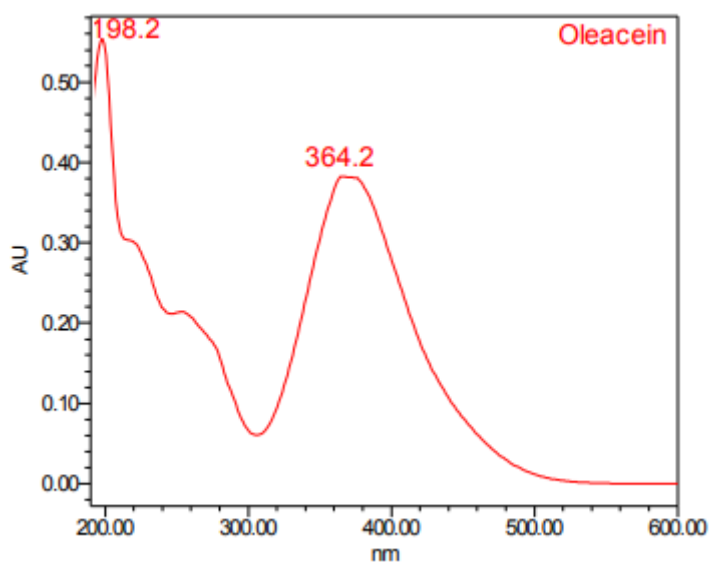


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83881_Oleacein_1001379



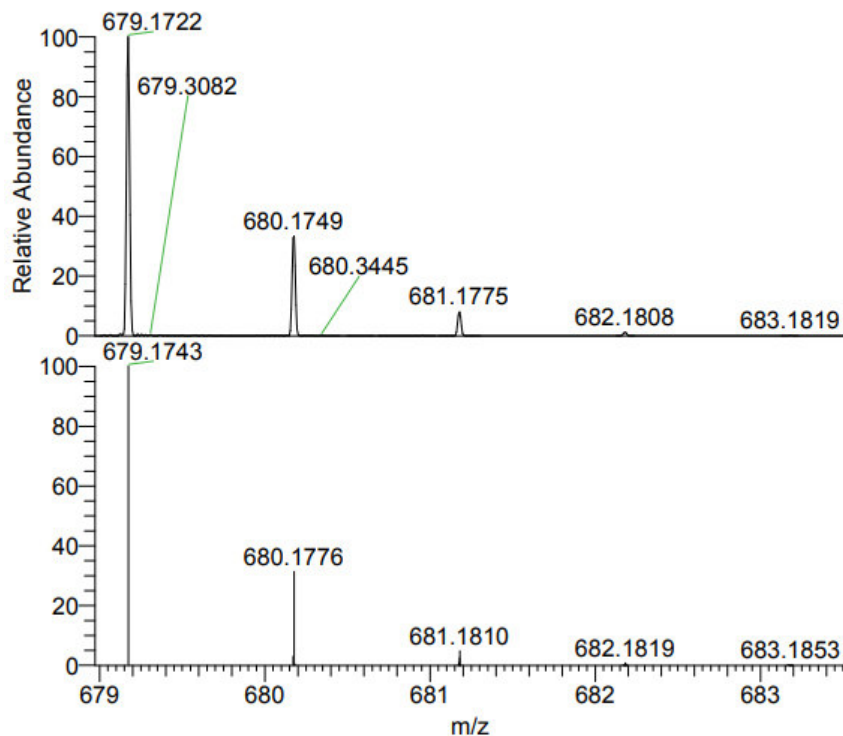
UV spectrum (derived from HPLC/PDA)





MS spectrum (ESI)

Detection: negative mode (compared with predicted spectrum)



NL:
7.55E6
240807_011#1227 RT: 13.93
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:
6.88E5
C₂₉ H₂₇ N₈ O₁₂:
C₂₉ H₂₇ N₈ O₁₂
pa Chrg 1



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NMR spectra

¹H-NMR

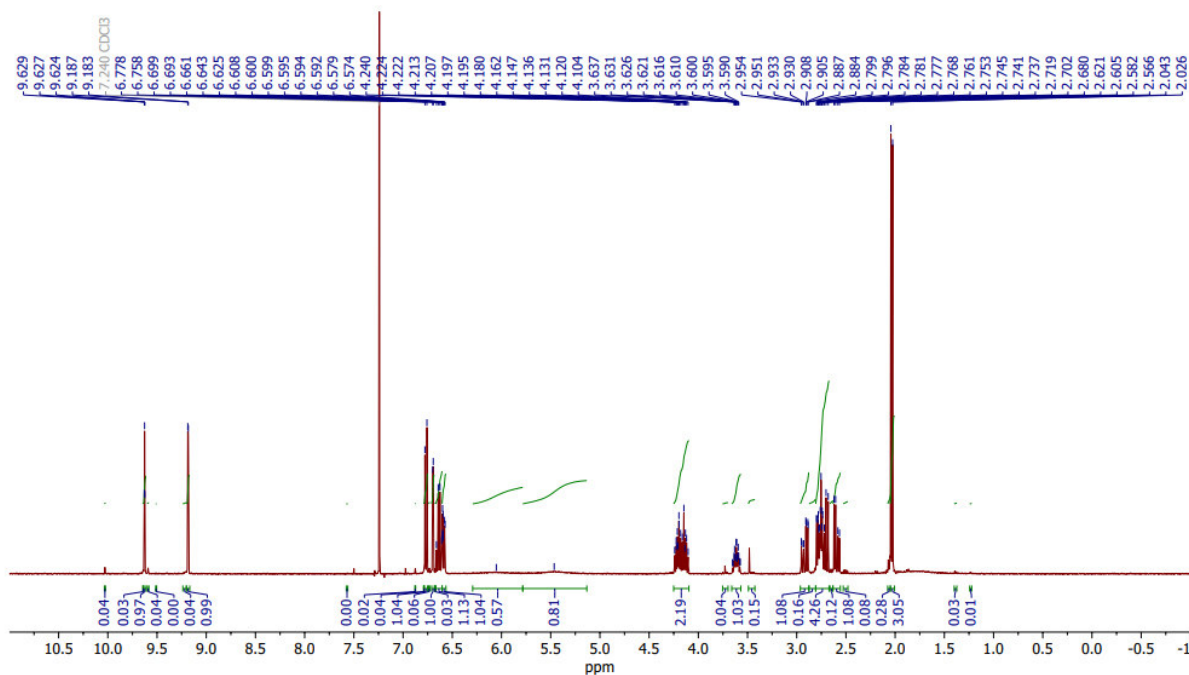
PhytoLab GmbH & Co. KG
Oleacein, Charge: 1001379
10.9 mg ad 0.7 ml CDCl₃

400 MHz ¹H-NMR, Agilent MR400



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¹³C-NMR

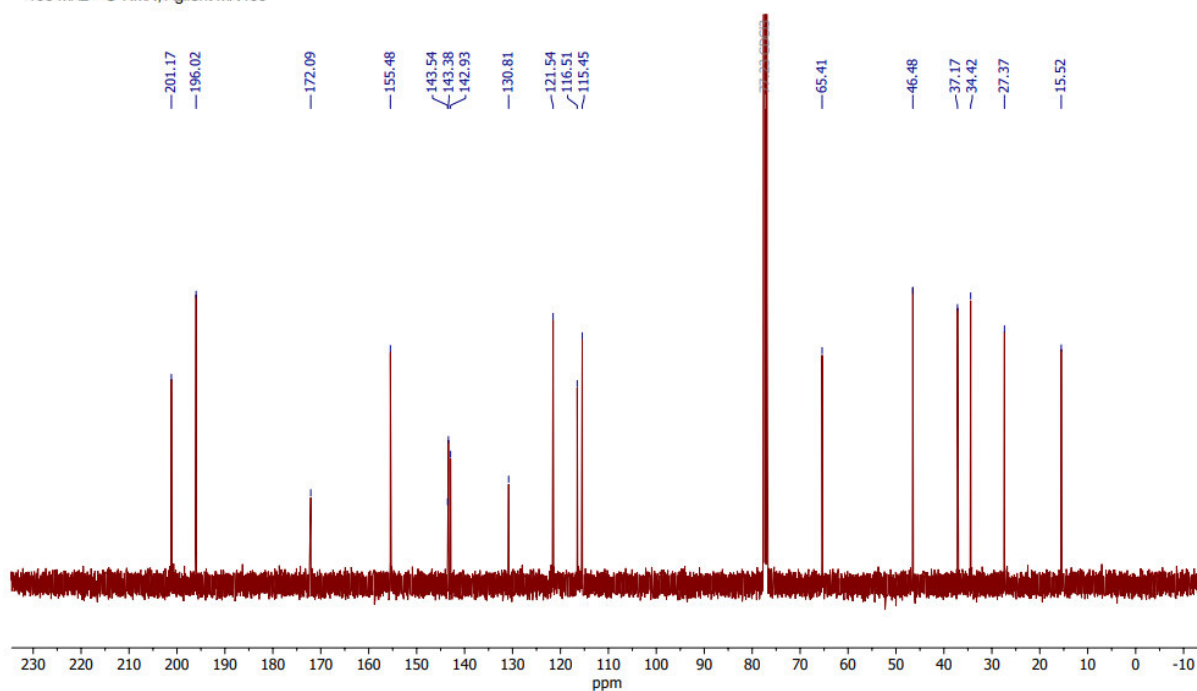
PhytoLab GmbH & Co. KG
Oleacein, Charge: 1001379
10.9 mg ad 0.7 ml CDCl₃

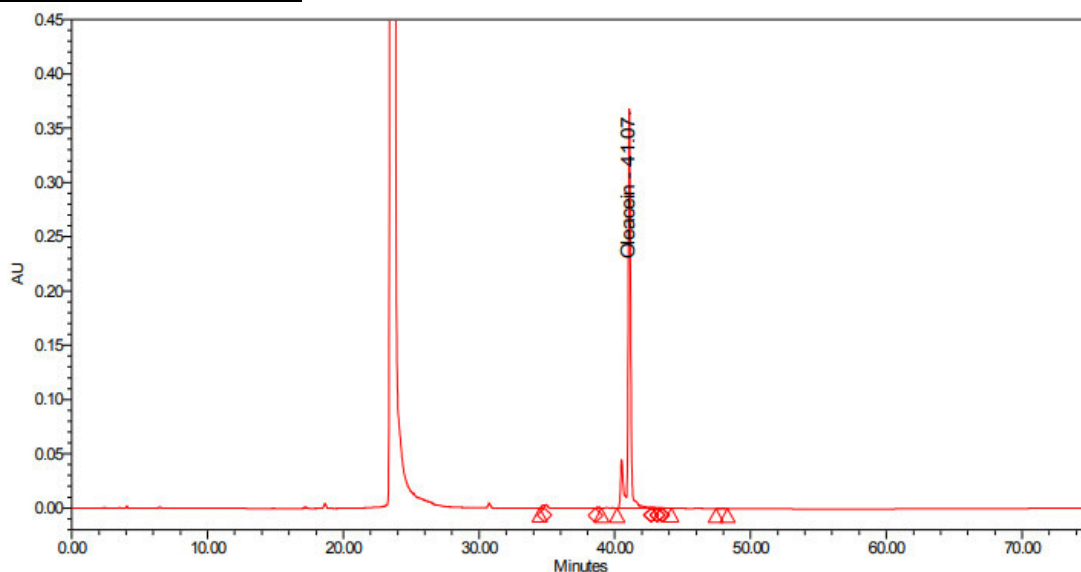
100 MHz ¹³C-NMR, Agilent MR400



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Chromatographic purity:**Peak Results**

	Name	RT	Area	Height	Chromatographic_Purity	% Area	Amount	Units	Manual
1		34.702	32775	2744	0.62	0.62			Yes
2		38.789	16981	1254	0.32	0.32			Yes
3	Oleacein	41.074	5166205	369988	98.28	98.28	5.240	mg/100ml	Yes
4		42.823	20409	942	0.39	0.39			Yes
5		43.184	9800	555	0.19	0.19			Yes
6		43.483	5259	336	0.10	0.10			Yes
7		47.889	5048	242	0.10	0.10			Yes

Analytical conditions

Column: Luna C18, 250x4,6mm, 5µm

Mobile Phase: eluent A: H₂O

eluent B: CH₃CN

Mode: gradient

Time [min]	Eluent A [%]	Eluent B [%]
0	100	0
50	5	95
60	5	95
65	100	0
75	100	0

Flow: 1.0 ml/min

Injection Volume: 20 µl

Column Temperature: 40 °C

Sample concentration: approx. 5.2 mg/100 ml

Sample preparation: dissolved in derivatization reagent (500 mg 2,4-DNPH in 100 mL CH₃CN + 0.1 mL formic acid, dissolve substance in reagent and stir 1 h at room temperature)

Detection: UV, 360 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.