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Certificate of analysis

Article: 84196 Carboxyatractyloside
 Material batch: 14765
 Sample-ID: 279505
 End of analysis: 08/2025
 Expiry date: 08/2026

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 (IR-spectroscopy, Ph.Eur. 10.3, 2.2.24 / USP43 NF37 <197>), 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 analysis) Mean value	%		9.7
Carboxyatractyloside (HPLC), method 1 (% AU), SOP 441844	%	≥ 90.00	98.46
Peakpurity, (HPLC), SOP 401367		conform	conform

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Test	Unit	Specified value	Testresult
Inorganic impurities, (ICP-MS), for reference substances, SOP 811701:	%		<0.1
Calcium			
Potassium	%		21.4
Magnesium	%		<0.1
Sulfur	%		5.4
Sodium	%		<0.1
Phosphorus	%		3.7
Aluminium	%		<0.1
Residual solvents, (headspace-GC), SOP 805765:	%		
Residual solvents (LOQ: 0.050)			<0.050
Phosphate (calculated from the Phosphor content as determined during ICP-MS), SOP 811702	%		11.44
Content, SOP 890002, calculated in (%): (100 - water - residual solvents - inorganic impurities - counterion) x chromatographic purity / 100. For detailed information refer to attached data sheet!	%		57

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.

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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.

The literature describes carboxyatractyloside predominantly as the dipotassium salt (CAS #33286-30-5) and not as the free carboxyatractylic acid (CAS # 77228-71-8). We adopted the description of this reference substance from the scientific literature; however, we consider potassium and other inorganic elements (except sulfur that is part of the molecule itself) to be impurities in the calculation of the absolute purity (SOP 890002). The content value given as the result of SOP 890002, therefore, refers to the free carboxyatractylic acid.

If quantitative data are to be given as carboxyatractyloside dipotassium salt, the absolute purity value (SOP 890002) would have to be multiplied by the factor resulting from the ratio of the molecular weights of carboxyatractyloside dipotassium salt ($C_{31}H_{44}O_{18}S_2K_2$; 847.00 g/mol) and carboxyatractylic acid ($C_{31}H_{46}O_{18}S_2$; 770.82 g/mol). Please make sure you are using the correct purity value in your calculation. We found hints that there may have been confusion in the literature between atractyloside (article 84195) and 4'-desulfocarboxyatractylic acid (article 85734). 4'-Desulfocarboxyatractylic acid is a derivative of carboxyatractyloside (article 84196).

Vestenbergsgreuth, 27/Aug/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.

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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.