

Analytical information

Name: Quality Controlled standard of 13,19-didesmethyl Spirolide C

Code: 00-13,19-didesMeC

Batch: 20-001

General description:

Product Specification	
MOLECULAR FORMULA:	C ₄₁ H ₆₀ NO ₇
MOLECULAR WEIGHT:	678.4364
MONOISOTOPIC MW	678.9171
CAS NUMBER:	908118-02-5
SOURCE/HOST:	Cultures of <i>Alexandrium ostenfeldii</i>
CONCENTRATION:	(7.53 ± 0.57) µg/mL [†]
PURITY:	≥ 95 % [‡]
FORMULATION:	Liquid. In methanol with TFA 0.05% v/v
SHIPPING:	SHIPPED ON ICE
LONG TERM STORAGE:	-20 °C
HAZARD:	See MSDS.

[†] 20-001 batch concentration of 13,19-didesmethyl Spirolide C was settled by UPLC MS/MS versus 13-desmethyl spirolide C calibration curve where the assumption of an equal response factor for toxin quantification was performed.

[‡] 13,19-didesmethyl Spirolide C was purified via preparative cromatography from batch cultures of the dinoflagellate *Alexandrium ostenfeldii*. Analytical UPLC-MS/MS were used to quantify and check purity.

Instructions for proper handling use: 00-13,19-didesMeC is presented in amber argon-filled glass sealed ampoules. This material contains toxic material, and should be handled with care. Read MSDS before using. Material Safety Data sheet for information regarding 00-13,19-didesMeC enclosed in the package. Use proper disposal methods.

Before opening an ampoule it must be guaranteed that the content is a liquid and properly mixed to ensure homogeneity. Sample aliquots for analysis should be withdrawn at 15 °C to 25 °C immediately after opening the ampoules and should be processed without delay for the certified value to be valid within the stated uncertainty. Ampoule should not remain open longer than few minutes due to solvent volatility and air contamination.

Instructions for appropriate conditions of storage: The original ampoule should be stored at temperatures below/at -20 °C (freezer) until use. Unopened ampoules should be stored upright under normal laboratory conditions inside the original container supplied.

Property values:

Date of analysis:	August, 21 st 2020
Concentration of <u>13,19-didesmethyl Spirolide C</u> in methanol with 0.05% Trifluoroacetic acid solution	(7.53 ± 0.57) µg / mL

Estimated uncertainty corresponds to a level of confidence in terms of one standard deviation.

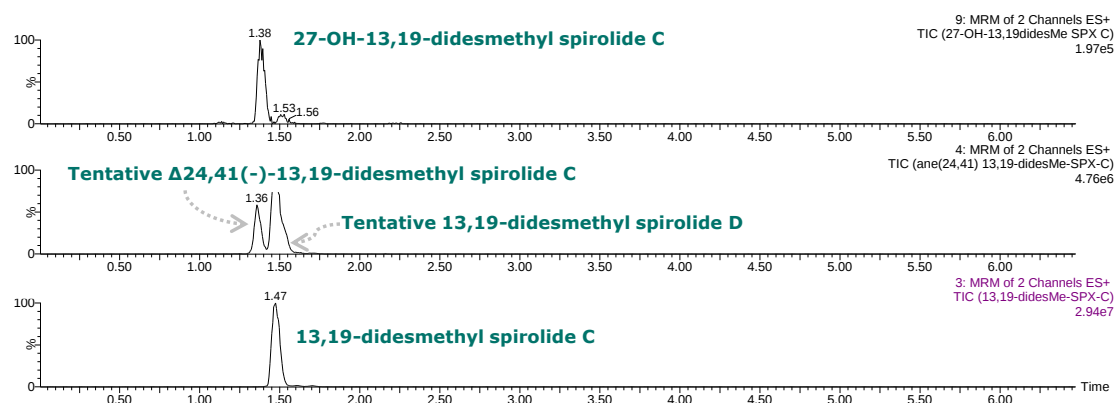


Figure 1. Analysis of the 00-13,19-didesMeC solution by UPLC-MS/MS.. Conditions: ACQUITY UPLC BEH C18 1.7 μ m, 100x2.1 mm, UPLC column. Elution conditions, gradient mode with mobile phases: (A) Water and (B) Aqueous 95% acetonitrile, both with 2mM ammonium formate and 50mM formic acid; Gradient: 0 min 30% B; 3.0 min 90% B; 4.5 min 90% B; 4.6 min 30% B; 6.5 min 30% B; flow rate: 0.40 mL/min. Temperature: 30°C. MS detector: Waters XEVO TQ using the typical MRM transitions of spiroside toxin group found in the bibliography.

Table 1. Impurities content[†] in Quality Controlled standard of 00-13,19-didesMeC, batch 20-001.

Compound	rt / min	Relative %	$\mu\text{g/mL}^{\dagger}$
Tentative $\Delta^{24,41}(-)$ -13,19-didesmethyl spiroside C	1.36	2.9 %	0.23 ± 0.02
27-OH-13,19-didesmethyl spiroside C	1.38	0.3 %	0.02 ± 0.01
Tentative 13,19-didesmethyl spiroside D	1.54	1.3 %	0.10 ± 0.01

[†] Impurities batch concentration was settled by UPLC MS/MS versus 13-desmethyl spiroside C calibration curve where the assumption of an equal response factor for toxin quantification was performed.

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This Analytical Information is only valid if the product was obtained directly from Laboratorio CIFGA S.A. or one of our authorized distributors.

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