

BDG SYNTHESIS

Certificate of Analysis

BDG Synthesis certifies that this reference material meets or exceeds the specifications stated herein.

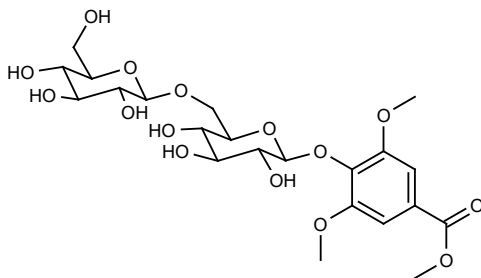
Neil Beare

Neil Beare, PhD, Director
23 November 2020

Name: Leptosperin

CAS Number: 1431845-42-9

Structure:



Molecular Weight: $C_{22}H_{32}O_{15} = 536.48$

Lot Number: BDG 11870

Appearance: White, crystalline solid

Corrected Purity: 99.7 % (HPLC) - 0.3 % (methanol) - 3.3 % (water) = 96.2 %

Re-test Date: 23 November 2021

Storage and Handling:

Temperature:	refrigerate for prolonged storage; may be handled and shipped at ambient temperature.
Humidity:	not believed to be hygroscopic; may be handled in normal laboratory atmosphere.
Light:	protect from strong sunlight.
Caution:	only experienced laboratory personnel should handle the material.

Identity and Purity

Proton NMR Spectrum

Identity: the signals are consistent with the proposed structure and in accord with literature where available.

Residual Solvents: a small amount of methanol (0.3 % w/w) is observed.

Impurities: a trace of an unidentified impurity is seen in the baseline.

Carbon-13 NMR Spectrum

Identity: the signals are consistent with the proposed structure and in accord with literature where available.

High-resolution Mass Spectrum (TOF MS ES+)

Found m/z 559.1638. $C_{22}H_{32}O_{15}Na$ $[M+Na]^+$ requires m/z 559.1639. The deviation of 0.2 ppm is within normally accepted limits for the establishment of identity by HRMS.

HPLC

A sharp, symmetrical peak is observed (99.7 %). Note: in the absence of reference materials for preparing calibration curves, it is assumed that all peaks have the same detector response. Where possible, the conditions of analysis follow a pharmacopeial or literature method, or have been adapted from same.

Elemental Analysis

	Found:	C 47.59, H 6.04 %
$C_{22}H_{32}O_{15} \cdot 1.0H_2O$	Requires:	C 47.65, H 6.18 %, H_2O 3.25 %
$C_{22}H_{32}O_{15}$	Requires:	C 49.25, H 6.01 %

The elemental analyses fall somewhat outside those expected for anhydrous material; the presence of water is reasonably expected from the method of purification and/or the type of material, and the "best-fit" hydrated molecular formula is given. In the absence of a Karl-Fischer water analysis, we recommend that the "best-fit" water content be used when determining corrected purity.

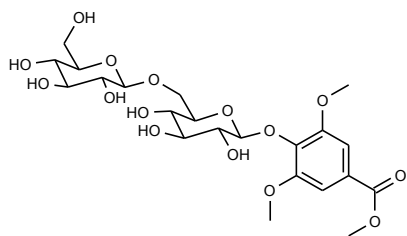
The available quantity of custom-synthesised material is always small, and this limits the extent and type of analytical data which can be obtained. This Certificate is presented in descriptive format for use by analytical chemists who are trained in the use of custom-synthesised materials. Custom materials often contain higher levels of residual solvents and/or water, and we urge you to use the corrected purity where needed rather than the raw HPLC purity. This compound is intended for use as an analytical reference material and it is not for human administration. Structures are shown with relative stereochemistry unless otherwise specified.

The re-test date is assigned from experience gained with the material in the laboratory and/or on storage. It is not possible to perform formal storage studies because of the small amount of material available.

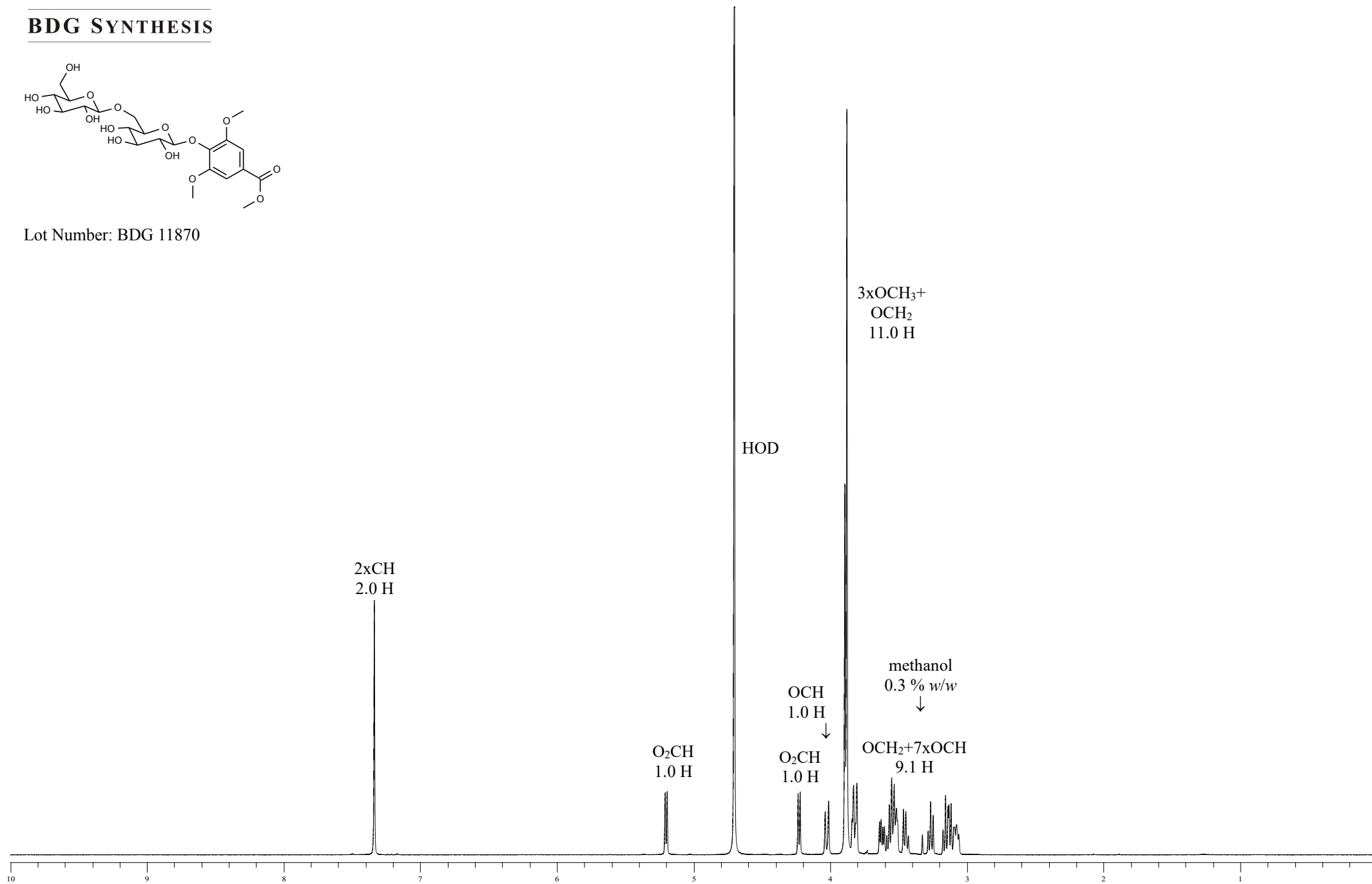


Proton NMR Spectrum of Leptosperin in D₂O

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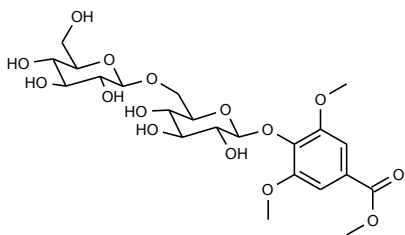
Lot Number: BDG 11870





Carbon-13 NMR Spectrum of Leptosperin in Methanol-d₄

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Lot Number: BDG 11870

