

BDG SYNTHESIS

Certificate of Analysis

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

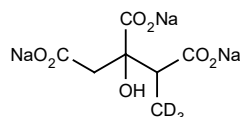
Neil Beare

Neil Beare, PhD, Director
24 September 2018

Name: Trisodium 2-methylcitrate-d₃

CAS Number: 117041-96-0 (unlabelled)

Structure:



Molecular Weight: C₇H₄D₃Na₃O₇ = 275.11

Lot Number: BDG 15987.3

Appearance: White, crystalline solid

Purity By HPLC: 97.3 %

Isotopic Purity: Under 0.5 % d₀

Re-test Date: 24 September 2023

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. Two sets of signals are observed due to the presence of diastereomers.

Isotopic Labelling: the signal at the site of deuteration is absent, compared with what would be expected for unlabelled material, indicating clean deuteration.

Residual Solvents: a trace (under 0.1 % w/w) of ethanol is observed.

Impurities: traces of unidentified impurities are seen in the baseline.

Carbon-13 NMR Spectrum

Identity: the signals are consistent with the proposed structure and in accord with literature where available. Two sets of signals are observed due to the presence of diastereomers.

Isotopic Labelling: the signal at the site of deuteration has collapsed to a small multiplet compared with what would be expected for unlabelled material, indicating clean deuteration.

High-resolution Mass Spectrum (TOF MS ES-)

Found m/z 208.0529. $C_7H_6D_3O_7 [M-3Na+2H]^-$ requires m/z 208.0537. The deviation of 3.8 ppm is within normally accepted limits for the establishment of identity by HRMS. No signal for d_0 material was seen (detection limit about 0.5 %).

HPLC

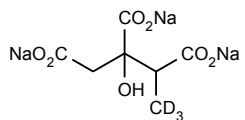
Two somewhat broadened, slightly asymmetrical peaks are observed (combined total = 97.3 %). These two peaks are observed due to the presence of diastereomers. Note: in the absence of reference materials for preparing calibration curves, it is assumed that all peaks have the same detector response. Where possible, the conditions of analysis follow a pharmacopoeial or literature method, or have been adapted from same.

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.

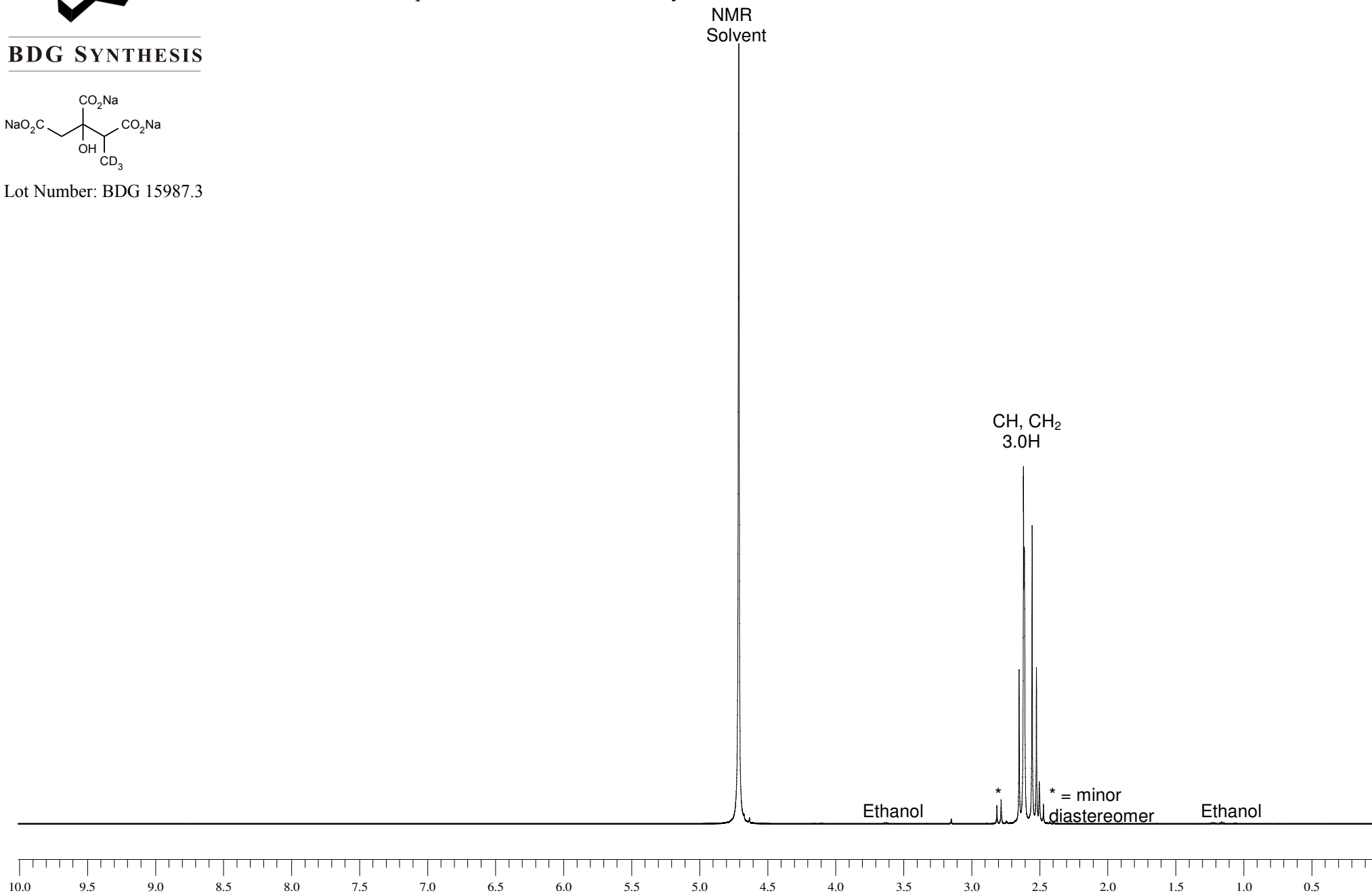


BDG SYNTHESIS



Lot Number: BDG 15987.3

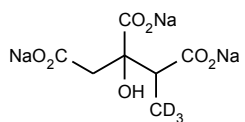
Proton NMR Spectrum of Trisodium 2-methylcitrate-d₃ in D₂O





Carbon-13 NMR Spectrum of Trisodium 2-methylcitrate-d₃ in D₂O

BDG SYNTHESIS



Lot Number: BDG 15987.3

