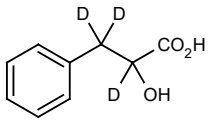
BDG SYNTHESIS

Certificate of Analysis

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

Neil Beare, PhD, Director
14 September 2018

Name:	**3-Phenyllactic acid-d_3**
CAS Number:	828-01-3 (unlabelled)
Structure:	
Molecular Weight:	$C_9H_7D_3O_3$ = 169.19
Lot Number:	BDG 17389.2
Appearance:	White, crystalline solid
Corrected Purity:	98.9 % (HPLC) - 0.2 % (benzene) = 98.7 %
Isotopic Purity:	Under 0.5 % d_0
Re-test Date:	14 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.

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Identity and Purity

Proton NMR Spectrum

Identity: the signals are consistent with the proposed structure and in accord with literature where available.
Isotopic Labelling: signals at the sites of deuteration are greatly diminished, compared with what would be expected for unlabelled material, indicating clean deuteration.
Residual Solvents: a small amount of benzene (0.2 % *w/w*) is observed.
Impurities: no significant impurities are evident in the spectrum.

Carbon-13 NMR Spectrum

Identity: the signals are consistent with the proposed structure and in accord with literature where available.
Isotopic Labelling: signals at the site of deuteration have collapsed to small multiplets compared with what would be expected for unlabelled material, indicating clean deuteration.

High-resolution Mass Spectrum (ESI-)

Found *m/z* 168.0735. $C_9H_6D_3O_3$ $[M-H]^-$ requires *m/z* 168.0740. The deviation of 3.0 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

A sharp, symmetrical peak is observed (98.9 %). 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 63.98, H 4.35, D 3.73 %
$C_9H_7D_3O_3$	Requires:	C 63.89, H 4.17, D 3.57 %

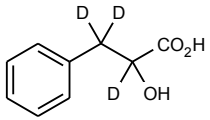
The elemental analyses fall within generally accepted limits for establishing the molecular formula given. The results may also be taken to imply the absence of significant quantities of water or inorganic salts (which have not been elsewhere tested for because of sample size limitations).

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

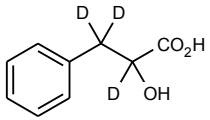
Proton NMR Spectrum of 3-Phenyllactic acid-d_3 in DMSO-d_6



Lot Number: BDG 17389.2

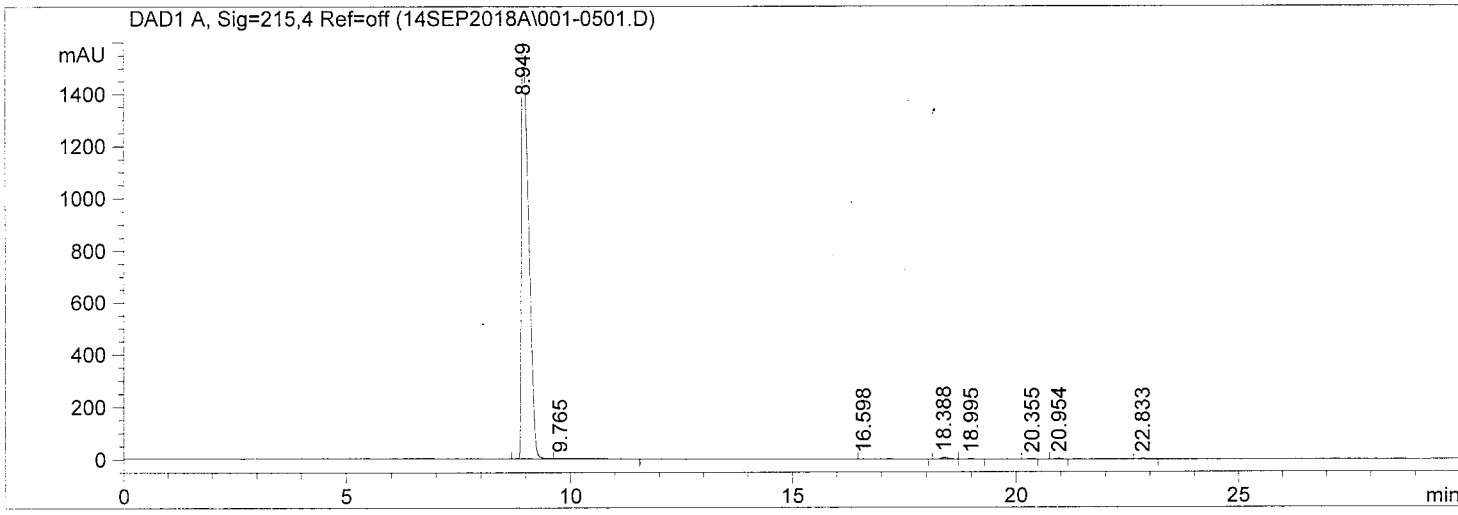
BDG SYNTHESIS

Carbon-13 NMR Spectrum of 3-Phenyllactic acid-d_3 in DMSO-d_6



Lot Number: BDG 17389.2

Injection Date : 9/14/2018 12:44:24 PM Inj : 1
Inj Volume : 10 µl
Acq. Method : C:\CHEM32\1\METHODS\2018\LC20031A.M
Last changed : 9/14/2018 11:23:14 AM by Bruce Hamilton
Analysis Method : C:\CHEM32\1\METHODS\2018\LC20031A.M
Last changed : 9/14/2018 4:57:30 PM by Bruce Hamilton
(modified after loading)
Method Info : BDG - Analysis of 3-Phenyllactic Acid-d3
Column : Phenomenex Luna C18(2) 5 um 250 x 4.6 mm : Guard C18RP 4 x 3 mm
Mobile Phase A: 95:5 20mM K2HPO4 pH=7.00 : Acetonitrile
Mobile Phase B: 70:30 20mM K2HPO4 pH=7.00 : Acetonitrile
Gradient (A:B) : T0=100:0, T20=0:100, T25=0:100, T26=100:0, T30=100:0
Flow : 1 ml/min., Column Temperature : 20 C, Injection : 10 ul,
Detection : UV at 215 nm, Sample Solvent : Water



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Area Percent Report

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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=215,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.949	BV R	0.1845	1.80094e4	1610.44104	98.9158
2	9.765	VB	0.9683	46.25925	5.63183e-1	0.2541
3	16.598	BB	0.3578	14.63413	5.08423e-1	0.0804
4	18.388	BB	0.1719	66.85037	6.19368	0.3672
5	18.995	BB	0.1160	9.49141	1.20400	0.0521
6	20.355	BB	0.0996	9.97858	1.53981	0.0548
7	20.954	BB	0.0997	21.84100	3.36632	0.1200
8	22.833	BB	0.1561	28.34320	2.66457	0.1557
Totals :				1.82068e4	1626.48102	

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*** End of Report ***