

## BDG SYNTHESIS

### Certificate of Analysis

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

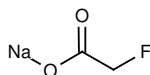
*Neil Beare*

Neil Beare, PhD, Director  
3 June 2015

**Name:** Sodium Fluoroacetate

**CAS Number:** 62-74-8

**Structure:**



**Molecular Weight:**  $C_2H_2FNaO_2 = 100.02$

**Lot Number:** BDG 16466.1

**Appearance:** White, crystalline solid

**Purity By NMR:** 99.0 %

**Re-test Date:** 3 June 2016

**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:	this compound is highly toxic, 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: traces (under 0.1 % w/w) of ethanol and diethyl ether are observed.

Impurities: traces of sodium bromoacetate and an unidentified impurity 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.

### High-resolution Mass Spectrum (ESI+)

Found  $m/z$  122.9833.  $C_2H_2FNa_2O_2$   $[M+Na]^+$  requires  $m/z$  122.9834. The deviation of 0.8 ppm is within normally accepted limits for the establishment of identity by HRMS.

### Elemental Analysis

	Found:	C 24.11, H 1.92 %
$C_2H_2FNaO_2$	Requires:	C 24.02, H 2.02 %

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).

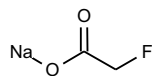
The available quantity of custom-synthesised material is always small, and this limits the extent and type of analytical data which can be obtained. This Certificate is presented in descriptive format for use by analytical chemists who are trained in the use of custom-synthesised materials. Custom materials 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.

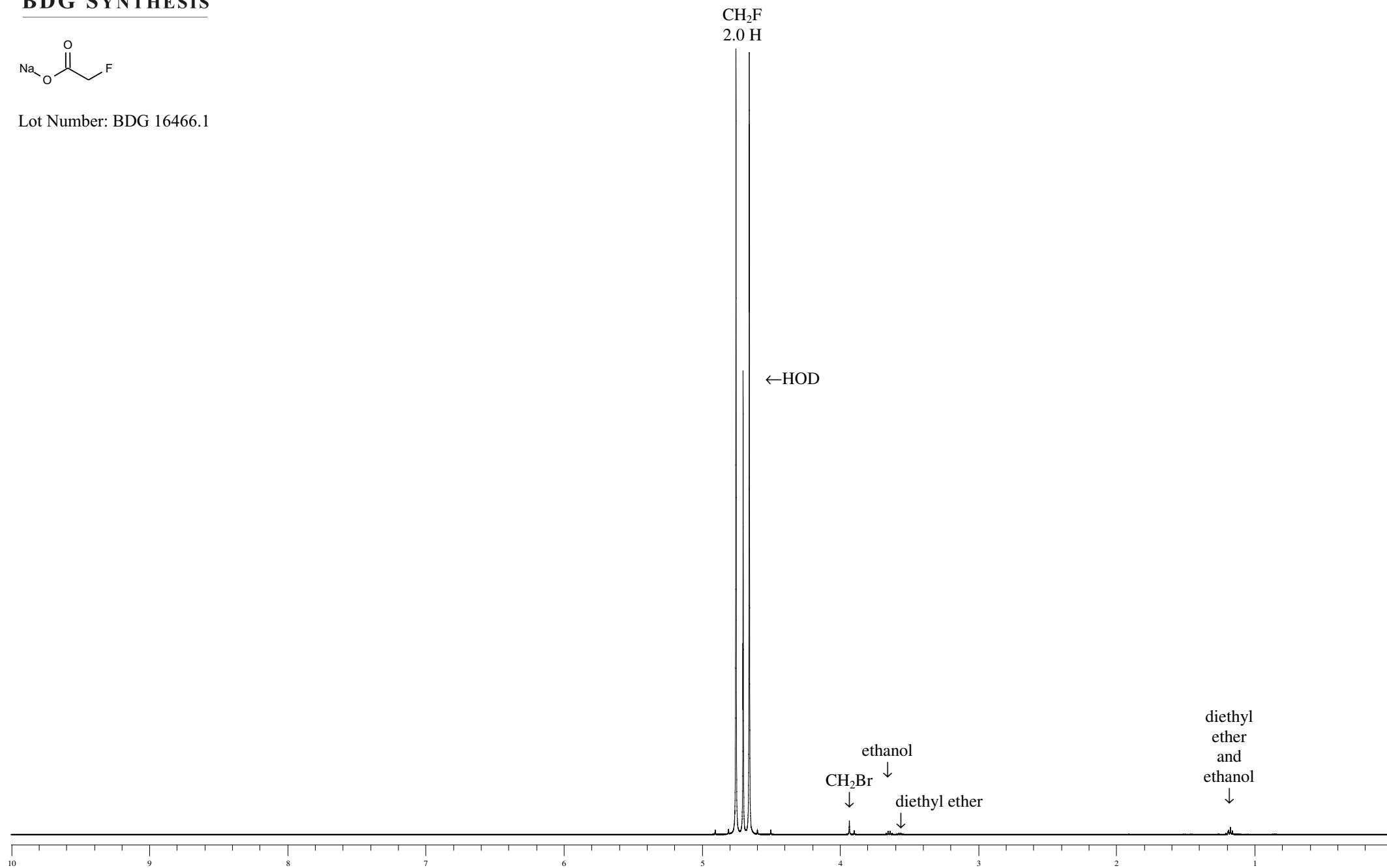


# Proton NMR Spectrum of Sodium Fluoroacetate in D<sub>2</sub>O

**BDG SYNTHESIS**



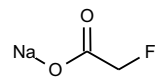
Lot Number: BDG 16466.1



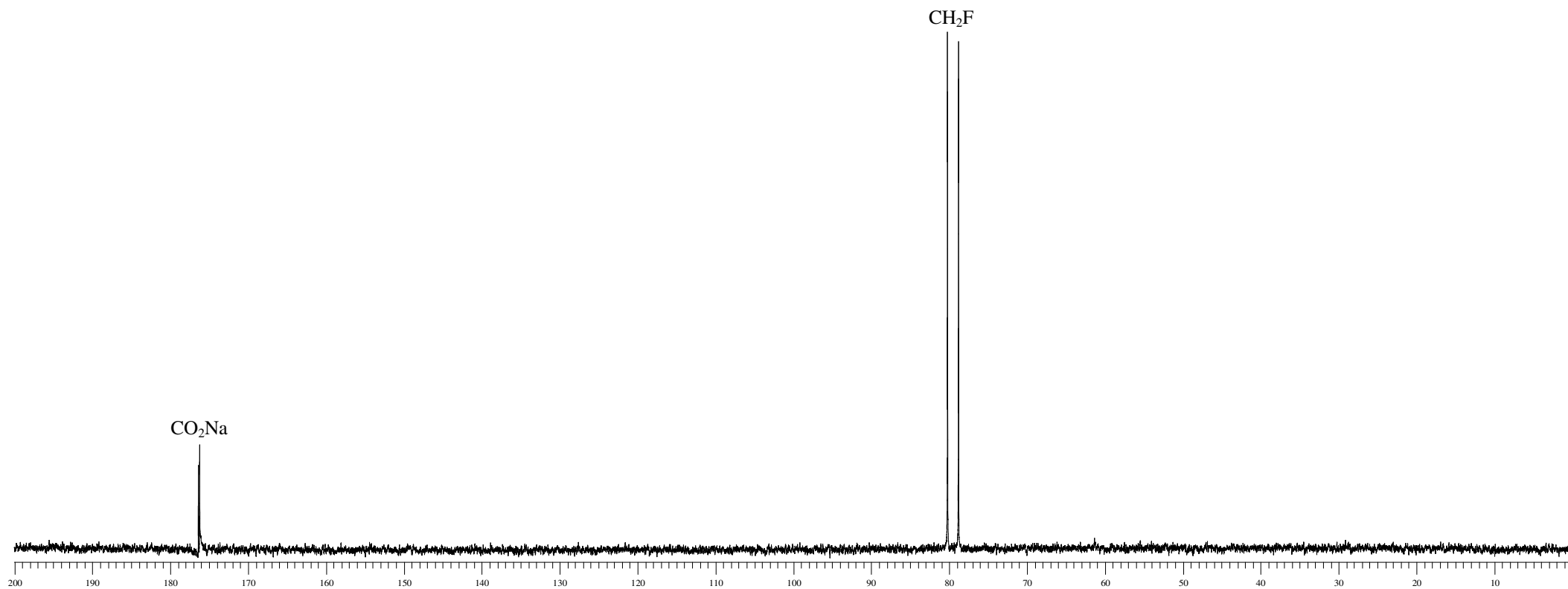


# Carbon-13 NMR Spectrum of Sodium Fluoroacetate in D<sub>2</sub>O

**BDG SYNTHESIS**



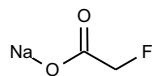
Lot Number: BDG 16466.1





# Proton NMR Spectrum of Sodium Fluoroacetate in D<sub>2</sub>O

**BDG SYNTHESIS**



Lot Number: BDG 16466.1

Note: \* denotes internal standard peaks (1-Methylnicotinamide iodide BDG 8678.2, 99.3 % pure). Used 5.05 mg of substrate and 13.07 mg internal standard. Purity calculated as 99 %.

