

BDG SYNTHESIS

Certificate of Analysis

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

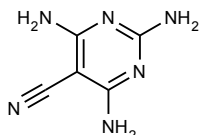
Barry Dent

Barry R. Dent, PhD, Director
25 October 2009

Name: 2,4,6-Triamino-5-pyrimidinecarbonitrile

CAS Number: 465531-97-9

Structure:



Molecular Weight: C₅H₆N₆ = 150.14

Lot Number: BDG 10631.2

Appearance: White, crystalline solid

Purity By HPLC: 98.2 %

Re-test Date: 25 October 2010

Storage and Handling:

Temperature:	ambient laboratory temperature; may be refrigerated.
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 trace (under 0.1 % w/w) of dimethyl sulfoxide 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.

High-resolution Mass Spectrum (ESI+)

Found m/z 151.0731. $C_5H_7N_6$ $[M+H]^+$ requires m/z 151.0732. The deviation of 0.7 ppm is within normally accepted limits for the establishment of identity by HRMS.

HPLC

A sharp, symmetrical peak is observed (98.2 %). 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 40.02, H 3.95, N 55.85 %
$C_5H_6N_6$	Requires:	C 40.00, H 4.03, N 55.97 %

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).

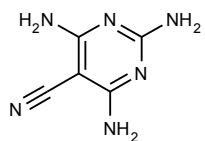
The available quantity of custom-synthesised material is always small, and this limits the extent and type of analytical data which can be obtained. This Certificate is presented in descriptive format for use by analytical chemists who are trained in the use of custom-synthesised materials. Custom materials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

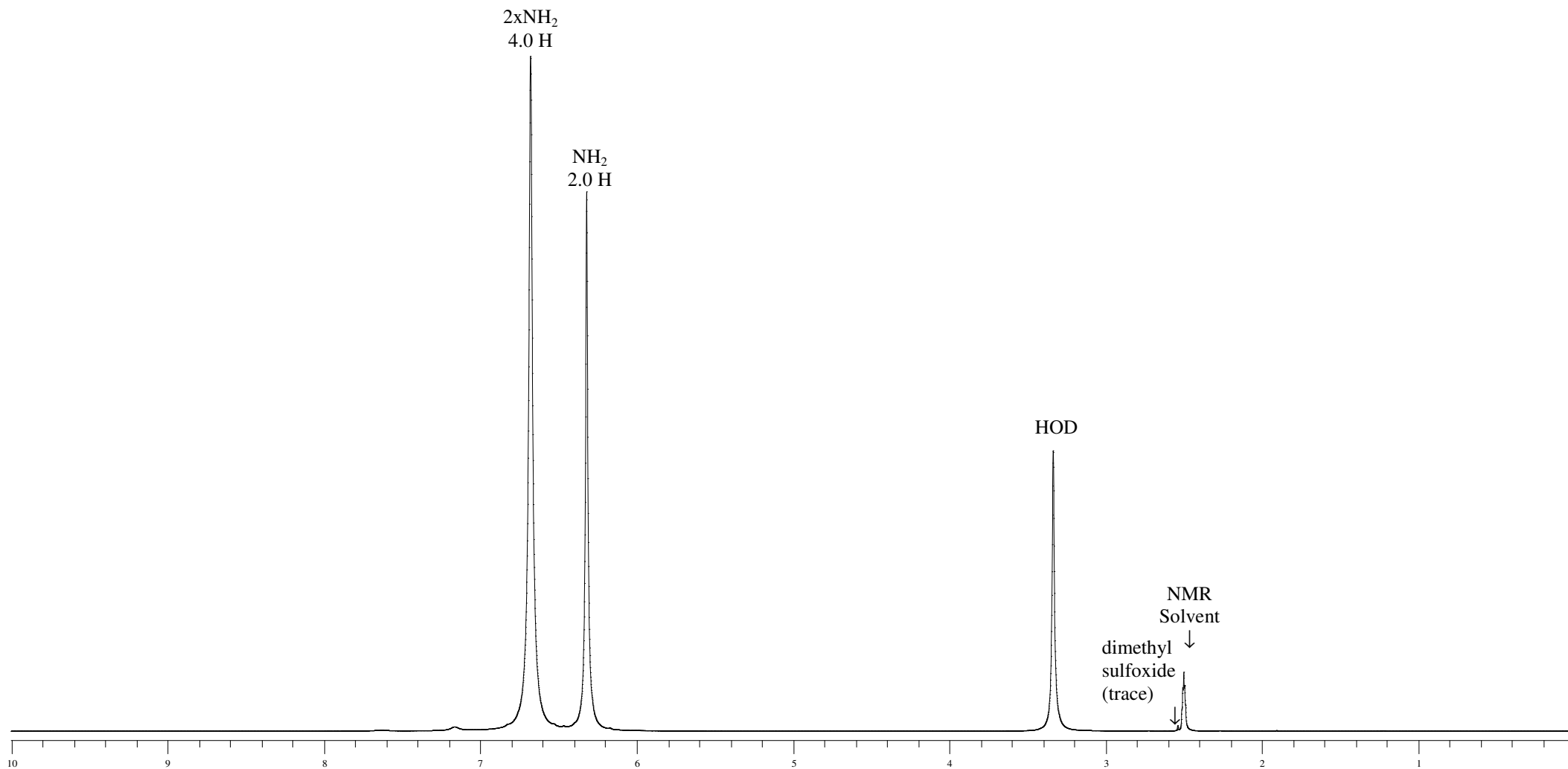


Proton NMR Spectrum of 2,4,6-Triamino-5-pyrimidinecarbonitrile in DMSO-d₆

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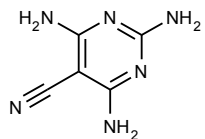
Lot Number: BDG 10631.2



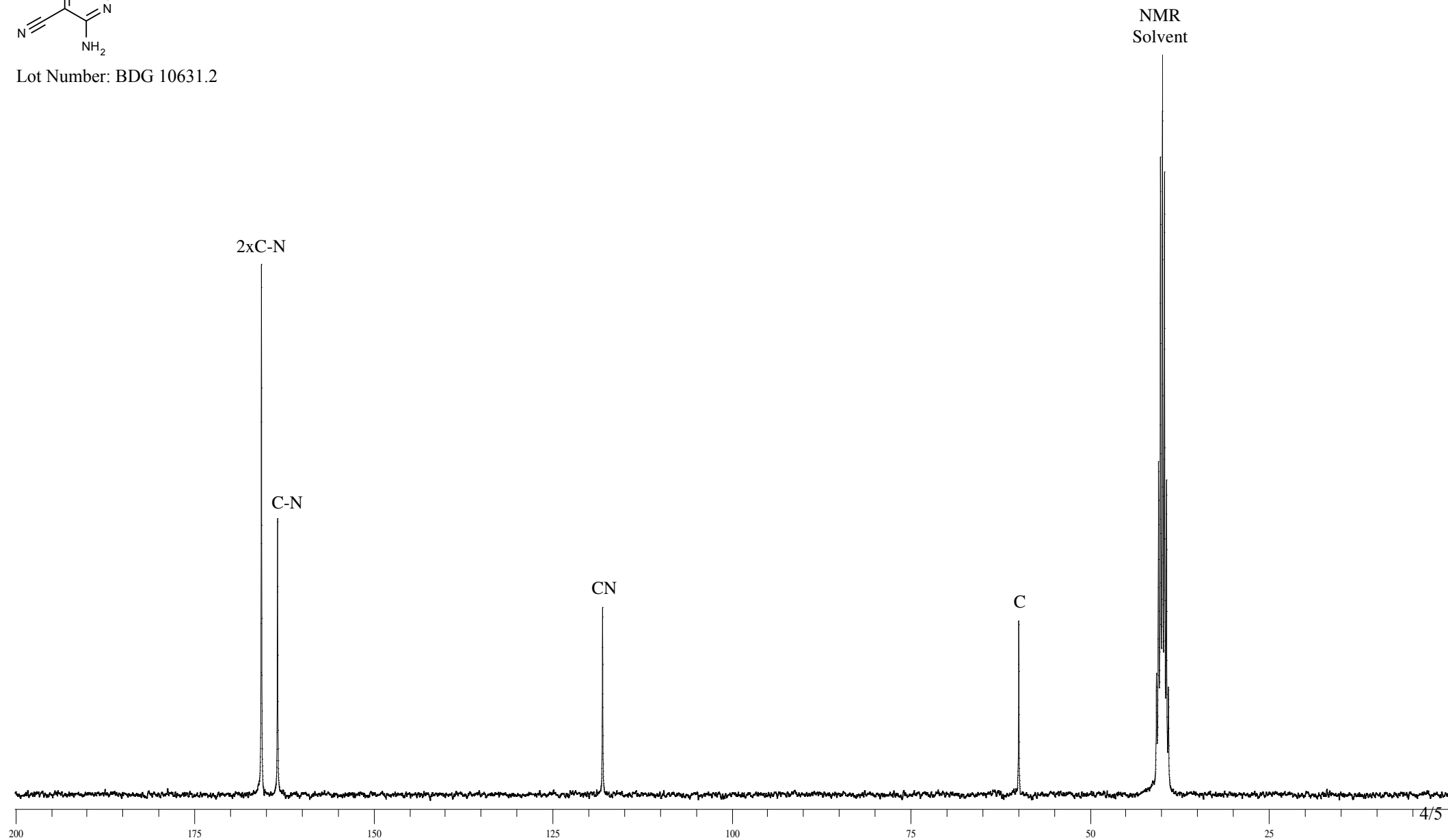


Carbon-13 NMR Spectrum of 2,4,6-Triamino-5-pyrimidinecarbonitrile in DMSO-d₆

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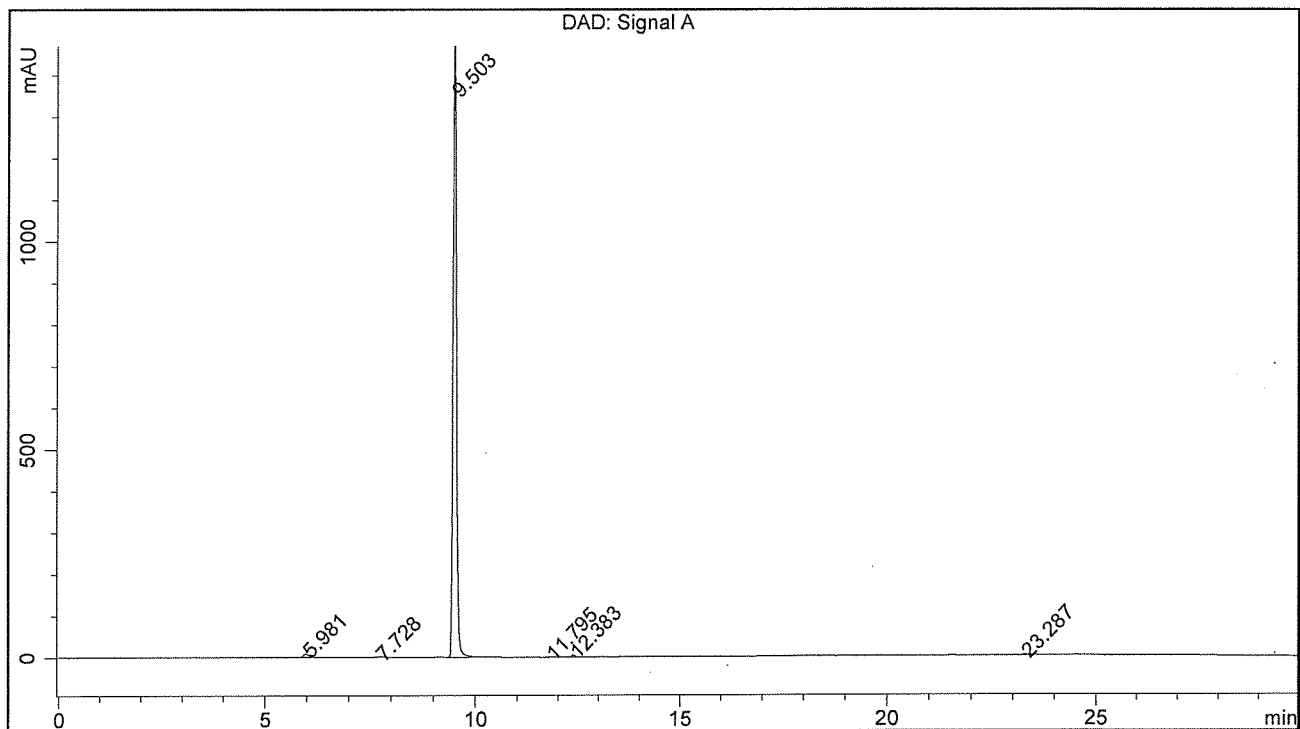
Lot Number: BDG 10631.2



BDG - Analysis of 2,4,6-Triamino-5-pyrimidinecarbonitrile

Column : Phenomenex Luna C18(2) 5um 250 x 4.6 mm
 Guard : Phenomenex Security Guard C18 RP 4 x 3 mm
 Mobile Phase A : 95:5 20 mM Potassium diHydrogen Phosphate pH=6.0 : Acetonitrile
 Mobile Phase B : 30:70 Water : Acetonitrile
 Gradient (A:B) : T0=100:0, T24=0:100, T27=100:0, T30=100:0
 Flow Rate : 1.0 mL/min Sample Solvent : Initial Mobile Phase
 Column Temperature : 20C Injection Volume : 10 uL Detection : UV 222 nm

Sample Name	BDG 10631.2	Instrument	AnalyticalLC01
Acquisition	25/10/2009, 14:21:06	Method (rev.)	LC10349b (9)
Sequence	BDG_25Oct2009j - Reprocessed	Vial Position	1
Operator	solvation010\cerityadmin	Injection	1 of 2



Area Percent Report

Peak#	RT	Peak Height	Peak Area	Width	Area %
1	5.98 min	8.5581	74.1618	0.1311 min	0.870 %
2	7.73 min	0.6733	25.9304	0.4653 min	0.304 %
3	9.50 min	1538.3725	8366.8179	0.0835 min	98.203 %
4	11.80 min	0.8117	3.6138	0.0679 min	0.042 %
5	12.38 min	5.6590	27.2189	0.0741 min	0.319 %
6	23.29 min	1.8319	22.1912	0.1633 min	0.260 %