

# Chemical Information:

Name: 1,3-Dimethyl-4-nitrobenzene  
CAS No.: 89-87-2  
Tox21\_ID No.: Tox21\_202223  
NTP\_CID No.: 53

Date of Analysis: 16 February 2007

Supplier: Sigma-Aldrich  
Lot No.: 01430KI  
MW: 151.16 g/mol

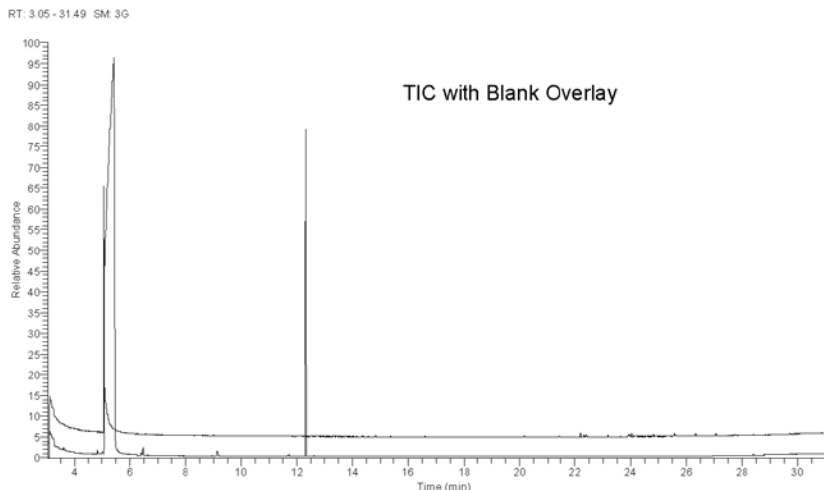
# Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) <sup>a</sup>
DMSO	5.44	Not applicable
1,3-Dimethyl-4-nitrobenzene	12.33	99.63

<sup>a</sup> Peaks comprising ≥ 0.5% of total area.

# GC/MS Instrument Parameters:

Instrument / Ionization	ThermoFinnigan TraceGC with ThermoFinnigan TraceMS / Electron Impact
Solvent	Dichloromethane (100 mM in DMSO, diluted 1/1000 with dichloromethane)
Column	J&W Scientific HP-5MS, 30 m x 0.25 mm ID, 0.25-μm film thickness
Carrier Gas	Helium at 1.0 mL/min
Oven Program	35°C, hold 2 min; ramp @ 10°C/min to 310°C, hold 2 min
Source Temperature	250°C
Auxiliary Temperature	250°C
Scan Range	50 – 250 amu
Injector Temperature	280°C
Injection Volume / Mode	2 μL / Splitless
Run Time	31.5 minutes
Data Analysis Software	Xcalibur, v 1.2 and NIST Library v 1.7, build 11/5/1999



07b1027 #1116 RT: 12.32 AM: 1 SB: 2 12.38 12.38 NL: 201EE  
T: 30.0 eV der360.00 Full ms [50.31-350.00]

