

Chemical Information:

Name: 4-Chloro-3-nitro-a,a,a-trifluorotoluene
CAS No.: 121-17-5 Supplier: Sigma-Aldrich
Tox21_ID No.: Tox21_201833 Lot No.: 15810DI
NTP_CID No.: 368 MW: 225.55 g/mol

Date of Analysis: 04 December 2007

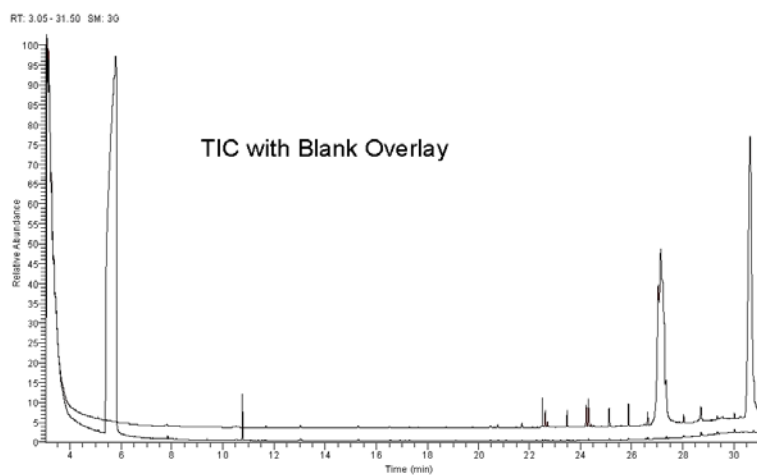
Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
DMSO	5.80	Not applicable
4-Chloro-3-nitro-a,a,a-trifluorotoluene	10.75	98.04
unknown	22.92	1.15
unknown	24.60	0.81

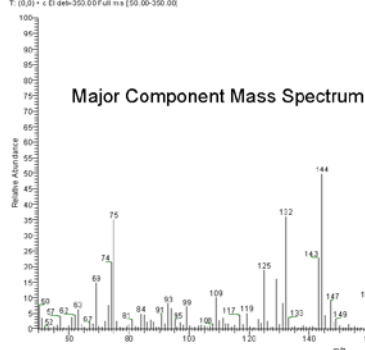
^a Peaks comprising $\geq 0.5\%$ of total area.

GC/MS Instrument Parameters:

Instrument / Ionization	Gas Chromatograph with Mass Spectrometer / 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- μ m 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 – 350 amu
Injector Temperature	250°C
Injection Volume / Mode	2 μ L / Splitless
Run Time	31.5 minutes
Data Analysis Software	Xcalibur, v 1.2 and NIST Library v 1.7, build 11/5/1999



070405 #229 RT: 10.74 MS: 1 SM: 3 10.87 10.84 NL: 4.72E5
T: (0.0) + 4.01e+003.00 Full MS (50.00-350.00)



NIST Reference Mass Spectrum

