

Chemical Information:

Name: 3-Nitro-a,a,a-trifluorotoluene
CAS No.: 98-46-4 Supplier: Sigma-Aldrich
Tox21_ID No.: Tox21_200760 Lot No.: 09010KO
NTP_CID No.: 340 MW: 191.11 g/mol

Date of Analysis: 10 April 2007

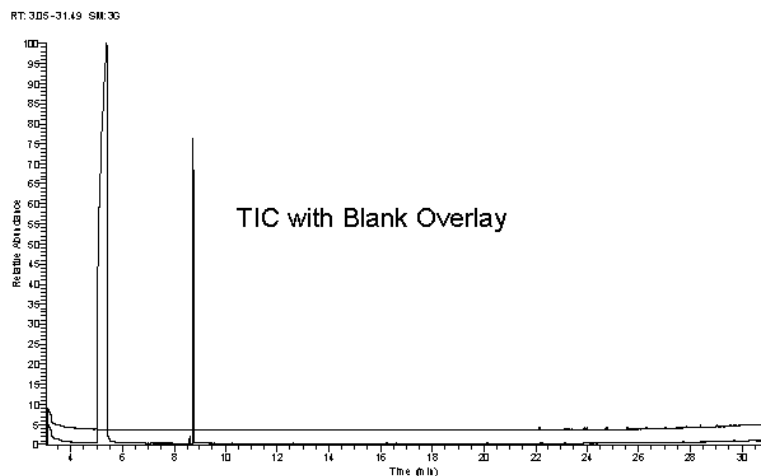
Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
DMSO	5.38	Not applicable
unknown	8.60	2.21
3-Nitro-a,a,a-trifluorotoluene	8.74	97.48

^a 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	250°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



01610000958 RT: 8.74 AU: 1 NL: 3.5256
T: 812 • C ESI+350.00 Full MS (50.00-250.00)

