

Chemical Information:

Name: 2,4,5-Trichloronitrobenzene
CAS No.: 89-69-0 Supplier: Sigma-Aldrich
Tox21_ID No.: Tox21_200937 Lot No.: 5028X
NTP_CID No.: 147 MW: 226.44 g/mol

Date of Analysis: 18 April 2007

Purity and Identity Results:

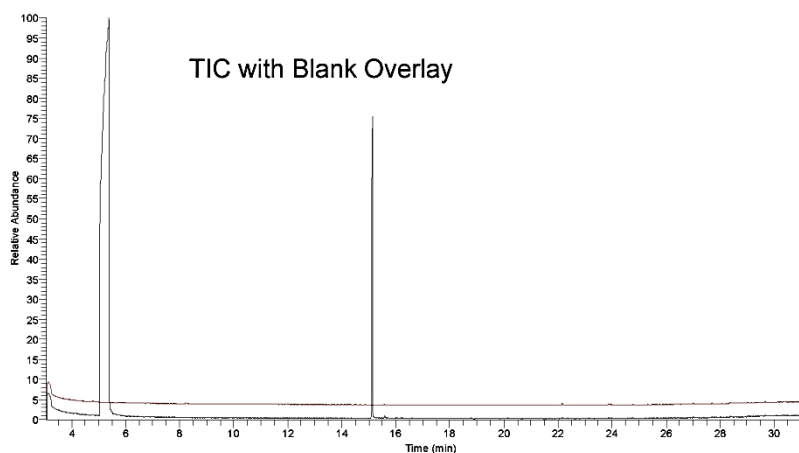
Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
DMSO	5.38	Not applicable
2,4,5-Trichloronitrobenzene	15.13	99.03
unknown	15.59	0.97

^a Peaks comprising ≥ 0.5% of total area.

GC/MS Instrument Parameters:

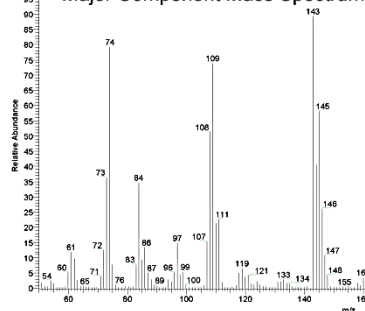
Instrument / Ionization	ThermoFinnigan TraceGC with ThermoFinnigan TraceMS / Electron Impact
Solvent	Dichloromethane (100 mM in DMSO, diluted 1/1000 with dichloromethane)
Column	J&W Scientific HP-5MS, 30 m x 0.25 mm ID, 0.25-μm film thickness
Carrier Gas	Helium at 1.0 mL/min
Oven Program	35°C, hold 2 min; ramp @ 10°C/min to 310°C, hold 2 min
Source Temperature	250°C
Auxiliary Temperature	250°C
Scan Range	50 – 350 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

RT: 3.05 - 31.50 SM 3G



07018a04 #1455 RT: 15.13 AU: 1 NL: 8.43E5
T: (0.0) * c E1 det=350.00 Full ms [50.00-350.00]

Major Component Mass Spectrum



NIST Reference Mass Spectrum

