

Chemical Information:

Name: beta_Nitrostyrene
CAS No.: 5153-67-3
Tox21_ID No.: Tox21_200772
NTP_CID No.: 547

Supplier: Sigma-Aldrich
Lot No.: 15020TC
MW: 149.15 g/mol

Date of Analysis: 27 March 2007

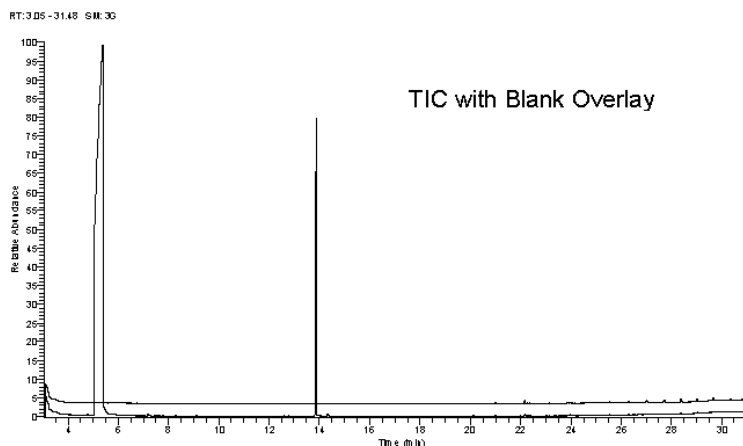
Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
DMSO	5.39	Not applicable
unknown	7.20	0.69
beta_Nitrostyrene	13.87	98.42
unknown	14.34	0.68

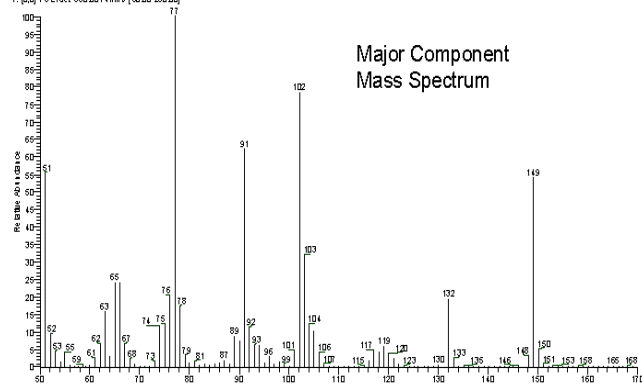
^a Peaks comprising ≥ 0.5% of total area.

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



07-027-00 #1304 RT: 13.87 MS: 1 NL: 23066
T: (0.0) + c E (0.0) 350.00 F (0.0) s (50.00-250.00)



NIST Reference Mass Spectrum

