

Chemical Information:

Name: 3-Methyl-4-nitrobenzoic acid
CAS No.: 3113-71-1 Supplier: Sigma-Aldrich
Tox21_ID No.: Tox21_200835 Lot No.: 15530DB
NTP_CID No.: 339 MW: 181.15 g/mol

Date of Analysis: 16 August 2007

Purity and Identity Results:

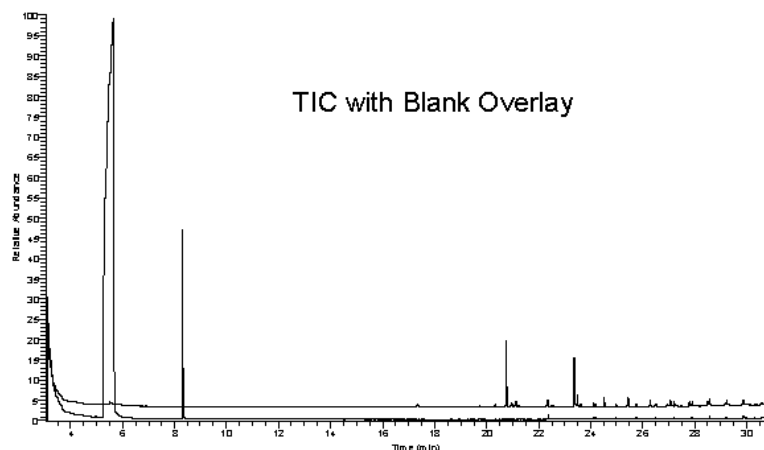
Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
DMSO	5.66	Not applicable
3-Methyl-4-nitrobenzoic acid	16.70	99.39

^a Peaks comprising ≥ 0.5% of total area.

GC/MS Instrument Parameters:

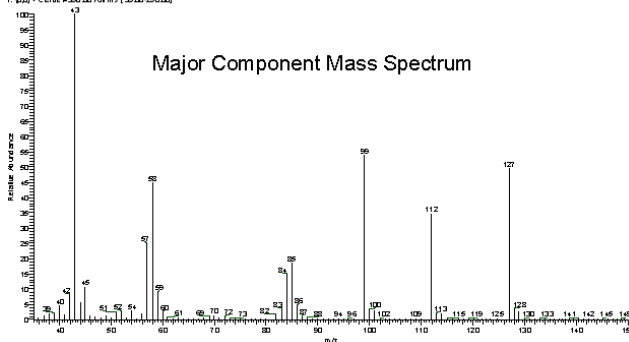
Instrument / Ionization	ThermoFinnigan TraceGC with ThermoFinnigan TraceMS / Electron Impact
Solvent	Dichloromethane (100 mM in DMSO, diluted 1/1000 with dichloromethane)
Column	J&W Scientific HP-5MS, 30 m x 0.25 mm ID, 0.25-μm film thickness
Carrier Gas	Helium at 1.0 mL/min
Oven Program	35°C, hold 2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

RT: 3.05 - 31.49 SM: 30

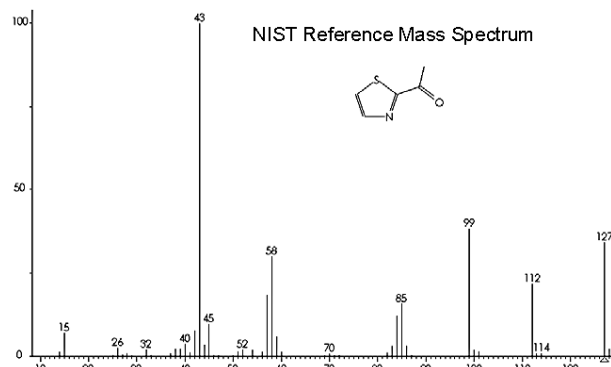


TIC with Blank Overlay

07/16/07 #1380 RT: 5.21 AU: 1 NL: 334.66
T: 212 °C ESI MS-TOF MS/MS (30.00-250.00)



Major Component Mass Spectrum



NIST Reference Mass Spectrum

