

Chemical Information:

Name: o-Chlorobenzoic acid
CAS No.: 118-91-2
Tox21_ID No.: Tox21_200286
NTP_CID No.: 1094

Date of Analysis: 29 March 2007

Supplier: Sigma-Aldrich
Lot No.: 10504HC_HIPS
MW: 156.57 g/mol

Purity and Identity Results:

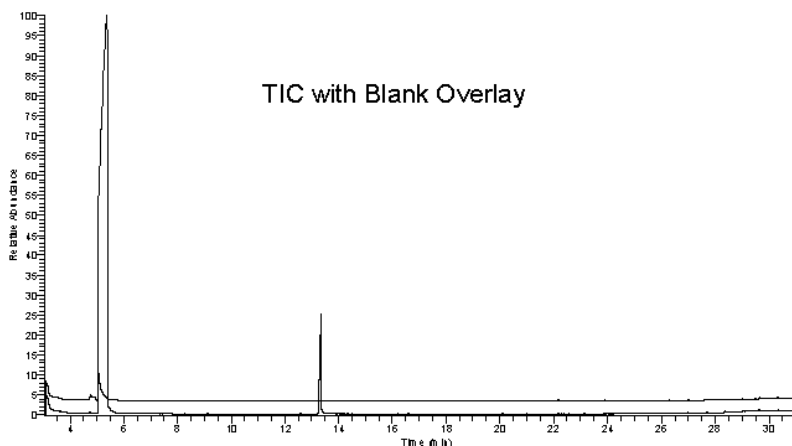
Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
DMSO	5.38	Not applicable
o-Chlorobenzoic acid	13.34	99.45

^a Peaks comprising ≥ 0.5% of total area.

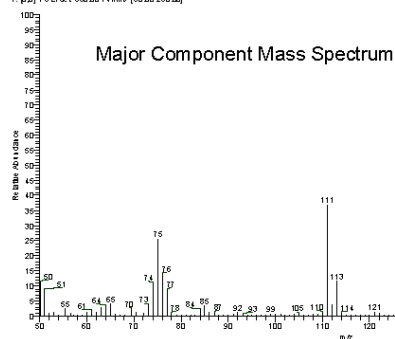
GC/MS Instrument Parameters:

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

RT: 3.05 - 31.48 SM: 30



01-02-2001 11:24:00 RT: 13.34 AU: 1.5185
T: (0.0) + c 01-02-2000 P: 0.00 (50.00-250.00)



NIST Reference Mass Spectrum

