

Chemical Information:

Name: 3,4-Dichlorobenzoic Acid
CAS No.: 51-44-5
Tox21_ID No.: Tox21_200322
NTP_CID No.: 305

Date of Analysis: 5 April 2007

Supplier: Sigma-Aldrich
Lot No.: 05224DS
MW: 191.01 g/mol

Purity and Identity Results:

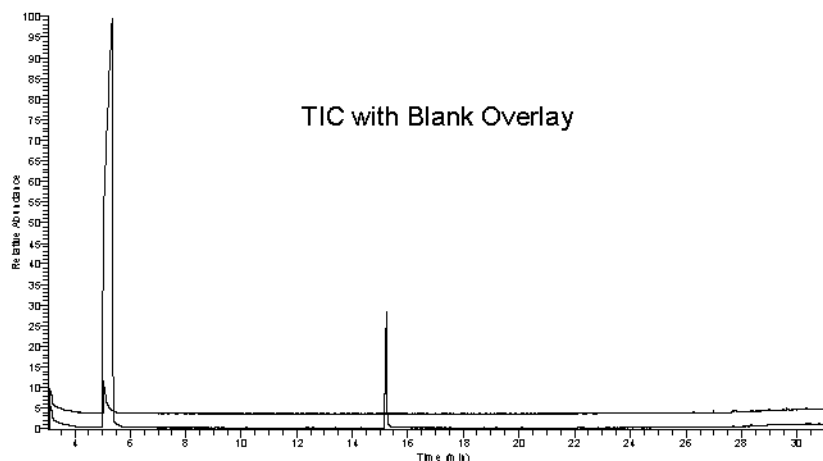
Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
DMSO	5.36	Not applicable
3,4-Dichlorobenzoic Acid	15.23	99.70

^a Peaks comprising $\geq 0.5\%$ of total area.

GC/MS Instrument Parameters:

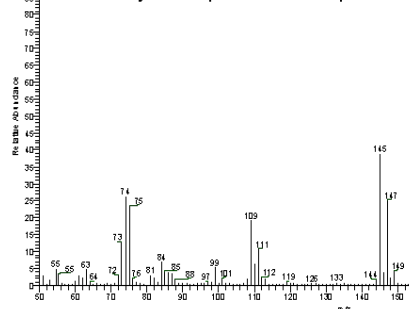
Instrument / Ionization	ThermoFinnigan TraceGC with ThermoFinnigan TraceMS / Electron Impact
Solvent	Dichloromethane (100 mM in DMSO, diluted 1/1000 with dichloromethane)
Column	J&W Scientific HP-5MS, 30 m x 0.25 mm ID, 0.25- μ m film thickness
Carrier Gas	Helium at 1.0 mL/min
Oven Program	35°C, hold 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 μ L / 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: 3G



07-05-07 14:56 RT: 15.22 AU: 1 NL: 1.00E5
T: (P) + C (I) + S (D) P (M) 150.00-250.00

Major Component Mass Spectrum



NIST Reference Mass Spectrum

