

Chemical Information:

Name: Benzoic acid
CAS No.: 65-85-0
Tox21_ID No.: Tox21_202403
NTP_CID No.: 525

Date of Analysis: 02 October 2007

Supplier: Sigma-Aldrich
Lot No.: 10507DD
MW: 122.12 g/mol

Purity and Identity Results:

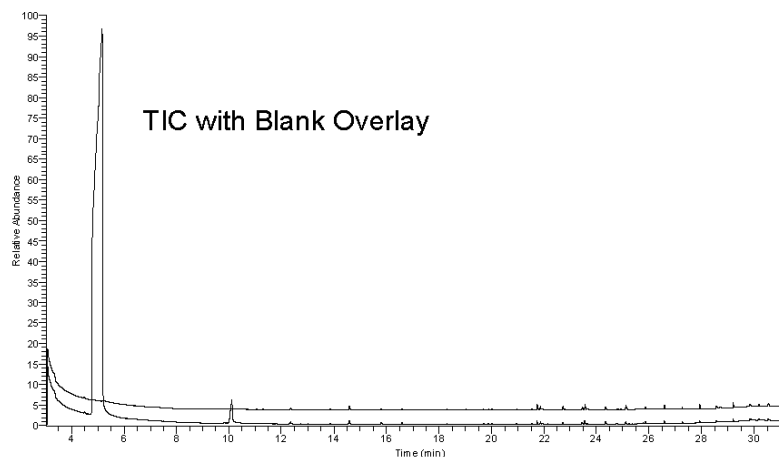
Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
DMSO	5.18	Not applicable
Benzoic acid	10.12	97.85
unknown	25.79	1.30

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

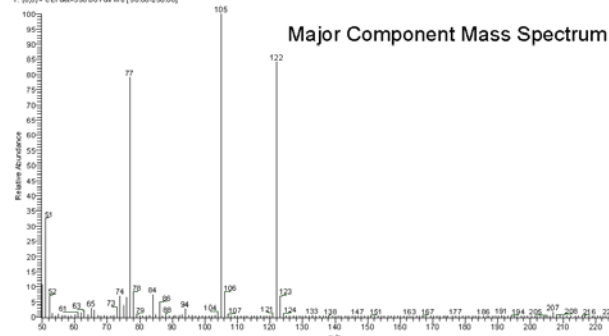
GC/MS Instrument Parameters:

Instrument / Ionization	Gas Chromatograph / Mass Spectrometer / 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: 30



07/02/13 #853 RT: 10.11 AU: 1 NL: 4.00E-5
T: (5.0) - cEI 06-350.00 Full MS (50.00-250.00)



NIST Reference Mass Spectrum

