

Chemical Information:

Name: p-Tolunitrile
CAS No.: 104-85-8
Tox21_ID No.: Tox21_200947
NTP_CID No.: 1241

Supplier: Sigma-Aldrich
Lot No.: 02310EC
MW: 117.15 g/mol

Date of Analysis: 10 July 2007

Purity and Identity Results:

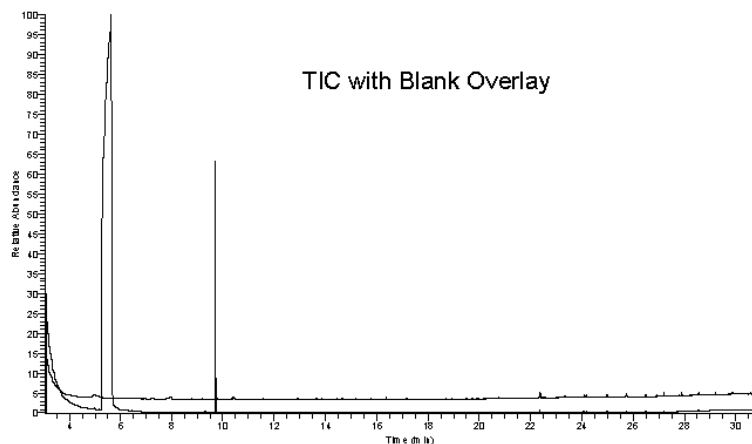
Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
DMSO	5.65	Not applicable
p-Tolunitrile	9.71	99.65

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

GC/MS Instrument Parameters:

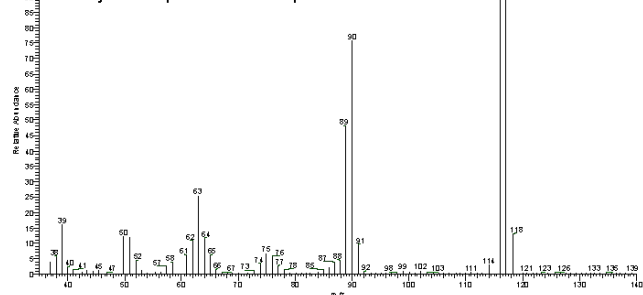
Instrument / Ionization	ThermoFinnigan TraceGC with ThermoFinnigan TraceMS / Electron Impact
Solvent	Dichloromethane (100 mM in DMSO, diluted 1/1000 with dichloromethane)
Column	J&W Scientific HP-5MS, 30 m x 0.25 mm ID, 0.25- μ m film thickness
Carrier Gas	Helium at 1.0 mL/min
Oven Program	35°C, hold 2 min; ramp @ 10°C/min to 310°C, hold 2 min
Source Temperature	250°C
Auxiliary Temperature	250°C
Scan Range	35 – 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 - 31.50 SM: 30



DTG16 #1762 RT: 9.70 AC: 1 NL: 4.5285
T: (0.0) v: 0.000000 F: 0.000000

Major Component Mass Spectrum



NIST Reference Mass Spectrum

