

Chemical Information:

Name: p-tert-Butyltoluene

Date of Analysis: 10 July 2007

CAS No.: 98-51-1

Supplier: Sigma-Aldrich

Tox21_ID No.: Tox21_202329

Lot No.: 15830LA

NTP_CID No.: 1237

MW: 148.24 g/mol

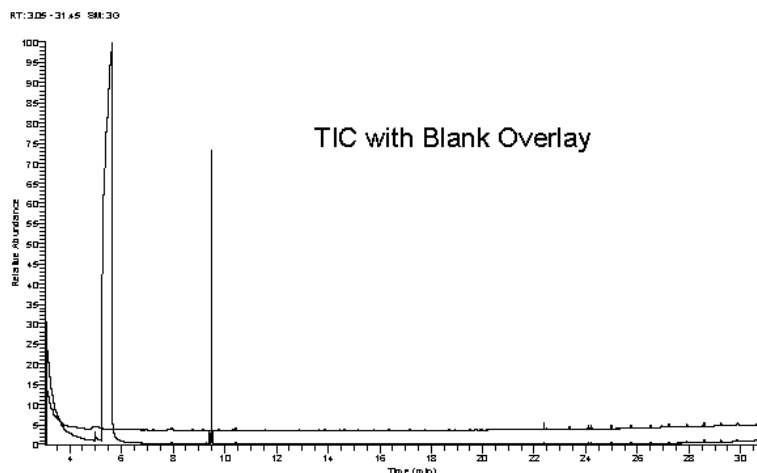
Purity and Identity Results:

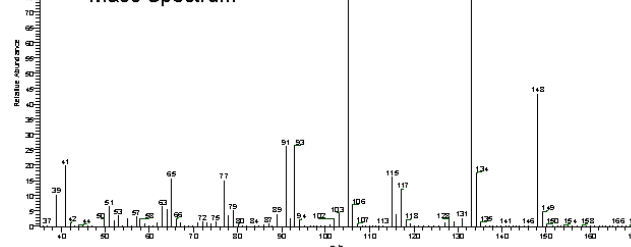
Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
DMSO	5.64	Not applicable
unknown	9.42	6.79
p-tert-Butyltoluene	9.50	95.99

^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


DTG101201002 RT: 9.42 AM: 1 ML: 0.2366
T: 0.74 * C: 0.166 * 200.00 * 1.0000 * 1 (30.00000000)

Major Component Mass Spectrum

NIST Reference Mass Spectrum
