

# Chemical Information:

Name: o-Tolunitrile  
CAS No.: 529-19-1  
Tox21\_ID No.: Tox21\_200324  
NTP\_CID No.: 1132

Supplier: Sigma-Aldrich  
Lot No.: 01914BB  
MW: 117.15 g/mol

Date of Analysis: 11 July 2007

## Purity and Identity Results:

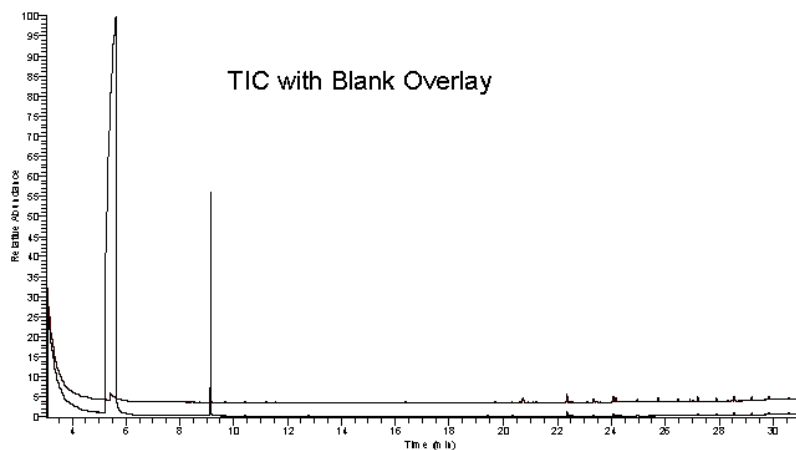
Peak Identity	Retention Time (min)	Purity (% Total Area) <sup>a</sup>
DMSO	5.63	Not applicable
o-Tolunitrile	9.14	100.00

<sup>a</sup> Peaks comprising  $\geq 0.5\%$  of total area.

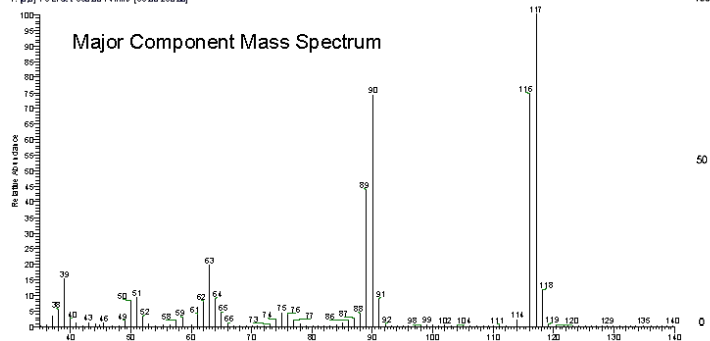
## GC/MS Instrument Parameters:

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- $\mu$ 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 $\mu$ 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 - 31.51 SM 30



01g1007\_070112080722#1604 RT: 9.13 AU: 1 NL: 3.31E6  
T: 0.01 uO 01 06 300.00 F4101 (35.00-250.00)



NIST Reference Mass Spectrum

