

Chemical Information:

Name: 2-Ethylhexanoic acid

Date of Analysis: 30 August 2007

CAS No.: 149-57-5

Supplier: Sigma-Aldrich

Tox21_ID No.: Tox21_201406

Lot No.: 15318TB

NTP_CID No.: 244

MW: 144.21 g/mol

Purity and Identity Results:

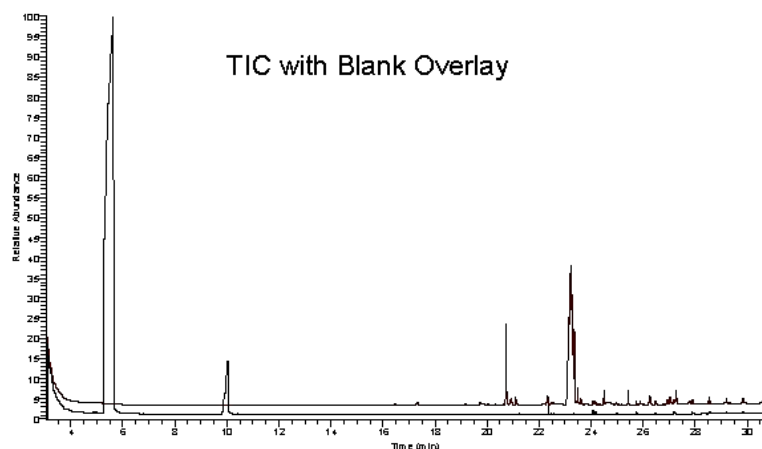
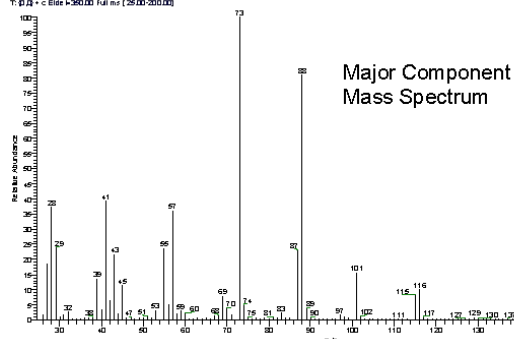
Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
DMSO	5.63	Not applicable
2-Ethylhexanoic acid	10.04	100.00

^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	25 – 200 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

RT: 3.05 - 31.43 SM: 30


07/02/08 RT: 10.04 AC: 1 NL: 13688
T: 0.04 c: 0.00000 Full MS (25.00-200.00)


NIST Reference Mass Spectrum

