

Chemical Information:

Name: 3-Cyclohexene-1-carboxaldehyde, 4-(4-hydroxy-4-methylpentyl)-
 Date of Analysis: 20 October 2010
 CAS No.: 31906-04-4 Supplier: Sigma-Aldrich
 Tox21_ID No.: Tox21_200394 Lot No.: 1050509
 NTP_CID No.: 3343 MW: 210.31 g/mol

Purity and Identity Results:

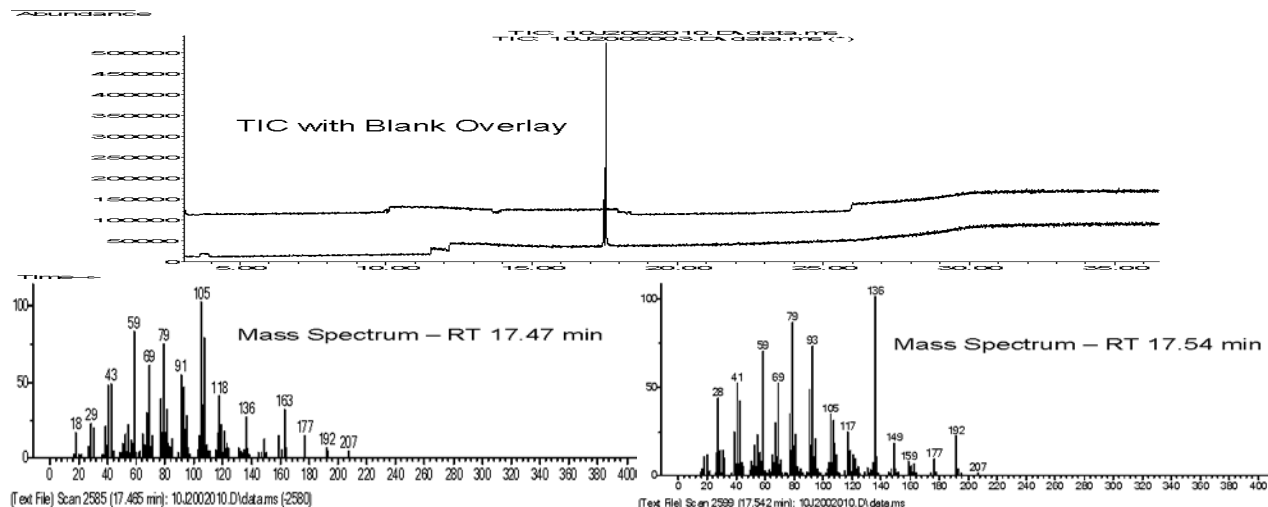
Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
3-Cyclohexene-1-carboxaldehyde, 3-(4-hydroxy-4-methylpentyl)-, Isomer 1	17.47	18.84
3-Cyclohexene-1-carboxaldehyde, 4-(4-hydroxy-4-methylpentyl)-, Isomer 2	17.54	81.16

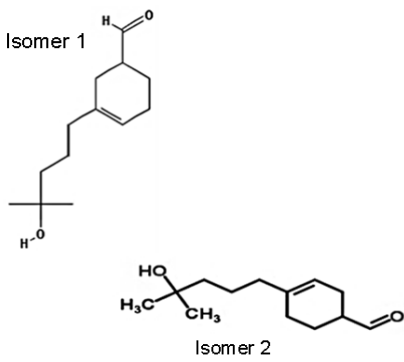
^a Peaks comprising ≥ 0.5% of total area.

COA indicates isomers.

GC/MS Instrument Parameters:

Instrument / Ionization	Gas Chromatograph with Mass Spectrometer / Electron Impact
Solvent	Methanol
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 7 min
Source Temperature	230°C
Auxiliary Temperature	250°C
Scan Range	15 – 500 amu
Injector Temperature	250°C
Injection Volume / Mode	1 μL / Split (100:1)
Data Analysis Software	MSD Chemstation, v D.03.00.SP1 and NIST Library v 2.0f, build 10/8/2008



m/z	Isomer 1 Fragment	Isomer 1	m/z	Isomer 2 Fragment
192	C ₁₃ H ₂₀ O		192	C ₁₃ H ₂₀ O
177	C ₁₂ H ₁₇ O		177	C ₁₂ H ₁₇ O
163	C ₁₁ H ₁₅ O		149	C ₁₀ H ₁₅ O
136	C ₉ H ₁₂ O		136	C ₉ H ₁₂ O
105	C ₇ H ₅ O		105	C ₇ H ₅ O
91	C ₇ H ₇		93	C ₇ H ₉
79	C ₆ H ₇		79	C ₆ H ₇
59	C ₃ H ₇ O		59	C ₃ H ₇ O