

# Chemical Information:

Name: Citral  
CAS No.: 5392-40-5  
Tox21\_ID No.: Tox21\_202093  
NTP\_CID No.: 641

Supplier: Aldrich Chemical Company  
Lot No.: 04402AQ  
MW: 152.23 g/mol

Date of Analysis: 08 December 2009

## Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) <sup>a</sup>
unknown	10.77	0.84
cis-Citral	11.65	35.57
trans-Citral	12.08	63.59

<sup>a</sup> Peaks comprising ≥ 0.5% of total area.

## GC/MS Instrument Parameters:

Instrument / Ionization	Gas Chromatograph with Mass Spectrometer / Electron Impact
Solvent	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 7 min
Source Temperature	250°C
Auxiliary Temperature	250°C
Scan Range	25 – 500 amu
Injector Temperature	250°C
Injection Volume / Mode	1 μL / Split (100:1)
Data Analysis Software	Xcalibur, v 1.2 and NIST Library v 2.0f, build 10/08/2008

