

# Chemical Information:

Name: Lime oil  
 CAS No.: 8008-26-2  
 Tox21\_ID No.: Tox21\_200691  
 NTP\_CID No.: 906

Supplier: Sigma-Aldrich  
 Lot No.: 02925KE  
 MW: Not applicable

Date of Analysis: 25 March 2010

## Purity and Identity Results:

Peak Identity <sup>a</sup>	Retention Time (min)	Purity (% Total Area) <sup>b</sup>
$\alpha$ -Pinene (80-56-8)	7.54	1.36
$\beta$ -Pinene (127-91-3)	8.31	1.99
$\beta$ -Myrcene (123-35-3)	8.53	1.05
7-Oxabicyclo[2.2.1]heptane, 1-methyl-4-(1-methylethyl)- (470-67-7)	8.96	2.69
Bicyclo[4.1.0]hept-2-ene, 3,7,7-trimethyl- (554-61-0)	8.98	2.79
Benzene, 1-methyl-2-(1-methylethyl)- (527-84-4)	9.12	2.91
D-Limonene (5989-27-5)	9.19	53.66
Eucalyptol (470-85-6)	9.25	2.82
$\gamma$ -Terpinene (99-85-4)	9.69	13.06
Cyclohexene, 3-methyl-6-(1-methylethylidene)- (586-63-0)	10.18	9.47
unknown	10.91	0.90
$\alpha$ -Terpineol (98-55-5)	11.78	5.86
unknown	11.89	1.42

<sup>a</sup> Lime oil is a mixture; total of identified components = 97.66%.

<sup>b</sup> Peaks comprising  $\geq 0.5\%$  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- $\mu$ 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 7 min
Source Temperature	230°C
Auxiliary Temperature	250°C
Scan Range	25 – 500 amu
Injector Temperature	250°C
Injection Volume / Mode	1 $\mu$ L / Split (100:1)
Data Analysis Software	MSD Chemstation, v E.02.00.SP2 and NIST Library v 2.0f, build 10/8/2008

