

### Chemical Information:

Name: alpha-Amylcinnamyl alcohol  
 CAS No.: 101-85-9 Supplier: Sigma Aldrich  
 Tox21\_ID No.: Tox21\_202715 Lot No.: 1425669  
 NTP\_CID No.: 6008 MW: 204.31 g/mol

Date of Analysis: 10 March 2017

### Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) <sup>a</sup>
Unknown	22.74	0.53
alpha-Amylcinnamyl alcohol	23.13	91.38
alpha-Amylcinnamyl alcohol	23.37	4.13
Unknown	24.04	3.96

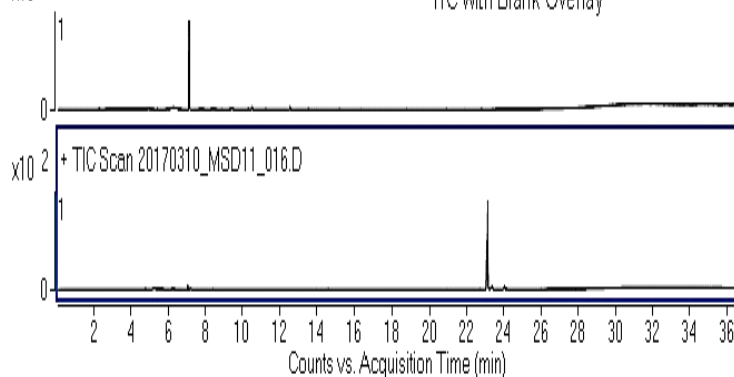
<sup>a</sup> Peaks comprising ≥ 0.5% of total area. Purity = 95.51%, total of isomers

### GC/MS Instrument Parameters:

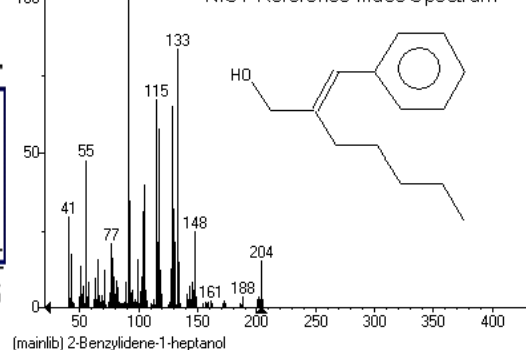
Instrument / Ionization	Gas Chromatograph with Mass Spectrometer / Electron Impact
Solvent	Methanol
Column	Restek Rtx-5MS with Integra-Guard, 30 m x 0.25 mm ID, 1-μm film thickness
Carrier Gas	Helium at 1.0 mL/min
Oven Program	35°C, hold 2 min; ramp @ 10°C/min to 310°C, hold 7 min
Source Temperature	250°C
Auxiliary Temperature	250°C
Scan Range	40 – 640 amu
Injector Temperature	250°C
Injection Volume / Mode	1 μL / Splitless
Data Analysis Software	MassHunter GC/MS Acquisition B.07.02.1938 / MassHunter Qualitative Analysis B.07.00 Build 7.0.7024.0 / NIST Library Version 2.2 Build 2014

x10<sup>2</sup> + TIC Scan 20170310\_MSD11\_007.D

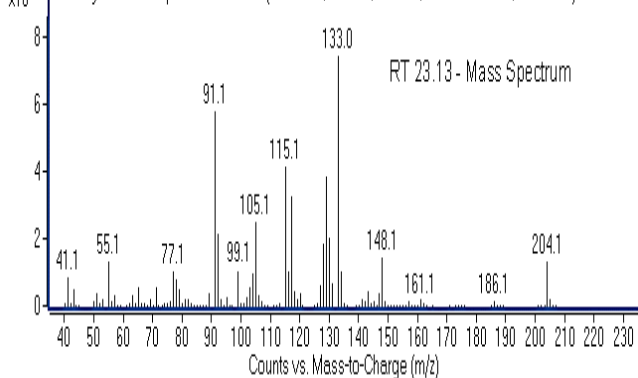
TIC with Blank Overlay



NIST Reference Mass Spectrum



x10<sup>5</sup> 2-Benzylidene-1-heptanol: + Scan (rt: 23.094, 23.101, 23.108, 23.115 ... min, 9 scans) 2017031...



x10<sup>4</sup> 2-Benzylidene-1-heptanol: + Scan (rt: 23.339, 23.346, 23.352, 23.359 ... min, 9 scans) 2017031...

