

# Chemical Information:

Name: Isophytol  
CAS No.: 505-32-8  
Tox21\_ID No.: Tox21\_200139  
NTP\_CID No.: 884

Date of Analysis: 10 October 2007

Supplier: Sigma-Aldrich  
Lot No.: 342024/1  
MW: 296.53 g/mol

## Purity and Identity Results:

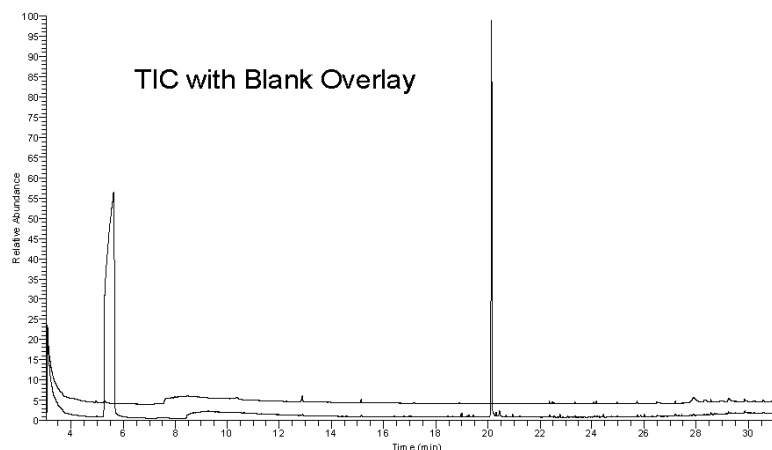
Peak Identity	Retention Time (min)	Purity (% Total Area) <sup>a</sup>
DMSO	5.63	Not applicable
Unknown	19.02	0.65
Isophytol	20.15	95.21
Unknown	20.45	1.24
Unknown	22.78	0.50

<sup>a</sup> Peaks comprising  $\geq 0.5\%$  of total area.

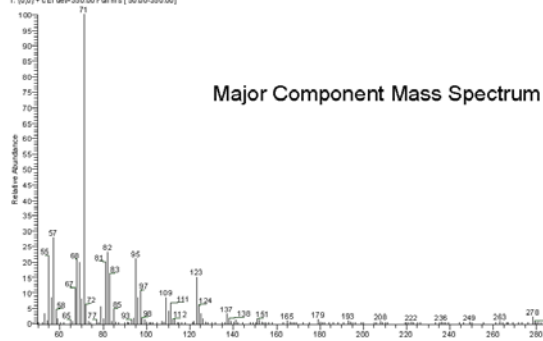
## GC/MS Instrument Parameters:

Instrument / Ionization	Gas Chromatograph / Mass Spectrometer / 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- $\mu$ 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 2 min
Source Temperature	250°C
Auxiliary Temperature	250°C
Scan Range	50 – 350 amu
Injector Temperature	250°C
Injection Volume / Mode	2 $\mu$ L / 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 - 31.49 SM: 3G



07101011 #2052 RT: 20.10 Rev 1 SM: 2 20.07, 20.20 NL: 2.87E5  
T: (0.0) + c1 dph-350.00 Full m/z (50.00-350.00)



## NIST Reference Mass Spectrum

