

Chemical Information:

Name: Safrole
CAS No.: 94-59-7
Tox21_ID No.: Tox21_202439
NTP_CID No.: 1265

Supplier: Sigma-Aldrich
Lot No.: 025K2613
MW: 162.19 g/mol

Date of Analysis: 16 April 2007

Purity and Identity Results:

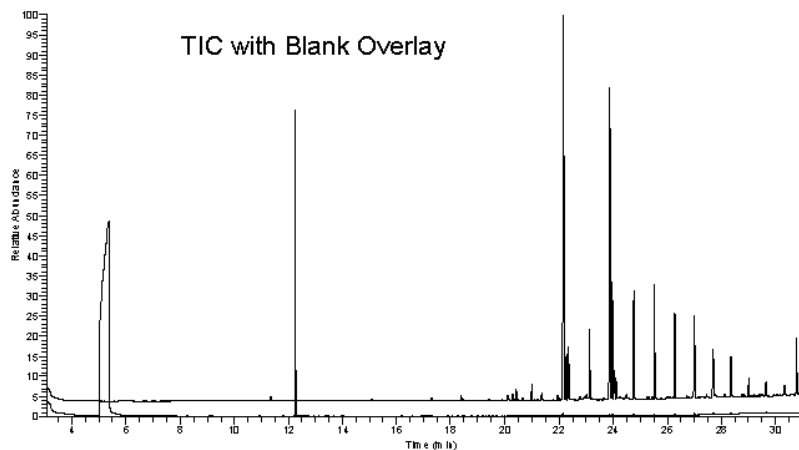
Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
DMSO	5.37	Not applicable
Safrole	12.26	99.97

^a Peaks comprising $\geq 0.5\%$ of total area.

GC/MS Instrument Parameters:

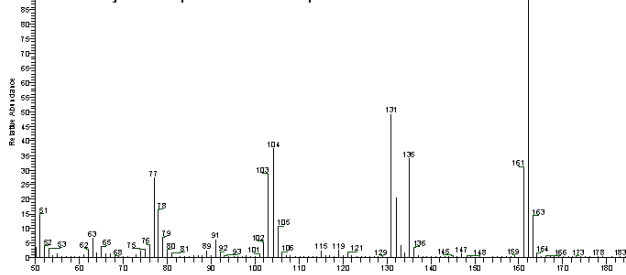
Instrument / Ionization	ThermoFinnigan TraceGC with ThermoFinnigan TraceMS / Electron Impact
Solvent	Dichloromethane (100 mM in DMSO, diluted 1/1000 with dichloromethane)
Column	J&W Scientific HP-5MS, 30 m x 0.25 mm ID, 0.25- μ m film thickness
Carrier Gas	Helium at 1.0 mL/min
Oven Program	35°C, hold 2 min; ramp @ 10°C/min to 310°C, hold 2 min
Source Temperature	250°C
Auxiliary Temperature	250°C
Scan Range	50 – 250 amu
Injector Temperature	250°C
Injection Volume / Mode	2 μ 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 - 31.50 SM: 3G



07/01/07 #1109 RT: 12.24 AC: 1 SE: 2 12.21, 12.30 NL: 32455
T: (P2) + c10e1p-350.00 F110.01 [50.00-250.00]

Major Component Mass Spectrum



NIST Reference Mass Spectrum

