

Chemical Information:

Name: Benzylideneacetone (Methyl styryl ketone)
CAS No.: 122-57-6 Supplier: Sigma-Aldrich
Tox21_ID No.: Tox21_201502 Lot No.: 04525KC
NTP_CID No.: 963 MW: 146.19 g/mol

Date of Analysis: 24 October 2007

Purity and Identity Results:

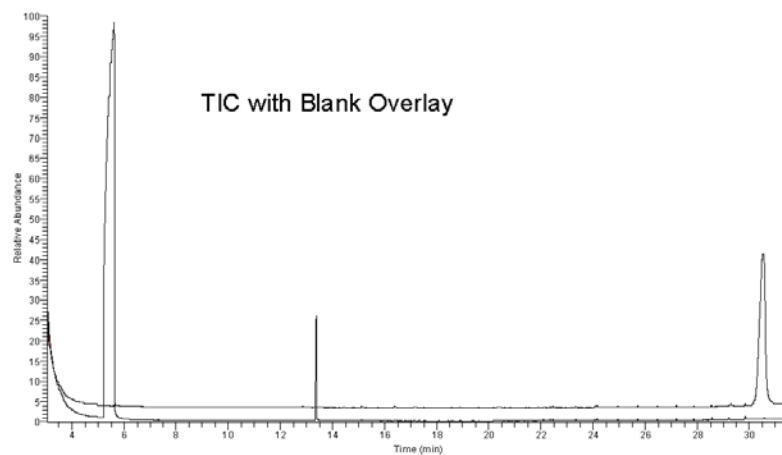
Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
DMSO	5.62	Not applicable
Benzylideneacetone	13.38	99.52

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

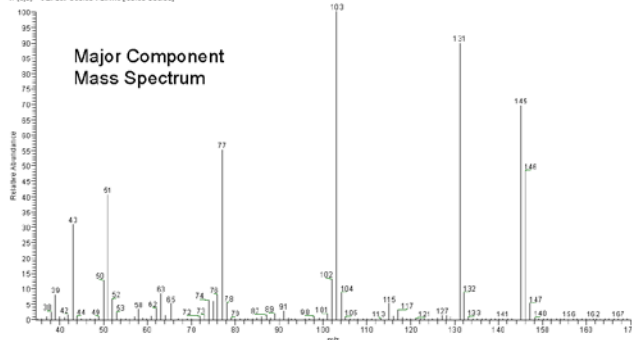
GC/MS Instrument Parameters:

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- 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	35 – 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 - 31.51 SM: 30



712419#271.7 RT: 13.38 AM: 1 SB: 2 1333 1342 NL: 20068
T: (E)-c Et dech-350.80 Full.ms [35.00-250.00]



NIST Reference Mass Spectrum

