

Chemical Information:

Name: Cyclohexanone
CAS No.: 108-94-1
Tox21_ID No.: Tox21_202121
NTP_CID No.: 663

Supplier: Sigma-Aldrich
Lot No.: 12419AD
MW: 98.14 g/mol

Date of Analysis: 24 October 2007

Purity and Identity Results:

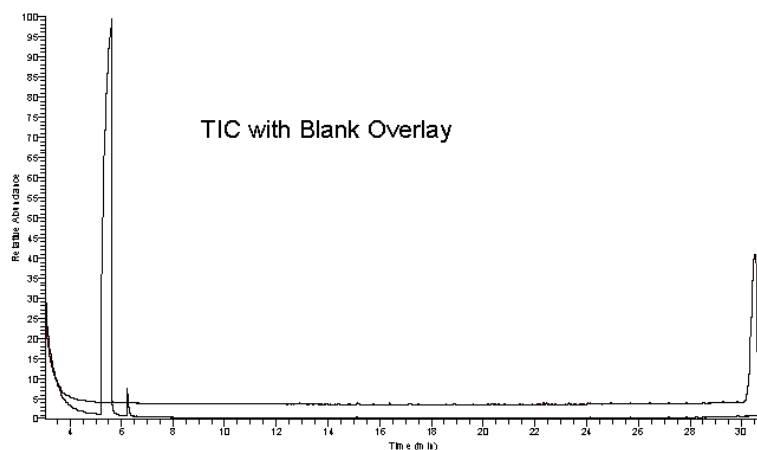
Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
DMSO	5.62	Not applicable
Cyclohexanone	6.23	99.70

^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: 36



DI: 24/11/06 RT: 6.23 AB: 1 NL: 9.36E5

T: (0.0) v: 0.0 w: 0.0000 F4: 0.00 F5: 0.000000

0 10 20 30 40 50 60 70 80 90 100

35 40 45 50 55 60 65 70 75 80 85 90 95 100

100 90 80 70 60 50 40 30 20 10 0

35 40 45 50 55 60 65 70 75 80 85 90 95 100

100 90 80 70 60 50 40 30 20 10 0

35 40 45 50 55 60 65 70 75 80 85 90 95 100

100 90 80 70 60 50 40 30 20 10 0

35 40 45 50 55 60 65 70 75 80 85 90 95 100

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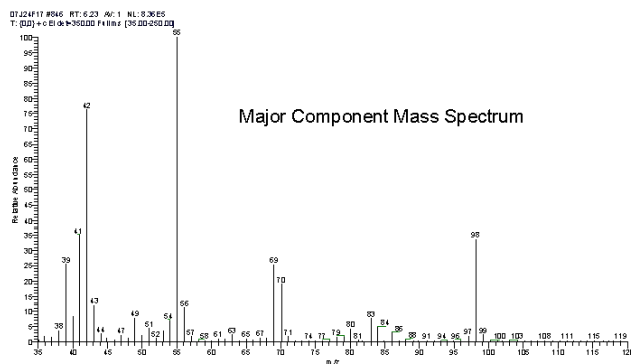
100 90 80 70 60 50 40 30 20 10 0

35 40 45 50 55 60 65 70 75 80 85 90 95 100

100 90 80 70 60 50 40 30 20 10 0

35 40 45 50 55 60 65 70 75 80 85 90 95 100

Major Component Mass Spectrum



NIST Reference Mass Spectrum

