

Chemical Information:

Name: 3-Pentenitrile
CAS No.: 4635-87-4
Tox21_ID No.: Tox21_200088
NTP_CID No.: 341

Supplier: Sigma-Aldrich
Lot No.: 321725/1
MW: 81.12 g/mol

Date of Analysis: 21 August 2007

Purity and Identity Results:

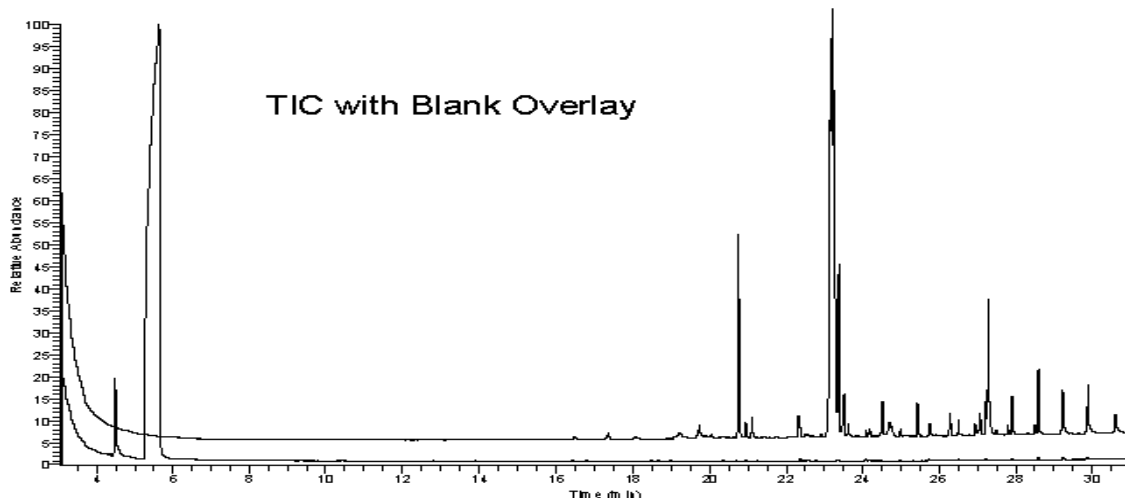
Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
unknown	4.37	0.87
3-Pentenitrile	4.48	98.36
DMSO	5.64	Not applicable

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

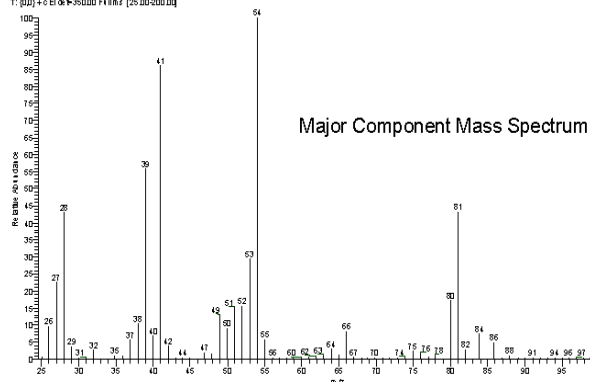
GC/MS Instrument Parameters:

Instrument / Ionization	Gas Chromatograph with 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	25 – 200 amu
Injector Temperature	250°C
Injection Volume / Mode	2 μ L / Splitless
Data Analysis Software	Xcalibur, v 1.2 and NIST Library v 1.7, build 11/5/1999

RT: 3.05 - 31.49 SM: 36



0712103 #078 RT: 4.48 AU: 1 NL: 2.8655
T: (0.0) +0.000000 Filter: (25.00-200.00)



NIST Reference
Mass Spectrum

