

Chemical Information:

Name: o-Nitroacetophenone

Date of Analysis: 11 July 2007

CAS No.: 577-59-3

Supplier: Sigma-Aldrich

Tox21_ID No.: Tox21_200072

Lot No.: 10604TR

NTP_CID No.: 1110

MW: 165.15 g/mol

Purity and Identity Results:

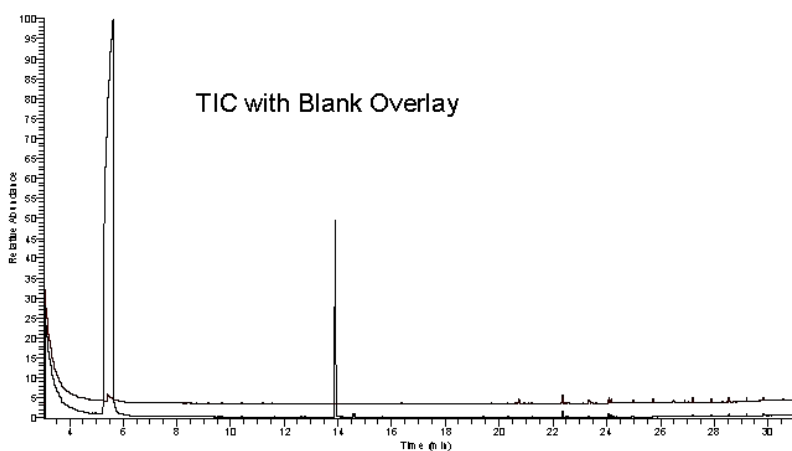
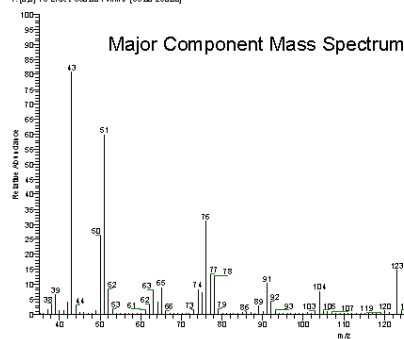
Peak Identity	Retention Time (min)	Purity (% Total Area) ^a	Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
DMSO	5.63	Not applicable	unknown	14.16	0.56
unknown	12.64	0.65	unknown	14.57	1.10
o-Nitroacetophenone	13.91	96.17	unknown	14.61	1.08

^a Peaks comprising ≥ 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-μm 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 μL / 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: 30


0191020_01012100722 #2048 RT: 13.91 AV: 1 NL: 3.0906
T: (0.0) +0.010-300.00 File # 2 (35.00-250.00)


NIST Reference Mass Spectrum

