

Chemical Information:

Name: 1-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-1-penten-3-one
CAS No.: 7779-30-8 Supplier: Sigma-Aldrich
Tox21_ID No.: Tox21_201216 Lot No.: S110305OB-7
NTP_CID No.: 4 MW: 206.32 g/mol

Date of Analysis: 13 August 2015

Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) ^a	Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
CAS 7779-30-8 ^b	26.48	70.84	Unknown	27.60	0.94
Unknown	25.55	2.20	CAS 127-43-5 ^c	27.91	20.54
Unknown	26.78	2.21	Unknown	28.23	1.73

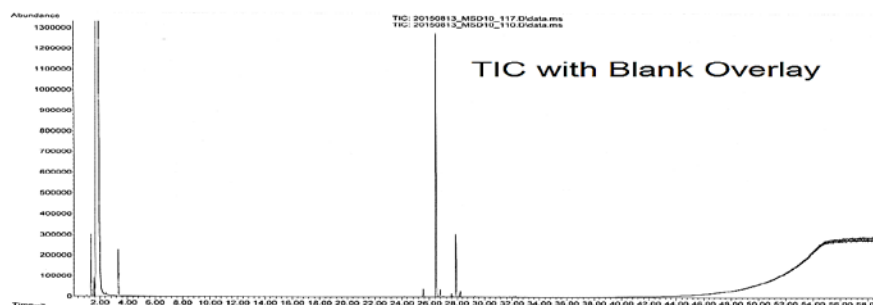
^a Peaks comprising $\geq 0.5\%$ of total area.

^b 1-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-1-penten-3-one

^c 1-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-1-penten-3-one

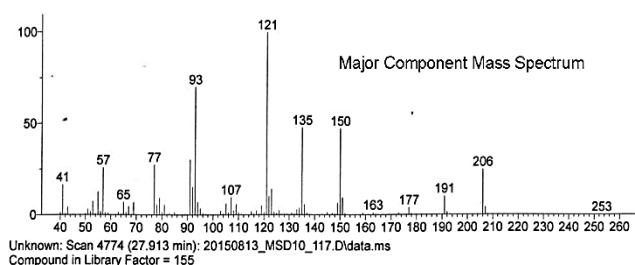
GC/MS Instrument Parameters:

Instrument / Ionization	Gas Chromatograph with Mass Spectrometer / Electron Impact
Solvent	Dichloromethane
Column	Rtx-5 MS, 30 m x 0.25 mm ID, 1- μ m film thickness
Carrier Gas	Helium at 2.0 mL/min
Oven Program	50°C, hold 0 min; ramp @ 5°C/min to 320°C, hold 5 min
Source Temperature	230°C
Auxiliary Temperature	250°C
Scan Range	40 – 550 amu
Injector Temperature	250°C
Injection Volume / Mode	1 μ L / Splitless
Data Analysis Software	MSD ChemStation, ver D.03.00.611, NIST Library ver 2.0d, build Dec 2005

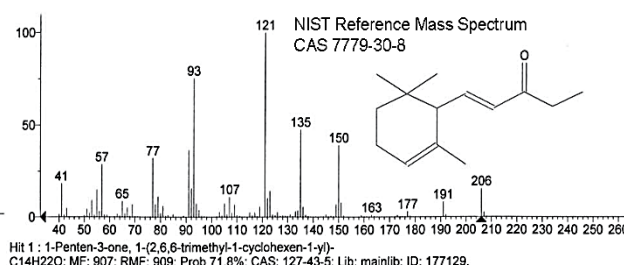


Unknown: Scan 4527 (26.474 min): 20150813_MSD10_117.D\data.ms (-4554)
Compound in Library Factor = 273

Hit 1: 1-Penten-3-one, 1-(2,6,6-trimethyl-2-cyclohexen-1-yl)-
C14H22O; MF: 941; RMF: 941; Prob 89.7%; CAS: 7779-30-8; Lib: mainlib; ID: 102833.



Unknown: Scan 4774 (27.913 min): 20150813_MSD10_117.D\data.ms
Compound in Library Factor = 155



Hit 1: 1-Penten-3-one, 1-(2,6,6-trimethyl-1-cyclohexen-1-yl)-
C14H22O; MF: 907; RMF: 909; Prob 71.8%; CAS: 127-43-5; Lib: mainlib; ID: 177129.

