

Chemical Information:

Name: 1-Iodohexadecane

Date of Analysis: 16 December 2016

CAS No.: 544-77-4

Supplier: Sigma-Aldrich

Tox21_ID No.: Tox21_202845

Lot No.: 15614AJV

NTP_CID No.: 6225

MW: 352.34 g/mol

Purity and Identity Results:

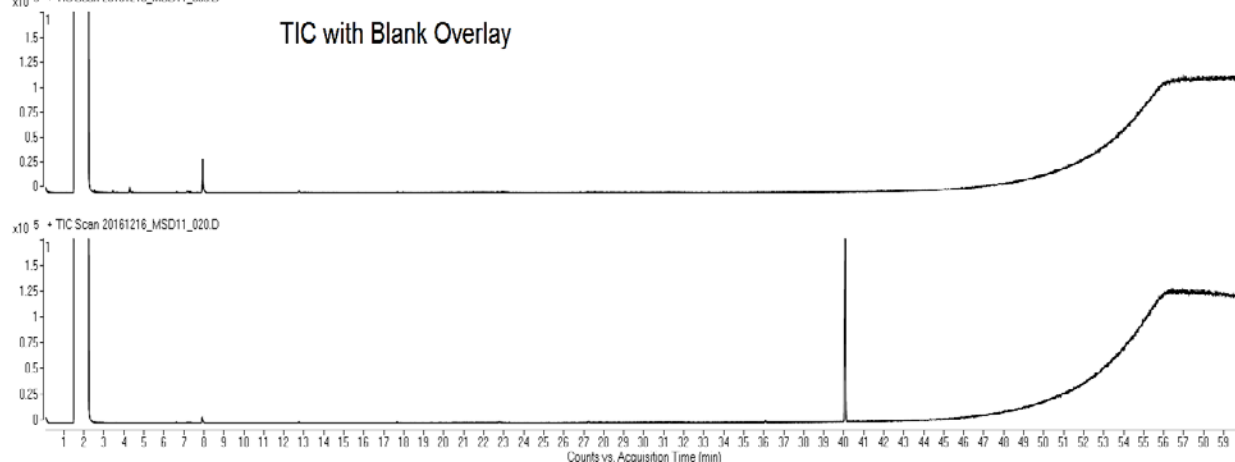
Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
Unknown	22.77	0.71
Unknown	27.24	0.64
Unknown	36.08	0.66
1-Iodohexadecane	40.07	97.99

^a Peaks comprising ≥ 0.5% of total area.

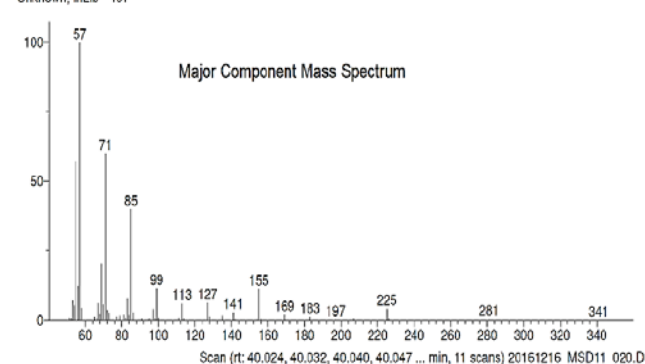
GC/MS Instrument Parameters:

Instrument / Ionization	Gas Chromatograph with Mass Spectrometer / Electron Impact
Solvent	Acetone
Column	Rtx-5 MS, 30 m x 0.25 mm ID, 1-μm film thickness
Carrier Gas	Helium at 1.5 mL/min
Oven Program	50°C, hold 2 min; ramp @ 5°C/min to 315°C, hold 5 min
Source Temperature	230°C
Auxiliary Temperature	250°C
Scan Range	50 – 400 amu
Injector Temperature	250°C
Injection Volume / Mode	1 μL / Splitless
Data Analysis Software	MassHunter GC/MS Acquisition B.07.02.1938 / MassHunter Qualitative Analysis B.07.00 Build 7.0.7024.0 / NIST Library Version 2.2f Build 2014

x10 5 • TIC Scan 20161216_MSD11_003.D



Unknown; InLib=197


Hexadecane, 1-iodo-
C16H33I; MF: 796; RMF: 800; Prob 1.61%; CAS: 544-77-4; Lib: mainlib; ID: 22883.
