

Chemical Information:

Name: Ethanone, 1-[(3R,3aR,7R,8aS)-2,3,4,7,8,8a-hexahydro-3,6,8,8-tetramethyl-1H-3a,7-methanoazulen-5-yl]-

Date of Analysis: 01 November 2016

CAS No.: 32388-55-9

Supplier: Sigma Aldrich

Tox21_ID No.: Tox21_202194

Lot No.: 08206PI

NTP_CID No.: 3751

MW: 246.39 g/mol

Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) ^a	Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
unknown	33.59	0.96	unknown	35.25	2.00
unknown	33.81	0.59	unknown	35.47	1.88
unknown	33.91	0.50	unknown	35.65	0.92
unknown	34.68	2.95	unknown	35.75	0.52
CAS# 32388-58-2 ^b	34.80	7.11	unknown	36.23	1.58
CAS# 32388-55-9	34.91	65.38	unknown	36.30	2.40
unknown ^c	35.16	6.90	unknown	36.63	2.42

^a Peaks comprising ≥ 0.5% of total area.

^b Ethanone, 1-(1,2,3,4,7,7a-hexahydro-1,4,4,5-tetramethyl-1,3a-ethano-3aH-inden-6-yl)-

^c Component was not identified; however, mass spectrum is similar to components at 34.80 and 34.91 minutes

GC/MS Instrument Parameters:

Instrument / Ionization	Gas Chromatograph with Mass Spectrometer / Electron Impact
Solvent	Methanol
Column	Restek Rtx-5MS with Integra-Guard, 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	40 – 650 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 2.2 Build 2014

