

### Chemical Information:

Name: Ethanone, 1-(1,2,3,4,5,6,7,8-octahydro-2,3,8,8-tetramethyl-2-naphthalenyl)-  
 Date of Analysis: 25 March 2010  
 CAS No.: 54464-57-2 Supplier: Toronto Research Chemicals  
 Tox21\_ID No.: Tox21\_201355 Lot No.: 15-SSR-21-1  
 NTP\_CID No.: 880 MW: 234.38 g/mol

### Purity and Identity Results:

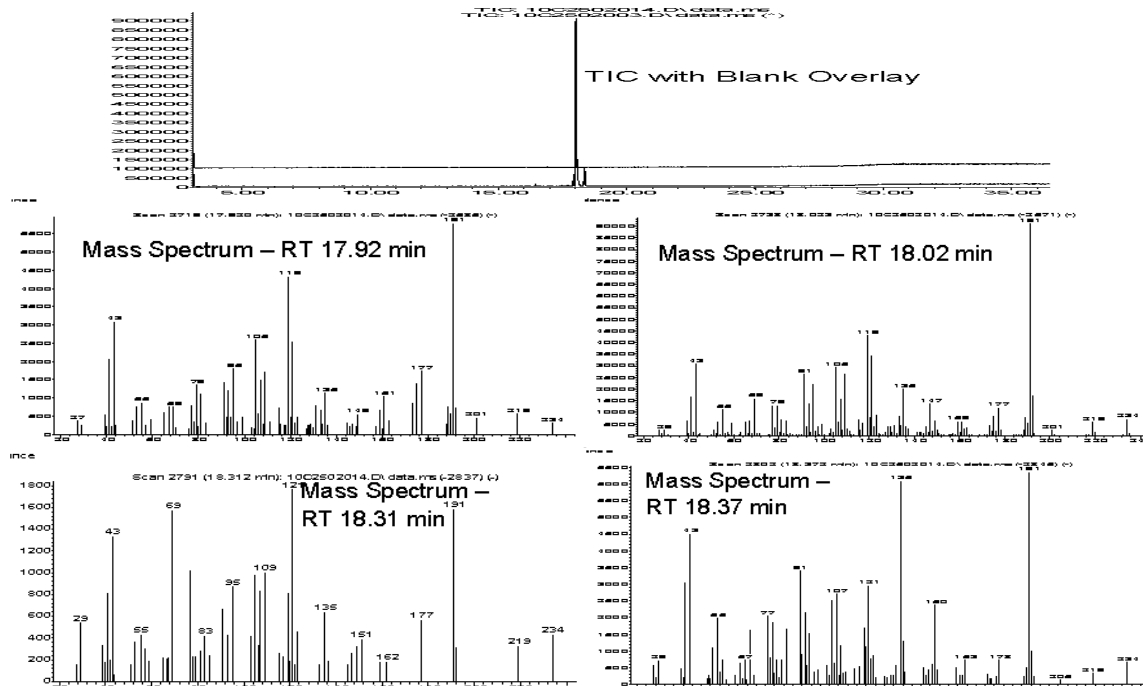
Peak Identity	Retention Time (min)	Purity (% Total Area) <sup>a</sup>	Peak Identity	Retention Time (min)	Purity (% Total Area) <sup>a</sup>
54464-57-2	17.92	4.56	54464-57-2	18.31	1.71
54464-57-2	18.02	86.53	54464-57-2	18.37	7.21

<sup>a</sup> Peaks comprising ≥ 0.5% of total area.

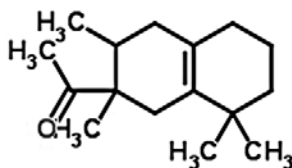
Similar mass spectra indicate the components are isomers, totaling 100%.

### GC/MS Instrument Parameters:

Instrument / Ionization	Gas Chromatograph with Mass Spectrometer / Electron Impact
Solvent	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 7 min
Source Temperature	230°C
Auxiliary Temperature	250°C
Scan Range	25 – 500 amu
Injector Temperature	250°C
Injection Volume / Mode	1 μL / Split (100:1)
Data Analysis Software	MSD Chemstation, v E.02.00.SP2 and NIST Library v 2.0f, build 10/8/2008



Mass ion (C<sub>16</sub>H<sub>26</sub>O) = m/z 234



m/z	Fragment	m/z	Fragment
219	C <sub>15</sub> H <sub>23</sub> O	105	C <sub>8</sub> H <sub>9</sub>
191	C <sub>14</sub> H <sub>23</sub>	91	C <sub>7</sub> H <sub>7</sub>
121	C <sub>9</sub> H <sub>13</sub>	55	C <sub>4</sub> H <sub>7</sub>
119	C <sub>9</sub> H <sub>11</sub>	43	C <sub>2</sub> H <sub>3</sub> O