

### Chemical Information:

Name: Melatonin  
CAS No.: 73-31-4  
Tox21\_ID No.: Tox21\_201527  
NTP\_CID No.: 932

Supplier: Sigma-Aldrich  
Lot No.: 068K1538  
MW: 232.28g/mol

Date of Analysis: 29 June 2016

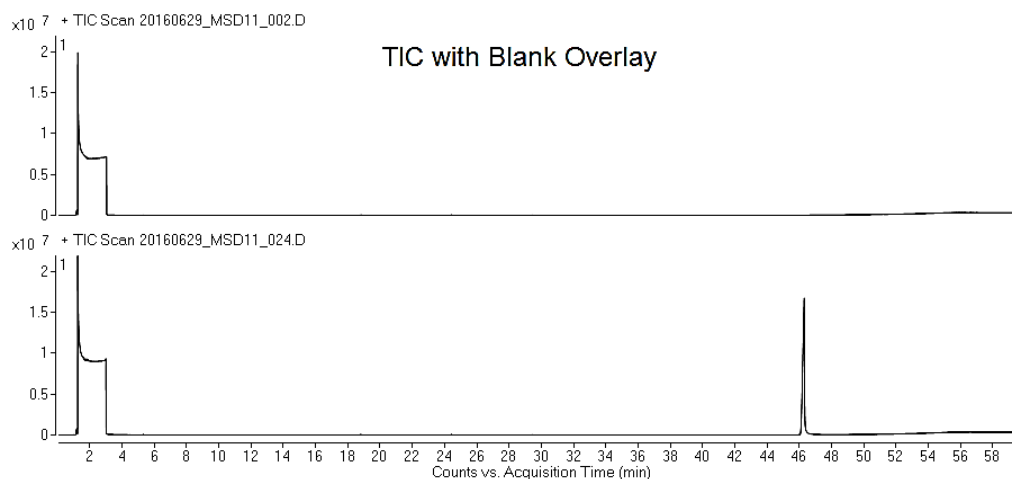
### Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) <sup>a</sup>
Melatonin	46.30	100.00

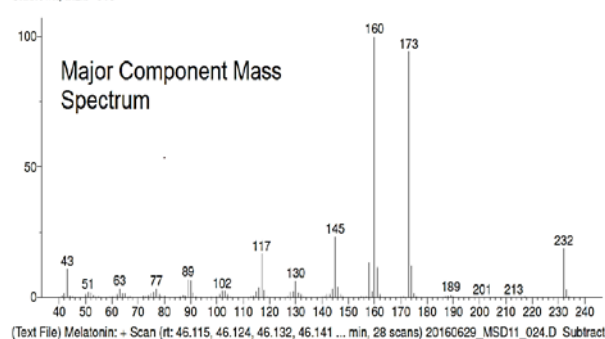
<sup>a</sup> Peaks comprising  $\geq 0.5\%$  of total area.

### GC/MS Instrument Parameters:

Instrument / Ionization	Gas Chromatograph with Mass Spectrometer / Electron Impact
Solvent	Ethanol
Column	Rtx-5 MS, 30 m x 0.25 mm ID, 1- $\mu$ m film thickness
Carrier Gas	Helium at 2.0 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 – 800 amu
Injector Temperature	250°C
Injection Volume / Mode	1 $\mu$ L / 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



Unknown; InLib=515



Hit 1: Melatonin  
C<sub>13</sub>H<sub>16</sub>N<sub>2</sub>O<sub>2</sub>; MF: 952; RMF: 955; Prob 93.8%; CAS: 73-31-4; Lib: repLib; ID: 21161.

