

# Chemical Information:

Name: 3-Methylcholanthrene

Date of Analysis: 14 December 2016

CAS No.: 56-49-5

Supplier: Sigma-Aldrich

Tox21\_ID No.: Tox21\_202592

Lot No.: MKBB1176

NTP\_CID No.: 4464

MW: 268.35 g/mol

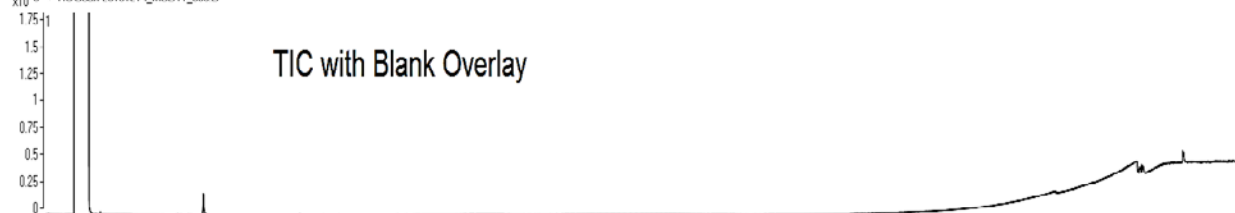
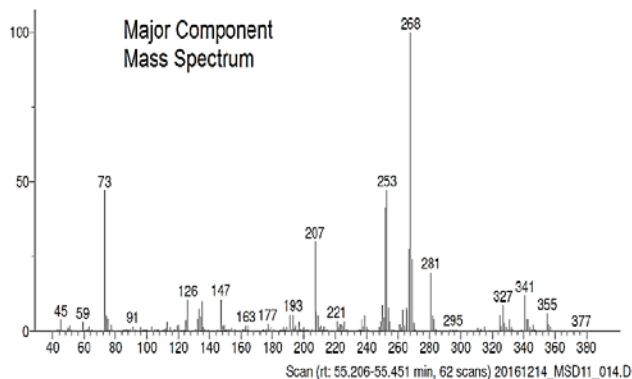
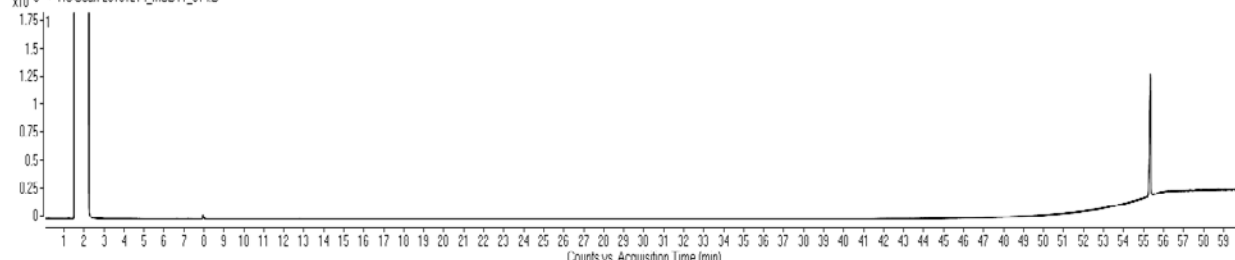
## Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) <sup>a</sup>
3-Methylcholanthrene	55.33	100.00

<sup>a</sup> 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	40 – 380 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<sup>6</sup> • TIC Scan 20161214\_MSD11\_003.D

x10<sup>6</sup> • TIC Scan 20161214\_MSD11\_014.D

Hit 1: 3-Methylcholanthrene  
C21H16; MF: 682; RMF: 836; Prob 22.8%; CAS: 56-49-5; Lib: replib; ID: 26794.
