

Chemical Information:

Name: 1-Benzoylacetone
CAS No.: 93-91-4
Tox21_ID No.: Tox21_202879
NTP_CID No.: 6311

Supplier: Sigma-Aldrich
Lot No.: 06702MH
MW: 162.19 g/mol

Date of Analysis: 16 December 2016

Purity and Identity Results:

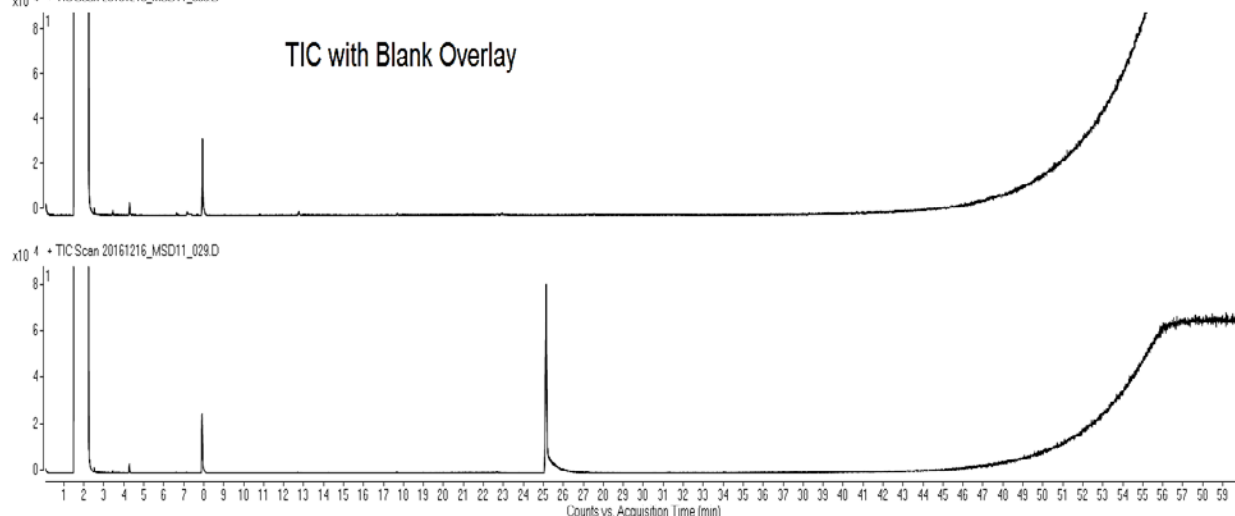
Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
1-Benzoylacetone	25.14	100.00

^a Peaks comprising $\geq 0.5\%$ of total area.

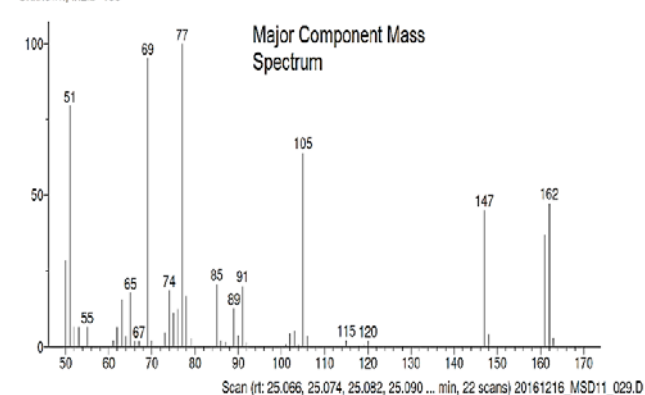
GC/MS Instrument Parameters:

Instrument / Ionization	Gas Chromatograph with Mass Spectrometer / Electron Impact
Solvent	Acetone
Column	Rtx-5 MS, 30 m x 0.25 mm ID, 1- μ m 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 μ 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 2.2f Build 2014

x10⁴ • TIC Scan 20161216_MSD11_003.D



Unknown; InLib=166



Hit 1: 1,3-Butanedione, 1-phenyl-
C10H10O2; MF: 847; RMF: 847; Prob 52.3%; CAS: 93-91-4; Lib: replib; ID: 13853.

