

# Chemical Information:

Name: Vanillin  
CAS No.: 121-33-5  
Tox21\_ID No.: Tox21\_201925  
NTP\_CID No.: 1393

Supplier: Sigma-Aldrich  
Lot No.: 01802PC  
MW: 152.15 g/mol

Date of Analysis: 14 September 2007

## Purity and Identity Results:

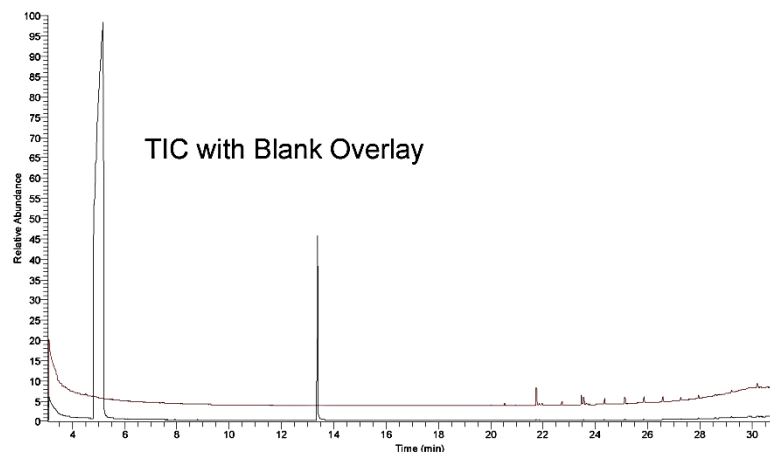
Peak Identity	Retention Time (min)	Purity (% Total Area) <sup>a</sup>
DMSO	5.17	Not applicable
Vanillin	13.38	99.46

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

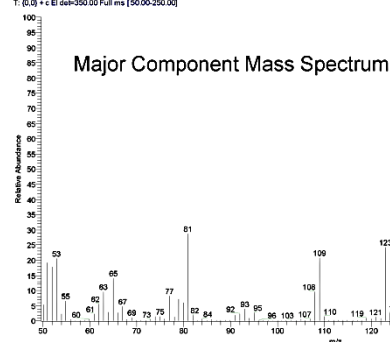
## GC/MS Instrument Parameters:

Instrument / Ionization	ThermoFinnigan TraceGC with ThermoFinnigan TraceMS / Electron Impact
Solvent	Dichloromethane (100 mM in DMSO, diluted 1/1000 with dichloromethane)
Column	J&W Scientific HP-5MS, 30 m x 0.25 mm ID, 0.25- $\mu$ m 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 2 min
Source Temperature	250°C
Auxiliary Temperature	250°C
Scan Range	50 – 250 amu
Injector Temperature	250°C
Injection Volume / Mode	2 $\mu$ L / Splitless
Run Time	31.5 minutes
Data Analysis Software	Xcalibur, v 1.2 and NIST Library v 1.7, build 11/5/1999

RT: 3.05 - 31.50 SM 3G



07111628 #1245 RT: 13.38 AU: 1 NL: 1.8058  
T: (0.0) \* c EI det-350.00 Full.ms [5000-250.00]



NIST Reference Mass Spectrum

