

### Chemical Information:

Name: Methyl coumarin  
CAS No.: 92-48-8  
Tox21\_ID No.: Tox21\_201810  
NTP\_CID No.: 417

Supplier: Sigma-Aldrich  
Lot No.: 10117PB  
MW: 160.17 g/mol

Date of Analysis: 26 September 2007

### Purity and Identity Results:

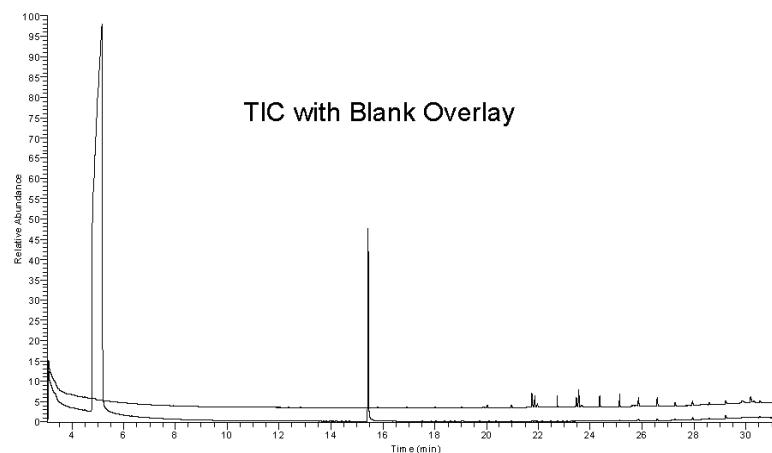
Peak Identity	Retention Time (min)	Purity (% Total Area) <sup>a</sup>
DMSO	5.16	Not applicable
Methyl coumarin	15.42	99.05
Unknown	19.03	0.51

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

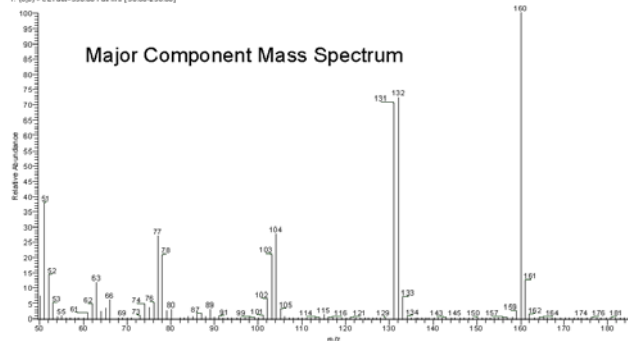
### GC/MS Instrument Parameters:

Instrument / Ionization	Gas Chromatograph / Mass Spectrometer / 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: 30



07/26/07 #1490 RT: 15.42 AUC: 1 NL: 27768  
T: 0.001 v: 0.01 (0.001) Full MS (100.00-250.00)



### NIST Reference Mass Spectrum

