

### Chemical Information:

Name: Methylbenzoate  
CAS No.: 93-58-3  
Tox21\_ID No.: Tox21\_201832  
NTP\_CID No.: 948

Supplier: Sigma-Aldrich  
Lot No.: 08309PC  
MW: 136.15 g/mol

Date of Analysis: 28 March 2007

### Purity and Identity Results:

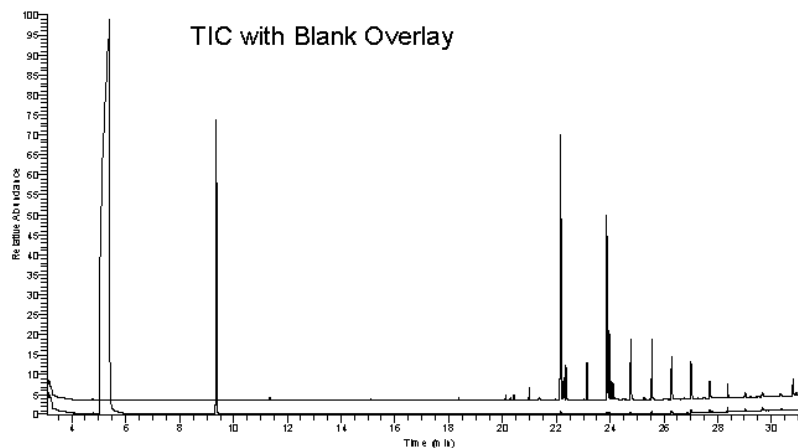
| Peak Identity  | Retention Time (min) | Purity (% Total Area) <sup>a</sup> |
|----------------|----------------------|------------------------------------|
| DMSO           | 5.43                 | Not applicable                     |
| Methylbenzoate | 9.36                 | 99.42                              |

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

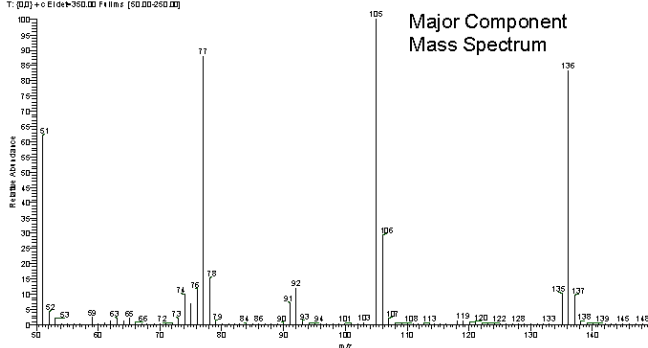
### GC/MS Instrument Parameters:

|                         |  |
|-------------------------|--|
| 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: 30



07-02814 #163 RT: 9.36 AM: 1 NL: 3.8566  
T: (02) +0-0100-300.00 File: 07-02814-001.D



NIST Reference Mass Spectrum

