

# Chemical Information:

Name: Theophylline  
CAS No.: 58-55-9  
Tox21\_ID No.: Tox21\_202375  
NTP\_CID No.: 1343

Supplier: Sigma  
Lot No.: 124K0570  
MW: 180.16 g/mol

Date of Analysis: 10 July 2007

## Purity and Identity Results:

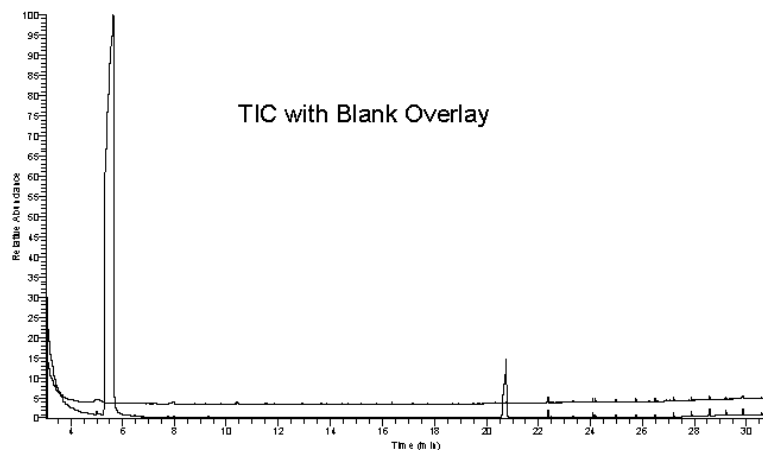
| Peak Identity | Retention Time (min) | Purity (% Total Area) <sup>a</sup> |
|---------------|----------------------|------------------------------------|
| DMSO          | 5.65                 | Not applicable                     |
| Theophylline  | 20.77                | 98.72                              |

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

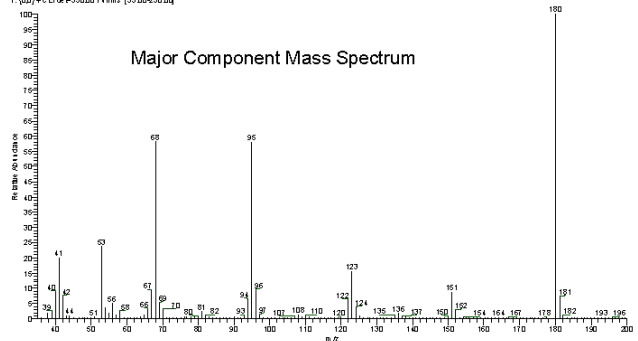
## GC/MS Instrument Parameters:

|                         |  |
|-------------------------|--|
| 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              | 35 – 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 - 31.49 S.M. 35



0101005 P4674 RT: 20.76 AU: 1.16485  
T: (0.0) + e- EI 6.30000 FWHM: [35.00-250.00]



NIST Reference Mass Spectrum

