

# Chemical Information:

Name: 1-Phenyl-3-methyl-5-pyrazolone  
CAS No.: 89-25-8 Supplier: Sigma-Aldrich  
Tox21\_ID No.: Tox21\_201747 Lot No.: 08210ED  
NTP\_CID No.: 08210ED MW: 174.20 g/mol

Date of Analysis: 16 August 2007

# Purity and Identity Results:

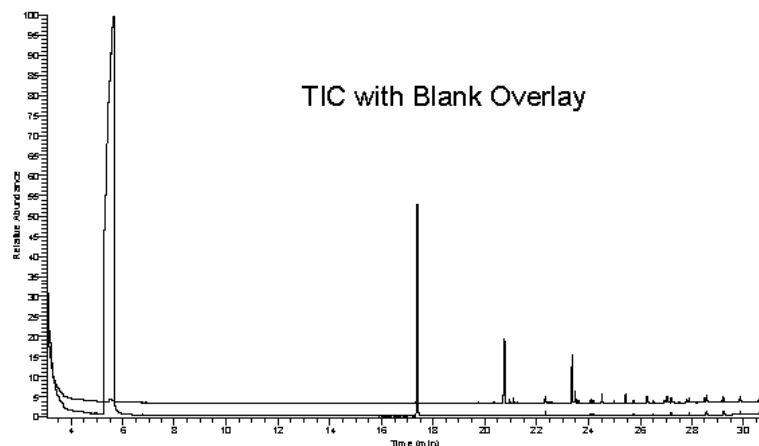
Peak Identity	Retention Time (min)	Purity (% Total Area) <sup>a</sup>
DMSO	5.66	Not applicable
1-Phenyl-3-methyl-5-pyrazolone	17.40	99.97

<sup>a</sup> Peaks comprising ≥ 0.5% of total area.

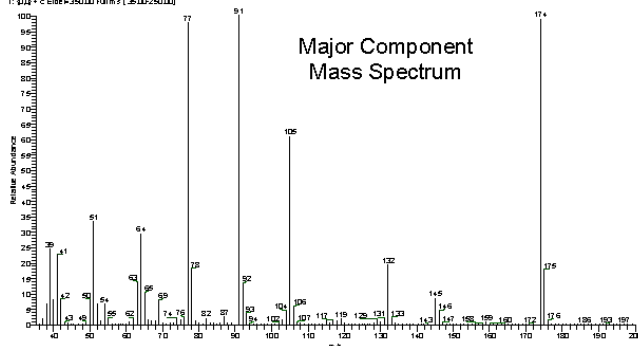
# GC/MS Instrument Parameters:

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-μm 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 μL / 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 - 31.51 SM: 30



07/16/07 07:07 RT: 17.39 AU: 1 NL: 3.0006  
T: 0.02 - c: 0.000000 Full Scan (35.000-250.00)



NIST Reference  
Mass Spectrum

