

Chemical Information:

Name: Phenylbutazone
CAS No.: 50-33-9
Tox21_ID No.: Tox21_201809
NTP_CID No.: 1186

Supplier: Sigma-Aldrich
Lot No.: 124K1625
MW: 308.37 g/mol

Date of Analysis: 28 June 2007

Purity and Identity Results:

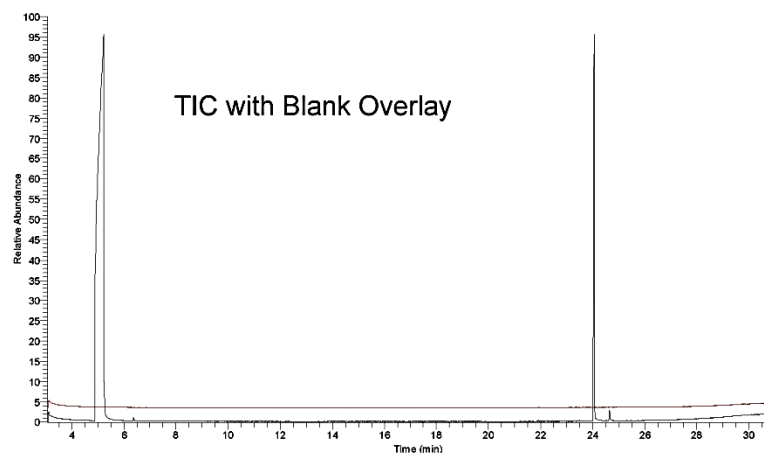
Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
DMSO	5.23	Not applicable
Phenylbutazone	24.06	96.98
unknown	24.65	2.74

^a Peaks comprising ≥ 0.5% of total area.

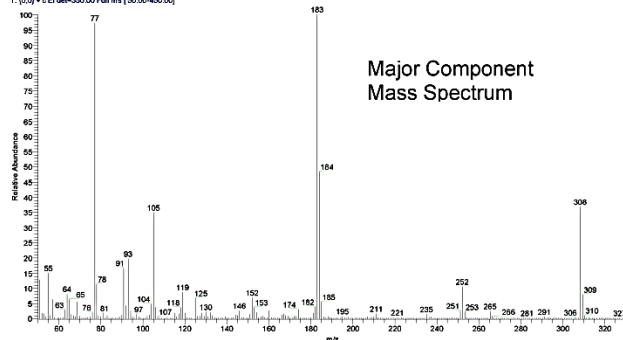
GC/MS Instrument Parameters:

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	50 – 450 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 - 31.52 SM 3G



070306 #2525 RT: 24.05 AU: 1 NL: 3.4868
T: (0.0) * e El det=350.00 Full ms [50.00-450.00]



NIST Reference Mass Spectrum

