

Chemical Information:

Name: 3-Propylidenephthalide
 CAS No.: 17369-59-4 Supplier: Sigma-Aldrich
 Tox21_ID No.: Tox21_201206 Lot No.: 11205DD
 NTP_CID No.: 344 MW: 174.20 g/mol

Date of Analysis: 14 August 2007

Purity and Identity Results:

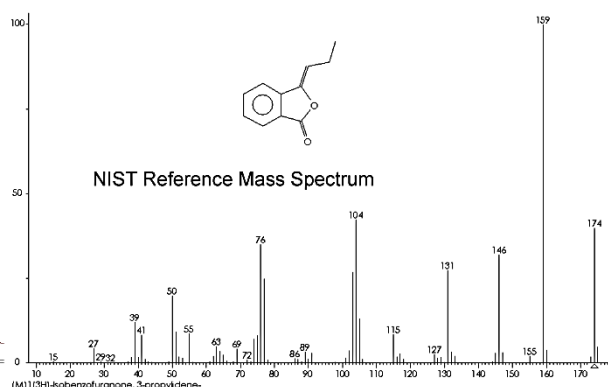
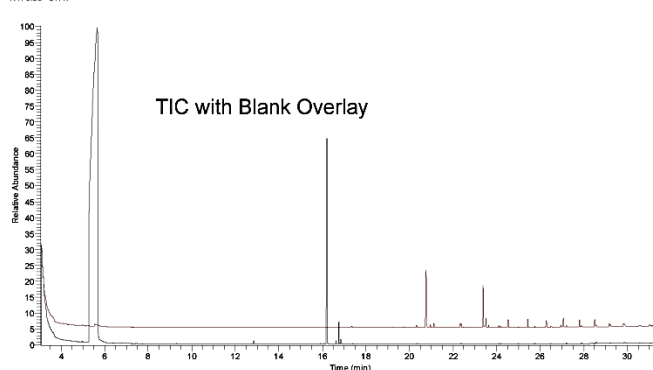
Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
DMSO	5.67	Not applicable
3-Propylidenephthalide	16.21	87.57
3-Propylidenephthalide	16.76	8.58

^a Peaks comprising $\geq 0.5\%$ of total area.

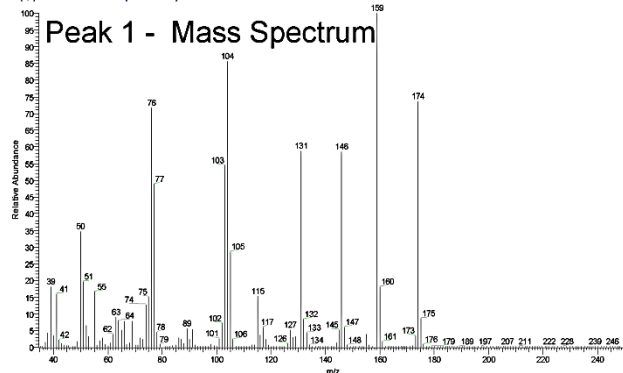
GC/MS Instrument Parameters:

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- μ 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 μ 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 - 31.47



071454 #0460 RT: 16.21 Av: 1 NL: 3.00E5
 T: (0.0) + c B de3-350.00 Full ms [35.00-250.00]



071454 #0603 RT: 16.76 Av: 1 NL: 6.03E5
 T: (0.0) + c B de3-350.00 Full ms [35.00-250.00]

