

Chemical Information:

Name: 4,7-Methanoisobenzofuran-1,3-dione,
3a,4,7,7a-tetrahydromethyl-, (3aR,4S,7R,7aS)-rel-
CAS No.: 25134-21-8 Supplier: Sigma Aldrich
Tox21_ID No.: Tox21_201205 Lot No.: 1317283
NTP_CID No.: 3246 MW: 178.18 g/mol

Date of Analysis: 03 August 2015

Purity and Identity Results:

Peak Identity ^a	Retention Time (min)	Purity (% Total Area) ^b	Peak Identity ^a	Retention Time (min)	Purity (% Total Area) ^b
Acetone	1.50	Not Applicable	Peak 1	23.16	4.89
Unknown	2.76	1.67	Peak 2	23.94	5.51
Unknown	2.82	1.41	Peak 3	24.76	45.30
			Peak 4	25.03	39.06

^a Peaks 1-4 were identified as isomers of 4,7-methanoisobenzofuran-1,3-dione, 3a,4,7,7a-tetrahydromethyl-

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

GC/MS Instrument Parameters:

Instrument / Ionization	Gas Chromatograph with Mass Spectrometer / Electron Impact
Solvent	Acetone (~ 400 $\mu\text{g/mL}$)
Column	Restek Rtx-5MS with Integra-Guard, 30 m x 0.25 mm ID, 1- μm film thickness
Carrier Gas	Helium at 2 mL/min
Oven Program	50°C, hold 2 min; ramp @ 5°C/min to 320°C, hold 5 min
Source Temperature	230°C
Auxiliary Temperature	250°C
Scan Range	40 – 600 amu
Injector Temperature	250°C
Injection Volume / Mode	1 μL / Split (10:1)
Data Analysis Software	MassHunter GC/MS Acquisition B.07.02.1938 / Chemstation Enhanced Data Analysis F.01.01.2317 / NIST Library Version 2.2 Build 2014

