

Chemical Information:

Name: 1,2,5,6,9,10-Hexabromocyclododecane Date of Analysis: 29 June 2016
CAS No.: 3194-55-6 Supplier: Sigma-Aldrich
Tox21_ID No.: Tox21_201402 Lot No.: MKAA0776
NTP_CID No.: 3043 MW: 641.70 g/mol

Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) ^a	Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
unknown	21.64	1.16	unknown	42.50	0.61
unknown	22.49	1.68	unknown	47.59	3.93
unknown	23.04	0.63	unknown	47.96	6.59
unknown	35.78	0.64	3194-55-6 ^b	52.22	4.19
unknown	36.52	0.94	unknown	52.48	0.84
unknown	36.74	1.07	unknown	52.59	1.96
unknown	36.92	1.37	3194-55-6 ^b	57.38	73.91

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

^b Two components were identified as the target, based on mass spectra, possibly isomers. Reported purity of the combined components: 78.10%.

GC/MS Instrument Parameters:

Instrument / Ionization	Gas Chromatograph with Mass Spectrometer / Electron Impact
Solvent	Ethanol
Column	Rtx-5 MS, 30 m x 0.25 mm ID, 1- μ m film thickness
Carrier Gas	Helium at 2.0 mL/min
Oven Program	50°C, hold 2 min; ramp @ 5°C/min to 315°C, hold 5 min
Source Temperature	230°C
Auxiliary Temperature	250°C
Scan Range	40 – 800 amu
Injector Temperature	250°C
Injection Volume / Mode	1 μ L / Splitless
Data Analysis Software	MassHunter GC/MS Acquisition B.07.02.1938 / MassHunter Qualitative Analysis B.07.00 Build 7.0.7024.0 / NIST Library Version 2.2 Build 2014

