

Chemical Information:

Name: Organofunctional Silane 45-49
CAS No.: 82985-35-1 Supplier: Sigma-Aldrich
Tox21_ID No.: Tox21_200368 Lot No.: 76197MJ
NTP_CID No.: 1125 MW: 341.55 g/mol

Date of Analysis: 13 May 2010

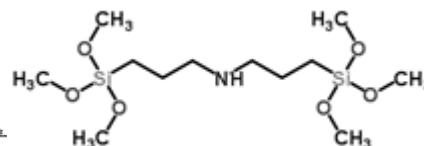
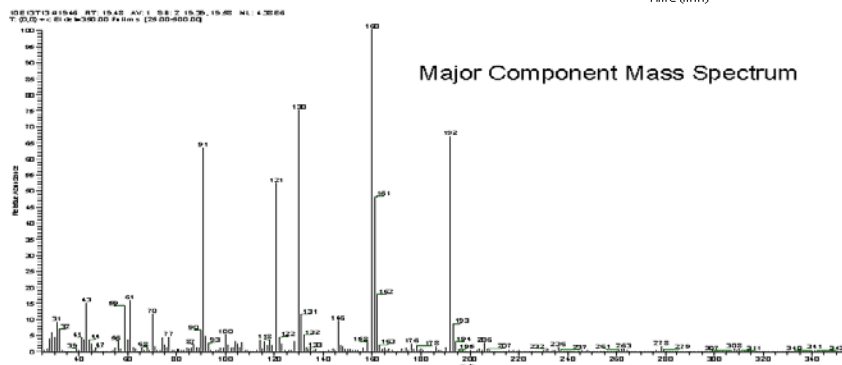
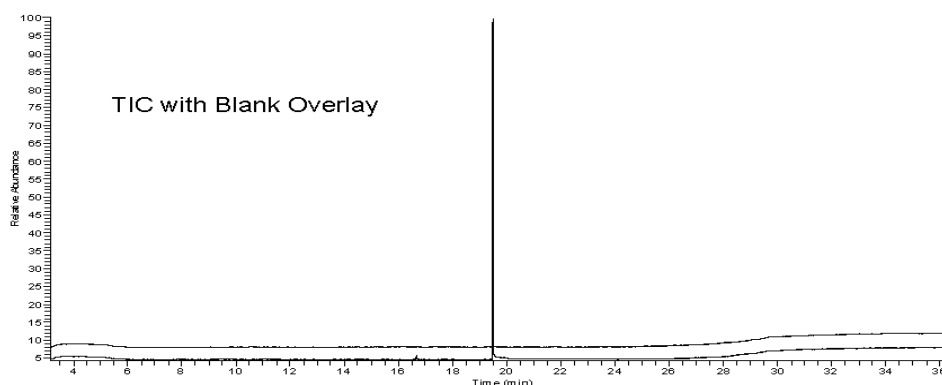
Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
unknown	16.68	1.59
Organofunctional Silane 45-49	19.48	98.41

^a Peaks comprising ≥ 0.5% of total area.

GC/MS Instrument Parameters:

Instrument / Ionization	Gas Chromatograph with Mass Spectrometer / Electron Impact
Solvent	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 7 min
Source Temperature	250°C
Auxiliary Temperature	250°C
Scan Range	25 – 500 amu
Injector Temperature	250°C
Injection Volume / Mode	1 μL / Split (100:1)
Data Analysis Software	Xcalibur ver 1.2, and NIST Library ver 2.0f, build 10/08/2008



Mass Ion (C₁₂H₃₁NO₆Si₂) = m/z 341

m/z	Fragment	m/z	Fragment
192	C ₇ H ₁₈ NO ₃ Si	121	C ₃ H ₉ O ₃ Si
160	C ₆ H ₁₄ NO ₂ Si	91	C ₂ H ₇ O ₂ Si
130	C ₄ H ₈ NO ₂ Si	31	CH ₃ O