SUPPLEMENTAL INFORMATION

Trisaminohexyl Isocyanurate, a Urinary Biomarker of HDI Isocyanurate Exposure

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Table S1. Gradient program for the NanoAcquity ultra-performance liquid chromatography system (Waters Corp., Milford, MA) using a Symmetry C18 trapping column, 5 μm, 180 μm × 20 mm (Waters Corp.) and an Atlantis dC18 analytical column, 3 μm, 100 μm × 100 mm (Waters Corp.). Mobile phase A consisted of 0.1% formic acid in deionized water and mobile phase B consisted of 0.1% formic acid in acetonitrile.

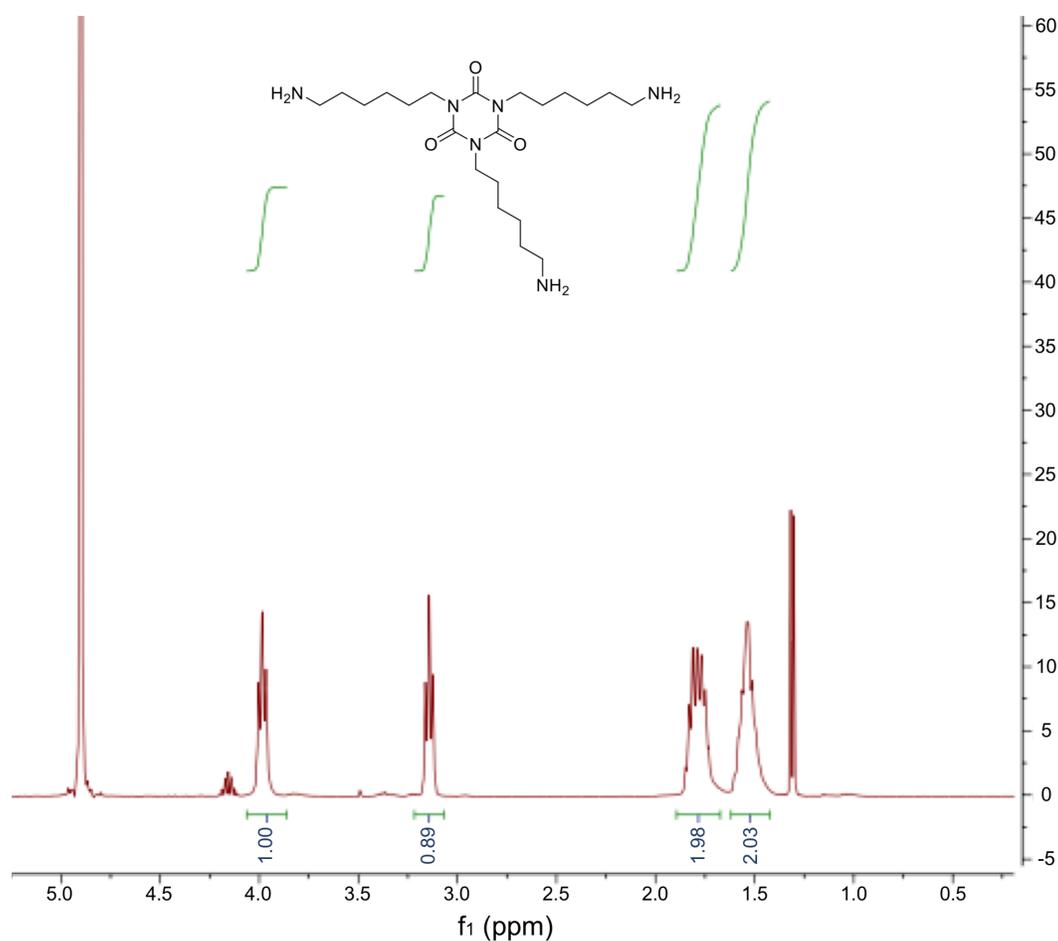| Mobile Phase A	Mobile Phase B	Time (min)	Flow Rate (nL/min)
95	5	0	600
10	90	17	600
10	90	29	600
95	5	30	600
95	5	44	600

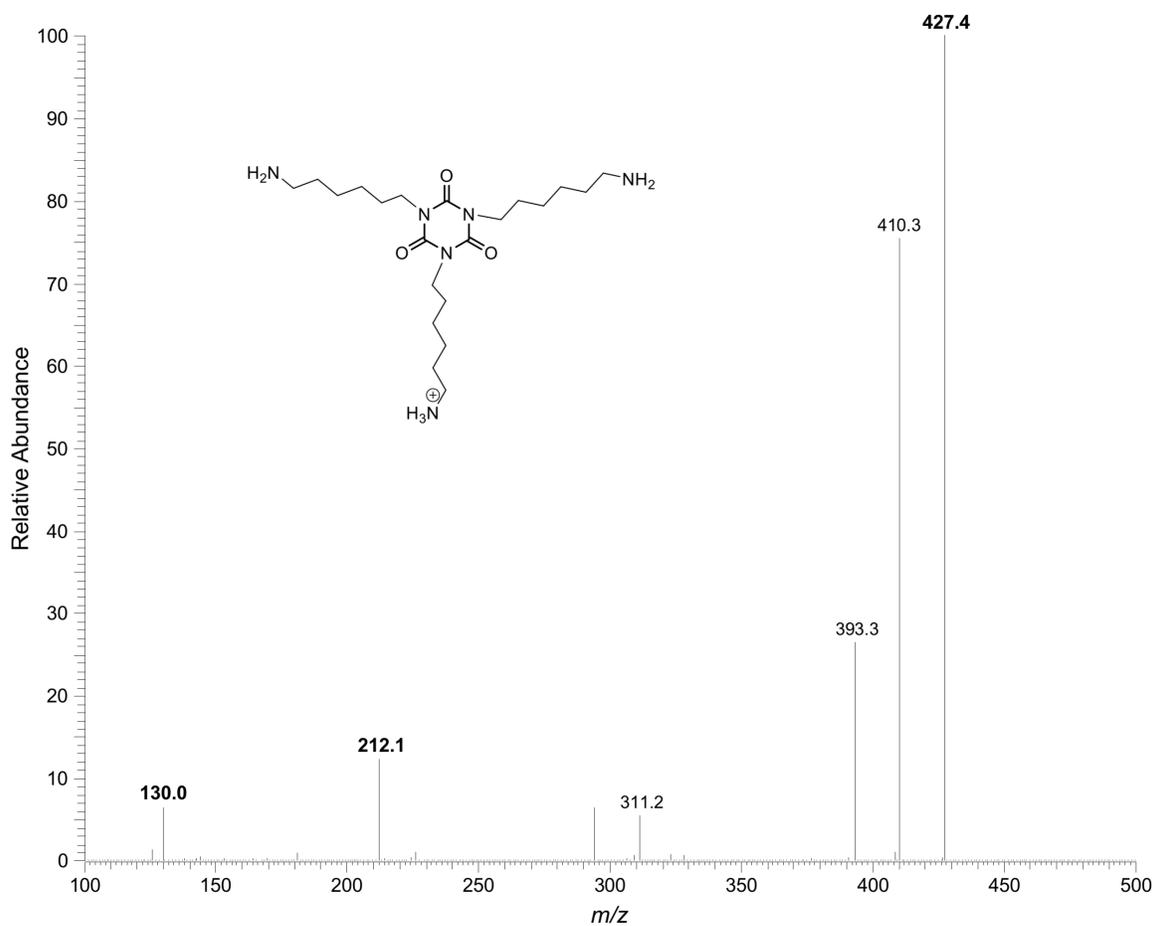**Figure S1**. Proton nuclear magnetic resonance spectrum for TAHI.

Figure S2. Fragmentation spectrum of precursor ion [M + H]⁺ for TAHI (*m/z* 427.3) obtained by nano-UPLC-ESI-MS/MS operated in positive ion-mode with nano-electrospray ionization (scan range, *m/z* 100-500; collision energy, 25 eV).
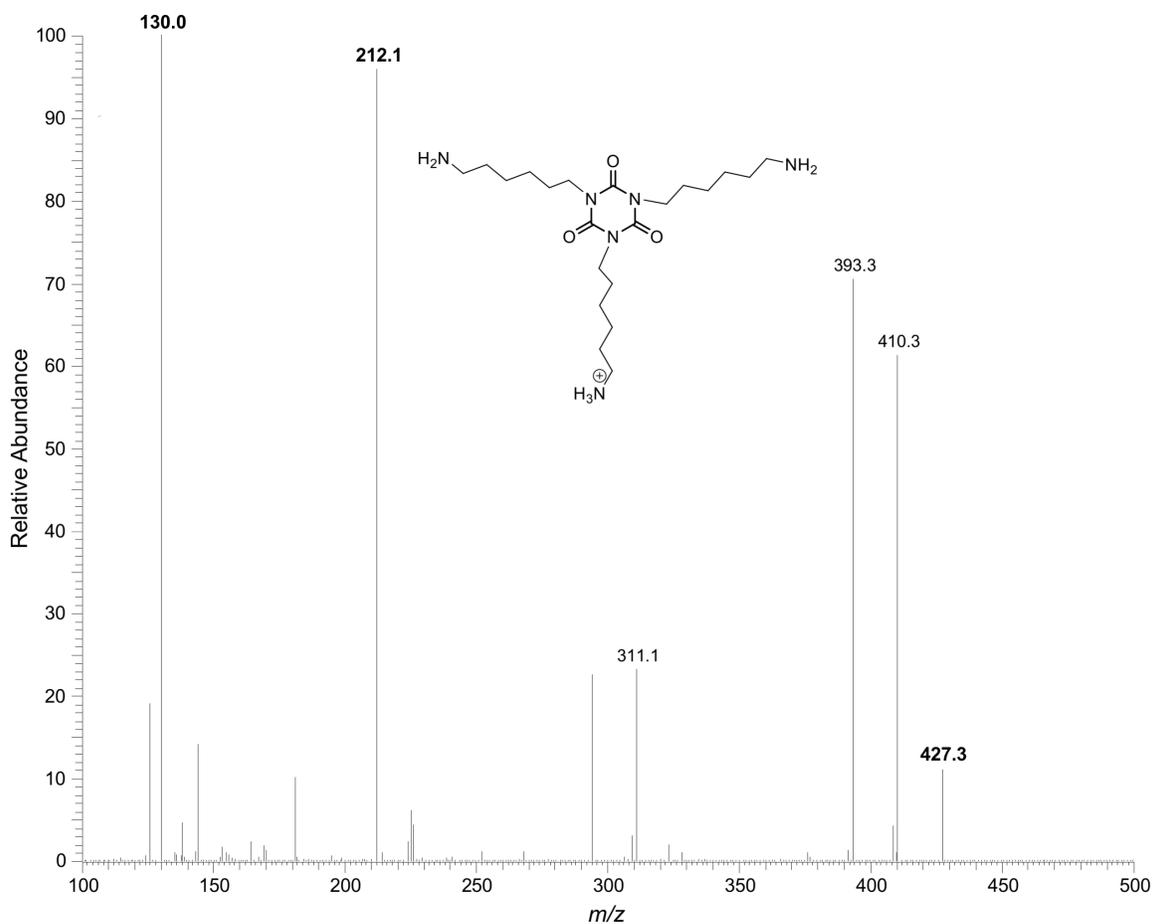
Figure S3. Fragmentation spectrum of precursor ion [M + H]⁺ for TAHI (*m/z* 427.3) obtained by nano-UPLC-ESI-MS/MS operated in positive ion-mode with nano-electrospray ionization (scan range, *m/z* 100-500; collision energy, 35 eV).
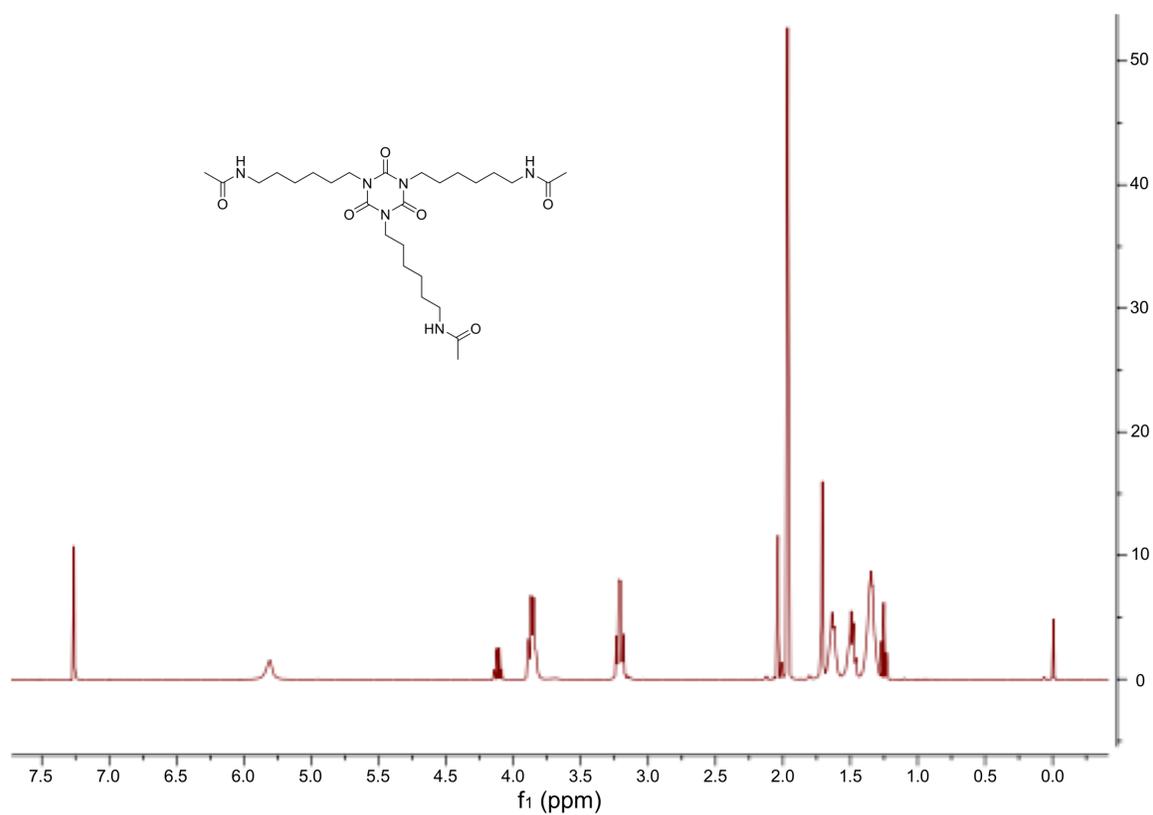
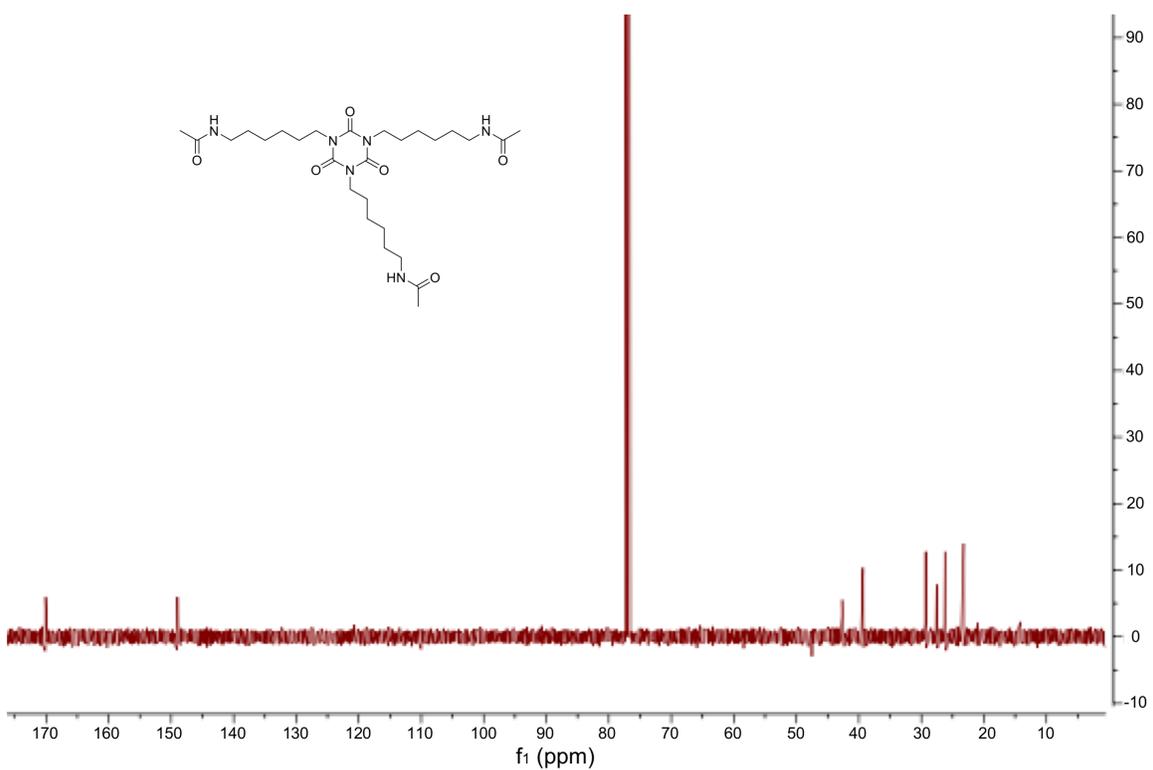**Figure S4**. Proton nuclear magnetic resonance spectrum for TAAHI.

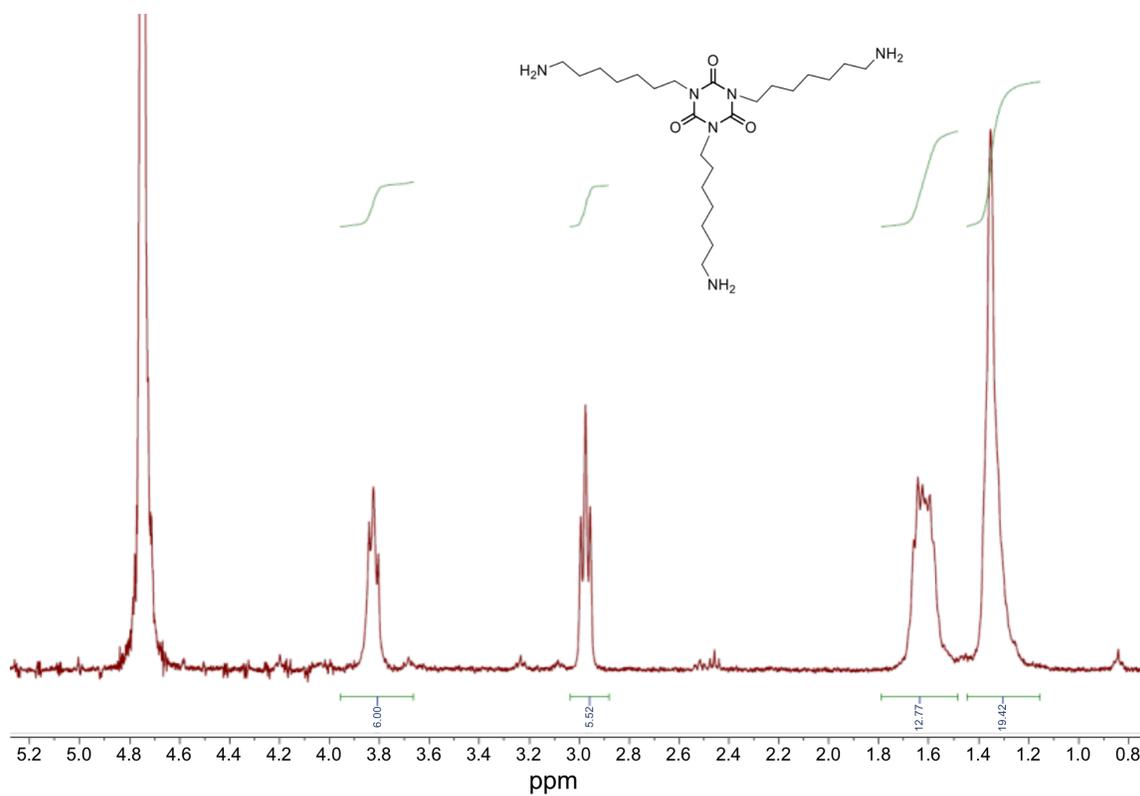**Figure S5**. Carbon-13 nuclear magnetic resonance spectrum for TAAHI.

Figure S6. Proton nuclear magnetic resonance spectrum for 7,7',7''-(2,4,6-trioxo-1,3,5-triazinane-1,3,5-triyl)triheptanenitrile.

Figure S7. Carbon-13 nuclear magnetic resonance spectrum for 7,7',7''-(2,4,6-trioxo-1,3,5-triazinane-1,3,5-triyl)triheptanenitrile.

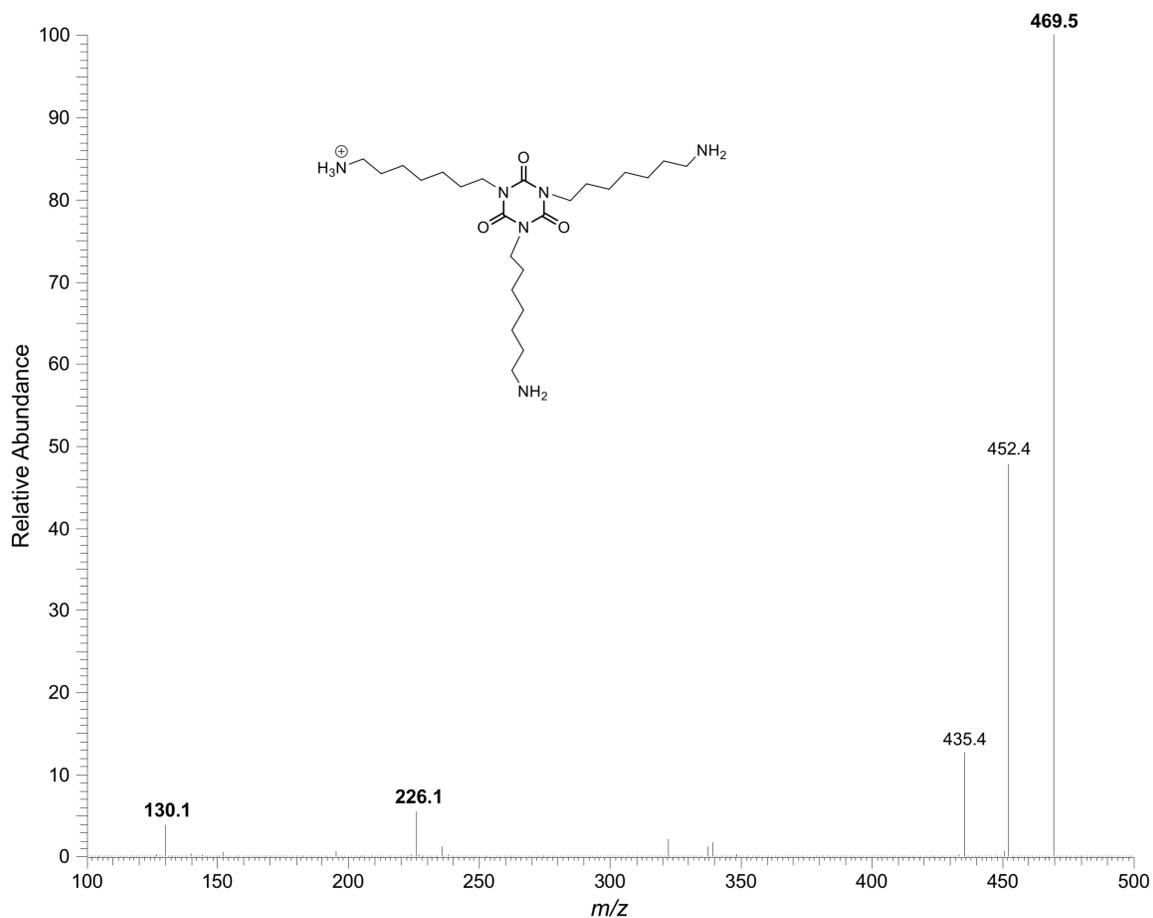**Figure S8**. Proton nuclear magnetic resonance spectrum for TAHpI.

Figure S9. Fragmentation spectrum of precursor ion [M + H]$^+$ for TAHpI (*m/z* 469.3) obtained by nano-UPLC-ESI-MS/MS operated in positive ion-mode with nano-electrospray ionization (scan range, *m/z* 100-500; collision energy, 25 eV).

Figure S10. Fragmentation spectrum of precursor ion [M + H]⁺ for TAHpI (*m/z* 469.3) obtained by nano-UPLC-ESI-MS/MS operated in positive ion-mode with nano-electrospray ionization (scan range, 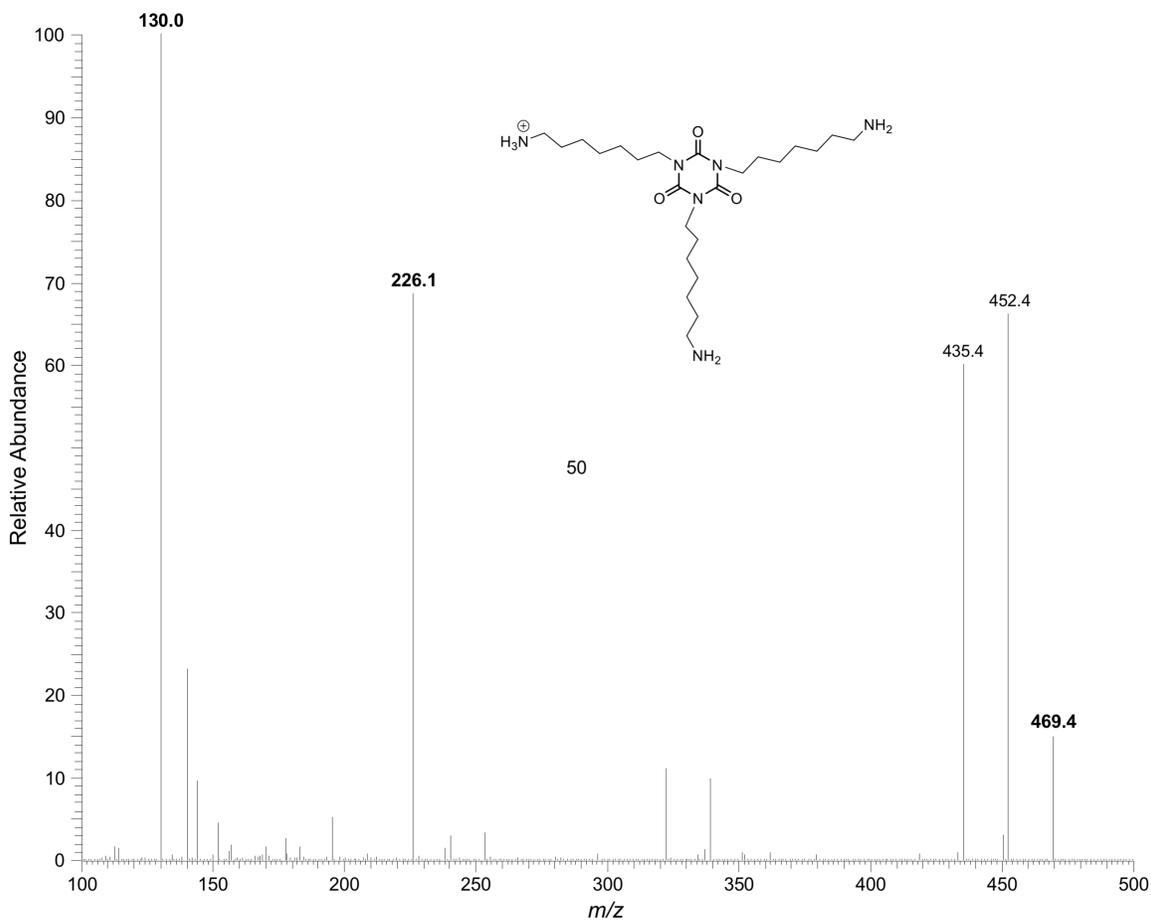*m/z* 100-500; collision energy, 35 eV).