

Characterization of the volatiles profiles of the eggs of forensically relevant *Lucilia sericata* and *Phormia regina* (Diptera: Calliphoridae) blow flies by SPME-facilitated GC-MS

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SUPPORTING MATERIAL

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Contained within are GC-MS chromatograms showing the analysis of two species of blow flies, *L. sericata* and *P. regina*. Additionally presented are head-to-tail plots of compound matches to spectral libraries and confirmation studies of analyzed authentic chemical standards, and a table containing GC-MS experimental parameters.

L. sericata eggs-Batch 1

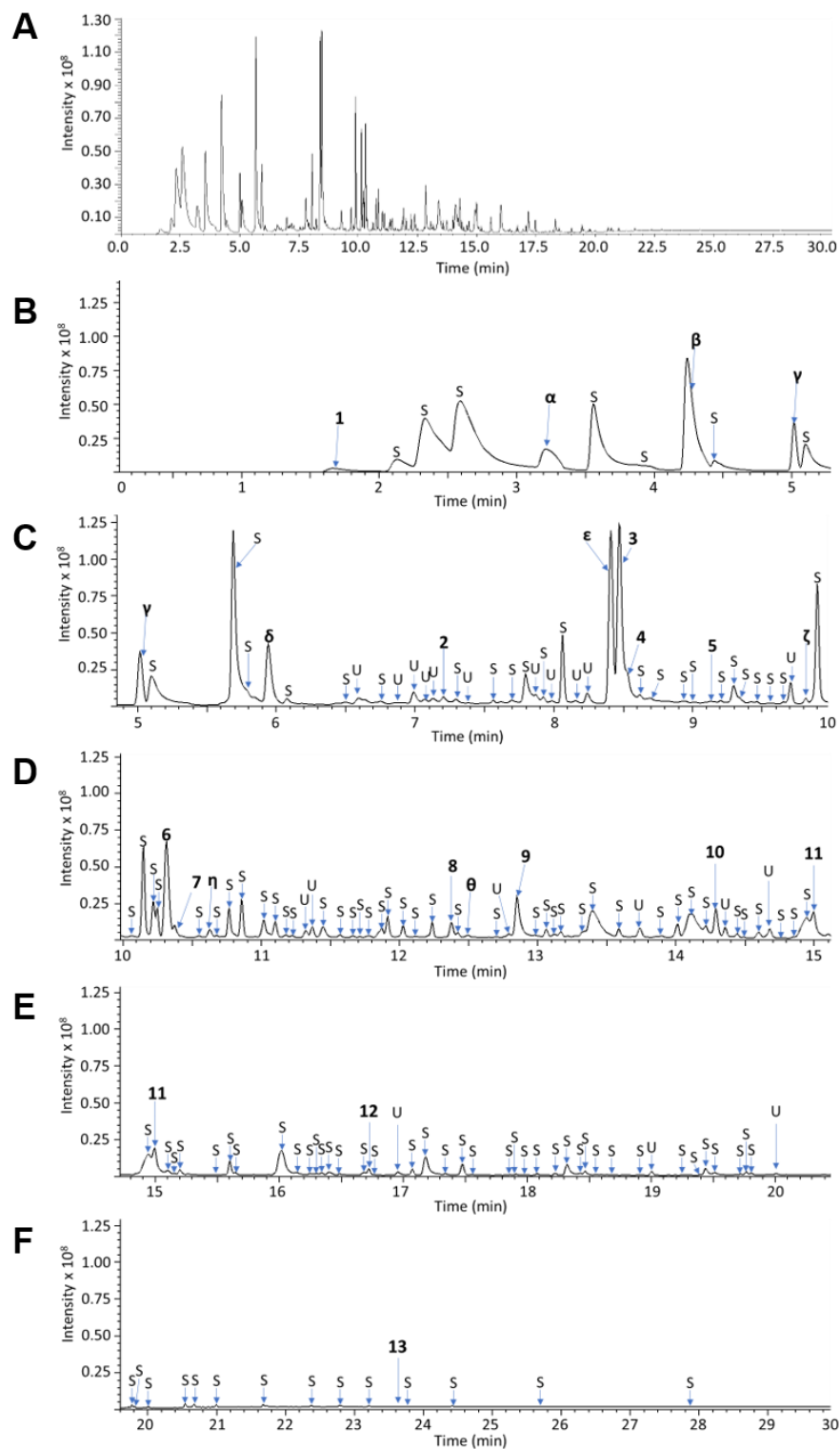


Figure S1. GC chromatograms of *L. sericata* eggs analyzed using a HP-FFAP column (Batch #1). Panel A shows the entire GC chromatogram, and panels B-F show magnifications of the chromatogram in 5-minute increments for clarity. The peaks are each assigned a number, the identities of which are listed in Table 1. Silanes derived from column bleed are labeled “S” and ubiquitous unnatural (synthetic) contaminants are labeled “U”.

L. sericata eggs-FFAP Column Spectra

Labeled peak in chromatogram

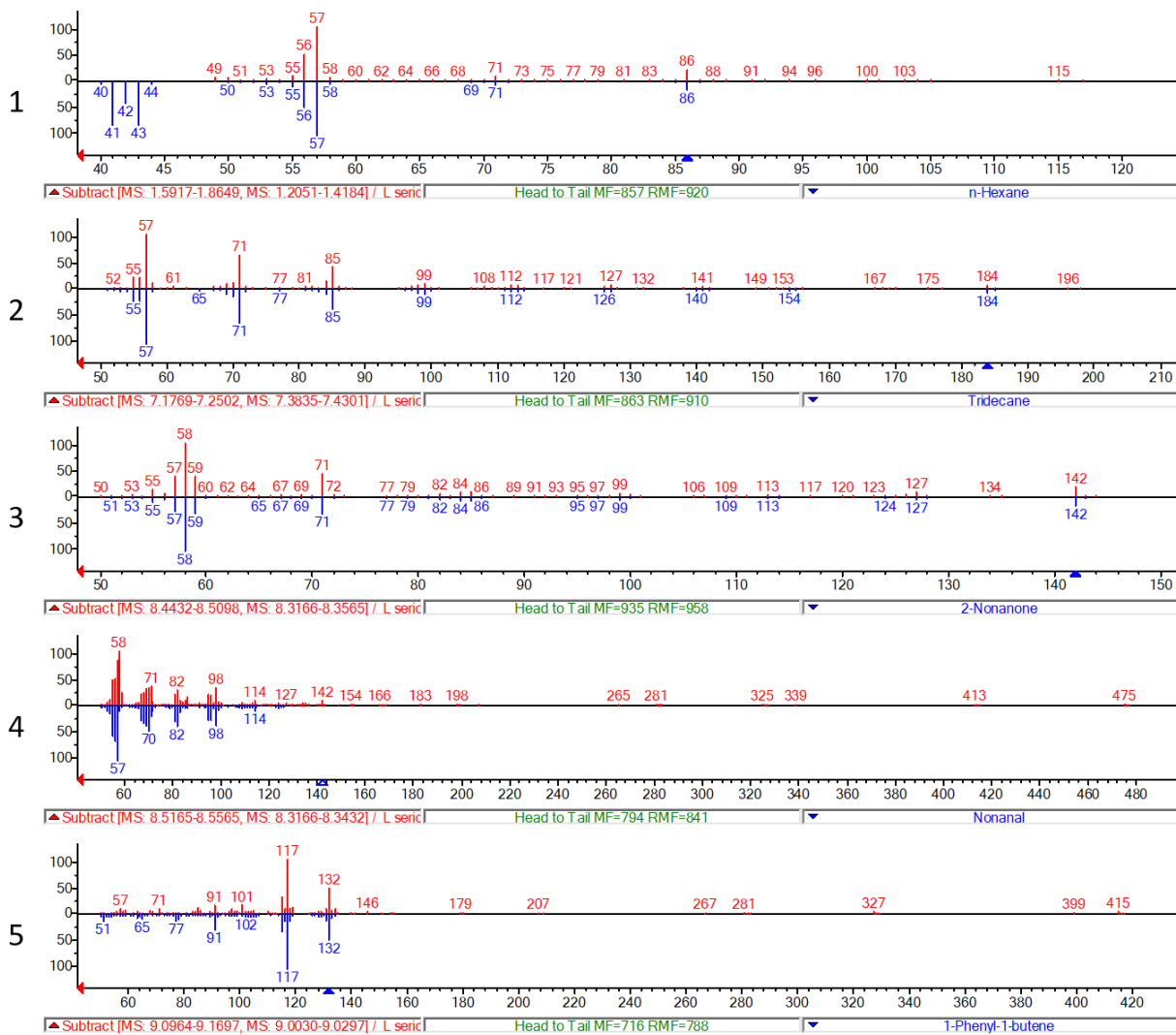


Figure S2. Head-to-tail plots showing the comparison of the GC-MS results of the analysis of *L. sericata* egg headspace using the HP-FFAP column, to library standards for the numbered peaks. In each case, the top spectrum is of the compound derived from the egg sample, and the bottom is that of the library match.

L. sericata eggs-FFAP Column Spectra

Labeled peak in chromatogram

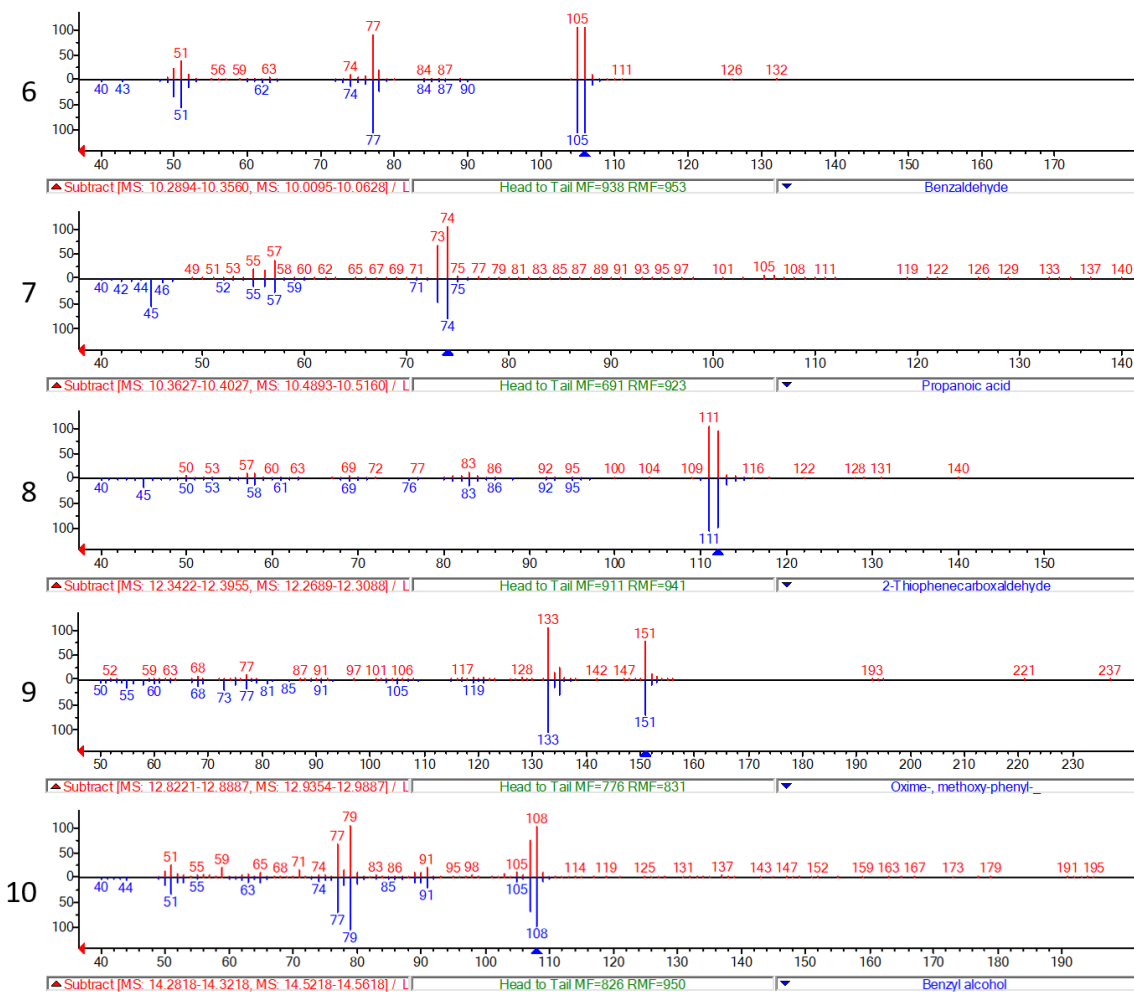


Figure S2 (continued). Head-to-tail plots showing the comparison of the GC-MS results of the analysis of *L. sericata* egg headspace using the HP-FFAP column, to library standards for the numbered peaks. In each case, the top spectrum is of the compound derived from the egg sample, and the bottom is that of the library match.

L. sericata eggs-FFAP Column Spectra

Labeled peak in chromatogram

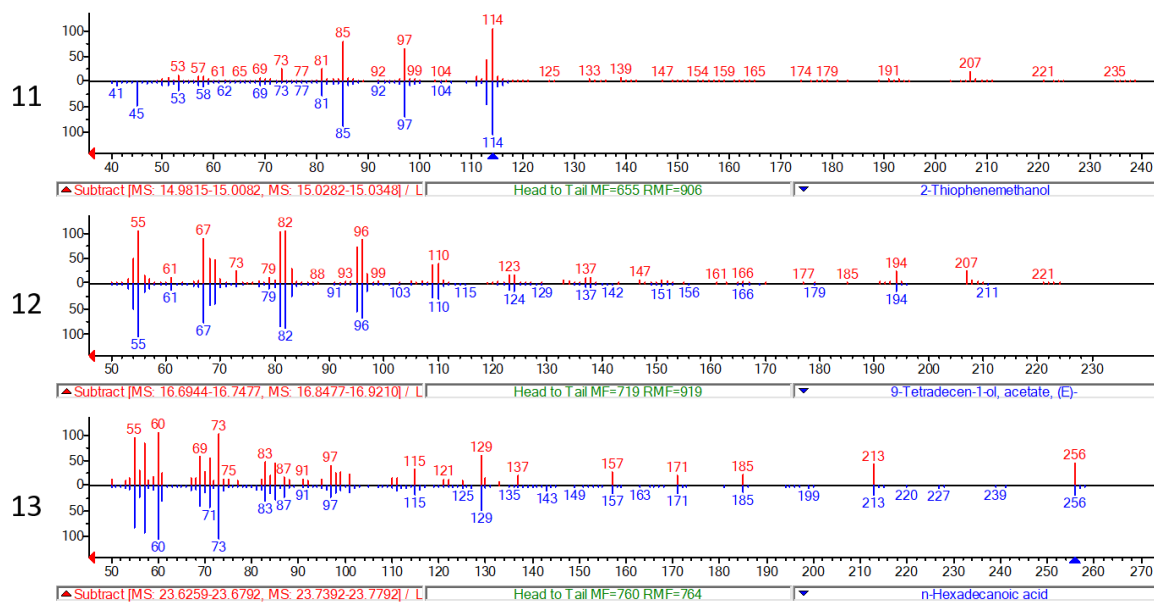


Figure S2 (continued). Head-to-tail plots showing the comparison of the GC-MS results of the analysis of *L. sericata* egg headspace using the HP-FFAP column, to library standards for the numbered peaks. In each case, the top spectrum is of the compound derived from the egg sample, and the bottom is that of the library match.

L. sericata eggs-FFAP Column Spectra-Batch 1

Labeled peak in chromatogram

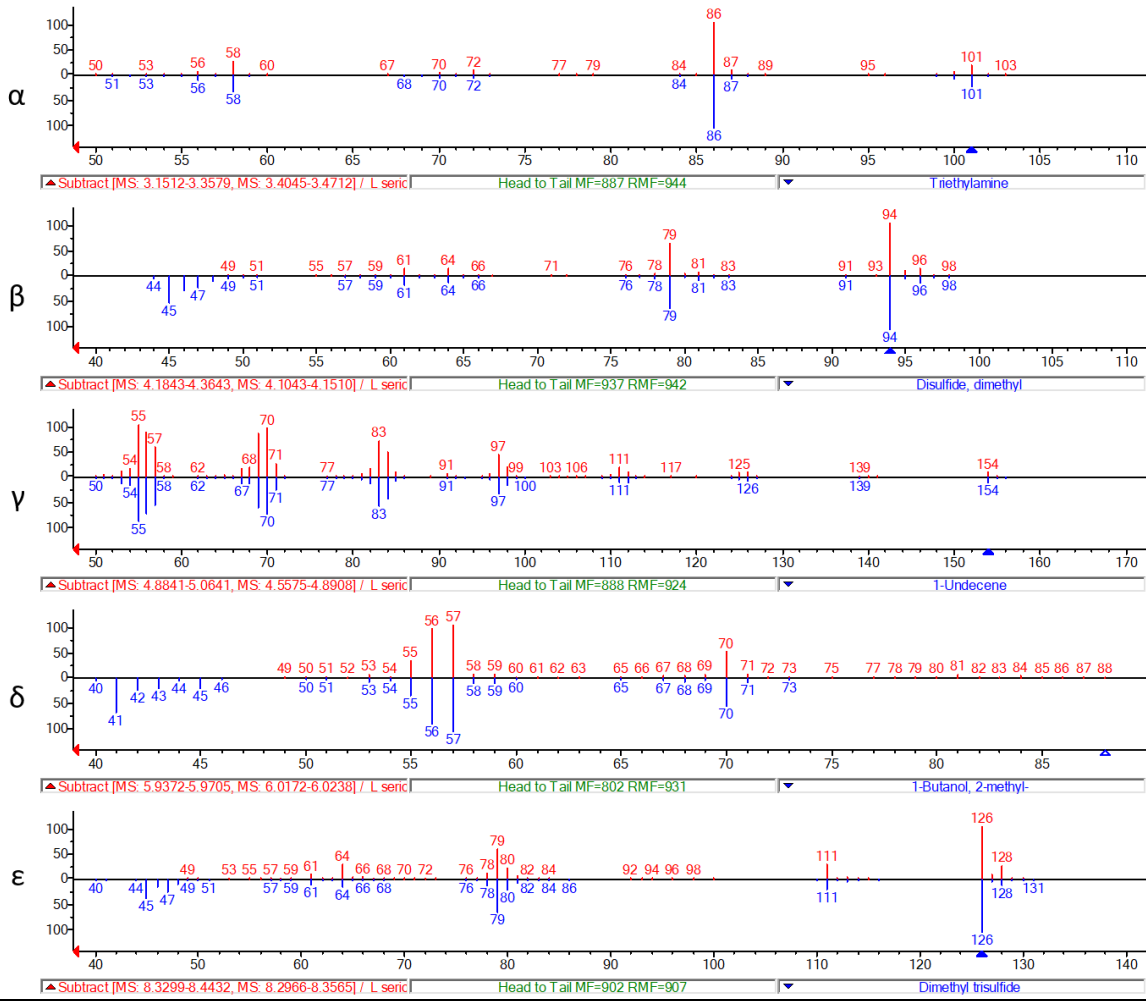


Figure S2 (continued). Head-to-tail plots showing the comparison of the GC-MS results of the analysis of *L. sericata* egg headspace using the HP-FFAP column, to library standards for the numbered peaks. In each case, the top spectrum is of the compound derived from the egg sample, and the bottom is that of the library match.

L. sericata eggs-FFAP Column Spectra-Batch 1

Labeled peak in chromatogram

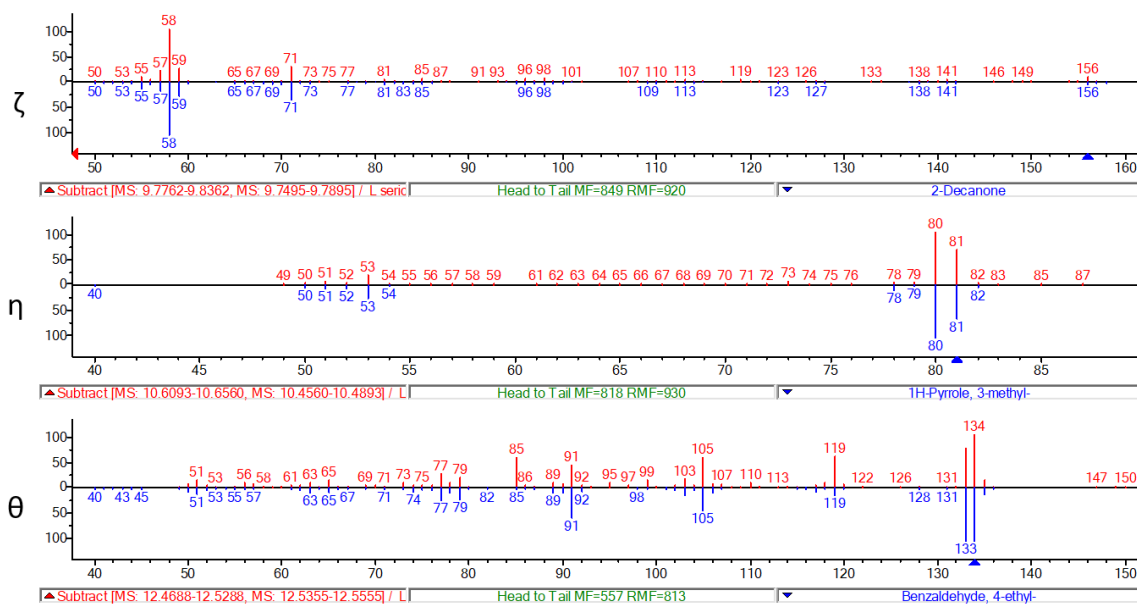


Figure S2 (continued). Head-to-tail plots showing the comparison of the GC-MS results of the analysis of *L. sericata* egg headspace using the HP-FFAP column, to library standards for the numbered peaks. In each case, the top spectrum is of the compound derived from the egg sample, and the bottom is that of the library match.

L. sericata eggs-FFAP Column Spectra-Batch 2

Labeled peak in chromatogram

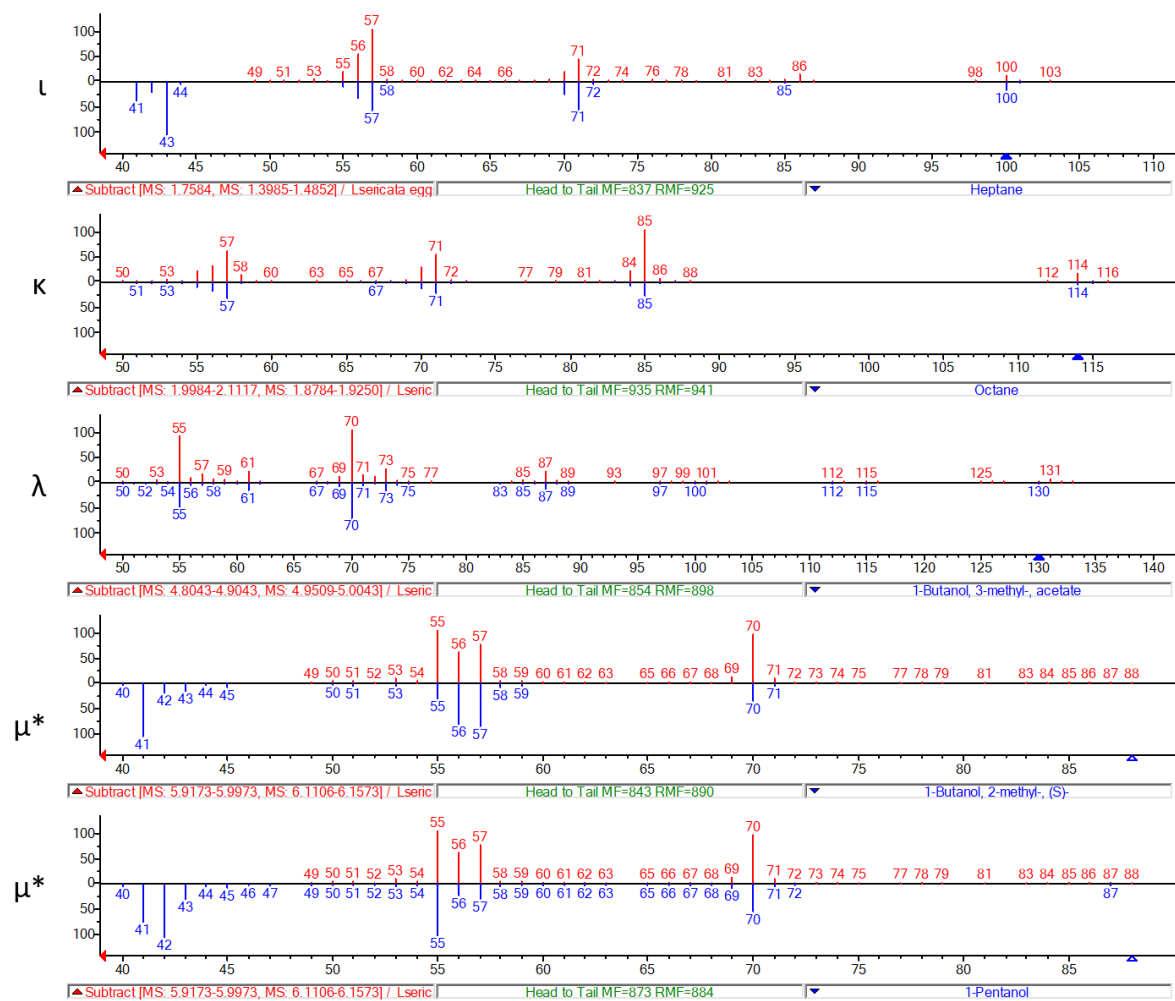


Figure S2 (continued). Head-to-tail plots showing the comparison of the GC-MS results of the analysis of *L. sericata* egg headspace using the HP-FFAP column, to library standards for the numbered peaks. In each case, the top spectrum is of the compound derived from the egg sample, and the bottom is that of the library match.

L. sericata eggs-FFAP Column Spectra-Batch 2

Labeled peak in chromatogram

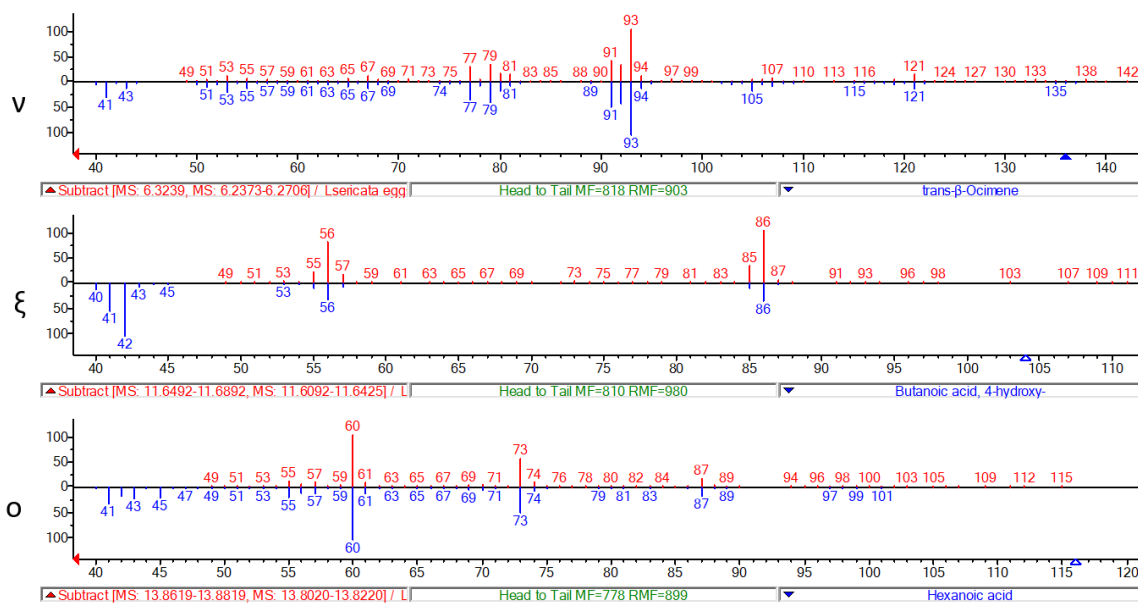


Figure S2 (continued). Head-to-tail plots showing the comparison of the GC-MS results of the analysis of *L. sericata* egg headspace using the HP-FFAP column, to library standards for the numbered peaks. In each case, the top spectrum is of the compound derived from the egg sample, and the bottom is that of the library match.

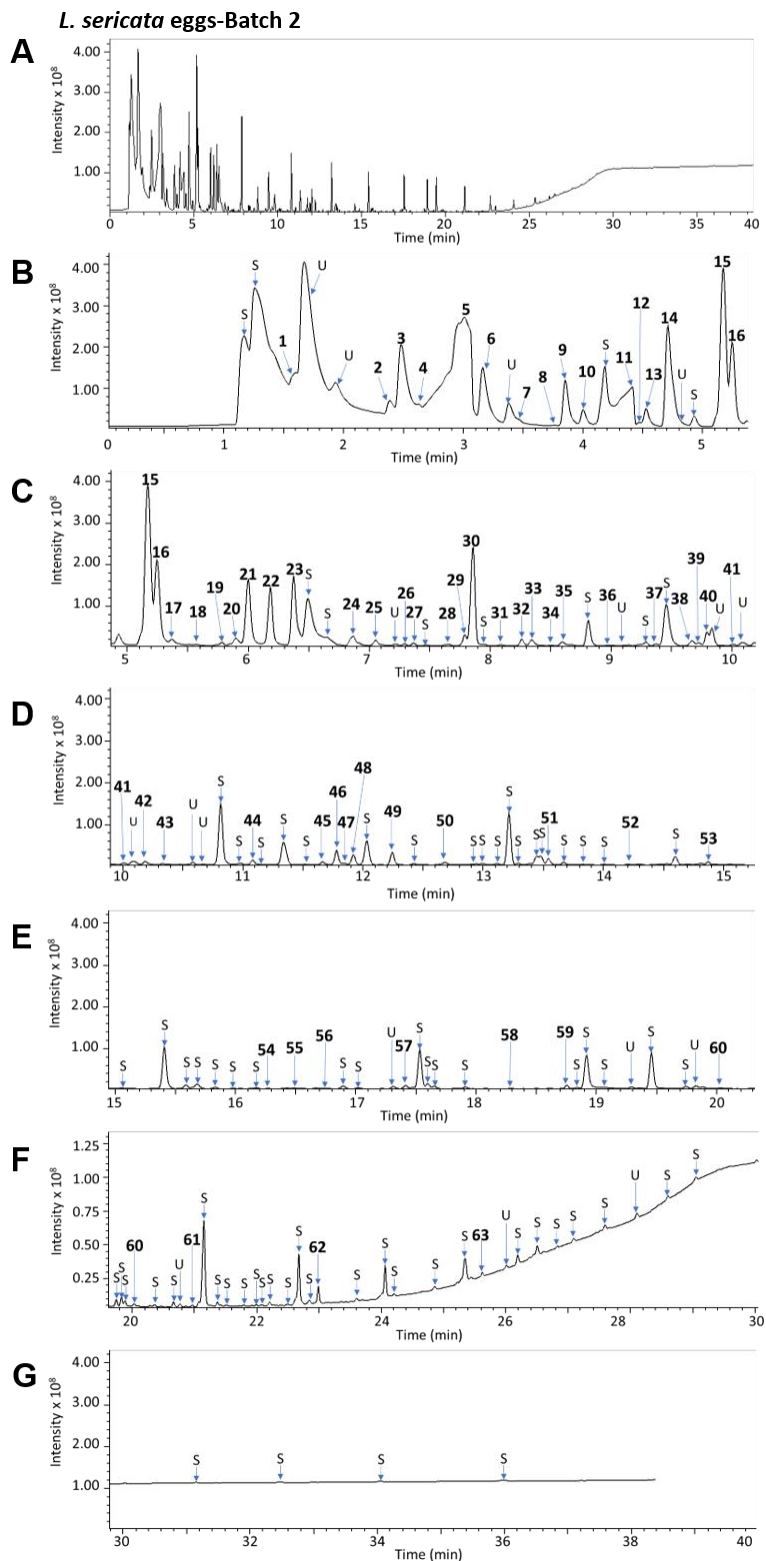


Figure S3. GC chromatograms of *L. sericata* eggs (Batch #2) analyzed by CP-Sil column. Panel A shows the entire GC chromatogram, and panels B-G show magnifications of the chromatogram in 5-minute increments for clarity. The peaks are each assigned a number, the identities of which are listed in Table 2. Silanes associated with column bleed are labeled “S” and ubiquitous unnatural products are labeled “U”.

L. sericata eggs-Amine Column Spectra

Labeled peak in chromatogram

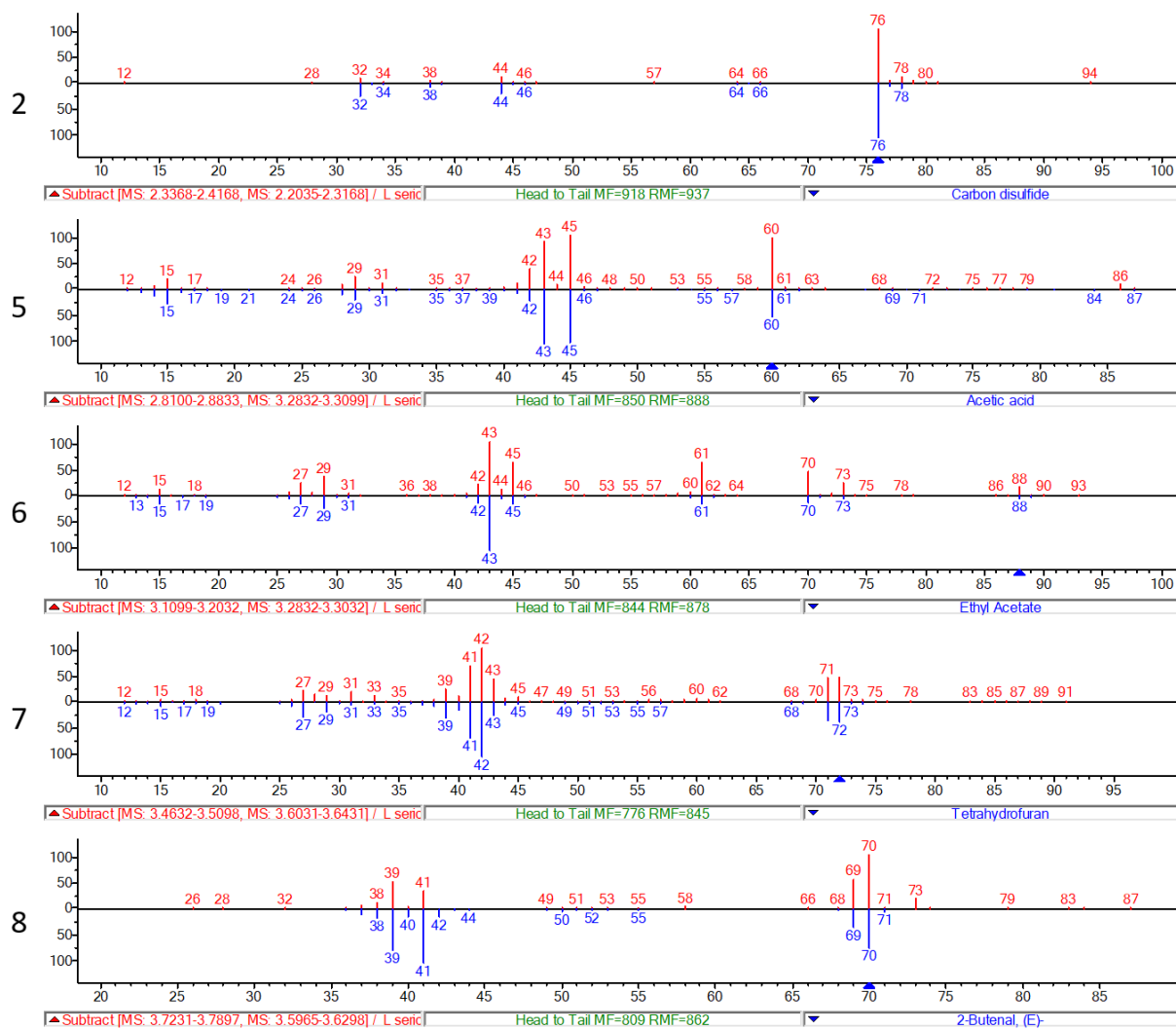


Figure S4. Head-to-tail plots showing the comparison of the GC-MS results of the analysis of *L. sericata* egg headspace using a CP-Sil column, to library standards for the numbered peaks. In each case, the top spectrum is of the compound derived from the egg sample, and the bottom is that of the library match.

L. sericata eggs-Amine Column Spectra

Labeled peak in chromatogram

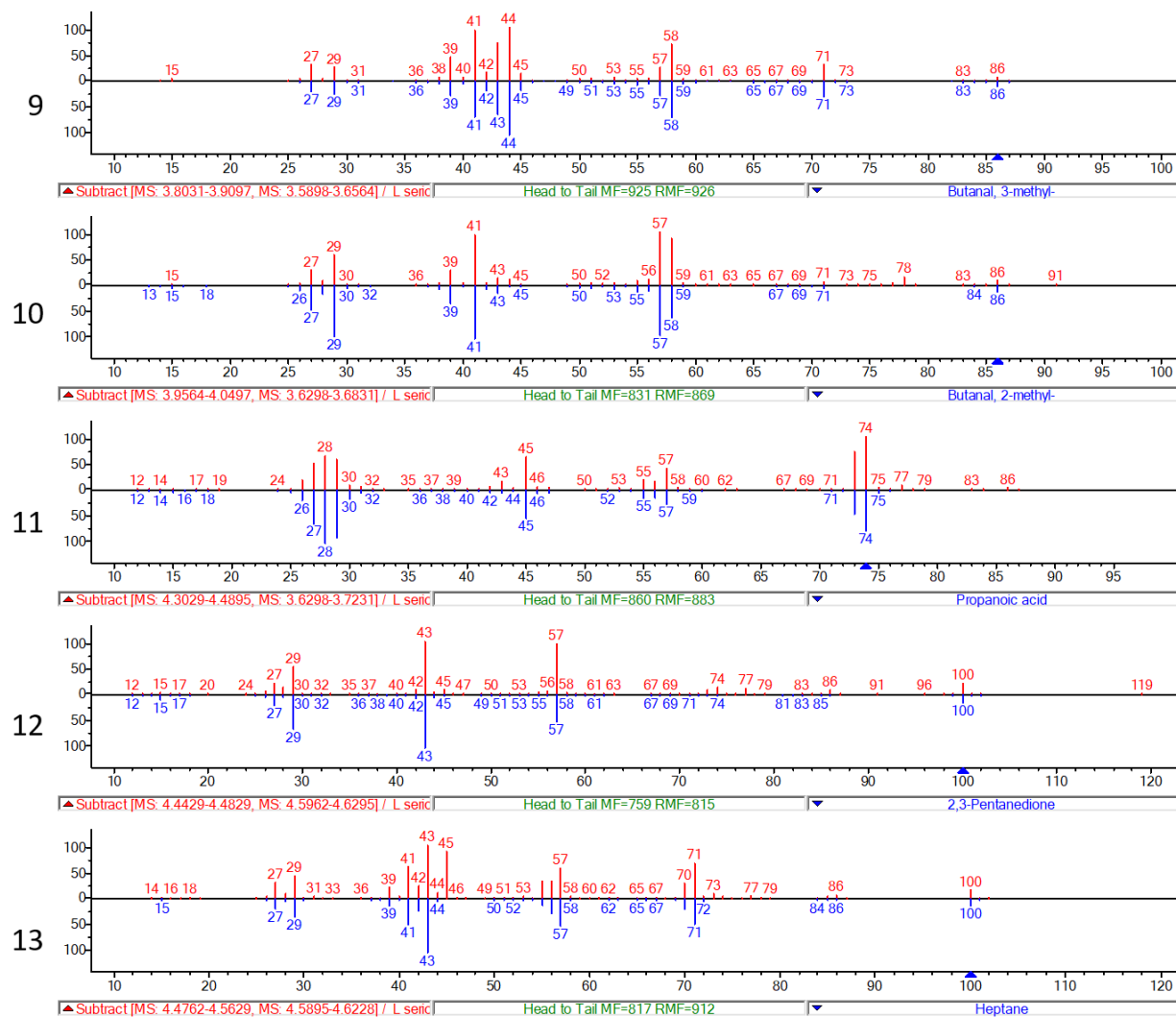


Figure S4 (continued). Head-to-tail plots showing the comparison of the GC-MS results of the analysis of *L. sericata* egg headspace using a CP-Sil column, to library standards for the numbered peaks. In each case, the top spectrum is of the compound derived from the egg sample, and the bottom is that of the library match.

L. sericata eggs-Amine Column Spectra

Labeled peak in chromatogram

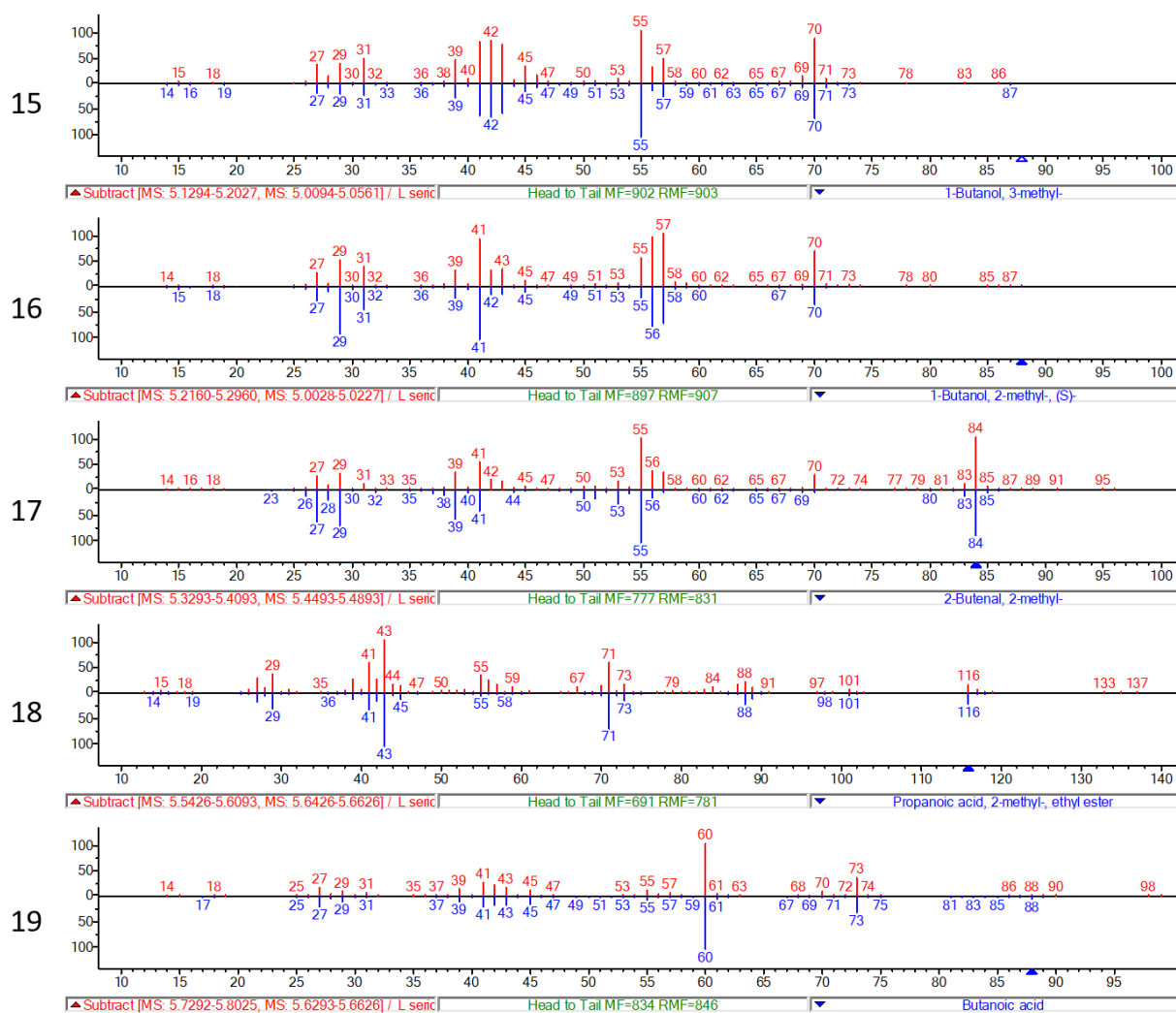


Figure S4 (continued). Head-to-tail plots showing the comparison of the GC-MS results of the analysis of *L. sericata* egg headspace using a CP-Sil column, to library standards for the numbered peaks. In each case, the top spectrum is of the compound derived from the egg sample, and the bottom is that of the library match.

L. sericata eggs-Amine Column Spectra

Labeled peak in chromatogram

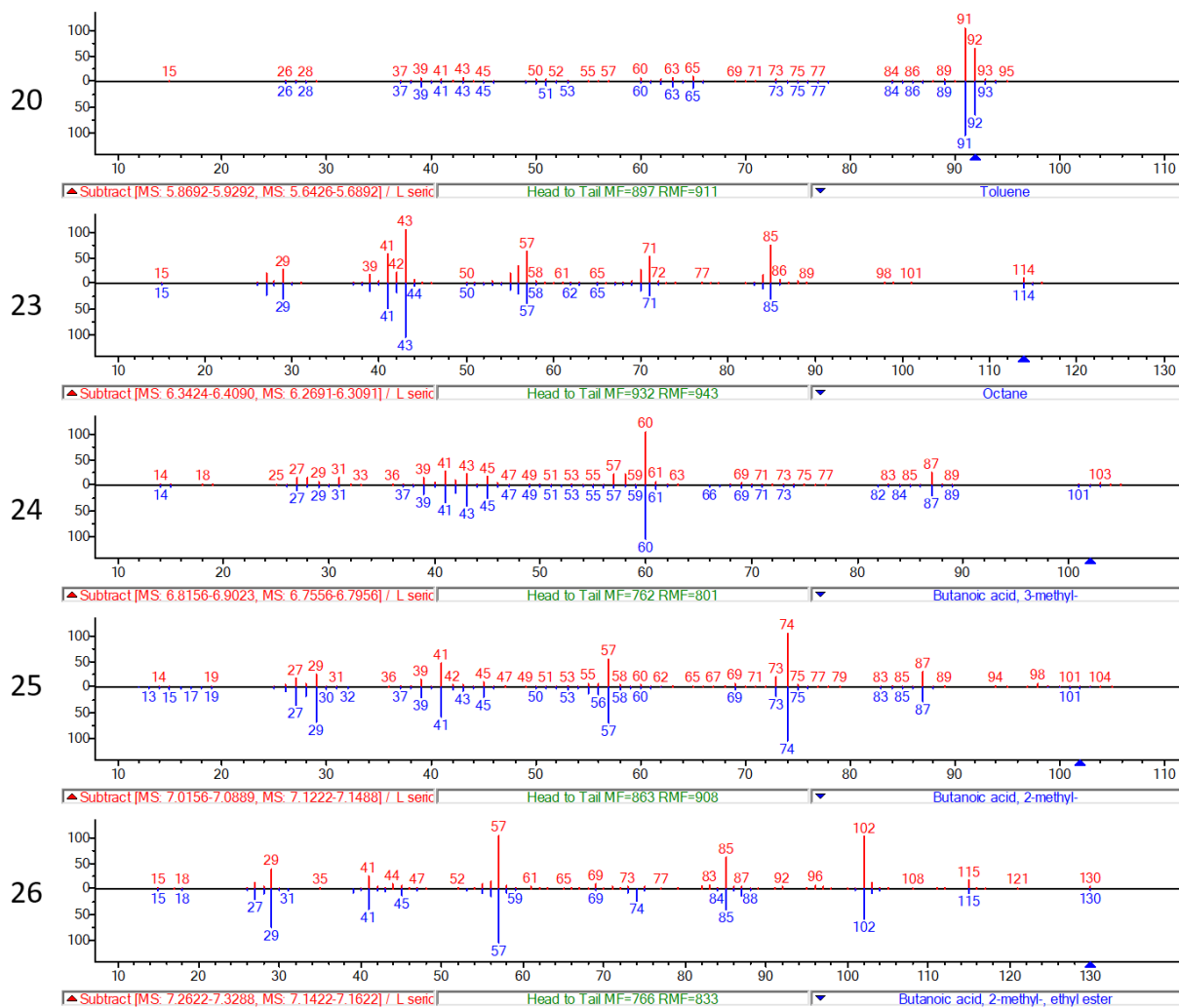


Figure S4 (continued). Head-to-tail plots showing the comparison of the GC-MS results of the analysis of *L. sericata* egg headspace using a CP-Sil column, to library standards for the numbered peaks. In each case, the top spectrum is of the compound derived from the egg sample, and the bottom is that of the library match.

L. sericata eggs-Amine Column Spectra

Labeled peak in chromatogram

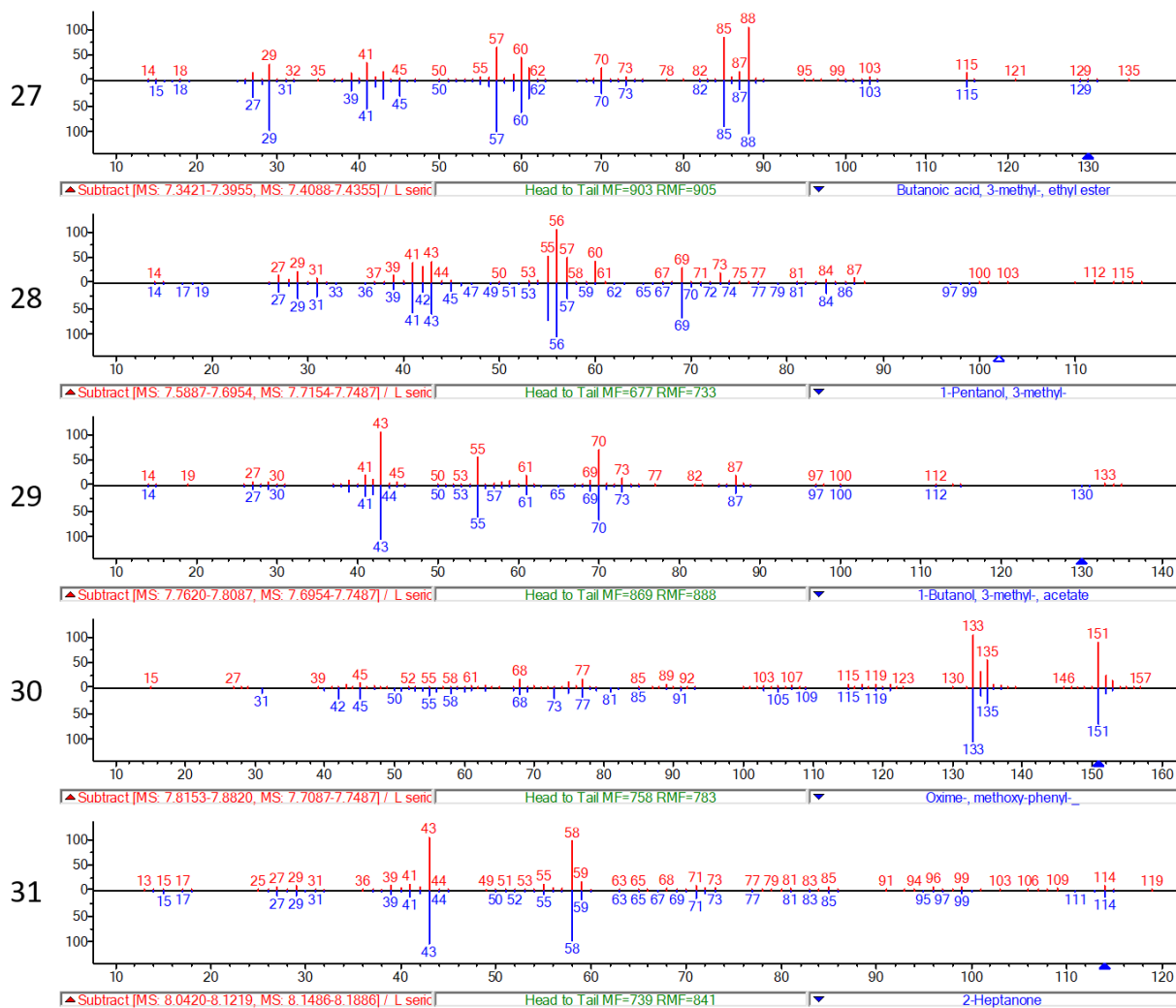


Figure S4 (continued). Head-to-tail plots showing the comparison of the GC-MS results of the analysis of *L. sericata* egg headspace using a CP-Sil column, to library standards for the numbered peaks. In each case, the top spectrum is of the compound derived from the egg sample, and the bottom is that of the library match.

L. sericata eggs-Amine Column Spectra

Labeled peak in chromatogram

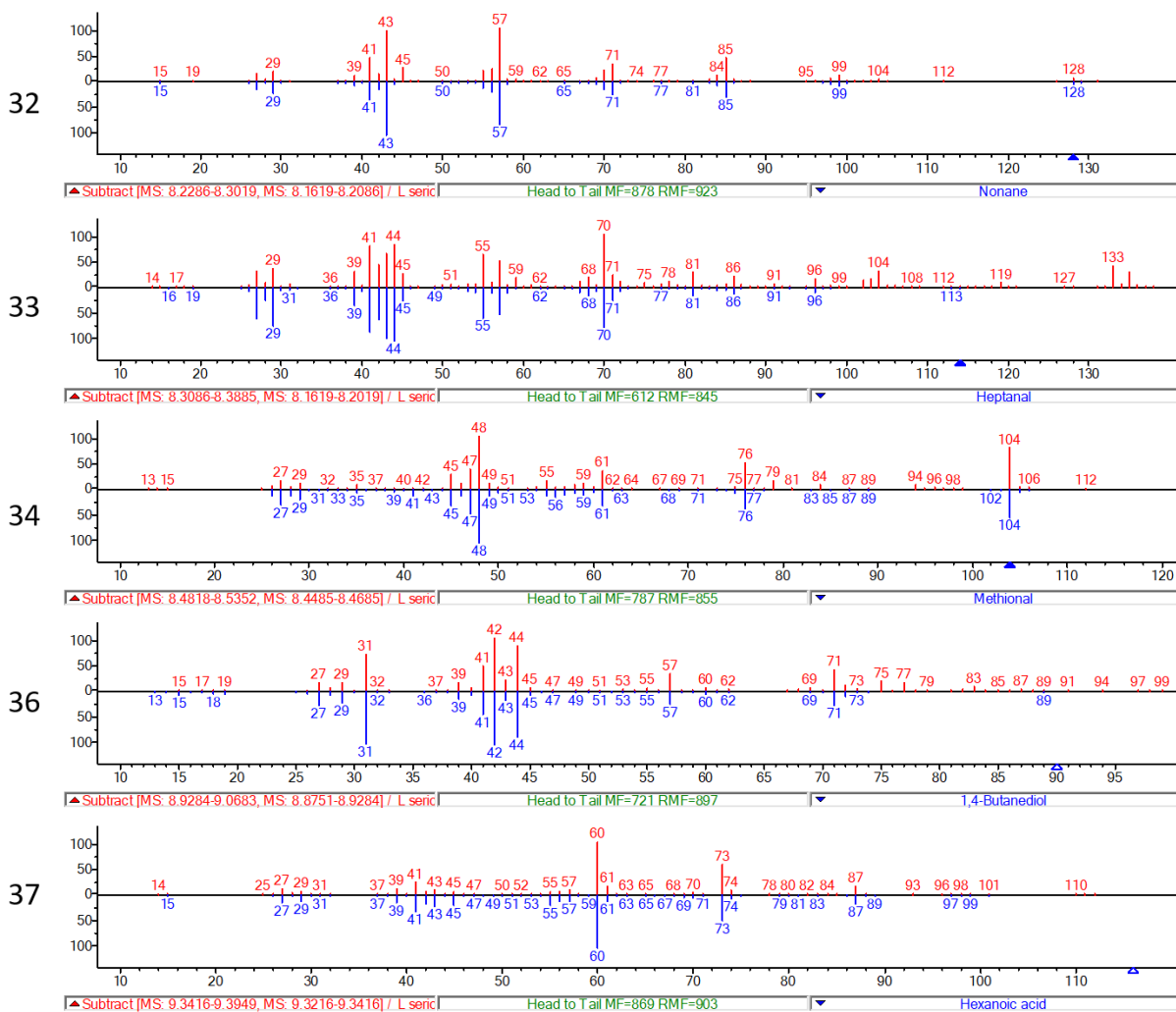


Figure S4 (continued). Head-to-tail plots showing the comparison of the GC-MS results of the analysis of *L. sericata* egg headspace using a CP-Sil column, to library standards for the numbered peaks. In each case, the top spectrum is of the compound derived from the egg sample, and the bottom is that of the library match.

L. sericata eggs-Amine Column Spectra

Labeled peak in chromatogram

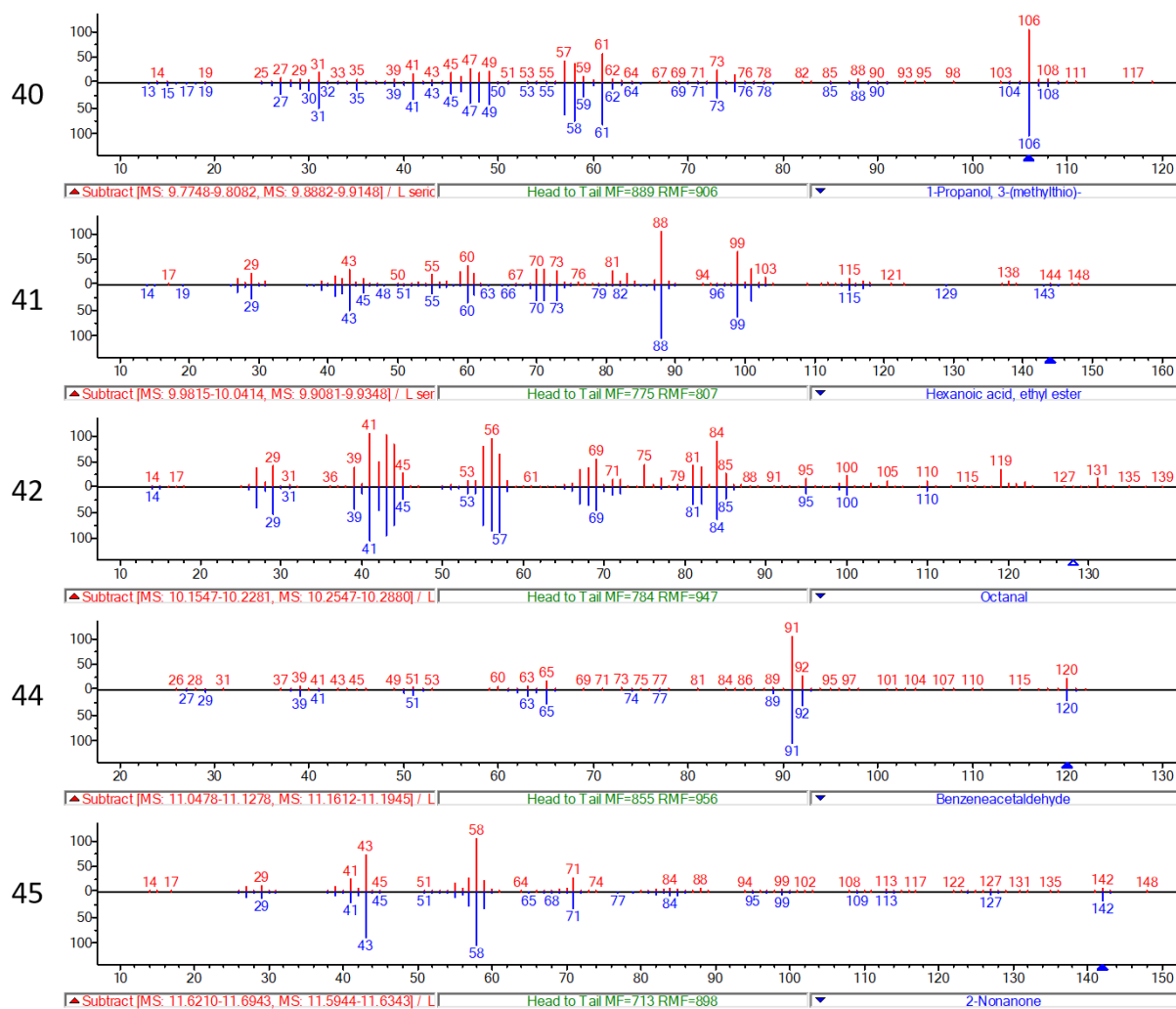


Figure S4 (continued). Head-to-tail plots showing the comparison of the GC-MS results of the analysis of *L. sericata* egg headspace using a CP-Sil column, to library standards for the numbered peaks. In each case, the top spectrum is of the compound derived from the egg sample, and the bottom is that of the library match.

L. sericata eggs-Amine Column Spectra

Labeled peak in chromatogram

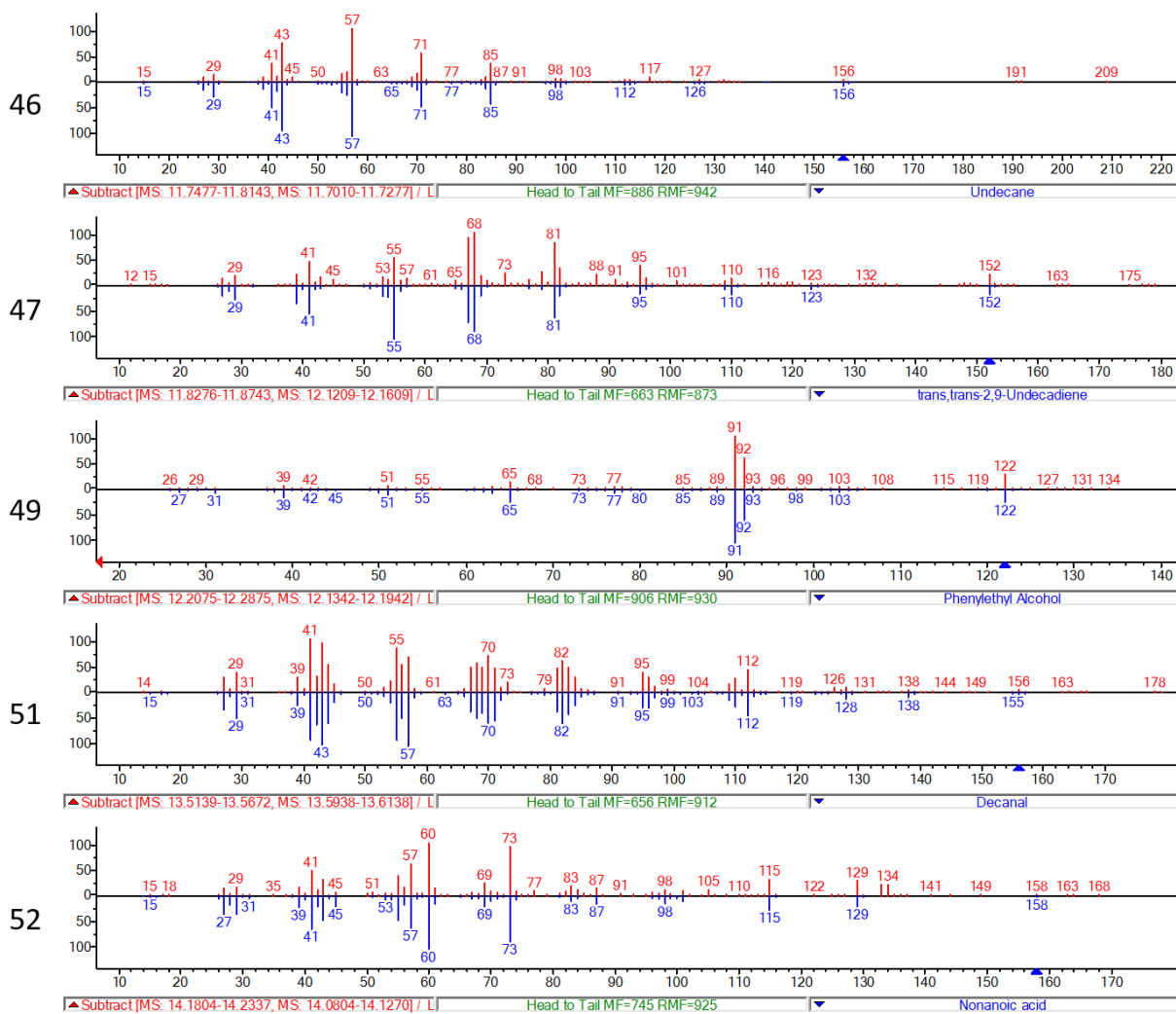


Figure S4 (continued). Head-to-tail plots showing the comparison of the GC-MS results of the analysis of *L. sericata* egg headspace using a CP-Sil column, to library standards for the numbered peaks. In each case, the top spectrum is of the compound derived from the egg sample, and the bottom is that of the library match.

L. sericata eggs-Amine Column Spectra

Labeled peak in chromatogram

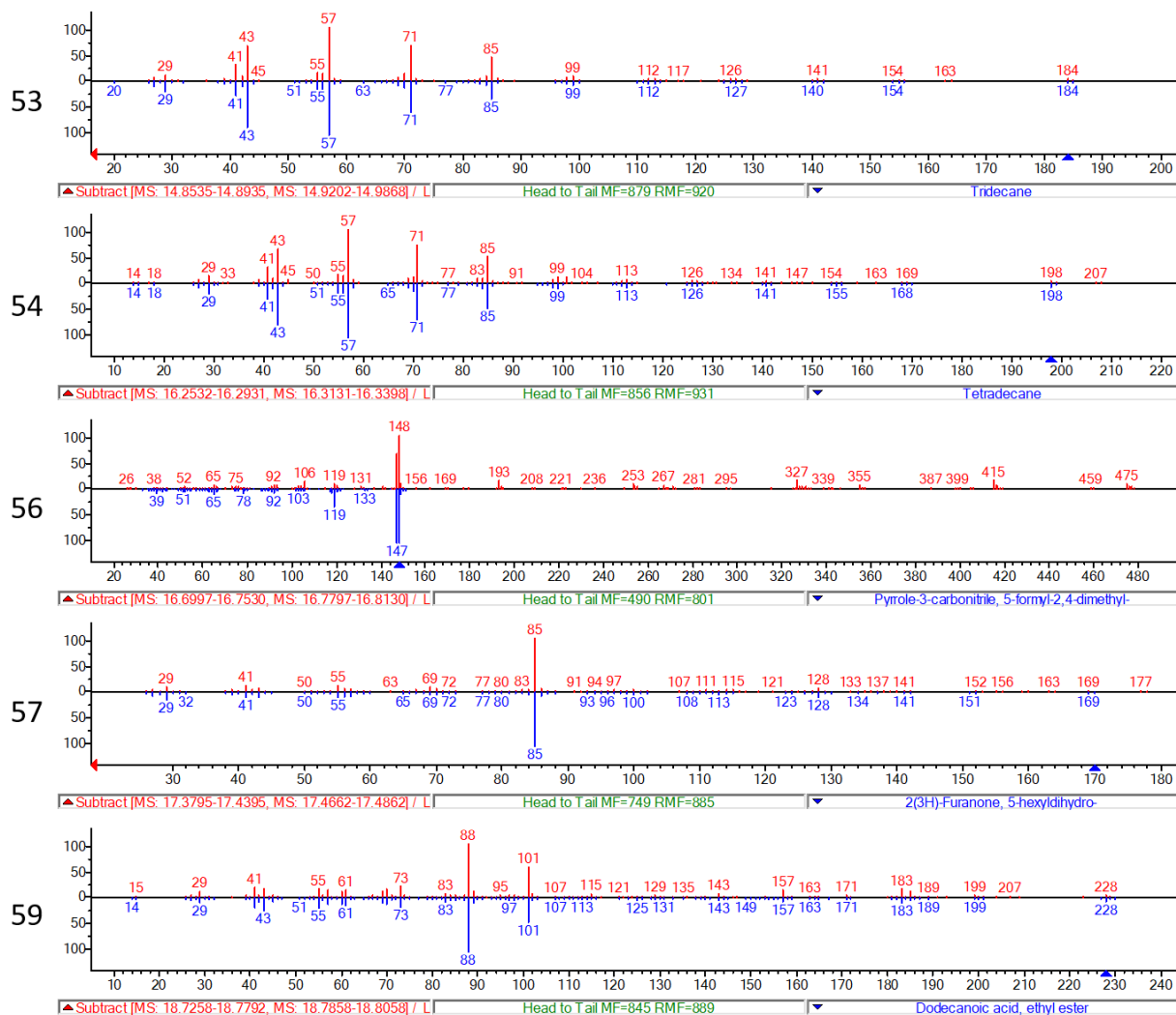


Figure S4 (continued). Head-to-tail plots showing the comparison of the GC-MS results of the analysis of *L. sericata* egg headspace using a CP-Sil column, to library standards for the numbered peaks. In each case, the top spectrum is of the compound derived from the egg sample, and the bottom is that of the library match.

L. sericata eggs-Amine Column Spectra

Labeled peak in chromatogram

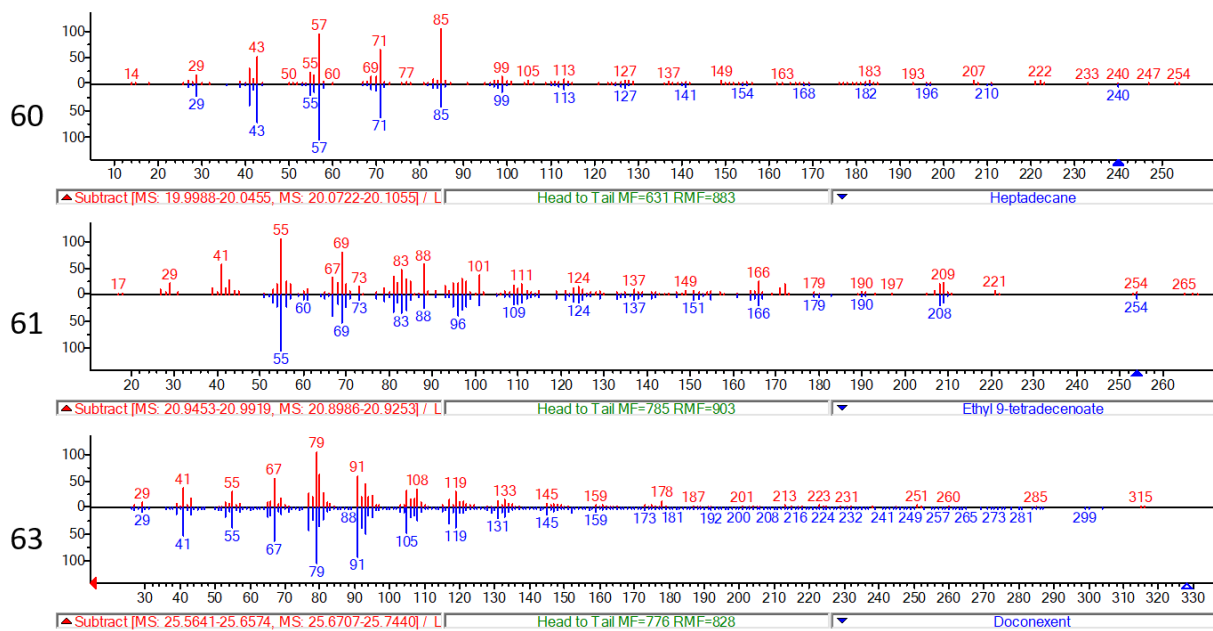


Figure S4 (continued). Head-to-tail plots showing the comparison of the GC-MS results of the analysis of *L. sericata* egg headspace using a CP-Sil column, to library standards for the numbered peaks. In each case, the top spectrum is of the compound derived from the egg sample, and the bottom is that of the library match.

L. sericata eggs-Amine Column Spectra

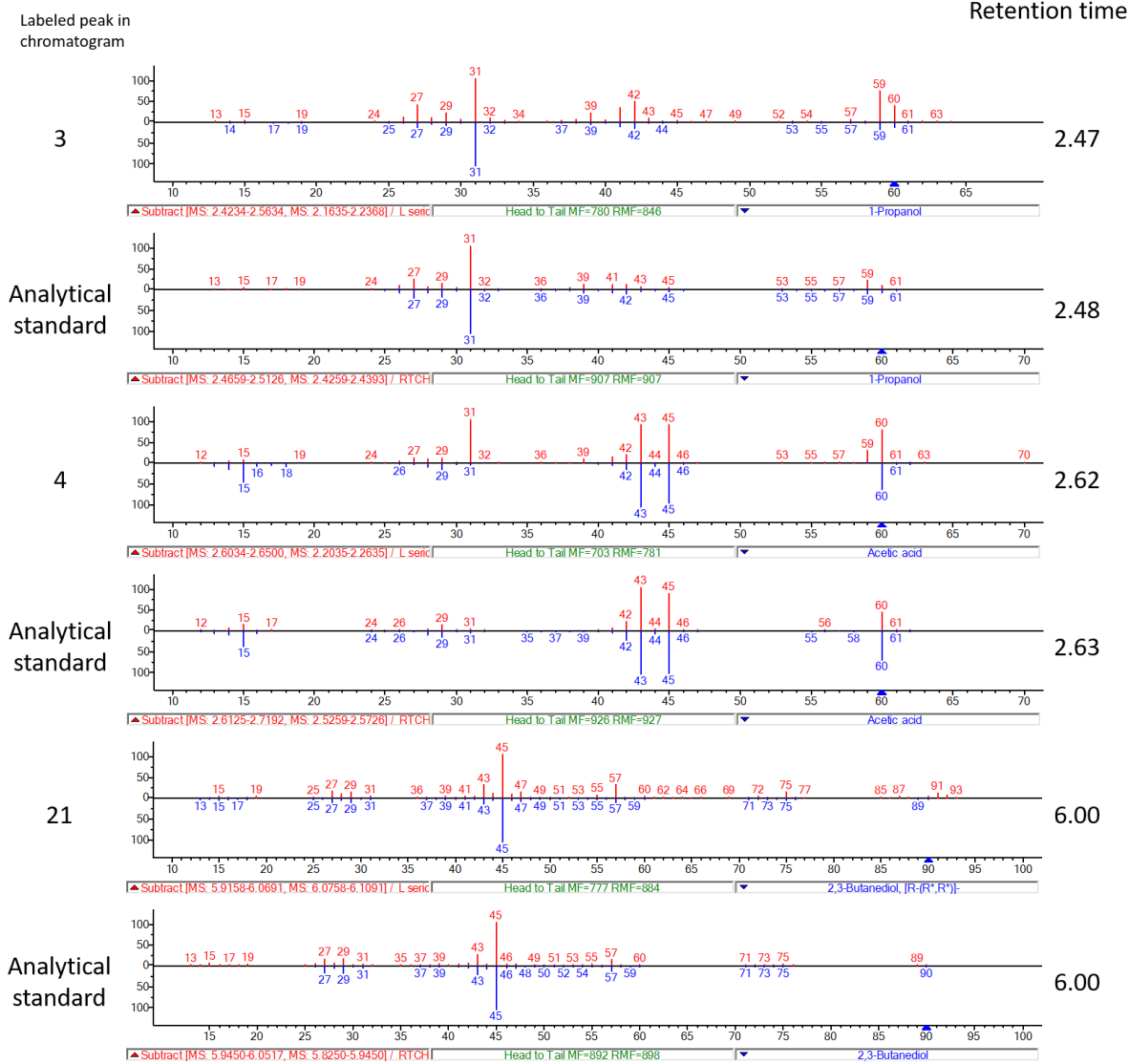


Figure S4 (continued). Head-to-tail plots showing the results of control experiments run for the confirmation of peak identities in *L. sericata* egg headspace analyzed by CP-Sil column. In each pair of spectra, the top is the compound observed in the egg headspace, and the bottom is that of the pure analytical standard, with their corresponding retention times.

L. sericata eggs-Amine Column Spectra

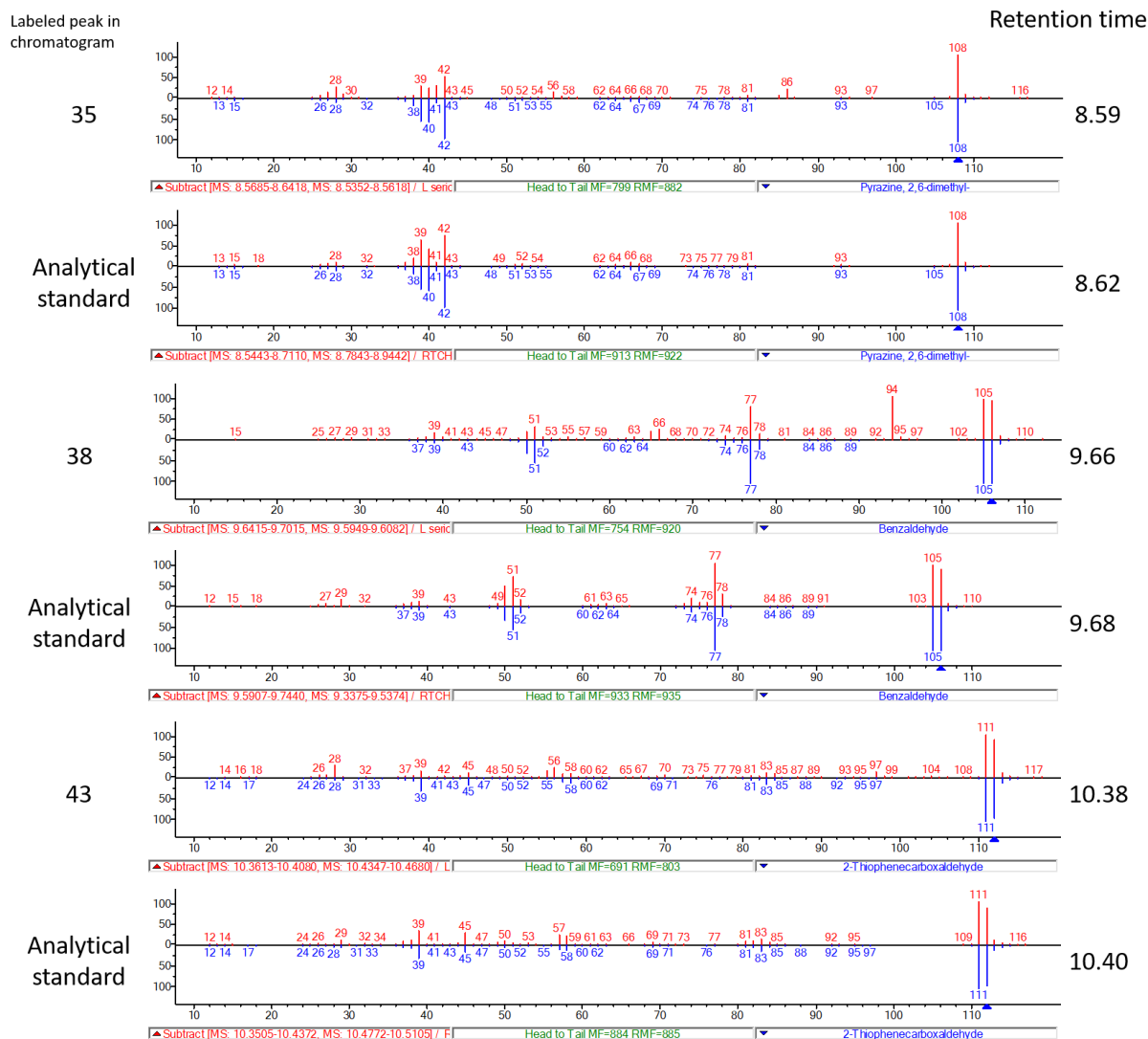


Figure S4 (continued). Head-to-tail plots showing the results of control experiments run for the confirmation of peak identities in *L. sericata* egg headspace analyzed by CP-Sil column. In each pair of spectra, the top is the compound observed in the egg headspace, and the bottom is that of the pure analytical standard, with their corresponding retention times.

L. sericata eggs-Amine Column Spectra

Retention time

Labeled peak in chromatogram

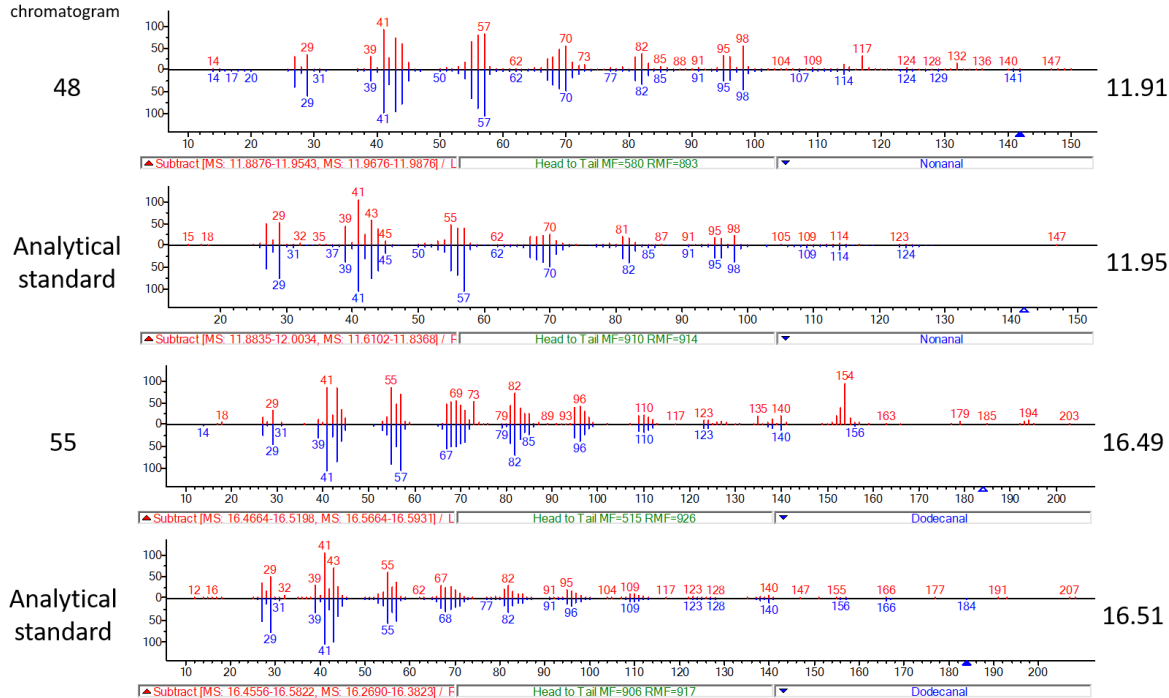


Figure S4 (continued). Head-to-tail plots showing the results of control experiments run for the confirmation of peak identities in *L. sericata* egg headspace analyzed by CP-Sil column. In each pair of spectra, the top is the compound observed in the egg headspace, and the bottom is that of the pure analytical standard, with their corresponding retention times.

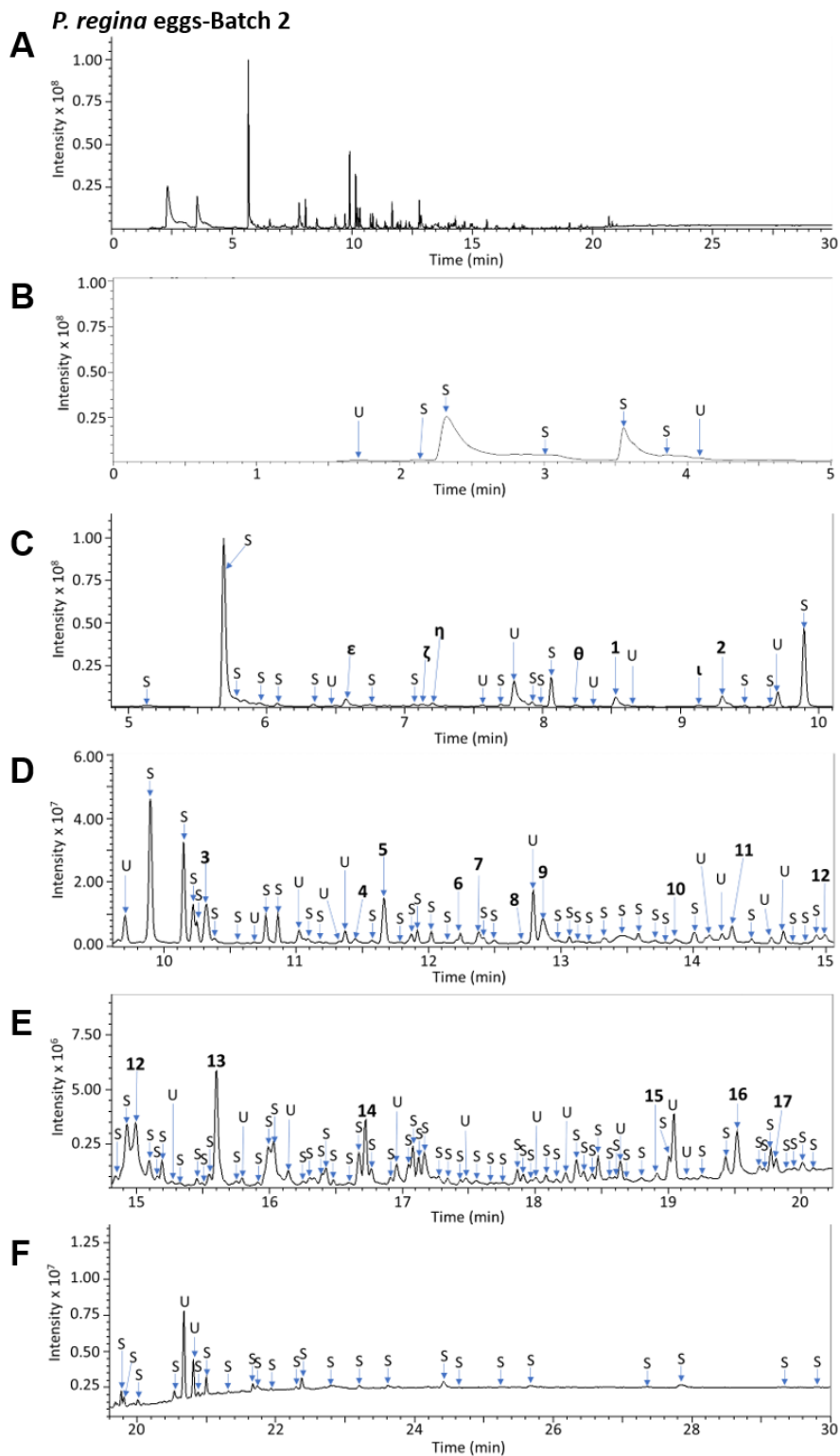


Figure S5. GC chromatogram of *P. regina* eggs analyzed by HP-FFAP column (Batch #2). Panel A shows the entire GC chromatogram, and panels B-F show magnifications of the chromatogram in 5-minute increments for clarity. The peaks are each assigned a number, the identities of which are listed in Table 3. Silanes derived from column bleed are labeled “S” and ubiquitous unnatural products are labeled “U”.

P. regina eggs-FFAP Column Spectra

Labeled peak in chromatogram

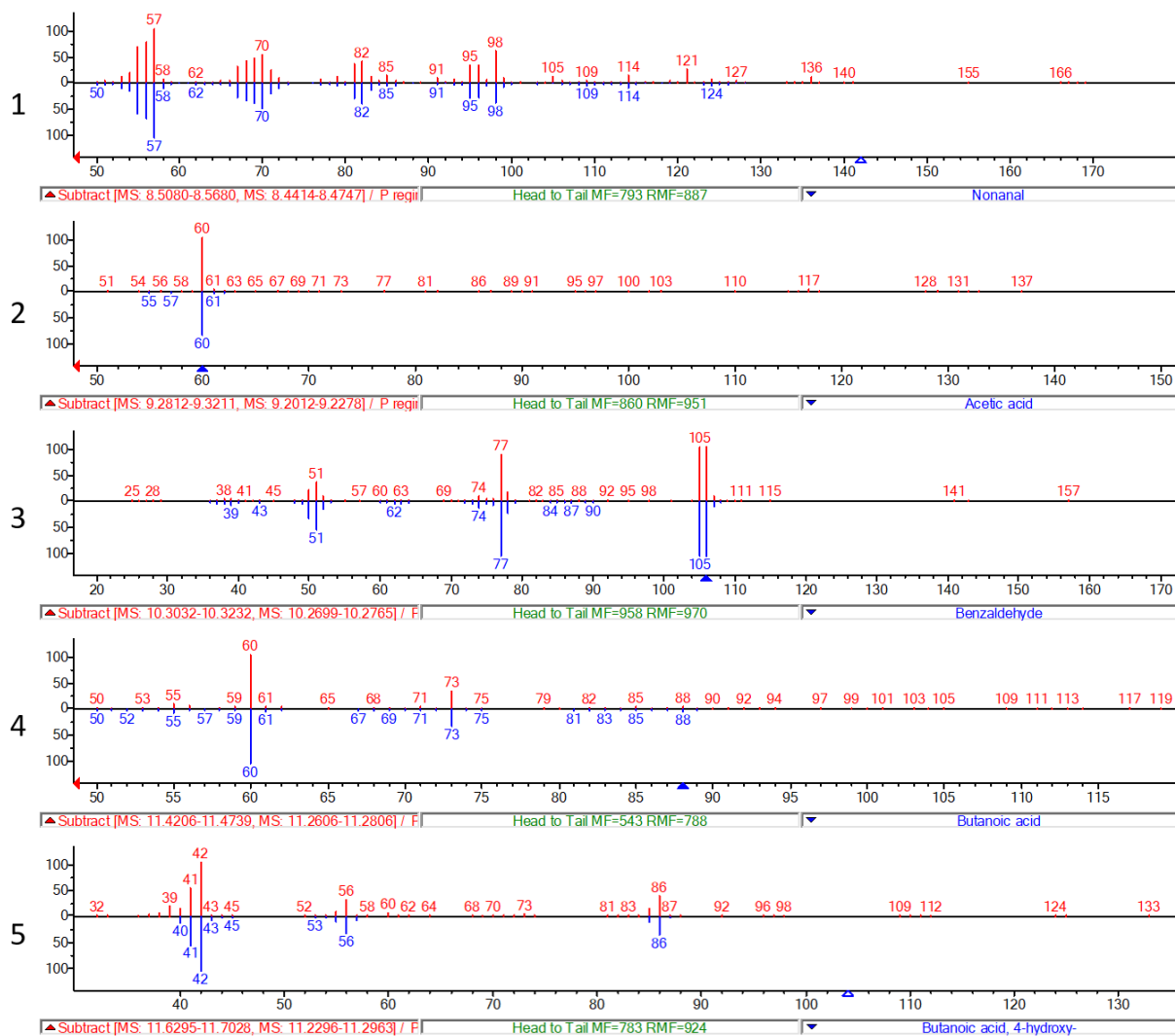


Figure S6. Head-to-tail plots showing the comparison of the GC-MS results of the analysis of *P. regina* egg headspace by HP-FFAP column, to library standards for the numbered peaks. In each case, the top spectrum is of the compound derived from the egg sample, and the bottom is that of the library match.

P. regina eggs-FFAP Column Spectra

Labeled peak in chromatogram

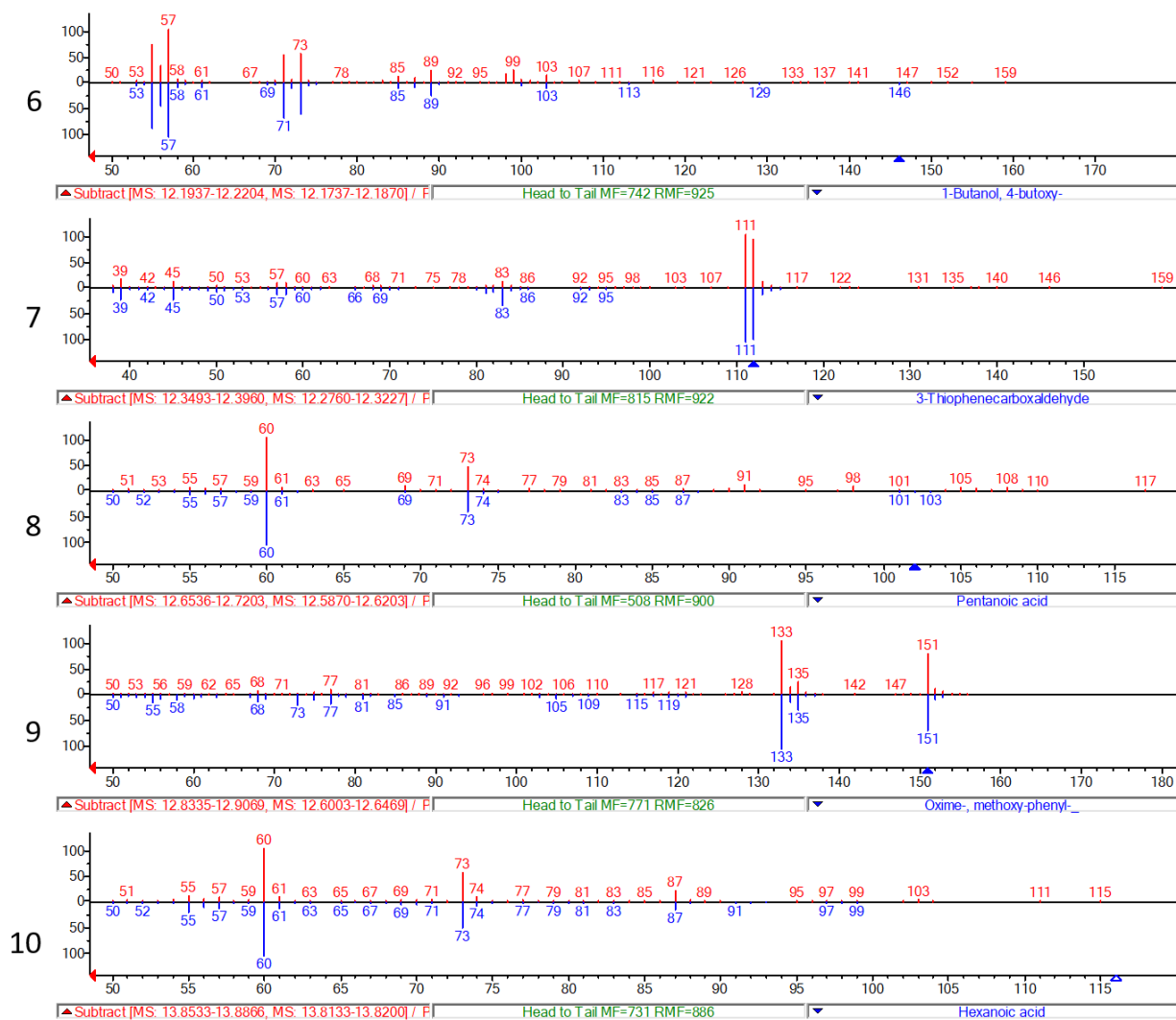


Figure S6 (continued). Head-to-tail plots showing the comparison of the GC-MS results of the analysis of *P. regina* egg headspace by HP-FFAP column, to library standards for the numbered peaks. In each case, the top spectrum is of the compound derived from the egg sample, and the bottom is that of the library match.

P. regina eggs-FFAP Column Spectra

Labeled peak in chromatogram

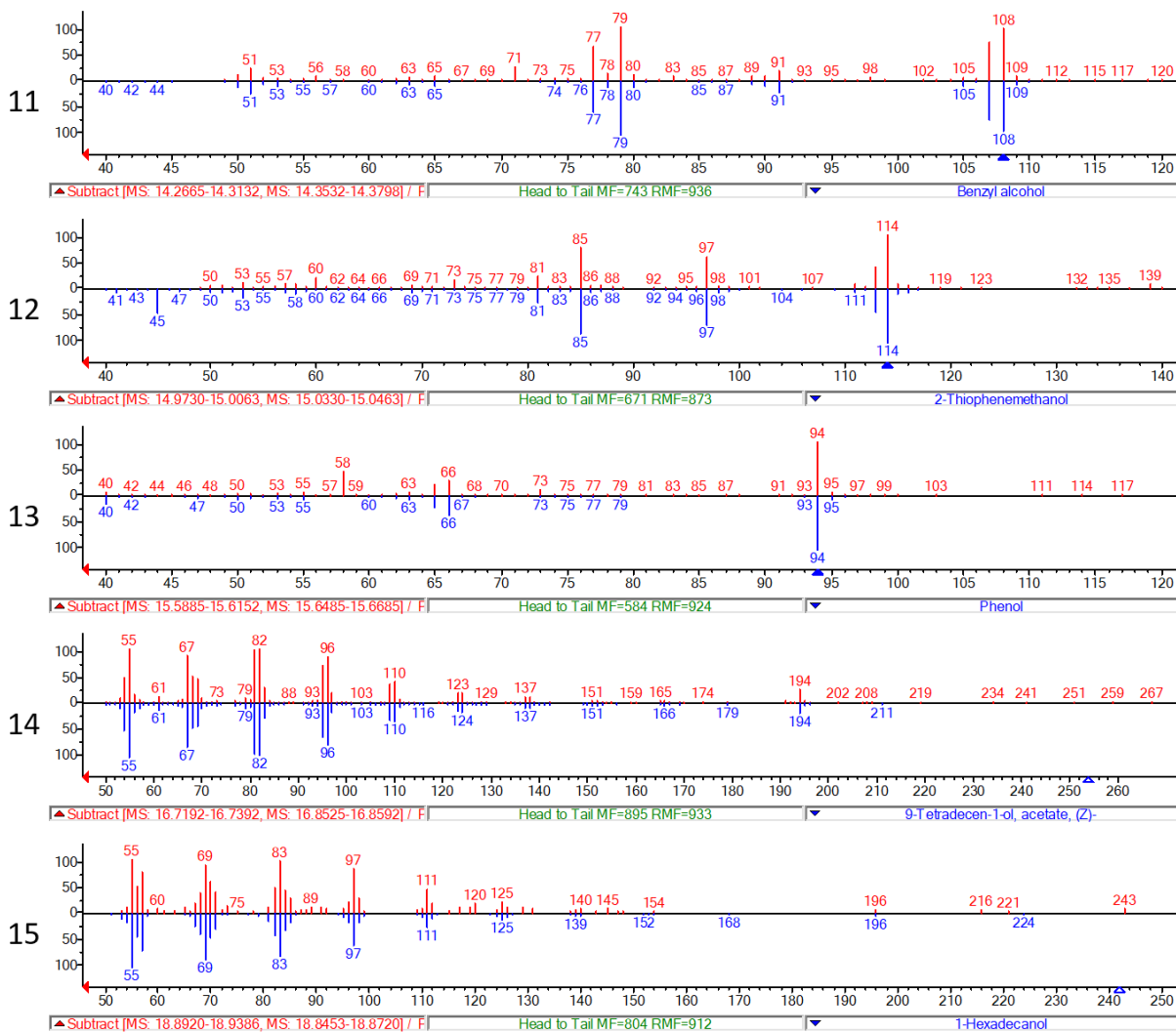


Figure S6 (continued). Head-to-tail plots showing the comparison of the GC-MS results of the analysis of *P. regina* egg headspace by HP-FFAP column, to library standards for the numbered peaks. In each case, the top spectrum is of the compound derived from the egg sample, and the bottom is that of the library match.

P. regina eggs-FFAP Column Spectra

Labeled peak in chromatogram

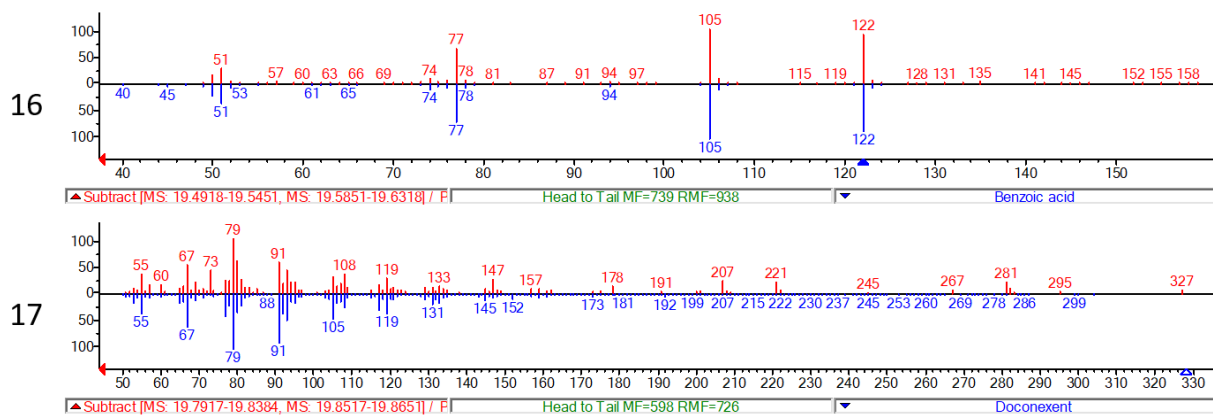


Figure S6 (continued). Head-to-tail plots showing the comparison of the GC-MS results of the analysis of *P. regina* egg headspace by HP-FFAP column, to library standards for the numbered peaks. In each case, the top spectrum is of the compound derived from the egg sample, and the bottom is that of the library match.

P. regina eggs-FFAP Column Spectra-Batch 1

Labeled peak in chromatogram

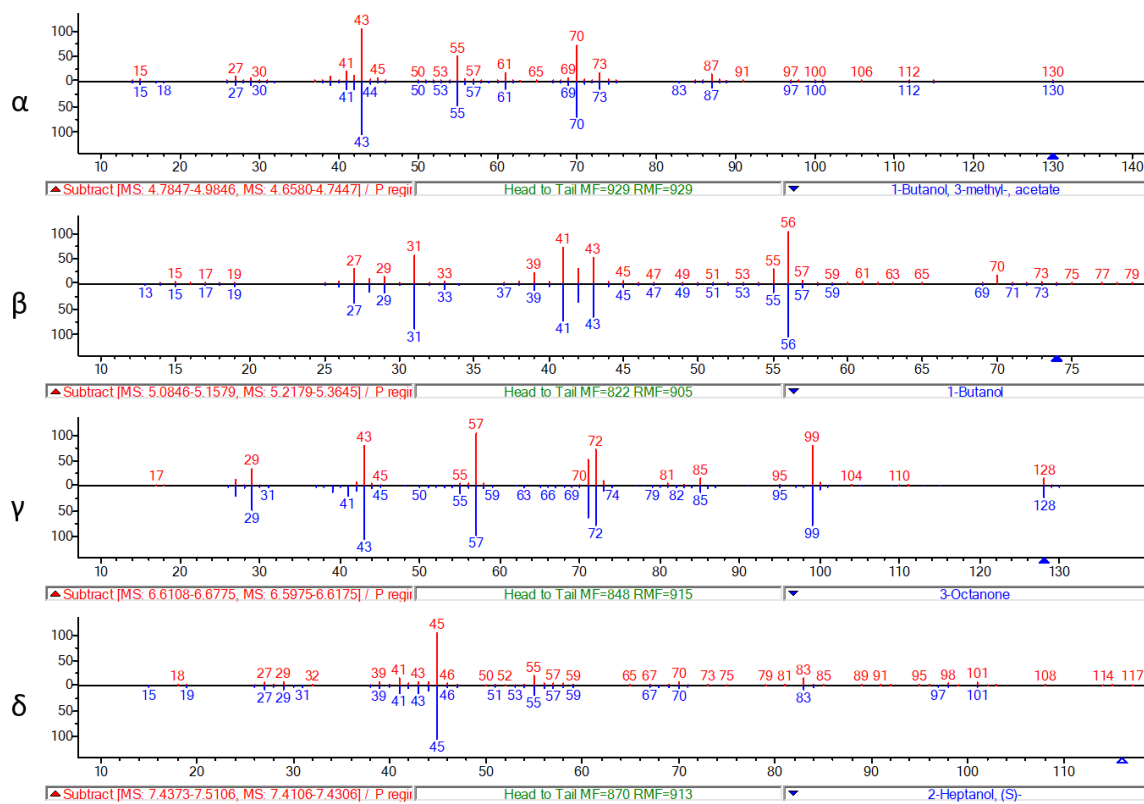


Figure S6 (continued). Head-to-tail plots showing the comparison of the GC-MS results of the analysis of *P. regina* egg headspace by HP-FFAP column, to library standards for the numbered peaks. In each case, the top spectrum is of the compound derived from the egg sample, and the bottom is that of the library match.

P. regina eggs-FFAP Column Spectra-Batch 2

Labeled peak in chromatogram

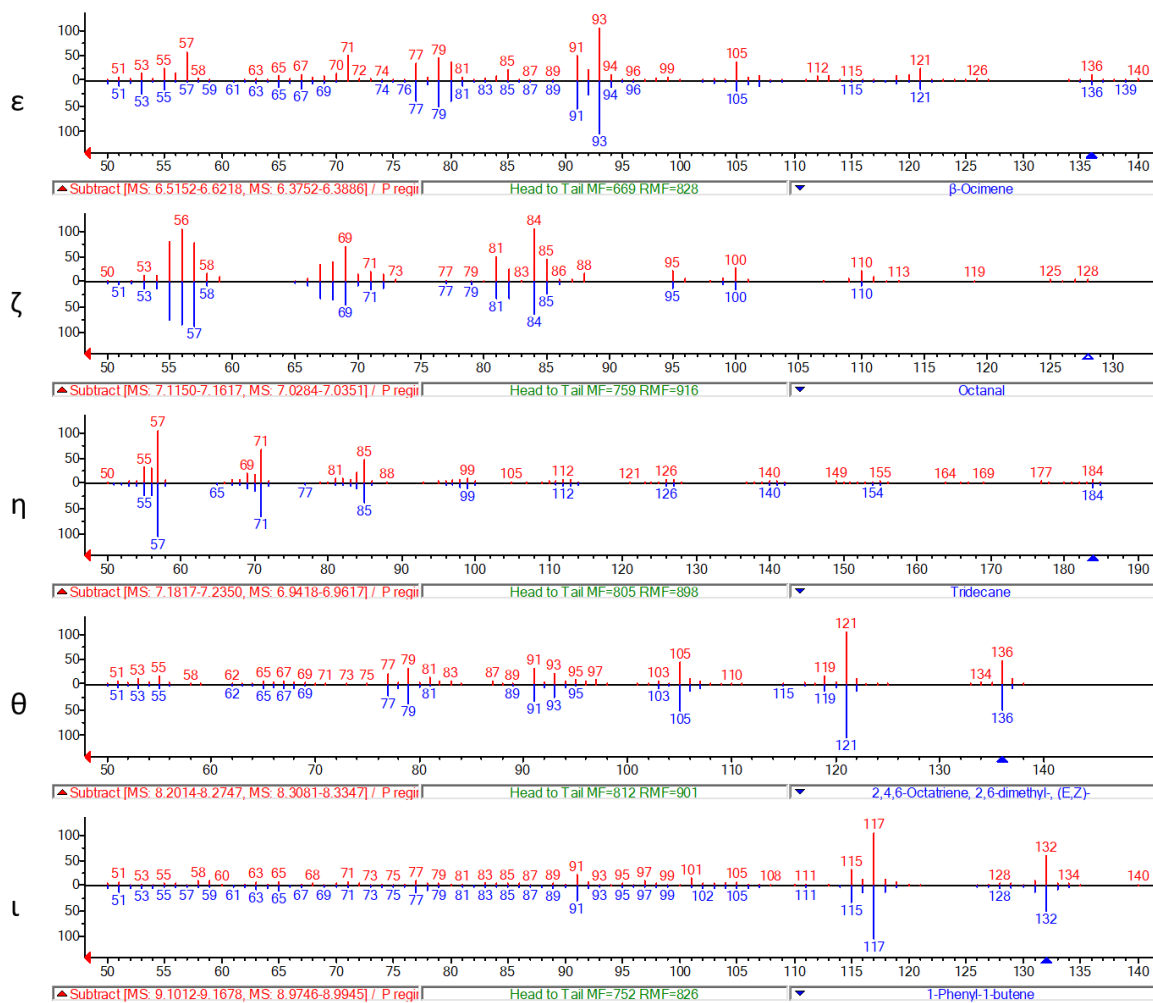


Figure S6 (continued). Head-to-tail plots showing the comparison of the GC-MS results of the analysis of *P. regina* egg headspace by HP-FFAP column, to library standards for the numbered peaks. In each case, the top spectrum is of the compound derived from the egg sample, and the bottom is that of the library match.

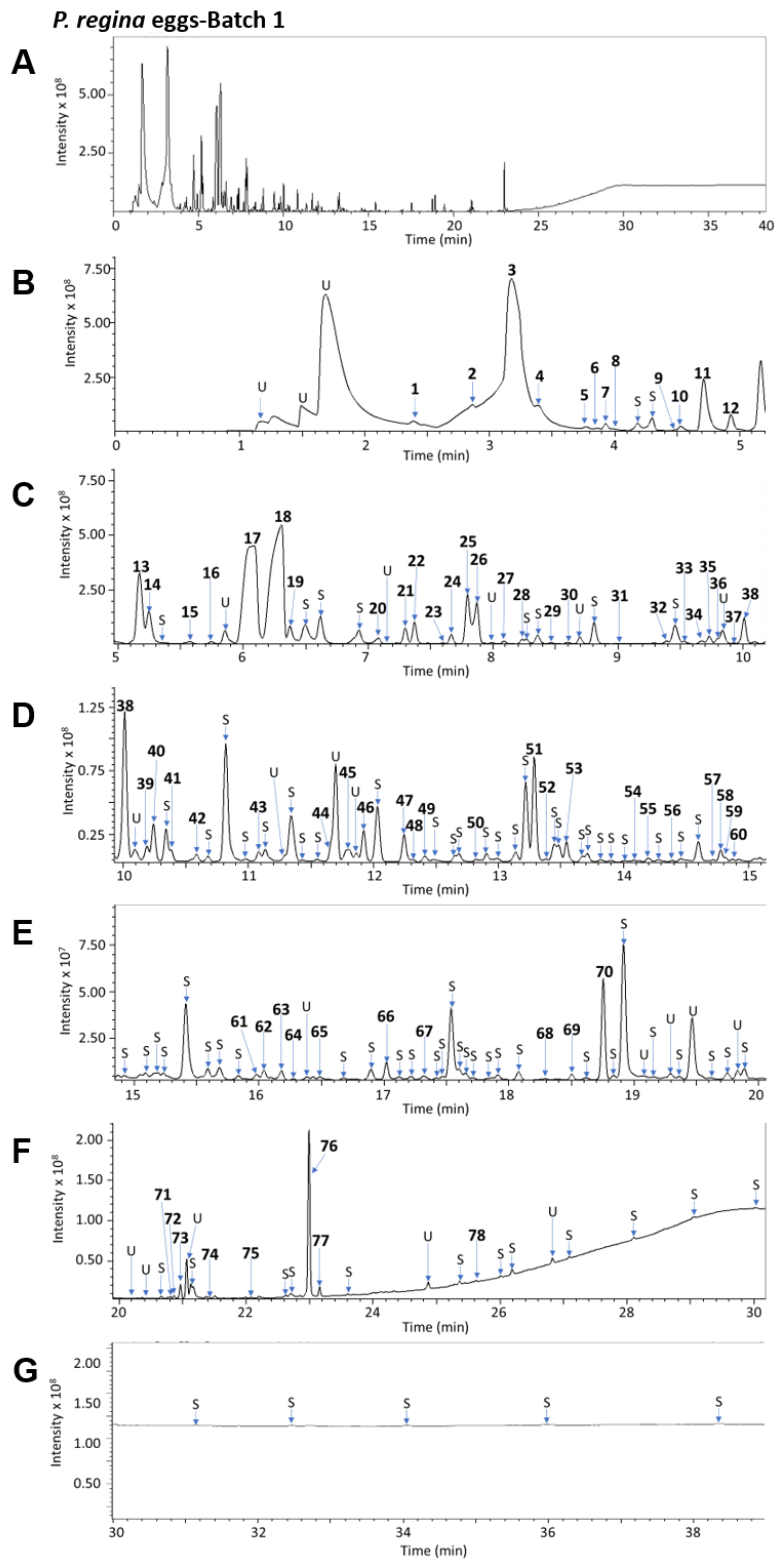


Figure S7. GC chromatogram of *P. regina* eggs (Batch #1) analyzed by CP-Sil column. Panel A shows the entire GC chromatogram, and panels B-G show magnifications of the chromatogram in 5-minute increments for clarity. The peaks are each assigned a number, the identities of which are listed in Table 4. Silanes associated with column bleed are labeled “S” and ubiquitous unnatural products are labeled “U”.

P. regina eggs-Amine Column Spectra

Labeled peak in chromatogram

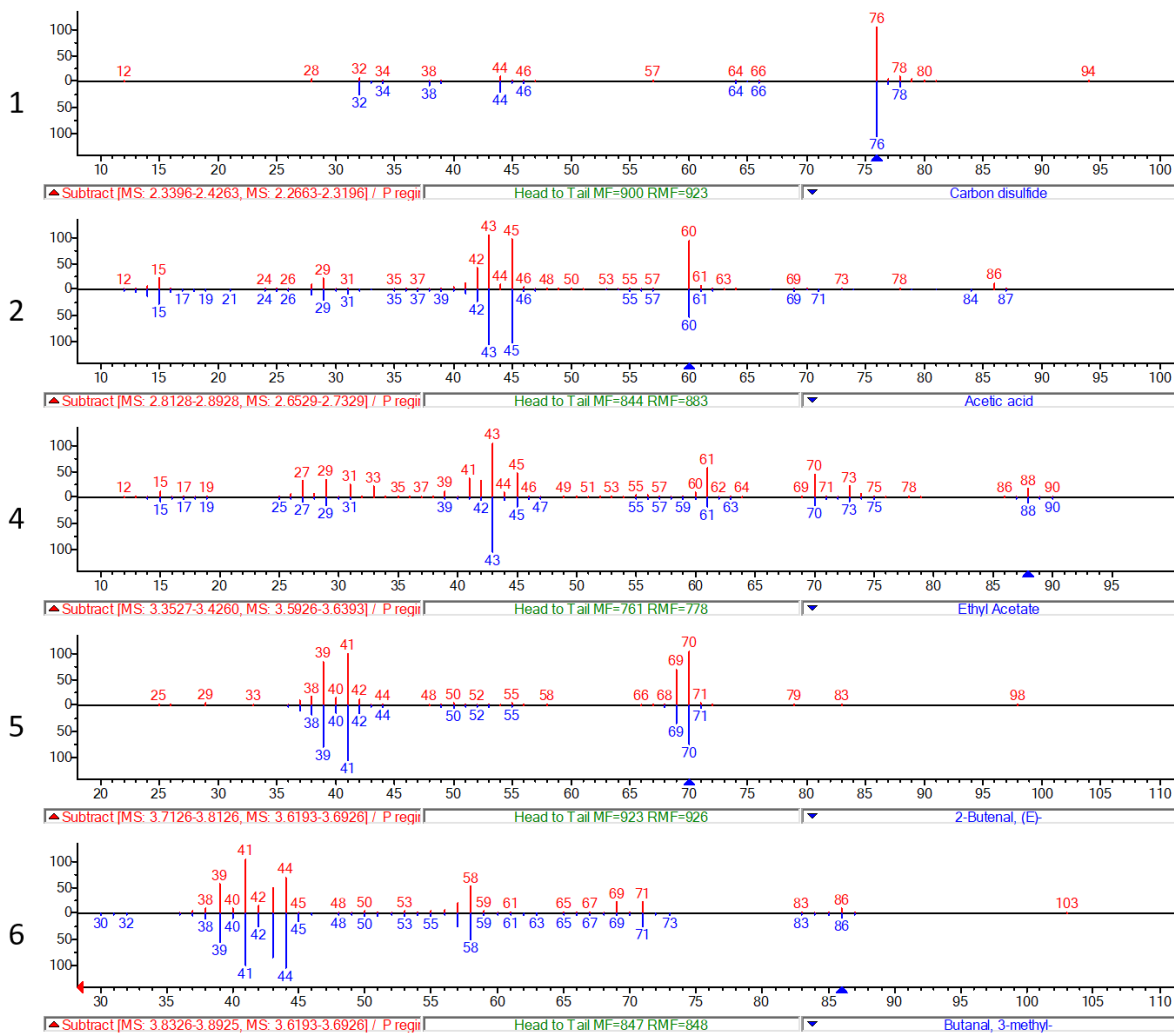


Figure S8. Head-to-tail plots showing the comparison of the GC-MS results of the analysis of *P. regina* egg headspace by CP-Sil column, to library standards for the numbered peaks. In each case, the top spectrum is of the compound derived from the egg sample, and the bottom is that of the library match.

P. regina eggs-Amine Column Spectra

Labeled peak in chromatogram

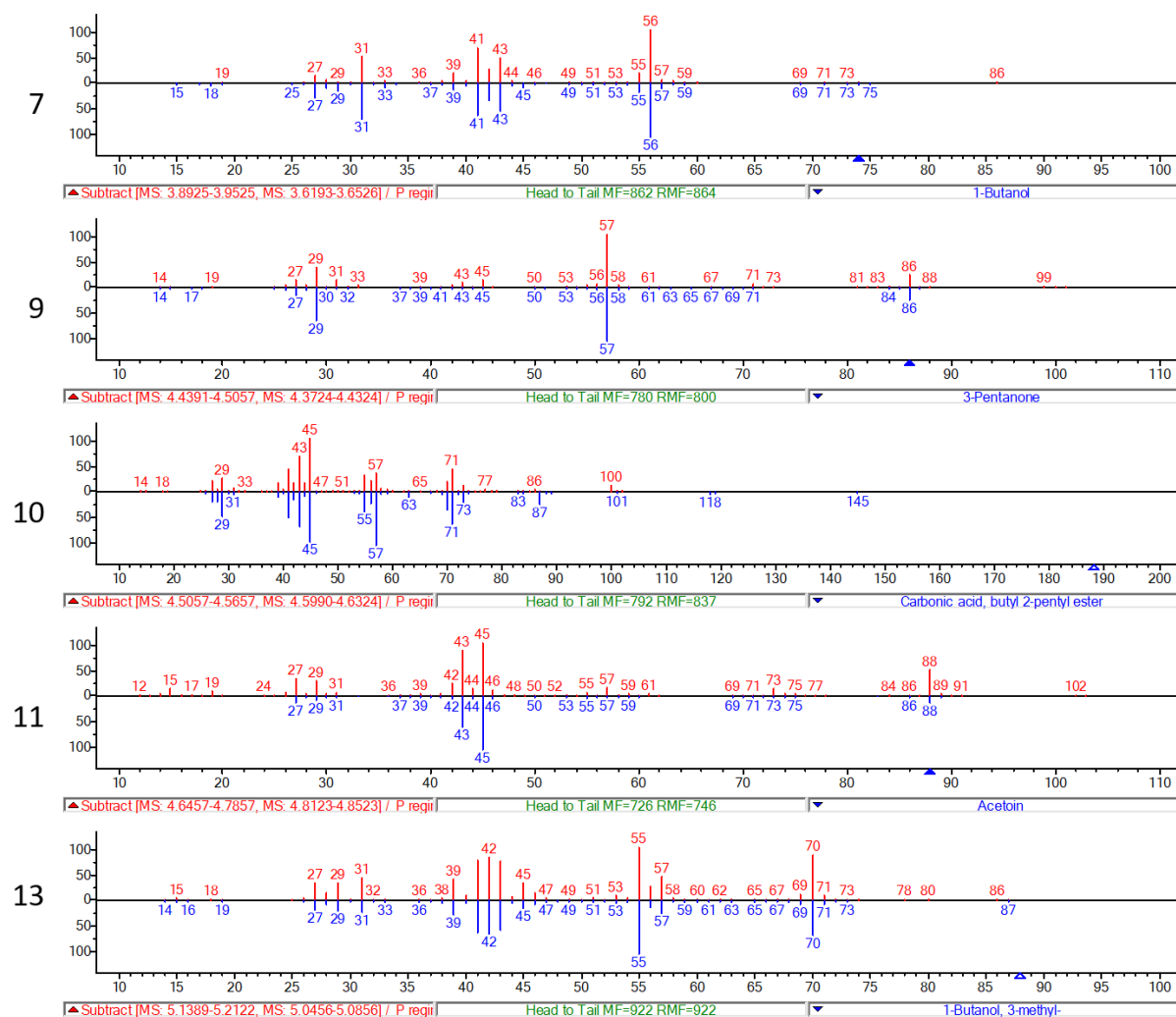


Figure S8 (continued). Head-to-tail plots showing the comparison of the GC-MS results of the analysis of *P. regina* egg headspace by CP-Sil column, to library standards for the numbered peaks. In each case, the top spectrum is of the compound derived from the egg sample, and the bottom is that of the library match.

P. regina eggs-Amine Column Spectra

Labeled peak in chromatogram

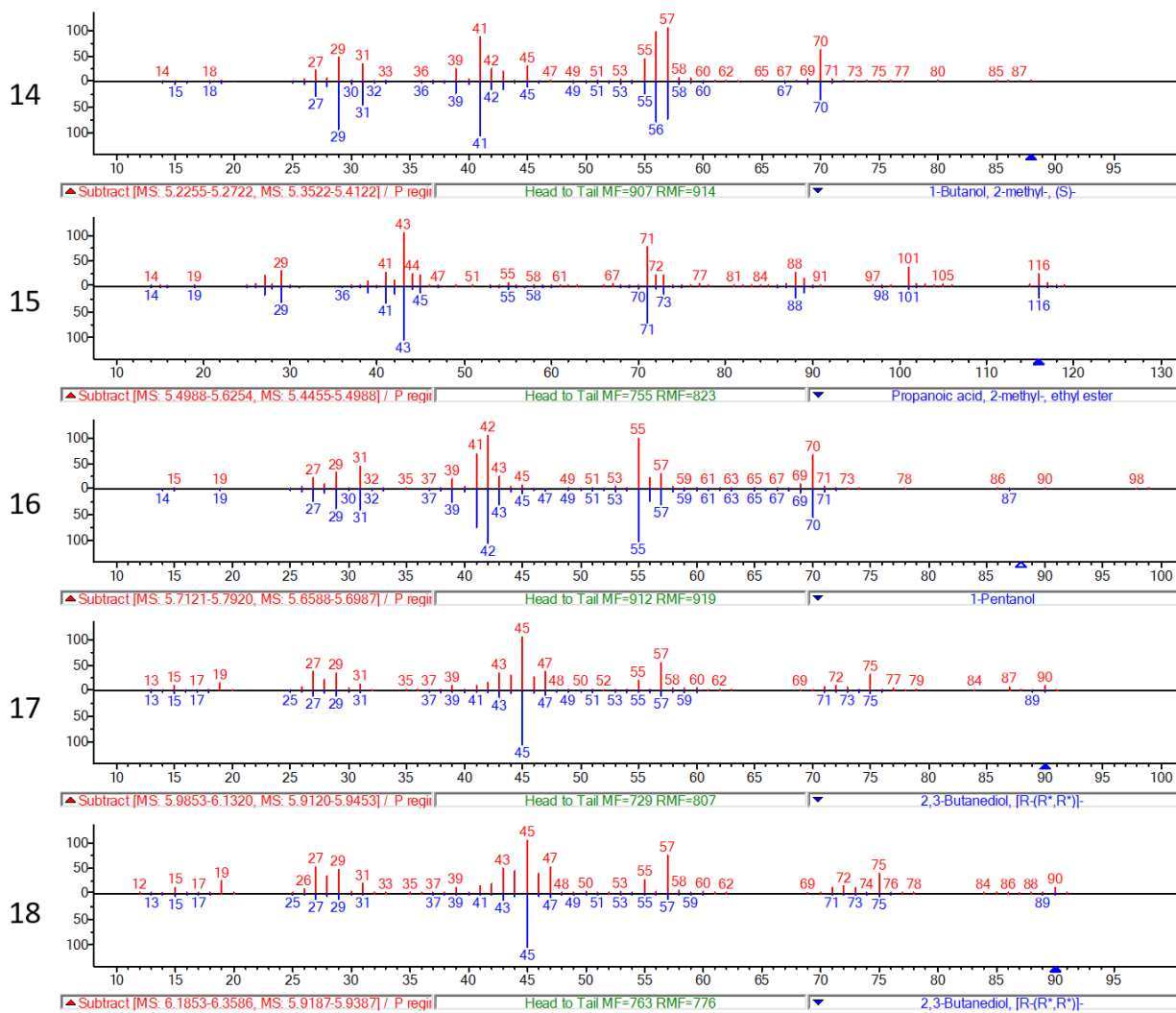


Figure S8 (continued). Head-to-tail plots showing the comparison of the GC-MS results of the analysis of *P. regina* egg headspace by CP-Sil column, to library standards for the numbered peaks. In each case, the top spectrum is of the compound derived from the egg sample, and the bottom is that of the library match.

P. regina eggs-Amine Column Spectra

Labeled peak in chromatogram

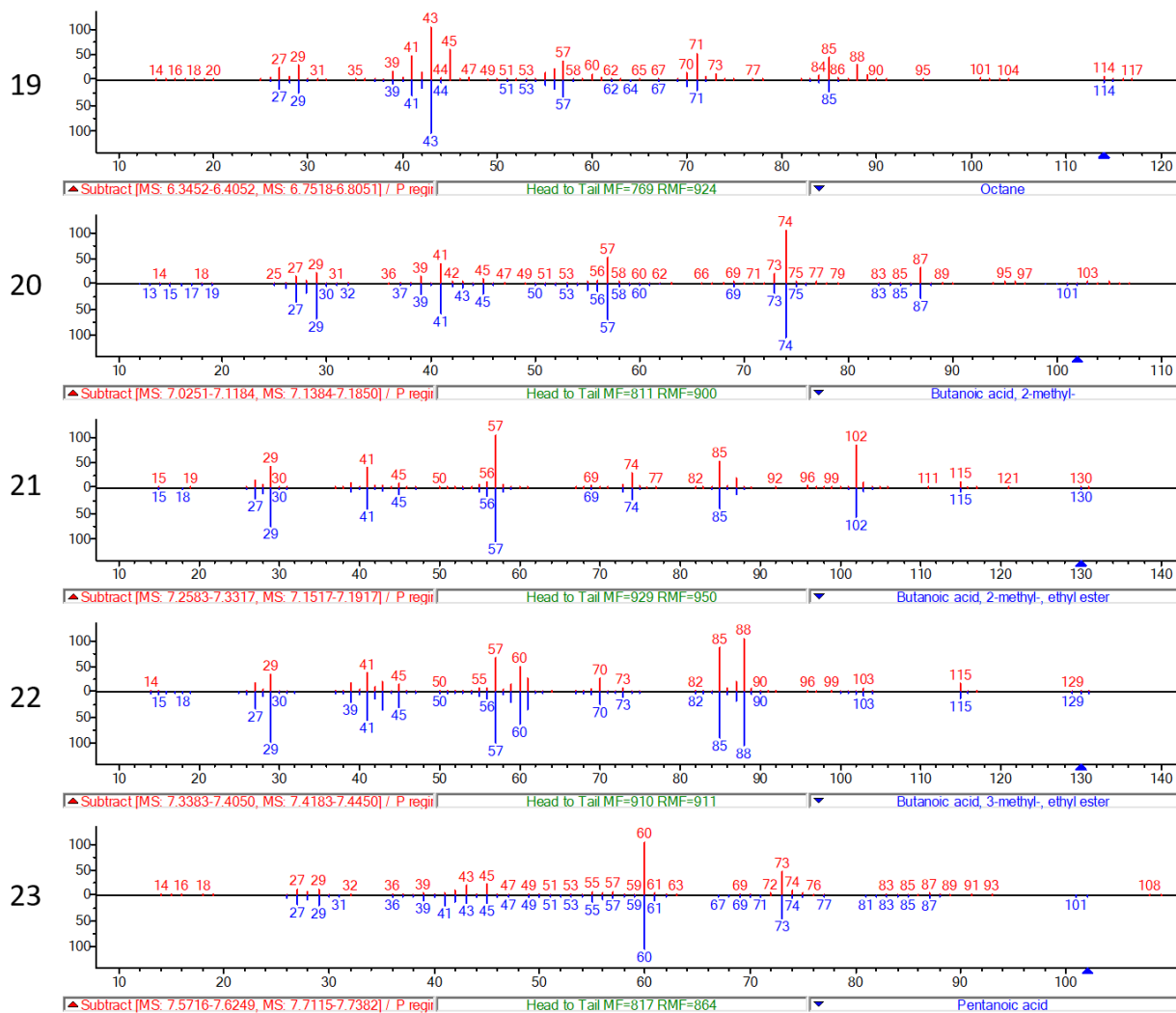


Figure S8 (continued). Head-to-tail plots showing the comparison of the GC-MS results of the analysis of *P. regina* egg headspace by CP-Sil column, to library standards for the numbered peaks. In each case, the top spectrum is of the compound derived from the egg sample, and the bottom is that of the library match.

P. regina eggs-Amine Column Spectra

Labeled peak in chromatogram

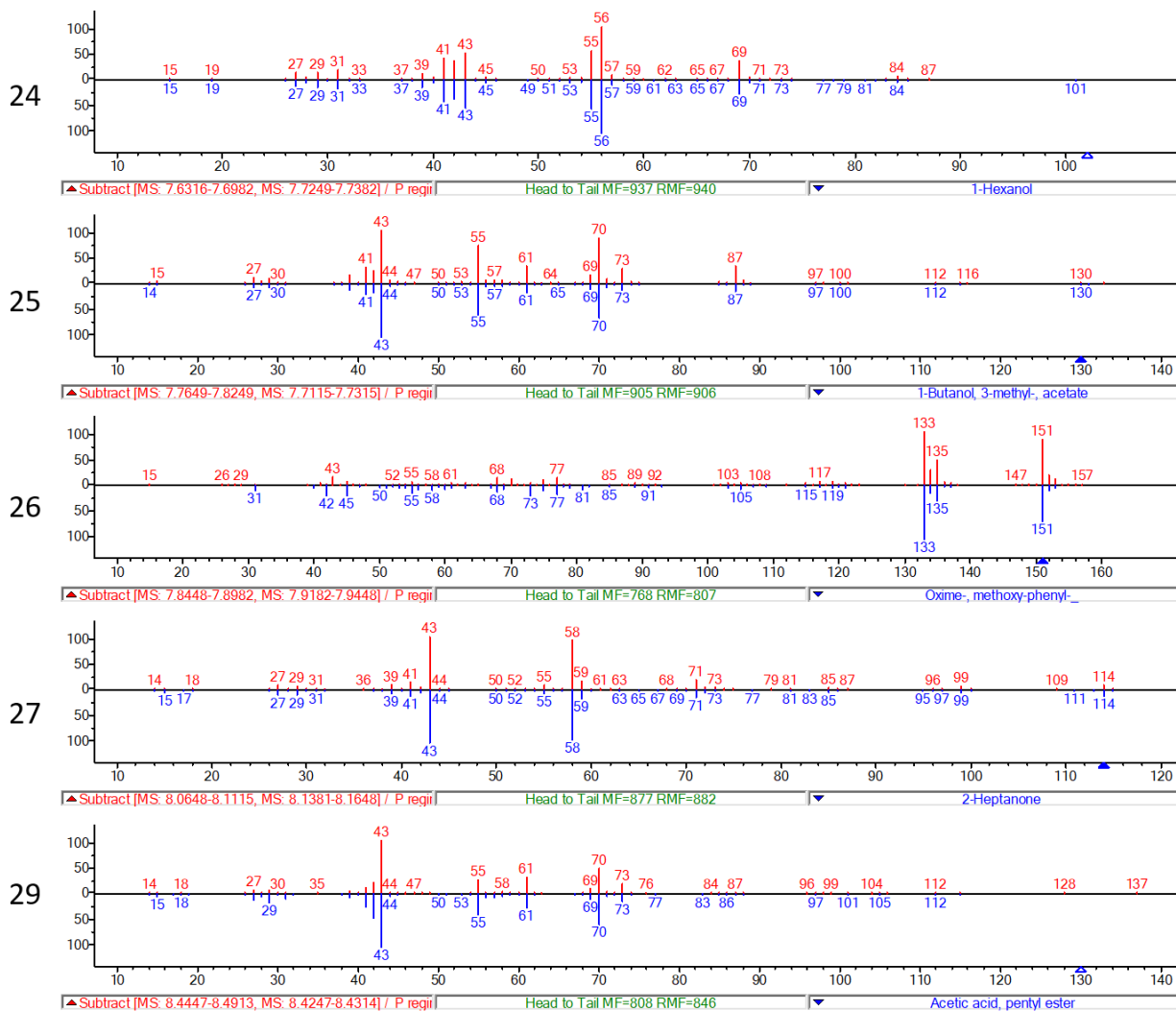


Figure S8 (continued). Head-to-tail plots showing the comparison of the GC-MS results of the analysis of *P. regina* egg headspace by CP-Sil column, to library standards for the numbered peaks. In each case, the top spectrum is of the compound derived from the egg sample, and the bottom is that of the library match.

P. regina eggs-Amine Column Spectra

Labeled peak in chromatogram

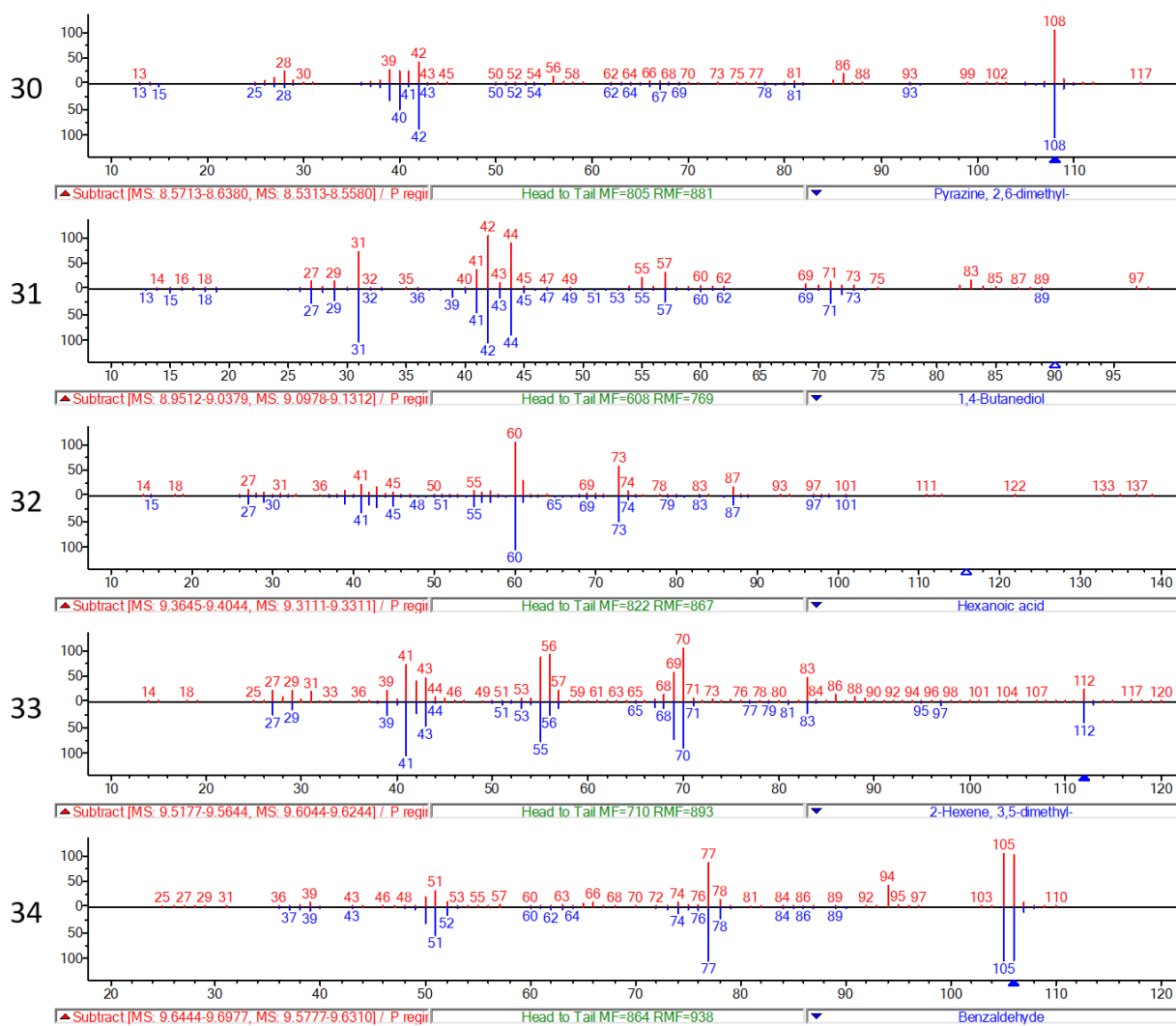


Figure S8 (continued). Head-to-tail plots showing the comparison of the GC-MS results of the analysis of *P. regina* egg headspace by CP-Sil column, to library standards for the numbered peaks. In each case, the top spectrum is of the compound derived from the egg sample, and the bottom is that of the library match.

P. regina eggs-Amine Column Spectra

Labeled peak in chromatogram

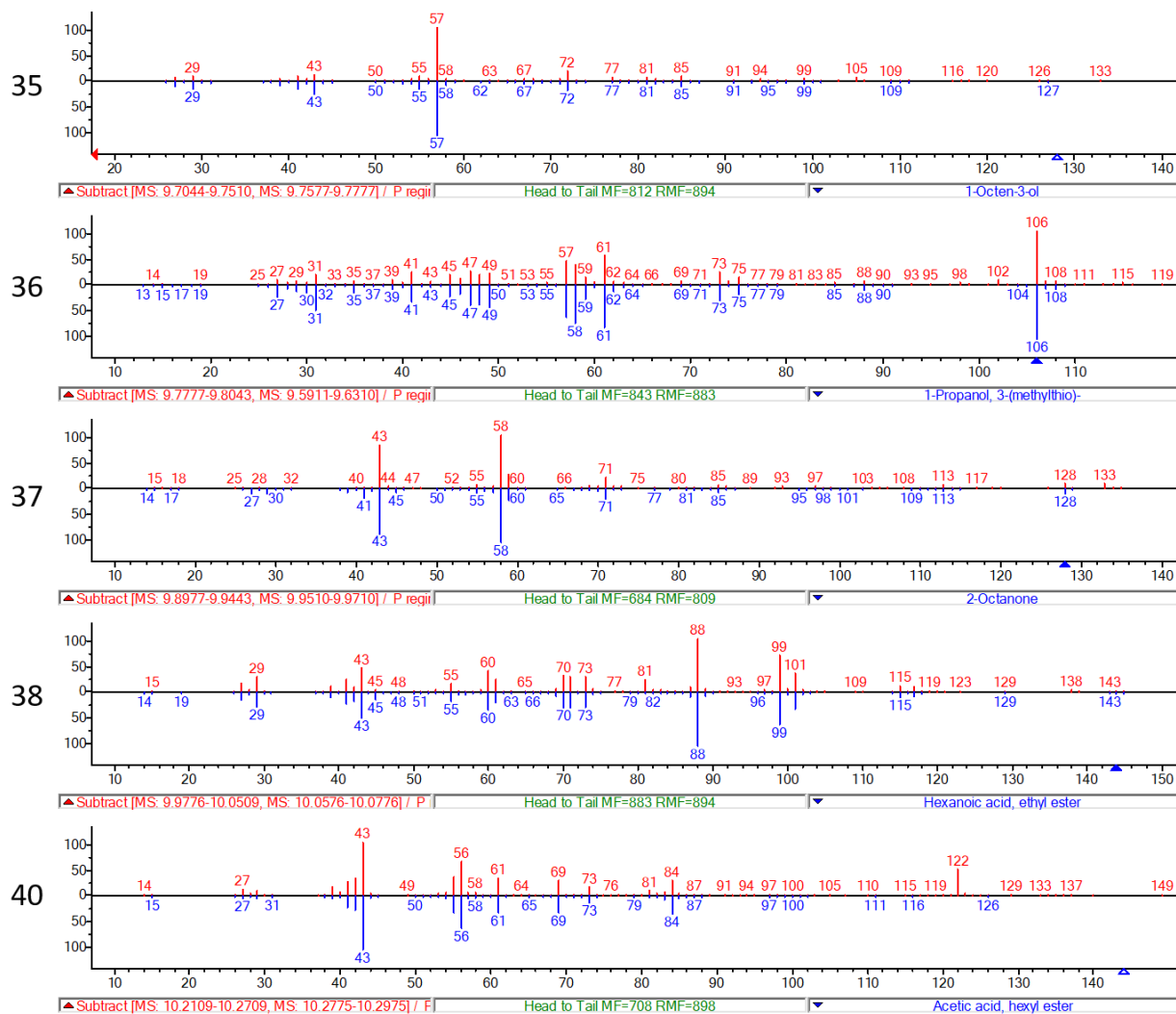


Figure S8 (continued). Head-to-tail plots showing the comparison of the GC-MS results of the analysis of *P. regina* egg headspace by CP-Sil column, to library standards for the numbered peaks. In each case, the top spectrum is of the compound derived from the egg sample, and the bottom is that of the library match.

P. regina eggs-Amine Column Spectra

Labeled peak in chromatogram

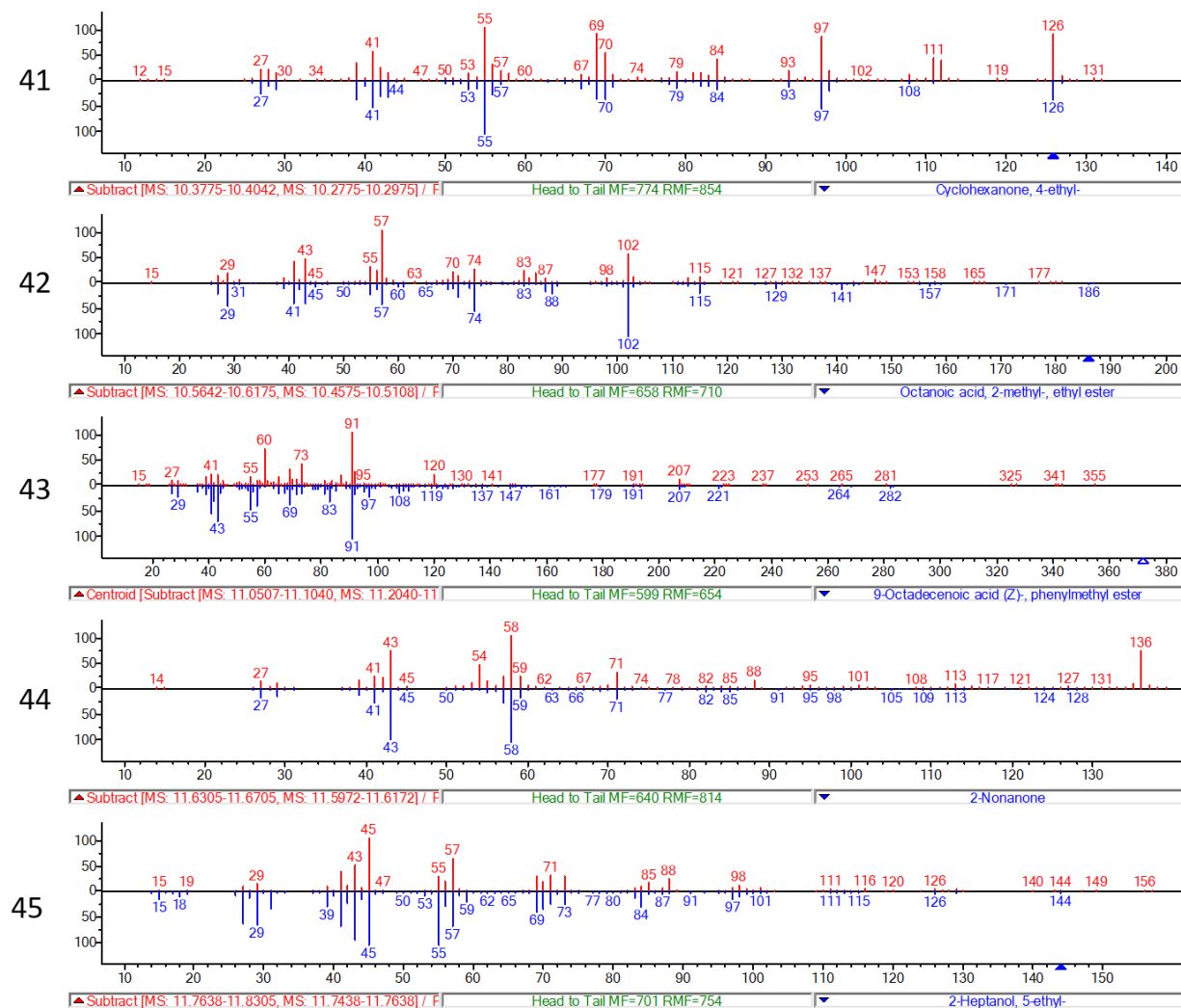


Figure S8 (continued). Head-to-tail plots showing the comparison of the GC-MS results of the analysis of *P. regina* egg headspace by CP-Sil column, to library standards for the numbered peaks. In each case, the top spectrum is of the compound derived from the egg sample, and the bottom is that of the library match.

P. regina eggs-Amine Column Spectra

Labeled peak in chromatogram

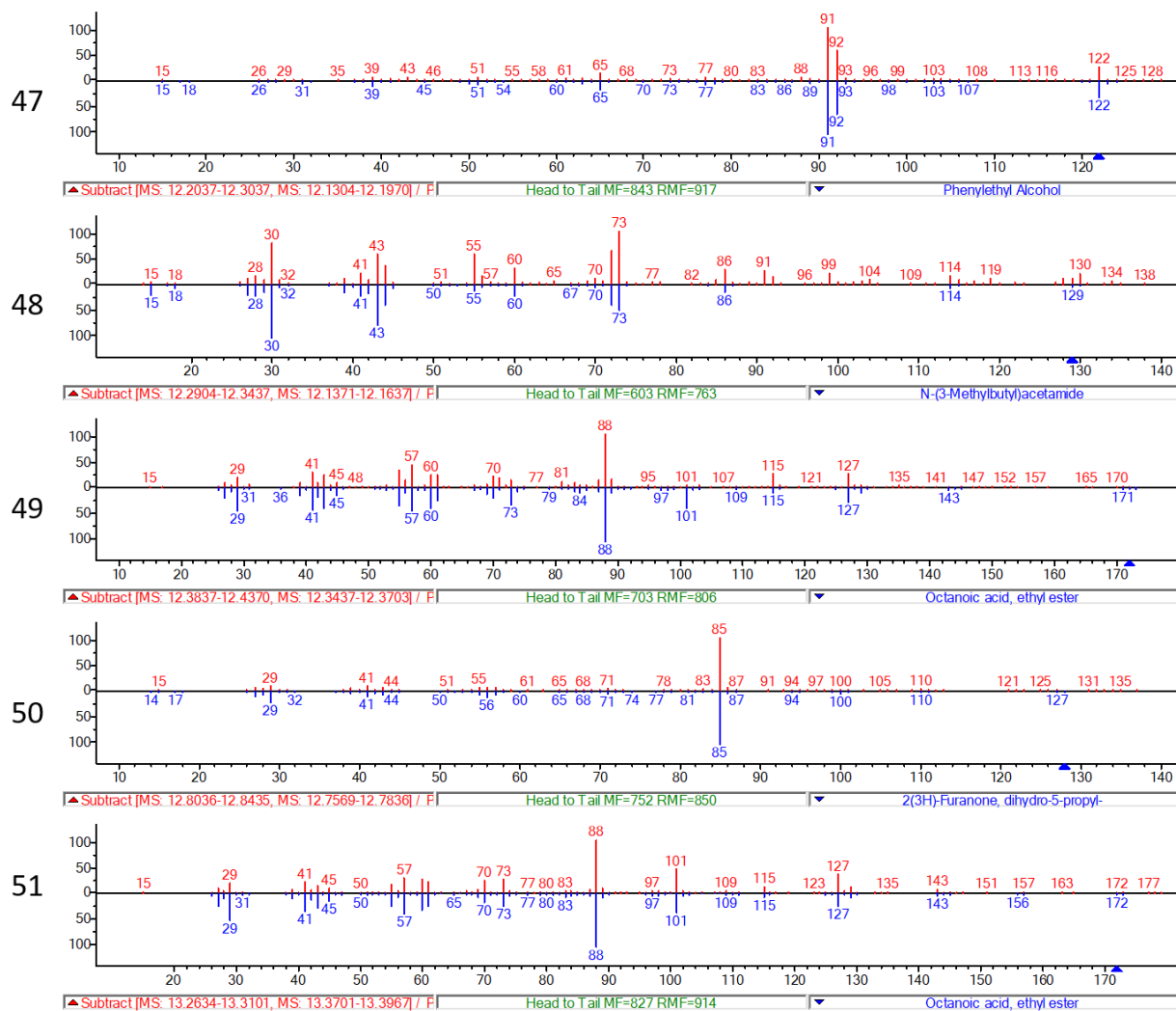


Figure S8 (continued). Head-to-tail plots showing the comparison of the GC-MS results of the analysis of *P. regina* egg headspace by CP-Sil column, to library standards for the numbered peaks. In each case, the top spectrum is of the compound derived from the egg sample, and the bottom is that of the library match.

P. regina eggs-Amine Column Spectra

Labeled peak in chromatogram

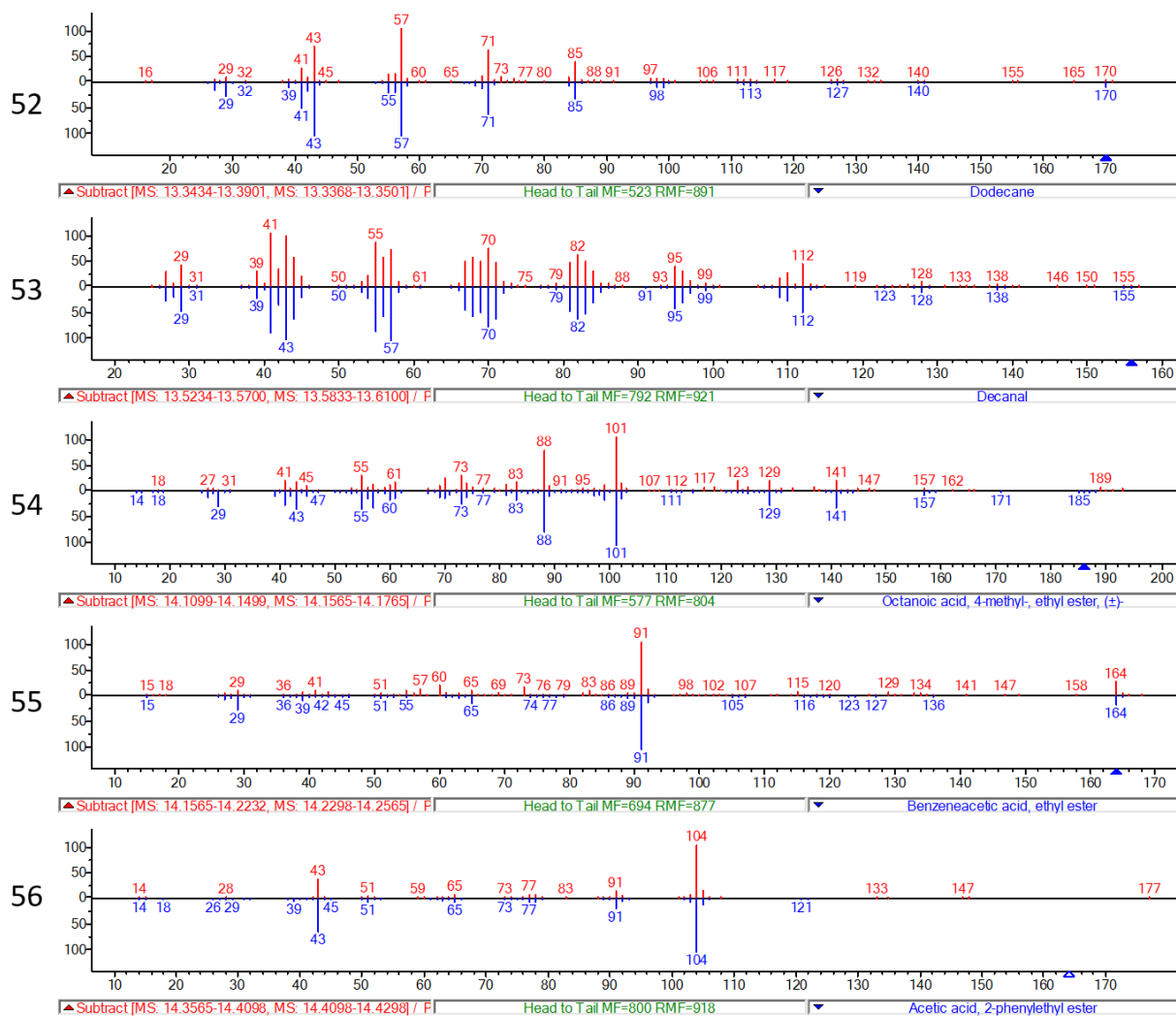


Figure S8 (continued). Head-to-tail plots showing the comparison of the GC-MS results of the analysis of *P. regina* egg headspace by CP-Sil column, to library standards for the numbered peaks. In each case, the top spectrum is of the compound derived from the egg sample, and the bottom is that of the library match.

P. regina eggs-Amine Column Spectra

Labeled peak in chromatogram

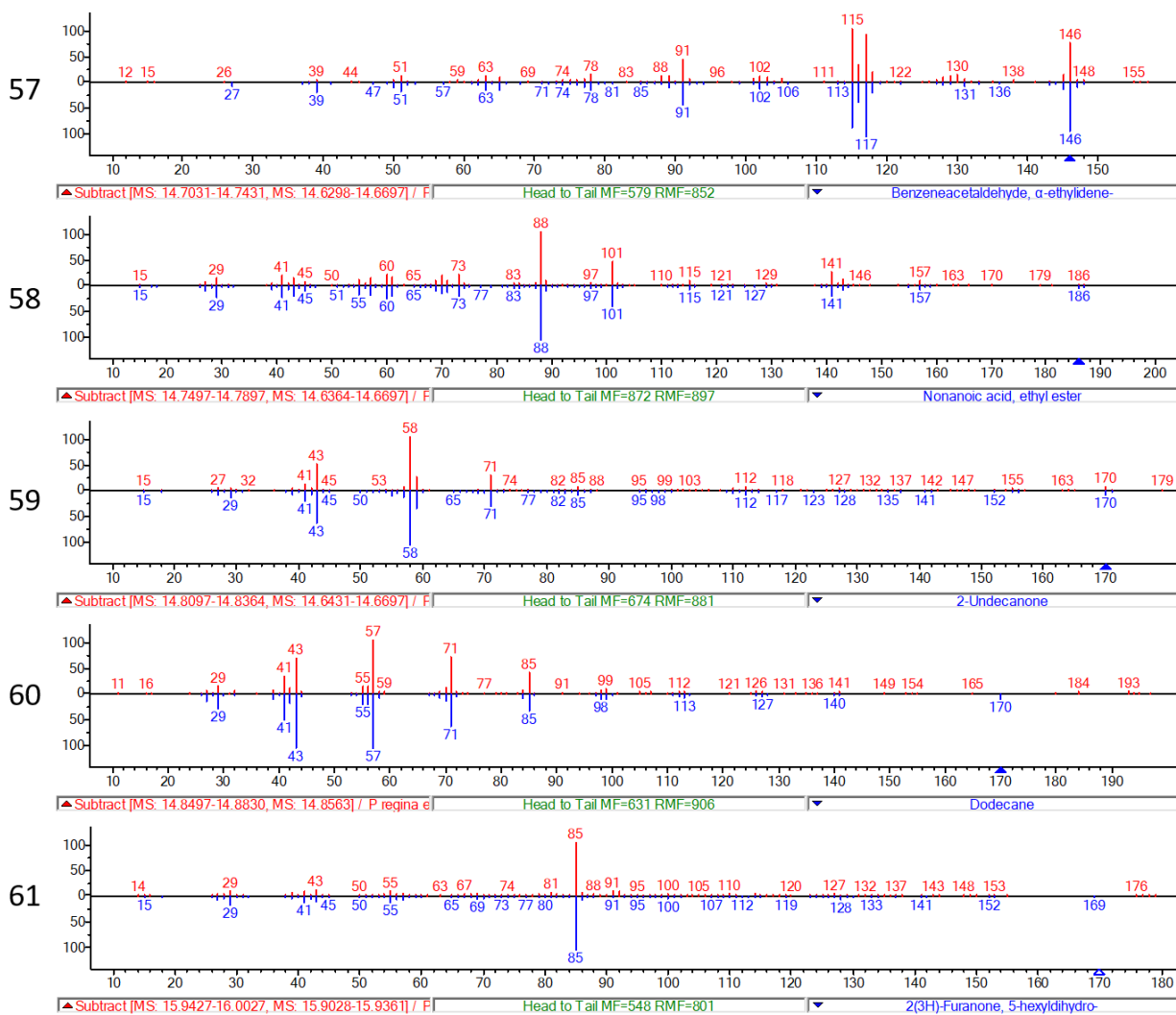


Figure S8 (continued). Head-to-tail plots showing the comparison of the GC-MS results of the analysis of *P. regina* egg headspace by CP-Sil column, to library standards for the numbered peaks. In each case, the top spectrum is of the compound derived from the egg sample, and the bottom is that of the library match.

P. regina eggs-Amine Column Spectra

Labeled peak in chromatogram

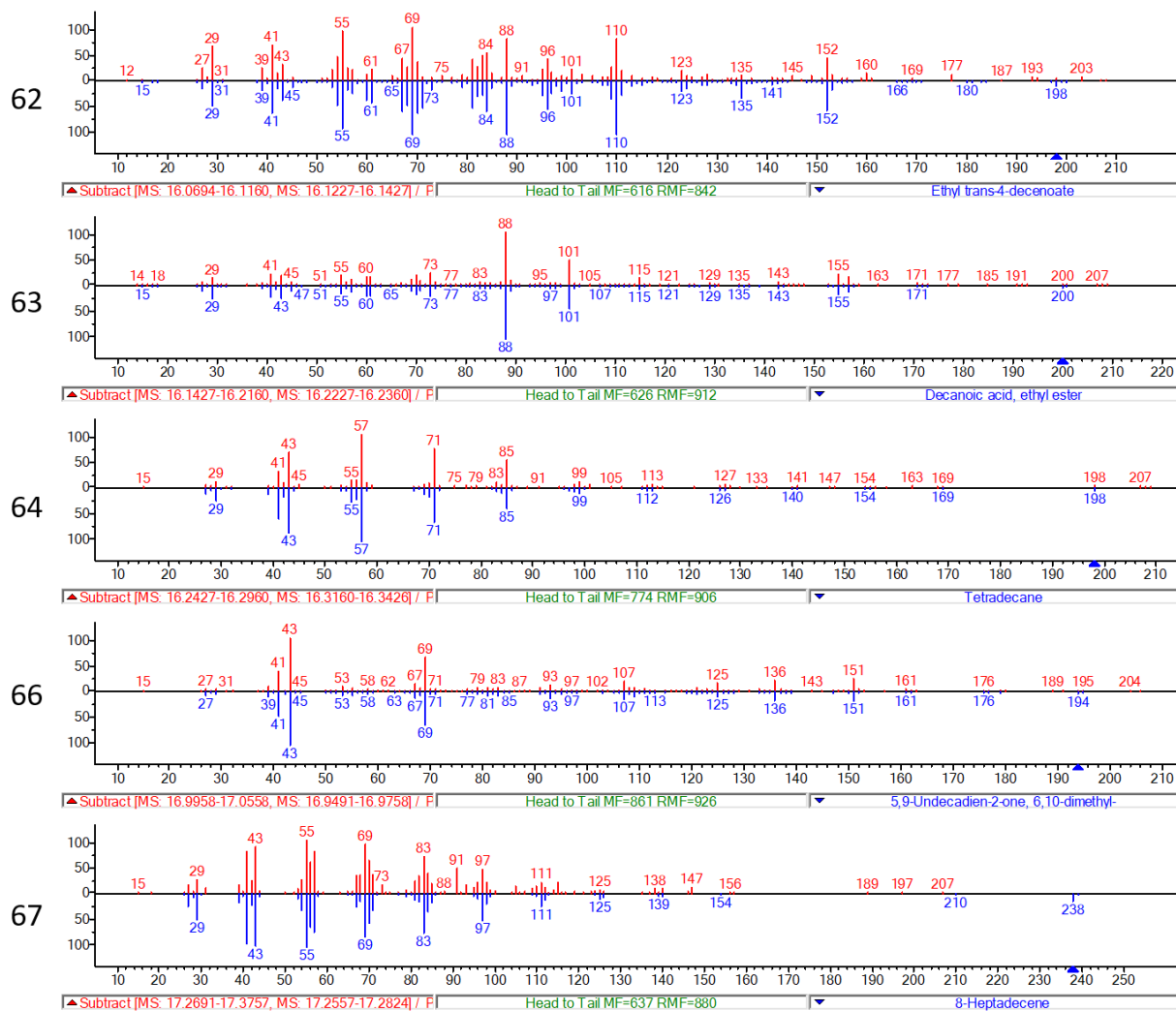


Figure S8 (continued). Head-to-tail plots showing the comparison of the GC-MS results of the analysis of *P. regina* egg headspace by CP-Sil column, to library standards for the numbered peaks. In each case, the top spectrum is of the compound derived from the egg sample, and the bottom is that of the library match.

P. regina eggs-Amine Column Spectra

Labeled peak in chromatogram

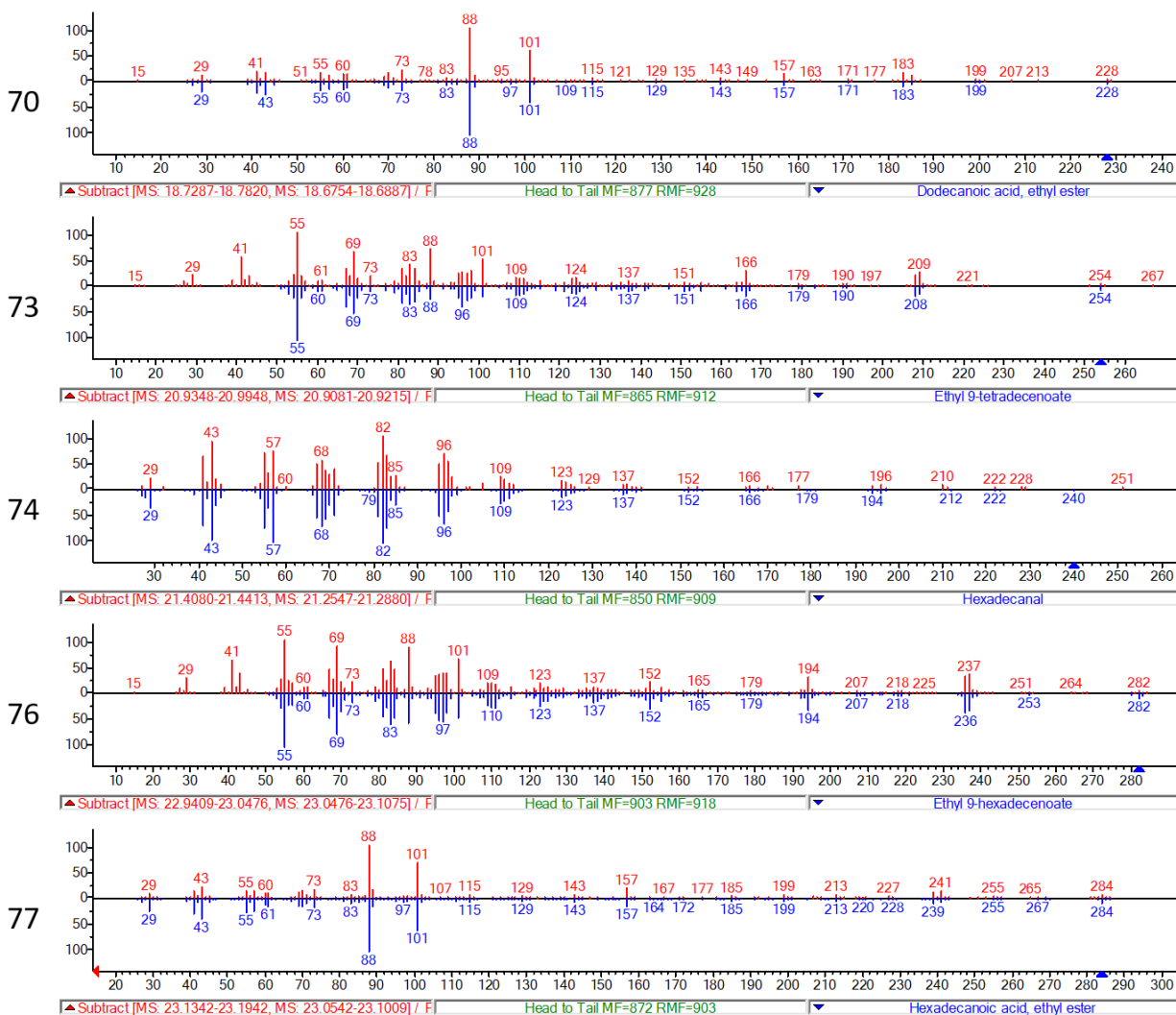


Figure S8 (continued). Head-to-tail plots showing the comparison of the GC-MS results of the analysis of *P. regina* egg headspace by CP-Sil column, to library standards for the numbered peaks. In each case, the top spectrum is of the compound derived from the egg sample, and the bottom is that of the library match.

P. regina eggs-Amine Column Spectra

Labeled peak in chromatogram

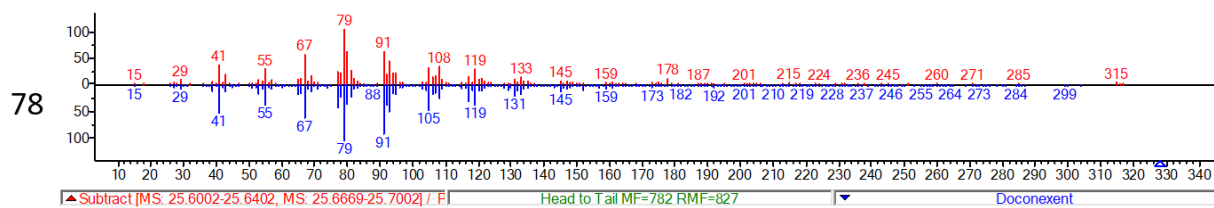


Figure S8 (continued). Head-to-tail plots showing the comparison of the GC-MS results of the analysis of *P. regina* egg headspace by CP-Sil column, to library standards for the numbered peaks. In each case, the top spectrum is of the compound derived from the egg sample, and the bottom is that of the library match.

P. regina eggs-Amine Column Spectra

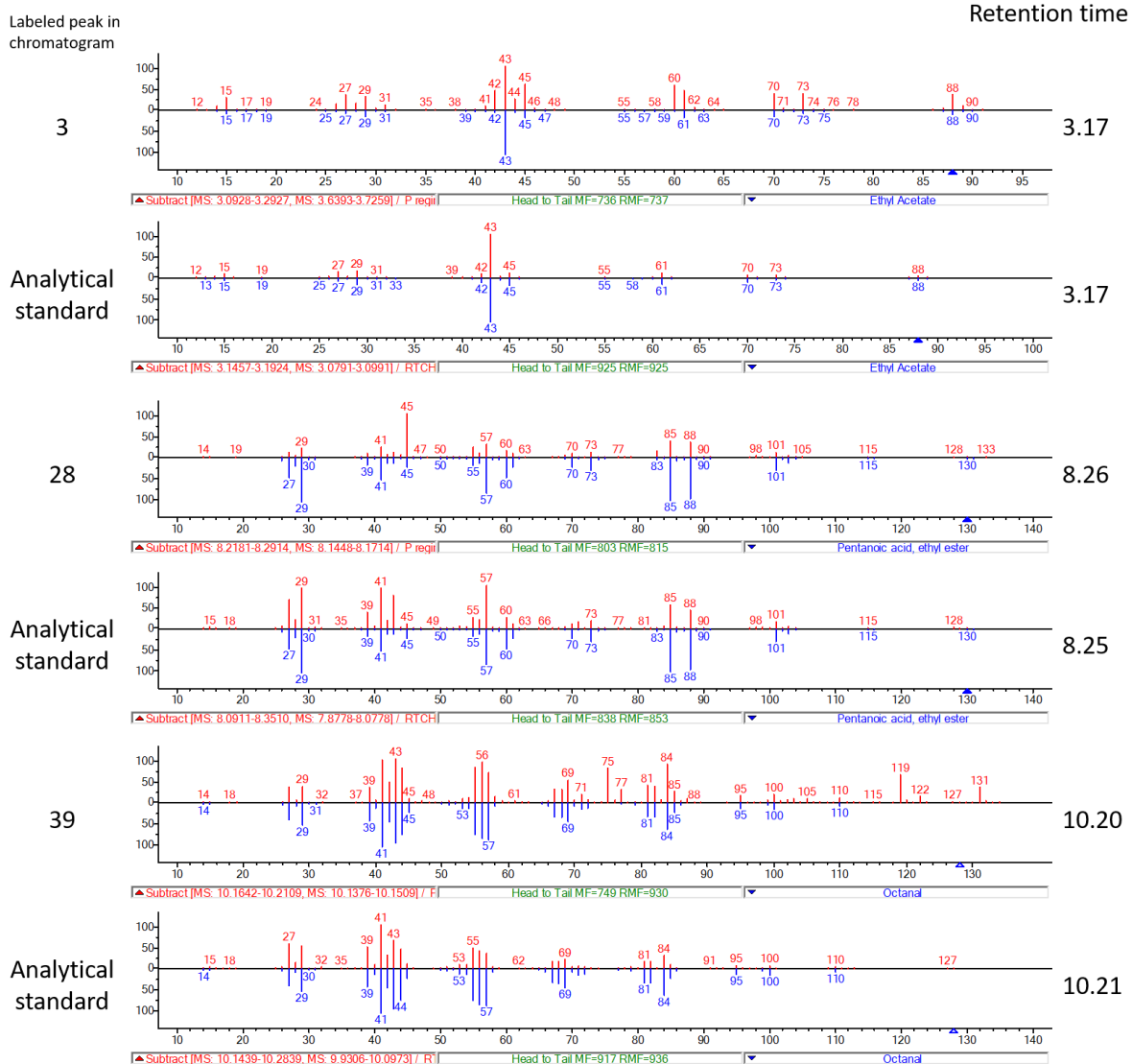


Figure S8 (continued). Head-to-tail plots showing the results of control experiments run for the confirmation of peak identities in *P. regina* egg headspace analyzed by CP-Sil column. In each pair of spectra, the top is the compound observed in the egg headspace, and the bottom is that of the analytical standard, with their corresponding retention times.

P. regina eggs-Amine Column Spectra

Labeled peak in chromatogram

Retention time

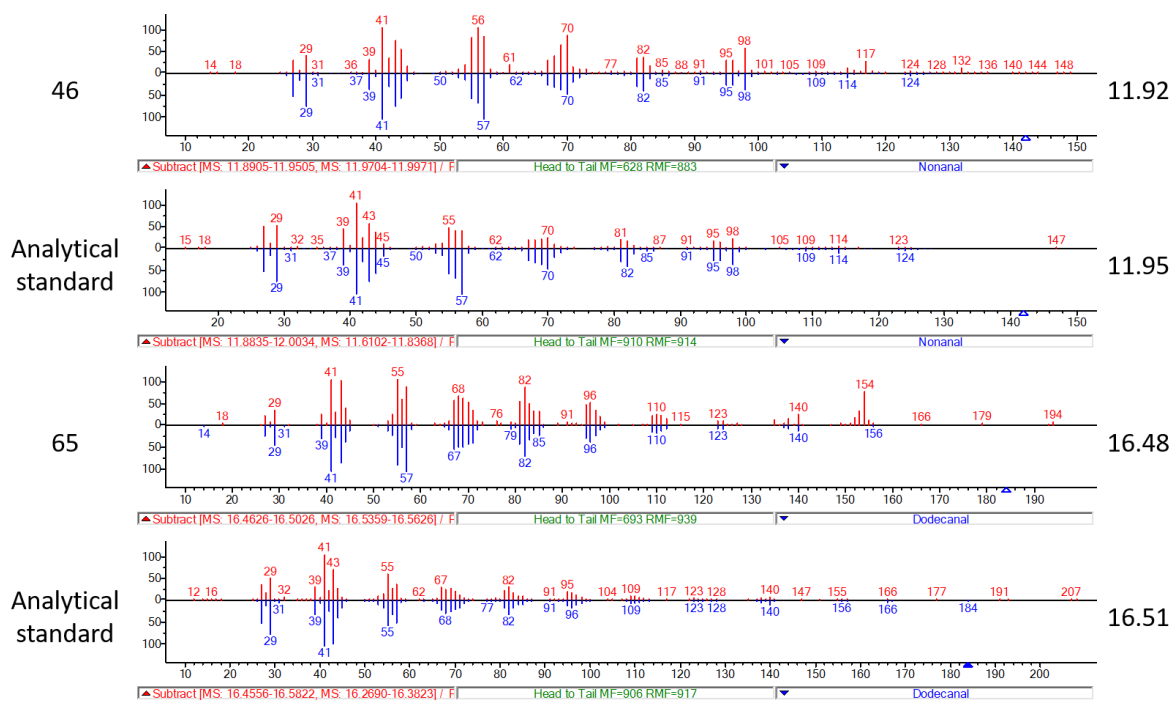


Figure S8 (continued). Head-to-tail plots showing the results of control experiments run for the confirmation of peak identities in *P. regina* egg headspace analyzed by CP-Sil column. In each pair of spectra, the top is the compound observed in the egg headspace, and the bottom is that of the analytical standard, with their corresponding retention times.

Tables

Table S1. GC-MS parameters for the analysis of the headspace of blow fly eggs.		
Column type	HP-FFAP 30 m x 0.25 mm, 0.25 μ m	CP-Sil 8 CB 30 m x 0.32 mm, 1.0 μ m
Helium flow rate (mL/min)	1.0	1.5
Oven program	40 °C (1 min hold), ramp 10 °C/min to 240 °C (9 min hold)	40 °C (1 min hold), ramp 10 °C/min to 320 °C (10 min hold)
Total run time (min)	30	39
Ion source temperature (°C)	200	250
GC-ITF temperature (°C)	240	280