

Supplementary material

Suspect Screening and Semi-Quantification of Macrolide Antibiotics in Municipal Wastewater by High-Performance Liquid Chromatography – Precursor Ion Scan Tandem Mass Spectrometry

Contents:

Figure S1. Collision-induced dissociation pathways of erythromycin.

Figure S2. Collision-induced dissociation pathways of clarithromycin.

Figure S3. Collision-induced dissociation pathways of azithromycin.

Figure S4. Collision-induced dissociation pathways of midecamycin.

Figure S5. Collision-induced dissociation pathways of spiramycin.

Figure S6. Collision-induced dissociation pathways of josamycin.

Figure S7. HPLC-MS/MS (PrecIS) chromatogram of the model mixture macrolides with concentrations close to LOQ.

Diagnostic ions: m/z 174 (red) and m/z 158 (black)

Figure S8. Extracted ion current HPLC-HRMS chromatograms of municipal wastewater (peak numbers and m/z values correspond to those listed in Figure 4 and in Table 4).

Table S1. Recoveries of the macrolides obtained by solid-phase extraction on an HLB stationary phase.

Table S2. Tandem mass spectra of the precursor ion candidates found in HPLC-MS/MS (PrecIS) chromatogram of municipal wastewater (compound numbers correspond to the peaks on Figure 4 and in Table 4).

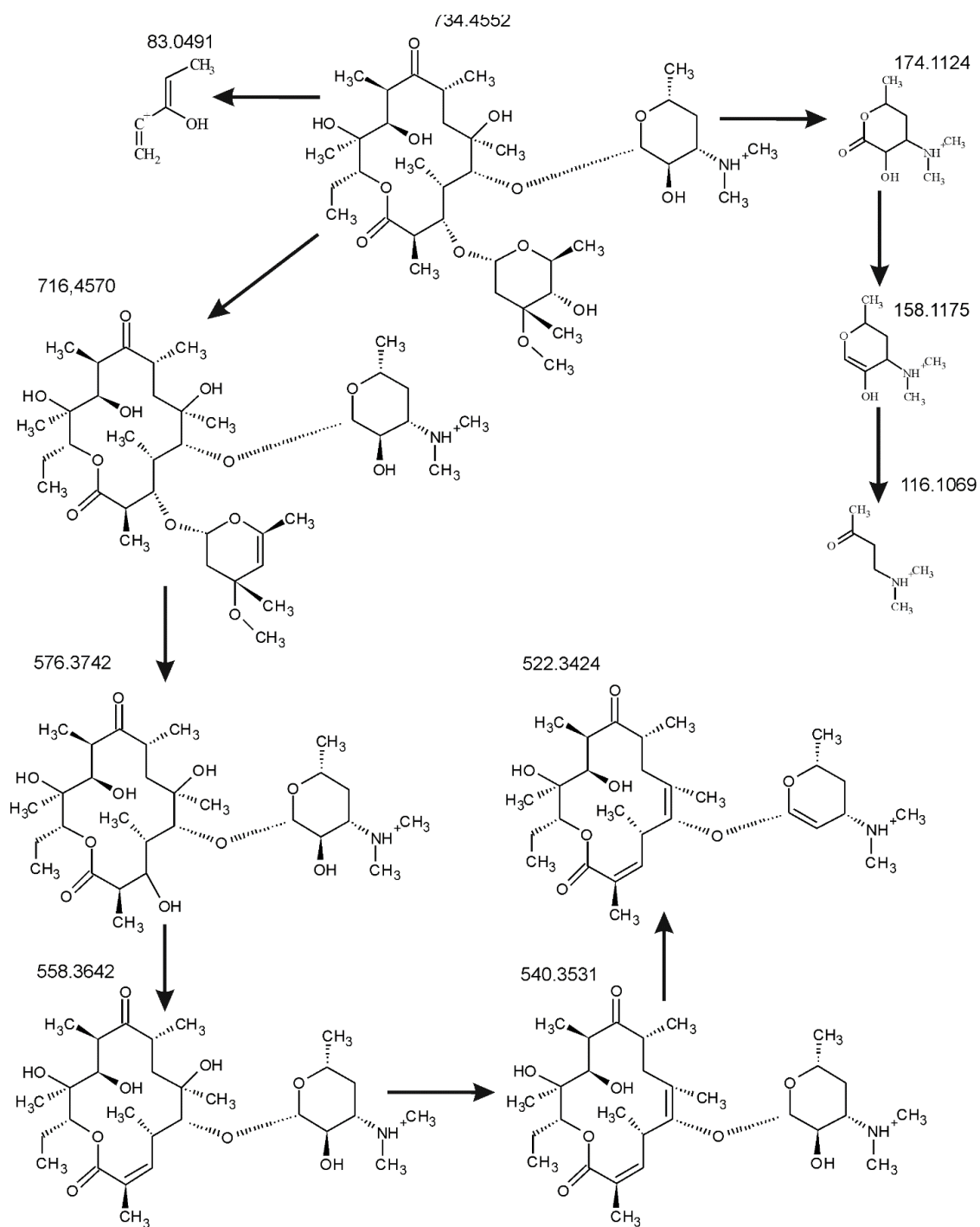


Figure S1. Collision-induced dissociation pathways of erythromycin.

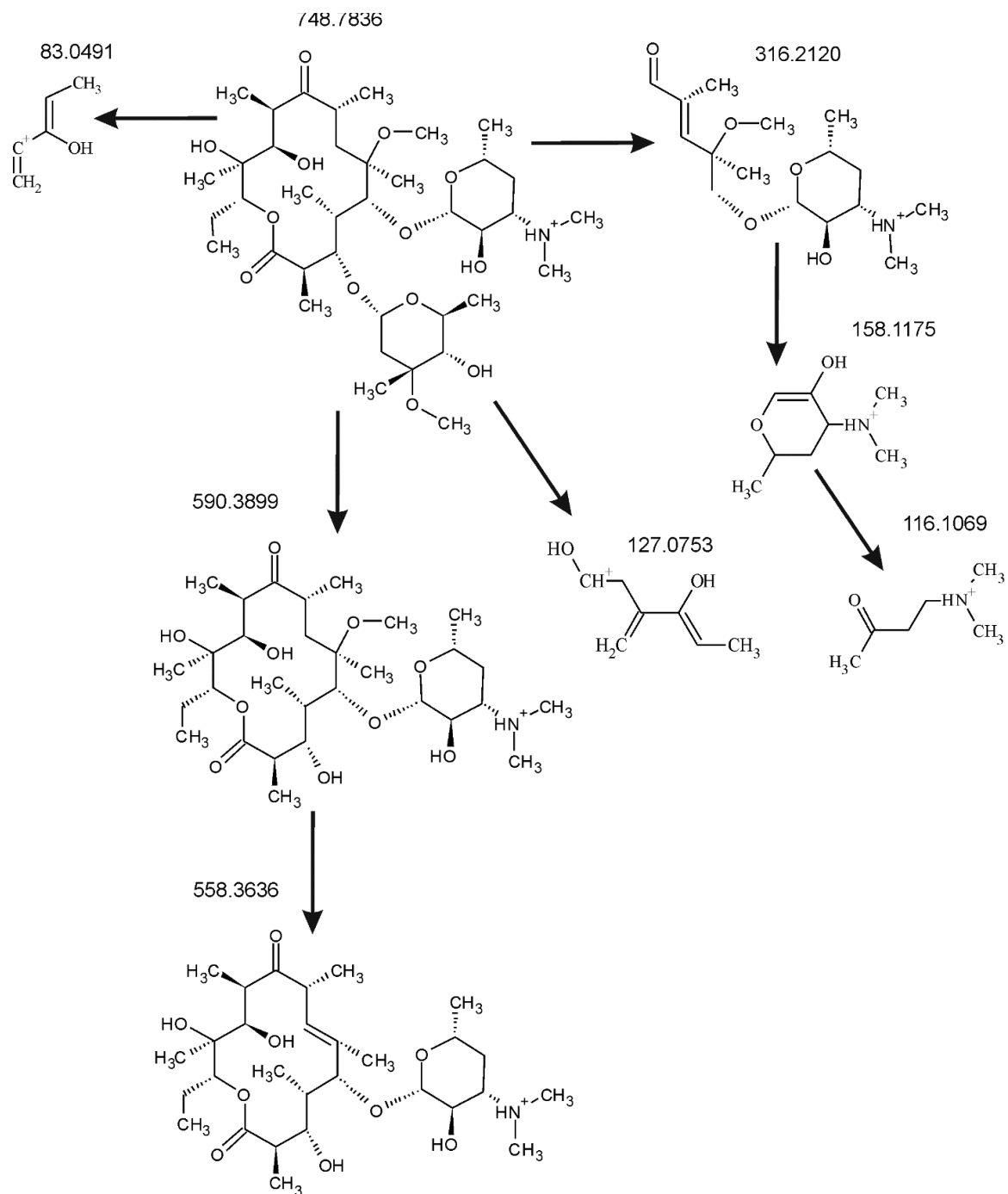


Figure S2. Collision-induced dissociation pathways of clarithromycin.

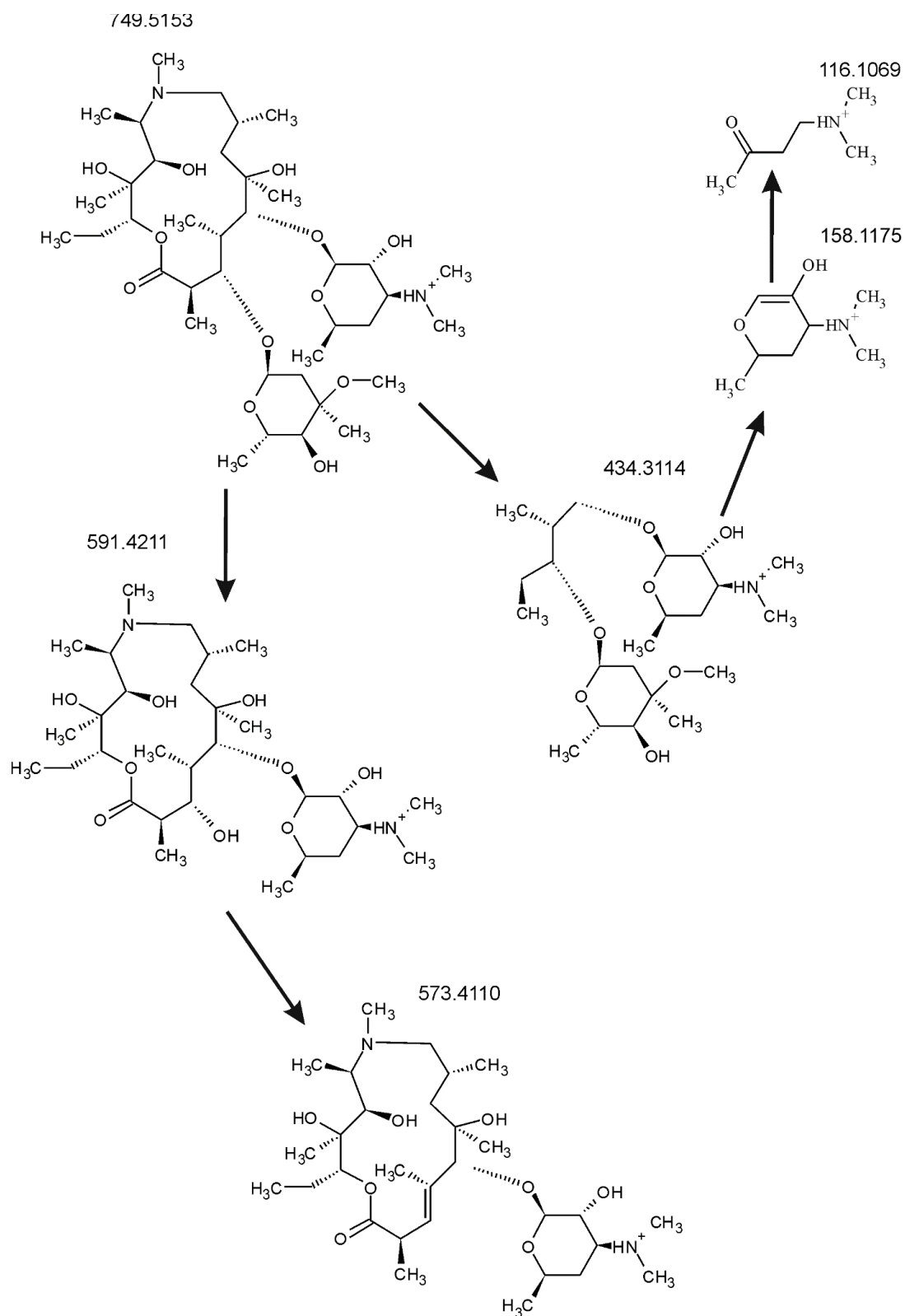


Figure S3. Collision-induced dissociation pathways of azithromycin.

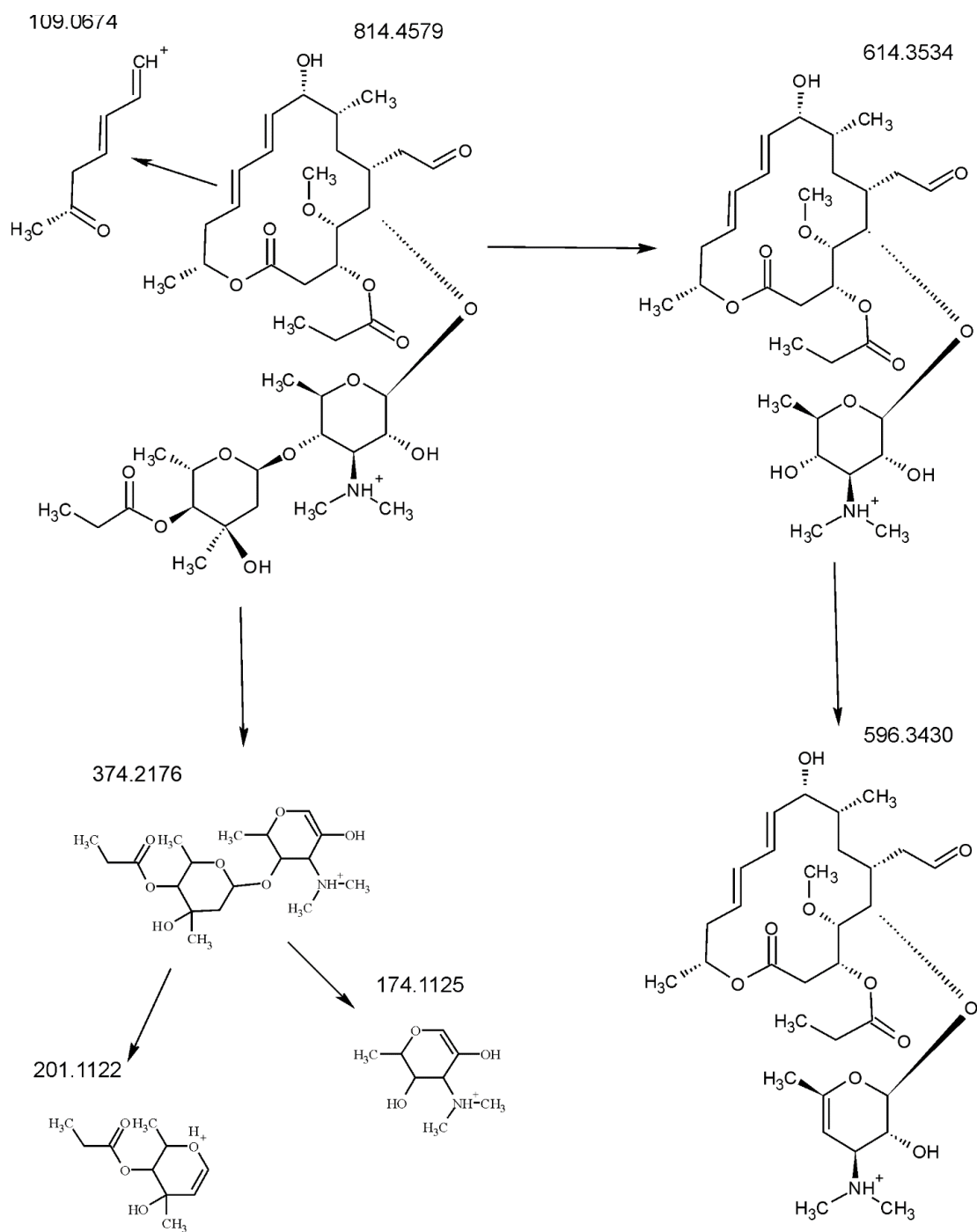


Figure S4. Collision-induced dissociation pathways of midecamycin.

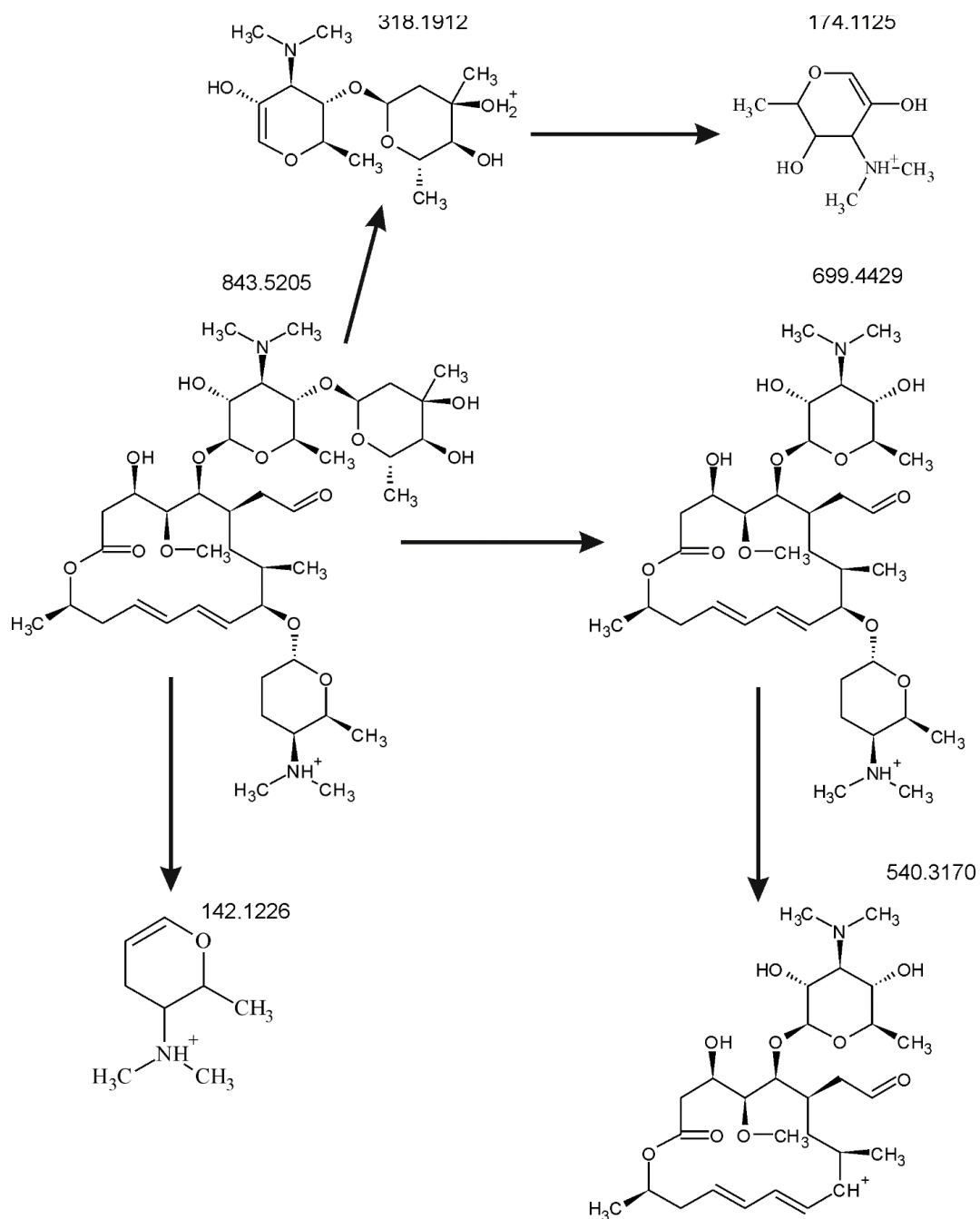


Figure S5. Collision-induced dissociation pathways of spiramycin.

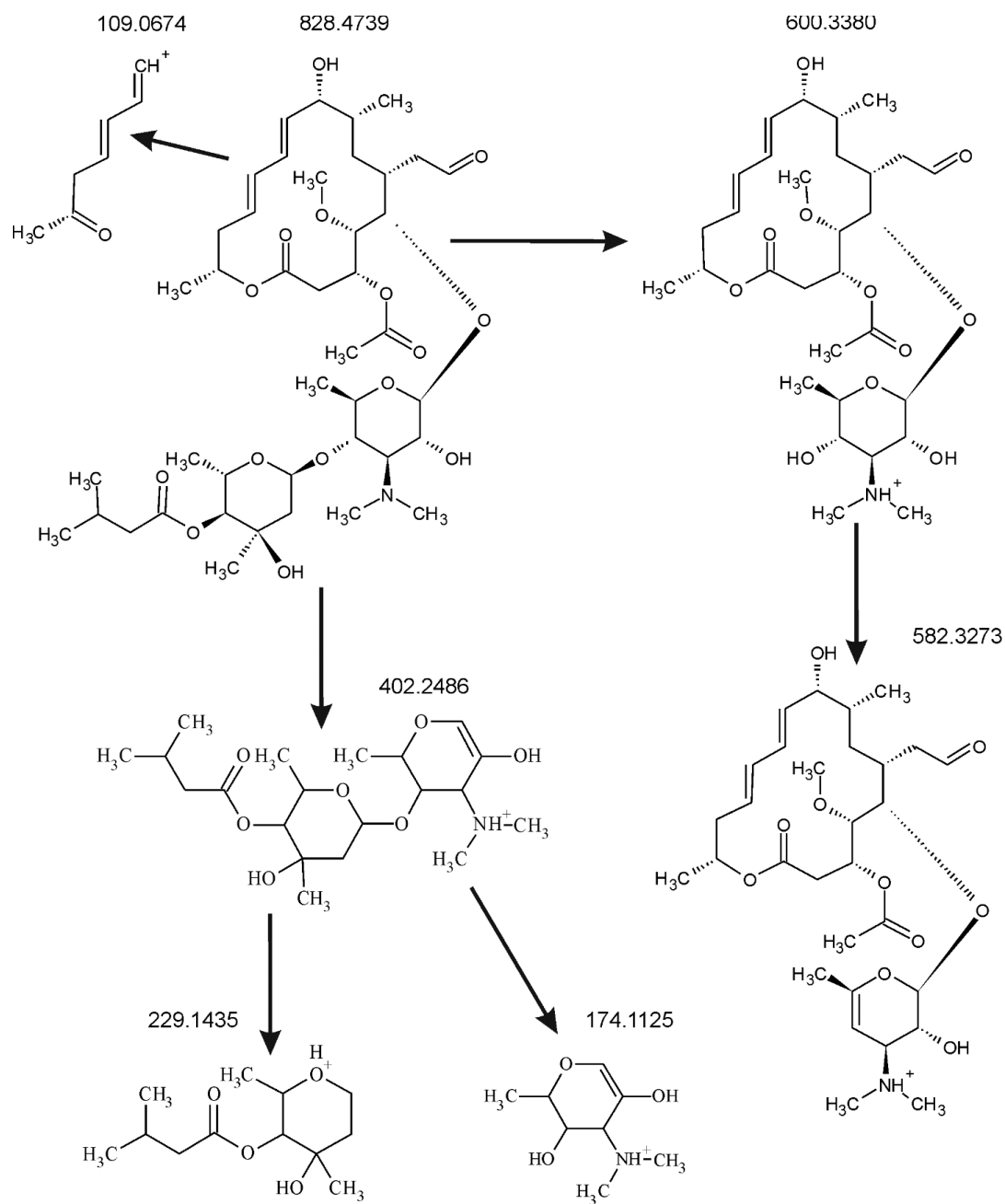


Figure S6. Collision-induced dissociation pathways of josamycin.

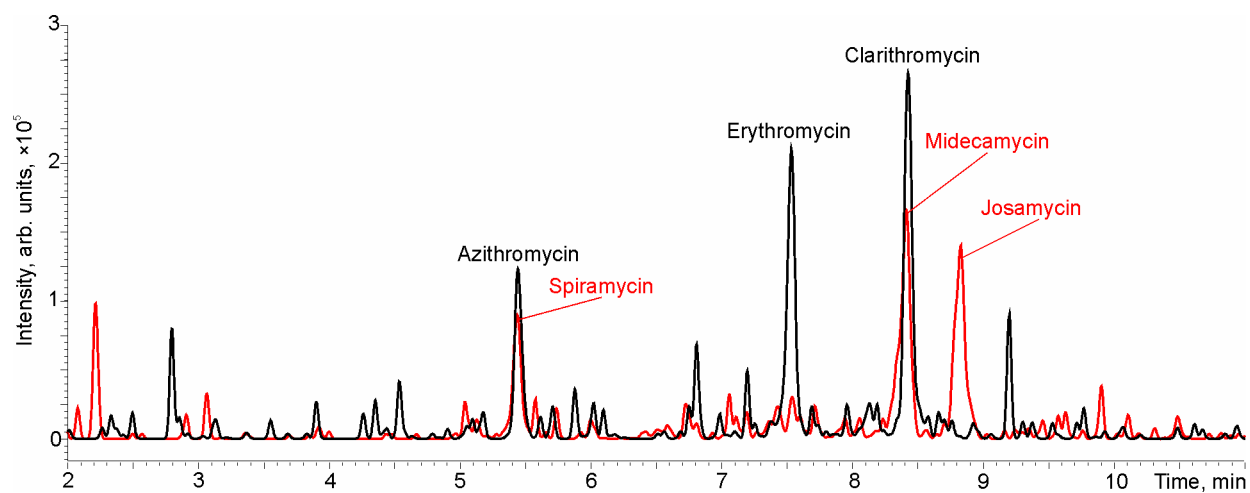


Figure S7. HPLC-MS/MS (PrecIS) chromatogram of the model mixture macrolides with concentrations close to LOQ.

Diagnostic ions: m/z 174 (red) and m/z 158 (black)

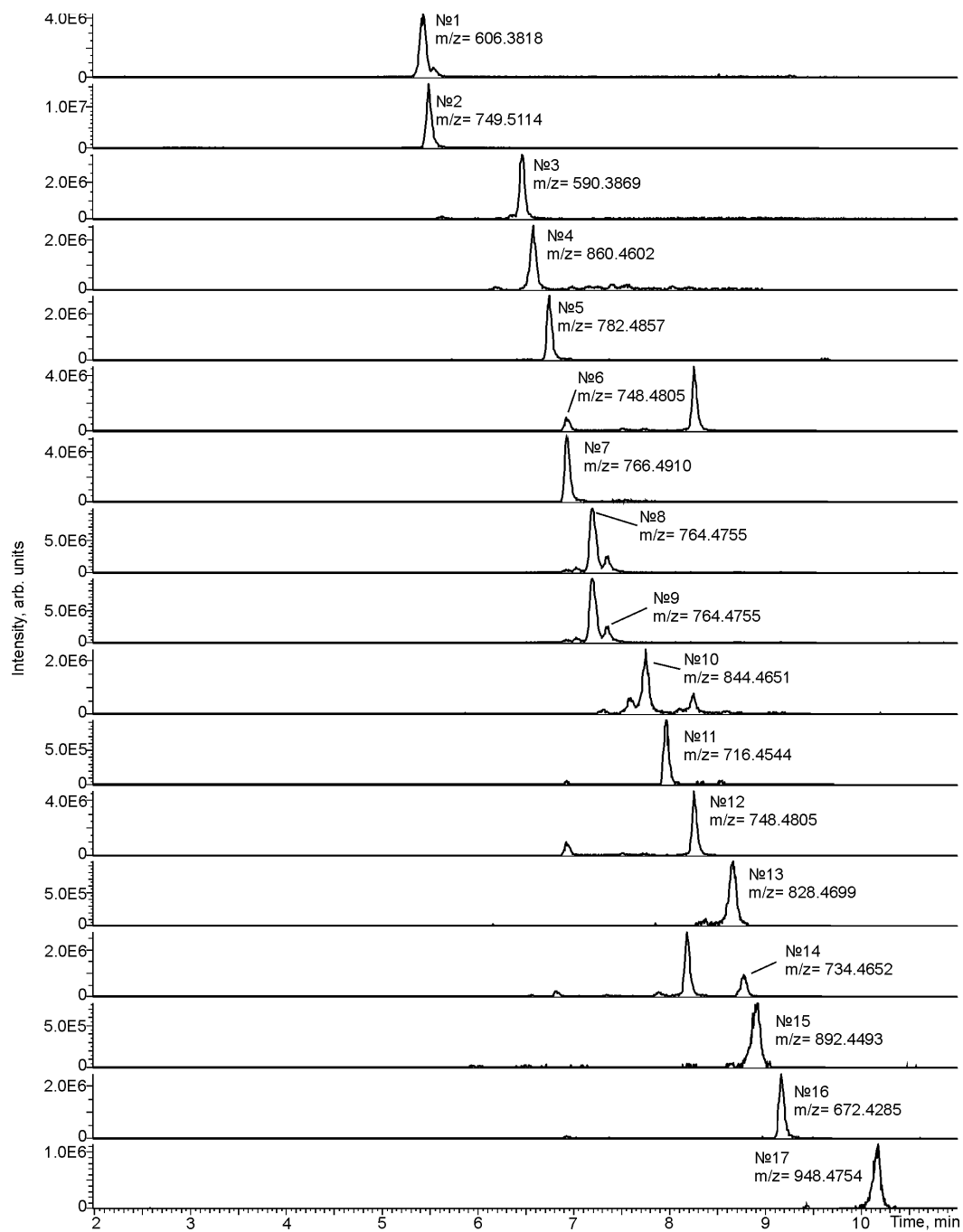
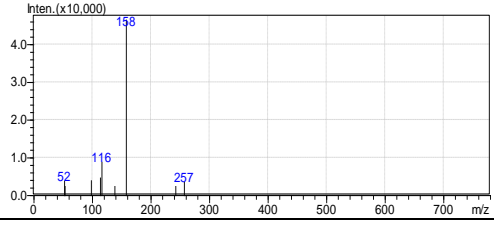
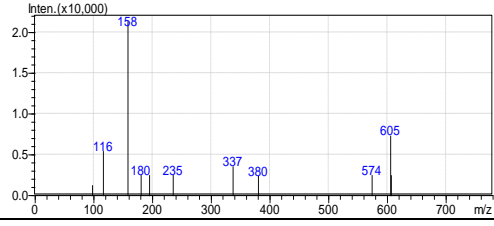
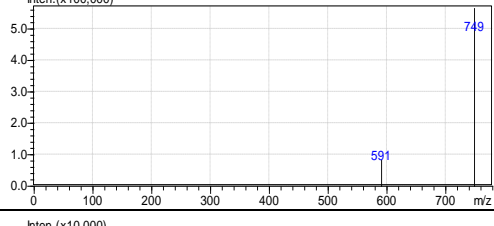
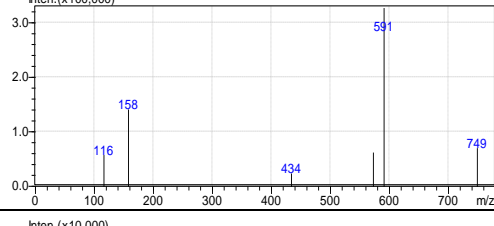
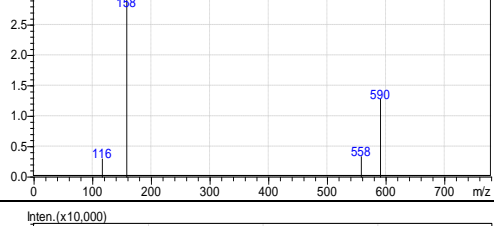
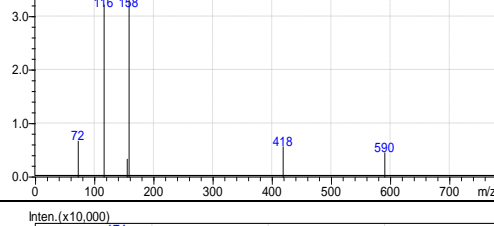
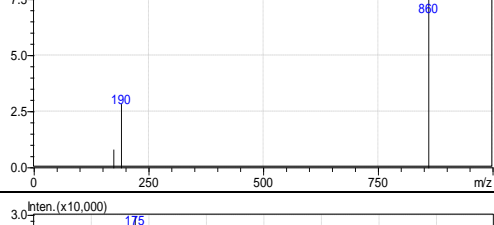
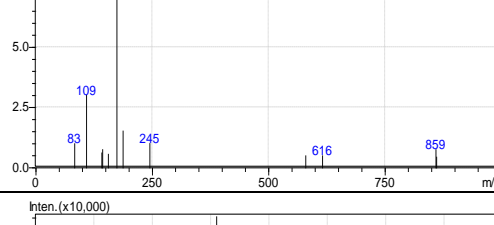
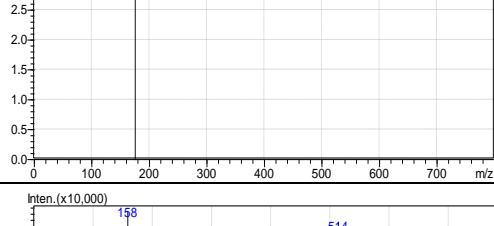
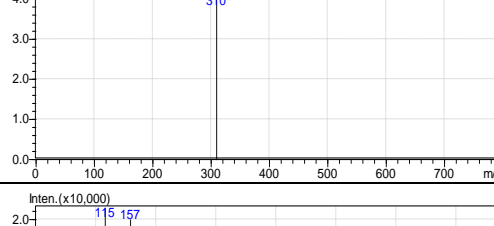
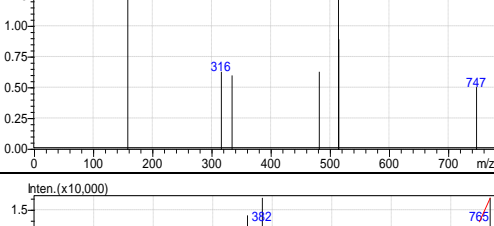
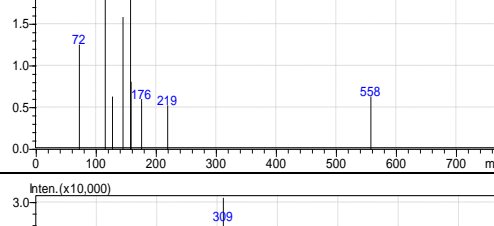
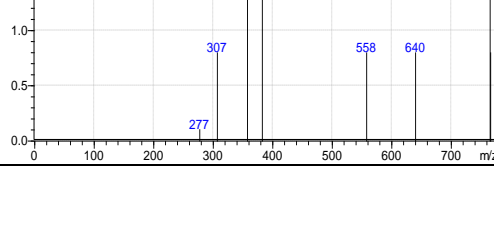
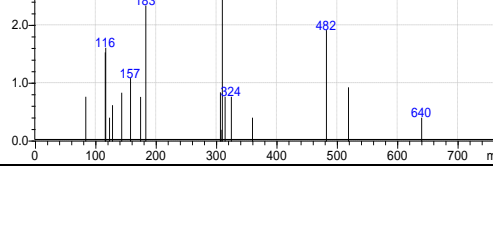


Figure S8. Extracted ion current HPLC-HRMS chromatograms of municipal wastewater (peak numbers and m/z values correspond to those listed in Figure 4 and in Table 4).

Table S1. Recoveries of the macrolides obtained by solid-phase extraction on an HLB stationary phase.

Compound	Recovery, %
Azithromycin	53.4±5.8
Spiramycin	58.9±2.8
Erythromycin	73.1±0.7
Midecamycin	82.1±0.2
Clarithromycin	93.8±2
Josamycin	84.7±1.2

Table S2. Tandem mass spectra of the precursor ion candidates found in HPLC-MS/MS (PrecIS) chromatogram of municipal wastewater (compound numbers correspond to the peaks on Figure 4 and in Table 4).

№	Precursor ion, m/z	Collision energy	
		20 eV	32 or 36 eV
1	606		
2	749		
3	590		
4	860		
5	782		
6	748		
7	766		

8	764	<p>Mass spectrum for compound 8, m/z 764. The x-axis is m/z from 0 to 750, and the y-axis is Intensity (x10,000) from 0.0 to 7.5. The base peak is at m/z 606. Other significant peaks are at m/z 158, 116, 316, 362, 538, 574, and 764.</p>	<p>Mass spectrum for compound 8, m/z 764. The x-axis is m/z from 0 to 750, and the y-axis is Intensity (x100,000) from 0.0 to 1.5. The base peak is at m/z 158. Other significant peaks are at m/z 116 and 363.</p>
9	764	<p>Mass spectrum for compound 9, m/z 764. The x-axis is m/z from 0 to 750, and the y-axis is Intensity (x10,000) from 0.0 to 2.5. The base peak is at m/z 138. Other significant peaks are at m/z 116, 556, 640, and 764.</p>	<p>Mass spectrum for compound 9, m/z 764. The x-axis is m/z from 0 to 750, and the y-axis is Intensity (x10,000) from 0.0 to 2.5. The base peak is at m/z 137. Other significant peaks are at m/z 115, 195, 208, 556, 574, and 604.</p>
10	844	<p>Mass spectrum for compound 10, m/z 844. The x-axis is m/z from 0 to 750, and the y-axis is Intensity (x10,000) from 0.0 to 1.5. The base peak is at m/z 417. Other significant peaks are at m/z 174, 109, 229, 362, 616, and 844.</p>	<p>Mass spectrum for compound 10, m/z 844. The x-axis is m/z from 0 to 750, and the y-axis is Intensity (x10,000) from 0.0 to 2.0. The base peak is at m/z 174. Other significant peaks are at m/z 116, 229, 367, 462, 681, and 674.</p>
11	716	<p>Mass spectrum for compound 11, m/z 716. The x-axis is m/z from 0 to 750, and the y-axis is Intensity (x10,000) from 0.0 to 2.0. The base peak is at m/z 717. Other significant peaks are at m/z 158, 174, 103, 345, 558, and 716.</p>	<p>Mass spectrum for compound 11, m/z 716. The x-axis is m/z from 0 to 750, and the y-axis is Intensity (x10,000) from 0.0 to 1.25. The base peak is at m/z 716. Other significant peaks are at m/z 188, 144, 83, 360, 558, and 716.</p>
12	748	<p>Mass spectrum for compound 12, m/z 748. The x-axis is m/z from 0 to 750, and the y-axis is Intensity (x10,000) from 0.0 to 2.0. The base peak is at m/z 590. Other significant peaks are at m/z 158, 117, 365, 483, 558, and 748.</p>	<p>Mass spectrum for compound 12, m/z 748. The x-axis is m/z from 0 to 750, and the y-axis is Intensity (x10,000) from 0.0 to 4.0. The base peak is at m/z 138. Other significant peaks are at m/z 83, 315, 437, 558, 670, and 748.</p>
13	828	<p>Mass spectrum for compound 13, m/z 828. The x-axis is m/z from 0 to 750, and the y-axis is Intensity (x10,000) from 0.0 to 3.0. The base peak is at m/z 828. Other significant peaks are at m/z 174 and 598.</p>	<p>Mass spectrum for compound 13, m/z 828. The x-axis is m/z from 0 to 750, and the y-axis is Intensity (x10,000) from 0.0 to 3.0. The base peak is at m/z 174. Other significant peaks are at m/z 83, 108, 229, 259, and 828.</p>
14	734	<p>Mass spectrum for compound 14, m/z 734. The x-axis is m/z from 0 to 750, and the y-axis is Intensity (x10,000) from 0.0 to 1.5. The base peak is at m/z 138. Other significant peaks are at m/z 60, 89, 198, 208, 428, 481, 576, 692, and 734.</p>	<p>Mass spectrum for compound 14, m/z 734. The x-axis is m/z from 0 to 750, and the y-axis is Intensity (x10,000) from 0.0 to 2.5. The base peak is at m/z 138. Other significant peaks are at m/z 116, 304, 576, and 734.</p>
15	892	<p>Mass spectrum for compound 15, m/z 892. The x-axis is m/z from 0 to 750, and the y-axis is Intensity (x10,000) from 0.0 to 3.0. The base peak is at m/z 892. Other significant peaks are at m/z 174, 109, and 229.</p>	<p>Mass spectrum for compound 15, m/z 892. The x-axis is m/z from 0 to 750, and the y-axis is Intensity (x10,000) from 0.0 to 4.0. The base peak is at m/z 174. Other significant peaks are at m/z 109, 229, 381, and 663.</p>

