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).

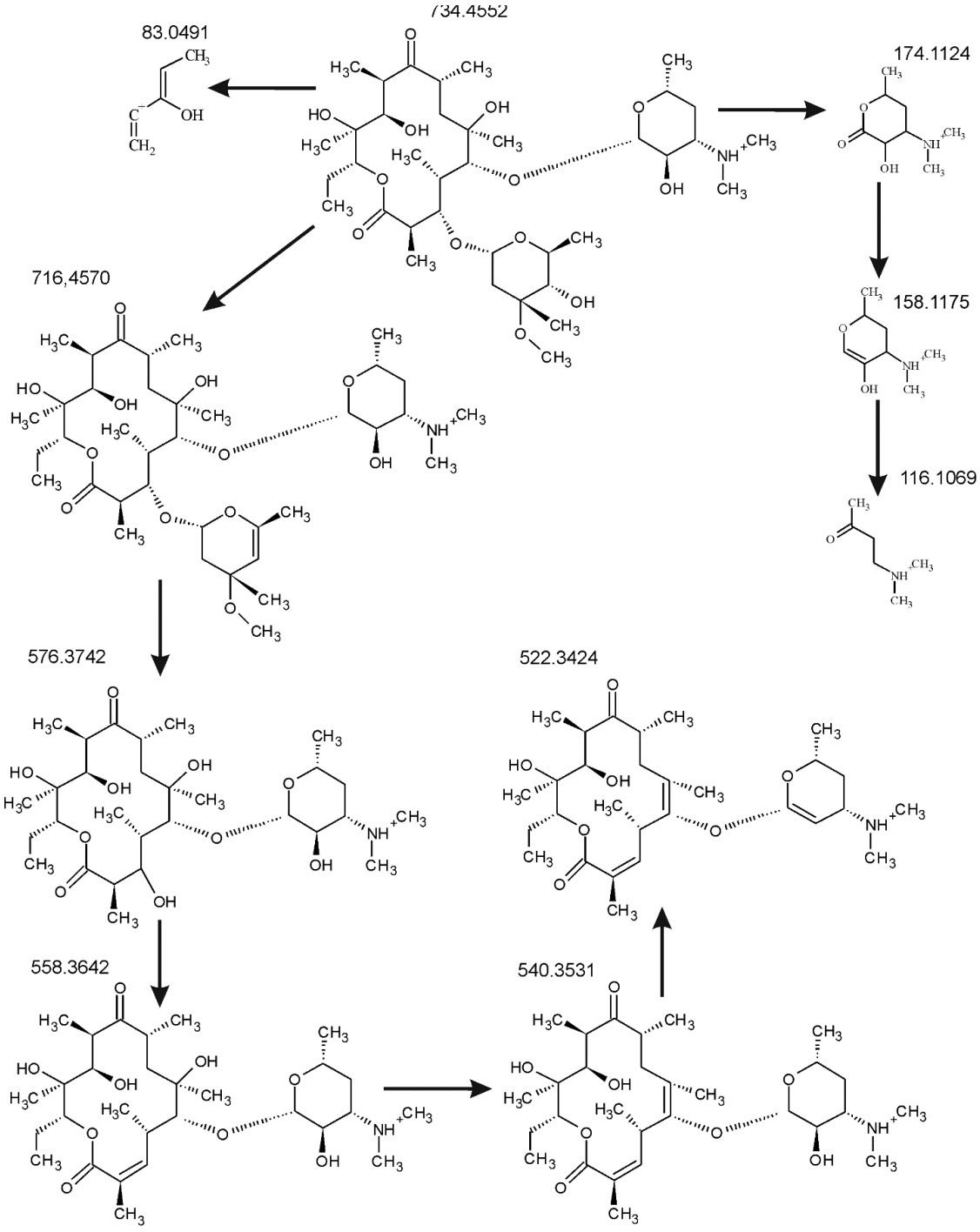


Figure S1. Collision-induced dissociation pathways of erythromycin.

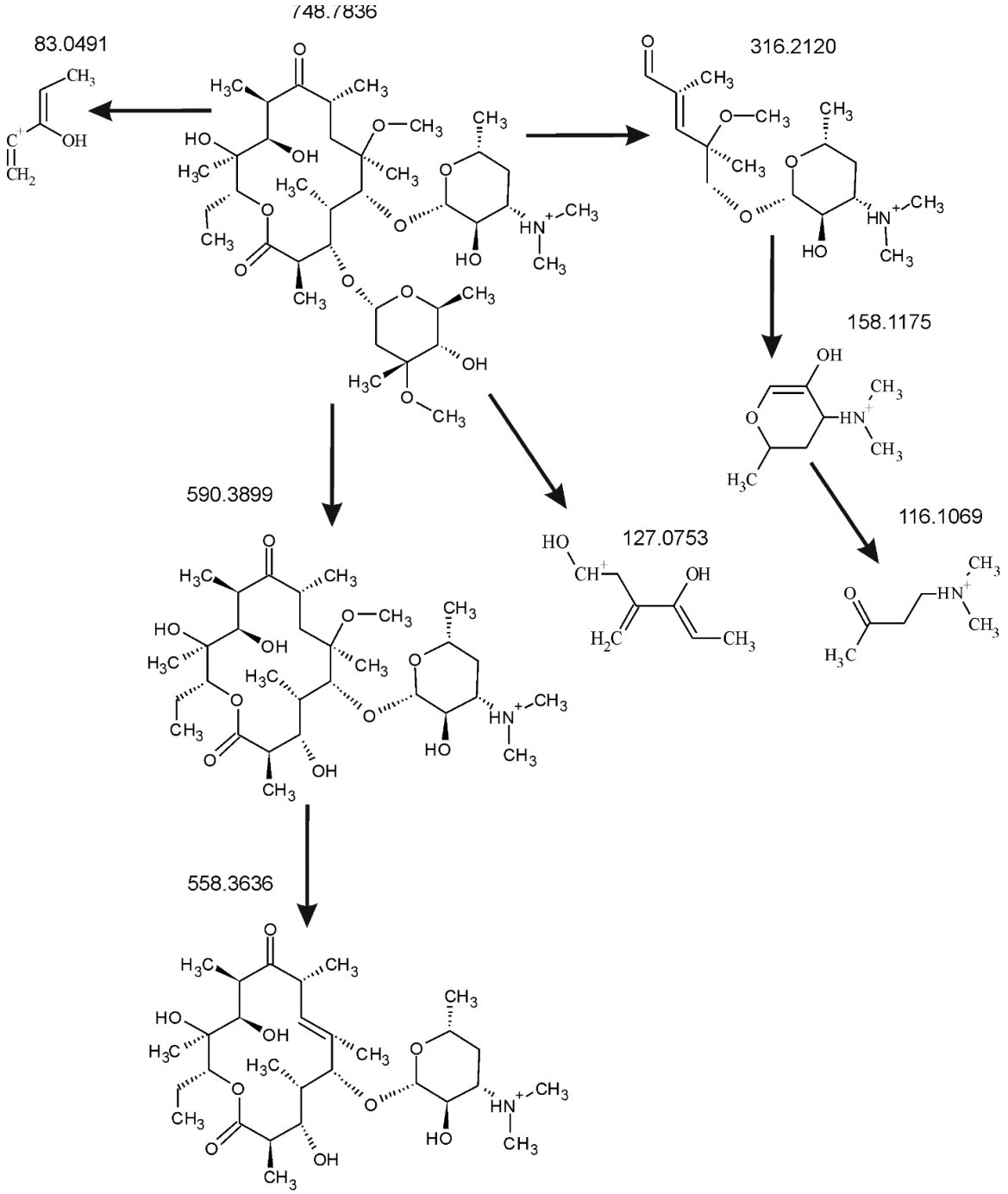


Figure S2. Collision-induced dissociation pathways of clarithromycin.

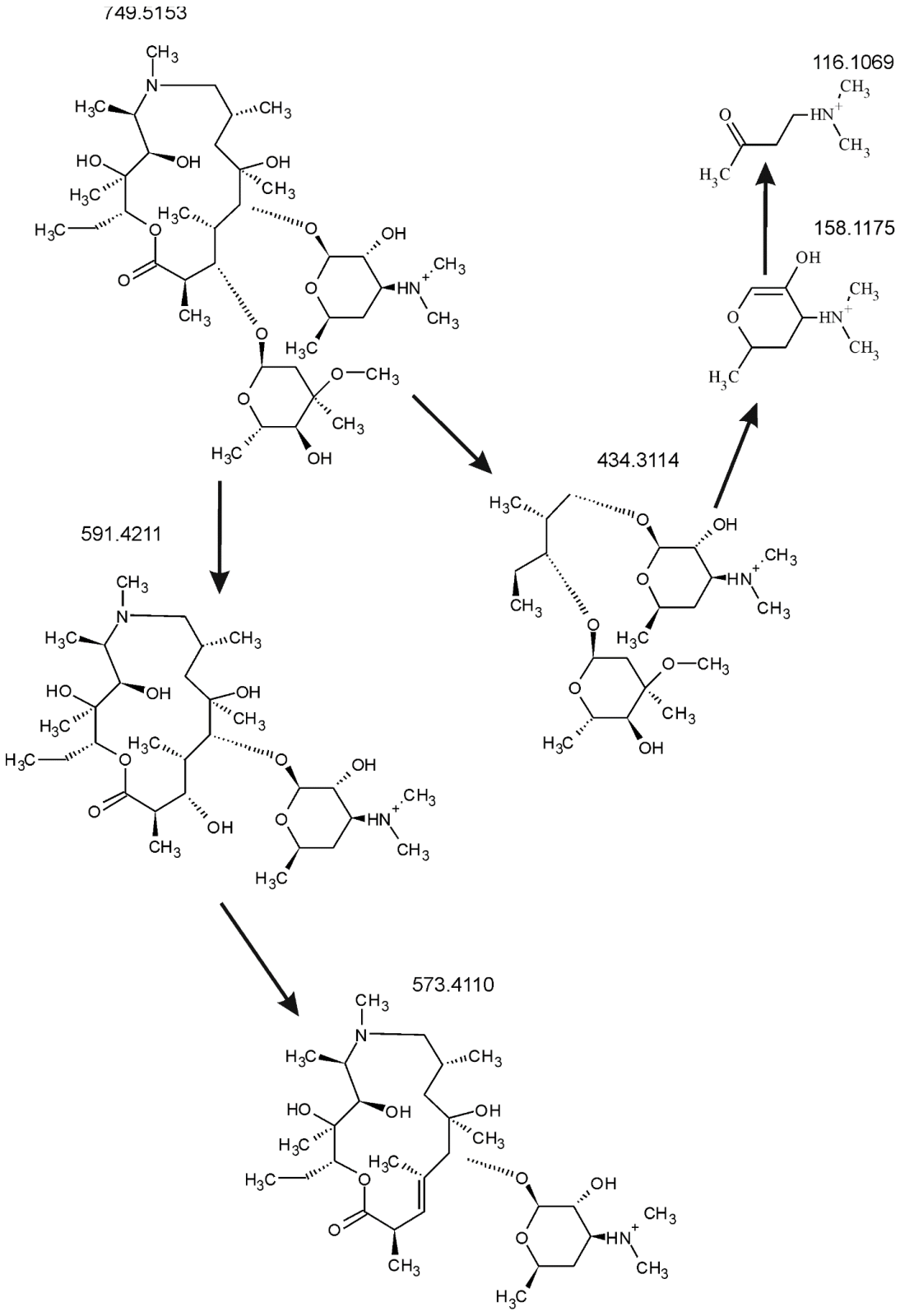


Figure S3. Collision-induced dissociation pathways of azithromycin.

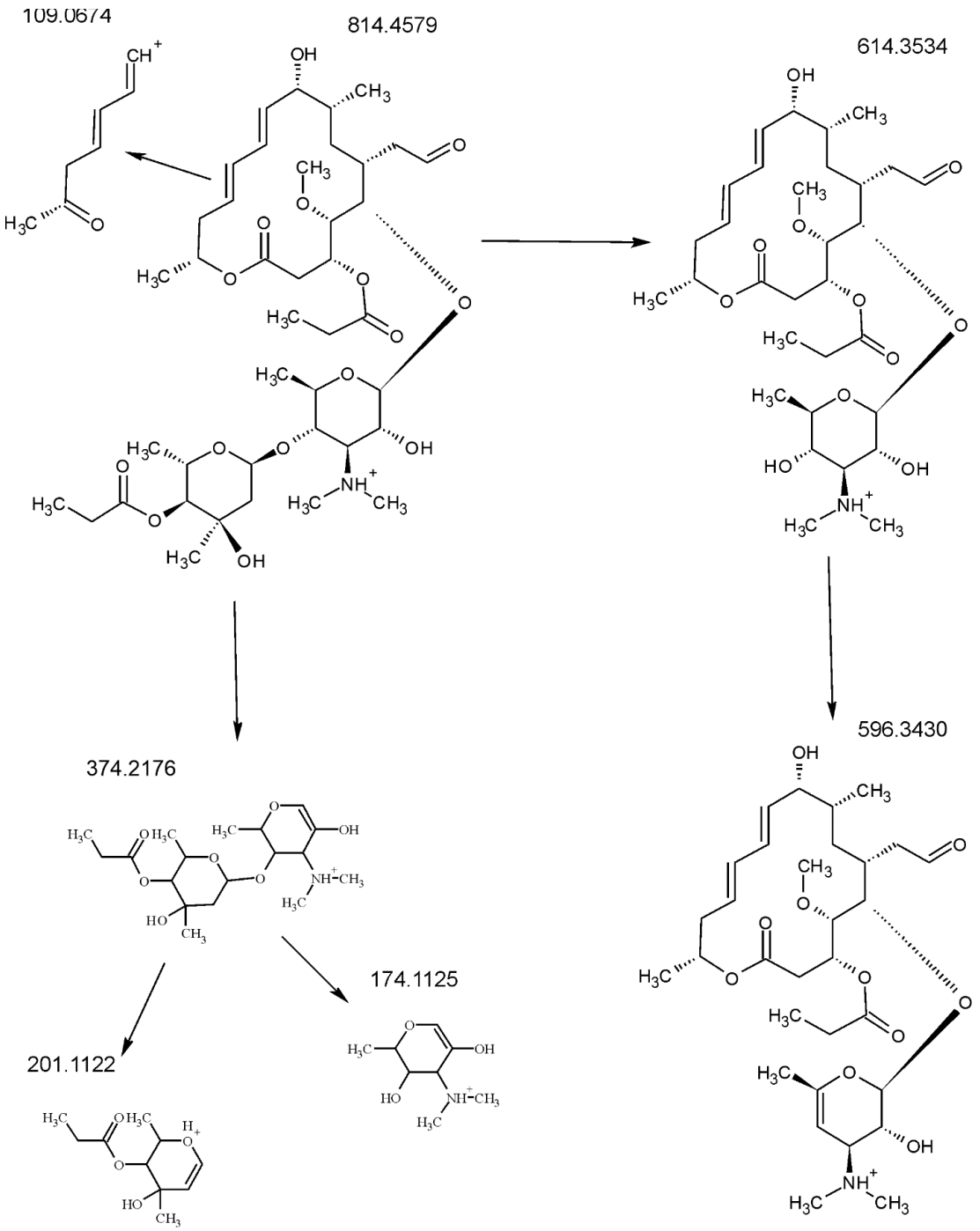


Figure S4. Collision-induced dissociation pathways of midecamycin.

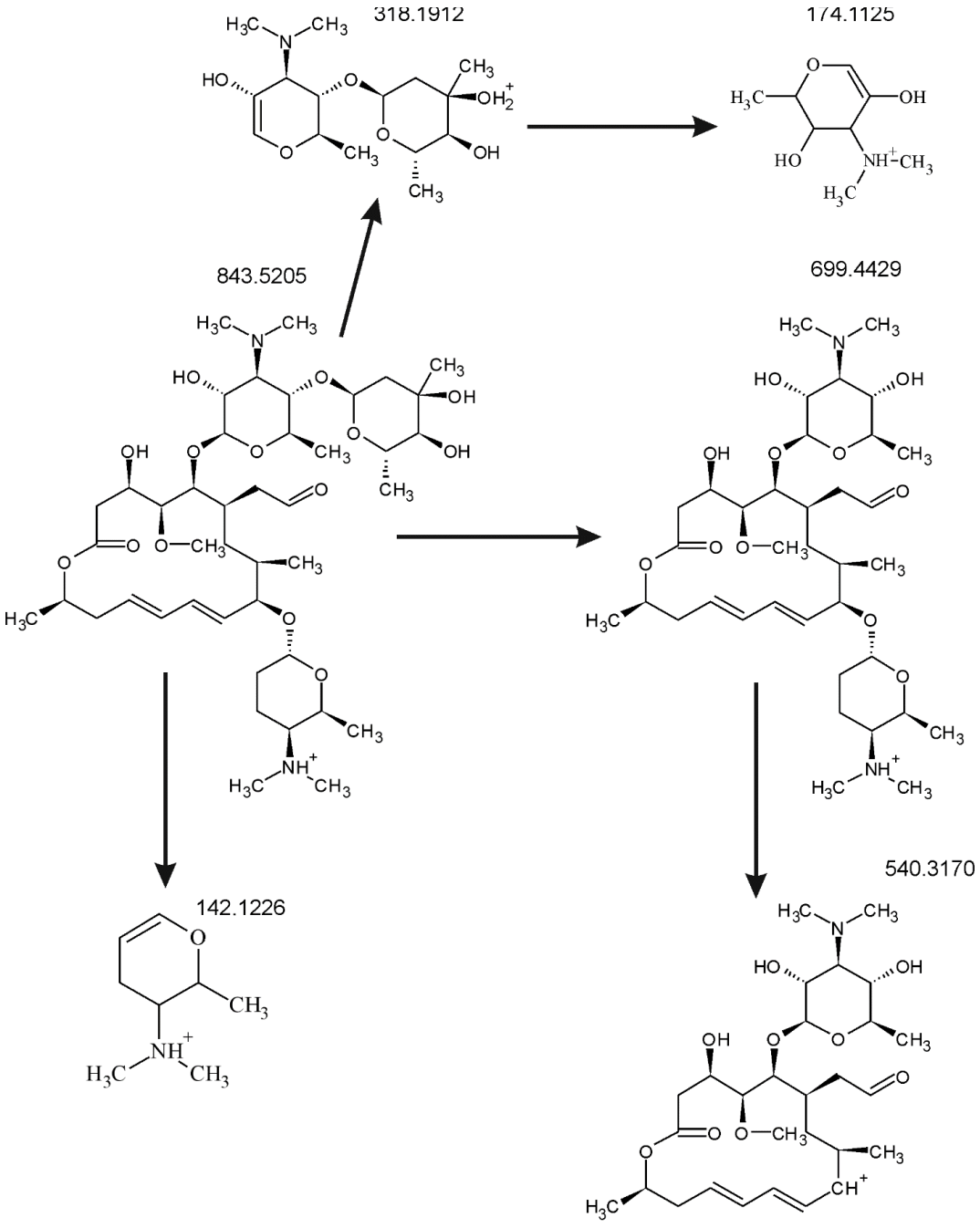


Figure S5. Collision-induced dissociation pathways of spiramycin.

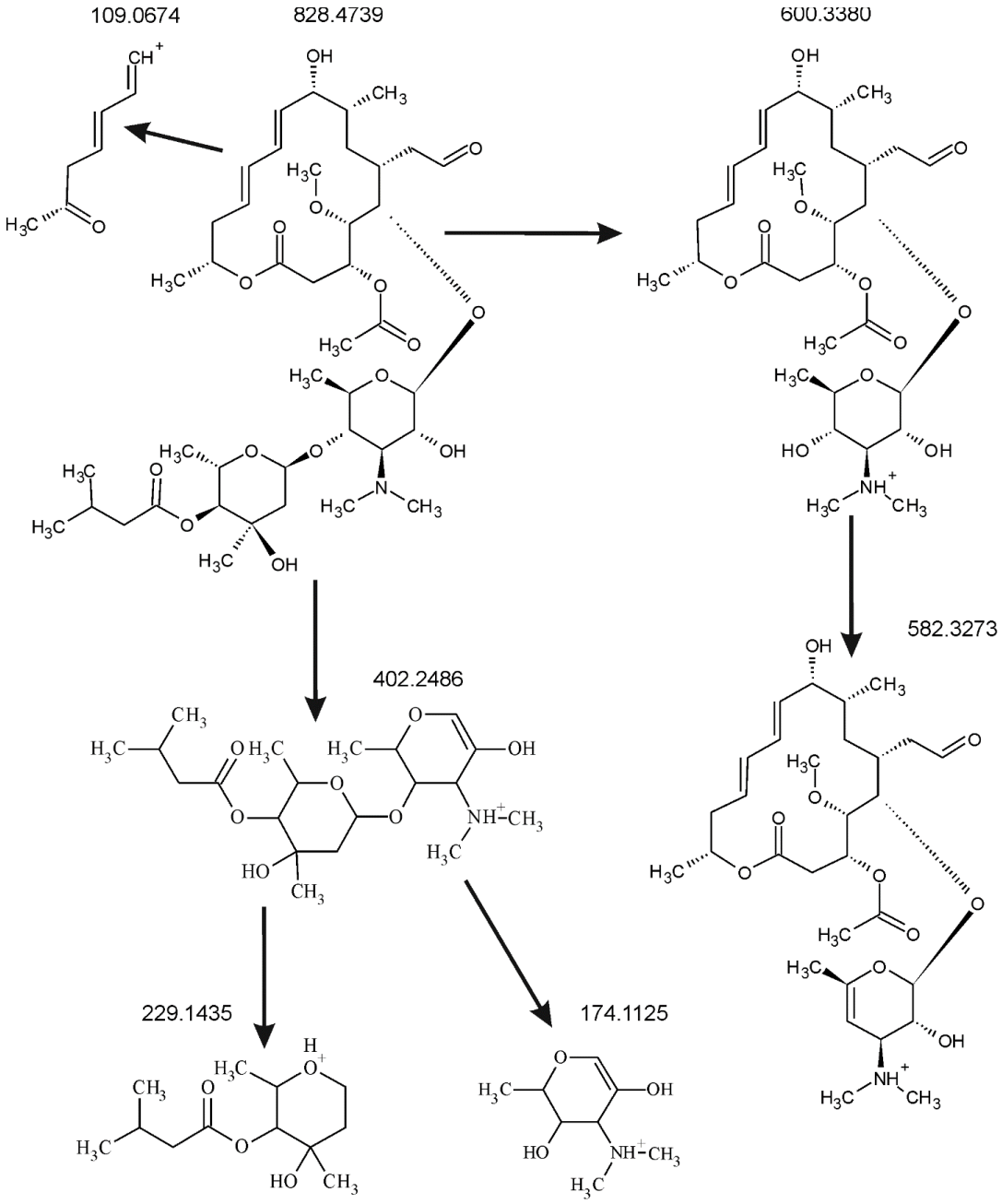


Figure S6. Collision-induced dissociation pathways of josamycin.

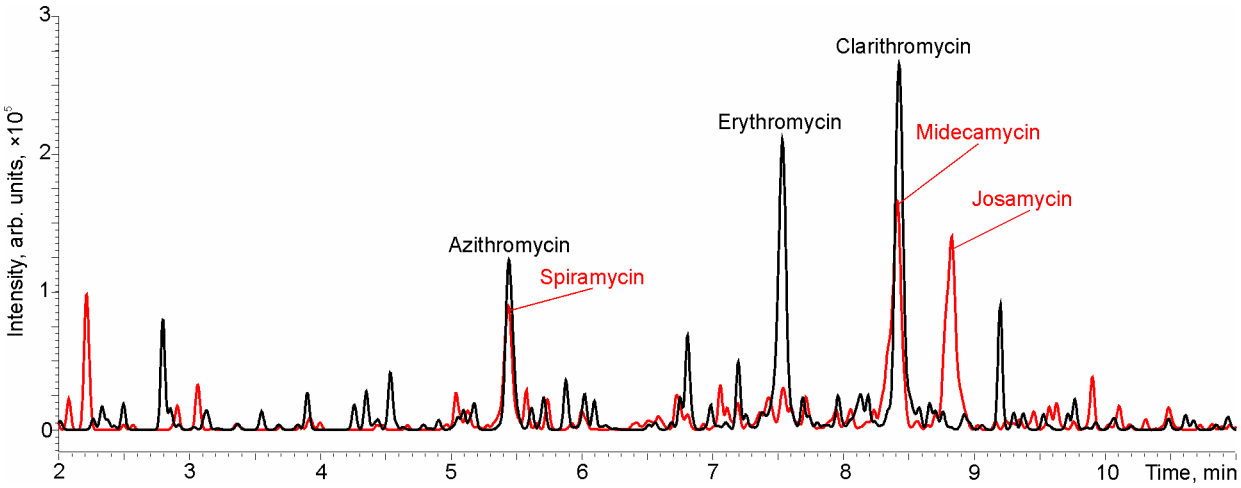


Figure S7. HPLC-MS/MS (PrecIS) chromatogram of the model mixture macrolides with concentrations close to LOQ. Diagnostic ions: *m*/*z* 174 (red) and *m*/*z* 158 (black)

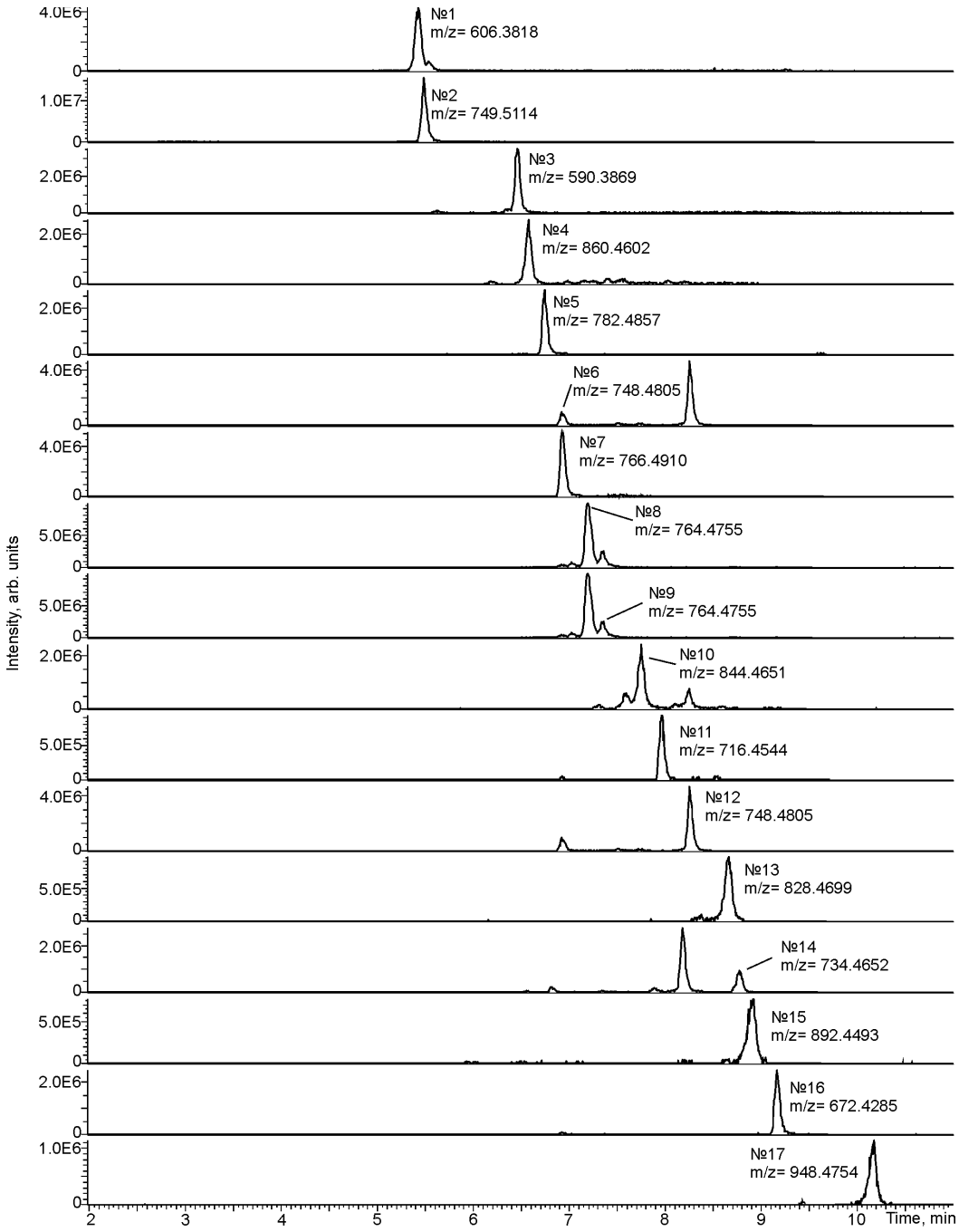
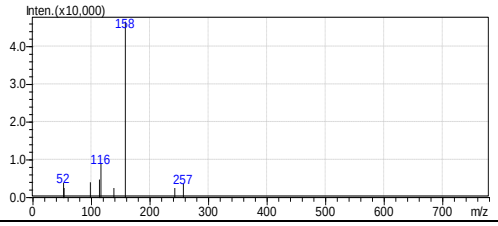
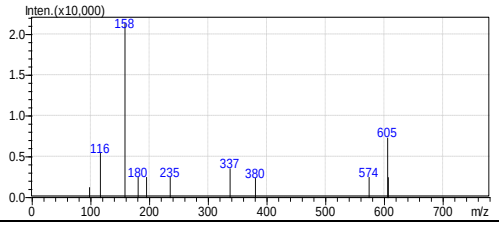
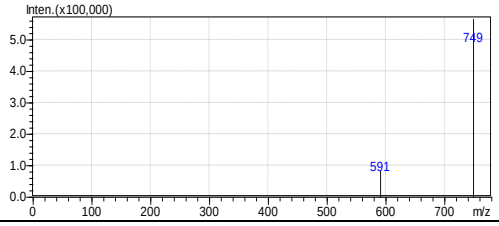
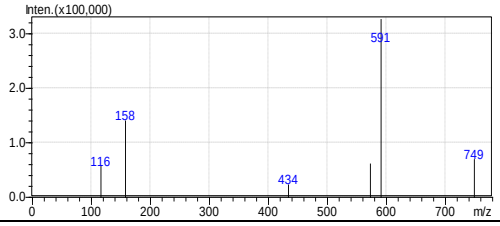
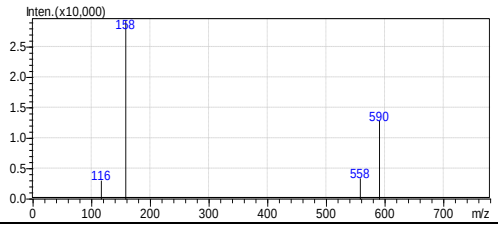
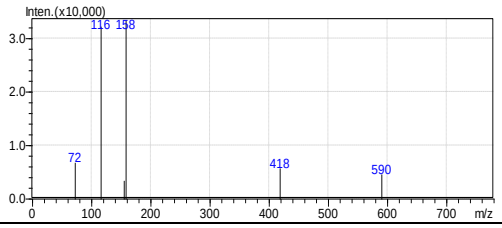
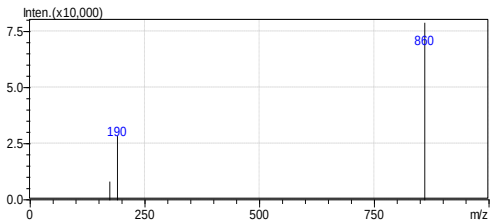
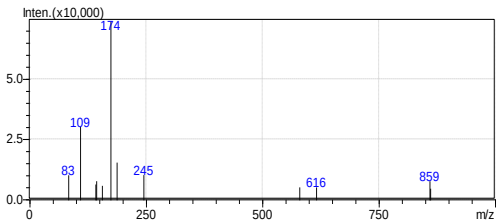
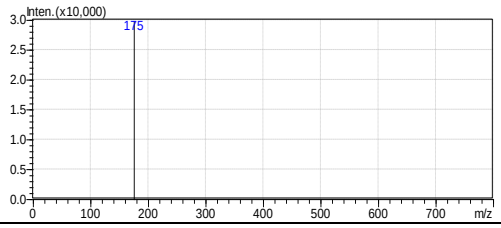
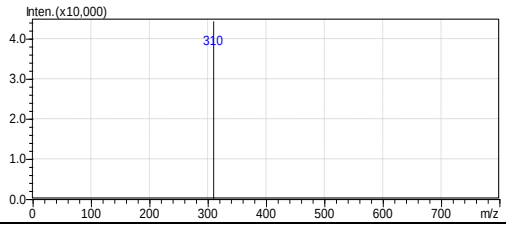
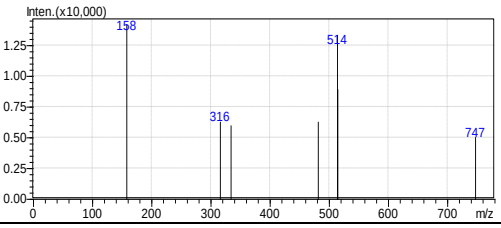
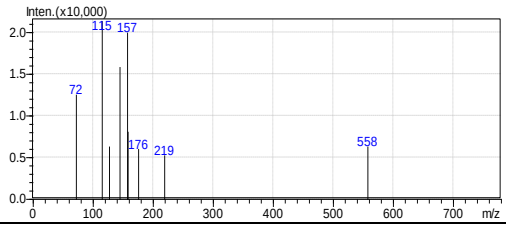
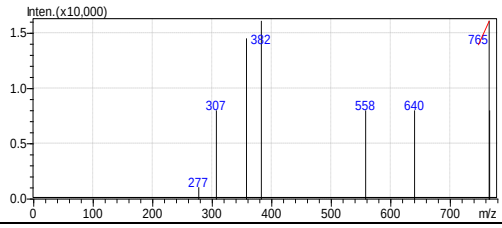
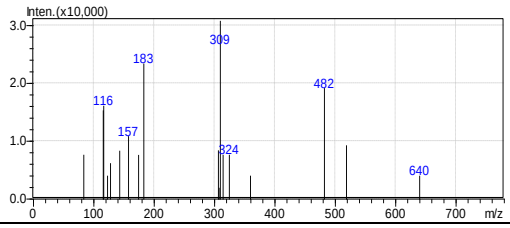


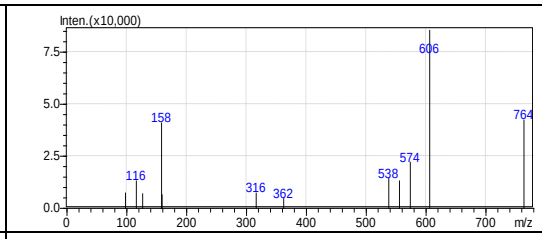
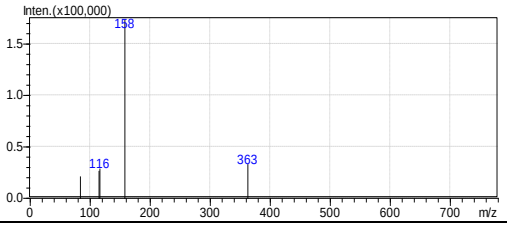
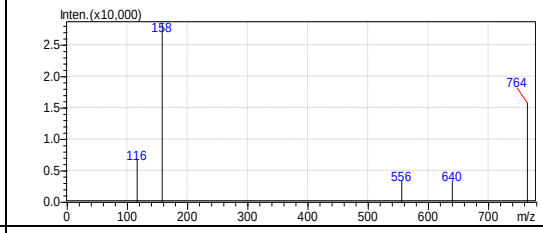
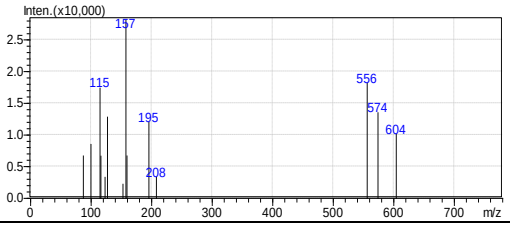
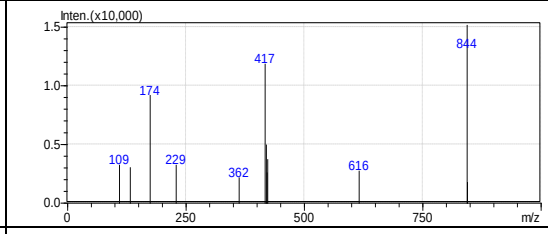
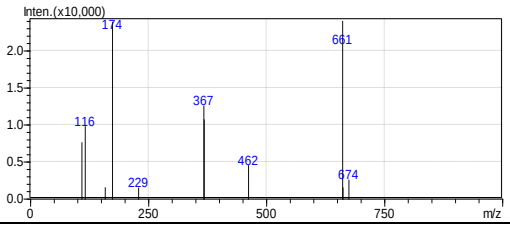
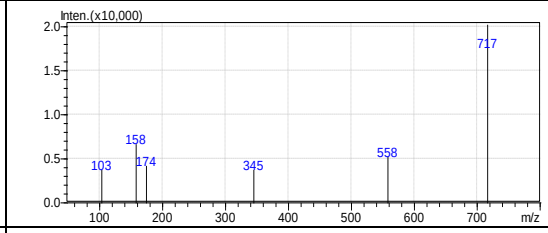
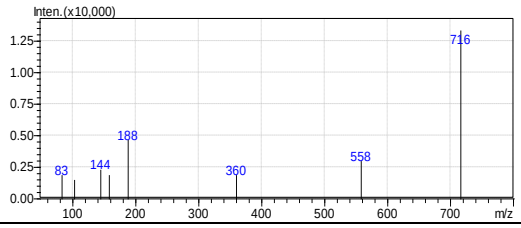
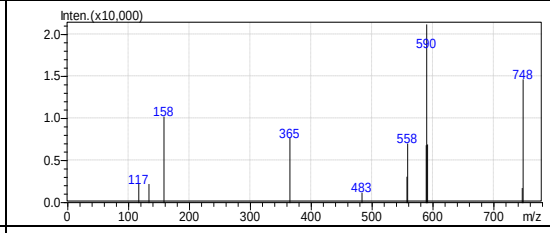
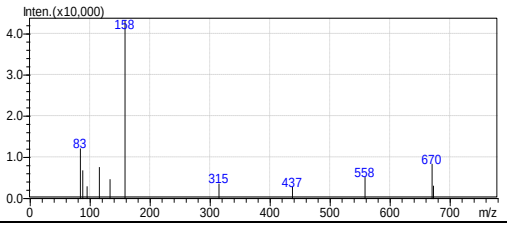
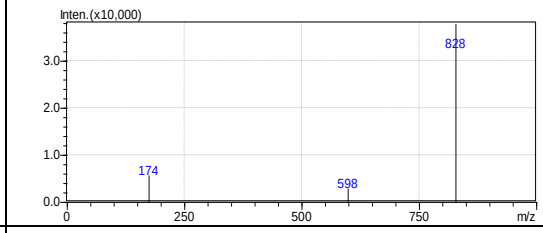
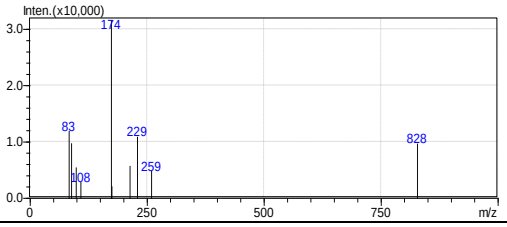
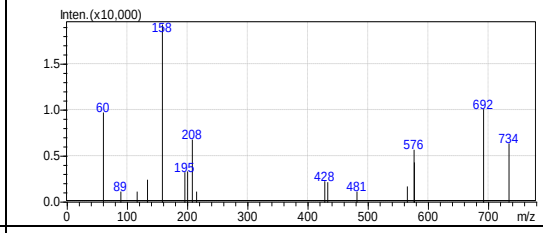
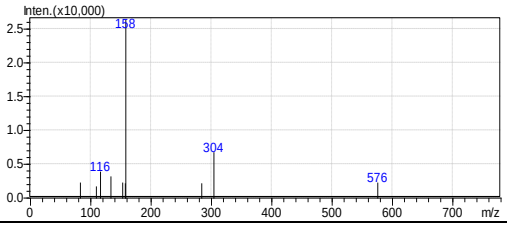
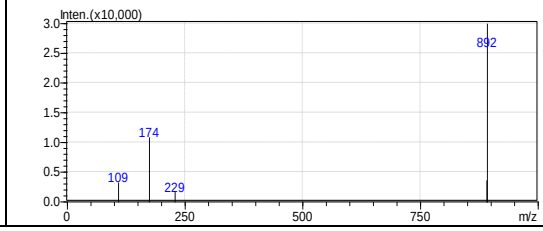
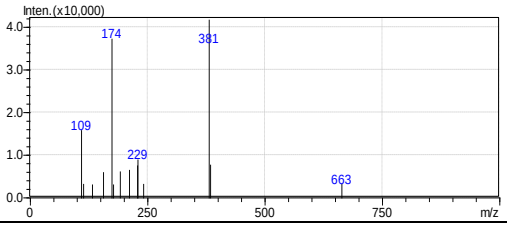
Figure S8. Extracted ion current HPLC-HRMS chromatograms of municipal wastewater (peak numbers and *m*/*z* values correspond to those listed in Figure 4 and in Table 4).

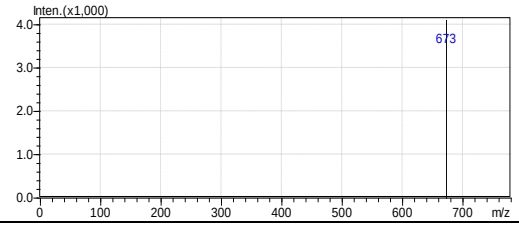
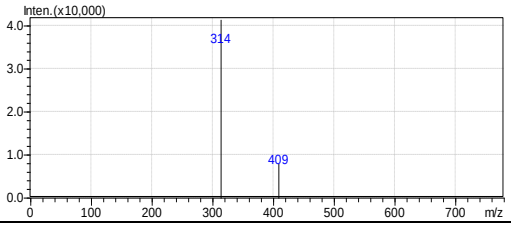
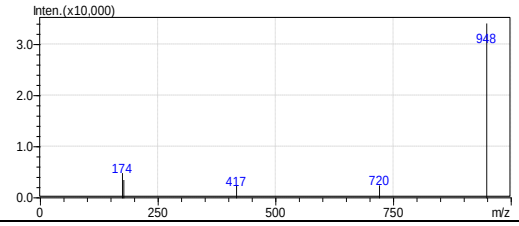
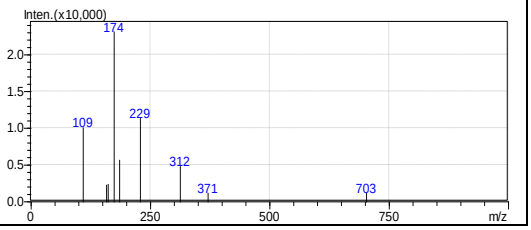
Table S1. Recoveries of the macrolides obtained by solid-phase extraction on an HLB stationary phase.

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		
9	764		
10	844		
11	716		
12	748		
13	828		
14	734		
15	892		

16	672	 Inten.(x1,000) 673 m/z	 Inten.(x10,000) 314 409 m/z
17	948	 Inten.(x10,000) 948 174 417 720 m/z	 Inten.(x10,000) 174 109 229 312 371 703 m/z