Supporting materials

This is the supporting information for "Combined LC-MS/MS and molecular networking approach reveals antioxidant and antimicrobial compounds from *Erismadelphus exsul bark*" including global molecular network data, antimicrobial activity and LC-MS spectra.

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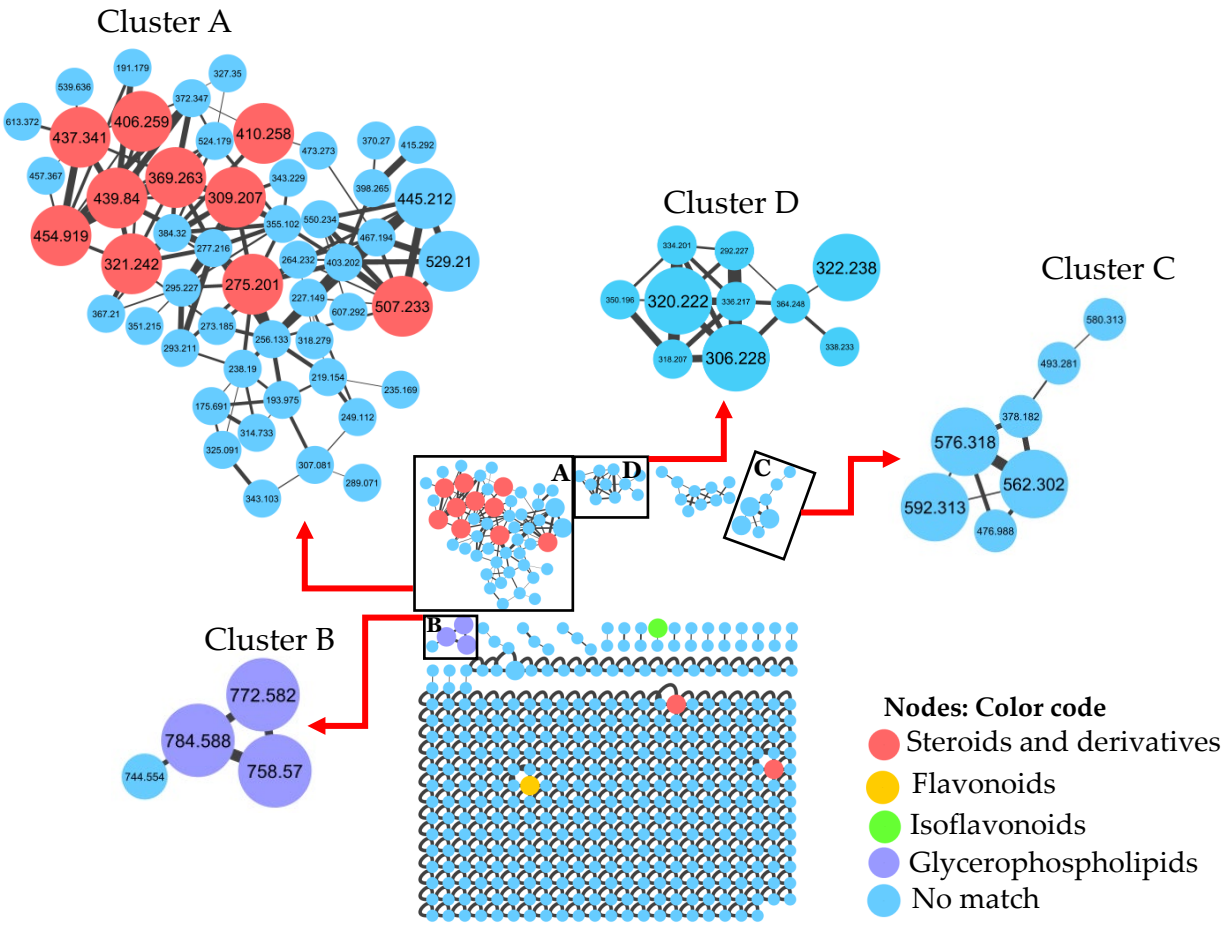


Figure S1. The molecular network of the ethanolic crude extract of *Erismadelphus exsul* obtained with the GNPS platform and visualized with the Cytoscape 3.9.0 software. The resulting analysis and parameters for the network can be accessed via this link : http://gnps.ucsd.edu/ProteoSAFe/status.jsp?task=f4b18f2a813c440bab3cf78abe5aa648.

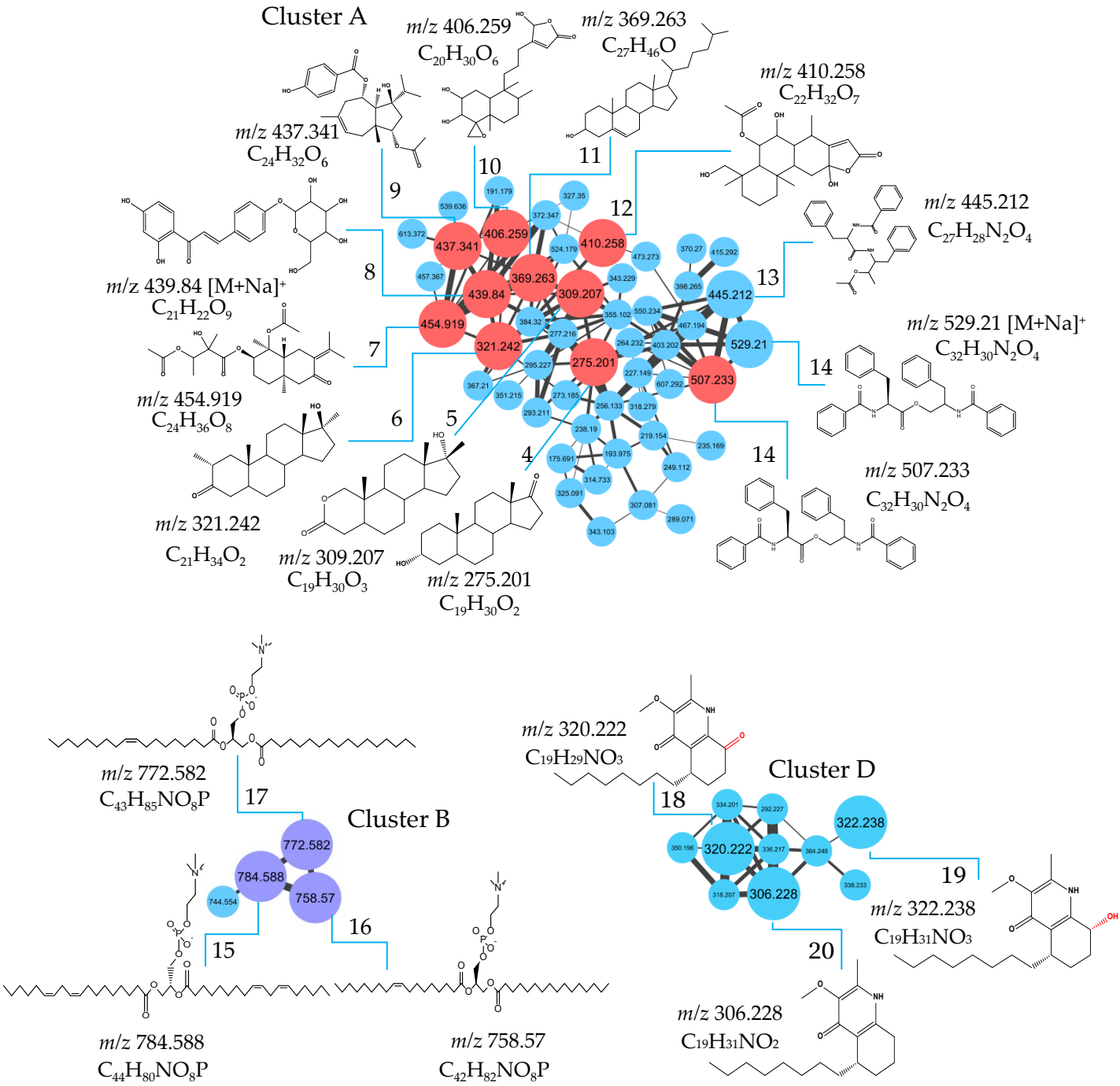


Figure S2. Shows the structures of the compounds identified on the molecular network **(4)** h_127_1_Androstenediol, **(5)** h_61_17_Epioxandrolone, **(6)** Methasteron, **(7)** [(1S,2R,4aR,8aR)-1-Acetyloxy-1,4a-dimethyl-6-oxo-7-propan-2-ylidene-2,3,4,5,8,8a-hexahydronaphthalen-2-yl]-3_acetyloxy-2-hydroxy-2-methylbutanoate, **(8)** Isoliquiritin, **(9)** [1S,3R,3aS,4S,8aR)-1-Acetyloxy-3-hydroxy-6,8a-dimethyl-3-propan-2-yl-1,2,3a,4,5,8-hexahydroazulen-4-yl]4-hydroxybenzoate, **(10)** 3-[2-(6,7-Dihydroxy-1,2,4a-trimethylspiro[3,4,6,7,8,8a-hexahydro-2H-naphthalene-5,2'-oxirane]-1-yl)ethyl]-2-hydroxy-2H-furan-5-one, **(11)** Cholesterol, **(12)** [6,10a-dihydroxy-4-(hydroxymethyl)-4,7,11b-

trimethyl-9-oxo-1,2,3,4a,5,6,6a,7,11,11a-decahydronaphtho[2,1-f][1]benzofuran-5-yl] acetate, **(13)** Asperglaucide, **(14)** Asperphenamate, **(15)** 1,2-Dilinoleoyl-sn-glycero-3-phosphofcholine, **(16)** 1-Palmitoyl-2-linoleoyl-sn-glycero-3-phosphocholine, **(17)** 1-Heptadecanoyl-2-(9Z-octadecenoyl)-sn-glycero-3-phosphocholine, Antidesmone (**18**), 8-Dihydroantidesmone (**19**) and 8-Deoxoantidesmone (**20**).

Table S1. *In vitro* colony diameters (mm) obtained using two independent experiments for *Phytophthora infestans* and *Zymoseptoria tritici* at different concentrations of crude extract and eight fractions from *Erismadelphus exsul* bark.

	Concentration (mg.L^{-1})													
	0		**31.5**		**62.5**		**125**		**250**		**500**		**1000**	
	Rep1	**Rep2**	**Rep1**	**Rep2**	**Rep1**	**Rep2**	**Rep1**	**Rep2**	**Rep1**	**Rep2**	**Rep1**	**Rep2**	**Rep1**	**Rep2**
Phytophthora infestans														
DMSO	**13.3** (0.2)	**13.3** (0.3)	**13.5** (1.3)	**13.5** (0.5)	**13.2** (0.3)	**13.2** (1.3)	**12.7** (1.0)	**12.8** (1.2)	**11.7** (2.4)	**12.3** (1.5)	**10.3** (3.0)	**10.2** (2.0)	**10.8** (2.1)	**10.0** (1.8)
Crude extract	**13.3** (0.2)	**13.3** (0.3)	**9.7** (2.8)	**9.5** (2.2)	**7.0** (3.0)	**7.2** (1.3)	**6.8** (2.3)	**7.5** (1.5)	**6.0** (2.5)	**4.8** (1.2)	**3.3** (1.9)	**2.2** (3.8)	**2.3** (4.0)	**2.3** (4.0)
F1	**13.3** (0.2)	**13.3** (0.3)	**12.2** (1.0)	**12.0** (1.0)	**9.5** (1.8)	**10.7** (2.3)	**8.0** (1.8)	**8.0** (3.6)	**3.5** (2.8)	**6.7** (2.4)	**1.0** (1.7)	**1.0** (1.7)	**0.7** (1.2)	**0.7** (1.2)
F2	**13.3** (0.2)	**13.3** (0.3)	**10.8** (2.8)	**11.7** (1.8)	**9.7** (2.8)	**9.0** (3.1)	**7.3** (2.5)	**7.8** (2.8)	**6.2** (2.8)	**7.5** (2.6)	**3.0** (3.6)	**2.0** (3.5)	**0.7** (1.2)	**1.3** (1.5)
F3	**13.3** (0.2)	**13.3** (0.3)	**9.7** (2.9)	**10.0** (1.7)	**9.3** (1.8)	**7.8** (1.5)	**8.7** (2.4)	**7.0** (0.5)	**4.5** (1.5)	**4.2** (4.0)	**1.0** (1.7)	**1.8** (3.2)	**0.0** (0.0)	**0.0** (0.0)
F4	**13.5** (1.1)	**14.3** (0.4)	**11.5** (3.9)	**12.0** (1.0)	**10.5** (3.0)	**10.5** (1.3)	**9.8** (2.9)	**8.7** (0.6)	7.5 (2.5)	**8.3** (1.6)	**6.2** (1.0)	**4.5** (1.5)	**3.7** (3.3)	**1.0** (0.0)
F5	**13.5** (1.1)	**14.3** (0.4)	**12.2** (1.9)	**11.8** (1.0)	**10.0** (2.6)	**10.8** (0.6)	**9.7** (0.23)	**9.8** (2.0)	**8.2** (1.4)	**9.3** (2.4)	**0.67** (1.2)	**7.7** (1.6)	**3.7** (3.5)	**2.3** (2.3)
F6	**13.5** (1.1)	**14.3** (0.4)	**11.7** (3.6)	**13.2** (3.5)	**9.8** (2.1)	**12.3** (3.8)	**10.2** (2.3)	**11.8** (1.0)	**8.2** (3.3)	**10.5** (1.3)	**4.8** (3.5)	**9.2** (0.8)	**6.0** (3.8)	**4.5** (1.3)
F7	**13.5** (1.1)	**14.3** (0.4)	**11.3** (2.9)	**13.8** (0.8)	**9.5** (4.0)	**12.0** (1.8)	**10.2** (3.3)	**12.2** (1.0)	**8.7** (3.3)	**10.0** (1.7)	**7.0** (5.3)	**7.2** (2.0)	**4.7** (4.1)	**3.8** (3.5)
F8	**13.5** (1.1)	**14.3** (0.4)	**11.8** (2.9)	**12.7** (1.9)	**10.8** (4.2)	**11.8** (1.0)	**9.5** (3.3)	**11.2** (1.4)	**7.5** (3.9)	**9.5** (1.8)	**7.3** (2.0)	**7.8** (2.5)	**4.5** (4.0)	**6.7** (1.5)
Zymoseptoria tritici														
DMSO	**9.8** (0.5)	**9.9** (0.2)	**9.0** (0.0)	**9.5** (0.7)	**9.3** (0.6)	**9.2** (0.3)	**9.8** (0.3)	**9.2** (0.3)	**9.3** (0.3)	**9.3** (0.3)	**9.5** (0.5)	**8.8** (0.3)	**8.8** (0.6)	**9.5** (0.7)
Crude extract	**9.8** (0.5)	**9.9** (0.2)	**7.8** (0.3)	**7.7** (0.3)	**7.0** (0.0)	**7.5** (0.0)	**6.8** (0.3)	**6.8** (0.3)	**6.2** (0.3)	**6.2** (0.3)	**5.8** (0.4)	**5.7** (0.3)	**5.0** (0.0)	**5.0** (0.0)
F1	**9.8** (0.5)	**9.9** (0.2)	**8.8** (0.3)	**10.0** (0.0)	**9.5** (0.5)	**9.0** (0.0)	**9.2** (0.3)	**9.5** (0.5)	**9.3** (0.3)	**9.2** (0.3)	**9.0** (0.0)	**8.8** (0.3)	**8.7** (0.3)	**8.7** (0.6)
F2	**9.8** (0.5)	**9.9** (0.2)	**8.0** (0.0)	**8.2** (0.3)	**7.0** (0.0)	**6.7** (0.6)	**6.2** (0.3)	**6.8** (0.3)	**6.0** (0.0)	**6.0** (0.0)	**5.0** (0.0)	**5.0** (0.0)	**3.8** (0.3)	**5.0** (0.0)
F3	**9.8** (0.5)	**9.9** (0.2)	**6.7** (0.3)	**7.0** (0.0)	**6.0** (0.0)	**6.0** (0.0)	**5.0** (0.0)	**5.3** (0.6)	**5.0** (0.0)	**5.0** (0.0)	**4.0** (0.0)	**4.0** (0.0)	**3.0** (0.0)	**3.5** (0.0)
F4	**9.8** (0.5)	**9.9** (0.2)	**8.3** (0.3)	**7.0** (0.0)	**7.0** (0.0)	**6.0** (0.0)	**6.3** (0.3)	**5.7** (0.6)	**6.0** (0.0)	**5.0** (0.0)	**5.0** (0.0)	**4.0** (0.0)	**4.5** (0.5)	**3.3** (0.3)
F5	**9.8** (0.5)	**9.9** (0.2)	**8.0** (0.0)	**7.3** (0.6)	**7.0** (0.0)	**6.8** (0.3)	**6.0** (0.0)	**6.0** (0.0)	**5.3** (0.6)	**5.7** (0.6)	**5.3** (0.3)	**5.0** (0.0)	**5.0** (0.0)	**4.7** (0.3)

F6	**9.8** (0.5)	**9.9** (0.2)	**8.3** (0.6)	**8.0** (0.0)	**7.0** (0.0)	**6.8** (0.3)	**6.3** (0.3)	**6.0** (0.0)	**6.0** (0.0)	**6.0** (0.0)	**5.3** (0.6)	**5.3** (0.6)	**5.0** (0.0)	**4.5** (0.5)
F7	**9.8** (0.5)	**9.9** (0.2)	**7.8** (0.3)	**6.2** (0.8)	**6.8** (0.3)	**7.2** (0.3)	**6.0** (0.0)	**6.0** (0.0)	**5.7** (0.3)	**5.3** (0.6)	**5.0** (0.0)	**4.8** (0.3)	**5.0** (0.0)	**5.0** (0.0)
F8	**9.8** (0.5)	**9.9** (0.2)	**7.8** (0.3)	**7.5** (0.5)	**6.8** (0.3)	**7.0** (0.0)	**6.3** (0.3)	**6.0** (0.0)	**6.0** (0.0)	**6.0** (0.0)	**5.8** (0.3)	**5.7** (0.3)	**5.2** (0.3)	**5.8** (0.3)

Rep 1: Repetition 1 ; Rep2: Repetition 2

Values in bold indicate means of *in vitro* colony diameters measured at three and eleven days after microplate inoculation with *P. infestans* and *Z. tritici*, respectively, while the values in brackets indicate the corresponding standard deviations obtained with three biological replicates for each tested concentration.

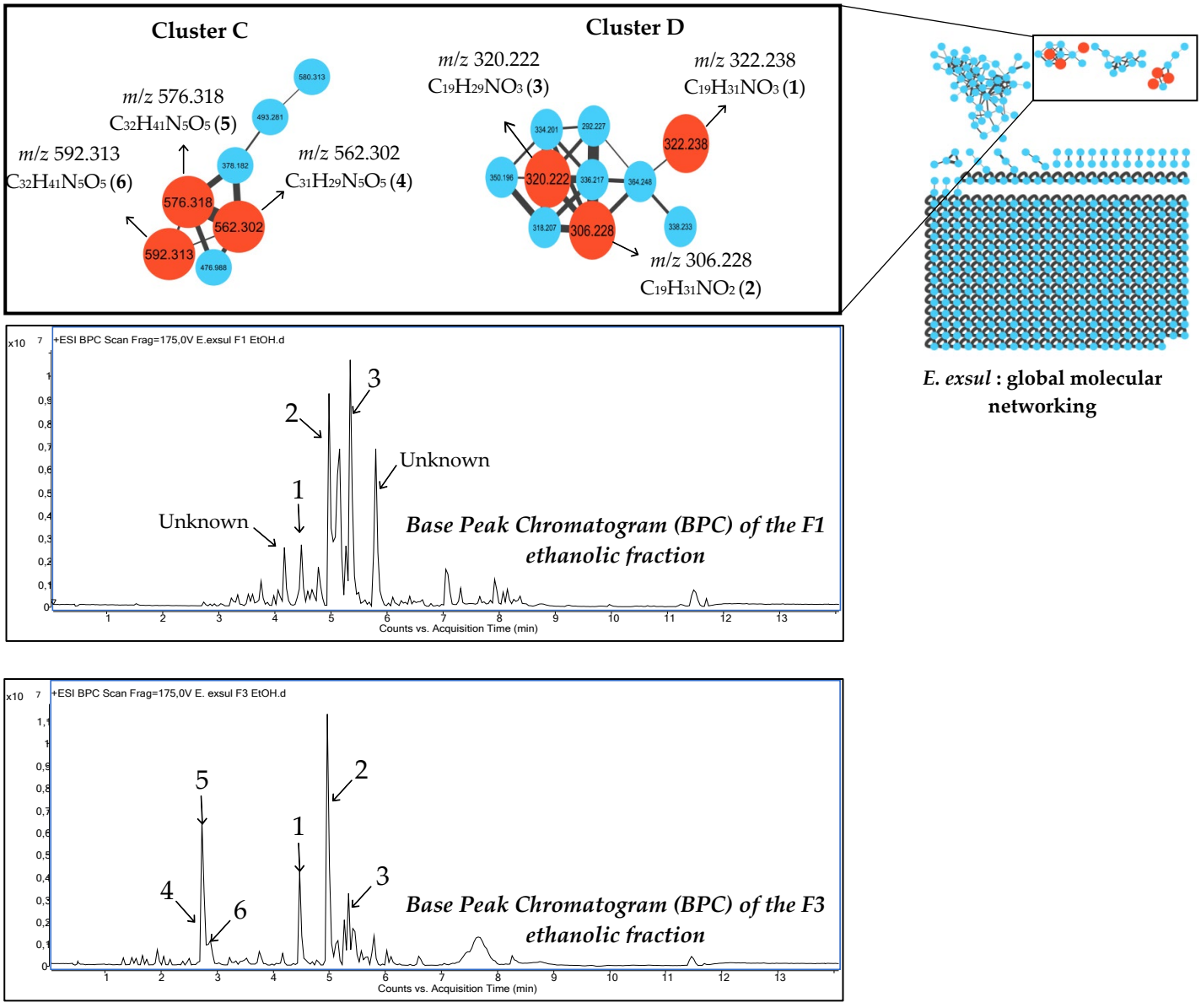
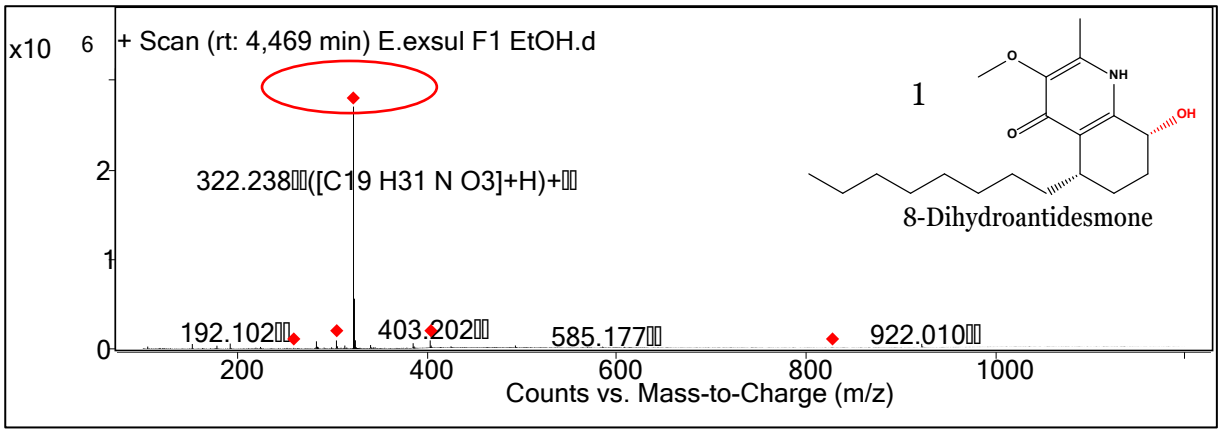
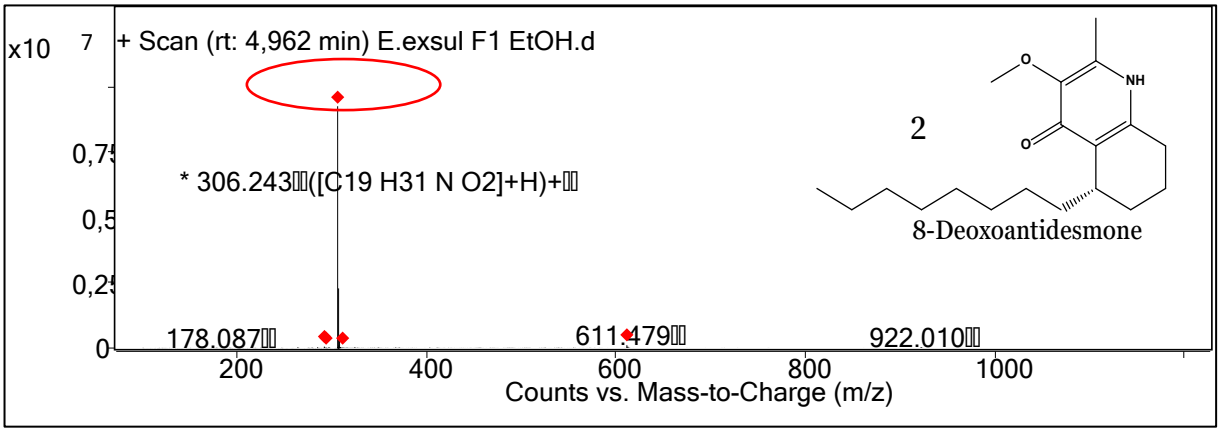
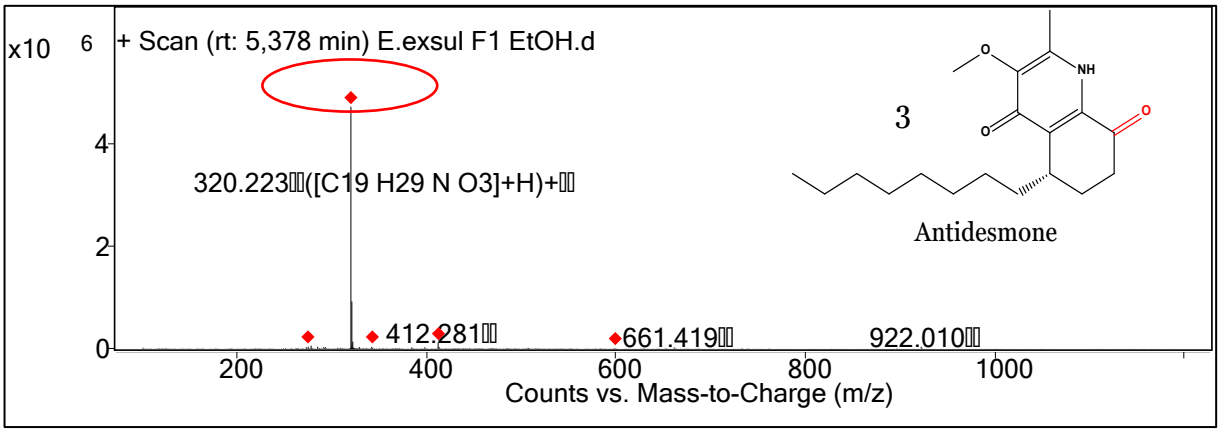


Figure S3. Focus on the cluster of antimicrobial ions of interest contained in fractions F1and F3.


x10 6
+ Scan (rt: 4,469 min) E.exsul F1 EtOH.d
322.238□□([C19 H31 N O3]+H)+□□
192.102□□
403.202□□
585.177□□
922.010□□
Counts vs. Mass-to-Charge (m/z)
1
8-Dihydroantidesmone


x10 7
+ Scan (rt: 4,962 min) E.exsul F1 EtOH.d
* 306.243□□([C19 H31 N O2]+H)+□□
178.087□□
611.479□□
922.010□□
Counts vs. Mass-to-Charge (m/z)
2
8-Deoxoantidesmone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+ Scan (rt: 5,378 min) E.exsul F1 EtOH.d
320.223□□([C19 H29 N O3]+H)+□□
412.281□□
661.419□□
922.010□□
Counts vs. Mass-to-Charge (m/z)
3
Antidesmone

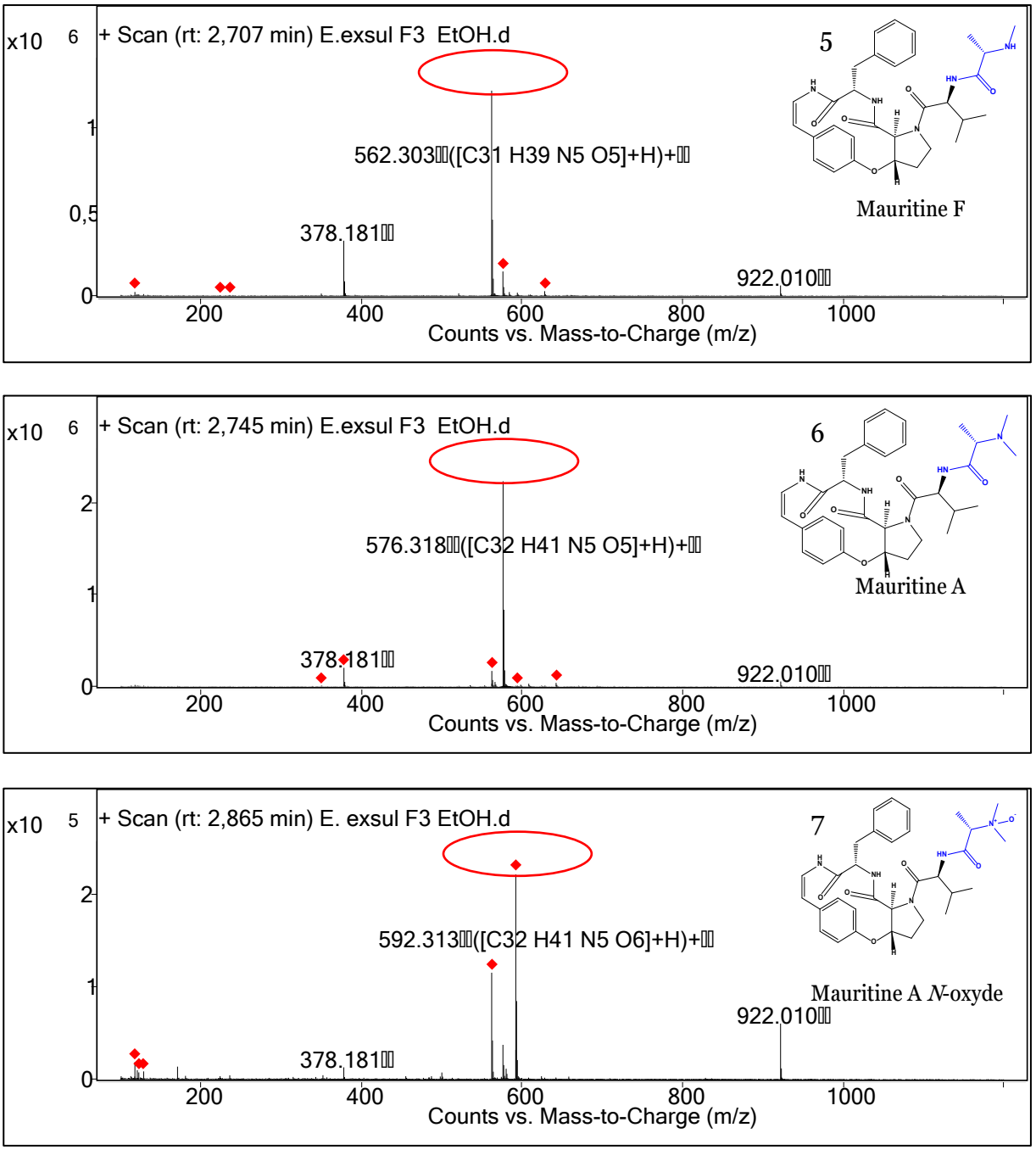

Figure S4. Mass spectra of the $[M+H]^+$ ions of Mauritine A , Mauritine F , Mauritine A N-oxide, 8-Dihydroantidesmone (2), 8-Deoxoantidesmone (3), and Antidesmone (4) obtained by LC–ESI–MS.