Supplementary Information

Comparative Metabolic Profiling in *Cololobus* Species across Habitats

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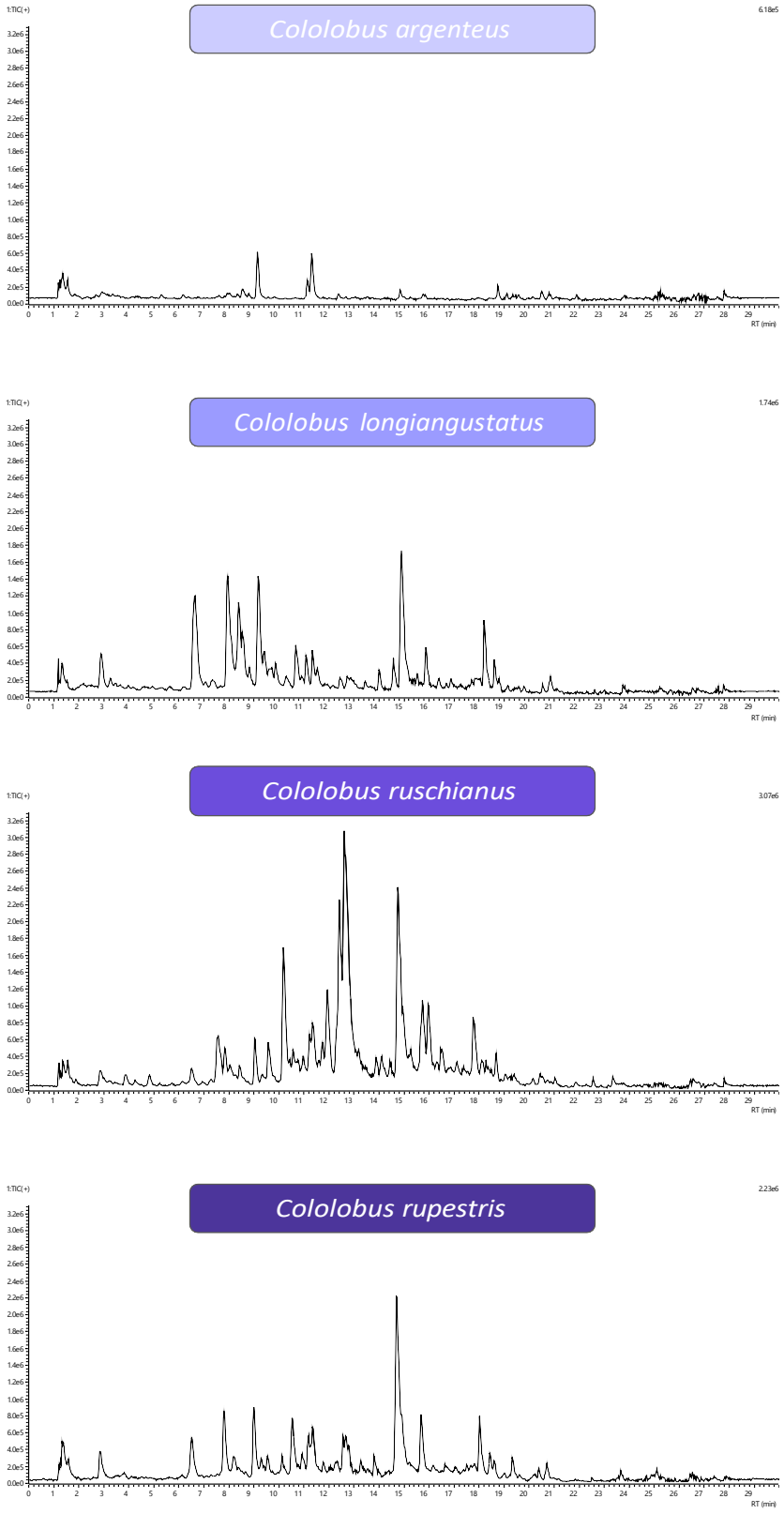

Figure S1. Total ion chromatograms of *Cololobus* species from Atlantic Forest inselbergs, analyzed by LC-MS/MS in positive ionization mode.

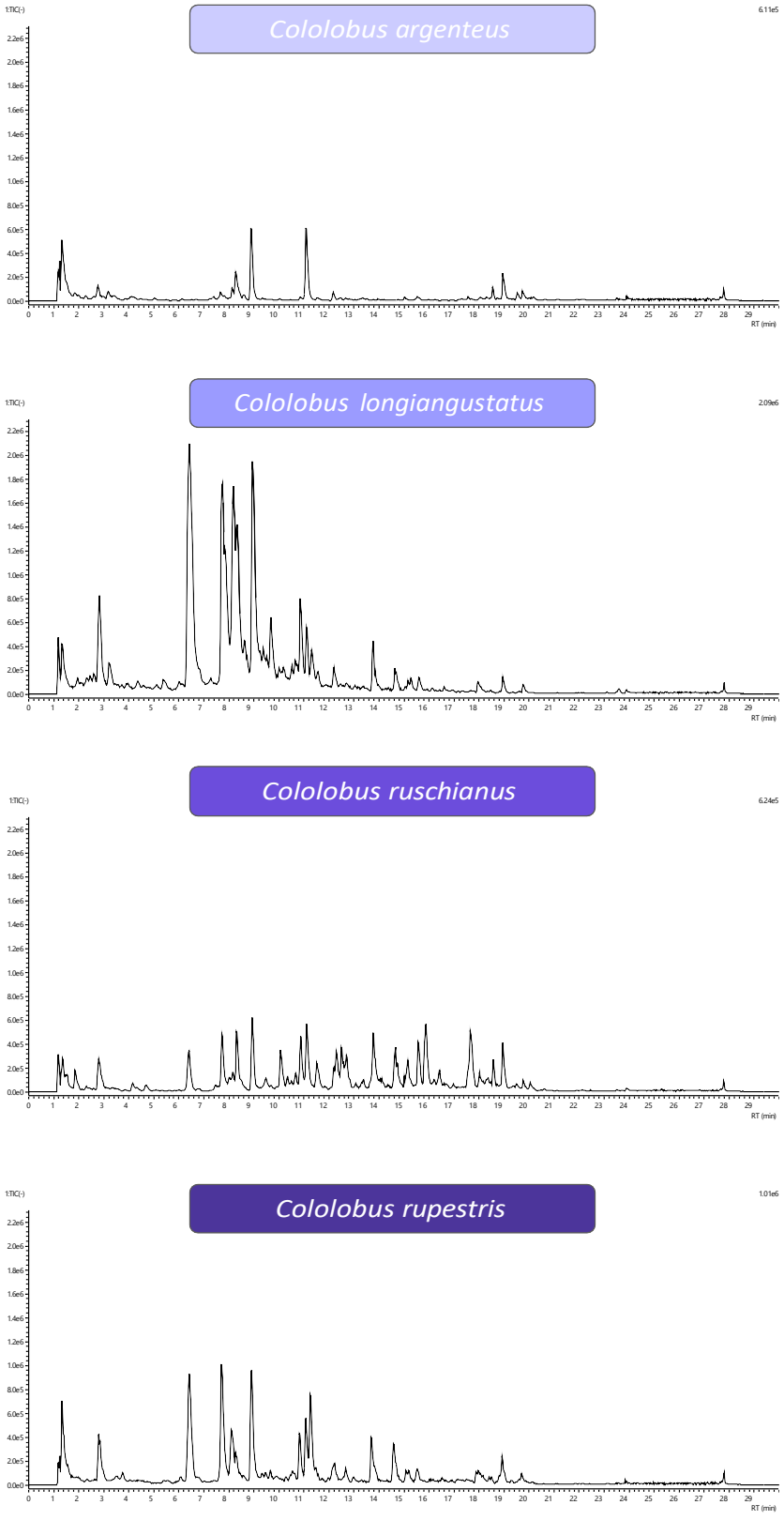

Figure S2. Total ion chromatograms of *Cololobus* species from Atlantic Forest inselbergs, analyzed by LC-MS/MS in negative ionization mode.

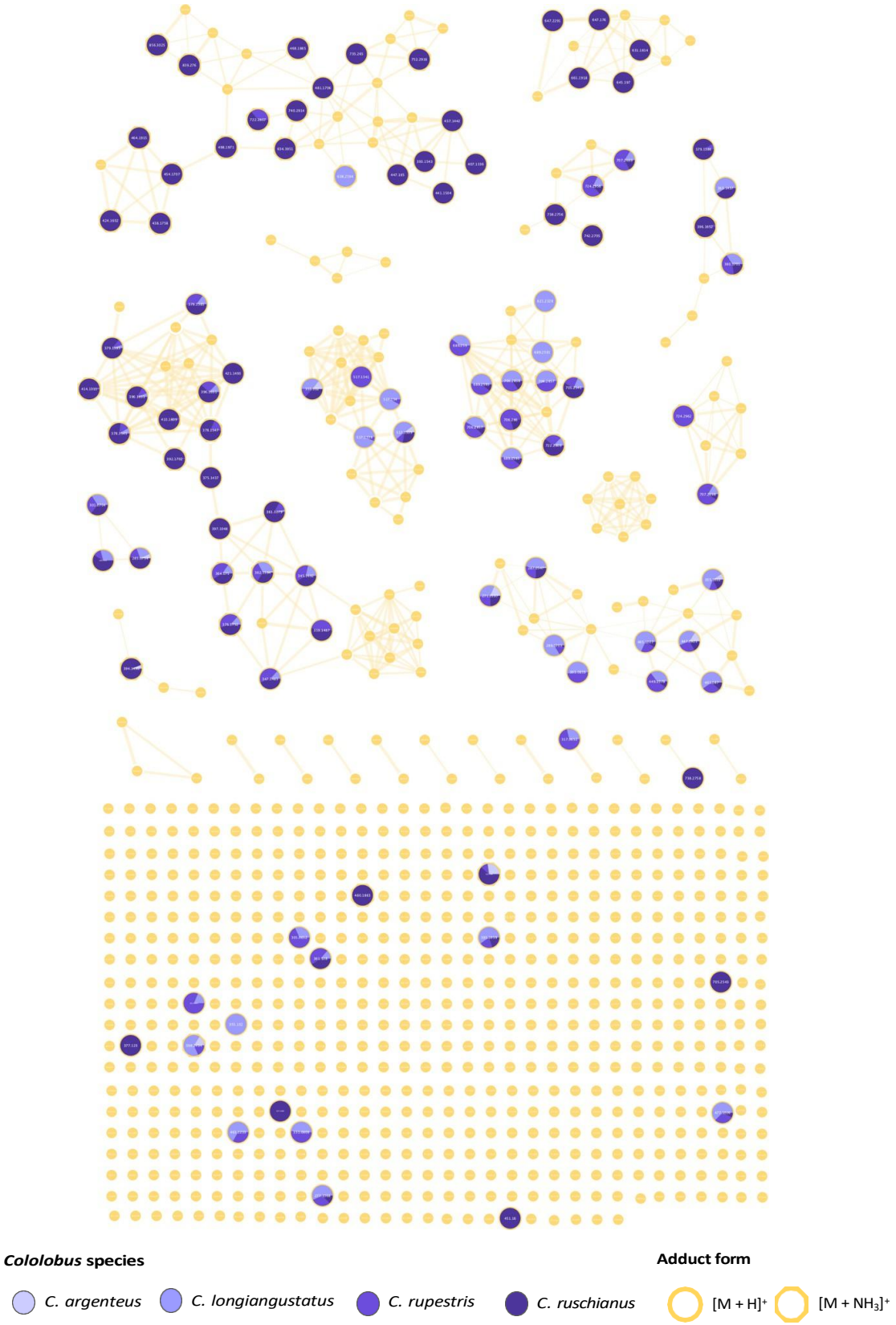

Figure S3. Molecular networking of *Cololobus* species from Atlantic Forest inselbergs, using LC-MS/MS data obtained in positive ionization mode.

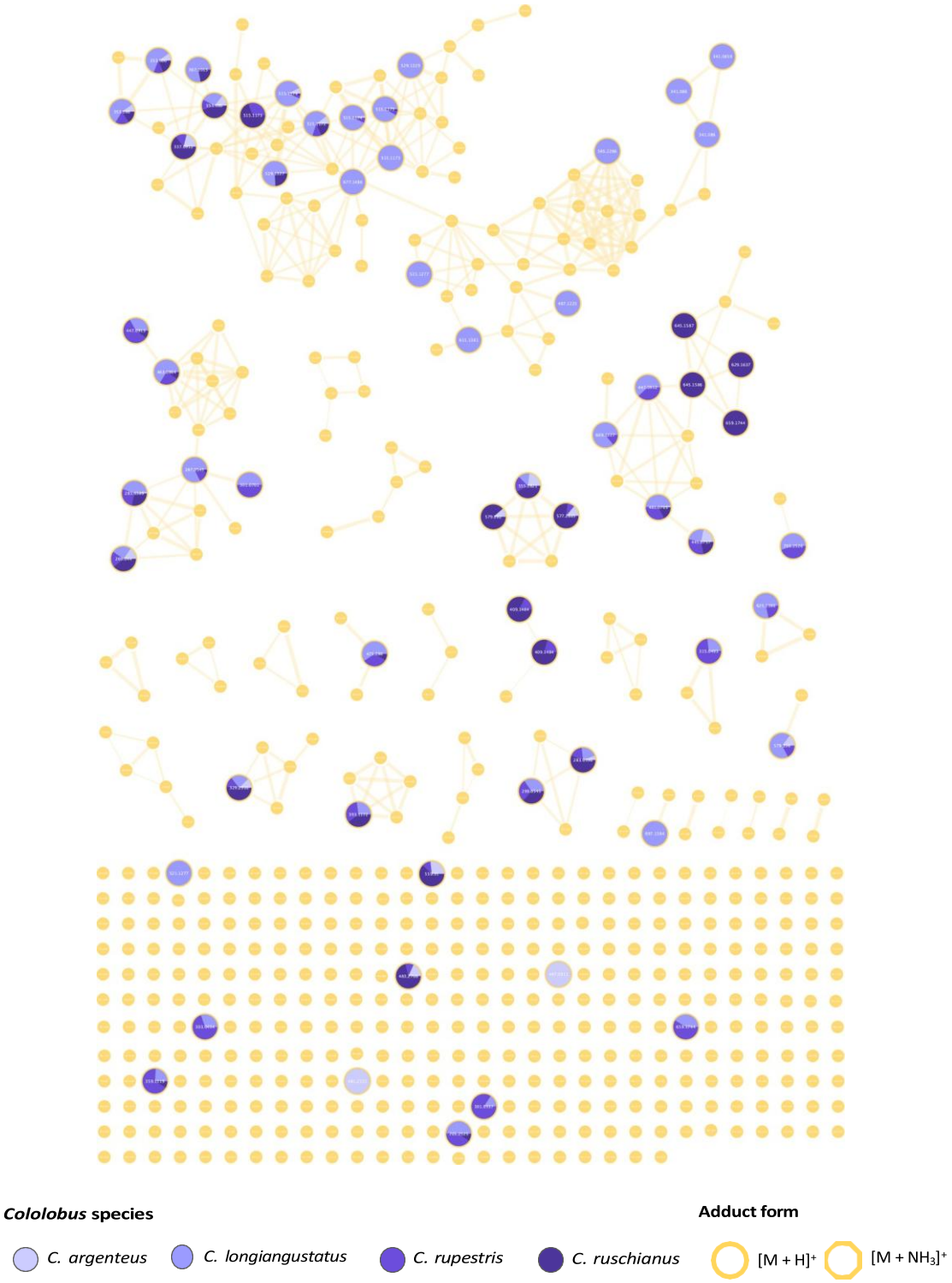

Figure S4. Molecular networking of *Cololobus* species from Atlantic Forest inselbergs, using LC-MS/MS data obtained in negative ionization mode.

Table S1. Information of plant material collection, including collector details, identification, collection date and geographical coordinates

Cololobus species	Collector name (collector number)	Identified by	Date	Location	Coordinates (latitude, longitude)	Collection code
Cololobus longiangustatus	C. Esgario, (23)	A. P. Fontana	July 16, 2006	Alto Misterioso, São Roque do Canaã, Espírito Santo, Brazil	–19.796944, –40.775278	MBML 29761
Cololobus rupestris	C.C. Chamas (161)	A. P. Fontana	May 23, 1994	Estação Biológica de Santa Lúcia, Santa Teresa, Espírito Santo, Brazil	–19.971389, –40.530278	MBML 11982
Cololobus ruschianus	Monge *et al*. (3320)	M. Monge	Oct 2, 2016	Vale do Canaã, Santa Teresa, Espírito Santo, Brazil	–19.911111, –40.60500	UEC 195464
Cololobus argenteus	Monge *et al*. (3585)	M. Monge	Jul 27, 2019	Pedra da Tartaruga, Águia Branca, Espírito Santo, Brazil	–18.983111, –40.740306	HUFU 3585

Table S2. Spectroscopic and spectrometric data of the detected metabolites in *Cololobus* species, along with the annotation given by the GNPS and class predictions generated in the SIRIUS

ID	Node ID	t_R / min	*m/z*	Fragmentation precursor ion → fragments	UV / nm	Formula	Error / ppm	GNPS annotation (cosine) Sirius NPC superclass (probability)	Metabolite name
	85P		355.1021 $[M + H]^+$	355.1021 → 163.0386 bp, 145.0280, 135.0431, 117.0331, 89.0380			–0.73	chlorogenic acid CCMSLIB00013639456 (0.953) phenylpropanoids (C6-C3) (0.998)	
1	51N	1.9	353.0859 $[M – H]^–$	353.0859 → 191.0546 bp, 179.0334, 173.0446, 161.0227, 135.0438, 134.0358, 127.0390, 111.0440, 93.0328, 85.0280	195, 218, 240 sh, 297 sh, 323	$C_{16}H_{18}O_9$	–5.41	5-*O*-caffeoylquinic acid CCMSLIB00005467735 (0.9945) phenylpropanoids (C6-C3) (0.999)	3-*O*-caffeoylquinic acid
2N	54N	2.0	341.0859 $[M – H]^–$	341.0860 → 203.0340, 179.0335, 161.0231 bp, 135.0440, 134.0353, 133.0286	197, 241 sh, 296, 322	$C_{15}H_{18}O_9$	–4.43	NCGC00380261-01 CCMSLIB00000848728 (0.5744) [a] phenylpropanoids (C6-C3) (0.996)	caffeoyl *O*-hexoside

3N	60N	2.2	341.0863 $[M - H]^-$	341.0860 → 221.0447, 179.0335, 177.0333, 161.0231, 135.0440 bp, 133.0286	199, 240 sh, 295, 323	$C_{15}H_{18}O_9$	–4.45	NCGC00380261-01 CCMSLIB00000848728 (0.6329) [a] Phenylpropanoids (C6-C3) (0.988)	caffeoyl *O*-hexoside
4N	71N	2.5	341.0860 $[M - H]^-$	341.0859 → 281.0653, 251.0559, 221.0439, 179.0337, 177.0539, 161.0232, 135.0439 bp, 134.0359, 133.0282	198, 241 sh, 298, 322	$C_{15}H_{18}O_9$	–5.31	NCGC00380261-01 CCMSLIB00000848728 (0.6989) [a] phenylpropanoids (C6-C3) (0.995)	caffeoyl *O*-hexoside
5	101P	2.6	355.1020 $[M + H]^+$	355.1021 → 163.0384 bp, 145.0270, 135.0440, 117.0328, 89.0378	218, 245 sh, 298 sh, 324	$C_{16}H_{18}O_9$	–1.15	chlorogenic_acid CCMSLIB00013639456 (0.9690) phenylpropanoids (C6-C3) (0.997)	4-*O*-caffeoylquinic acid
	74N	2.6	353.0861 $[M - H]^-$	353.0860 → 191.0547, 179.0338, 173.0442, 161.0219, 155.0329, 135.0439 bp, 134.0360, 127.0380, 93.0334			–4.84	chlorogenic acid CCMSLIB00010152869 (0.9552) phenylpropanoids (C6-C3) (0.999)	

	111P		355.1021 $[M + H]^+$	355.1021 → 163.0384 bp, 145.0278, 135.0435, 117.0331, 89.0379	195, 217, 243 sh, 299 sh, 325		–0.73	chlorogenic_acid CCMSLIB00013639456 (0.4119) Phenylpropanoids (C6-C3) (0.994)	
6		2.9		353.0498 → 191.0547 bp, 177.0178, 173.0443, 161.0231, 155.0338, 135.0439, 127.0388, 109.0284, 93.0334, 87.0077, 85.0283		$C_{16}H_{18}O_9$			5-*O*-caffeoylquinic acid
	84N		353.0861 $[M – H]^–$				–4.84	chlorogenic acid CCMSLIB00010152869 (0.9585) phenylpropanoids (C6-C3) (0.997)	
7N	116N	4.1	337.0912 $[M – H]^–$	337.0911 → 191.0546 bp, 173.0440, 163.0386, 127.0385, 119.0489, 93.0335, 85.0276	220, 297 sh, 310	$C_{16}H_{18}O_8$	–5.01	coumaroyl quinic acid CCMSLIB00005747504 (0.9766) phenylpropanoids (C6-C3) (0.996)	5-*p*-coumaroylquinic acid
8N	118N	4.3	515.1170 $[M – H]^–$	515.1170 → 353.0860, 335.0747, 191.0545 bp, 179.0335, 135.0437	220, 296 sh, 323	$C_{25}H_{24}O_{12}$	–1.02	1,4-dicaffeoylquinic acid CCMSLIB00010012012 (0.9602) phenylpropanoids (C6-C3) (0.998)	1,3-*O*-dicaffeoylquinic acid

9P	152P	4.7	595.1655 $[M + H]^+$	595.1655 → 457.1124 bp, 427.1007, 409.0890, 379.0808, 337.0690, 325.0701	220, 289 sh, 328	$C_{27}H_{30}O_{15}$	–0.42	PR303371 CCMSLIB00005745586 (0.6605) flavonoids (0.918)	apigenin *C*-hexose- hexoside
10N	135N	5.0	367.1016 $[M – H]^–$	367.1015 → 193.0489, 191.0547 bp, 173.0447, 134.0360, 93.0333	211, 291 sh, 325	$C_{17}H_{20}O_9$	–6.43	feruloyl quinic acid CCMSLIB00005749052 (0.9807) phenylpropanoids (C6-C3) (0.994)	5-*O*-feruloylquinic acid
11N	140N	5.4	625.1384 $[M – H]^–$	625.1382 → 463.0857, 449.1069, 287.0543 bp, 175.0235, 151.0024, 135.0440, 113.0233	212, 285 326 sh	$C_{27}H_{30}O_{17}$	–4.19	– flavonoids (1.000)	eriodictyol *O*-hexose-*O*-hexuroside
12	171P	6.1	305.0652 $[M + H]^+$	305.0652 → 231.0646, 153.0177 bp, 149.0230, 123.0441	223, 290, 328 sh	$C_{15}H_{12}O_7$	–0.59	taxifolin CCMSLIB00004719703 (0.9369) flavonoids (0.993)	dihydroquercetin

	151N		303.0492 $[M-H]^-$	303.0496 → 285.0386, 241.0503, 217.0495, 201.0174, 199.0389, 177.0176, 175.0389, 151.0029, 150.0312, 153.0182, 149.0234, 125.0233 bp, 123.0443, 121.0287, 109.0277			–6.04	taxifolin CCMSLIB00004691353 (0.9320) flavonoids (0.997)	
13N	154N	6.2	521.1279 $[M-H]^-$	521.1278 → 323.0749, 179.0345, 161.0227, 135.0438 bp, 133.0277	224, 289, 328	$C_{24}H_{26}O_{13}$	–4.14	salviaflaside CCMSLIB00004711942 (0.6667) phenylpropanoids (C6-C3) (0.686)	rosmarinic acid *O*-hexoside
14	180P	6.5	465.1027 $[M+H]^+$	465.1027 → 289.0703 bp, 271.0600, 205.0495, 187.0387, 179.0334, 163.0385, 153.0177, 145.0280, 135.0437,	197, 225sh, 283, 327 sh	$C_{21}H_{20}O_{12}$	–0.06	NCGC00385261-01 CCMSLIB00000847602 (0.9389) [a] flavonoids (0.999)	eriodictyol *O*-hexuronoside

				123.0435, 123.0435,				
				117.0329, 111.0067, 89.0377				
	169N		463.0866 $[M-H]^-$	463.0869 → 329.0648, 287.0544, 269.0440, 217.0129, 175.0234, 151.0024 bp, 125.0439, 113.0233, 107.0127, 99.0075, 95.0126, 85.0284, 83.0129			–3.46	(2*S*)-eriodictoyl-7-*O*-beta-*D*-glucopyranosiduronic acid CCMSLIB00012404887 (0.9235) flavonoids (1.000)
15N	188N	7.2	521.1284 $[M-H]^-$	521.1277 → 197.0440, 179.0331, 161.0229 bo	218, 289, 324	$C_{24}H_{26}O_{13}$	–3.19	salviaflaside CCMSLIB00004711942 (0.7767) stilbenoids (0.958) [a]	rosmarinic acid *O*-hexoside

16P	222P 227P	7.5	396.1652 $[M + NH_4]^+$ 379.1386 $[M + H]^+$	396.1652 → 379.1389, 277.1069, 259.0962, 241.0857, 231.1014 bp, 213.0907, 203.0700, 185.0956, 175.0751, 157.1009, 147.0801, 129.0694, 119.0851, 91.0535	218, 266	$C_{19}H_{22}O_8$	–0.23 –0.42	NCGC00386023 - CCMSLIB00012450934 (0.6809) 222P sesquiterpenoids (0.967) 227P sesquiterpenoids (0.936)	putative vernodalinol
				379.1387 → 259.0961, 231.1009 bp, 213.0909, 185.0952, 175.0749, 157.1014, 147.0799, 129.0692, 119.0852, 115.0538					
17	239P	7.7	463.0868 $[M + H]^+$	463.0868 → 287.0545 bp, 269.0444, 241.0490, 179.0334, 161.0229, 153.0177, 135.0435,	203, 254, 265 sh, 347	$C_{21}H_{18}O_{12}$	–0.39	luteolin 7-glucuronide CCMSLIB00012320258 (0.9970) flavonoids (1.000)	luteolin *O*-hexuronoside

				117.0330				
	204N		461.0702 $[M - H]^-$	461.0703 → 357.0593, 327.0496, 285.0387 bp, 241.0488, 217.0489, 199.0385, 175.0386, 151.0023, 133.0282, 121.0275, 109.0289, 107.0128			–5.01	luteolin 7-glucuronide CCMSLIB00012318865 (0.9723) flavonoids (0.999)	
18	256P	7.9	517.1336 $[M + H]^+$	517.1336 → 499.1233, 319.0805, 163.0385 bp, 145.0279, 135.0437, 117.0330, 89.0379	218, 241 sh, 298 sh, 325	$C_{25}H_{24}O_{12}$	–0.83	19870-46-3 CCMSLIB00012337965 (0.9849) phenylpropanoids (C6-C3) (0.988)	3,4-*O*-dicaffeoylquinic acid

	229N		515.1177 $[M - H]^-$	515.1175 → 353.0859, 335.0755, 299.0547, 255.0643, 203.0334, 191.0547, 179.0336, 173.0442 bp, 161.0230, 155.0337, 135.0440, 133.0283, 127.0393, 111.0444, 107.0491, 93.0334			–3.48	isochlorogenic acid C CCMSLIB00012404413 (0.9569) phenylpropanoids (C6-C3) (0.999)	
19P	262P 258P	8.0	394.1496 $[M + NH_4]^+$ 377.1230 $[M + H]^+$	394.1295 → 377.1235, 275.0908, 257.0813, 229.0858 bp, 211.0751, 201.0907, 183.0799, 173.0956, 155.0848	-	$C_{19}H_{20}O_8$	–0.30 –0.21	262P sesquiterpenoids (0.628) 258P flavonoids (0.378)	hirsutinolide-type STL
20	273P	8.1	449.1080 $[M + H]^+$	449.1079 → 287.0552, 273.0754 bp, 153.0178, 147.0436, 119.0487, 91.0532	194, 218, 285, 328	$C_{21}H_{20}O_{11}$	0.29	flavonoids (1.000)	naringenin *O*-hexuronoside

	247N	447.0913 $[M - H]^-$	447.0914 → 271.0595 bp, 227.0700, 187.0381, 175.0235, 151.0024, 143.0498, 119.0490, 113.0232, 107.0128, 99.0074, 93.0331, 85.0279			–4.45	29741-09-1 CCMSLIB0001243 6403 (0.8159) [a] flavonoids (1.000)	
	275P	517.1336 $[M + H]^+$	517.1336 → 499.1241, 319.0805, 163.0384 bp, 145.0279, 135.0436, 117.0333, 89.0379			–0.87	19870-46-3 CCMSLIB00012337967 (0.9627) phenylpropanoids (C6-C3) (0.790)	
21	262N	515.1178 $[M - H]^-$	515.1177 → 353.0859, 335.0751, 191.0546 bp, 179.0336, 173.0442, 161.0231, 155.0335, 135.0439, 127.0388, 111.0442, 107.0490, 93.0335,	8.2	193, 218, 241 sh, 299 sh, 326	$C_{25}H_{24}O_{12}$	3-*O*-caffeoylquinic acid CCMSLIB00005467731 (0.9838) phenylpropanoids (C6-C3) (0.998)	3,5-*O*-dicaffeoylquinic acid

			85.0283					
22	288P	8.3	517.1341 [M + H]$^+$	517.1341 → 499.1239, 319.0793, 163.0386 bp, 145.0279, 135.0441, 117.0332, 89.0380	193, 218, 240 sh, 299 sh, 328	$C_{25}H_{24}O_{12}$	–0.27	19870-46-3 CCMSLIB00012337965 (0.9807) phenylpropanoids (C6-C3) (0.984)	1,5-*O*-dicaffeoylquinic acid
	270N		515.1177 [M – H]$^-$	515.1177 → 353.0859, 335.0751, 191.0547 bp, 179.0336, 173.0442, 161.0230, 155.0333, 135.0439, 127.0388, 111.0442, 109.0282, 93.0335, 87.0076, 85.0283			–0.27	NCGC00380583-01 CCMSLIB00000846311 (0.9980) phenylpropanoids (C6-C3) (0.998)	

23	310P	8.6	598.2492 $[M + NH_4]^+$	598.2491 → 401.1599, 383.1488, 265.1065, 235.0960, 217.0856, 205.0854 bp, 190.0620, 173.0592, 167.0699, 145.0629	-	$C_{28}H_{36}O_{13}$	–0.37	acanthoside B CCMSLIB00012430652 (0.8291) lignans (0.999)	acanthoside B
	292N		579.2053 $[M – H]^–$	579.2059 → 417.1533 bp, 402.1302, 387.1073, 181.0492, 166.0259, 161.0229, 151.0025			–5.11	acanthoside B CCMSLIB00012400440 (0.8847) lignans (1.000)	
24	322P	8.9	447.0922 $[M + H]^+$	447.0920 → 271.0597 bp, 229.0499, 153.0176, 119.0486	210, 222, 267, 336	$C_{21}H_{18}O_{11}$	0.022	29741-09-1 CCMSLIB00012436403 (0.9977) flavonoids (0.998)	apigenin *O*-hexuronoside
	314N		445.0756 $[M – H]^–$	445.0755 → 269.0438 bp, 225.0540, 175.0236, 159.0438, 149.0230, 117.0334, 113.0231, 107.0128,			–4.61	HexA-apigenin CCMSLIB00004683272 (0.9909) flavonoids (0.995)	

				99.0074, 85, 0279					
25N	297N	8.8	447.0912 $[M - H]^-$	447.0900 → 285.0389 bp, 271.491, 151.0027, 133.286	217, 289 sh, 332	$C_{21}H_{20}O_{11}$	–4.68	kaempferol-3-*O*-glucoside CCMSLIB00000222087 (0.9914) flavonoids (0.999)	luteolin *O*-hexoside
26	327P	9.0	517.1338 $[M + H]^+$	517.1341 → 499.1243, 319.0812, 163.0385 bp, 145.0279, 135.0437, 117.0330, 107.0484, 89.0380	197, 218, 299 sh, 328	$C_{25}H_{24}O_{12}$	–0.42	19870-46-3 CCMSLIB00012337965 (0.9850) phenylpropanoids (C6-C3) (0.984)	1,4-*O*-dicaffeoylquinic acid

	323N		515.1176 [M – H]⁻	515.1176 → 353.0859, 335.0754, 317.0648, 299.0544, 255.0646, 227.0702, 203.0334, 191.0546, 179.0336, 173.0442 bp, 161.0231, 155.0337, 137.0232, 135.0439, 134.0360, 127.0389, 111.0440, 109.0284, 107.0490, 93.0334, 85.0282			–3.69	3,4-dicaffeoylquinic acid CCMSLIB00012415410 (0.9757) phenylpropanoids (C6-C3) (0.999)	
27N	343N	9.2	487.1224 [M – H]⁻	487.1225 → 443.1327, 323.0755, 280.0560, 221.0442, 179.0334, 177.0547, 163.0387, 161.0230 bp, 135.0439,	216, 280, 324 sh	$C_{24}H_{24}O_{11}$	–4.49	5-hydroxy-7-*O*-(6-*O*-*p*-*cis*- coumaroyl-beta-*D*- glucopyranosyl)chromone CCMSLIB00016039119 (0.9466) [a] phenylpropanoids (C6-C3) (0.605)	caffeoyl-hexose derivative

				133.0284, 132.0204, 119.0490					
28P	338P	9.3	277.1067 $[M + H]^+$	277.1067 → 233.0803 bp, 191.0711, 163.0748, 145.0651, 128.0607, 115.0537, 91.0534, 77.0378	221, 273	$C_{15}H_{16}O_5$	–1.26	– sesquiterpenoids (0.828)	putative vernolepin
29	350P	9.4	477.1024 $[M + H]^+$	477.1024 → 301.0700 bp, 286.0467, 258.0518	218, 292 sh, 332	$C_{22}H_{20}O_{12}$	–0.73	6-*O*-methylscutellarin CCMSLIB00012430935 (0.9254) flavonoids (0.998)	luteolin *O*-methyl *O*-hexuroside
	348N		475.0863 $[M – H]^–$	475.0861 → 299.0547 bp, 284.0309, 256.0375, 175.0249, 113.0233			–4.54	(2*S*,3*S*,4*S*,5*R*,6*S*)-3,4,5-trihydroxy-6-[5-hydroxy-2-(4-hydroxyphenyl)-6-methoxy-4-oxochromen-7-yl]oxyoxane-2-carboxylic acid CCMSLIB00004720057 (0.9813) Flavonoids (1.000)	

30N	358N	9.5	447.0914 $[M - H]^-$	447.0914 → 285.0389 bp, 151.0023, 133.0282	224, 267 sh, 295 sh, 332	$C_{21}H_{20}O_{11}$	–4.21	luteolin-4'-*O*-glucoside CCMSLIB00005746260 (0.9939) flavonoids (0.965)	luteolin *O*-hexoside
31P	351P	9.5	463.1233 $[M + H]^+$	463.1234 → 301.0703 bp, 287.0551, 286.0466, 258.0519	224, 291 sh, 328	$C_{22}H_{22}O_{11}$	–1.06	Peonidin 3-galactoside CCMSLIB0000313 6790 (0.9763) flavonoids (0.986)	luteolin *O*-methyl-*O*-hexoside
32P	358P 359P	9.6	396.1652 $[M + NH_4]^+$ 379.1387 $[M + H]^+$	396.1653 → 379.1387, 259.0962 bp, 241.0857, 231.1013, 213.0907, 203.1061, 185.0958, 161.0594, 142.0774, 133.0644, 128.0616, 105.0693	221, 273	$C_{19}H_{22}O_8$	–0.13 –0.08	NCGC00386023 CCMSLIB00012450933 (0.7320) 358P sesquiterpenoids (0.983) 359P sesquiterpenoids (0.953)	putative vernocinerascolide
33	372P	9.7	289.0702 $[M + H]^+$	289.0702 → 271.0509, 187.0385, 179.0333, 163.0384, 153.0177 bp, 145.0278, 135.0435, 123.0433, 117.0329, 97.0277,	199, 223, 288, 327 sh	$C_{15}H_{12}O_6$	–1.66	eriodictyol CCMSLIB00000223053 (0.9578) flavonoids (0.909)	eriodictyol

				89.0380, 77.0381					
	364N		287.0548 $[M-H]^-$	575.1173 → 287.0543; 193.0503, 161.0233, 151.0024 bp, 135.0439, 125.0233, 107.0128			–4.02	eriodictyol CCMSLIB00000222042 (0.9634) flavonoids (0.915)	
34N	378N	9.9	529.1325 $[M-H]^-$	529.1327 → 367.1016, 193.0491, 191.0547 bp, 173.0428, 134.0358	226, 292 sh, 328	$C_{26}H_{26}O_{12}$	–5.01	NCGC00385740-01 CCMSLIB00012414008 (0.2677) phenylpropanoids (C6-C3) (0.959)	*O*-caffeoyl-*O*-feruloylquinic acid
35N	393N	10.1	515.1172 $[M-H]^-$	515.1164 → 353.0859, 203.0340, 191.0546, 179.0337, 173.0443, 161.0229, 155.0340, 135.0439, 93.0330	226, 295 sh, 325	$C_{25}H_{24}O_{12}$	–4.47	3,4-dicaffeoylquinic acid CCMSLIB00012415410 (0.9740) phenylpropanoids (C6-C3) (0.999)	4,5-*O*-dicaffeoylquinic acid

36P	408P 407P	10.1	396.1650 $[M + NH_4]^+$ 379.1385 $[M + H]^+$	379.1387 → 259.0960, 241.0844, 231.1017, 213.0898, 203.1069, 185.0956, 170.0720, 161.0587, 157.1009, 142.0774, 133.0640, 129.0692, 115.0538, 105.0693, 91.0544	211, 269	$C_{19}H_{22}O_8$	–0.57 –0.52	NCGC00386023 CCMSLIB00012450937 (0.7094) 408P sesquiterpenoids (0.971) 407P sesquiterpenoids (0.987)	putative hydroxyvernolide
37N	397N	10.2	565.2264 $[M – H]^–$	565.2265 bp → 403.1952, 179.0334, 161.0230, 135.0438, 133.0284	226, 294 sh, 325	$C_{26}H_{26}O_{12}$	–4.64	4-(acetyloxy)-2,3-bis[(4-hydroxy-3-methoxyphenyl)methyl]butyl (2*E*)-3-(3,4-dihydroxyphenyl)prop-2-enoate CCMSLIB00005724424 (0.8673) phenylpropanoids (C6-C3) (0.901)	caffeoyl-hexose derivative
38N	400N	10.3	529.1330 $[M – H]^–$	529.1328 → 367.1013, 193.0476, 173.0440 bp	225, 292, 325	$C_{26}H_{26}O_{12}$	–4.06	NCGC00385740-01! CCMSLIB00012414008 (0.9404) phenylpropanoids (C6-C3) (0.998)	*O*-caffeoyl-*O*-feruloylquinic acid

39P	418P 417P	10.4	454.1707 $[M + NH_4]^+$ 437.1442 $[M + H]^+$	454.1708 → 437.1439, 419.1334 bp, 379.1390, 259.0964, 241.0850, 231.1011, 213.0908, 185,0955, 161.0594, 157.1007, 142.0772, 133.0646, 129.0695, 105.0695	220, 266	$C_{21}H_{24}O_{10}$	–0.09	– 418P sesquiterpenoids (0.695) 417P monoterpenoids (0.905) [a]	putative STL
40P	428P 438P	10.5	380.1709 $[M + NH_4]^+$ 363.1436 $[M + H]^+$	363.1437 → 277.1071, 259.0966, 241.0850, 231.1014, 213.0906 bp, 203.1069, 191.0695, 185.0959, 175.0745, 173.0591, 163.0748, 157.1010, 147.0800, 145.0641, 142.0773, 129.0695, 128.0610, 119.0848,	216, 265	$C_{19}H_{22}O_7$	–0.63	– 428 sesquiterpenoids (0.964) 438 sesquiterpenoids (0.956)	putative dihydrovernodalin

				115.0538, 105.0694, 91.0536					
41N	409N	10.5	609.1228 $[M - H]^-$	609.1226 → 447.0912, 323.0755, 285.0389 bp, 221.0441, 179.0336, 161.0233, 151.0026, 135.0439, 133.0284	211, 263, 328	$C_{30}H_{26}O_{14}$	–3.58	– flavonoids (0.998)	luteolin *O*-hexose-hexoside
	442P		303.0495 $[M + H]^+$	303.0498 → 229.0482, 153.0179, 137.0237		$C_{15}H_{10}O_7$	–0.69	quercetin CCMSLIB00003138830 (0.9793) flavonoids (0.988)	
42	412N	10.7	301.0336 $[M - H]^-$	301.0338 → 273.0394, 245.0431, 229.0496, 193.0120, 178.9974, 159.0448, 151.0024 bp, 149.0229, 121.0284, 109.0283, 107.0127, 93.0334, 83.0135, 65.0027	215, 263, 363	$C_{15}H_{10}O_7$	–5.91	quercetin CCMSLIB00004719957 (0.9650) flavonoids (0.998)	quercetin

43P	445P 444P	10.7	498.1970 $[M + NH_4]^+$ 481.1707 $[M + H]^+$	498.1970 → 481.1700, 463.1600, 433.1494, 389.1238, 379.1388, 259.0963 bp, 241.0859, 231.1014, 213.0906, 203.2065, 185.0957 481.1705 → 379.1382, 259.0963 bp, 231.1022, 213.0907, 185.0962	221, 269	$C_{23}H_{28}O_{11}$	0.04 0.60	– 445P sesquiterpenoids (0.809) 444P sesquiterpenoids (0.232)	glaucolide-type STL
44N	419N	10.7	409.1483 $[M – H]^–$	409.1483 → 277.1062, 191.0701 bp, 190.0631, 189.0536, 173.0590, 147.0802	-	$C_{20}H_{26}O_9$	–5.16	– fluorenes (0.488)	-
45N	425N	10.8	611.1384 $[M – H]^–$	611.1379 bp → 475.0888, 449.1069, 323.0754, 287.0542, 221.0439, 179.0336,	220, 287, 328	$C_{30}H_{28}O_{14}$	–3.65	– flavonoids (0.999)	flavonoid caffeoyl-hexose derivative

				177.0177, 161.0231, 151.0024, 135.0439,					
				133.0288, 125.0232, 107.0126					
46P	459P 458P	10.9	468.1865 $[M + NH_4]^+$ 451.1600 $[M + H]^+$	468.1866 → 415.1378, 379.1379, 259.0964 bp, 231.1010, 213.0905, 185.0960, 161.0600, 135.0441	221	$C_{22}H_{26}O_{10}$	0.192	– 459P sesquiterpenoids (0.355) 458P tryptophan alkaloids (0.335) [a]	putative STL

	470P		287.0548 $[M + H]^+$	287.0548 → 269.0439, 241.0494, 213.0549, 161.0229, 153.0179, 135.0436, 117.0332, 89.0380, 68.9965			0.66	luteolin CCMSLIB00006381253 (0.6195) flavonoids (0.999)	
47	427N	11.0	285.0390 $[M – H]^–$	285.0390 → 267.0281, 257.0438, 241.0489, 217.0493, 199.0386, 175.0387, 171.0436, 151.0024, 149.0231, 133.0283, 132.0206, 1221.0284, 115.0176, 107.0128, 105.0338, 93.0336, 89.0383, 83.0129, 65.0022	211, 251, 265 sh, 292 sh, 345	$C_{15}H_{10}O_6$	–4.10	luteolin CCMSLIB00010012027 (0.9319) flavonoids (0.995)	luteolin

48P	495P 494P	11.2	424.1602 $[M + NH_4]^+$ 407.1336 $[M + H]^+$	407.1336 → 389.1246, 259.0967, 241.0867, 231.1010, 213.0907, 185.0960 bp, 161.0593, 157.1013, 142.0769, 141.0685, 133.0645	220, 269	$C_{20}H_{22}O_9$	0.09 0.02	– 495P sesquiterpenoids (0.724) 494P sesquiterpenoids (0.834)	putative STL
49P	513P 510P	11.3	378.1547 $[M + NH_4]^+$ 361.1280 $[M + H]^+$	378.1547 → 361.1280, 277.1064, 259.0961 bp, 241.0856, 231.1013, 213.0907, 203.1064, 185.0956, 167.0848, 161.0593, 157.1008, 142.0774, 133.0642, 115.0642, 105.0693	221	$C_{19}H_{20}O_7$	–0.08	– 513P sesquiterpenoids (0.973) 510P sesquiterpenoids (0.947)	putative STL

50	516P	11.3	317.0652 $[M + H]^+$	317.0652 → 302.0418 bp, 301.0339, 285.0391, 274.0469, 257.0438, 245.0439, 228.0412, 217.0496, 200.0466, 193.0125, 135.0178, 137.0228, 109.0278	209, 256, 267 sh, 293 sh, 356	$C_{16}H_{12}O_7$	–1.10	3-methylquercetin CCMSLIB00004718195 (0.6217) flavonoids (0.999)	quercetin 3-*O*-methyl ether
	458N		315.0494 $[M – H]^–$	315.0493 → 300.0259 bp, 271.0234, 255.0285, 243.0284, 227.0337, 215.0338, 199.0388, 187.0386, 183.0439, 171.0440, 164.0101, 148.0155, 143.0492, 135.0078, 133.0296, 120.0207, 108.0208, 107.0125			–5.02	3-*O*-methylquercetin CCMSLIB00012410990 (0.8843) flavonoids (0.999)	

51N	462N	11.4	677.1484 $[M-H]^-$	677.1486 → 515.1170 bp, 353.0858, 335.0763, 191.0549, 179.0334, 173.0441, 135.0439	221, 289, 324	$C_{34}H_{30}O_{15}$	–4.15	NCGC00169736-02 CCMSLIB00000845611 (0.9335) phenylpropanoids (C6-C3) (0.999)	3,4,5-tri-*O*-caffeoylquinic acid
52N	467N	11.5	409.1482 $[M-H]^-$	409.1483 → 277.1064 bp, 215.1059, 191.0697, 190.0620, 175.0747, 173.0594, 161.0595, 147.0802, 132.0567, 119.0852	-	$C_{20}H_{26}O_9$	–5.40	– flavonoids (0.102)	-
53N	472N	11.6	697.1385 $[M-H]^-$	697.1385 → 653.1485 bp, 491.1175, 365.0862, 287.0543, 179.0335, 161.0231, 151.0024, 135.0439, 133.0285, 125.0230	221, 287 sh, 325	$C_{33}H_{30}O_{17}$	–3.61	– flavonoids (0.952)	-

54P	533P 536P	11.7	410.1811 $[M + NH_4]^+$ 393.1543 $[M + H]^+$	410.1811 → 393.1539, 259.0962 bp, 241.0841, 231.1013, 213.0906, 203.1065, 185.0956, 161.0594, 142.0775, 133.0643, 129.0689, 105.0693	-	$C_{20}H_{24}O_8$	0.34	– 533P sesquiterpenoids (0.970) 536P sesquiterpenoids (0.791)	putative STL
55P	553P 552P	11.8	438.1757 $[M + NH_4]^+$ 421.1496 $[M + H]^+$	438.1758 → 421.1499, 403.1384 bp, 259.0962, 241.0858, 231.1016, 213.0903, 203.1065, 198.0671, 185.0956, 167.0857, 161.0593, 157.1003, 152.0614, 142.0769, 137.0593, 133.0643, 129.0696, 105.0692	220, 269	$C_{21}H_{24}O_9$	–0.25 0.64	– 553P sesquiterpenoids (0.930) 552P sesquiterpenoids (0.990)	putative STL

56P	557P 562P	11.9	392.1703 $[M + NH_4]^+$ 375.1436 $[M + H]^+$	392.1704 → 375.1437, 357.1336, 277.1069, 259.0963 bp, 241.0857, 231.1013, 213.0907, 203.1063, 185.0957, 167.0852, 161.0592, 142.0773, 133.0643, 129.0695, 115.0538, 105.0694	222, 269	$C_{20}H_{22}O_7$	–0.15 –0.61	– 557P sesquiterpenoids (0.996) 562P sesquiterpenoids (0.952)	putative STL
57	587P	12.2	271.0596 $[M + H]^+$	271.0596 → 243.0636, 153.0177 bp, 145.0273, 119.0482, 115.0537, 91.0535	220, 268, 332	$C_{15}H_{10}O_5$	–1.73	apigenin CCMSLIB00005757475 (0.5205) flavonoids (0.948)	apigenin

	486N		269.0439 $[M - H]^-$	269.0440 → 227.0337, 225.0538, 224.0474, 201.0544, 181.0648, 159.0439, 151.0024, 149.0232, 121.0282, 117.0334, 107.0128, 105.0334, 93.0331, 89.0387, 83.0130, 65.0024			–6.13	apigenin CCMSLIB00004683313 (0.9637) flavonoids (0.900)	
58N	489N	12.2	359.1120 $[M + H]^+$	359.1122 → 289.0708 bp, 151.0392, 85.0280	218, 266, 332	$C_{19}H_{20}O_7$	–4.54	– anthranilic acid alkaloids (0.070) [a]	-

59P	614P 599P	12.4	414.1312 $[M + NH_4]^+$ 397.1048 $[M + H]^+$	414.1313 → 397.1050, 277.1071, 259.0963 bp, 241.0856, 231.1014, 213.0908, 203.1063, 185.0957, 161.0593, 142.0773, 133.0644, 129.0695, 115.0537, 105.0693, 91.0536	-	$C_{19}H_{21}O_7$	–0.01 –0.55	– 614 sesquiterpenoids (0.911) 599 coumarins (0.399)	putative STL
60P	620P 643P	12.6	378.1546 $[M + NH_4]^+$ 361.1282 $[M + H]^+$	378.1547 → 361.1282, 259.0962, 241.0857, 231.1013, 213.0907, 203.1063, 185.0957, 167.0852, 161.0592, 142.0772, 129.0694, 115.0537, 105.0693, 91.0535, 77.0380	216, 269	$C_{19}H_{20}O_7$	–0.72 –0.38	– 620P sesquiterpenoids (0.950) 643P sesquiterpenoids (0.973)	putative vernodalin
61P	661P	12.8	480.1863 $[M + NH_4]^+$	480.1862 → 463.1604,	-	$C_{23}H_{26}O_{10}$	–0.29	– sesquiterpenoids	putative STL

			435.1648,					
			463.1604 [M + H]+	417.1554, 379.1388, 259.0965, 241.0859, 231.1012, 213.0908 bp, 185.0956, 161.0593, 157.1006, 142.0774, 133.0646, 129.0691, 105.0691			(0.338)	
62	688P	13.0	303.0860 [M + H]+	303.0859 → 167.0333 bp, 163.0338, 117.0333, 89.0374	222, 273, 332	$C_{16}H_{14}O_6$	–1.02	NCGC00384501-01 CCMSLIB00000848380 (0.9277) flavonoids (0.948)	eriodictyol *O*-methyl
	527N		301.0699 [M – H]–	301.0701 → 165.0181, 149.9945, 135.0439 bp, 134.0362, 121.0284, 109.0277			–6.18	blumeatin CCMSLIB00012343132 (0.9087) flavonoids (0.992)	

63P	690P	13.1	441.1503 $[M + NH_4]^+$ 424.1240 $[M + H]^+$	441.1504 → 424.1238, 378.1277, 259.0952 bp, 241.0853, 232.0733, 231.1011, 213.0906, 203.1063, 185.0956, 161.0593, 157.1010, 142.0774, 133.0640, 129.0707 424.1238 → 383.1105 bp, 231.1020, 213.0899, 185.0956, 161.0594, 142.0776	222, 269	$C_{19}H_{21}NO_{10}$	–0.27	sesquiterpenoids (0.920)	putative STL
64	693P	13.3	331.0808 $[M + H]^+$	331.0814 bp → 316.0575, 301.0340, 273.0372, 245.0427, 217.0485	222, 288, 332	$C_{17}H_{14}O_7$	–1.33	3,4'-dDimethoxy-5,7,3'-trihydroxyflavone CCMSLIB00003138441 (0.9565) coumarins (0.393) [a]	tricetin *O*-dimethyl ether

65	716P	13.8	301.0705 $[M + H]^+$	301.0705 → 286.0467, 258.0519 bp, 229.0496, 213.0545, 203.0336, 184.0519, 167.0336, 136.0514, 124.0149, 96.0201	221, 267, 347	$C_{16}H_{12}O_6$	–0.60	5,7-dihydroxy-2-(4-hydroxyphenyl)-3-methoxy-4*H*-chromen-4-one CCMSLIB00000424755 (0.1985) flavonoids (1.000)	luteolin *O*-methyl ether
	535N		299.0547 $[M – H]^–$	299.0546 → 284.0311 bp, 256.0363, 227.0336, 211.0387, 183.0438, 151.0025, 133.0283, 107.0127, 83.0128, 63.0233			–4.72	chrysoeriol CCMSLIB00012330010 (0.5476) flavonoids (0.999)	

66P	723P 722P	14.1	464.1915 $[M + NH_4]^+$ 447.1652 $[M + H]^+$	464.1914 → 447.1649, 429.1544, 259.0966 bp, 241.0855, 231.1010, 213.0904, 203.1065, 198.0671, 185.0955, 167.0851, 161.0593, 157.1011, 142.0776, 133.0643, 129.0694, 105.0695	222	$C_{23}H_{26}O_9$	–0.04 0.47	– 723P sesquiterpenoids (0.863) 722P sesquiterpenoids (0.588)	putative STL
67N	563N	14.7	393.1171 $[M + H]^+$	393.1170 → 307.0811, 235.0597 bp, 191.0701, 173.0589, 149.0599, 147.0804, 113.0234	214, 268	$C_{19}H_{22}O_9$	–5.09	– flavonoids (0.910)	-

68P	777P 770P	14.8	362.1594 $[M + NH_4]^+$ 345.1335 $[M + H]^+$	362.1594 → 345.1332, 259.0959, 241.0855, 231.1010, 213.0907, 198.0672, 185.0958 bp, 170.0718, 157.1007, 152.0616, 142.0773, 141.0695, 129,0692, 128.0617, 115.0536, 105.0695, 91.0538 345.1334 → 259.0963, 241.0855, 231.1011, 213.0906, 198.0671, 185.0957 bp, 167.0851, 152.0615, 142.0772, 129.0694, 115.0537, 105.0693, 91.0535	222, 269	$C_{19}H_{20}O_6$	–1.21 0.67	NCGC00381113 CCMSLIB00000850132 (0.8944) 777P sesquiterpenoids (0.943) 770P sesquiterpenoids (0.592)	putative hirsutinolide-type STL

69P	786P 785P	15.0	364.1753 $[M + NH_4]^+$ 347.1488 $[M + H]^+$	347.1487 → 259.0961, 241.0859, 231.1015, 213.0907, 198.0673, 185.0958 bp, 167.0851, 152.0614, 142.0771, 141.0694, 129.0694, 128.0616, 115.0537, 105.0693, 91.0535	222, 269	$C_{19}H_{22}O_6$	–0.55 –0.43	– 786P sesquiterpenoids (0.963) 785P sesquiterpenoids (0.974)	putative STL
70	794P	15.1	285.0753 $[M + H]^+$	285.0754 → 270.0520, 242.0569 bp, 213.0542, 197.0589, 187.0378, 167.0338, 153.0175, 124.0149, 119.0438, 96.0200	221, 269, 332	$C_{16}H_{12}O_5$	–1.58	5-hydroxy-2-(4-hydroxyphenyl)-7-methoxy-4*H*-chromen-4-one CCMSLIB00006410039 (0.6124) flavonoids (0.998)	apigenin *O*-methyl ether

	569N		283.0597 $[M-H]^-$	283.0594 → 268.0361, 239.0334, 211.0385, 195.0439, 183.0437, 167.0490, 151.0025, 130.0412, 117.0334, 107.0125, 83.0128, 65.0023			–5.30	genkwanin CCMSLIB00012289023 (0.8058) flavonoids (0.998)	
71N	570N	15.2	659.1747 $[M-H]^-$	659.1741 bp → 641.1644, 615.1843, 533.1435, 507.1634, 315.0496, 300.0259, 271.0232, 151.0024, 125.0233	-	$C_{35}H_{32}O_{13}$	–3.50	lignans (0.988)	-

72P	806P 805P	15.4	638.2598 $[M + NH_4]^+$ 621.2329 $[M + H]^+$	621.2329 → 603.2220, 585.2126, 557.2164, 507.1996, 345.1320, 327.1248, 281.1146, 259.0965 bp, 241.0850, 231.1014, 213.0908, 203.1057, 185.0957, 161.0591	-	$C_{34}H_{36}O_{11}$	–0.30 –0.47	806P aminosugars and aminoglycosides (0.722) [a] 805P monoterpenoids (0.704) [a]	putative STL dimer
73P	815P	15.5	738.2761 $[M + H]^+$	738.2758 → 720.2654 bp, 702.2541, 480.1874, 462.1762, 430.1859, 416.1699, 390.1547, 372.1441, 239.0965, 241.0854, 231.1011, 213.0909, 203.1061, 185.0956, 175.1108,	222, 268	$C_{38}H_{43}NO_{14}$	0.61	tryptophan alkaloids (0.118)	-

				161.0592, 157.1010				
74	813P 819P	15.6	724.2963 $[M + NH_4]^+$ 707.2669 $[M + H]^+$	707.2697 → 621.2330 bp, 603.2219, 575.2280, 413.1591, 327.1217, 309.1114, 299.1265, 281.1171, 277.1068, 259.0957, 231.1013, 213.0913, 203.0702, 185.0939, 175.0747, 147.0801	222, 268	$C_{38}H_{42}O_{13}$	– 813P –0.10 0.04 819P	aromatic polyketides (0.237) [a] triterpenoids (0.426) [a]	putative STL dimer
	579N		705.2522 $[M – H]^–$	705.2524 → 429.1528, 343.1166 bp, 299.1273, 275.0907, 255.1375, 237.1268, 231.1012, 219.0662, 217.0488, 213.0901, 211.1117, 201.0905, 185.0961, 173.0591,			–4.41	sesquiterpenoids (0.246)	

			145.0647, 123.0441					
75	821P	15.7	647.1763 $[M + H]^+$	647.1760 → 545.1423, 389.0866, 343.0809 bp, 325.0702, 287.0545, 259.0966 241.0857, 231.1012, 213.0907, 185.0955, 161.0593, 157.1007, 142.0773, 133.0644, 129.0696, 105.0692	221, 268, 343	$C_{34}H_{30}O_{13}$	0.59	– sesquiterpenoids (0.295)	putative STL dimer
	588N		645.1586 $[M – H]^–$	645.1585 → 387.0700, 341.0647, 285.0387 bp, 151.0029			0.59	– flavonoids (0.420) [a]	

76P	834P 826P	15.8	376.1752 $[M + NH_4]^+$ 359.1487 $[M + H]^+$	359.1487 → 259.0965, 241.0860, 231.1018, 213.0909, 198.0672, 185.0958 bp, 167.0852, 152.0619, 142.0773, 141.0692, 129.0693, 128.0615, 115.0536, 105.0693, 91.0535	221, 268	$C_{20}H_{22}O_6$	–0.77 –0.72	NCGC00380702-01 CCMSLIB00000856030 (0.7566) 834P sesquiterpenoids (0.927) 826P sesquiterpenoids (0.958)	putative STL
77	852P	16.0	647.1759 $[M + H]^+$	647.1760 → 629.1655, 389.0867, 343.0810, 287.0547 bp, 257.0447, 241.0859, 231.1014, 213.0908, 198.0673, 185.0957, 161.0592, 142.0771, 133.0643, 129.0693, 105.0694, 91.0546	-	$C_{34}H_{30}O_{13}$	–0.03	– sesquiterpenoids (0.920)	putative STL dimer

				645.1606 → 387.0700, 369.0595, 341.0642, 325.0698, 311.0537, 285.0387 bp, 284.0307, 281.0450, 231.1005, 175.0381					
	580N		645.1588 $[M - H]^-$				–4.01	– flavonoids (0.994) [a]	
78P	884P 883P	16.3	856.3024 $[M + NH_4]^+$	856.3033 → 839.2764, 821.2653 bp,	223, 269	$C_{42}H_{46}O_{18}$	0.16 0.23	– 884P+ oligopeptides (0.996) [a]	putative STL dimer
			839.2755 $[M + H]^+$	461.1439, 415.1391, 259.0965, 231.1019, 213.0905				883P macrolides (0.895) [a]	

79	888P	16.5	631.1813 $[M + H]^+$	631.1814 bp → 373.0915, 327.0863, 309.0755, 281.0798, 271.0601, 241.0859, 231.1012, 213.0903, 203.1061, 198.0672, 185.0959, 171.0797, 161.0591, 157.1005, 142.0774, 133.0645, 129.0689, 105.0693	-	$C_{34}H_{30}O_{12}$	0.54	– monoterpenoids (0.979) [a]	putative STL dimer
	606N		629.1638 $[M – H]^–$	629.1636 → 601.1681, 371.0747, 325.0700, 309.0753, 269.0438 bp, 268.0361			–4.21	– flavonoids (0.760) [a]	

80	893P 894P	16.6	724.2962 $[M + NH_4]^+$ 707.2702 $[M + H]^+$	724.2962 → 707.2698, 621.2332, 603.2228 bp, 517.1868, 489.1904, 277.1073, 259.0961, 257.0804, 231.1008	-	$C_{38}H_{42}O_{13}$	–0.18 0.51	– 893P saccharides (0.766) [a] 894P	putative STL dimer
	607N		705.2529 $[M – H]^–$	705.2527 → 619.2160 bp, 533.1799			–3.35	saccharides (0.319)* – aromatic polyketides (0.551) [a]	
81P	904P	16.8	740.2915 $[M + NH_4]^+$ 723.2653 $[M + H]^+$	740.2914 → 723.2653, 705.2542 bp, 637.2277, 619.2191, 259.0963, 241.0854, 231.1016, 213.0910, 185.0957, 161.0597	-	$C_{38}H_{42}O_{14}$	0.23	– saccharides (0.578) [a]	putative STL dimer

82P	917P 916P	17.0	722.2810 $[M + NH_4]^+$ 705.2542 $[M + H]^+$	722.2811 → 705.2545 bp, 603.2229, 585.2125, 557.2171, 327.1228, 309.1119, 299.1262, 281.1167, 263.1051, 259.0961, 241.0859, 231.1013, 213.0907, 203.1064, 185.0958, 161.0590, 157.1010	-	$C_{38}H_{40}O_{13}$	0.46 –0.01	– 917P monoterpenoids (0.637) [a] 916P saccharides (0.273) [a]	putative STL dimer
83P	932P	17.3	738.2755 $[M + NH_4]^+$ 721.2502 $[M + H]^+$	738.2757 → 721.2502, 635.2123 bp, 617.2008, 259.0977, 257.0805, 239.0704, 229.0862, 213.0903, 187.0753	-	$C_{38}H_{40}O_{14}$	–0.22	– aminosugars and aminoglycosides (0.847) [a]	putative vernodalidimer A

84P	937P 936P	17.4	752.2922 $[M + NH_4]^+$ 735.2657 $[M + H]^+$	752.2916 → 735.2657 bp, 459.1652, 431.1703, 259.0961, 241.0861, 231.1013, 213.0905, 203.1061, 185.0956, 161.0589	-	$C_{39}H_{42}O_{14}$	1.20	– 937P macrolides (0.821) [a] 936P monoterpenoids (0.691) [a]	putative STL dimer
85P	941P 940P	17.5	722.2810 $[M + NH_4]^+$ 705.2544 $[M + H]^+$	722.2811 → 705.2544 bp, 687.2434, 603.2221, 601.2072, 327.1245, 281.1169, 259.0969, 241.0853, 231.1017, 213.0919, 185.0959	-	$C_{38}H_{40}O_{13}$	0.35	– 941P monoterpenoids (0.199) [a] 940P monoterpenoids (0.880) [a]	putative STL dimer
86P	953P	17.6	689.2584 $[M + H]^+$	689.2592 bp → 603.2225, 557.2185, 259.0962, 241.0856, 213.0897, 185.0960, 161.0582	-	$C_{38}H_{40}O_{12}$	–1.19	monoterpenoids (0.751) [a]	putative STL dimer

87N	616N	17.6	577.2661 $[M - H]^-$	577.2662 bp → 299.0427, 277.2165, 225.0059, 206.9957, 164.9848, 152.9850, 148.9900, 134.9736, 125.0228, 94.9793, 80.9640	-	$C_{30}H_{42}O_{11}$	1.14	– glycerolipids (0.622)	-
88	959P	17.7	661.1917 $[M + H]^+$	661.1920 bp → 559.1599, 403.1022, 357.0968, 301.0704, 300.0626, 271.0599, 241.0857, 231.1014, 213.0904, 203.1062, 185.0957, 167.0853, 161.0590, 133.0642	222, 268, 341	$C_{35}H_{32}O_{13}$	0.12	– monoterpenoids (0.964)	-

	625N		659.1744 $[M - H]^-$	659.1741 → 401.0856, 383.0751, 355.0803, 339.0855, 325.0700, 312.0619, 299.0543 bp, 298.0465, 284.0309, 275.0906, 255.0283, 231.1013			–3.96	nucleosides (0.151)
89P	971P 972P	17.8	706.2858 $[M + NH_4]^+$ 689.2591 $[M + H]^+$	689.2591 bp → 603.2226, 557.2160, 327.1230, 259.0960, 241.0851,	-	$C_{38}H_{40}O_{12}$	–0.01 –0.19	– 971P aromatic polyketides (0.788) [a]	putative STL dimer
				231.1004, 213.0906, 203.1057, 185.0958, 161.0591				972P monoterpenoids (0.692) [a]	

90P	973P	17.8	742.2700 $[M + NH_4]^+$ 725.2442 $[M + H]^+$	742.2705 → 725.2442, 639.2074 bp, 361.1280, 261.0752, 259.0963, 243.0664, 241.0855, 231.1015, 215.0685, 213.0901, 185.0957	-	$C_{37}H_{40}O_{15}$	–0.73	– naphthalenes (0.462) [a]	putative STL dimer
91P	975P	17.9	299.0911 $[M + H]^+$	299.0913 bp → 284.0676, 256.0727, 241.0484, 213.0547, 167.0336, 133.0645, 124.0150	-	$C_{17}H_{14}O_5$	–0.87	di-*O*-methylapigenin CCMSLIB00006421404 (0.5961) flavonoids (1.000)	apigenin *O*-dimethyl ether
92P	984P 983P	18.1	706.2856 $[M + NH_4]^+$ 689.2588 $[M + H]^+$	689.2594 bp → 603.2232, 585.2150, 557.2162, 327.1223, 259.0962, 241.0857, 231.1015, 213.0906, 185.0957, 161.0597	-	$C_{38}H_{40}O_{12}$	–0.28 –0.61	– 984P triterpenoids (0.774) [a] 983P monoterpenoids (0.306) [a]	putative STL dimer

93P	994P	18.2	645.1972 $[M + H]^+$	645.1970 bp → 559.1591, 287.1073, 341.1019, 301.0706, 285.0756, 259.0965, 241.0858, 231.1013, 213.0905, 203.1061, 185.0956, 161.0594, 142.0773, 133.0644, 105.0689	223	$C_{35}H_{32}O_{12}$	0.82	– monoterpenoids (0.982) [a]	putative STL dimer
94P	998P 1004	18.4	706.2855 $[M + NH_4]^+$ 689.2590 $[M + H]^+$	689.2591 bp → 603.2227, 585.2123, 557.2181, 413.1592, 299.1273, 259.0960, 241.0854, 231.1006, 213.0902, 203.1058, 185.0958, 161.0591, 129.0688	-	$C_{38}H_{40}O_{12}$	–0.37 –0.31	– 998P aromatic polyketides (0.761) [a] 1004P monoterpenoids (0.788) [a]	putative STL dimer

95N	641N	18.4	579.2825 $[M - H]^-$	579.2819 bp → 299.0426, 279.2310, 225.0060, 206.0059, 164.9852, 152.9852, 148.9907, 134.9742, 94.9793, 80.9640	-	$C_{30}H_{44}O_{11}$	2.43	– glycerolipids (0.954)	-
96N	645N	18.5	559.3099 $[M - H]^-$	559.3099 → 513.3042, 277.2155 bp, 253.0913, 235.0812, 161.0444	-	$C_{28}H_{48}O_{11}$	–4.45	NCGC00380867 CCMSLIB00012420826 (0.9966) glycerolipids (1.000)	-
97P	1007P 1012P	18.6	706.2859 $[M + NH_4]^+$ 689.2595 $[M + H]^+$	689.2592 → 603.2221, 413.1591, 259.0961 bp, 241.0856, 231.1015, 213.0909, 203.1059, 185.0959, 161.0593	-	$C_{38}H_{40}O_{12}$	0.09 0.29	1007P triterpenoids (0.437) [a] 1012P monoterpenoids (0.785) [a]	putative STL dimer

98P	1010P 1009	18.7	532.348 $[M + NH_4]^+$	532.3480 → 387.2538, 353.2687 bp, 335.2581, 261.2216, 243.2106, 187.1484, 173.1325, 163.1472, 159.1153, 149.1322, 145.1011, 135.1166, 131.0856, 121.1004, 107.0851, 105.0693, 95.0847, 93.0693	-	$C_{27}H_{46}O_9$	0.08	NCGC00380867 CCMSLIB00000852864 (0.8805) glycerolipids (0.999)	-
99N	651N	18.9	555.2822 $[M – H]^–$	555.2819 bp → 299.0424, 255.2314, 225.0058, 206.9954, 164.9849, 152.9850, 148.9902, 134.9746, 125.0234,	279	$C_{28}H_{44}O_{11}$	1.64	– glycerolipids (0.966)	-

				106.9797, 94.9795, 80.9640					
100N	654N	19.5	481.2549 $[M - H]^-$	481.2553 → 253.2161, 245.0413, 227.0305, 171.0048, 152.9944 bp	-	$C_{36}H_{34}O$	2.51	– glycerophospholipids (1.000)	-
101N	664N	20.1	483.2708 $[M - H]^-$	483.2705 → 255.2313 bp, 227.0323, 152.9943	-	$C_{36}H_{36}O$	3.00	– cyclic polyketides (0.023)	-
102P	1104P 1103P	23.3	634.3950 $[M + NH_4]^+$ 617.3679 $[M + H]^+$	634.3953 → 617.3679, 599.3577, 259.0964 bp, 241.0850, 231.1007, 213.0907, 203.1068, 185.0960, 161.0592	-	$C_{35}H_{52}O_9$	0.13	– 1104P oligopeptides (0.958)[a] 1103P monoterpenoids (0.272) [a]	putative STL dimer

[a]Indicates compounds wrongly annotated or classified by GNPS or SIRIUS tools, respectively. ID: identification of the metabolite. ID node: identification of the node in the molecular networks where P represents the nodes of data obtained in the positive ionization mode and N represents the nodes of data obtained in the negative ionization mode; t_R: retention time; *m/z*: mass-to-charge ratio; $[M + H]^+$: protonated molecule; $[M - H]^-$: deprotonated molecule; $[M + NH_4]^+$: ammonium adduct; UV: maximum absorption in the ultraviolet wavelength region; STL: sesquiterpene lactones.