

Table S1 Detected chemical constituents in wastewaters from *Rosa damascena* (RDAM), *R. gallica* (RGAL), *R. centifolia* (RCEN) and *R. alba* (RALB) by UHPLC-HRMS/MS analysis.

No	Compound name	RT (min)	Found mass	Species	Formula	MS/MS (intensity)	Wastewater from			
							RDAM ¹	RGAL ¹	RCEN ¹	RALB ¹
1	Gallic acid	1.66	169.0132	[M-H] ⁻	C ₇ H ₅ O ₅	125.023 (100)	3.85	9.28	4.57	5.63
2	Glucogallin	2.67	331.0674	[M-H] ⁻	C ₁₃ H ₁₅ O ₁₀	169.0132 (100), 125.023 (60)	0.01	1.54	<0.01	0.1
3	Bis-galloyl-hexose	2.89	483.0781	[M-H] ⁻	C ₂₀ H ₁₉ O ₁₄	331.0675 (30), 313.0571 (20), 169.0131 (100), 125.0231 (75)	1.41	0.02	2.09	0.6
4	Protocatechuic acid	3.25	153.0182	[M-H] ⁻	C ₇ H ₅ O ₄	109.0280 (100)	<0.01	0.5	0.08	-
5	Bis-galloyl-hexose	3.67	483.0784	[M-H] ⁻	C ₂₀ H ₁₉ O ₁₄	331.0668 (10), 313.0569 (70), 169.0133 (100), 125.0231 (60)	0.23	-	0.42	-
6	Bis-galloyl-hexose	3.85	483.0784	[M-H] ⁻	C ₂₀ H ₁₉ O ₁₅	331.0671 (15), 313.0568 (20), 271.0462 (25), 211.0243 (30), 169.0132 (90), 125.0230 (70)	0.2	0.23	0.2	0.23
7	Corilagin	4.33	633.0739	[M-H] ⁻	C ₂₇ H ₂₁ O ₁₈	481.0622 (10), 300.9991 (100), 275.0197 (20)	0.23	-	0.45	-
8	Methylgalloyl-hexoside	4.66	345.0829	[M-H] ⁻	C ₁₄ H ₁₇ O ₁₀	183.0290 (100)	0.65	3.12	0.26	0.24

9	Protocatechuic acid glucoside	4.93	315.0726	$[M-H]^-$	$C_{13}H_{15}O_9$	153.0183 (100)	-	0.3	0.04	-
10	Proantocianidin B2	5.52	577.1357	$[M-H]^-$	$C_{30}H_{25}O_{12}$	425.0893 (10), 407.0768 (60), 425.0893 (80), 161.0232 (20), 125.0230 (100)	<0.01	0.75	0.01	-
11	Bis-galloyl-quinic acid	5.61	495.0785	$[M-H]^-$	$C_{21}H_{19}O_{14}$	343.0672 (100), 191.0553 (80), 169.0132 (80), 169.0132 (100), 125.0230 (40)	-	<0.01	-	0.3
12	Proantocianidin B-type dimer	5.92	577.1357	$[M-H]^-$	$C_{30}H_{25}O_{13}$	407.0772 (50), 289.0717 (70), 125.0231 (100)	<0.01	0.13	<0.01	0.04
13	HHDP-di-galloyl-glucose	5.96	785.0849	$[M-H]^-$	$C_{34}H_{25}O_{22}$	483.0774 (10), 300.9993 (100), 275.0202 (40), 249.0405 (30), 169.0133 (15), 125.0230 (10)	<0.01	-	0.72	-
14	Bis-galloyl-hexose	6.04	483.0785	$[M-H]^-$	$C_{20}H_{19}O_{14}$	313.0571 (20), 271.0463 (80), 211.0243 (100), 193.0135 (45), 169.0131 (80), 125.0231 (70), 107.0124 (20)	0.11	<0.01	<0.01	<0.01
15	Bis-galloyl-quinic acid	6.12	495.0785	$[M-H]^-$	$C_{21}H_{19}O_{14}$	343.0670 (70), 325.0572 (10), 191.0550 (15), 169.0133 (100), 125.0230 (40)	-	<0.01	-	0.3
16	Catechin	6.18	289.0719	$[M-H]^-$	$C_{15}H_{13}O_6$	245.0816 (50), 203.0707 (30), 179.0342 (20), 151.0389 (20), 123.0439 (40), 109.0280 (60)	0.4	5.16	0.74	2.2
17	Chlorogenic acid	6.70	353.0880	$[M-H]^-$	$C_{16}H_{17}O_9$	191.0554 (100), 179.0340 (10), 173.0446 (15), 135.0439 (10)	<0.01	<0.01	<0.01	<0.01
18	Brevifolincarboxylic acid	6.99	291.0149	$[M-H]^-$	$C_{13}H_7O_8$	247.0245 (100), 219.0293 (10), 191.0341 (20), 173.0235 (10), 145.0282 (10)	<0.01	1.08	<0.01	1.34

19	Tris-galoyl-hexose	7.02	635.0892	$[M-H]^-$	$C_{27}H_{23}O_{18}$	465.0671 (75), 421.0781 (10), 313.0570 (45), 169.0131 (100), 125.0231 (65)	1.67	-	2.26	-
20	HHDP-di-galloyl-glucose	8.29	785.0848	$[M-H]^-$	$C_{34}H_{25}O_{22}$	483.0786 (10), 300.9992 (100), 275.0202 (35), 249.0406 (25), 169.0132 (13), 125.0230 (15)	0.53	-	1.31	-
21	Epicatechin	8.66	289.0721	$[M-H]^-$	$C_{15}H_{13}O_6$	245.0092 (70), 217.0136 (20), 189.0184 (15), 173.0234 (20), 161.0233 (18), 145.0282 (35), 117.0332 (17)	<0.01	0.35	<0.01	<0.01
22	Digalloyl deoxyhexose	8.70	467.0831	$[M-H]^-$	$C_{20}H_{19}O_{13}$	423.0932 (25), 315.0726 (20), 169.0131 (40), 152.0103 (35), 125.0230 (30), 108.0202 (45)	-	-	-	0.31
23	Phenylethyl-hexoside-pentoside	8.89	461.1669	$[M+FA-H]^-$	$C_{20}H_{29}O_{12}$	415.1608 (100), 269.1029 (70), 169.0132 (15), 161.0446 (30), 101.0229 (40)	-	-	-	0.15
24	Phenylethyl-hexoside-pentoside	9.49	461.1667	$[M+FA-H]^-$	$C_{20}H_{29}O_{12}$	415.1614 (10), 191.0554 (55), 179.0552 (25), 149.0444 (80), 131.0337 (80)	2.12	-	0.48	0.49
25	1'-Monodecarboxyvaloneic acid dilactone	9.88	469.0051	$[M+FA-H]^-$	$C_{21}H_9O_{13}$	425.0151 (15), 299.9913 (100), 270.9887 (10)	<0.01	<0.01	<0.01	<0.01
26	Ellagic acid hexoside	9.92	463.0522	$[M-H]^-$	$C_{20}H_{15}O_{13}$	300.9990 (100)	-	2.41	-	-
27	Ellagic acid hexoside	10.46	463.0521	$[M-H]^-$	$C_{20}H_{15}O_{13}$	300.9992 (100)	<0.01	0.27	<0.01	<0.01
28	Phenylethyl-hexoside-pentoside	10.49	461.1666	$[M+FA-H]^-$	$C_{20}H_{29}O_{12}$	415.1609 (20), 179.0551 (20), 149.0444 (70), 131.0337 (30)	1.74	<0.01	0.05	<0.01
29	Quercetine-3-O-hexoside-hexoside	11.20	625.1409	$[M-H]^-$	$C_{27}H_{29}O_{17}$	300.0277 (100), 271.0247 (45), 255.0296 (20), 243.0296 (16)	-	-	-	6.96

30	Quercetine-3-O-hexoside-hexoside	11.42	625.1408	[M-H] ⁻	C ₂₇ H ₂₉ O ₁₇	300.0277 (100), 271.0247 (45), 255.0296 (20), 243.0296 (16)	-	-	-	6.2
31	Isorhamnetin-3-O-gentiobioside	12.40	639.1573	[M-H] ⁻	C ₂₈ H ₃₁ O ₁₇	314.0435 (60), 299.0200 (100), 271.0250 (35), 215.0345 (20)	0.32	0.75	-	0.13
32	Kaempferol-3-O-hexoside-hexoside	12.78	609.1463	[M-H] ⁻	C ₂₇ H ₂₉ O ₁₆	284.0328 (100), 255.0298 (60), 227.0346 (45)	-	-	-	0.57
33	Ellagoyl-pentoside	12.93	433.0414	[M-H] ⁻	C ₁₉ H ₁₃ O ₁₂	300.9991 (100), 271.0612 (10), 216.0057 (10)	<0.01	0.12	0.25	-
34	Kaempferol-3-O-hexoside-hexoside	13.01	609.1461	[M-H] ⁻	C ₂₇ H ₂₉ O ₁₆	284.0327 (100), 255.0296 (60), 227.0345 (40)	-	-	-	4.63
35	Quercetine-3-O-pentoside-hexoside	13.29	595.1309	[M-H] ⁻	C ₂₆ H ₂₇ O ₁₆	300.0277 (100), 271.0247 (40), 255.0297 (20), 243.0296 (10)	-	-	-	0.53
36	Ellagoyl-pentoside	13.35	433.0414	[M-H] ⁻	C ₁₉ H ₁₃ O ₁₂	299.9911 (100), 216.0060 (10)	0.09	0.09	0.06	-
37	Ellagic acid	13.56	300.9988	[M-H] ⁻	C ₁₄ H ₅ O ₈	300.9990 (100), 283.9963 (90), 257.0085 (20), 245.0088 (5), 229.0138 (70), 201.0183 (80) 185.0236 (70), 173.0233 (75), 157.0283 (45), 145.0282 (75)	10.98	16.88	12.89	14.12
38	Rutin	13.80	609.1463	[M-H] ⁻	C ₂₇ H ₂₉ O ₁₆	300.0279 (100), 271.0251 (50), 255.0300 (25), 243.0297 (15), 151.0024 (10)	<0.01	-	-	<0.01
39	Hyperoside	13.89	463.0883	[M-H] ⁻	C ₂₁ H ₁₉ O ₁₂	300.0274 (100), 271.0251 (45), 255.0300 (20), 243.0297 (15), 151.0025 (10)	5.67	4.69	5.8	3.68
40	Miquelianin	13.97	477.0671	[M-H] ⁻	C ₂₁ H ₁₇ O ₁₃	301.0356 (100), 178.9977 (15), 151.0024 (25)	<0.01	<0.01	<0.01	8.64

41	Isoquercitrin	14.25	463.0883	[M-H] ⁻	C ₂₁ H ₁₉ O ₁₂	300.0275 (100), 271.0252 (50), 255.0300 (25), 243.0298 (15), 151.0025 (10)	5.98	0.43	5.89	3.57
42	Quercetin-3-O-pentoside	15.01	433.0777	[M-H] ⁻	C ₂₀ H ₁₇ O ₁₁	300.0276 (100), 271.0247 (50), 255.0296 (20), 243.0297 (15), 151.0025 (10)	0.5	-	1.82	0.12
43	Quercetin-3-O-galloyl-hexoside	15.11	615.0997	[M-H] ⁻	C ₂₈ H ₂₃ O ₁₆	301.0356 (100), 193.0138 (10), 178.9976 (15), 151.0025 (30)	0.58	0.37	-	0.16
44	Kaempferol-3-O-pentoside-hexoside	15.20	579.1360	[M-H] ⁻	C ₂₆ H ₂₇ O ₁₅	284.0327 (100), 255.0297 (55), 227.0346 (40)	-	-	-	0.36
45	Kaempferol-3-O-galactoside	15.48	447.0933	[M-H] ⁻	C ₂₁ H ₁₉ O ₁₁	284.0328 (85), 255.0297 (80), 227.0346 (75)	4.63	1.6	0.95	1.33
46	Kaempferol-hexoside-methylpentoside	15.76	593.1514	[M-H] ⁻	C ₂₇ H ₂₉ O ₁₅	285.0404 (100), 255.0298 (45), 227.0345 (30)	2.07	-	<0.01	<0.01
47	Avicularin	15.78	433.0776	[M-H] ⁻	C ₂₀ H ₁₇ O ₁₁	301.0351 (100), 271.0252 (45), 255.0301 (25), 243.0298 (15), 178.9977 (10), 151.0025 (15)	<0.01	3.09	5.18	4.3
48	Quercetin-hexoside-methylpentoside	15.90	609.1460	[M-H] ⁻	C ₂₇ H ₂₉ O ₁₆	301.0354 (100), 271.0248 (30), 255.0298 (20), 243.0296 (10), 178.9979 (15), 151.0025 (30)	1.09	<0.01	-	-
49	Kaempferol-3-O-glucoside	16.24	447.0933	[M-H] ⁻	C ₂₁ H ₁₉ O ₁₁	284.0326 (78), 255.0297 (80), 227.0346 (78), 183.0444 (10)	16.53	1.02	2.98	6
50	Kaempferol-galloyl-hexoside	17.22	599.1047	[M-H] ⁻	C ₂₈ H ₂₃ O ₁₅	313.0568 (15), 285.0406 (100), 151.0024 (10)	1.29	-	-	0.23
51	Kaempferol-pentoside	17.36	417.0828	[M-H] ⁻	C ₂₀ H ₁₇ O ₁₀	284.0326 (85), 255.0298 (80), 227.0346 (83), 183.0444 (10)	2.15	<0.01	0.84	<0.01

52	Eschweilenol A	17.49	425.0152	[M-H] ⁻	C ₂₀ H ₉ O ₁₁	299.9911 (100), 270.9887 (10), 216.0058 (10)	-	4.72	1.2	2.78
53	Kampferol-3-O-arabinoside	18.01	417.0828	[M-H] ⁻	C ₂₀ H ₁₇ O ₁₀	284.0325 (100), 255.0298 (95), 227.0346 (90), 183.0444 (10)	5.32	2.49	2.49	2.81
54	Kaempferol-hexoside-methylpentoside	18.08	593.1514	[M-H] ⁻	C ₂₇ H ₂₉ O ₁₅	285.0404 (100), 229.0504 (10)	<0.01	<0.01	-	-
55	Kaempferol-3-O-rhamnoside	18.78	431.0983	[M-H] ⁻	C ₂₁ H ₁₉ O ₁₀	285.0402 (100), 255.0297 (65), 227.0346 (60), 183.0445 (10)	5.4	0.81	4.6	1.24
56	Quercetin-3-acetyl-hexoside-methylpentoside	19.50	651.1574	[M-H] ⁻	C ₂₉ H ₃₁ O ₁₇	301.0354 (100), 271.0251 (35), 255.0299 (20), 243.0296 (10), 178.9975 (20), 151.0024 (35)	0.62	0.12	-	-
57	Kaempferol-galloyl-pentose	19.60	569.0943	[M-H] ⁻	C ₂₇ H ₂₁ O ₁₄	285.0404 (100), 229.0503 (10)	<0.01	-	0.05	-
58	Quercetin-p-coumaroyl-hexoside	20.91	609.1255	[M-H] ⁻	C ₃₀ H ₂₅ O ₁₄	463.0883 (65), 300.0275 (100), 271.0252 (50), 255.0300 (25), 243.0297 (15), 178.9975 (10), 151.0024 (15)	0.19	0.17	0.7	0.35
59	Quercetin	21.33	301.0355	[M-H] ⁻	C ₁₅ H ₉ O ₇	178.9977 (25), 151.0025 (70), 121.0281 (20), 107.0124 (25), 65.0017 (25)	-	0.16	1.25	0.55
60	Kaempferol-3-acetyl-hexoside-methylpentoside	21.76	635.1618	[M-H] ⁻	C ₂₉ H ₃₁ O ₁₆	285.0402 (100), 229.0503 (10)	0.06	<0.01	-	-
61	Eschweilenol B isomer	21.82	422.9996	[M-H] ⁻	C ₂₀ H ₇ O ₁₁	376.9933 (70), 311.0203 (70), 299.9909 (70), 293.0093 (65), 270.9884 (100)	<0.01	1.83	2.95	2.07
62	Kaempferol-galloyl-pentose	22.25	569.0941	[M-H] ⁻	C ₂₇ H ₂₁ O ₁₄	285.0405 (100), 229.0504 (10)	0.16	-	<0.01	-

63	Eschweilenol B isomer	22.71	422.9999	[M-H] ⁻	C ₂₀ H ₇ O ₁₁	376.9946 (70), 311.0197 (100), 299.9907 (55), 293.0095 (85), 270.9887 (85)	<0.01	0.21	0.26	0.39
64	Kaempferol-p-coumaroyl-hexoside	23.17	593.1303	[M-H] ⁻	C ₃₀ H ₂₅ O ₁₃	447.0940 (10), 285.0404 (100), 255.0299 (55), 227.0346 (45), 145.0285 (10)	2.72	0.83	1.09	1.14
65	Kaempferol-p-coumaroyl-hexoside	23.66	593.1305	[M-H] ⁻	C ₃₀ H ₂₅ O ₁₃	447.0932 (10), 285.0402 (100), 255.0297 (55), 227.0346 (40), 145.0282 (10)	0.21	-	-	0.1
66	Kaempferol	25.57	285.0407	[M-H] ⁻	C ₁₅ H ₉ O ₆	285.0407 (100), 255.0288 (25), 239.0343 (40), 227.0351 (30), 211.0394 (35), 185.0599 (50), 159.0438 (45), 143.0489 (60), 135.0072 (20)	0.56	-	0.2	0.04

¹ The values are calculated by normalization method and represent the percent of the area of the base peak. The raw data were processed with Thermo Scientific Freestyle software package.