

Supplementary data for article:

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Supplementary Table 2: Gas chromatographic and mass spectral data

peak no.	retention index RI		mass spectrometric fragmentation <i>m/z (relative intensity)</i>	identified as
	measured	authentic reference*		
1	917	920	110 ([M+2] ⁺ , 5), 108 (M ⁺ ,100), 82 (20), 80 (22), 54 (34)	1,4-benzoquinone
2	977	978	95 ([M+1] ⁺ , 5), 94 (M ⁺ ,100), 66 (16), 65 (14), 57 (5), 55 (3)	phenol
3	1015	1014	122 (M ⁺ , 100), 94 (54), 82 (28), 68 (16), 66 (22), 54 (31)	2-methyl-1,4-benzoquinone
4	1071	1071	108 (M ⁺ , 100), 107 (82), 90 (6), 80 (6), 79 (11), 77 (13)	<i>p</i> -cresol
5	1108	1103 ^a	136 (M ⁺ , 77), 108 (100), 107 (38), 82 (24), 79 (40), 65 (7), 54 (31)	2-ethyl-1,4-benzoquinone
6	1120	1120	138 (M ⁺ ,100), 110 (11), 83 (15), 82 (40), 81 (20), 55 (11), 54 (10)	2-hydroxy-3-methyl-1,4-benzoquinone
7	1177	1178 ^b	122 (M ⁺ , 36), 108 (9), 107 (100), 91 (6), 77 (16), 65 (5), 51 (4)	<i>p</i> -ethylphenol
8	1182	1183	152 (M ⁺ , 100), 151 (20), 137 (5), 123 (7), 122 (47), 109 (13), 94 (5), 83 (8), 82 (12), 81 (7), 67 (8), 66 (15), 54 (10), 53 (12)	2-methoxy-3-methyl-1,4-benzoquinone
9	1191	-	152 (M ⁺ , 100), 137 (3), 123 (3), 109 (6), 96 (7), 95 (14), 83 (8), 82 (13), 81 (12), 78 (13), 69 (18), 55 (11)	unidentified
10	1243	-	166 (M ⁺ , 100), 151 (70), 138 (10), 133 (17), 123 (62), 121 (13), 95 (18), 82 (9), 79 (11), 69 (10), 67 (11), 54 (10)	2-ethyl-3-methoxy-1,4-benzoquinone
11	1245	-	138 (M ⁺ , 61), 123 (14), 110 (64), 108 (62), 95 (37), 82 (38), 69 (100), 54 (35), 53 (28), 52 (23)	2-methoxy-1,4-benzoquinone
12	1317	-	150 (M ⁺ , 16), 122 (69), 94 (37), 82 (100), 68 (18), 66 (43), 65 (9), 54 (93), 53 (19), 40 (24)	unidentified
13	1319	1320	168 (M ⁺ , 64), 153 (31), 125 (17), 123 (100), 97 (13), 95 (15), 82 (36), 69 (65), 54 (37), 53 (13)	2,3-dimethoxy-1,4-benzoquinone
14	1341	1341	124 (M ⁺ ,100), 123 (44), 107 (13), 105 (6), 95 (29), 77 (15), 69 (4), 67 (13), 57 (16)	2-methylhydroquinone
15	1341	-	152 (M ⁺ ,78), 137 (15), 124 (41), 123 (36), 122 (29), 109 (11), 84 (10), 69 (100), 66 (24), 56 (4)	2-methoxy-5-methyl-1,4-benzoquinone
16	1346	-	152 (M ⁺ , 70), 137 (14), 124 (87), 123 (18), 122 (68), 109 (22), 96 (16), 94 (12), 81 (8), 69 (100), 66 (28), 53 (26)	2-methoxy-6-methyl-1,4-benzoquinone
17	1349	-	151 (M ⁺ ,62), 120 (20), 119 (100), 92 (28), 91 (4), 65 (4), 63 (5)	unidentified
18	1375	1373 ^c	170 (M ⁺ , 100), 155 (50), 123 (6), 112 (14), 109 (24), 95 (5), 81 (4), 57 (16)	2,3-dimethoxyhydroquinone
19	1386	1390 ^c	152 (M ⁺ , 100), 151 (88), 136 (9), 121 (15), 66 (13), 65 (11)	2-methyl-3,4-methylenedioxyphenole
20	1411	-	154 (M ⁺ ,100), 139 (27), 128 (13), 126 (50), 111 (15), 98 (5), 97 (5), 85 (1), 82 (75), 72 (15), 57 (7), 54 (51)	2-hydroxy-3-methoxy-1,4-benzoquinone
21	1421	1420	182 (M ⁺ , 84), 167 (45), 153 (22), 139 (25), 137 (100), 136 (20), 121 (10), 111 (20), 108 (6), 96 (11), 83 (39), 69 (17), 68 (21),	2,3-dimethoxy-5-methyl-1,4-benzoquinone

22	1422	-	67 (9) 165 (M ⁺ , 100), 134 (17), 133 (26), 132 (36), 116 (5), 106 (8), 105 (49), 104 (44), 91 (3), 78 (8), 77 (15), 66 (4)	unidentified
23	1436	1409 ^a	138 (M ⁺ , 57), 124 (8), 123 (100), 91 (5), 77 (6), 67 (9), 65 (6), 55 (5)	2-ethyl-hydroquinone
24	1449	-	184 (M ⁺ , 100), 182 (8), 169 (71), 154 (11), 141 (12), 137 (20), 126 (41), 123 (19), 69 (11), 83 (12), 69 (23)	dimethoxy-methylhydroquinone /isomer 1
25	1455	1456	152 (M ⁺ , 58), 122 (6), 121 (100), 93 (12), 92 (1), 65 (6)	methylparaben
26	1465	-	166 (M ⁺ , 93), 165 (20), 152 (9), 151 (100), 121 (23), 77 (10), 65 (9), 53 (10)	2,3,5,6-tetramethylhydroquinone
27	1499	-	184 (M ⁺ , 50), 169 (100), 141 (7), 139 (2), 127 (2), 123 (22), 113 (9), 87 (20), 85 (15), 69 (4), 68 (3), 54 (6)	dimethoxy-hydroxy-benzoquinone isomer
27	1511	-	182 (M ⁺ , 100), 167 (13), 149 (14), 139 (79), 137 (8), 111 (32), 109 (24), 96 (11), 94 (15), 83 (90), 69 (79), 67 (21), 55 (14), 53 (22), 41 (10)	2,6-dimethoxy-3-methyl-1,4-benzoquinone
29	1518	-	168 (M ⁺ , 100), 153 (23), 140 (70), 125 (23), 112 (9), 97 (14), 96 (12), 85 (24), 72 (11), 68 (34)	2-hydroxy-3-methoxy-5-methyl-1,4-benzoquinone
30	1522	-	196 (M ⁺ , 97), 182 (22), 181 (59), 153 (31), 151 (100), 125 (33), 123 (18), 97 (57), 82 (26), 69 (24), 53 (31)	2,3-dimethoxy-5,6-dimethyl-1,4-benzoquinone
31	1532	-	214 (M ⁺ , 73), 169 (19), 168 (37), 167 (11), 155 (8), 138 (45), 137 (15), 136 (15), 127 (100), 114 (8), 99 (22), 68 (16), 59 (24)	unidentified
32	1535	-	199 ([M+1] ⁺ , 10), 198 (M ⁺ , 90), 184 (9), 183 (100), 168 (24), 151 (5), 140 (5), 123 (9), 69 (5)	2,3-dimethoxy-5,6-dimethylhydroquinone
33	1598	-	200 (M ⁺ , 100), 185 (15), 151 (50), 139 (4), 123 (18), 85 (2), 69 (4)	unidentified
34	1606	-	198 (M ⁺ , 100), 183 (83), 165 (27), 155 (16), 153 (10), 152 (5), 137 (32), 127 (20), 123 (4), 109 (7), 99 (27), 96 (7), 87 (22), 83 (5), 72 (3), 68 (10)	dimethoxy-hydroxy-methyl-benzoquinone isomer 1
35	1653	-	184 (M ⁺ , 100), 182 (28), 169 (43), 141 (54), 139 (34), 126 (33), 111 (20), 83 (37), 69 (56), 67 (19), 53 (21)	dimethoxy-methylhydroquinone isomer 2
36	1680	-	198 (M ⁺ , 100), 183 (21), 180 (3), 170 (7), 165 (7), 155 (26), 152 (4), 140 (4), 137 (4), 127 (15), 125 (5), 112 (3), 109 (8), 99 (17), 85 (14), 83 (14), 72 (6)	dimethoxy-hydroxy-methyl-benzoquinone isomer 2
37	1691	-	198 (M ⁺ , 100), 183 (69), 180 (7), 170 (32), 169 (26), 165 (8), 155 (12), 151 (6), 127 (14), 125 (43), 112 (9), 109 (4), 99 (27), 85 (33), 83 (44), 82 (4), 72 (4), 67 (11)	dimethoxy-hydroxy-methyl-benzoquinone isomer 3

*Authentic standards (materials and methods) were used for index-calculation. In cases where no standards were available, we compared the RIs measured for particular secretion components to RIs reported in literature, as ^aRocha et al. (2013), ^bEl-Sayed et al. (2005), ^cVujisić et al. (2011).