

**Table S1:** sample list (wine)

<b>Number</b>	<b>Colour</b>	<b>Cultivar</b>	<b>production</b>	<b>Vintage</b>	<b>Origin</b>
1	W	Welschriesling	Conventional	14	Burgenland
2	W	Welschriesling	Conventional	14	Lower Austria
3	W	Welschriesling	Conventional	14	Lower Austria
4	W	Chardonnay	Conventional	13	Vienna
5	W	Welschriesling	Conventional	14	Lower Austria
6	W	Welschriesling	Conventional	14	Lower Austria
7	W	Welschriesling	Conventional	14	Burgenland
8	W	Welschriesling	Conventional	14	Burgenland
9	W	Welschriesling	Conventional	14	Burgenland
10	W	Welschriesling	Conventional	14	Styria
11	W	Chardonnay	Conventional	12	Lower Austria
12	W	Chardonnay	Conventional	14	Burgenland
13	W	Rheinriesling	Conventional	16	Styria
14	W	Gelber Muskateller	Conventional	14	Styria
15	W	Chardonnay	Conventional	14	Burgenland
16	W	Rotgipfler	Conventional	13	Lower Austria
17	W	Chardonnay	organic	15	Burgenland
18	W	Welschriesling	Conventional	14	Styria
19	W	Roter Veltliner	Conventional	14	Lower Austria
20	W	Rheinriesling	Conventional	14	Styria
21	W	Chardonnay	Conventional	14	Styria
22	W	Sauvignon blanc	Conventional	14	Styria
23	W	Traminer	Conventional	14	Styria
24	W	Rheinriesling	Conventional	14	Lower Austria
25	W	Weißburgunder	Conventional	14	Styria
26	W	GT	Conventional	14	Lower Austria
27	W	Chardonnay	Conventional	14	Lower Austria
28	W	Sauvignon blanc	Conventional	14	Styria
29	W	Rheinriesling	organic	13	Lower Austria
30	W	Chardonnay	Conventional	14	Kärnten
31	W	Sauvignon blanc	Conventional	14	Lower Austria
32	W	Chardonnay	Conventional	14	Burgenland

33	W	Weißburgunder	Conventional	14	Lower Austria
34	Rosé	Cabernet Sauvignon	Conventional	14	Lower Austria
35	W	Welschriesling	Conventional	14	Styria
36	W	Weißburgunder	Conventional	13	Lower Austria
37	W	Grüner Veltliner	biodynamic	14	Styria
38	W	Grüner Veltliner	Conventional	14	Styria
39	W	Grüner Veltliner	Conventional	14	Styria
40	W	Grüner Veltliner	Conventional	14	Styria
41	W	Weißburgunder	Conventional	14	Burgenland
42	W	Chardonnay	Conventional	14	Styria
43	W	Chardonnay	Conventional	14	Burgenland
44	W	Sauvignon blanc	Conventional	14	Burgenland
45	W	Viennaer Gemischter Satz	Conventional	14	Vienna
46	W	Rotgipfler	Conventional	13	Lower Austria
47	W	Grüner Veltliner	Conventional	13	Lower Austria
48	W	Grüner Veltliner	Conventional	13	Lower Austria
49	W	Welschriesling	Conventional	13	Burgenland
50	W	Welschriesling	Conventional	13	Lower Austria
51	W	Welschriesling	Conventional	13	Lower Austria
52	W	Grüner Veltliner DAC	Conventional	13	Lower Austria
53	W	Chardonnay	Conventional	13	Lower Austria
54	W	Chardonnay	Conventional	13	Burgenland
55	W	Chardonnay	Conventional	13	Vienna
56	W	Grüner Veltliner	Conventional	13	Lower Austria
57	W	Chardonnay	Conventional	13	Burgenland
58	W	Grüner Veltliner	Conventional	13	Lower Austria
59	W	Welschriesling	Conventional	13	Lower Austria
60	W	Muskat Ottonellrillon	Conventional	13	Styria
61	W	Grüner Veltliner DAC	Conventional	14	Lower Austria
62	W	Grüner Veltliner DAC	Conventional	13	Lower Austria
63	W	Grüner Veltliner	Conventional	13	Lower Austria
64	W	Grüner Veltliner	Conventional	13	Lower Austria
65	W	Grüner Veltliner	Conventional	12	Lower Austria
66	W	Grüner Veltliner	Conventional	13	Lower Austria
67	Rosé	Zweigelt	Conventional	13	Lower Austria

68	W	Grüner Veltliner	Conventional	13	Lower Austria
69	W	Chardonnay	Conventional	13	Lower Austria
70	W	Grüner Veltliner DAC	Conventional	13	Lower Austria
71	W	Chardonnay	Conventional	13	Lower Austria
72	W	Grüner Veltliner	Conventional	13	Lower Austria
73	W	Cuvée	Conventional	13	Lower Austria
74	W	Traminer Beereauslese	Conventional	15	Lower Austria
75	W	Muskat Otonell	Conventional	13	Burgenland
76	W	Muskat Otonell	Conventional	13	Styria
77	W	Chardonnay	Conventional	13	Lower Austria
78	W	Chardonnay	Conventional	12	Burgenland
79	W	Chardonnay	Conventional	11	Lower Austria
80	W	Chardonnay	Conventional	13	Lower Austria
81	W	Chardonnay	Conventional	13	Lower Austria
82	W	Chardonnay	Conventional	12	Lower Austria
83	W	Welschriesling	Conventional	13	Burgenland
84	W	Welschriesling	Conventional	13	Burgenland
85	Rosé	Zweigelt	Conventional	13	Lower Austria
86	W	Grüner Veltliner	Conventional	13	Lower Austria
87	W	Grüner Veltliner	Conventional	13	Lower Austria
88	W	Grüner Veltliner	Conventional	13	Lower Austria
89	W	Grüner Veltliner	Conventional	14	Lower Austria
90	W	Grüner Veltliner	Conventional	13	Lower Austria
91	W	Traminer	organic	13	Burgenland
92	W	Cuvée	Conventional	13	Burgenland
93	W	Sauvignon blanc	Conventional	13	Lower Austria
94	W	Chardonnay	Conventional	13	Lower Austria
95	W	Neuburger	Conventional	13	Burgenland
96	W	Grüner Veltliner	organic	13	Lower Austria
97	W	Grüner Veltliner	Conventional	13	Lower Austria
98	W	Grüner Veltliner	Conventional	13	Lower Austria
99	W	Grüner Veltliner	Conventional	13	Lower Austria
100	W	Chardonnay	Conventional	13	Lower Austria
101	W	Chardonnay	Conventional	13	Lower Austria
102	W	Chardonnay	Conventional	13	Lower Austria

103	W	Chardonnay	Conventional	13	Lower Austria
104	W	Chardonnay	Conventional	13	Lower Austria
105	W	Chardonnay	Conventional	13	Burgenland
106	W	Chardonnay	Conventional	13	Burgenland
107	W	Grüner Veltliner	Conventional	13	Lower Austria
108	W	Grüner Veltliner	Conventional	18	Lower Austria
109	W	Grüner Veltliner	Conventional	18	Lower Austria
110	W	Grüner Veltliner	Conventional	18	Lower Austria
111	W	Grüner Veltliner	Conventional	18	Lower Austria
112	W	Grüner Veltliner	Conventional	18	Vienna
113	W	Gemischter Satz	Conventional	18	Lower Austria
114	W	Gelber Muskateller	Conventional	18	Lower Austria
115	W	Welschriesling	Conventional	18	Lower Austria
116	W	Grüner Veltliner	Conventional	18	Lower Austria
117	W	Gemischter Satz	Conventional	18	Vienna
118	W	Grüner Veltliner	Conventional	18	Lower Austria
119	R	Zweigelt/ME	Conventional	17	Lower Austria
120	R	Zweigelt/ME	Conventional	18	Lower Austria
121	R	Zweigelt	Conventional	18	Lower Austria
122	R	Zweigelt	organic	18	Lower Austria
123	W	Weißburgunder	organic	17	Lower Austria
124	R	Zweigelt	Conventional	16	Lower Austria
125	W	Grüner Veltliner	Conventional	18	Lower Austria
126	R	Zweigelt	Conventional	17	Lower Austria
127	R	Merlot	Conventional	16	Lower Austria
128	W	Grüner Veltliner	Conventional	17	Lower Austria
129	W	Grüner Veltliner	Conventional	17	Lower Austria
130	W	Grüner Veltliner	Conventional	17	Lower Austria
131	W	Grüner Veltliner	Conventional	18	Lower Austria
132	W	Grüner Veltliner	organic	18	Lower Austria
133	W	Grüner Veltliner	Conventional	18	Lower Austria
134	W	Grüner Veltliner	Conventional	18	Lower Austria
135	W	Grüner Veltliner	Conventional	15	Lower Austria
136	W	Weißburgunder	Conventional	17	Lower Austria
137	W	Chardonnay	Conventional	17	Lower Austria

138	W	Grüner Veltliner	Conventional	17	Lower Austria
139	W	Gelber Muskateller	Conventional	17	Lower Austria
140	W	Welschriesling	Conventional	17	Lower Austria
141	W	Weißburgunder	Conventional	18	Lower Austria
142	W	Weißburgunder	Conventional	18	Lower Austria
143	W	Weißburgunder	Conventional	18	Lower Austria
144	W	Weißburgunder	Conventional	18	Lower Austria
145	W	Weißburgunder	Conventional	18	Lower Austria
146	W	Weißburgunder	Conventional	18	Lower Austria
147	W	Grüner Veltliner	Conventional	17	Lower Austria
148	W	Grüner Veltliner	Conventional	17	Lower Austria
149	W	Weißburgunder	Conventional	17	Vienna
150	W	Gelber Muskateller	Conventional	17	Lower Austria
151	Rosé	Syrah	Conventional	17	Lower Austria
152	R	Zweigelt	Conventional	16	Lower Austria
153	W	Grüner Veltliner	Conventional	17	Lower Austria
154	W	Grüner Veltliner	Conventional	17	Lower Austria
155	R	Zweigelt	Conventional	17	Lower Austria
156	W	Grüner Veltliner	organic	17	Lower Austria
157	W	Grüner Veltliner	Conventional	17	Lower Austria
158	W	Welschriesling	Conventional	17	Lower Austria
159	W	Syrah	Conventional	17	Lower Austria
160	R	Zweigelt	Conventional	16	Lower Austria
161	W	Gelber Muskateller	Conventional	17	Lower Austria
162	W	Weißburgunder	Conventional	17	Lower Austria
163	W	Welschriesling	Conventional	17	Lower Austria
164	W	Grüner Veltliner	biodynamic	17	Lower Austria
165	W	Müller Thurgau	Conventional	17	Lower Austria
166	W	Chardonnay	Conventional	17	Lower Austria
167	W	Gelber Muskateller	Conventional	17	Lower Austria
168	W	Grüner Veltliner	organic	17	Lower Austria
169	W	Grüner Veltliner	Conventional	17	Vienna
170	W	Gelber Muskateller	organic	17	Lower Austria
171	W	Sauvignon blanc	Conventional	17	Vienna
172	W	Grüner Veltliner	Conventional	17	Lower Austria

173	W	Rheinriesling	Conventional	17	Vienna
174	W	Gemischter Satz	Conventional	17	Vienna
175	W	Rheinriesling	Conventional	17	Vienna
176	W	Grüner Veltliner	Conventional	17	Lower Austria
177	W	Müller Thurgau	Conventional	17	Lower Austria
178	W	Grüner Veltliner	Conventional	17	Lower Austria
179	W	Grüner Veltliner	Conventional	17	Lower Austria
180	W	Gelber Muskateller	organic	17	Lower Austria
181	W	Grüner Veltliner	Conventional	17	Lower Austria
182	W	Grüner Veltliner	Conventional	17	Lower Austria
183	W	Sauvignon blanc	Conventional	17	Lower Austria
184	W	Grüner Veltliner	Conventional	17	Lower Austria
185	W	Roter Veltliner	Conventional	17	Lower Austria
186	W	Syrah	Conventional	17	Styria
187	W	Sauvignon blanc	organic	17	Lower Austria
188	W	Grüner Veltliner	Conventional	17	Lower Austria
189	W	Grüner Veltliner	Conventional	17	Lower Austria
190	W	Chardonnay	Conventional	17	Lower Austria
191	W	Grüner Veltliner	Conventional	17	Lower Austria
192	Rosé	Zweigelt	Conventional	17	Lower Austria
193	R	Zweigelt	Conventional	17	Lower Austria
194	W	Welschriesling	Conventional	17	Lower Austria
195	W	Weißburgunder	Conventional	17	Styria
196	W	Grüner Veltliner	Conventional	17	Lower Austria
197	R	Sankt Laurent	Conventional	17	Lower Austria
198	R	Zweigelt	Conventional	15	Lower Austria
199	R	Cabernet Sauvignon	Conventional	17	Lower Austria
200	R	Merlot	Conventional	17	Lower Austria
201	R	Zweigelt	Conventional	17	Lower Austria
202	W	Gemischter Satz	Conventional	17	Lower Austria
203	W	Rheinriesling	organic	17	Lower Austria
204	W	Welschriesling	Conventional	17	Lower Austria
205	W	Grüner Veltliner	Conventional	17	Lower Austria
206	W	Welschriesling	Conventional	17	Lower Austria
207	W	Grüner Veltliner	Conventional	17	Lower Austria

208	W	Grüner Veltliner	Conventional	17	Lower Austria
209	W	Grüner Veltliner	Conventional	17	Lower Austria
210	W	Chardonnay	Conventional	17	Lower Austria
211	R	Sankt Laurent	Conventional	16	Lower Austria
212	Rosé	Blauburgunder	Conventional	17	Lower Austria
213	W	Chardonnay	Conventional	17	Lower Austria
214	W	Grüner Veltliner	Conventional	16	Lower Austria
215	W	Grüner Veltliner	Conventional	17	Lower Austria
216	R	Cuvée	Conventional	17	Lower Austria
217	R	Blaufränkisch	Conventional	17	Lower Austria
218	W	Welschriesling	Conventional	17	Lower Austria
219	W	Rheinriesling	Conventional	17	Lower Austria
220	W	Zierfandler/Rotgipfler	Conventional	17	Lower Austria
221	W	Zierfandler/Rotgipfler	Conventional	17	Lower Austria
222	W	Rheinriesling	organic	17	Lower Austria
223	R	Rösler	organic	15	Lower Austria
224	W	Grüner Veltliner	Conventional	17	Lower Austria
225	W	Chardonnay	Conventional	17	Lower Austria
226	W	Chardonnay	Conventional	17	Lower Austria
227	W	Grüner Veltliner	Conventional	17	Lower Austria
228	W	Grüner Veltliner	Conventional	17	Lower Austria
229	W	Sauvignon blanc	Conventional	17	Styria
230	W	Grüner Veltliner	Conventional	17	Lower Austria
231	R	Zweigelt	Conventional	17	Lower Austria
232	R	Zweigelt	Conventional	17	Lower Austria
233	R	Cuvée	Conventional	17	Lower Austria
234	W	Grüner Veltliner	Conventional	17	Lower Austria
235	W	Rheinriesling	organic	17	Lower Austria
236	R	Merlot	Conventional	16	Lower Austria
237	W	Grüner Veltliner	Conventional	17	Lower Austria
238	Rosé	Zweigelt	organic	17	Lower Austria
239	W	Sauvignon blanc	Conventional	17	Lower Austria
240	R	Zweigelt	Conventional	16	Lower Austria
241	R	Cabernet Sauvignon	Conventional	17	Burgenland
242	R	Cabernet Sauvignon	Conventional	15	Burgenland

243	R	Merlot	Conventional	15	Burgenland
244	R	Zweigelt	Conventional	15	Burgenland
245	R	Blauburgunder	Conventional	15	Burgenland
246	R	Blaufränkisch	Conventional	16	Burgenland
247	R	Blaufränkisch	Conventional	15	Burgenland
248	R	Blaufränkisch	organic	16	Burgenland
249	R	Blaufränkisch	biodynamic	15	Burgenland
250	R	Blauburger	Conventional	17	Burgenland

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**Table S2:** sample list (must and fermenting must: all conventional)

Number	Colour	Cultivar	Kind of product	Vintage	Origin
1	W	Grüner Veltliner	must	19	Burgenland
2	W	Grüner Veltiner	must	19	Burgenland
3	W	Grüner Veltliner	must	19	Lower Austria
4	W	Grüner Veltliner	must	19	Vienna
5	W	Welschriesling	must	19	Burgenland
6	W	Welschriesling	must	19	Styria
7	W	Welschriesling	must	19	Styria
8	R	Zweigelt	must	19	Burgenland
9	R	Zweigelt	must	19	Burgenland
10	R	Zweigelt	must	19	Burgenland
11	R	Zweigelt	must	19	Burgenland
12	W	Chardonnay	must	19	Burgenland
13	W	Cuvée	must	19	Burgenland
14	W	Gemischter Satz	must	19	Vienna
15	W	Chardonnay	must	19	Burgenland
16	R	Blauer Portugieser	must	19	Lower Austria
17	R	Blauer Portugieser	must	19	Lower Austria
18	W	Chardonnay	must	19	Burgenland
19	W	Cuvée	must	19	Burgenland
20	R	Blauer Portugieser	must	19	Lower Austria
21	R	Blauburger	must	19	Lower Austria
22	R	Blauburger	must	19	Lower Austria
23	R	Cuvée	must	19	Burgenland
24	R	Cuvée	must	19	Burgenland
25	R	Cuvée	must	19	Burgenland
26	W	Traminer	must	19	Lower Austria
27	W	Chardonnay	must	19	Burgenland
28	W	Sauvignon blanc	must	19	Lower Austria
29	W	Sauvignon blanc	must	19	Lower Austria
30	W	Chardonnay	must	19	styria
31	R	Blauburger	must	19	Lower Austria
32	R	Zweigelt	must	19	Burgenland
33	W	Zweigelt	must	19	Lower Austria

34	Rosé	Cabernet Sauvignon	must in fermentation	19	Lower Austria
35	W	Welschriesling	must in fermentation	19	Lower Austria
36	W	Weißburgunder	must in fermentation	19	Lower Austria
37	W	Grüner Veltliner	must in fermentation	19	Lower Austria
38	W	Grüner Veltliner	must in fermentation	19	Lower Austria
39	W	Grüner Veltliner	must in fermentation	19	Burgenland
40	W	Grüner Veltliner	must in fermentation	19	Burgenland
41	W	Weißburgunder	must in fermentation	19	Burgenland
42	W	Chardonnay	must in fermentation	19	Burgenland
43	W	Chardonnay	must in fermentation	19	Burgenland
44	W	Sauvignon blanc	must in fermentation	19	Lower Austria
45	W	Viennaer Gemischter Satz	must in fermentation	19	Lower Austria
46	W	Rotgipfler	must in fermentation	19	Vienna
47	W	Grüner Veltliner	must in fermentation	19	Lower Austria
48	W	Grüner Veltliner	must in fermentation	19	Burgenland
49	W	Welschriesling	must in fermentation	19	Burgenland
50	W	Welschriesling	must in fermentation	19	Lower Austria
51	W	Welschriesling	must in fermentation	19	Burgenland
52	W	Grüner Veltliner DAC	must in fermentation	19	Vienna
53	W	Chardonnay	must in fermentation	19	Lower Austria
54	W	Chardonnay	must in fermentation	19	Burgenland
55	W	Chardonnay	must in fermentation	19	Burgenland

56	W	Grüner Veltliner	must in fermentation	19	Lower Austria
57	W	Chardonnay	must in fermentation	19	Lower Austria
58	W	Sauvignon blanc	must in fermentation	19	Styria
59	W	Sauvignon blanc	must in fermentation	19	Styria
60	W	Sauvignon blanc	must in fermentation	19	Styria
61	W	Rheinriesling	must in fermentation	19	Lower Austria
62	W	Grüner Veltliner	must in fermentation	19	Lower Austria
63	W	Grüner Veltliner	must in fermentation	19	Lower Austria
64	W	Gemischter Satz	must in fermentation	19	Lower Austria
65	W	Gemischter Satz	must in fermentation	19	Lower Austria
66	W	Grüner Veltliner	must in fermentation	19	Lower Austria
67	R	Zweigelt	must in fermentation	19	Burgenland
68	R	Zweigelt	must in fermentation	19	Lower Austria
69	R	Blauer Portugieser	must in fermentation	19	Lower Austria
70	R	Syrah	must in fermentation	19	Burgenland
71	W	Chardonnay	must in fermentation	19	Burgenland
72	W	Cuvée	must in fermentation	19	Burgenland
73	W	Cuvée	must in fermentation	19	Lower Austria
74	R	Zweigelt	must in fermentation	19	Burgenland
75	R	Blauburger	must in fermentation	19	Burgenland
76	R	Pinot Noir	must in fermentation	19	Lower Austria
77	R	Merlot	must in fermentation	19	Lower Austria

78

W

Chardonnay

must in  
fermentation

19

Lower Austria

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**Table S3:** Calibration and validation data of the pesticide method

Compound Name	RT [min]	MS-Ms Transitions (m/z) Lehotay et al.*1	CE (V)	R^2	Recovery [%] WW	Recovery [%] RW	Intraday repeatability [% RSD]	LOD [µg/l]	LOQ [µg/l]
Pirimethanil	16,16	198 → 183 198 → 158 198 → 118	15 20 35	0,9991	62,5	60,1	12,4	2,4	11,7
Chlorpyrifos-methyl	18,11	286 → 93 125 → 47 79 → 47	25 15 10	0,9970	92,7	70,1	28,8	1,7	8,4
Metalaxyl	18,64	234 → 146 234 → 174 220 → 192	10 20 5	0,9954	85,7	86,2	19,7	1,5	7,4
Chlorpyrifos	19,99	199 → 171 314 → 258 197 → 169	15 15 15	0,9998	75,9	78,6	5,5	3,7	18,1
Cyprodinil	20,90	224 → 208 226 → 225 225 → 224	10 10 20	0,9975	67,1	64,9	17,2	2,2	10,8
Penconazol	21,22	248 → 192 248 → 157 159 → 89	15 25 35	0,9991	98,9	110,7	8,9	2,8	14,0
Fluopyram	21,64	173 → 125 173 → 145	25 25	0,9963	96,9	101,0	6,1	2,0	10,0
Folpet	21,67	260 → 232 262 → 130 260 → 130	15 5 15	0,9962	82,2	88,5	11,9	3,3	16,2
Mepanipyrim	22,60	221 → 220 223 → 222 222 → 207	10 15 15	0,9977	82,7	92,1	14,8	0,8	4,0
Napropamid	22,96	128 → 72 271 → 72 128 → 100	15 10 5	0,9972	93,1	101,9	9,8	1,9	9,4
Fludioxonil	23,39	248 → 182 248 → 154 248 → 127	10 20 30	0,9948	85,4	86,8	9,6	1,8	8,7
Myclobutanil	23,73	179 → 90 179 → 125 150 → 123	10 30 15	0,9952	104,9	85,6	9,3	2,4	11,9

Kresoxim-methyl	24,07	116 → 63 131 → 89 116 → 89	30 15 30	0,9967	82,5	79,7	9,6	2,7	13,3
Cyflufenamid	24,40	118 → 90 188 → 88 118 → 89	35 10 25	0,9988	76,3	79,5	12,2	2,3	11,0
Benalaxyl	25,98	148 → 105 266 → 148 148 → 105	5 20 35	0,9944	83,0	72,9	13,0	2,5	12,5
Quinoxifen	26,04	272 → 237 307 → 237 237 → 208	20 10 20	0,9950	116,3	118,9	5,5	1,8	8,9
Fenhexamid	26,19	177 → 113 97 → 78 172 → 145	15 25 10	0,9371	91,2	80,7	16,0	2,0	9,7
Trifloxystrobin	26,48	116 → 63 172 → 145 116 → 89	15 15 30	0,9962	76,9	84,6	9,1	2,1	10,3
Tebuconazol	26,75	125 → 99 250 → 125 125 → 89	20 20 15	0,9956	87,6	73,7	19,8	2,3	11,5
TPP IST	27,04	233 → 215 326 → 325 215 → 168	5 10 15	IST					
Fenpyrazamin	30,60	230 → 188 230 → 160 230 → 132	5 10 15	0,9947	92,0	95,9	11,7	1,9	9,6
Boscalid	33,36	140 → 76 140 → 112 112 → 76	10 25 15	0,9964	79,0	82,6	14,2	2,2	10,6
Cypermethrin	33,49	163 → 127 165 → 91 163 → 91	15 5 15	0,9986	72,2	84,4	10,9	2,1	10,3
Indoxacarb	36,51	203 → 106 203 → 134 203 → 78	15 25 30	0,9999	81,7	77,4	8,8	1,7	8,4

\*1 Lehotay, S. J.; Kok, A. D.; Hiemstra, M.; Bodegraven, P. V. Validation of a fast and easy method for the determination of residues from 229 pesticides in fruits and vegetables using gas and liquid chromatography and mass spectrometric detection. *J. AOAC Int.* **2005.**, 88(2), 595–614.

**Table S4.** Information concerning calibration and validation of the volatile compound.

<b>Volatile substance (µg/L)</b>	<b>Meth od</b>	<b>abbrevi ation</b>	<b>Quantif ier</b>	<b>Qualif ier</b>	<b>Internal standard</b>	<b>calibration area</b>	<b>linearity</b>	<b>RI</b>	<b>reference RI</b>	<b>repeatability</b>	<b>LOQ</b>	<b>LOD</b>
(Z)-linalool oxide	FM	FM1	59	94, 111	3,4-dimethylanisole	0.9-174.3	0.998	1 070	1065-1098 a	5.8 %	0.87	0.26
(E)-linalool oxide	FM	FM2	59	94, 111	3,4-dimethylanisole	0.9-175.7	0.998	1 087	1065-1098 a	6.0 %	0.88	0.26
linalool	FM	FM3	71	93, 67	3,4-dimethylanisole	0.8-160	0.998	1 101	1074-1112 a	7.0 %	0.80	0.24
hotrienol	FM	FM4	71	82, 67	3,4-dimethylanisole	0.5-108.1	0.999	1 104	1101-1109 a	5.7 %	0.54	0.16
(Z)-rose oxide	FM	FM5	139	69, 154	3,4-dimethylanisole	0.6-113.2	0.998	1 110	1097-1121 a		0.57	0.17
(E)-rose oxide	FM	FM6	139	69, 154	3,4-dimethylanisole	0.1-10.8	0.999	1 123			0.05	0.02
(E)-limonene oxide	FM	FM7	94	67, 109	3,4-dimethylanisole	0.8-153.9	0.998	1 132			0.77	0.23
beta-terpineol	FM	FM8	93	121, 136	3,4-dimethylanisole	0.1-11.8	0.997	1 144	1127-1188 a		0.06	0.02
nerol oxide	FM	FM9	68	83	3,4-dimethylanisole	0.6-118.0	0.998	1 146	1137-1172 a	4.1 %	0.59	0.18
lavandulol	FM	FM10	69	111, 123	3,4-dimethylanisole	0.7-147.0	0.998	1 160	1140-1185 a	15.3 %	0.74	0.22
alpha-terpineol	FM	FM11	93	121, 136	3,4-dimethylanisole	0.4-86.0	0.998	1 194	1150-1224 a	13.3 %	0.40	0.12
gamma-terpineol	FM	FM12	121	136, 93	3,4-dimethylanisole	0.1-28.4	0.997	1 198	1177-1218 a		0.14	0.04
nerol	FM	FM13	69	93, 95	3,4-dimethylanisole	0.7-134.0	0.998	1 228	1204-1254 a	16.5 %	0.67	0.20
citronellol	FM	FM14	69	95, 93	3,4-dimethylanisole	0.7-148.0	0.998	1 229	1206-1238 a	12.2 %	0.74	0.22
geraniol	FM	FM15	69	93, 123	3,4-dimethylanisole	0.7-131.0	0.998	1 256	1221-1277 a	4.8 %	0.66	0.20

1-propanol (mg/L)	MV	HA1	31	42	d10-butanol	0.09-496.01	0.999	1035	1002-1073 b	8.2 %	0.010	0.003
isobutanol (mg/L)	MV	HA2	42	31	d10-butanol	0.91-91.79	0.999	1088	1043-1124 b	5.7 %	0.918	0.275
isoamyl alcohol (mg/L)	MV	HA3	70	43	d10-butanol	10.42-521.24	0.999	1206	1163-1255 b	7.8 %	10.42 5	3.127
1-butanol (mg/L)	MV	HA4	56	41	d10-butanol	0.06-2.79	0.998	1142	1110-1179 b	7.6 %	0.063	0.019
(Z)-3-hexen-1-ol (mg/L)	MV	C6-1	82	67, 55	d5-ethyl hexanoate	0.01-0.20	0.999	1371	1346-1426 b	11.0 %	0.010	0.003
1-hexanol (mg/L)	MV	C6-26	69	55	d13-hexanol	0.01-6.48	0.998	1352	1314-1396 b	2.8 %	0.013	0.004
ethyl acetate (mg/L)	MV	EE1	61	43	d5-ethyl octanoate	9.83-196.57	0.999	892	854-914 b	7.0 %	9.829	2.949
ethyl lactate (mg/L)	MV	EE2	45	75	d5-ethyl octanoate	0.10-51.78	0.998	1335	1316-1353 b	6.5 %	0.104	0.031
ethyl propanoate (mg/L)	MV	EE3	57	75	d5-ethyl hexanoate	9.80-980.00	0.998	952	915-976 b	10.6 %	0.010	0.003
diethyl succinate (mg/L)	MV	MiE1	101	129	d5-ethyl octanoate	0.1-9.9	0.997	1668	1658-1714 b	11.3 %	0.099	0.030
ethyl butanoate	MME	EE4	71	88, 43	d5-ethyl valerate	12.5-2500.0	0.998	802	770-818 a	3.4 %	12.50	3.75
ethyl isovalerate	MME	EE5	88	85, 57	d5-ethyl valerate	0.3-49.8	0.998	852	824-859 a	3.3 %	0.25	0.07
ethyl valerate	MME	EE6	85	88, 57	d5-ethyl valerate	0.1-10.4	0.998	901	871-929 a	4.4 %	0.13	0.04
ethyl hexanoate	MME	EE7	88	99, 43	d5-ethyl hexanoate	13.2-2641.0	0.999	1001	976-1014 a	3.1 %	13.21	3.96
ethyl heptanoate	MME	EE8	88	113	d5-ethyl valerate	0.1-10.5	0.999	1098	1080-1099 a	3.9 %	0.05	0.02



ethyl octanoate	MME	EE9	88	101, 127	d5-ethyl octanoate	16.4-3280.0	0.999	1202	1173-1202 a	2.6 %	16.40	4.92
ethyl decanoate	MME	EE10	88	101	d5-ethyl decanoate	16.9-3385.8	0.999	1399	1367-1405 a	8.2 %	16.93	5.08
ethyl dodecanoate	MME	EE11	88	101, 157	d5-ethyl decanoate	0.3-50.8	0.998	1595	1566-1596 a	15.7 %	0.25	0.08
ethyl tetradecanoate	MME	EE12	TIC	TIC	d5-ethyl decanoate	0.3-49.9	0.998	1795	1769-1799 a	11.9 %	0.25	0.07
ethyl hexadecanoate	MME	EE13	88	101, 157	d5-ethyl decanoate	3.9-55.9	0.998	1990	1966-2013 a	13.0 %	3.92	1.18
methyl isovalerate	MME	ME1	74	85, 57	d5-ethyl valerate	0.1-10.4	0.999	774	766-778 a		0.05	0.02
methyl hexanoate	MME	ME2	74	87, 43	d5-ethyl valerate	0.1-10.6	0.999	924	902-931 a	3.9 %	0.05	0.02
methyl octanoate	MME	ME3	74	87, 127	d5-ethyl hexanoate	0.1-8.7	0.999	1124	1105-1138 a	6.6 %	0.04	0.01
methyl decanoate	MME	ME4	74	87, 143	d5-ethyl octanoate	0.1-10.6	0.999	1325	1304-1329 a	5.9 %	0.05	0.02
methyl dodecanoate	MME	ME5	74	87, 143	d5-ethyl decanoate	0.2-41.9	0.998	1525	1503-1527 a		0.21	0.06
methyl tetradecanoate	MME	ME6	74	87, 143	d5-ethyl decanoate	0.2-48.6	0.998	1727	1699-1738 a		0.24	0.07
isoamyl acetate	MME	ISAE1	43	70	d5-ethyl valerate	1.0-11.6	0.996	877	851-885 a	4.1 %	0.98	0.29
isoamyl butanoate	MME	ISAE2	71	70, 43	d5-ethyl hexanoate	0.1-9.6	0.999	1057	1041-1086 a	7.2 %	0.05	0.01
isoamyl isovalerate	MME	ISAE3	85	70	d5-ethyl octanoate	0.1-9.2	0.998	1105	1081-1105 a		0.05	0.01

isoamyl hexanoate	MME	ISAE4	70	43, 99	d5-ethyl octanoate	0.1-10	0.997	1254	1238-1254 a	5.9 %	0.05	0.02
isoamyl octanoate	MME	ISAE5	70	127	d5-ethyl octanoate	0.1-10.1	0.997	1448	1450 a	13.8 %	0.05	0.02
ethyl benzoate	MME	ArE1	105	122	d5-ethyl hexanoate	0.1-14.3	0.999	1173	1138-1206 a	6.3 %	0.07	0.02
ethyl phenylacetate	MME	ArE2	91	91	d5-ethyl octanoate	0.1-13.0	0.996	1244	1209-1251 a	9.5 %	0.07	0.02
isobutyl acetate	MME	HAA1	43	56	d5-ethyl valerate	12.7-2540.0	0.998	771	741-788 a	8.3 %	12.70	3.81
2-methylbutyl acetate	MME	HAA2	43	70	d5-ethyl valerate	13.4-2680.0	0.997	878	863-892 a	3.7 %	13.40	4.02
hexyl acetate	MME	HAA3	43	56, 61	d5-ethyl hexanoate	13.2-2630.0	0.999	1013	987-1025 a	3.2 %	13.15	3.95
isobutyl propionate	MME	MiE2	57	29	d5-ethyl valerate	0.3-52.1	0.998	866	843-866 a	8.3 %	0.26	0.08
butyl isobutanoate	MME	MiE3	43	71	d5-ethyl hexanoate	1.0-11.0	0.999	953	952-955 a	9.5 %	0.98	0.30
pentyl butanoate	MME	MiE4	43	71, 70	d5-ethyl hexanoate	0.1-10.8	0.999	1095	1062-1098 a	12.1 %	0.05	0.02
hexyl 2-methylbutanoate	MME	MiE5	99	56, 117	d5-ethyl hexanoate	0.1-10.2	0.999	1237	1204-1247 a		0.05	0.02
propyl isovalerate	MME	MiE6	85	103	d5-ethyl hexanoate	0.1-10.0	0.998	950	928-951 a		0.05	0.02
butyl butanoate	MME	MiE7	71	88	d5-ethyl hexanoate	13.0-2600.0	0.999	996	969-996 a	0.9 %	13.00	3.90
propyl octanoate	MME	MiE8	145	127, 61	d5-ethyl octanoate	0.1-10.4	0.997	1292	1290 a	4.8 %	0.05	0.02
isobutyl octanoate	MME	MiE9	57	56	d5-ethyl decanoate	0.1-9.8	0.998	1349	1348-1370 a	14.9 %	0.05	0.01

(Data in empty fields could not be collected because it was not available or not detectable in the validation wine.)

a Kovats RI according to the RI calculation of Van Den Dool and Kratz, non-polar column, temperature ramp + custom temperature program (@nist database: <https://webbook.nist.gov/chemistry/>)  
b Kovats RI

according to the RI calculation of Van Den Dool and Kratz, polar column, temperature ramp + custom temperature program (@nist database: <https://webbook.nist.gov/chemistry/>)

FM=method for free monoterpenes, MV=method for main volatile substances, MME=method for major and minor esters, NOR=method for C13-norisoprenoids, MP=method for methoxypyrazines, OV=method for volatile phenols, oak volatiles, lactones and some carbonyl compounds

**Table S5:** volatile profiles of the white wines before and after fining

[illegible]

	ohne Mittel	Absolut	Reskue	CarboTec	NaCalit	Purity D	Flowpure	Grandeco	Granucol	
alpha-Terpineol (µg/l)	6,1a		5,6b	6,1a	6,1a	5,5b	5,8ab	5,6b	4,3c	5,8ab
gamma-Terpineol (µg/l)	<0,14		<0,14	<0,14	<0,14	<0,14	<0,14	<0,14	<0,14	<0,14
Nerol (µg/l)	2,2a		1,7cd	2,3a	2,2a	2,0ab	2,2a	1,8bc	1,5d	1,5d
Citronellol (µg/l)	0,7a		0,7a	0,7a	0,7ab	0,6ab	0,7ab	0,7ab	0,5b	0,6ab
Geraniol (µg/l)	11,5a		11,1a	11,5a	11,3a	8,9bc	9,6b	9,7b	8,2c	8,7bc
Higher Alcohols										
Propanol1 (mg/l)	23,83a		22,17abc	22,67abc	22,93ab	20,43c	20,57bc	21,93abc	20,63bc	22,55abc
Isobutanol (mg/l)	25,17a		23,67bc	24,90ab	24,20abc	23,53bc	24,23abc	23,37c	23,50bc	24,75abc
Isoamylalkohol (mg/l)	120,37a		117,07a	118,93a	120,17a	120,40a	121,67a	119,83a	119,73a	122,60a
Butanol 1 (mg/l)	0,20a		0,20a	0,20a	0,20a	0,20a	0,20a	0,20a	0,20a	0,20a
C6-alcohols										
cis-3-Hexen-1ol (mg/l)	0,01a		0,01a	0,01a	0,01a	0,01a	0,01a	0,01a	0,01a	0,01a
1-Hexanol (mg/l)	0,50a		0,50a	0,50a	0,50a	0,50a	0,49a	0,50a	0,48a	0,49a
Major ethyl esters										
ethyl acetate (mg/l)	21,23a		21,03a	20,90ab	20,47ab	20,87ab	19,77b	20,80ab	20,17ab	20,83ab

	ohne Mittel	Absolut	Reskue	CarboTec	NaCalit	Purity D	Flowpure	Grandeco	Granucol
ethyl lactate (mg/l)	4,70a	4,37ab	3,40e	3,97bcd	4,07bc	3,53de	3,83cde	3,70cde	3,60de
ethyl propanoate (mg/l)	0,13a	0,10a	0,10a	0,10a	0,10a	0,10a	0,10a	0,10a	0,10a
diethyl succinate (mg/l)	1,07a	0,90b	1,00a	0,80c	0,90b	1,00a	1,00a	1,00a	0,83a
Minor ethyl esters									
ethyl butanoate (µg/l)	373,8a	343,0b	348,1b	346,5b	369,2a	310,7d	369,1a	367,3a	322,5c
ethyl isovalerate (µg/l)	5,5a	5,2a	4,7b	4,8b	5,4a	4,7b	5,3a	5,2a	4,6b
ethyl valerate (µg/l)	0,5a	0,5a	0,5a	0,5a	0,5a	0,4b	0,5a	0,5a	0,5a
ethyl hexanoate (µg/l)	633,1	591,8ab	557,4ab	580,6ab	628,5a	511,8bc	616,1a	531,0b	453,8c
ethyl heptanoate (µg/l)	0,8a	0,2d	0,8a	0,7ab	0,7ab	0,5c	0,7ab	0,7ab	0,6bc
ethyl octanoate (µg/l)	1788,3a	1498,0c	1591,7bc	1533,0c	1777,9a	1351,4d	1635,7b	1363,0d	1194,7e
ethyl decanoate (µg/l)	1189,0a	889,7d	831,0d	848,4d	1203,7a	676,0e	1055,2b	972,3c	707,4e
ethyl dodecanoate (µg/l)	63,0a	59,0ab	47,6c	55,5abc	61,6ab	54,1bc	60,2ab	53,8bc	27,5d

	ohne Mittel	Absolut	Reskue	CarboTec	NaCalit	Purity D	Flowpure	Grandeco	Granucol
ethyl tetradecanoate (µg/l)	11,3a	4,3f	6,0d	7,4c	10,2b	7,9c	5,6de	4,6ef	3,1g
ethyl hexadecanoate (µg/l)	36,9a	22,3c	33,9ab	32,6ab	34,4ab	30,0b	32,7ab	30,4b	7,8d
<b>Methyl esters</b>									
methyl isovalerate (µg/l)	<0,05	<0,05	<0,05	<0,05	<0,05	<0,05	<0,05	<0,05	<0,05
methyl hexanoate (µg/l)	1,7a	1,6a	1,6a	1,5a	1,7a	1,3a	1,7a	1,6a	1,5a
methyl octanoate (µg/l)	1,3a	1,1b	1,1b	1,1b	1,3a	1,0bc	1,1b	1,1b	0,9c
methyl decanoate (µg/l)	0,8a	0,8ab	0,8ab	0,7b	0,8a	0,7ab	0,8ab	0,7ab	0,8ab
methyl dodecanoate (µg/l)	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
methyl tetradecanoate (µg/l)	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
<b>Isoamyl esters</b>									
isoamyl acetate (µg/l)	2468,7a	2306,2bc	2253,0bc	2206,7c	2459,2a	2049,4d	2369,8ab	2310,1bc	2074,4d

	ohne Mittel	Absolut	Reskue	CarboTec	NaCalit	Purity D	Flowpure	Grandeco	Granucol
isoamyl butanoate (µg/l)	0,1a	0,1a	0,1a	0,1a	0,1a	0,1a	0,1a	0,1a	0,1a
isoamyl isovalerate (µg/l)	<0,05	<0,05	<0,05	<0,05	<0,05	<0,05	<0,05	<0,05	<0,05
isoamyl hexanoate (µg/l)	2,3a	2,2a	2,0b	2,2ab	2,3a	2,2ab	2,3a	2,2a	2,3a
isoamyl octanoate (µg/l)	2,4a	2,1bc	1,9c	1,6d	2,4a	2,1bc	2,3ab	2,2ab	1,6d
<b>Aromatic esters</b>									
ethyl benzoate (µg/l)	0,1a	0,1a	0,1a	0,1a	0,1a	0,1a	0,1a	0,1a	0,1a
ethyl phenylacetate (µg/l)	1,4a	0,9d	1,1c	1,2b	1,3b	0,8d	1,1c	0,9d	0,9d
<b>Higher alcohol acetate</b>									
isobutyl acetate (µg/l)	108,0a	98,2bcd	100,1bcd	97,0cd	103,2abc	98,6bcd	105,6ab	104,7abc	93,9d
2-methylbutyl acetate (µg/l)	317,9a	303,6bc	291,2de	286,9e	313,3ab	267,6f	298,7cd	297,7cd	248,5g
hexyl acetate (µg/l)	214,8a	194,2bc	190,0c	182,5cd	211,7a	172,5de	205,7ab	160,8e	160,3e



Miscellaneous minor esters									
isobutyl propionate (µg/l)	19,6a	19,1ab	18,9ab	17,9bc	19,2ab	17,1c	18,5ab	19,2ab	18,7ab
butyl isobutanoate (µg/l)	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
pentyl butanoate (µg/l)	0,2a	0,2a	0,2a	0,2a	0,2a	0,2a	0,2a	0,2a	0,2a
hexyl 2-methylbutanoate (µg/l)	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
propyl isovalerate (µg/l)	<0,05	<0,05	<0,05	<0,05	<0,05	<0,05	<0,05	<0,05	<0,05
butyl butanoate (µg/l)	15,6a	14,0b	14,2b	12,9c	15,2a	10,2e	9,5f	12,1d	12,1d
propyl octanoate (µg/l)	1,8a	1,7ab	1,5cd	1,6bc	1,7ab	1,3de	1,1f	1,3de	1,2ef
isobutyl octanoate (µg/l)	0,3a	<0,05	<0,05	0,1b	0,2b	<0,05	<0,05	<0,05	<0,05

**Table S6::** volatile profiles of the red wines before and after fining

	ohne Mittel	Absolut	Reskue	CarboTec	NaCalit	Purity D	Flowpure	Grandeco	Granucol
Free Monoterpens									
cis- Linalooloxid (µg/l)	6,3a	5,3ab	6,1ab	5,2b	6,2ab	6,3a	5,4ab	5,4ab	6,3a
trans- Linalooloxid (µg/l)	2,6a	2,6a	2,6a	2,4ab	2,6a	2,6a	2,6a	2,3b	2,6a
Linalool (µg/l)	13,8a	12,0ab	12,1ab	11,6ab	13,0ab	13,8a	13,2ab	8,7b	11,4ab
Hotrienol (µg/l)	2,4a	2,0ab	2,3a	2,0ab	2,4a	2,4a	2,1ab	1,8b	2,4a
cis-Rosenoxid (µg/l)	0,2a	0,2a	0,2a	0,2a	0,2a	0,2a	0,2a	0,1b	0,2a
trans- Rosenoxid (µg/l)	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
trans- Limonenoxid (µg/l)	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
beta-Terpineol (µg/l)	0,2a	0,1a	0,2a	0,1a	0,2a	0,2a	0,1a	0,1a	0,1a
Neroloxid (µg/l)	1,4a	1,2ab	1,3ab	1,3ab	1,4ab	1,4a	1,3ab	0,9c	1,2b

	ohne Mittel	Absolut	Reskue	CarboTec	NaCalit	Purity D	Flowpure	Grandeco	Granucol
Lavandulool (µg/l)	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
alpha- Terpineol (µg/l)	5,2a	4,8a	4,7a	4,8a	5,2a	5,2a	5,0a	3,8b	5,0a
gamma- Terpineol (µg/l)	0,3a	0,2ab	0,1ab	0,2ab	0,2ab	0,2ab	0,2ab	0,1b	0,2ab
Nerol (µg/l)	0,9a	0,8ab	0,9ab	0,7ab	0,9ab	0,7ab	0,9ab	0,7ab	0,6b
Citronellol (µg/l)	2,2a	1,9ab	1,7abc	2,1ab	1,9ab	2,0ab	2,0ab	1,4c	1,6bc
Geraniol (µg/l)	7,2a	6,0abc	5,6abc	6,8ab	6,3ab	6,7ab	6,8ab	4,6c	5,3bc
Higher Alcohols									
Propanol1 (mg/l)	28,66a	26,18a	24,89a	26,78a	27,27a	27,80a	24,98a	24,31a	28,45a
Isobutanol (mg/l)	51,10a	48,15a	47,33a	48,81a	50,24a	48,76a	48,38a	48,45a	50,75a
Isoamylalkohol (mg/l)	274,39a	274,39a	273,13a	273,40a	274,39a	272,14a	274,39a	274,39a	274,39a
Butanol 1 (mg/l)	1,09a	1,03ab	1,01b	1,06ab	1,08ab	1,06ab	1,04ab	1,07ab	1,08ab

	ohne Mittel	Absolut	Reskue	CarboTec	NaCalit	Purity D	Flowpure	Grandeco	Granucol
C6-alcohols									
cis-3- Hexen- 1ol (mg/l)	0,03a	0,03a	0,03a	0,03a	0,03a	0,03a	0,03a	0,03a	0,03a
1- Hexano l (mg/l)	0,13a	0,13a	0,12b	0,13a	0,13a	0,13a	0,13a	0,13a	0,13a
Major ethyl esters									
ethyl acetate (mg/l)	79,88a	79,87a	75,59a	77,19a	77,10a	79,25a	79,87a	73,96a	79,52a
ethyl lactate (mg/l)	203,08a	167,56ab	158,64ab	186,06ab	147,99b	163,22ab	175,82ab	152,93ab	154,26ab
ethyl propanoate (mg/l)	0,19a	0,19a	0,19a	0,19a	0,18a	0,19a	0,19a	0,18a	0,19a
diethyl succinate (mg/l)	5,21a	5,18a	4,93a	4,54a	4,95a	4,09a	4,55a	5,03a	4,13a
Minor ethyl esters									
ethyl butanoate (µg/l)	124,4a	122,2a	119,7ab	115,5abc	107,9bcd	108,1bcd	124,4a	97,5d	105,9
ethyl isovalerate (µg/l)	24,8a	24,2a	23,6ab	23,4ab	21,6bc	21,4bc	24,8a	19,3c	21,2bc

ohne Mittel	Absolut	Reskue	CarboTec	NaCalit	Purity D	Flowpure	Grandeco	Granucol	
ethyl valerate (µg/l)	2,0a	2,0a	1,9ab	1,8ab	1,8ab	1,8ab	2,0a	1,6b	1,8ab
ethyl hexanoate (µg/l)	182,1a	166,4ab	144,7c	168,8ab	153,3bc	153,8bc	181,4a	117,1d	141,9c
ethyl heptanoate (µg/l)	0,5a	0,4ab	0,4ab	0,1c	0,5a	0,4ab	0,5a	0,3b	0,3ab
ethyl octanoate (µg/l)	175,3a	150,6b	107,2e	145,0bc	131,7cd	137,4bc	168,4a	88,6f	120,1de
ethyl decanoate (µg/l)	83,2a	67,2b	53,2cd	63,1b	51,5d	60,3bc	82,1a	38,0e	49,8d
ethyl dodecanoate (µg/l)	4,5a	4,4ab	3,8b	4,2ab	2,5c	2,5c	4,4a	2,0cd	1,9d
ethyl tetradecanoate (µg/l)	5,8a	2,9cd	2,4de	2,2de	3,1cd	3,8bc	4,8ab	2,3de	1,4e
ethyl hexadecanoate (µg/l)	14,2a	12,4a	8,4b	8,6b	9,1b	10,0b	14,1a	8,4b	2,9c

[illegible]

	ohne Mittel	Absolut	Reskue	CarboTec	NaCalit	Purity D	Flowpure	Grandeco	Granucol
Isoamyl esters									
isoamyl acetate (µg/l)	260,2a	254,9a	244,2ab	245,5ab	224,5bc	224,0bc	260,2a	199,1c	222,6bc
isoamyl butanoate (µg/l)	0,2a	0,2ab	0,1a	0,2ab	0,1a	0,1a	0,2a	0,1a	0,1a
isoamyl isovalerate (µg/l)	0,2a	0,1a	0,2a	0,2a	0,2a	0,1a	0,2a	0,1a	0,1a
isoamyl hexanoate (µg/l)	0,3a	0,3a	0,3a	0,3a	0,3a	0,3a	0,3a	0,3a	0,3a
isoamyl octanoate (µg/l)	0,3a	0,3a	0,3ab	0,3ab	0,2b	0,2b	0,3a	0,2b	0,2b
Aromatic esters									
ethyl benzoate (µg/l)	0,6a	0,4abcd	0,3cd	0,4bcd	0,5ab	0,5abc	0,6a	0,3d	0,3d
ethyl phenylacetate (µg/l)	6,4a	5,2b	4,2c	4,5c	5,3b	5,6b	6,3a	3,5d	4,0cd
	ohne Mittel	Absolut	Reskue	CarboTec	NaCalit	Purity D	Flowpure	Grandeco	Granucol
Higher alcohol acetate									

isobutyl acetate (µg/l)	106,6a	104,1a	102,9a	98,4ab	98,7ab	97,4ab	106,6a	90,4b	93,0b
2-methylbutyl acetate (µg/l)	66,7a	62,9ab	61,7ab	63,7ab	56,8bc	56,5bc	65,4a	51,1c	51,8c
hexyl acetate (µg/l)	40,1a	38,6a	30,6bc	36,6ab	33,3ab	33,0ab	39,7a	24,6c	29,4bc

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Miscellaneous minor esters

isobutyl propionate (µg/l)	0,8a	0,8a	0,8a	0,8a	0,8a	0,7a	0,8a	0,7a	0,8a
butyl isobutanoate (µg/l)	1,7a	1,7a	1,7a	1,7a	1,7a	1,5ab	1,6ab	1,6ab	1,5b
pentyl butanoate (µg/l)	0,2a	0,2a	0,2a	0,2a	0,2a	0,2a	0,2a	0,2a	0,2a
hexyl 2-methylbutanoate (µg/l)	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
propyl isovalerate (µg/l)	0,3a	0,3a	0,3a	0,3a	0,3a	0,3a	0,2a	0,3a	0,2a
butyl butanoate (µg/l)	16,8a	13,4bcd	13,0bcd	15,0abc	13,8abcd	13,9abcd	16,4ab	10,9d	12,8cd
propyl octanoate (µg/l)	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.

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ohne Mittel	Absolut	Reskue	CarboTec	NaCalit	Purity D	Flowpure	Grandeco	Granucol
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isobutyl octanoate (µg/l)	0,2a	<0,05	<0,05	<0,05	<0,05	0,1b	0,1b	<0,05	<0,05
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