Chemical characterization and sensory evaluation of a phenolic-rich melanoidin isolate contributing to coffee astringency

Department of Food Science & Technology, The Ohio State University, 2015 Fyffe Rd., Columbus, OH 43210-1007, USA, peterson.892@osu.edu, +1-614-688-2723

Supplemental Data

Table S1. Signal Detection Response Matrix. Letters a-l represent group response frequencies for each response type (adapted from O'Mahony, 1992).

	Different (Sure)	Different (Unsure)	Different (Guess)	Same (Guess)	Same (Unsure)	Same (Sure)
Stimulus	a	b	c	d	e	f
Blind Control	g	h	i	j	k	l

Equation S1. R-index equation. Variables refer to response frequencies represented in Table S1. (reproduced from O'Mahony 1992)

$$R = \frac{a(h+i+j+k+l) + b(i+j+k+l) + c(j+k+l) + d(k+l) + e(l) + f + \frac{1}{2(ag+bh+ci+dj+ek+fl)}}{(a+b+c+d+e+f)(g+h+i+j+k+l)}$$

Table S2. Mass-to-charge (*m/z*), mass error (err ppm), and molecular formula for upper quartile (75-100th percentile) of FT-ICR MS data for F9.6.4 ordered by relative intensity. Columns six and seven indicate calculated molecular ratios corresponding to van Krevelen diagram coordinates (O/C = oxygen to carbon, H/C = hydrogen to carbon) (Figure 4). Compounds located within the polyphenolic region of the van Krevelen plot are highlighted in gray.

Ion Intensity Rank (out of 319)	Observed *m/z*	calc. *m/z*	err ppm	sum formula	O/C	H/C
1	557.1663	557.1665	0.298	$C_{28}H_{29}O_{12}$	0.429	1.036
2	253.2173	253.2173	-0.160	$C_{16}H_{29}O_{2}$	0.125	1.813
3	269.2486	269.2486	0.046	$C_{17}H_{33}O_{2}$	0.118	1.941
4	465.3043	465.3042	-0.265	$C_{19}H_{41}N_{6}O_{7}$	0.368	2.158
5	513.1400	513.1402	0.452	$C_{26}H_{25}O_{11}$	0.423	0.962
6	241.2173	241.2173	-0.118	$C_{15}H_{29}O_{2}$	0.133	1.933
7	511.4729	511.4732	0.520	$C_{32}H_{63}O_{4}$	0.125	1.969
8	399.1846	399.1845	-0.195	$C_{12}H_{27}N_{6}O_{9}$	0.750	2.250
9	227.2017	227.2017	0.002	$C_{14}H_{27}O_{2}$	0.143	1.929
10	527.1557	527.1559	0.314	$C_{27}H_{27}O_{11}$	0.407	1.000
11	539.5043	539.5045	0.316	$C_{34}H_{67}O_{4}$	0.118	1.971
12	415.1034	415.1035	0.197	$C_{21}H_{19}O_{9}$	0.429	0.905
13	425.3635	425.3636	0.324	$C_{26}H_{49}O_{4}$	0.154	1.885
14	439.1397	439.1398	0.380	$C_{24}H_{23}O_{8}$	0.333	0.958
15	383.1135	383.1136	0.333	$C_{21}H_{19}O_{7}$	0.333	0.905
16	467.1346	467.1348	0.441	$C_{25}H_{23}O_{9}$	0.360	0.920
17	425.1241	425.1242	0.270	$C_{23}H_{21}O_{8}$	0.348	0.913
18	437.1241	437.1242	0.290	$C_{24}H_{21}O_{8}$	0.333	0.875
19	397.1292	397.1293	0.107	$C_{22}H_{21}O_{7}$	0.318	0.955
20	479.1346	479.1348	0.349	$C_{26}H_{23}O_{9}$	0.346	0.885
21	413.1241	413.1242	0.257	$C_{22}H_{21}O_{8}$	0.364	0.955
22	509.1451	509.1453	0.416	$C_{27}H_{25}O_{10}$	0.370	0.926
23	371.1135	371.1136	0.285	$C_{20}H_{19}O_{7}$	0.350	0.950
24	409.1292	409.1293	0.295	$C_{23}H_{21}O_{7}$	0.304	0.913
25	523.1609	523.1610	0.174	$C_{28}H_{27}O_{10}$	0.357	0.964
26	469.1502	469.1504	0.355	$C_{25}H_{25}O_{9}$	0.360	1.000
27	770.3153	770.3155	0.322	$C_{39}H_{44}N_{7}O_{10}$	0.256	1.128
28	395.1136	395.1136	0.189	$C_{22}H_{19}O_{7}$	0.318	0.864
29	427.1397	427.1398	0.255	$C_{23}H_{23}O_{8}$	0.348	1.000
30	493.1503	493.1504	0.276	$C_{27}H_{25}O_{9}$	0.333	0.926
31	535.1608	535.1610	0.355	$C_{29}H_{27}O_{10}$	0.345	0.931
32	497.1452	497.1453	0.156	$C_{26}H_{25}O_{10}$	0.385	0.962
33	483.1295	483.1297	0.393	$C_{25}H_{23}O_{10}$	0.400	0.920
34	367.3581	367.3582	0.050	$C_{24}H_{47}O_{2}$	0.083	1.958
35	353.1029	353.1031	0.365	$C_{20}H_{17}O_{6}$	0.300	0.850
36	521.1452	521.1453	0.175	$C_{28}H_{25}O_{10}$	0.357	0.893
37	539.1557	539.1559	0.327	$C_{28}H_{27}O_{11}$	0.393	0.964
38	511.1609	511.1610	0.190	$C_{27}H_{27}O_{10}$	0.370	1.000
39	465.1553	465.1555	0.384	$C_{26}H_{25}O_{8}$	0.308	0.962

Continued

Table S2 continued

40	525.1400	525.1402	0.505	$C_{27}H_{25}O_{11}$	0.407	0.926
41	369.0979	369.0980	0.301	$C_{20}H_{17}O_{7}$	0.350	0.850
42	507.1658	507.1661	0.439	$C_{28}H_{27}O_{9}$	0.321	0.964
43	411.1448	411.1449	0.298	$C_{23}H_{23}O_{7}$	0.304	1.000
44	385.1292	385.1293	0.105	$C_{21}H_{21}O_{7}$	0.333	1.000
45	339.1999	339.1998	-0.562	$C_{11}H_{27}N_{6}O_{6}$	0.545	2.455
46	695.5466	695.5467	0.267	$C_{41}H_{75}O_{8}$	0.195	1.829
47	367.1186	367.1187	0.371	$C_{21}H_{19}O_{6}$	0.286	0.905
48	495.1659	495.1661	0.316	$C_{27}H_{27}O_{9}$	0.333	1.000
49	397.3322	397.3323	0.448	$C_{24}H_{45}O_{4}$	0.167	1.875
50	463.1396	463.1398	0.484	$C_{26}H_{23}O_{8}$	0.308	0.885
51	505.1503	505.1504	0.139	$C_{28}H_{25}O_{9}$	0.321	0.893
52	355.1187	355.1187	0.088	$C_{20}H_{19}O_{6}$	0.300	0.950
53	341.1030	341.1031	0.218	$C_{19}H_{17}O_{6}$	0.316	0.895
54	401.1241	401.1242	0.122	$C_{21}H_{21}O_{8}$	0.381	1.000
55	537.1765	537.1766	0.284	$C_{29}H_{29}O_{10}$	0.345	1.000
56	471.1295	471.1297	0.331	$C_{24}H_{23}O_{10}$	0.417	0.958
57	387.1085	387.1085	0.191	$C_{20}H_{19}O_{8}$	0.400	0.950
58	441.1554	441.1555	0.164	$C_{24}H_{25}O_{8}$	0.333	1.042
59	519.1660	519.1661	0.200	$C_{29}H_{27}O_{9}$	0.310	0.931
60	357.0979	357.0980	0.353	$C_{19}H_{17}O_{7}$	0.368	0.895
61	491.1346	491.1348	0.394	$C_{27}H_{23}O_{9}$	0.333	0.852
62	439.3791	439.3793	0.478	$C_{27}H_{51}O_{4}$	0.148	1.889
63	547.1608	547.1610	0.308	$C_{30}H_{27}O_{10}$	0.333	0.900
64	381.0979	381.0980	0.202	$C_{21}H_{17}O_{7}$	0.333	0.810
65	465.1190	465.1191	0.176	$C_{25}H_{21}O_{9}$	0.360	0.840
66	421.1292	421.1293	0.166	$C_{24}H_{21}O_{7}$	0.292	0.875
67	533.1452	533.1453	0.271	$C_{29}H_{25}O_{10}$	0.345	0.862
68	279.2329	279.2330	0.104	$C_{18}H_{31}O_{2}$	0.111	1.722
69	399.1449	399.1449	0.097	$C_{22}H_{23}O_{7}$	0.318	1.045
70	681.5309	681.5311	0.320	$C_{40}H_{73}O_{8}$	0.200	1.825
71	343.1186	343.1187	0.246	$C_{19}H_{19}O_{6}$	0.316	1.000
72	525.1765	525.1766	0.240	$C_{28}H_{29}O_{10}$	0.357	1.036
73	453.3949	453.3949	0.162	$C_{28}H_{53}O_{4}$	0.143	1.893
74	267.2330	267.2330	-0.146	$C_{17}H_{31}O_{2}$	0.118	1.824
75	329.1030	329.1031	0.180	$C_{18}H_{17}O_{6}$	0.333	0.944
76	481.4261	481.4262	0.286	$C_{30}H_{57}O_{4}$	0.133	1.900
77	415.1397	415.1398	0.399	$C_{22}H_{23}O_{8}$	0.364	1.045
78	411.3478	411.3480	0.333	$C_{25}H_{47}O_{4}$	0.160	1.880
79	507.1295	507.1297	0.320	$C_{27}H_{23}O_{10}$	0.370	0.852