

**Table S1** Summary table of correlation coefficients between agglomerative hierarchical clusters and phytochemical variables within a PCA of consumer liking scores.

Variables	Mouthfeel liking C1	Mouthfeel liking C2 <sup>*A</sup>	Mouthfeel liking C3	Taste liking C1*	Taste liking C2	Purchase intent C1	Purchase intent C2 <sup>*A</sup>	Purchase intent C3	Bitter perception C1*	Bitter perception C2 <sup>*A</sup>	Hotness perception C1 <sup>*A</sup>	Hotness perception C2*	Hotness perception C3 <sup>*A</sup>	Sweetness perception C2 <sup>*A</sup>	Sweetness perception C3*	Pepper perception C1*	Pepper perception C3 <sup>*A</sup>
<i>Glucosinolates</i>																	
4-hydroxyglucobrassicin	-0.206	-0.670	0.289	-0.190	-0.098	-0.249	0.702	-0.683	-0.375	-0.206	0.317	0.455	<b>0.805</b>	-0.400	<b>-0.826</b>	0.663	0.203
Glucotropaeolin	0.441	<b>0.789</b>	<b>-0.854</b>	0.686	-0.603	0.551	-0.339	0.555	0.223	-0.600	-0.166	-0.127	-0.295	0.159	0.272	-0.043	-0.053
Glucoraphanin	0.344	0.190	0.042	0.261	0.199	0.521	-0.102	-0.210	-0.742	0.135	-0.232	-0.133	0.195	0.535	0.115	-0.095	0.490
Glucoberverin	-0.273	0.454	0.019	-0.214	0.331	-0.001	-0.228	0.082	0.256	0.648	0.246	-0.705	-0.365	0.489	0.364	-0.481	-0.332
Glucosativin	<b>-0.766</b>	-0.737	0.407	-0.678	-0.006	<b>-0.841</b>	0.365	-0.484	0.300	0.540	0.730	-0.315	0.420	-0.344	-0.532	-0.020	-0.125
DMB	0.095	-0.432	0.093	-0.055	-0.184	-0.021	-0.105	-0.330	-0.630	0.358	-0.038	-0.186	0.431	0.557	-0.318	0.042	0.328
Glucosylsucin	0.107	-0.370	0.167	-0.067	-0.028	0.015	0.544	-0.403	-0.387	-0.344	-0.125	<b>0.764</b>	0.444	-0.041	-0.656	<b>0.896</b>	-0.217
Glucorucin	0.306	0.491	-0.394	0.358	-0.198	0.521	-0.402	0.045	-0.455	0.269	-0.071	-0.614	0.016	<b>0.894</b>	0.186	-0.291	0.236
Glucoraphenin	0.397	0.140	-0.180	0.265	-0.140	0.416	-0.385	-0.012	-0.640	0.244	-0.300	-0.292	0.084	<b>0.851</b>	0.089	-0.134	0.295
Glucobarin	0.070	-0.468	0.330	-0.044	0.144	-0.252	-0.364	0.230	0.017	0.036	-0.292	0.055	-0.165	-0.514	0.441	-0.590	0.648
Total GSL	-0.447	-0.671	0.288	-0.452	-0.115	-0.503	0.170	-0.557	-0.241	0.628	0.504	-0.427	0.570	0.216	-0.541	-0.021	0.144
<i>Flavonols</i>																	
Myricetin	0.517	0.518	-0.440	0.638	-0.209	0.504	-0.521	0.591	0.040	-0.491	-0.422	-0.062	-0.387	-0.163	0.667	-0.495	0.528
Kaempferol-3-glucoside	-0.115	-0.261	-0.064	-0.202	-0.290	-0.185	0.003	-0.239	-0.197	0.373	0.166	-0.220	0.271	0.598	-0.450	0.245	-0.278
Isorhamnetin-3-glucoside	-0.463	-0.312	0.066	-0.334	-0.162	-0.487	-0.250	-0.119	0.181	0.708	0.516	<b>-0.859</b>	0.126	0.155	-0.014	-0.611	0.187
Kaempferol-3,4'-diglucoside	0.121	0.167	-0.169	0.049	-0.118	0.176	-0.410	0.023	-0.311	0.504	-0.056	-0.566	-0.042	<b>0.869</b>	0.110	-0.279	0.021
Isorhamnetin-3,4'-diglucoside	0.229	-0.304	0.275	0.044	0.170	0.181	-0.111	-0.287	-0.748	0.254	-0.240	-0.035	0.306	0.355	-0.011	-0.119	0.597
Kaempferol-3-diglucoside-7-glucoside	0.078	-0.199	0.534	-0.242	0.620	-0.085	-0.293	0.138	-0.118	0.372	-0.446	0.117	-0.384	0.049	0.501	-0.384	0.122
Quercetin-3,3',4'-triglucoside	-0.152	0.148	0.314	-0.142	0.544	-0.095	-0.296	0.252	0.302	0.320	-0.041	-0.321	-0.469	-0.298	0.705	<b>-0.767</b>	0.241
Kaempferol-3-(2-sinapoyl-glucoside)-4'-glucoside	-0.504	-0.010	0.196	-0.380	0.250	-0.529	-0.288	0.306	<b>0.782</b>	0.470	0.322	-0.565	-0.485	-0.413	0.511	<b>-0.793</b>	-0.104
Quercetin-3,4'-diglucoside-3'-(6-caffeoyl-glucoside)	-0.156	-0.355	0.517	-0.362	0.465	-0.292	-0.346	0.000	-0.092	0.674	-0.114	-0.329	-0.198	0.118	0.395	-0.629	0.280
Total Flav.	-0.026	-0.164	0.255	-0.185	0.236	-0.074	-0.398	-0.034	-0.278	0.664	-0.092	-0.485	-0.086	0.493	0.281	-0.531	0.266
<i>Amino acids</i>																	
Alanine	0.191	0.453	0.115	0.121	0.499	0.323	-0.370	0.303	-0.017	0.182	-0.322	-0.197	-0.503	0.150	0.725	-0.552	0.174
Valine	0.456	0.217	0.170	0.276	0.418	0.506	-0.143	0.074	-0.495	-0.145	-0.545	0.289	-0.151	0.129	0.405	-0.098	0.396
Leucine	0.177	0.699	-0.465	0.360	-0.160	0.564	-0.180	-0.031	-0.300	0.174	0.147	-0.632	0.051	<b>0.773</b>	0.099	-0.167	0.071
Threonine	0.533	0.591	-0.179	0.498	0.195	<b>0.755</b>	-0.185	0.115	-0.507	-0.212	-0.427	0.043	-0.127	0.398	0.383	-0.081	0.336
Serine	0.129	0.750	-0.495	0.395	-0.162	0.533	0.288	-0.035	0.017	-0.422	0.194	-0.015	0.075	0.147	-0.134	0.366	-0.243
Proline	-0.510	-0.378	0.369	-0.537	0.232	-0.716	-0.381	0.230	0.617	0.674	0.225	-0.539	-0.398	-0.282	0.416	<b>-0.803</b>	-0.034
Asparagine	0.268	-0.239	0.423	0.026	0.452	0.026	-0.129	0.222	-0.091	-0.245	-0.578	0.579	-0.287	-0.513	0.448	-0.170	0.366
Aspartic Acid	0.585	0.449	-0.167	0.544	0.114	0.719	-0.286	0.146	-0.573	-0.235	-0.480	0.024	-0.080	0.312	0.426	-0.208	0.573
Glutamic Acid	0.281	0.380	-0.020	0.148	0.256	0.388	-0.440	0.172	-0.316	0.348	-0.327	-0.336	-0.303	0.667	0.476	-0.394	0.124
Glutamine	0.646	0.494	-0.196	0.573	0.117	0.680	-0.451	0.398	-0.367	-0.323	-0.636	0.100	-0.333	0.178	0.644	-0.333	0.515
Total AA	0.449	0.657	-0.202	0.450	0.208	0.664	-0.354	0.264	-0.301	-0.076	-0.379	-0.174	-0.307	0.383	0.576	-0.347	0.309
<i>Free sugars</i>																	
Fructose	-0.047	0.191	-0.240	-0.016	-0.177	-0.283	-0.547	<b>0.755</b>	<b>0.850</b>	-0.038	-0.153	-0.170	-0.749	-0.270	0.578	-0.511	-0.343
Glucose	-0.506	-0.309	-0.036	-0.336	-0.297	-0.619	-0.187	0.057	0.530	0.444	0.518	-0.637	-0.006	-0.159	-0.045	-0.467	-0.057
Galactose	-0.267	-0.091	-0.157	-0.208	-0.282	-0.505	-0.483	0.485	0.733	0.280	0.131	-0.452	-0.458	-0.120	0.309	-0.545	-0.263
Sucrose	0.221	0.227	-0.473	0.253	-0.470	0.529	-0.150	0.519	0.486	-0.570	-0.241	0.359	0.350	-0.188	0.047	0.263	-0.447
Total Sugar	-0.342	-0.146	-0.175	-0.214	-0.355	-0.533	-0.329	0.342	0.699	0.234	0.287	-0.459	-0.274	-0.196	0.131	-0.439	-0.222
<i>Organic acids</i>																	
Malic Acid	0.463	-0.053	-0.064	0.446	-0.095	0.280	-0.356	0.299	-0.259	-0.419	-0.464	0.187	-0.073	-0.360	0.434	-0.382	<b>0.823</b>
Citric Acid	0.528	<b>0.879</b>	-0.718	0.593	-0.338	0.612	-0.348	0.641	0.228	-0.557	-0.424	0.125	-0.538	0.331	0.377	0.115	-0.388
Total OA	0.683	0.329	-0.374	0.695	-0.240	0.540	-0.501	0.571	-0.156	-0.653	-0.640	0.238	-0.305	-0.210	0.589	-0.325	0.640
<i>Headspace VOCs</i>																	
(E)-4-oxohex-2-enal (C1)	0.527	0.006	-0.167	0.434	-0.178	0.180	-0.459	0.637	0.115	-0.631	-0.676	0.472	-0.419	-0.494	0.544	-0.255	0.417
4-isothiocyanato-1-butene (C2)	0.246	-0.057	-0.190	0.189	-0.309	0.279	-0.202	-0.246	-0.701	0.283	-0.045	-0.367	0.389	<b>0.818</b>	-0.230	0.005	0.340
1-penten-3-ol (C3)	0.176	<b>0.809</b>	-0.196	0.170	0.321	0.393	-0.218	0.446	0.326	-0.062	-0.260	-0.034	-0.669	0.244	0.567	-0.142	-0.480
1-penten-3-one (C4)	0.183	0.460	0.024	0.116	0.386	0.260	0.153	0.308	0.315	-0.476	-0.350	0.607	-0.481	-0.332	0.311	0.273	-0.440
2-(1,1-dimethylethyl)-1H-indole (C5)	-0.179	0.031	0.387	-0.295	0.538	0.116	0.510	-0.584	-0.412	0.341	0.172	0.103	0.292	0.391	-0.353	0.447	-0.296
2-methyl-2-butenal (C6)	-0.362	0.515	0.023	-0.254	0.369	0.054	0.241	-0.186	0.233	0.430	0.418	-0.401	-0.134	0.394	-0.023	0.053	-0.627
2-hexenal (C7)	-0.269	0.455	0.049	-0.223	0.371	0.097	0.469	-0.231	0.199	0.123	0.290	0.050	-0.071	0.230	-0.210	0.455	<b>-0.783</b>
(E)-2-hexenal (C8)	-0.333	0.539	-0.035	-0.250	0.313	0.004	0.072	-0.004	0.374	0.446	0.331	-0.437	-0.309	0.412	0.111	-0.060	-0.701
(Z)-2-penten-1-ol (C9)	-0.154	0.577	0.022	-0.161	0.432	0.177	0.168	-0.019	0.208	0.245	0.111	-0.107	-0.312	0.391	0.105	0.158	-0.706
(E)-2-pentenal (C10)	-0.174	0.289	0.143	-0.198	0.401	0.011	0.523	-0.074	0.348	-0.228	0.063	0.515	-0.185	-0.231	-0.151	0.582	<b>-0.772</b>
(E,E)-2,4-hexadienal (C11)	-0.148	0.561	-0.076	-0.132	0.280	0.172	-0.001	-0.010	0.132	0.412	0.163	-0.381	-0.267	0.614	0.115	-0.009	-0.596
5-ethyl-2(5H)-furanone (C12)	-0.037	0.260	0.068	-0.235	0.290	-0.035	-0.027	0.206	0.306	0.170	-0.199	0.190	-0.478	0.341	0.119	0.236	<b>-0.840</b>
3-hexen-1-ol (C14)	0.611	0.435	-0.295	0.627	-0.059	0.555	-0.416	0.541	-0.089	-0.603	-0.596	0.245	-0.374	-0.231	0.636	-0.313	0.519
3-hexenal (C15)	0.258	<b>0.792</b>	-0.226	0.317	0.256	0.631	0.136	0.057	-0.115	-0.247	-0.140	0.109	-0.196	0.306	0.182	0.232	-0.263
(Z)-3-hexenal (C16)	<b>-0.810</b>	0.004	0.530	-0.711	0.691	-0.488	0.390	-0.384	0.457	<b>0.760</b>	0.696	-0.479	-0.060	-0.121	-0.030	-0.217	-0.483
3-octyne (C17)	0.316	0.086	0.208	0.219	0.379	0.239	-0.252	0.292	-0.097	-0.232	-0.481	0.258	-0.323	-0.384	0.611	-0.400	0.515
3-pentanone (C18)	0.430	0.347	-0.227	0.294	-0.027	0.300	-0.019	0.468	0.226	-0.694	-0.575	<b>0.773</b>	-0.451				

5-nonanone oxime (C21)	0.144	-0.416	0.124	0.092	-0.119	0.038	0.557	-0.369	-0.365	-0.589	-0.084	<b>0.790</b>	0.536	-0.445	-0.582	0.746	0.172
1-isothiocyanato-3-methylbutane (C23)	-0.485	-0.595	0.554	-0.480	0.304	-0.337	<b>0.937</b>	<b>-0.913</b>	-0.315	0.117	0.540	0.346	<b>0.794</b>	-0.317	<b>-0.869</b>	0.701	-0.071
Ethylidene-cyclopropane (C24)	-0.231	0.061	0.168	-0.413	0.272	-0.233	-0.009	0.046	0.285	0.444	0.008	-0.042	-0.332	0.413	-0.006	0.139	<b>-0.798</b>
2-ethyl-furan (C26)	0.002	-0.462	0.045	-0.166	-0.270	-0.202	-0.117	-0.198	-0.339	0.341	-0.019	-0.116	0.282	0.498	-0.354	0.129	0.000
3-methyl-furan (C27)	0.310	0.410	-0.161	0.224	0.105	0.162	<b>-0.846</b>	<b>0.793</b>	0.332	0.104	-0.520	-0.303	<b>-0.840</b>	0.120	<b>0.979</b>	<b>-0.841</b>	0.128
Hexyl isothiocyanate (C29)	-0.327	-0.699	0.132	-0.205	-0.346	-0.433	0.201	-0.476	-0.214	0.217	0.489	-0.277	0.681	-0.203	-0.541	-0.031	0.483
2-oxo-methyl ester hexanoic acid (C30)	-0.136	0.088	0.135	-0.349	0.267	-0.318	-0.339	0.471	0.610	0.325	-0.235	0.006	-0.732	0.133	0.411	-0.200	-0.739
Pentyl isothiocyanate (C31)	-0.565	-0.613	0.151	-0.383	-0.273	-0.543	0.471	-0.618	-0.016	0.281	0.749	-0.280	0.717	-0.208	-0.750	0.202	0.087
Iberverin (C33)	-0.372	-0.608	0.101	-0.219	-0.334	-0.335	0.514	-0.710	-0.321	0.138	0.626	-0.147	<b>0.881</b>	-0.096	<b>-0.844</b>	0.356	0.263
Propanoic acid anhydride (C34)	-0.504	0.116	0.201	-0.546	0.340	-0.396	-0.045	0.021	0.511	0.709	0.323	-0.456	-0.368	0.328	0.103	-0.199	-0.751
4-methyl-2-(2-methyl-propenyl)-pyridine (C35)	-0.529	0.214	0.364	-0.527	0.624	-0.177	0.471	-0.370	0.242	0.513	0.443	-0.151	-0.061	0.187	-0.165	0.219	-0.734
Pyrrolidine-1-dithiocarboxylic acid 2-oxocyclopentyl ester (C36)	-0.323	-0.702	0.136	-0.246	-0.346	-0.386	0.381	-0.633	-0.340	0.204	0.508	-0.140	<b>0.809</b>	-0.029	<b>-0.778</b>	0.285	0.278
3-ethyl-thiophene (C37)	-0.180	0.149	0.125	-0.210	0.256	0.073	-0.025	-0.308	-0.288	0.676	0.237	-0.563	0.103	0.720	-0.042	-0.157	-0.108
Tetrahydrothiophene (C38)	-0.276	<b>-0.790</b>	0.212	-0.225	-0.295	-0.412	0.361	-0.571	-0.319	0.095	0.404	0.002	<b>0.765</b>	-0.243	-0.689	0.235	0.405
[Unknown 2] (C39)	-0.437	0.461	0.099	-0.334	0.434	-0.030	0.299	-0.206	0.308	0.446	0.454	-0.358	-0.148	0.293	-0.036	0.067	-0.681
[Unknown 8] (C40)	-0.469	-0.018	0.032	-0.255	-0.021	-0.070	<b>0.757</b>	<b>-0.787</b>	-0.204	0.224	<b>0.775</b>	-0.216	0.714	0.218	<b>-0.832</b>	0.587	-0.295
[Unknown 9] (C41)	-0.253	0.165	0.054	-0.336	0.178	-0.160	-0.182	0.021	0.184	0.659	0.153	-0.481	-0.266	0.633	0.085	-0.170	-0.554
Vinylfuran (C42)	0.358	0.036	-0.205	0.183	-0.225	0.126	0.048	0.290	0.096	-0.592	-0.476	<b>0.764</b>	-0.198	-0.063	-0.129	0.615	-0.460
<i>Polyatomic ions</i>																	
Chloride	0.068	-0.739	0.189	-0.014	-0.270	-0.144	0.267	-0.469	-0.592	-0.133	0.014	0.313	0.707	-0.140	-0.588	0.359	0.531
Nitrate	0.382	0.090	0.194	0.202	0.356	0.428	0.350	-0.137	-0.433	-0.506	-0.454	<b>0.817</b>	0.077	-0.142	-0.066	0.564	0.041
Phosphate	-0.237	-0.556	0.659	-0.354	0.508	-0.248	0.725	-0.560	-0.210	-0.148	0.096	0.698	0.421	-0.642	-0.435	0.529	0.065
Sulphate	-0.041	-0.213	0.515	-0.256	0.572	-0.064	0.563	-0.241	-0.044	-0.268	-0.205	<b>0.871</b>	0.020	-0.441	-0.199	0.618	-0.331
<i>Compound ratios</i>																	
Total Sugar:GSL ratio	0.194	0.550	-0.555	0.362	-0.356	0.131	-0.488	0.751	0.650	-0.371	-0.174	-0.155	-0.623	-0.190	0.551	-0.384	-0.165
Glucose:GSL	0.096	0.528	-0.521	0.319	-0.334	0.091	-0.458	0.659	0.635	-0.263	-0.034	-0.312	-0.540	-0.201	0.529	-0.479	-0.073
Fructose:GSL	0.307	0.588	-0.492	0.398	-0.230	0.210	-0.533	<b>0.838</b>	0.619	-0.444	-0.366	0.009	-0.748	-0.219	0.683	-0.379	-0.164
Galactose:GSL	0.063	0.358	-0.427	0.162	-0.317	-0.107	-0.636	<b>0.791</b>	0.753	-0.089	-0.152	-0.313	-0.715	-0.124	0.614	-0.573	-0.221
Sucrose:GSL	0.431	0.569	-0.623	0.521	-0.428	0.377	-0.191	0.600	0.362	<b>-0.761</b>	-0.360	0.367	-0.413	-0.133	0.224	0.222	-0.299
Sugar:ITC ratio	0.227	0.637	-0.567	0.292	-0.306	0.153	-0.603	<b>0.820</b>	0.649	-0.194	-0.279	-0.202	<b>-0.777</b>	0.151	0.595	-0.349	-0.436
Acid:sugar ratio	0.534	0.155	0.056	0.386	0.215	0.591	0.217	-0.108	-0.614	-0.547	-0.514	0.699	0.144	-0.009	-0.015	0.459	0.286

Numbers in bold indicate a significant correlation (Pearson  $n-1$ ); green = significance at  $P<0.05$ ; orange = significance at  $P<0.01$ . \* = significant differences observed between rocket accessions; ^ = agglomerative hierarchical cluster with <20 individuals