

# **A Chemometrics-driven Strategy for the Bioactivity Evaluation of Complex Multicomponent Systems and the Effective Selection of Bioactivity-predictive Chemical Combinations**

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The authors declare no conflict of interest.

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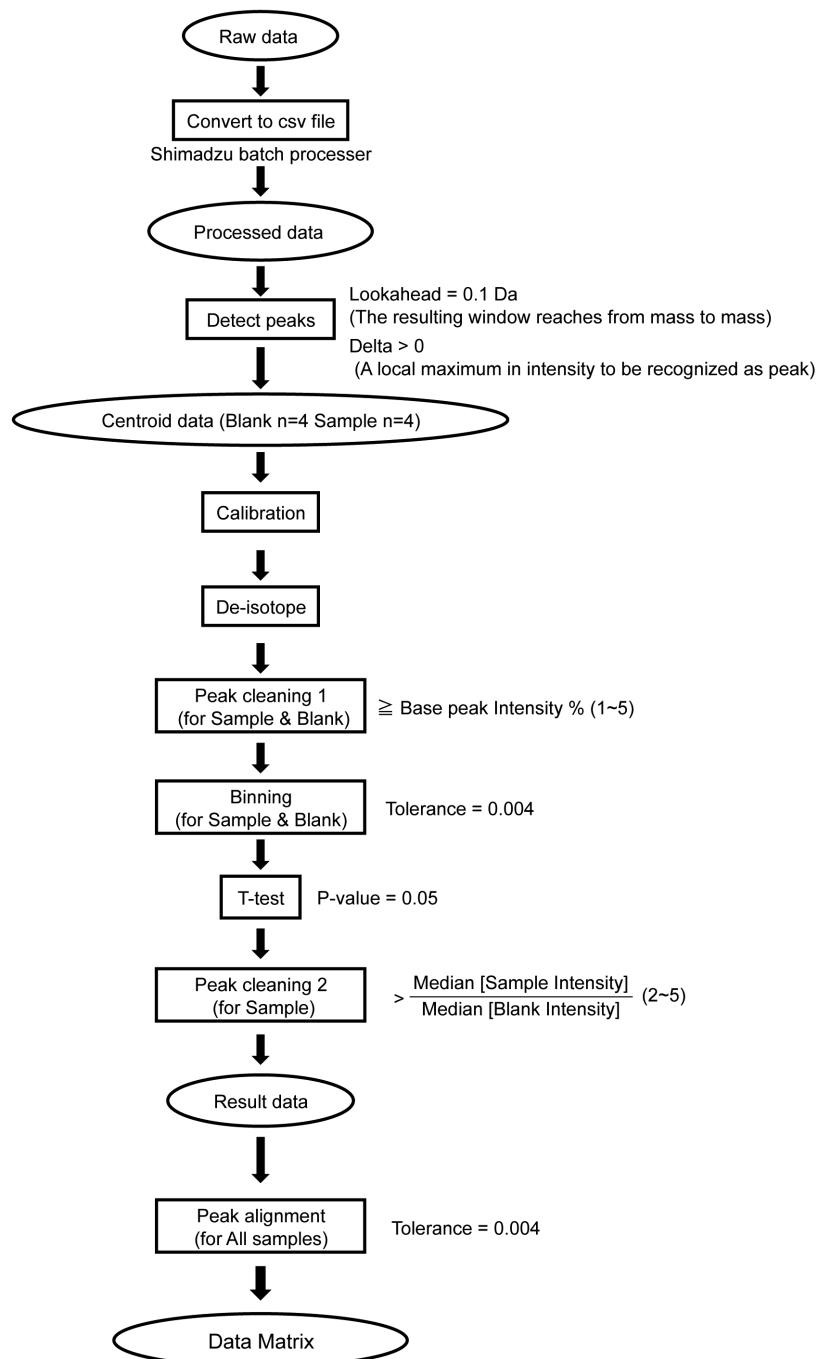
**Supplementary Table S6.** Selected peaks with the highest VIP values ( $>1$ ) contributing to the construction of OPLS regression models in LC–MS datasets.

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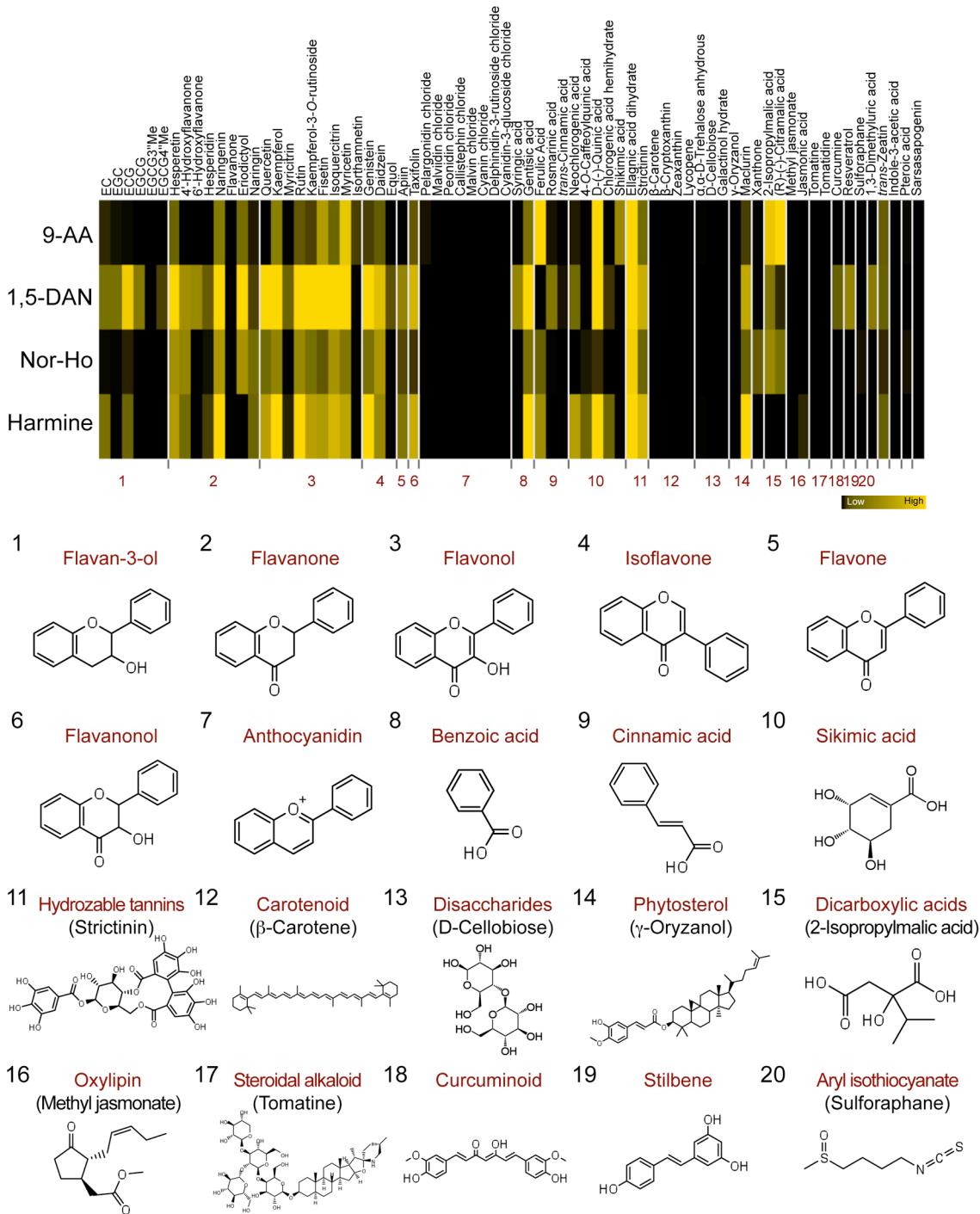
## Supplementary methods

**LC–MS analysis.** All GTEs were subjected to LC–MS analysis using a LCMS-IT-TOF instrument (Shimadzu, Kyoto, Japan). The instrument was fitted with a Luna C18(2) column (250 mm × 1.0 mm, 5 µm particle size, Phenomenex, Torrance, CA) maintained at 40°C. The mobile phase solvents were 0.1% aqueous formic acid (solvent A) and methanol (solvent B). Solvent B was 5% for 2.0 min, increased linearly from 5% to 60% over 6.0 min, and further increased from 60% to 100% at 13.0 min, and 100% holding for 4.5 min. Flow rate was constant (0.1 mL/min). The MS instrument was operated using an ESI source in both positive and negative ionization modes with survey scans acquired from *m/z* 100 to 700. Ionization parameters were as follows: capillary voltage, 4.5 kV and –3.5 kV; nebulizer gas flow, 1.5 L/min; CDL temperature, 250°C; heat block temperature, 250°C. Individual GTEs were diluted 1:50 in distilled water, and then 2.5 µM 4 hydroxybenzophenone was added as an internal standard. Samples were filtered through a 0.22-µm PTFE filter, and 5 µL was injected onto the column for each run.

## Supplementary Figures and Tables

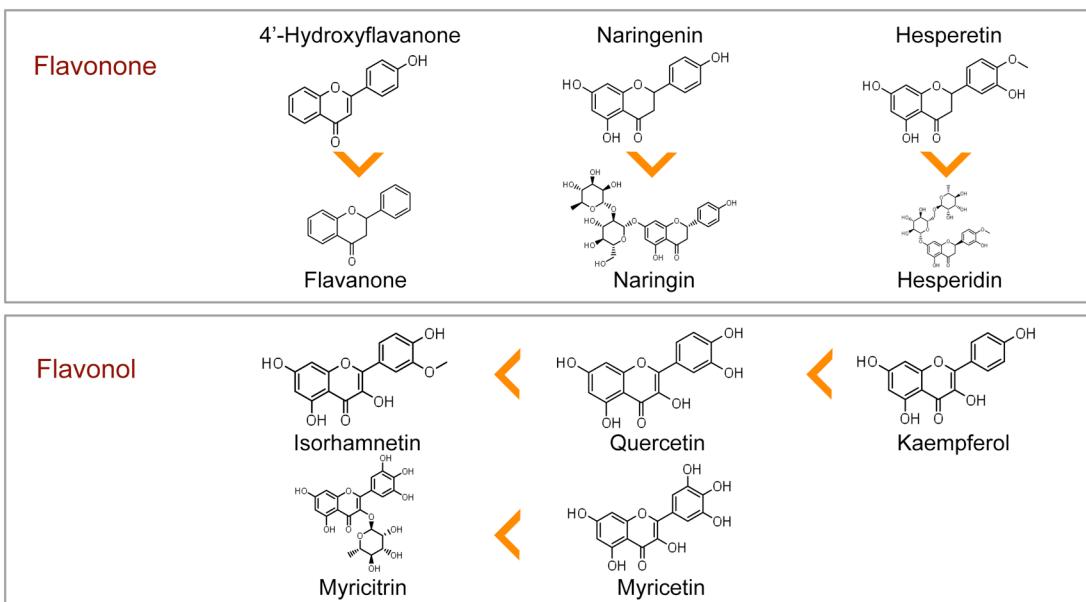


**Supplementary Figure S1.** The schematic flow of the peak picking and alignment of non-targeted MALDI-MS data.

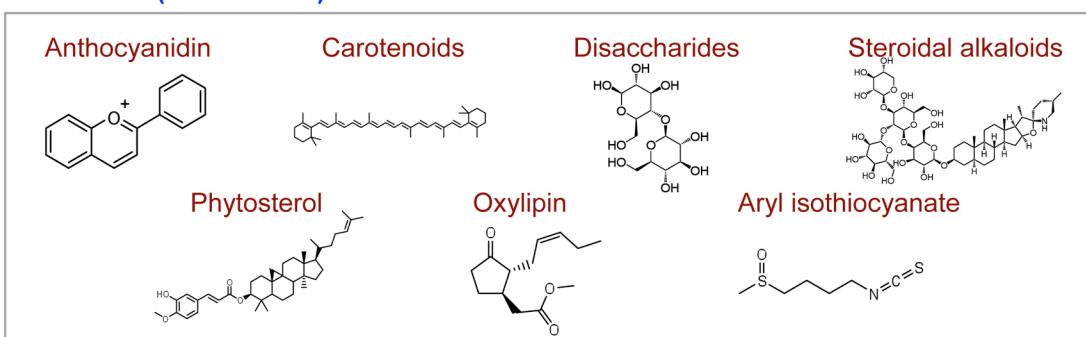


**Supplementary Figure S2. Heatmap representation of the ionization of the representative phytochemicals by MALDI-MS using four matrices dissolved in MeOH solution.** Heatmap analysis showing the different ionization rates of the 72 phytochemicals by the 4 matrices dissolved in 100% MeOH solution. In addition, 20 representative chemical structures of phytochemicals are illustrated.

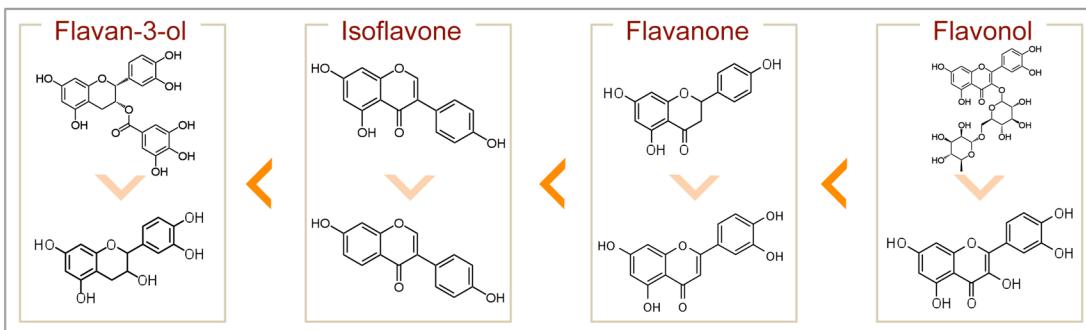
### A Detection (High)



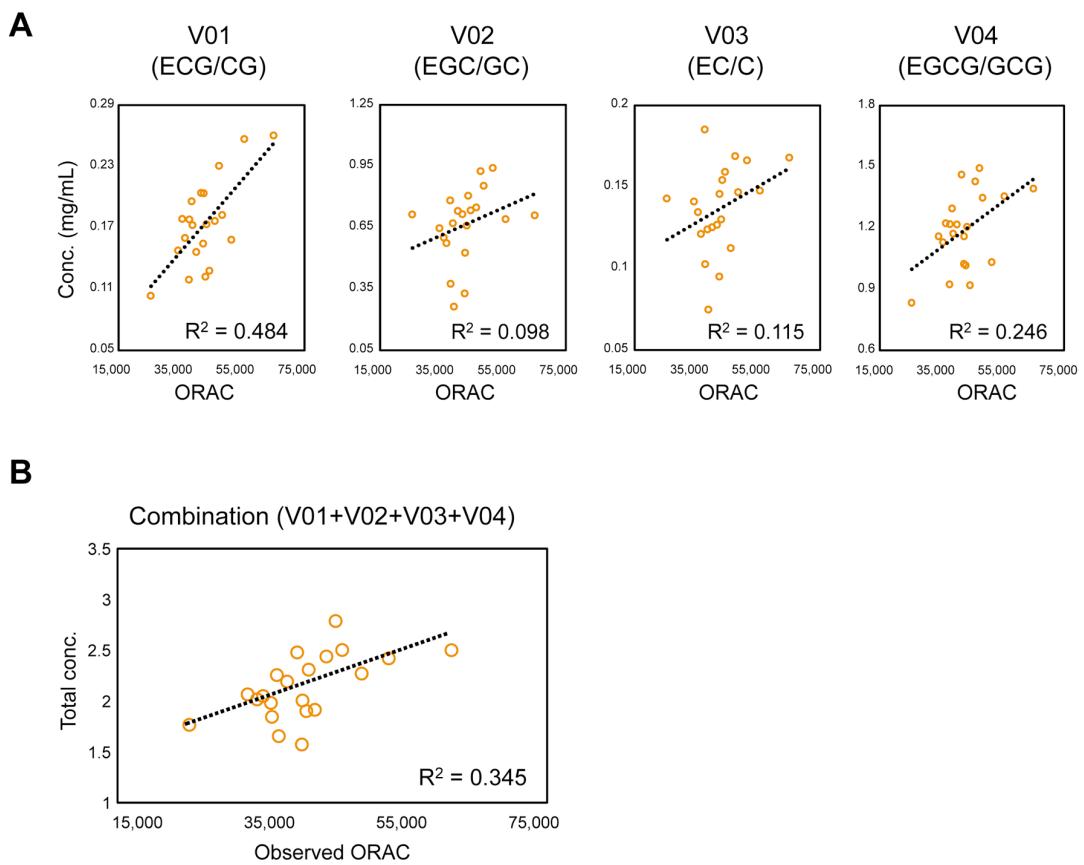
### Detection (Zero or Low)



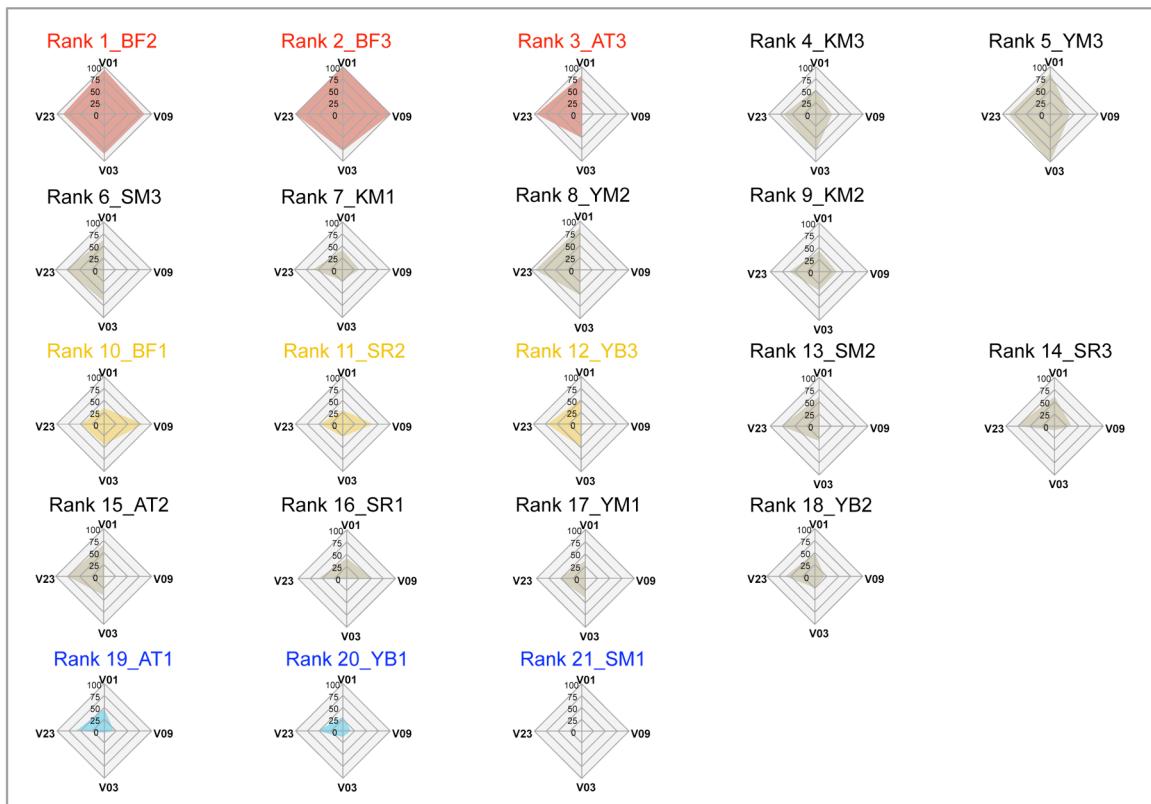
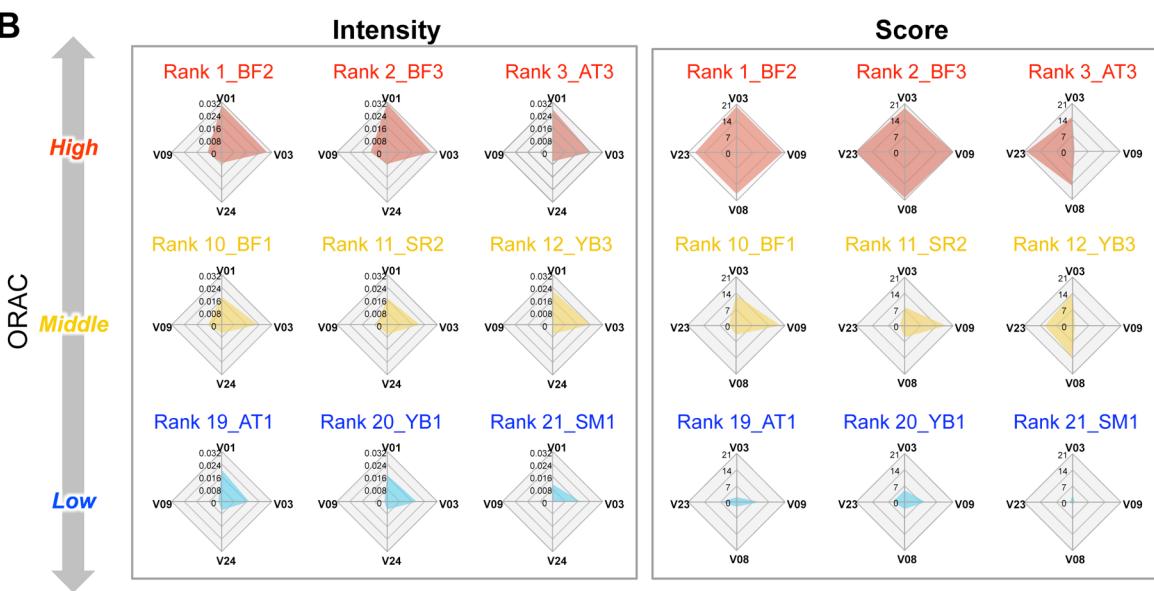
### B 1,5-DAN



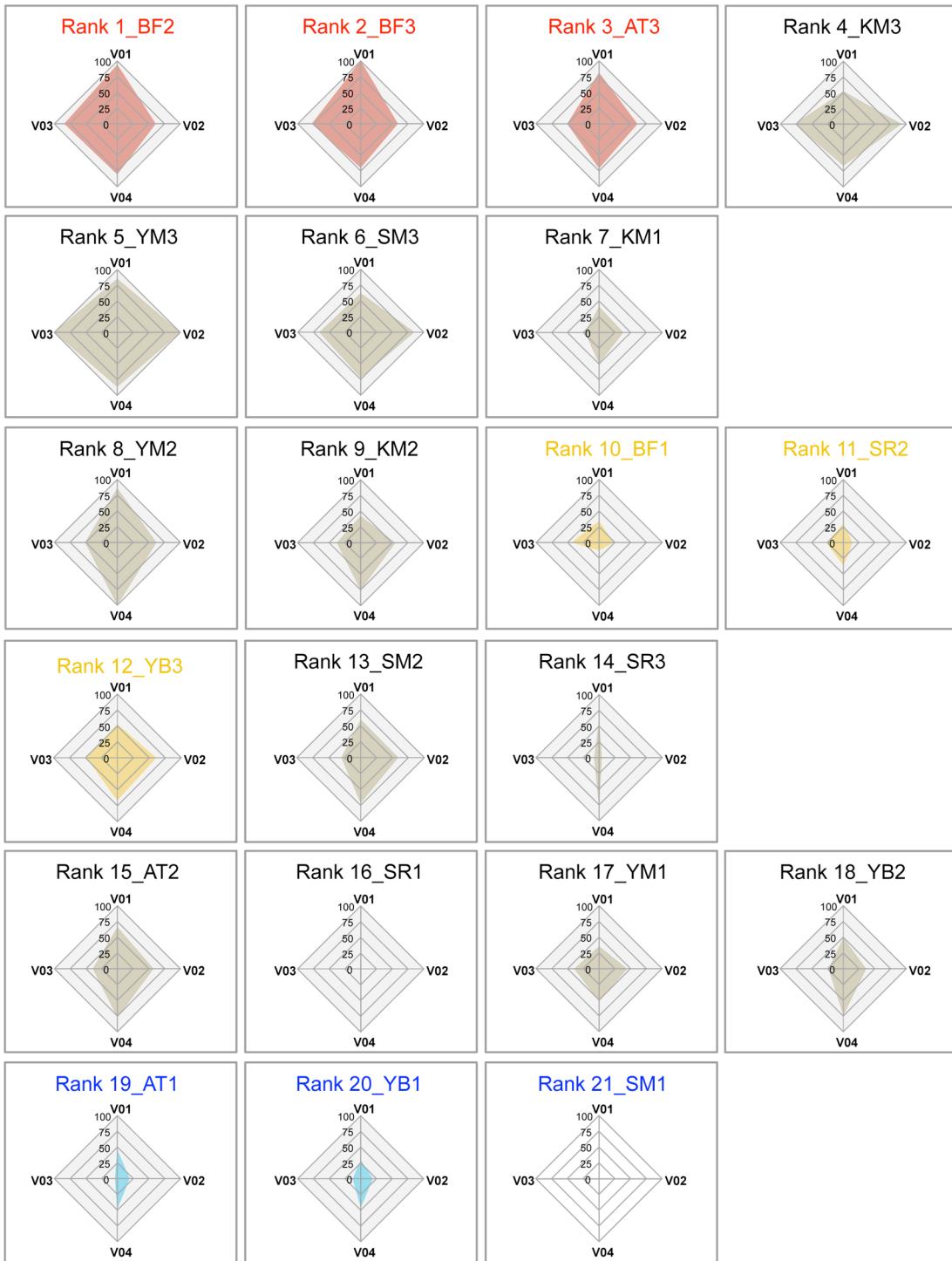
**Supplementary Figure S3. The representative relationship between the chemical structure and the ionization efficiency of phytochemicals.** Among the phytochemicals with different detectability, their representative relationships with the ionization efficiency are shown under conditions observed in (A) four matrices or (B) 1,5-DAN alone. The ionization efficacy of the phytochemicals is partially dependent on the position and the number of glycosylation, methylation, and hydroxylation.



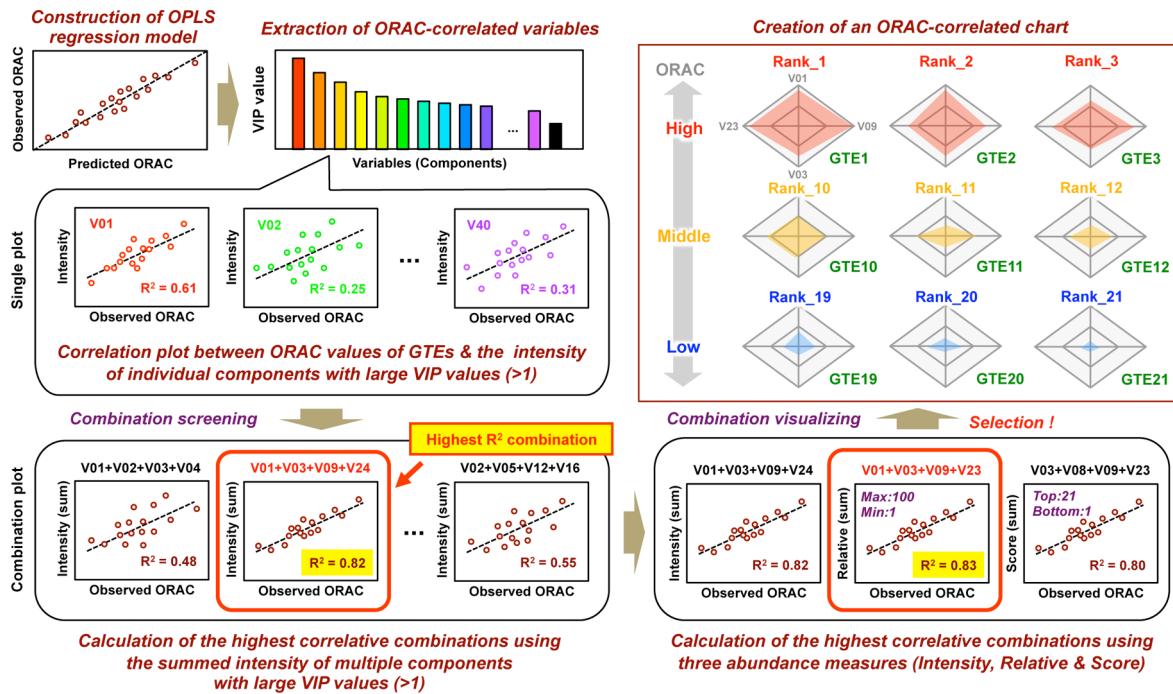
**Supplementary Figure S4. The correlation plot of the highest VIP-valued compounds at the concentration level of GTEs.** (A) Correlations between ORAC and the concentration of each of the top-4 components with the largest VIP values ( $>1$ ). (B) Correlations between ORAC and the summed concentrations of the top-4-VIP components.

**A****B**

**Supplementary Figure S5. The chart visualization of the observed ORAC values of GTEs using the selected combinations with the highest correlation values.** (A) Observed ORAC values of GTEs visualized as radar charts using information from the 4 selected components (V01+V03+V09+V23). Charts for all GTEs are shown. (B) A representative section of the charts for nine GTEs is also illustrated using the Intensity data of the combination (V01+V03+V09+V24) or the Score data of the combination (V03+V08+V09+V23)



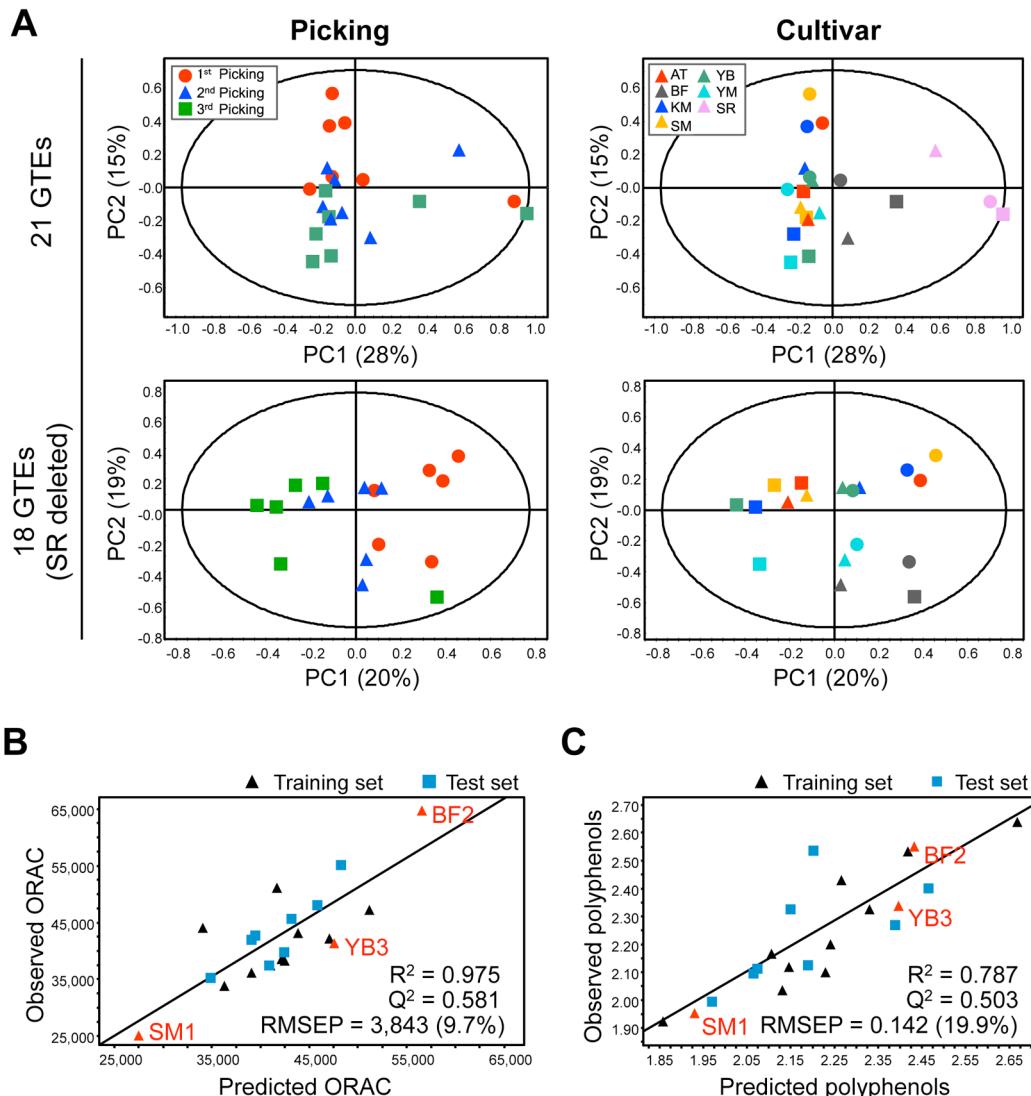
**Supplementary Figure S6. The chart visualization of the observed ORAC values of GTEs using the selected combination with low correlation value.** Observed ORAC values of GTEs visualized as radar charts using information from the 4 selected components (V01+V02+V03+V04) with low correlation value. Charts for all GTEs are shown.



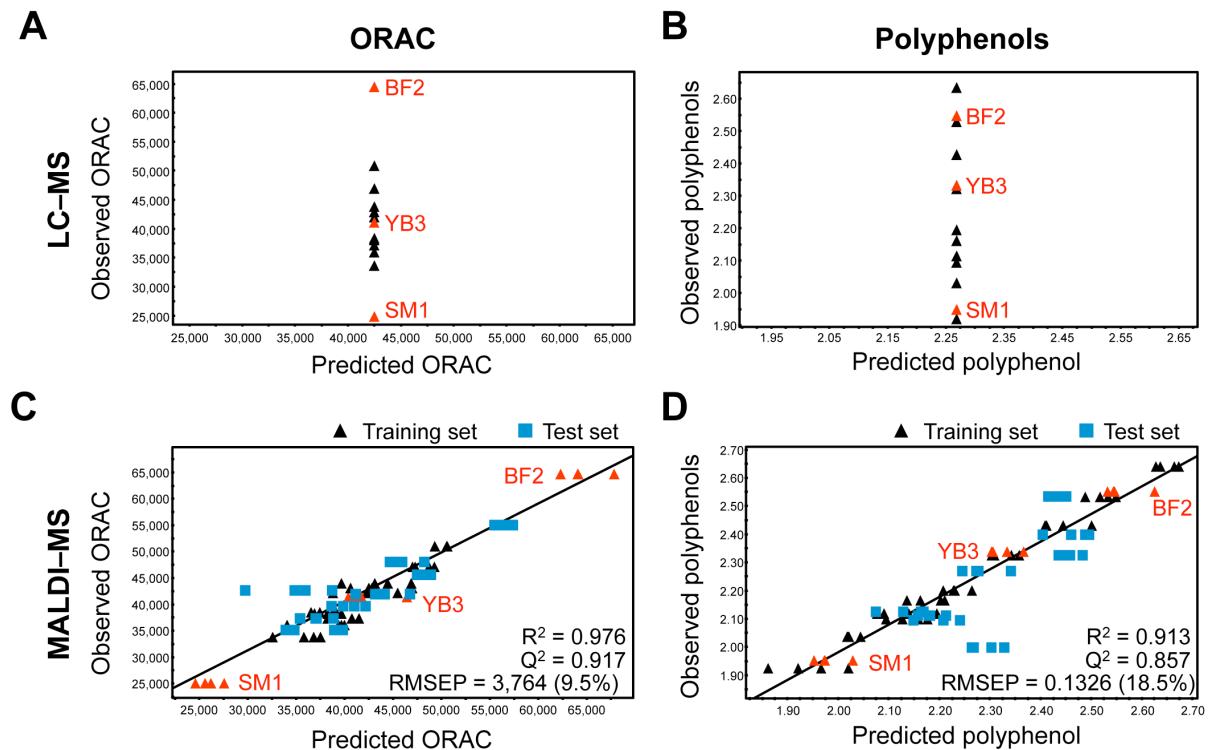
**Supplementary Figure S7. Scheme of chemometrics-driven selection of GTE bioactivity-correlated chemical combinations.**

<i>In View of Pharmaceutical, Nutraceutical, &amp; Food Functionality Researches</i>		<i>In View of Metabolomics Research</i>	
	Conventional strategy	Novel strategy (MALDI-MS-MP)	Conventional strategy (LC-MS-MP or GC-MS-MP)
Evaluation target	Single	Multiple	
Evaluation unit	Absolute quantity	Compositional balance	
Narrowing candidate components contributed to bioactivity	Multiple steps	One step	
Decision process of combination of multiple components	Hypothesis or experiment-driven	Hypothesis-generating or data-driven	
Bioassay validation (Frequency; labor-intensive)	High	Low	
	○	✗	Direct analysis of crude sample
	◎	△	Rapid & high-throughput
	◎	△	Extensibility of sample number (>1,000)
	○	○	Theoretical presentation of combination for bioactivity
	△	◎	Detective performance of small molecules

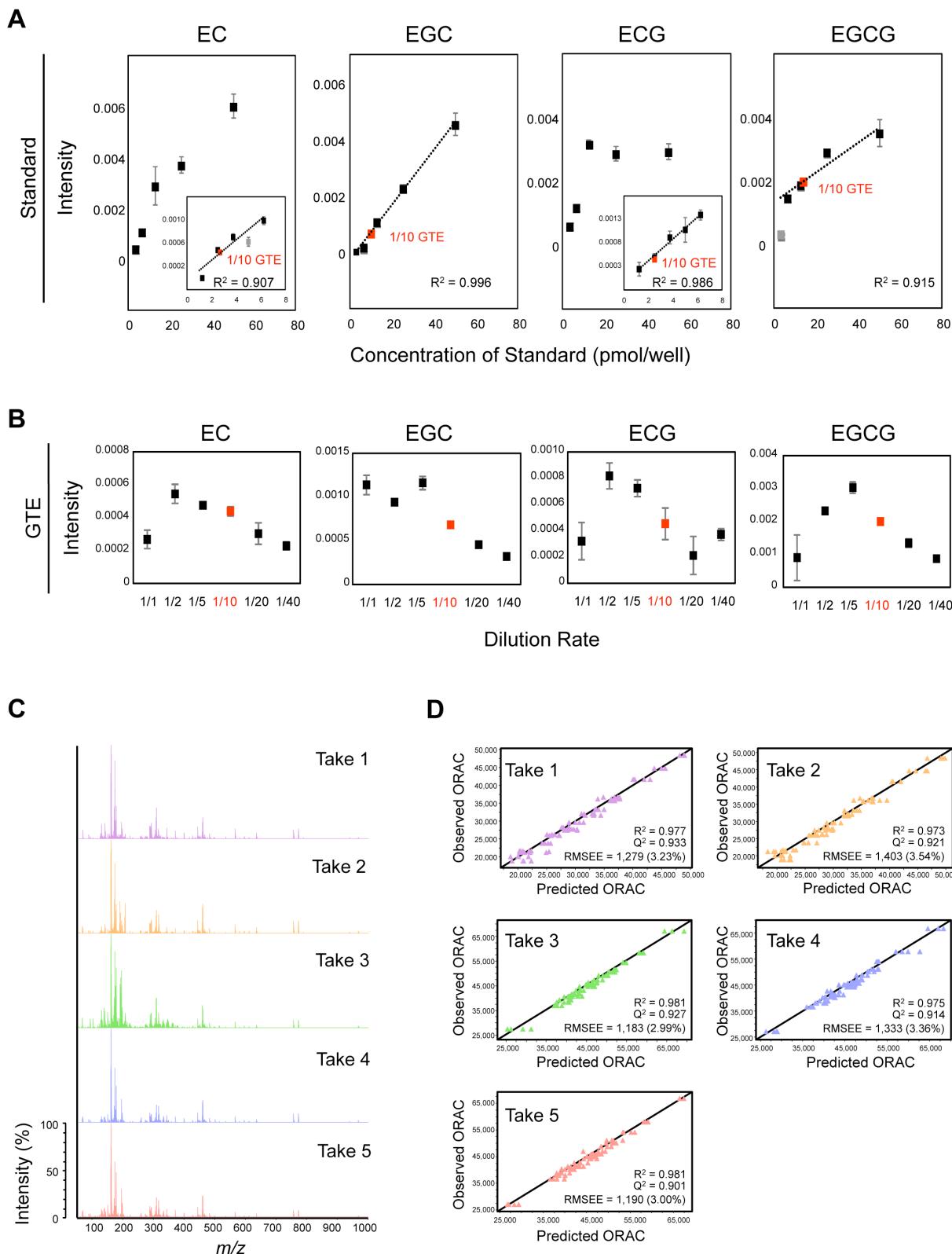
**Supplementary Figure S8. Comparison of the MALDI-MS-MP system with the conventional strategy in view of 2 distinct research fields.**



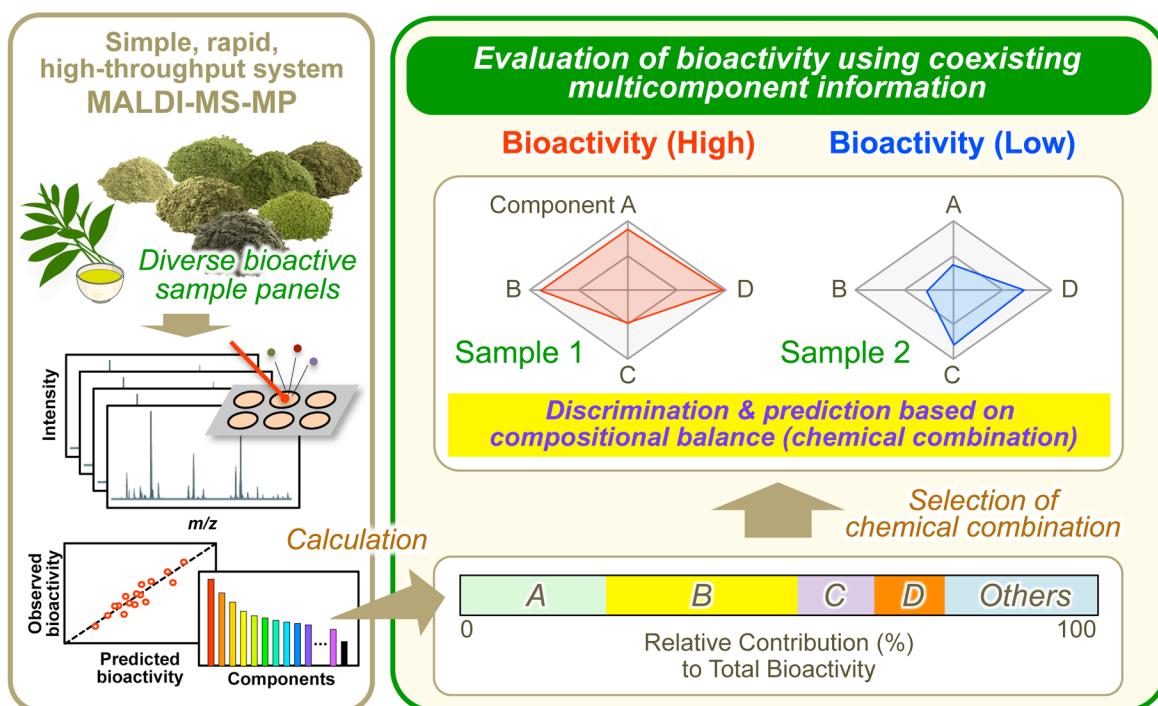
**Supplementary Figure S9. LC–MS-MP of 21 GTEs for evaluating their quality and bioactivity.** (A) PCA score plot of LC–MS datasets of 21 GTEs showing different clusters of MS profiles, based on the attributes of picking seasons and cultivars. (B) Models for predicting (B) ORAC or (C) total polyphenol content were calculated from the LC–MS datasets of 21 GTEs, including 13 training (black triangles) and 8 test (blue squares) sets.



**Supplementary Figure S10. The effect of components with the highest VIP values (>1) on the construction of OPLS regression models.** Models for predicting ORAC (A, C) or total polyphenol content (B, D) were calculated from the LC-MS (A, B) or MALDI-MS (C, D) datasets of 21 GTEs, including 13 training (black triangles) and 8 test (blue squares) sets. These models were constructed using datasets excluding components with the highest VIP values (>1).



**Supplementary Figure S11. The evaluation of the robustness of the present MALDI-MS-MP system.** (A) The calibration curve from the representative GTE components (EGCG, EGC, ECG, and EC at the standard level) in MALDI-MS system. In EC and EGCG, the coefficient of determination ( $R^2$ ) was calculated using datasets excluding the value of grey square symbol. Red square symbol indicates the data corresponding to 1/10 GTE sample. (B) Plots of these four compounds detected in a dilution series of the representative GTE (YB1). Data are shown as mean  $\pm$  SD ( $n=3-5$ ). (C) Verification of the repeatability of MS data acquired on a different day using the representative GTE (YB1). (D) OPLS regression models using such MS datasets.



**Supplementary Figure S12.** Graphical representation of MALDI-MS-MP system for the bioactivity evaluation of diverse bioactive sample panels representing multicomponent systems and the effective selection of bioactivity-predictive chemical combinations.

**Supplementary Table S1. The ionization rates of the representative phytochemicals for MALDI matrix screening.**

	<i>m/z</i>		Acetone				MeOH			
	Theoretical	Observed [M-H] <sup>-</sup>	9AA	1,5-DAN	Nor-Ho	Harmine	9AA	1,5-DAN	Nor-Ho	Harmine
EC	290.08	289.07	0.0016	0.0045	0.0006	0.0062	0.0011	0.0070	0.0005	0.0072
EGC	306.08	305.15	0.0003	0.0083	0.0001	0.0022	0.0005	0.0067	0.0003	0
ECG	442.09	441.17	0.0018	0.0123	0.0048	0.0058	0.0004	0.0282	0.0010	0.0046
EGCG	458.08	457.13	0.0002	0.0066	0.0009	0.0007	0	0.0092	0.0001	0
EGCG3'Me	472.10	471.12	0	0.0034	0.0002	0.0002	0	0	0.0001	0
EGCG4'Me	472.10	471.03	0	0.0033	0.0008	0.0004	0	0.0019	0.0001	0
Hesperetin	302.08	301.05	0.0095	0.0574	0.0154	0.0245	0.0049	0.0559	0.0147	0.0174
4'-Hydroxyflavanone	240.08	239.11	0.0026	0.0182	0.0086	0.0125	0	0.0144	0.0125	0.0060
6'-Hydroxyflavanone	240.08	239.07	0	0.0157	0.0001	0.0007	0	0.0127	0	0
Hesperidin	610.19	609.28	0.0008	0.0039	0.0005	0.0028	0	0.0036	0.0006	0.0018
Naringenin	272.07	271.09	0.0170	0.0524	0.0450	0.0444	0.0092	0.0683	0.0164	0.0582
Flavanone	224.08	223.10	0.0008	0.0010	0.0001	0	0	0	0.0001	0
Eriodictyol	288.07	287.12	0.0151	0.0500	0.0119	0.0658	0.0065	0.0520	0.0151	0
Naringin	580.18	579.23	0.0017	0.0059	0.0056	0.0033	0.0009	0.0020	0.0062	0.0049
Quercetin	302.04	301.08	0.0146	0.0364	0.0143	0.0245	0	0.0687	0.0054	0.0182
Kaempferol	286.05	285.09	0.0192	0.0559	0.0251	0.0399	0.0103	0.0538	0.0116	0.0344
Myricitrin	464.10	463.19	0.0012	0.0034	0.0004	0.0052	0	0.0045	0.0002	0.0009
Rutin	610.15	609.23	0.0112	0.0702	0.0189	0.0316	0.0030	0.0486	0.0126	0.0302
Kaempferol-3-O-rutinoside	594.16	593.23	0.0075	0.0410	0.0162	0.0183	0.0020	0.0328	0.0067	0.0185
Fisetin	286.05	285.10	0.0294	0.0339	0.0086	0.0183	0.0170	0.0372	0.0031	0.0168
Isoquercitrin	464.10	463.20	0.0165	0.0276	0.0179	0.0190	0.0048	0.0438	0.0151	0.0231
Myricetin	318.04	317.09	0.0275	0.0474	0.0179	0.0179	0.0264	0.0511	0.0088	0.0192
Iisorhamnetin	316.06	315.08	0.0017	0	0	0	0.0018	0	0	0
Genistein	270.05	269.11	0.0037	0.0488	0.0145	0.0221	0.0019	0.0448	0.0071	0.0427
Daidzein	254.06	253.10	0.0035	0.0289	0.0148	0.0112	0.0034	0.0247	0.0159	0.0125
Equol	242.09	241.08	0	0.0080	0	0	0	0.0026	0	0.0001
Apilin	564.15	563.27	0.0023	0.0089	0.0076	0.0043	0	0.0120	0.0022	0.0085
Taxifolin	304.06	303.11	0.0074	0.0149	0.0085	0.0209	0.0031	0.0227	0.0015	0.0210
Pelargonidin chloride	306.03	305.04	0.0006	0	0	0	0.0007	0	0	0
Malvidin chloride	366.05	365.06	0	0	0	0.0002	0	0	0	0
Peonidin chloride	336.04	335.11	0.0004	0	0	0.0002	0	0	0	0
Callistephin chloride	468.08	-	0	0	0	0	0	0	0	0
Malvin chloride	690.16	-	0	0	0	0	0	0	0	0
Cyanin chloride	646.13	-	0	0	0	0	0	0	0	0
Delphinidin-3-rutinoside chloride	646.13	-	0	0	0	0	0	0	0	0
Cyanidin-3-glucoside chloride	484.08	483.04	0.0002	0	0	0	0	0	0	0
Syringic acid	198.05	197.12	0	0.0161	0.0018	0	0	0.0123	0	0
Gentisic acid	154.03	152.94	0.0135	0.0311	0.0065	0.0565	0.0072	0.0833	0.0071	0.0522
Ferulic Acid	194.06	193.06	0.2511	0	0.0036	0.0161	0.2590	0	0.0038	0.0138
Rosmarinic acid	360.08	359.16	0.0026	0	0.0015	0.0076	0.0007	0.0081	0.0003	0
trans-Cinnamic acid	148.05	146.99	0	0.0010	0	0	0	0.0007	0	0
Neochlorogenic acid	354.10	353.12	0.0030	0.0092	0.0017	0.0164	0.0009	0.0059	0	0.0177
4-O-Caffeoylquinic acid (Chlorogenic acid)	354.10	353.13	0.0024	0.0011	0.0004	0.0123	0	0	0.0008	0.0046
D-(+)-Quinic acid	192.06	190.99	0.0857	0.0226	0.0072	0.0692	0.0581	0.0402	0.0014	0.0309
Chlorogenic acid hemihydrate	354.10	353.12	0.0022	0.0011	0.0009	0.0112	0	0.0014	0.0002	0.0047
Shikimic acid	174.06	173.04	0.0081	0	0.0034	0	0.0132	0	0	0
Ellagagic acid dihydrate	302.01	301.04	0.0620	0.0431	0.0404	0.0660	0.0648	0.0471	0.0285	0.0700
Strictinin	634.08	633.14	0.0073	0.0105	0.0083	0.0217	0.0057	0.0213	0.0043	0.0231
β-Carotene	536.44	535.38	0	0.0001	0	0	0	0	0	0
β-Cryptoxanthin	552.44	-	0	0	0	0	0	0	0	0
Zeaxanthin	568.43	-	0	0	0	0	0	0	0	0
Lycopene	536.44	-	0	0	0	0	0	0	0	0
α,α-D-Trehalose anhydrous	342.12	341.07	0	0	0.0001	0	0.0003	0	0	0.0003
D-Cellobiose	342.12	341.15	0.0002	0	0	0	0	0	0	0
Galactinol hydrate	342.12	341.09	0.0002	0	0	0	0	0	0	0
γ-Oryzanol	602.44	601.33	0	0.0010	0	0.0001	0.0002	0	0	0
Maclurin	262.05	261.07	0.0050	0.0266	0.0059	0.0456	0.0018	0.0199	0.0041	0.0307
Xanthone	196.06	195.07	0	0	0.0112	0	0	0	0.0036	0
2-Isopropylmalic acid	176.07	175.03	0.0353	0.0112	0.0129	0.0717	0.0269	0.0085	0.0126	0
(R)(-)-Citramalic acid	148.04	146.95	0.0696	0.0012	0.0154	0	0.0815	0.0011	0.0069	0
Methyl jasmonate	224.14	223.10	0.0011	0	0	0	0	0	0	0
Jasmonic acid	210.13	209.09	0.0030	0.0093	0.0004	0.0070	0	0	0	0.0011
Tomatine	1033.55	1032.49	0	0.0004	0.0002	0	0	0	0.0001	0
Tomatidine	415.35	-	0	0	0	0	0	0	0	0
Curcumine	368.13	367.08	0.0003	0	0.0001	0	0.0002	0.0037	0.0001	0
Resveratrol	228.08	227.17	0	0.0189	0.0002	0.0076	0	0.0121	0	0
Sulforaphane	177.03	175.92	0	0	0.0010	0	0	0	0.0006	0
1,3-Dimethyluric acid	196.06	195.08	0	0.0397	0	0.0611	0	0.0100	0	0
trans-Zeatin	219.11	218.17	0.0046	0.0113	0	0.0139	0.0035	0.0041	0.0012	0.0041
Indole-3-acetic acid	175.06	173.97	0	0	0	0.0005	0	0	0	0
Pteroi acid	312.10	311.21	0	0	0.0014	0.0103	0.0004	0	0.0006	0
Sarsasapogenin	416.33	415.12	0	0	0	0	0	0	0	0

**Supplementary Table S2. MALDI-MS datasets of 21 GTEs for multivariate statistical analyses.**

Name	AT1	AT2	AT3	BF1	BF2	BF3	KM1	KM2	KM3	SM1	SM2	SM3	SR1	SR2	SR3	YB1	YB2	YB3	YM1	YM2	YM3
ORAC	35.647	38.661	51.482	42.552	65.085	55.612	44.400	43.107	48.544	25.445	40.191	46.160	37.930	42.436	38.953	34.246	36.545	41.729	37.746	43.496	47.566
Polyphenol	1.93	2.11	2.54	2.04	2.56	2.54	2.00	2.11	2.41	1.96	2.13	2.33	2.44	2.33	2.17	2.12	2.13	2.34	2.21	2.28	2.65
(m/z)	70.98	0.0022	0.0029	0.0033	0.0017	0.0001	0.0020	0.0018	0.0020	0.0026	0.0040	0.0018	0.0025	0.0001	0.0030	0.0029	0.0015	0.0022	0.0022	0.0019	0.0020
112.97	0.0001	0.0001	0.0032	0.0001	0.0001	0.0001	0.0001	0.0001	0.0030	0.0001	0.0001	0.0001	0.0001	0.0059	0.0051	0.0001	0.0001	0.0001	0.0001	0.0001	
116.99	0.0066	0.0038	0.0001	0.0080	0.0031	0.0027	0.0051	0.0051	0.0026	0.0073	0.0077	0.0001	0.0071	0.0046	0.0039	0.0051	0.0056	0.0044	0.0060	0.0039	0.0001
122.99	0.0060	0.0076	0.0061	0.0056	0.0068	0.0054	0.0065	0.0068	0.0054	0.0060	0.0060	0.0089	0.0060	0.0055	0.0053	0.0055	0.0081	0.0090	0.0061	0.0071	0.0076
124.01	0.0080	0.0102	0.0089	0.0073	0.0096	0.0097	0.0071	0.0088	0.0092	0.0071	0.0085	0.0131	0.0081	0.0079	0.0083	0.0073	0.0105	0.0121	0.0080	0.0097	0.0104
125.02	0.0165	0.0201	0.0180	0.0151	0.0212	0.0205	0.0157	0.0189	0.0194	0.0156	0.0175	0.0265	0.0180	0.0186	0.0184	0.0155	0.0215	0.0241	0.0178	0.0194	0.0211
126.97	0.0085	0.0043	0.0001	0.0068	0.0051	0.0001	0.0066	0.0045	0.0001	0.0072	0.0036	0.0040	0.0065	0.0070	0.0038	0.0061	0.0069	0.0047	0.0073	0.0038	0.0040
128.00	0.0043	0.0018	0.0001	0.0167	0.0064	0.0024	0.0074	0.0061	0.0001	0.0152	0.0034	0.0001	0.0053	0.0061	0.0037	0.0093	0.0055	0.0021	0.0121	0.0030	0.0024
131.98	0.0055	0.0045	0.0036	0.0065	0.0061	0.0023	0.0069	0.0066	0.0048	0.0083	0.0048	0.0021	0.0059	0.0054	0.0039	0.0072	0.0094	0.0061	0.0047	0.0044	0.0066
132.97	0.0242	0.0127	0.0062	0.0282	0.0191	0.0129	0.0208	0.0180	0.0078	0.0217	0.0177	0.0053	0.0189	0.0249	0.0175	0.0174	0.0243	0.0112	0.0172	0.0144	0.0076
134.99	0.0044	0.0040	0.0001	0.0042	0.0001	0.0001	0.0001	0.0001	0.0075	0.0036	0.0037	0.0089	0.0073	0.0049	0.0001	0.0058	0.0053	0.0001	0.0001	0.0001	0.0001
136.99	0.0158	0.0199	0.0187	0.0158	0.0220	0.0205	0.0175	0.0210	0.0233	0.0191	0.0181	0.0276	0.0161	0.0200	0.0161	0.0156	0.0208	0.0248	0.0198	0.0194	0.0244
138.00	0.0092	0.0121	0.0113	0.0093	0.0129	0.0124	0.0103	0.0123	0.0135	0.0105	0.0110	0.0169	0.0084	0.0102	0.0087	0.0090	0.0119	0.0144	0.0111	0.0115	0.0144
138.77	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0017	0.0001	0.0001	0.0021	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0019	0.0001
139.78	0.0023	0.0023	0.0020	0.0021	0.0023	0.0022	0.0021	0.0022	0.0022	0.0021	0.0001	0.029	0.0188	0.0001	0.0001	0.0020	0.0025	0.0028	0.0021	0.0021	0.0026
144.99	0.0001	0.0001	0.0001	0.0182	0.0083	0.0001	0.0133	0.0082	0.0001	0.0217	0.0001	0.0001	0.0001	0.0001	0.0197	0.0001	0.0243	0.0001	0.0001	0.0001	0.0001
145.99	0.0107	0.0062	0.0051	0.0114	0.0074	0.0052	0.0119	0.0100	0.0071	0.0150	0.0081	0.0036	0.0096	0.0081	0.0063	0.0115	0.0106	0.0086	0.0129	0.0091	0.0076
149.00	0.0026	0.0030	0.0025	0.0035	0.0030	0.0025	0.0032	0.0030	0.0034	0.0025	0.0025	0.0035	0.0028	0.0025	0.0037	0.0040	0.0030	0.0024	0.0032	0.0024	0.0032
150.00	0.0062	0.0068	0.0063	0.0071	0.0092	0.0078	0.0070	0.0074	0.0062	0.0061	0.0081	0.0063	0.0075	0.0057	0.0066	0.0075	0.0084	0.0079	0.0071	0.0087	0.0087
151.00	0.0049	0.0053	0.0047	0.0049	0.0057	0.0054	0.0049	0.0054	0.0053	0.0050	0.0045	0.0066	0.0053	0.0073	0.0052	0.0047	0.0057	0.0068	0.0057	0.0051	0.0059
151.96	0.0037	0.0042	0.0040	0.0035	0.0046	0.0042	0.0036	0.0039	0.0045	0.0035	0.0044	0.0071	0.0059	0.0058	0.0058	0.0037	0.0046	0.0053	0.0037	0.0040	0.0050
152.95	0.0050	0.0061	0.0053	0.0044	0.0058	0.0058	0.0046	0.0061	0.0041	0.0052	0.0078	0.0062	0.0066	0.0059	0.0045	0.0059	0.0067	0.0047	0.0056	0.0066	0.0066
154.90	0.0063	0.0064	0.0048	0.0062	0.0050	0.0048	0.0050	0.0058	0.0050	0.0054	0.0048	0.0052	0.0067	0.0095	0.0073	0.0055	0.0065	0.0064	0.0059	0.0054	0.0060
157.87	0.0100	0.0096	0.0088	0.0079	0.0107	0.0099	0.0093	0.0100	0.0096	0.0001	0.0111	0.0091	0.0001	0.0103	0.0100	0.0097	0.0110	0.0099	0.0112	0.0109	0.0103
158.62	0.0001	0.0001	0.0001	0.0015	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0019	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001
159.67	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0074	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001
160.13	0.0096	0.0070	0.0042	0.0072	0.0063	0.0044	0.0077	0.0078	0.0050	0.0097	0.0069	0.0001	0.0103	0.0001	0.0053	0.0097	0.0090	0.0057	0.0099	0.0071	0.0056
160.83	0.0001	0.0001	0.0058	0.0001	0.0001	0.0064	0.0001	0.0001	0.0001	0.0063	0.0061	0.0001	0.0001	0.0063	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001
161.17	0.0083	0.0074	0.0055	0.0067	0.0060	0.0064	0.0067	0.0065	0.0087	0.0087	0.0001	0.0055	0.0001	0.0054	0.0070	0.0054	0.0071	0.0067	0.0082	0.0063	0.0064
161.97	0.0042	0.0040	0.0032	0.0035	0.0034	0.0036	0.0038	0.0038	0.0034	0.0044	0.0034	0.0035	0.0037	0.0032	0.0032	0.0039	0.0040	0.0035	0.0043	0.0039	0.0035
162.64	0.0001	0.0058	0.0053	0.0001	0.0059	0.0058	0.0001	0.0058	0.0056	0.0001	0.0058	0.0057	0.0001	0.0001	0.0058	0.0055	0.0001	0.0059	0.0063	0.0061	0.0060
163.05	0.0050	0.0001	0.0028	0.0054	0.0001	0.0039	0.0048	0.0044	0.0035	0.0069	0.0038	0.0042	0.0001	0.0001	0.0001	0.0055	0.0001	0.0052	0.0001	0.0001	0.0039
163.31	0.0001	0.0035	0.0001	0.0027	0.0031	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0034	0.0033	0.0032	0.0001	0.0039	0.0001	0.0037	0.0001
163.76	0.0029	0.0028	0.0026	0.0028	0.0030	0.0027	0.0027	0.0025	0.0027	0.0027	0.0027	0.0027	0.0028	0.0024	0.0026	0.0030	0.0032	0.0029	0.0030	0.0026	0.0026
164.04	0.0023	0.0020	0.0001	0.0029	0.0031	0.0001	0.0021	0.0001	0.0032	0.0028	0.0018	0.0001	0.0027	0.0027	0.0001	0.0027	0.0027	0.0029	0.0029	0.0001	0.0039
164.45	0.0045	0.0046	0.0042	0.0036	0.0047	0.0046	0.0044	0.0046	0.0043	0.0001	0.0048	0.0044	0.0048	0.0048	0.0045	0.0048	0.0050	0.0047	0.0051	0.0049	0.0047
165.05	0.0136	0.0151	0.0122	0.0150	0.0164	0.0149	0.0131	0.0164	0.0148	0.0158	0.0139	0.0151	0.0158	0.0184	0.0159	0.0128	0.0172	0.0171	0.0151	0.0134	0.0155
165.60	0.0025	0.0024	0.0025	0.0022	0.0024	0.0028	0.0023	0.0024	0.0026	0.0021	0.0023	0.0025	0.0027	0.0024	0.0026	0.0025	0.0027	0.0026	0.0026	0.0026	0.0025
166.02	0.0201	0.0266	0.0267	0.0216	0.0276	0.0264	0.0235	0.0272	0.0331	0.0220	0.0288	0.0288	0.0189	0.0217	0.0198	0.0208	0.0238	0.0272	0.0247	0.0270	0.0322
166.26	0.0001	0.0043	0.0039	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0041	0.0001	0.0001	0.0041	0.0001	0.0001	0.0041	0.0001	0.0001	0.0001	0.0001	0.0001
167.02	0.0335	0.0428	0.0393	0.0317	0.0412	0.0405	0.0332	0.0413	0.0419	0.0293	0.0416	0.0425	0.0355	0.0349	0.0389	0.0326	0.0401	0.0414	0.0363	0.0424	0.0440
167.46	0.0019	0.0020	0.0020	0.0016	0.																

(continued)

Name	AT1	AT2	AT3	BF1	BF2	BF3	KM1	KM2	KM3	SM1	SM2	SM3	SR1	SR2	SR3	YB1	YB2	YB3	YM1	YM2	YM3
ORAC	35,647	38,661	51,482	42,552	65,085	55,612	44,400	43,107	48,544	25,445	40,191	46,160	37,930	42,436	38,953	34,246	36,545	41,729	37,746	43,496	47,566
Polyphenol	1.93	2.11	2.54	2.04	2.56	2.54	2.00	2.11	2.41	1.96	2.13	2.33	2.44	2.33	2.17	2.12	2.13	2.34	2.21	2.28	2.65
306.80	0.0001	0.0019	0.0019	0.0015	0.0001	0.0018	0.0001	0.0001	0.0019	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	
307.24	0.0044	0.0053	0.0050	0.0040	0.0001	0.0001	0.0049	0.0051	0.0001	0.0043	0.0001	0.0001	0.0039	0.0040	0.0037	0.0044	0.0049	0.0052	0.0051	0.0051	0.0001
307.82	0.0021	0.0028	0.0031	0.0020	0.0001	0.0027	0.0024	0.0025	0.0033	0.0022	0.0021	0.0030	0.0020	0.0021	0.0001	0.0021	0.0022	0.0027	0.0023	0.0027	0.0028
308.24	0.0027	0.0030	0.0028	0.0025	0.0024	0.0027	0.0029	0.0030	0.0029	0.0026	0.0024	0.0021	0.0025	0.0021	0.0001	0.0027	0.0028	0.0028	0.0033	0.0031	0.0029
308.82	0.0001	0.0018	0.0022	0.0001	0.0001	0.0017	0.0001	0.0023	0.0001	0.0001	0.0020	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001
309.20	0.0057	0.0068	0.0061	0.0053	0.0059	0.0061	0.0058	0.0066	0.0067	0.0001	0.0062	0.0061	0.0001	0.0051	0.0050	0.0058	0.0064	0.0066	0.0062	0.0072	0.0070
317.52	0.0020	0.0001	0.0084	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0089	0.0124	0.0123	0.0135	0.0017	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001
319.16	0.0052	0.0060	0.0054	0.0047	0.0053	0.0056	0.0050	0.0054	0.0058	0.0042	0.0052	0.0061	0.0057	0.0049	0.0001	0.0051	0.0058	0.0060	0.0052	0.0059	0.0061
337.23	0.0001	0.0001	0.0001	0.0036	0.0043	0.0001	0.0001	0.0001	0.0001	0.0031	0.0001	0.0001	0.0001	0.0045	0.0046	0.0032	0.0001	0.0001	0.0001	0.0001	0.0001
338.28	0.0025	0.0021	0.0019	0.0019	0.0031	0.0023	0.0024	0.0021	0.0020	0.0001	0.0023	0.0001	0.0022	0.0001	0.0001	0.0030	0.0029	0.0024	0.0024	0.0024	0.0023
339.30	0.0001	0.0001	0.0001	0.0001	0.0001	0.0054	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0053	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001
354.53	0.0019	0.0001	0.0001	0.0014	0.0001	0.0017	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0018	0.0001	0.0001	0.0020	0.0001	0.0001	0.0001
413.46	0.0001	0.0001	0.0001	0.0017	0.0021	0.0021	0.0001	0.0001	0.0001	0.0001	0.0024	0.0024	0.0021	0.0001	0.0024	0.0001	0.0001	0.0024	0.0001	0.0001	0.0001
423.19	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0033	0.0027	0.0031	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001
429.43	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0029	0.0026	0.0024	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001
431.61	0.0001	0.0001	0.0001	0.0001	0.0001	0.0024	0.0001	0.0031	0.0026	0.0001	0.0032	0.0031	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001
439.11	0.0001	0.0019	0.0022	0.0001	0.0019	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0018	0.0001	0.0001	0.0020	0.0001	0.0001
440.09	0.0037	0.0046	0.0059	0.0030	0.0054	0.0061	0.0038	0.0038	0.0042	0.0001	0.0047	0.0048	0.0036	0.0030	0.0048	0.0033	0.0038	0.0043	0.0033	0.0056	0.0053
441.14	0.0202	0.0244	0.0274	0.0177	0.0301	0.0313	0.0192	0.0195	0.0215	0.0110	0.0231	0.0236	0.0193	0.0169	0.0231	0.0169	0.0209	0.0216	0.0182	0.0285	0.0283
443.22	0.0034	0.0040	0.0043	0.0023	0.0031	0.0034	0.0035	0.0036	0.0036	0.0001	0.0040	0.0039	0.0026	0.0023	0.0025	0.0035	0.0036	0.0036	0.0031	0.0039	0.0034
444.26	0.0020	0.0022	0.0024	0.0017	0.0001	0.0023	0.0021	0.0020	0.0020	0.0001	0.0022	0.0019	0.0001	0.0001	0.0020	0.0001	0.0021	0.0001	0.0025	0.0021	0.0021
445.25	0.0023	0.0022	0.0021	0.018	0.0023	0.0023	0.0024	0.0024	0.0021	0.0001	0.0022	0.0001	0.0001	0.0001	0.0025	0.0022	0.0021	0.0025	0.0027	0.0023	
447.28	0.0036	0.0034	0.0037	0.0024	0.0033	0.0038	0.0051	0.0039	0.0036	0.0001	0.0036	0.0039	0.0000	0.0054	0.0046	0.0048	0.0036	0.0041	0.0032	0.0035	0.0031
448.28	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0018	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001
449.22	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0028	0.0022	0.0022	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001
455.12	0.0061	0.0080	0.0079	0.0048	0.0077	0.0080	0.0068	0.0082	0.0070	0.0041	0.0077	0.0063	0.0057	0.0043	0.0064	0.0064	0.0078	0.0070	0.0062	0.0096	0.0084
456.09	0.0144	0.0179	0.0179	0.0109	0.0181	0.0175	0.0154	0.0182	0.0161	0.0097	0.0172	0.0164	0.0138	0.0122	0.0177	0.0146	0.0173	0.0163	0.0145	0.0214	0.0190
457.20	0.0411	0.0488	0.0472	0.0315	0.0497	0.0468	0.0413	0.0483	0.0458	0.0284	0.0472	0.0475	0.0408	0.0379	0.0494	0.0404	0.0480	0.0460	0.0420	0.0549	0.0513
459.33	0.0049	0.0058	0.0056	0.0039	0.0055	0.0056	0.0050	0.0057	0.0052	0.0001	0.0054	0.0050	0.0044	0.0033	0.0001	0.0050	0.0057	0.0056	0.0050	0.0063	0.0060
460.45	0.0033	0.0036	0.0034	0.0027	0.0037	0.0035	0.0036	0.0034	0.0034	0.0001	0.0035	0.0034	0.0001	0.0029	0.0032	0.0035	0.0036	0.0036	0.0039	0.0037	
461.40	0.0042	0.0046	0.0039	0.0034	0.0042	0.0039	0.0045	0.0050	0.0041	0.0001	0.0044	0.0042	0.0027	0.0032	0.0029	0.0027	0.0045	0.0045	0.0043	0.0050	0.0047
462.39	0.0026	0.0027	0.0025	0.0022	0.0025	0.0024	0.0029	0.0030	0.0023	0.0001	0.0026	0.0001	0.0024	0.0001	0.0020	0.0030	0.0027	0.0025	0.0030	0.0032	0.0027
463.38	0.0065	0.0066	0.0085	0.0039	0.0049	0.0051	0.0085	0.0052	0.0066	0.0077	0.0064	0.0075	0.0199	0.0168	0.0183	0.0068	0.0055	0.0065	0.0055	0.0054	0.0048
464.45	0.0025	0.0025	0.0029	0.0019	0.0021	0.0020	0.0031	0.0022	0.0024	0.0001	0.0025	0.0001	0.0001	0.0001	0.0001	0.0026	0.0022	0.0024	0.0024	0.0023	0.0020
465.44	0.0024	0.0024	0.0023	0.0018	0.0001	0.0019	0.0001	0.0026	0.0023	0.0001	0.0022	0.0001	0.0035	0.0026	0.0031	0.0025	0.0022	0.0024	0.0024	0.0024	
473.39	0.0001	0.0018	0.0023	0.0001	0.0001	0.0016	0.0001	0.0018	0.0001	0.0024	0.0023	0.0001	0.0001	0.0001	0.0018	0.0001	0.0018	0.0001	0.0001	0.0001	0.0001
478.23	0.0001	0.0001	0.0017	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0022	0.0001	0.0001	0.0001	0.0001	0.0001
479.57	0.0083	0.0101	0.0206	0.0001	0.0001	0.0091	0.0088	0.0001	0.0139	0.0001	0.0102	0.0194	0.0302	0.0244	0.0329	0.0077	0.0001	0.0148	0.0001	0.0076	0.0086
494.26	0.0020	0.0018	0.0019	0.0020	0.0001	0.0018	0.0019	0.0021	0.0001	0.0001	0.0027	0.0001	0.0001	0.0001	0.0001	0.0001	0.0027	0.0001	0.0001	0.0024	0.0001
495.36	0.0021	0.0018	0.0018	0.0019	0.0001	0.0001	0.0021	0.0001	0.0001	0.0025	0.0001	0.0020	0.0001	0.0001	0.0025	0.0001	0.0001	0.0020	0.0001	0.0001	0.0001
505.35	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0028	0.0043	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001
511.27	0.0032	0.0019	0.0001	0.0024	0.0034	0.0037	0.0033	0.0043	0.0032												

**Supplementary Table S3. The top-40 VIP-valued components highly contributing to the construction of OPLS regression model and their correlations with ORAC values.**

Variables	VIP	m/z	(Name)	AT1	AT2	AT3	BF1	BF2	BF3	KM1	KM2	KM3	SM1	SM2	SM3	SR1	SR2	SR3	YB1	YB2	YB3	YM1	YM2	YM3	Correlation with ORAC	
V01	3.11	441.14	(ORAC)	35,647	38,661	51,482	42,552	65,085	55,612	44,400	43,107	48,544	25,445	40,191	46,160	37,930	42,436	38,963	34,246	36,545	41,729	37,746	43,496	47,566	R <sup>2</sup> (Slope)	
V02	3.06	305.19		0.0202	0.0244	0.0274	0.0177	0.0301	0.0313	0.0192	0.0195	0.0215	0.0110	0.0231	0.0236	0.0193	0.0169	0.0231	0.0169	0.0209	0.0216	0.0182	0.0285	0.0283	0.616 (+)	
V03	2.86	289.19		0.0174	0.0226	0.0247	0.0232	0.0291	0.0281	0.0201	0.0224	0.0280	0.0177	0.0213	0.0264	0.0171	0.0207	0.0181	0.0184	0.0203	0.0239	0.0228	0.0243	0.0313	0.615 (+)	
V04	2.31	457.20		0.0411	0.0488	0.0472	0.0315	0.0497	0.0468	0.0413	0.0483	0.0458	0.0284	0.0472	0.0475	0.0408	0.0379	0.0494	0.0404	0.0480	0.0460	0.0420	0.0549	0.0513	0.253 (+)	
V05	2.26	209.19		0.0085	0.0001	0.0001	0.0096	0.0001	0.0001	0.0076	0.0001	0.0001	0.0087	0.0001	0.0001	0.0085	0.0001	0.0001	0.0075	0.0087	0.0001	0.0078	0.0001	0.0001	0.332 (-)	
V06	2.21	287.18		0.0184	0.0246	0.0244	0.0187	0.0253	0.0271	0.0203	0.0237	0.0150	0.0235	0.0269	0.0211	0.0202	0.0229	0.0193	0.0224	0.0251	0.0207	0.0261	0.0268	0.487 (+)		
V07	2.10	167.02		0.0335	0.0428	0.0391	0.0317	0.0412	0.0405	0.0332	0.0413	0.0419	0.0293	0.0416	0.0425	0.0355	0.0349	0.0389	0.0326	0.0401	0.0414	0.0363	0.0424	0.0440	0.283 (+)	
V08	1.99	288.20		0.0094	0.0132	0.0138	0.0097	0.0140	0.0156	0.0101	0.0122	0.0140	0.0073	0.0125	0.0164	0.0101	0.0100	0.0121	0.0096	0.0113	0.0133	0.0104	0.0139	0.0146	0.516 (+)	
V09	1.90	183.10		0.0021	0.0001	0.0001	0.0087	0.0090	0.0104	0.0037	0.0038	0.0036	0.0001	0.0001	0.0056	0.0067	0.0037	0.0018	0.0021	0.0001	0.0001	0.0001	0.0001	0.0044	0.296 (+)	
V10	1.90	166.02		0.0201	0.0266	0.0267	0.0216	0.0276	0.0264	0.0235	0.0272	0.0331	0.0220	0.0284	0.0288	0.0189	0.0217	0.0198	0.0208	0.0238	0.0272	0.0247	0.0270	0.0332	0.281 (+)	
V11	1.83	145.99		0.0107	0.0062	0.0051	0.0114	0.0074	0.0052	0.0119	0.0100	0.0071	0.0150	0.0081	0.0036	0.0096	0.0081	0.0063	0.0115	0.0106	0.0086	0.0129	0.0091	0.0076	0.396 (-)	
V12	1.82	177.14		0.0072	0.0001	0.0001	0.0070	0.0001	0.0046	0.0066	0.0001	0.0001	0.0091	0.0001	0.0074	0.0073	0.0064	0.0063	0.0001	0.0001	0.0074	0.0001	0.242 (-)			
V13	1.81	134.99		0.0044	0.0040	0.0001	0.0042	0.0001	0.0001	0.0001	0.0001	0.0001	0.0075	0.0034	0.0037	0.0089	0.0073	0.0049	0.0001	0.0058	0.0053	0.0001	0.0001	0.0001	0.310 (-)	
V14	1.78	168.06		0.0359	0.0455	0.0422	0.0336	0.0443	0.0441	0.0349	0.0443	0.0419	0.0311	0.0441	0.0475	0.0424	0.0446	0.0519	0.0349	0.0441	0.0458	0.0382	0.0443	0.0441	0.153 (+)	
V15	1.77	144.99		0.0001	0.0001	0.0001	0.0162	0.0083	0.0001	0.0133	0.0082	0.0001	0.0217	0.0001	0.0001	0.0001	0.0017	0.0001	0.0001	0.0001	0.0001	0.00243	0.0001	0.0001	0.105 (-)	
V16	1.75	175.44		0.0028	0.0019	0.0017	0.0128	0.0001	0.0019	0.0018	0.0018	0.0019	0.0017	0.0181	0.0001	0.0222	0.0001	0.0001	0.0020	0.0020	0.0020	0.0021	0.0023	0.0021	0.0001	0.190 (-)
V17	1.72	116.99		0.0066	0.0038	0.0001	0.0080	0.0031	0.0027	0.0051	0.0051	0.0026	0.0073	0.0077	0.0001	0.0071	0.0046	0.0039	0.0051	0.0056	0.0044	0.0060	0.0039	0.0001	0.368 (-)	
V18	1.71	128.00		0.0043	0.0018	0.0001	0.0167	0.0064	0.0024	0.0074	0.0061	0.0001	0.0152	0.0034	0.0001	0.0053	0.0061	0.0037	0.0093	0.0055	0.0021	0.0121	0.0030	0.0024	0.182 (-)	
V19	1.66	132.97		0.0242	0.0127	0.0063	0.0282	0.0191	0.0129	0.0208	0.0180	0.0078	0.0217	0.0177	0.0053	0.0189	0.0249	0.0175	0.0174	0.0243	0.0112	0.0172	0.0144	0.0076	0.149 (-)	
V20	1.57	126.97		0.0085	0.0043	0.0001	0.0068	0.0051	0.0001	0.0066	0.0045	0.0001	0.0072	0.0036	0.0040	0.0065	0.0070	0.0038	0.0061	0.0069	0.0047	0.0073	0.0038	0.0040	0.336 (-)	
V21	1.56	136.99		0.0158	0.0199	0.0187	0.0158	0.0220	0.0205	0.0175	0.0210	0.0233	0.0191	0.0181	0.0276	0.0161	0.0200	0.0161	0.0156	0.0208	0.0248	0.0198	0.0194	0.0244	0.162 (+)	
V22	1.53	160.13		0.0098	0.0070	0.0044	0.0072	0.0063	0.0044	0.0077	0.0078	0.0050	0.0097	0.0061	0.0001	0.0103	0.0001	0.0053	0.0097	0.0090	0.0057	0.0098	0.0071	0.0056	0.247 (-)	
V23	1.51	440.09		0.0037	0.0046	0.0059	0.0030	0.0054	0.0061	0.0038	0.0034	0.0042	0.0001	0.0047	0.0048	0.0036	0.0030	0.0048	0.0033	0.0038	0.0043	0.0033	0.0056	0.0053	0.544 (+)	
V24	1.51	271.20		0.0053	0.0056	0.0058	0.0053	0.0068	0.0074	0.0052	0.0052	0.0056	0.0001	0.0052	0.0059	0.0059	0.0058	0.0059	0.0051	0.0053	0.0059	0.0054	0.0061	0.0063	0.494 (+)	
V25	1.49	307.24		0.0044	0.0053	0.0053	0.0040	0.0001	0.0001	0.0049	0.0051	0.0001	0.0043	0.0001	0.0001	0.0039	0.0040	0.0037	0.0044	0.0049	0.0052	0.0051	0.0051	0.0001	0.315 (-)	
V26	1.48	939.15		0.0028	0.0069	0.0055	0.0017	0.0058	0.0065	0.0001	0.0039	0.0056	0.0001	0.0053	0.0033	0.0001	0.0080	0.0065	0.0001	0.0030	0.0029	0.0044	0.0046	0.0067	0.256 (+)	
V27	1.46	157.87		0.0100	0.0096	0.0088	0.0079	0.0107	0.0099	0.0093	0.0100	0.0096	0.0001	0.0111	0.0091	0.0001	0.0103	0.0100	0.0097	0.0112	0.0109	0.0103	0.170	0.247 (+)		
V28	1.44	456.09		0.0144	0.0179	0.0176	0.0109	0.0181	0.0175	0.0154	0.0182	0.0161	0.0097	0.0172	0.0164	0.0138	0.0122	0.0177	0.0148	0.0173	0.0163	0.0145	0.0214	0.0190	0.247 (-)	
V29	1.36	138.00		0.0092	0.0121	0.0113	0.0093	0.0129	0.0124	0.0103	0.0123	0.0135	0.0105	0.0110	0.0169	0.0084	0.0102	0.0087	0.0090	0.0119	0.0144	0.0111	0.0115	0.0144	0.202 (+)	
V30	1.36	162.64		0.0001	0.0058	0.0053	0.0001	0.0059	0.0058	0.0001	0.0058	0.0056	0.0001	0.0058	0.0057	0.0001	0.0059	0.0055	0.0001	0.0059	0.0063	0.0061	0.0060	0.180 (+)		
V31	1.25	940.09		0.0001	0.0047	0.0034	0.0001	0.0034	0.0001	0.0023	0.0034	0.0001	0.0020	0.0001	0.0045	0.0037	0.0001	0.0001	0.0001	0.0001	0.0026	0.0025	0.0042	0.259 (+)		
V32	1.25	923.16		0.0001	0.0031	0.0025	0.0001	0.0030	0.0035	0.0001	0.0001	0.0021	0.0001	0.0019	0.0001	0.0001	0.0035	0.0026	0.0001	0.0001	0.0001	0.0001	0.0028	0.304 (+)		
V33	1.22	125.02		0.0165	0.0201	0.0180	0.0151	0.0212	0.0205	0.0157	0.0189	0.0194	0.0156	0.0175	0.0265	0.0180	0.0186	0.0184	0.0155	0.0241	0.0218	0.0194	0.0211	0.161	0.247 (+)	
V34	1.21	204.14		0.0159	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0094	0.247 (-)	
V35	1.15	207.19		0.0038	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0054	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.269 (-)	
V36	1.15	304.16		0.0072	0.0097	0.0097	0.0068	0.0089	0.0098	0.0081	0.0091	0.0101	0.0069	0.0088	0.0101	0.0066	0.0064	0.0068	0.0073	0.0079	0.0086	0.0081	0.0097	0.0107	0.319 (+)	
V37	1.13	309.20		0.0057	0.0068	0.0061	0.0053	0.0059	0.0061	0.0058	0.0066	0.0067	0.0001	0.0062	0.0001	0.0051	0.0050	0.0050	0.0064	0.0066	0.0062	0.0072	0.0070	0.200 (+)		
V38	1.09	459.33		0.0049	0.0058	0.0056	0.0039	0.0055	0.0056	0.0050	0.0057	0.0052	0.0001	0.0054	0.0050	0.0044	0.0033	0.0001	0.0050	0.0057	0.0056	0.0050	0.0063	0.0060	0.220 (+)	
V39	1.08	150.00		0.0062	0.006																					

**Supplementary Table S4. Combinations of multiple components with the highest VIP values (>1) and their correlation values using three abundance measures.**

Combinations using the Intensity data	R <sup>2</sup>	Combinations using the Relative data	R <sup>2</sup>	Combinations using the Score data	R <sup>2</sup>	Combinations of the top-4 VIP components	R <sup>2</sup> (Intensity)	R <sup>2</sup> (Relative)	R <sup>2</sup> (Score)	
1 V01 V03 V09 V24 0.828		1 V01 V03 V09 V23 0.835		1 V03 V09 V23 - 0.812		V01 V02 V03 V04	0.486	0.561	0.510	
2 V01 V03 V09 V39 0.828		2 V03 V08 V09 V23 0.826		2 V03 V09 V23 - 0.803		V01 V02 V04	0.493	0.588	0.560	
3 V01 V03 V09 V23 0.825		3 V03 V09 V23 - 0.804		3 V03 V09 V23 - 0.793		V01 V03 V04	0.453	0.635	0.516	
4 V01 V03 V09 V37 0.825		4 V01 V02 V09 V24 0.823		4 V01 V03 V09 V23 0.793		V01 V02 V04	0.567	0.626	0.530	
5 V01 V03 V09 V38 0.818		5 V01 V09 V23 V39 0.821		5 V02 V03 V09 V23 0.792		V02 V03 V04	-	0.403	0.479	0.472
6 V03 V08 V09 V23 0.815		6 V02 V09 V23 - 0.821		6 V01 V03 V09 V23 0.787		V01 V02 V03	-	0.439	0.524	0.478
7 V03 V08 V09 V32 0.814		7 V01 V08 V08 V09 0.820		7 V01 V03 V09 V23 0.784		V01 V02 V03	-	0.721	0.722	0.643
8 V03 V08 V23 V38 0.813		8 V01 V08 V09 V24 0.815		8 V03 V09 V23 - 0.784		V01 V04	-	0.434	0.561	0.455
9 V01 V03 V08 V09 0.813		9 V01 V09 V10 V24 0.817		9 V02 V09 V23 0.782		V02 V03	-	0.358	0.451	0.487
10 V01 V09 V29 0.812		10 V02 V08 V23 V24 0.815		10 V03 V06 V09 V23 0.781		V02 V04	-	0.325	0.330	0.336
11 V01 V03 V09 V36 0.810		11 V03 V09 V23 V24 0.814		11 V03 V08 V09 V23 0.780		V03 V04	-	0.493	0.573	0.503
12 V01 V09 V36 0.810		12 V01 V09 V23 V29 0.813		12 V01 V09 V23 V39 0.778		V01 V03 V08 V10	-	0.772	0.772	0.726
13 V01 V06 V09 V33 0.809		13 V01 V08 V09 V23 0.809		13 V01 V09 V23 - 0.773		V01 V02 V03	-	0.488	0.533	0.484
14 V01 V08 V09 V30 0.808		14 V03 V09 V09 V23 0.813		14 V01 V02 V09 0.772		V01 V02 V04	-	0.721	0.722	0.643
15 V01 V09 V29 0.807		15 V08 V09 V23 V39 0.813		15 V01 V09 V23 V39 0.772		V01 V02 V03	-	0.434	0.561	0.455
16 V01 V09 V24 V29 0.807		16 V01 V09 V10 V23 0.812		16 V01 V03 V06 V09 0.772		V01 V02 V03	-	0.439	0.524	0.478
17 V03 V08 V09 V24 0.807		17 V01 V03 V09 V09 0.810		17 V03 V09 V23 V24 0.771		V01 V02 V04	-	0.721	0.722	0.643
18 V03 V08 V09 V31 0.805		18 V01 V03 V09 V09 0.810		18 V02 V09 V23 V39 0.771		V01 V02 V04	-	0.434	0.561	0.455
19 V08 V09 V23 V35 0.804		19 V01 V03 V09 V39 0.795		19 V01 V09 V23 V39 0.770		V01 V02 V04	-	0.487	0.533	0.484
20 V03 V09 V23 V28 0.804		20 V03 V08 V09 V24 0.809		20 V03 V09 V23 V29 0.767		V01 V02 V03	-	0.493	0.541	0.487
21 V01 V09 V23 V29 0.802		21 V09 V10 V23 - 0.809		21 V02 V03 V09 V24 0.765		V02 V03 V04	-	0.325	0.330	0.336
22 V08 V09 V23 V36 0.802		22 V01 V09 V21 V23 0.807		22 V09 V10 V23 - 0.758		V03 V04 V05	-	0.493	0.573	0.503
23 V01 V09 V09 V29 0.802		23 V03 V09 V23 V28 0.805		23 V01 V09 V20 V08 0.757		V01 V02 V03	-	0.281	0.281	0.271
24 V01 V09 V09 V29 0.802		24 V01 V09 V29 V09 0.757		24 V01 V09 V20 V08 0.757		V01 V02 V03	-	0.281	0.281	0.271
25 V03 V09 V23 V38 0.801		25 V03 V04 V09 V23 0.804		25 V03 V09 V10 V20 0.756		V03 V04 V05	-	0.323	0.330	0.336
26 V03 V06 V09 V23 0.800		26 V09 V10 V23 V24 0.803		26 V03 V09 V10 V23 0.756		V03 V04 V05	-	0.468	0.468	0.468
27 V03 V09 V23 V36 0.799		27 V01 V09 V24 V29 0.803		27 V09 V10 V23 V24 0.756		V01 V02 V03	-	0.494	0.494	0.426
28 V03 V09 V29 V32 0.799		28 V01 V09 V10 V09 0.801		28 V02 V09 V23 V24 0.755		V01 V02 V03	-	0.256	0.252	0.252
29 V01 V09 V23 V36 0.795		29 V01 V09 V24 V31 0.801		29 V01 V09 V23 V31 0.755		V01 V02 V03	-	0.261	0.261	0.261
30 V01 V09 V10 V24 0.798		30 V01 V09 V24 V31 0.800		30 V03 V08 V09 V28 0.754		V03 V04 V05	-	0.268	0.247	0.273
31 V01 V03 V09 V09 0.797		31 V09 V23 C29 V39 0.798		31 V03 V08 V09 0.796		V03 V04 V05	-	0.268	0.202	0.276
32 V01 V09 V23 V39 0.796		32 V01 V08 V09 - 0.796		32 V02 V03 V08 V09 0.754		V02 V03 V04	-	0.180	0.182	0.182
33 V01 V09 V38 V39 0.796		33 V03 V09 V24 V26 0.794		33 V02 V03 V08 V09 0.753		V02 V03 V04	-	0.259	0.264	0.264
34 V01 V09 V23 V28 0.795		34 V03 V09 V23 V28 0.795		34 V01 V09 V09 V39 0.751		V01 V02 V03 V04	-	0.304	0.304	0.307
35 V03 V09 V23 V28 0.795		35 V03 V09 V23 V28 0.793		35 V01 V09 V09 V09 0.751		V01 V02 V03 V04	-	0.161	0.161	0.235
36 V01 V03 V09 V27 0.794		36 V01 V09 V24 V36 0.793		36 V01 V09 V09 V09 0.751		V01 V02 V03 V04	-	0.319	0.319	0.291
37 V03 V06 V09 V24 0.793		37 V09 V23 V39 - 0.792		37 V01 V03 V09 V36 0.751		V01 V02 V03 V04	-	0.200	0.200	0.068
38 V01 V09 V37 V39 0.791		38 V01 V09 V28 V08 0.792		38 V01 V09 V02 V08 0.751		V01 V02 V03 V04	-	0.220	0.220	0.137
39 V03 V09 V23 V09 0.791		39 V01 V03 V09 V24 0.750		39 V01 V03 V09 V24 0.750		V01 V02 V03 V04	-	0.368	0.368	0.316
Among 15,290 combinations of 2-4 components, the representative combinations with higher correlation values ( $R^2 > 0.75$ ) are shown.										
These data are showing correlation values of positively correlated components (Slope > 0) among the top-40 components with large VIP values (>1).										
(Continued)										
(Continued)	Combinations using the Intensity data	R <sup>2</sup>	Combinations using the Relative data	R <sup>2</sup>	Combinations using the Score data	R <sup>2</sup>	Combinations of the top-4 VIP components	R <sup>2</sup> (Intensity)	R <sup>2</sup> (Relative)	R <sup>2</sup> (Score)
51 V03 V09 V23 V37 0.788		51 V09 V23 V24 V29 0.787		51 V03 V09 V23 V37 0.787		V03 V04 V05	0.616	0.483	(+)	
52 V03 V09 V24 V36 0.787		52 V03 V09 V24 V36 0.786		52 V03 V09 V23 V37 0.786		V02 V03 V04	0.254	0.254	0.326	
53 V01 V09 V21 V31 0.786		53 V01 V09 V21 V31 0.785		53 V01 V09 V23 V37 0.785		V01 V02 V03	0.615	0.602	(+)	
54 V01 V09 V21 V31 0.787		54 V01 V09 V21 V31 0.787		54 V01 V09 V23 V37 0.787		V01 V02 V03	0.253	0.253	0.209	
55 V01 V09 V21 V31 0.787		55 V01 V09 V21 V31 0.787		55 V01 V09 V23 V37 0.787		V01 V02 V03	0.267	0.267	0.267	
56 V03 V09 V23 V37 0.786		56 V03 V09 V23 V37 0.786		56 V03 V09 V23 V37 0.786		V03 V04 V05	0.759	0.759	0.759	
57 V01 V09 V23 V37 0.786		57 V01 V09 V23 V37 0.786		57 V01 V09 V23 V37 0.786		V01 V02 V03	0.759	0.759	0.759	
58 V01 V09 V23 V38 0.786		58 V01 V09 V21 V24 0.785		58 V01 V09 V21 V24 0.785		V01 V02 V03	0.759	0.759	0.759	
59 V01 V09 V36 V39 0.785		59 V01 V09 V36 V39 0.784		59 V01 V09 V36 V39 0.784		V01 V02 V03	0.759	0.759	0.759	
60 V01 V09 V10 V23 0.785		60 V01 V09 V10 V23 0.785		60 V01 V09 V10 V23 0.787		V01 V02 V03	0.761	0.761	0.761	
61 V01 V08 V09 V23 0.784		61 V01 V08 V09 V23 0.784		61 V01 V08 V09 V23 0.783		V01 V02 V03	0.761	0.761	0.761	
62 V01 V09 V21 V31 0.784		62 V01 V08 V09 V10 0.783		62 V01 V08 V09 V10 0.783		V01 V02 V03	0.762	0.762	0.762	
63 V01 V09 V23 V31 0.784		63 V01 V09 V23 V31 0.784		63 V01 V09 V23 V31 0.783		V01 V02 V03	0.763	0.763	0.763	
64 V01 V09 V36 V37 0.784		64 V01 V09 V36 V37 0.784		64 V01 V09 V36 V37 0.784		V01 V02 V03	0.764	0.764	0.764	
65 V01 V09 V28 V32 0.784		65 V01 V09 V28 V32 0.784		65 V01 V09 V28 V32 0.784		V01 V02 V03	0.765	0.765	0.765	
66 V03 V08 V09 V23 0.784		66 V03 V08 V09 V23 0.784		66 V03 V08 V09 V23 0.784		V03 V04 V05	0.766	0.766	0.766	
67 V03 V09 V28 V39 0.783		67 V01 V08 V09 V24 0.781		67 V01 V08 V09 V24 0.781		V01 V02 V03	0.767	0.767	0.767	
68 V01 V09 V10 V23 0.783		68 V01 V09 V10 V23 0.783		68 V01 V09 V10 V23 0.783		V01 V02 V03	0.768	0.768	0.768	
69 V01 V03 V09 V30 0.783		69 V01 V03 V09 V30 0.783		69 V01 V03 V09 V30 0.783		V01 V02 V03	0.769	0.769	0.769	
70 V03 V08 V09 V30 0.783		70 V03 V08 V09 V30 0.783		70 V03 V08 V09 V30 0.783		V03 V04 V05	0.770	0.770	0.770	
71 V01 V09 V24 V38 0.783		71 V01 V09 V24 V38 0.783		71 V01 V09 V24 V38 0.783		V01 V02 V03	0.771	0.771	0.771	
72 V06 V09 V23 V39 0.783		72 V01 V03 V09 V36 0.780		72 V01 V03 V09 V36 0.780		V01 V02 V03	0.772	0.772	0.772	
73 V08 V09 V32 V38 0.783		73 V09 V23 V28 V39 0.780		73 V09 V23 V28 V39 0.780		V09 V10 V11 V12	-	0.773	0.773	0.773
74 V01 V08 V09 V29 0.783		74 V01 V02 V09 V09 0.780		74 V01 V02 V09 V09 0.780		V01 V02 V03	-	0.774	0.774	0.774
75 V01 V09 V28 V38 0.783		75 V01 V09 V28 V38 0.783		75 V01 V09 V28 V38 0.783		V01 V02 V03	-	0.775	0.775	0.775
76 V01 V09 V28 V38 0.783		76 V01 V09 V28 V38 0.783		76 V01 V09 V28 V38 0.783		V01 V02 V03	-	0.776	0.776	0.776
77 V03 V08 V09 V24 0.782		77 V09 V24 V36 - 0.778		77 V09 V24 V36 - 0.778		V09 V10 V11 V12	-	0.777	0.777	0.777
78 V03 V09 V29 V31 0.781		78 V02 V09 V24 - 0.778		78 V02 V09 V24 - 0.778		V02 V03 V04	-	0.778	0.778	0.778
79 V09 V10 V23 V34 0.781		79 V09 V10 V23 V39 0.777		79 V09 V10 V23 V39 0.777		V09 V10 V11 V12	-	0.779	0.779	0.779
80 V01 V09 V21 V31 0.781		80 V01 V09 V21 V31 0.779		80 V01 V09 V21 V31 0.779		V01 V02 V03	-	0.780	0.780	0.780
81 V01 V09 V36 V37 0.780		81 V01 V09 V36 V37 0.780		81 V01 V09 V36 V37 0.780		V01 V02 V03	-	0.781	0.781	0.781
82 V03 V06 V09 V36 0.780		82 V03 V06 V09 V36 0.780		82 V03 V06 V09 V36 0.780		V03 V04 V05	-	0.782	0.782	0.782
83 V09 V23 V36 V39 0.780		83 V09 V23 V36 V39 0.780		83 V09 V23 V36 V39 0.780		V09 V10 V11 V12	-	0.783	0.783	0.783
84 V01 V08 V09 V37 0.779		84 V02 V09 V23 V39 0.776		84 V02 V09 V23 V39 0.776		V02 V03 V04	-	0.784	0.784	0.784
85 V01 V09 V32 V37 0.779		85 V01 V09 V32 V37 0.779		85 V01 V09 V32 V37 0.779		V01 V02 V03	-	0.785	0.785	0.785
86 V01 V09 V33 V37 0.779		86 V01 V09 V33 V37								

**Supplementary Table S5. LC-MS datasets of 21 GTEs for multivariate statistical analyses.**

<i>m/z</i>	R.T.	Polar.	(Name)	AT1	AT2	AT3	BF1	BF2	BF3	KM1	KM2	KM3	SM1	SM2	SM3	SR1	SR2	SR3	YB1	YB2	YB3	YM1	YM2	YM3	
(Polyphenol)				35,647	38,661	51,482	42,852	60,085	58,543	44,400	43,107	48,544	25,445	40,191	46,160	37,930	42,436	38,953	34,246	58,545	41,729	37,746	43,496	47,566	
125.03	8.909	-		0.00007	0.00008	0.00008	0.00014	0.00009	0.00008	0.00002	0.00002	0.00009	0.00003	0.00007	0.00004	0.00005	0.00002	0.00004	0.00005	0.00005	0.00009	0.00005	0.00009	0.00005	
133.02	2.142	-		0.000051	0.00023	0.00013	0.00044	0.00018	0.00017	0.00049	0.00028	0.00012	0.00027	0.00031	0.00011	0.00012	0.00021	0.00013	0.00055	0.0024	0.0004	0.00043	0.00031	0.00006	
135.03	2.325	-		0.000011	0.00005	0.00005	0.00003	0.00000	0.00000	0.00013	0.00004	0.00002	0.00009	0.00005	0.00005	0.00002	0.00003	0.00001	0.00009	0.00006	0.00006	0.00006	0.00006	0.00006	
136.04	2.378	-		0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	
139.04	8.917	+		0.00302	0.00400	0.00406	0.00363	0.00328	0.00342	0.00318	0.00363	0.00421	0.00314	0.00392	0.00432	0.00364	0.00295	0.00359	0.00374	0.00425	0.00446	0.00325	0.00400	0.00452	
146.96	13.209	-		0.00003	0.00005	0.00000	0.00002	0.00007	0.00002	0.00004	0.00004	0.00005	0.00008	0.00003	0.00003	0.00003	0.00003	0.00005	0.00005	0.00005	0.00002	0.00002	0.00003	0.00003	0.00003
147.04	9.514	+		0.00127	0.00193	0.00218	0.00279	0.00109	0.00100	0.00240	0.00172	0.0190	0.0193	0.0135	0.0053	0.0343	0.0264	0.0201	0.0164	0.0109	0.0112	0.0044	0.0007	0.0012	0.0012
150.08	2.173	+		0.00400	0.00178	0.00083	0.00480	0.0221	0.0147	0.0433	0.0024	0.0092	0.0489	0.0247	0.0148	0.0172	0.00468	0.0266	0.0058	0.0046	0.0255	0.0122	0.0006	0.0006	0.0006
163.08	12.362	+		0.00000	0.0024	0.00000	0.0001	0.00025	0.00008	0.0011	0.00009	0.00028	0.0024	0.0011	0.00000	0.0015	0.0015	0.00015	0.0015	0.0041	0.0031	0.0001	0.0001	0.0001	
163.13	11.066	+		0.00152	0.0125	0.00138	0.0197	0.0089	0.0198	0.0193	0.0137	0.00119	0.0115	0.0145	0.0164	0.0149	0.0161	0.0131	0.0059	0.0155	0.0017	0.0006	0.0006	0.0006	0.0006
166.03	8.481	+		0.00007	0.00009	0.00009	0.00008	0.00008	0.00010	0.00008	0.00009	0.00010	0.00004	0.00004	0.00009	0.00009	0.00007	0.00011	0.0008	0.00008	0.00001	0.00001	0.00001	0.00001	0.00001
166.08	6.24	+		0.00013	0.00054	0.00000	0.00011	0.00078	0.00010	0.00008	0.00033	0.00176	0.0019	0.00009	0.0048	0.00000	0.00006	0.00001	0.0041	0.0019	0.0123	0.00000	0.00011	0.00233	
169.02	6.749	+		0.00000	0.00091	0.00001	0.00001	0.0002	0.0002	0.0002	0.00002	0.00001	0.00007	0.00009	0.00002	0.00002	0.00004	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
169.05	8.906	+		0.00005	0.00023	0.00012	0.00041	0.00024	0.00015	0.00008	0.00016	0.00016	0.00008	0.00019	0.00018	0.00004	0.00014	0.00028	0.00008	0.0012	0.0014	0.00012	0.00012	0.00001	
169.08	3.039	+		0.00003	0.00034	0.00001	0.00017	0.00024	0.00024	0.00002	0.00001	0.00002	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	
171.07	10.651	-		0.00002	0.00001	0.00002	0.00002	0.00001	0.00000	0.00002	0.00001	0.00004	0.00001	0.0021	0.00001	0.00003	0.00002	0.00001	0.00001	0.00000	0.00000	0.00000	0.00000	0.00001	
173.04	2.13	-		0.00012	0.00002	0.00001	0.00011	0.00003	0.00003	0.00001	0.00002	0.00002	0.00004	0.00009	0.00000	0.00010	0.00003	0.00002	0.0013	0.00013	0.00002	0.00001	0.00001	0.00001	
173.05	2.112	-		0.00009	0.00003	0.00003	0.00004	0.00000	0.00000	0.00000	0.00000	0.00004	0.00003	0.00003	0.00004	0.00003	0.00001	0.00003	0.00002	0.00001	0.00001	0.00001	0.00001	0.00001	
173.06	2.945	-		0.00003	0.00000	0.00000	0.00000	0.00003	0.00002	0.00000	0.00000	0.00000	0.00005	0.00005	0.00005	0.00005	0.00005	0.00006	0.00006	0.00006	0.00006	0.00006	0.00006	0.00006	
173.10	2.166	-		0.00014	0.00048	0.00018	0.0210	0.0085	0.0046	0.0148	0.0084	0.0022	0.0020	0.0080	0.0045	0.0066	0.0048	0.0164	0.0085	0.0222	0.0006	0.0164	0.0096	0.0036	
173.22	2.161	-		0.00012	0.00000	0.00000	0.0036	0.00000	0.00000	0.0018	0.0003	0.0001	0.0021	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	
175.03	2.67	-		0.00069	0.00000	0.00000	0.0043	0.00000	0.00000	0.0054	0.00000	0.00000	0.00000	0.0012	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00123	0.00000	0.00000	0.00000	
176.04	2.802	-		0.00001	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000		
176.05	2.145	-		0.00002	0.00002	0.00002	0.00002	0.00002	0.00002	0.00002	0.00002	0.00002	0.00002	0.00002	0.00002	0.00002	0.00002	0.00002	0.00002	0.00002	0.00002	0.00002	0.00002		
176.09	16.183	-		0.00008	0.0008	0.00008	0.00008	0.00008	0.00008	0.00008	0.00008	0.00008	0.00008	0.00008	0.00008	0.00008	0.00008	0.00008	0.00008	0.00008	0.00008	0.00008	0.00008		
176.93	4.443	-		0.00005	0.00005	0.00012	0.00008	0.00008	0.00008	0.00008	0.00008	0.00008	0.00008	0.00008	0.00008	0.00008	0.00008	0.00008	0.00008	0.00008	0.00008	0.00008	0.00008		
179.00	8.669	-		0.00008	0.00013	0.00010	0.0022	0.00023	0.00025	0.00008	0.00009	0.00005	0.00004	0.00034	0.00007	0.0024	0.0018	0.0028	0.0005	0.003	0.003	0.0034	0.0005	0.0005	
179.04	2.346	-		0.00009	0.00001	0.00013	0.00053	0.00018	0.00014	0.00087	0.00019	0.00008	0.00008	0.00008	0.00008	0.00008	0.00008	0.00008	0.00008	0.00008	0.00008	0.00008	0.00008		
179.07	2.947	-		0.00052	0.00044	0.00034	0.00044	0.00044	0.00044	0.00005	0.00021	0.00086	0.0018	0.0008	0.0003	0.00056	0.00050	0.0035	0.0055	0.00000	0.00000	0.00000	0.00000		
179.10	11.744	-		0.00008	0.00089	0.00001	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000		
179.16	11.708	-		0.00001	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000		
179.17	1.477	-		0.00001	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000		
179.20	1.477	-		0.00002	0.00004	0.00004	0.00002	0.00004	0.00002	0.00002	0.00002	0.00002	0.00002	0.00002	0.00002	0.00002	0.00002	0.00002	0.00002	0.00002	0.00002	0.00002	0.00002		
179.23	14.789	-		0.00040	0.0036	0.0028	0.0042	0.0005	0.0035	0.0042	0.0002	0.0042	0.0038	0.003	0.0041	0.0008	0.0001	0.0002	0.0003	0.0004	0.0005	0.0006	0.0007		
179.25	12.542	+		0.00169	0.00103	0.0153	0.0168	0.00130	0.00173	0.0009	0.0286	0.00168	0.0019	0.0008	0.0000	0.0286	0.00155	0.00166	0.0008	0.0000	0.00129	0.00005	0.00005		
179.26	12.652	+		0.00169	0.00103	0.0153	0.0168	0.00130	0.00173	0.0009	0.0286	0.00168	0.0019	0.0008	0.0000	0.0286	0.00155	0.00166	0.0008	0.0000	0.001				

(continued)

	(Name)	A1	A2	A3	BF1	BF2	BF3	KM1	KM2	KM3	SM1	SM2	SM3	SR1	SR2	SR3	YB1	YB2	YB3	YM1	YM2	YM3		
m/z	R.T.	Polar.	(ORAC)	35.647	36.861	51.482	42.852	65.085	55.612	44.400	43.107	48.544	25.445	40.191	46.160	37.930	42.436	38.953	34.246	36.545	41.729	37.746	43.496	47.566
303.21	18.293	-	0.00014	0.0099	0.00125	0.00004	0.0001	0.0001	0.00149	0.0059	0.00167	0.00149	0.00118	0.00088	0.00006	0.00050	0.00069	0.00116	0.001	0.0183	0.00098	0.00098		
303.23	16.157	+	0.00040	0.0104	0.0089	0.00119	0.0135	0.0052	0.00153	0.00111	0.0098	0.00270	0.00068	0.0199	0.0097	0.00171	0.00161	0.00017	0.0183	0.0062	0.0000	0.0079	0.0069	
303.60	11.705	-	0.00005	0.00043	0.00004	0.00013	0.0059	0.0009	0.0008	0.0029	0.0007	0.0018	0.0001	0.0009	0.00032	0.0000	0.0021	0.0007	0.0000	0.0019	0.0003	0.0004		
304.06	7.816	-	0.00074	0.0079	0.00109	0.00033	0.0075	0.0065	0.0069	0.0016	0.00008	0.0043	0.0078	0.0067	0.0009	0.00050	0.0084	0.0068	0.0048	0.00075	0.00088	0.00147	0.0061	0.0091
304.07	8.225	-	0.00003	0.00028	0.00024	0.00005	0.0060	0.0009	0.0009	0.0018	0.0008	0.0003	0.00123	0.00069	0.0000	0.0008	0.00011	0.0008	0.0000	0.0001	0.0000	0.00079	0.00079	
304.91	8.354	-	0.00013	0.00109	0.00182	0.00083	0.0287	0.0077	0.0051	0.0043	0.0138	0.0103	0.0047	0.0048	0.0057	0.0051	0.0093	0.0118	0.0189	0.0058	0.0256	0.0155	0.0000	0.0000
305.06	8.485	-	0.04370	0.05556	0.06960	0.04580	0.05230	0.04240	0.05740	0.05240	0.0700	0.05677	0.05875	0.0590	0.02510	0.02700	0.01980	0.04570	0.04300	0.05830	0.07100	0.05880	0.07140	
305.08	7.747	-	0.00021	0.0018	0.0020	0.0017	0.0049	0.0051	0.0049	0.0030	0.0008	0.0002	0.0009	0.0009	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	
305.07	10.455	-	0.00008	0.0006	0.0034	0.0005	0.0009	0.0009	0.0009	0.0058	0.00023	0.0000	0.0033	0.0000	0.0008	0.0000	0.0001	0.0016	0.0010	0.0000	0.0000	0.0000	0.0000	
305.08	12.266	-	0.00044	0.00072	0.00117	0.0002	0.0001	0.0009	0.0007	0.0006	0.00027	0.00006	0.0004	0.0035	0.0008	0.0001	0.00048	0.00067	0.00008	0.0001	0.00052	0.00067		
305.19	16.358	-	0.00004	0.00037	0.00095	0.0009	0.0005	0.0005	0.0009	0.0016	0.00043	0.00078	0.0067	0.0009	0.00050	0.0084	0.0068	0.0048	0.00073	0.00088	0.0009	0.0003	0.0008	
307.04	8.441	-	0.00015	0.00181	0.00228	0.00146	0.0140	0.00191	0.0174	0.0259	0.0184	0.00208	0.0196	0.0075	0.0081	0.0017	0.0182	0.0191	0.0238	0.0193	0.0246	0.0117	0.0000	
307.31	8.476	-	0.000143	0.00181	0.00228	0.00146	0.0175	0.00203	0.0184	0.0259	0.0184	0.00208	0.0196	0.0075	0.0081	0.0017	0.0182	0.0191	0.0238	0.0193	0.0246	0.0117	0.0000	
307.40	8.478	-	0.000154	0.00188	0.00241	0.00160	0.0185	0.0048	0.0203	0.0184	0.00208	0.0192	0.0077	0.0081	0.0016	0.0194	0.0151	0.0203	0.0186	0.0210	0.0257	0.0117	0.0000	
307.07	2.244	-	0.00001	0.0000	0.0005	0.0023	0.0000	0.0001	0.0000	0.0006	0.0004	0.0001	0.0000	0.0000	0.0001	0.0002	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	
307.08	8.494	-	0.00012	0.0017	0.0022	0.0022	0.0170	0.0047	0.0220	0.0170	0.0040	0.0019	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	
307.14	10.499	-	0.00073	0.0135	0.0041	0.0022	0.003	0.0015	0.0028	0.0038	0.0050	0.0080	0.0004	0.0016	0.0042	0.0059	0.0011	0.0049	0.0048	0.0031	0.0052	0.0049	0.0023	
307.59	2.371	-	0.00169	0.0090	0.0083	0.00161	0.0052	0.0008	0.00136	0.0030	0.00114	0.00182	0.0008	0.0003	0.0005	0.0005	0.0005	0.0005	0.0018	0.00125	0.0000	0.0000	0.0000	
307.85	3.475	-	0.00000	0.0003	0.0001	0.0001	0.0000	0.0004	0.0002	0.0001	0.0000	0.0002	0.0000	0.0000	0.0003	0.0003	0.0003	0.0003	0.0000	0.0001	0.0000	0.0001	0.0000	
307.86	5.333	-	0.00006	0.0001	0.0002	0.0002	0.0004	0.0005	0.0006	0.0006	0.0000	0.0001	0.0010	0.0000	0.0007	0.0007	0.0007	0.0005	0.0004	0.0002	0.0003	0.0003		
307.86	3.864	-	0.00006	0.0001	0.0002	0.0002	0.0004	0.0005	0.0006	0.0006	0.0000	0.0001	0.0010	0.0000	0.0007	0.0007	0.0005	0.0004	0.0004	0.0002	0.0003	0.0003		
307.86	6.73	-	0.00011	0.0005	0.0006	0.0010	0.0000	0.0001	0.0001	0.0009	0.0000	0.0001	0.0002	0.0000	0.0001	0.0013	0.0003	0.0004	0.0005	0.0006	0.0010	0.0001	0.0000	
309.09	11.188	+	0.00000	0.00000	0.00000	0.00000	0.00195	0.0258	0.0291	0.0000	0.0000	0.0069	0.0000	0.0039	0.0038	0.0129	0.0258	0.0000	0.0034	0.0263	0.0247	0.0265	0.0000	
309.20	13.390	+	0.00000	0.00000	0.00000	0.00000	0.00174	0.0236	0.0275	0.0000	0.0000	0.0069	0.0000	0.0038	0.0037	0.0129	0.0275	0.0000	0.0034	0.0266	0.0251	0.0276	0.0000	
309.20	15.654	+	0.00000	0.00000	0.00000	0.00000	0.00203	0.0238	0.0278	0.0000	0.0000	0.0069	0.0000	0.0038	0.0037	0.0130	0.0278	0.0000	0.0034	0.0267	0.0252	0.0282	0.0000	
312.17	16.696	-	0.00006	0.0008	0.0003	0.0000	0.00192	0.023	0.0013	0.0000	0.0000	0.006	0.0000	0.003	0.0004	0.0000	0.0000	0.0001	0.0001	0.0001	0.0001	0.0000	0.0000	
312.18	17.533	+	0.00000	0.00000	0.00000	0.00000	0.00195	0.0238	0.0278	0.0000	0.0000	0.0069	0.0000	0.0038	0.0037	0.0132	0.0278	0.0000	0.0034	0.0268	0.0253	0.0283	0.0000	
312.19	18.293	-	0.00000	0.00000	0.00000	0.00000	0.00203	0.0238	0.0278	0.0000	0.0000	0.0069	0.0000	0.0038	0.0037	0.0133	0.0278	0.0000	0.0034	0.0268	0.0253	0.0283	0.0000	
312.20	18.635	+	0.00000	0.00000	0.00000	0.00000	0.00203	0.0238	0.0278	0.0000	0.0000	0.0069	0.0000	0.0038	0.0037	0.0133	0.0278	0.0000	0.0034	0.0268	0.0253	0.0283	0.0000	
313.00	13.744	-	0.00000	0.00000	0.00000	0.00000	0.00203	0.0238	0.0278	0.0000	0.0000	0.0069	0.0000	0.0038	0.0037	0.0133	0.0278	0.0000	0.0034	0.0268	0.0253	0.0283	0.0000	
313.10	15.261	-	0.00000	0.00000	0.00000	0.00000	0.00203	0.0238	0.0278	0.0000	0.0000	0.0069	0.0000	0.0038	0.0037	0.0133	0.0278	0.0000	0.0034	0.0268	0.0253	0.0283	0.0000	
313.16	15.306	-	0.00000	0.00000	0.00000	0.00000	0.00203	0.0238	0.0278	0.0000	0.0000	0.0069	0.0000	0.0038	0.0037	0.0133	0.0278	0.0000	0.0034	0.0268	0.0253	0.0283	0.0000	
313.24	15.117	-	0.00000	0.00000	0.00000	0.00000	0.00203	0.0238	0.0278	0.0000	0.0000	0.0069	0.0000	0.0038	0.0037	0.0133	0.0278	0.0000	0.0034	0.0268	0.0253	0.0283	0.0000	
315.07	8.005	-	0.00002	0.00203	0.00000	0.00006	0.0010	0.0000	0.0000	0.0006	0.00203	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000		
315.09	15.429	-	0.00000	0.00000	0.00000	0.00000	0.00198	0.0238	0.0278	0.0000	0.0000	0.0069	0.0000	0.0038	0.0037	0.0133	0.0278	0.0000	0.0034	0.0268	0.0253	0.0283	0.0000	
315.10	17.877	-	0.00000	0.00000	0.00000	0.00000	0.00203	0.0238	0.0278	0.0000	0.0000	0.0069	0.0000	0.0038	0.0037	0.0133	0.0278	0.0000	0.0034	0.0268	0.0253	0.0283	0.0000	
315.18	21.175	-	0.00000	0.00000	0.00000	0.00000	0.00203	0.0238	0.0278	0.0000	0.0000	0.0069	0.0000	0.0038	0.0037	0.0133	0.0278	0.0000	0.0034	0.0268	0.0253	0.0283	0.0000	
315.19	22.393	-	0.00000	0.00000	0.00000	0.00000	0.00203	0.0238	0.0278	0.0000	0.0000	0.0069	0.0000	0.0038	0.0037	0.0133	0.0278	0.0000	0.0034	0.0268	0.0253	0.0283	0.	

*(continued)*

**Supplementary Table S6.** Selected peaks with the highest VIP values ( $>1$ ) contributing to the construction of OPLS regression models in LC–MS datasets.

**Supplementary Table S7.** Selected peaks with the highest VIP values (>1) contributing to the construction of the polyphenol-predictive OPLS regression model in MALDI-MS datasets.

Variables	m/z	VIP	(Name)	AT1	AT2	AT3	BF1	BF2	BF3	KM1	KM2	KM3	SM1	SM2	SM3	SR1	SR2	SR3	YB1	YB2	YB3	YM1	YM2	YM3
V01	170.08	3.52	(Polyphenol)	1.93	2.11	2.54	2.04	2.56	2.54	2.00	2.11	2.41	1.96	2.13	2.33	2.44	2.33	2.17	2.12	2.13	2.34	2.21	2.28	2.65
V02	305.19	3.20		0.04070	0.05580	0.05710	0.04220	0.05710	0.05640	0.04840	0.05490	0.06950	0.04650	0.05640	0.06680	0.03360	0.03900	0.03480	0.04070	0.04740	0.05710	0.05080	0.05760	0.07250
V03	132.97	2.69		0.02420	0.01270	0.00620	0.02820	0.01910	0.01290	0.02080	0.01800	0.00780	0.02170	0.01770	0.00530	0.01890	0.02490	0.01750	0.01740	0.02430	0.01120	0.01720	0.01440	0.00760
V04	289.19	2.33		0.01740	0.02280	0.02420	0.02320	0.02910	0.02810	0.0210	0.02240	0.02800	0.01770	0.02130	0.02640	0.01710	0.02070	0.01810	0.01880	0.02030	0.02390	0.02260	0.02430	0.03130
V05	441.14	2.32		0.02020	0.02440	0.02740	0.01770	0.03010	0.03130	0.01920	0.01950	0.02150	0.01100	0.02310	0.02360	0.01930	0.01690	0.02310	0.01690	0.02090	0.02160	0.01820	0.02850	0.02830
V06	167.02	2.16		0.03350	0.04280	0.03930	0.03170	0.04120	0.04050	0.03320	0.04130	0.04190	0.02830	0.04160	0.04250	0.03550	0.03490	0.03890	0.03260	0.04010	0.04140	0.03630	0.04240	0.04400
V07	287.18	2.08		0.01840	0.02460	0.02430	0.01870	0.02530	0.02710	0.02030	0.02370	0.02530	0.01500	0.02350	0.02690	0.02110	0.02020	0.02290	0.01930	0.02240	0.02510	0.02070	0.02610	0.02680
V08	457.20	2.02		0.04110	0.04880	0.04720	0.03150	0.04970	0.04680	0.04130	0.04830	0.04580	0.02840	0.04720	0.04750	0.04080	0.03790	0.03940	0.04040	0.04800	0.04600	0.04200	0.05490	0.05130
V09	166.02	2.01		0.02010	0.02660	0.02670	0.02160	0.02760	0.02640	0.02350	0.02720	0.03310	0.02200	0.02880	0.01890	0.02170	0.01980	0.02080	0.02380	0.02720	0.02470	0.02700	0.03320	
V10	168.06	2.00		0.03590	0.04550	0.04220	0.03360	0.04430	0.04410	0.03490	0.04430	0.04190	0.03110	0.04410	0.04750	0.04240	0.04460	0.05190	0.03490	0.04410	0.04580	0.03820	0.04430	0.04410
V11	136.99	2.00		0.01580	0.01990	0.01870	0.01580	0.02200	0.02050	0.01750	0.02100	0.02330	0.01910	0.01810	0.02760	0.01610	0.02000	0.01610	0.01560	0.02080	0.02480	0.01980	0.01940	0.02440
V12	116.99	1.99		0.00660	0.00380	0.00310	0.00800	0.00310	0.00270	0.00510	0.00260	0.00730	0.00770	0.00110	0.00260	0.00460	0.00390	0.00510	0.00560	0.00440	0.00600	0.00390	0.00010	
V13	176.01	1.88		0.00480	0.00450	0.00010	0.00470	0.00010	0.00320	0.00440	0.00460	0.00010	0.00010	0.00010	0.00010	0.00450	0.00100	0.00400	0.00440	0.00500	0.00010	0.00490	0.00410	0.00010
V14	209.19	1.82		0.00850	0.00010	0.00100	0.00960	0.00010	0.00110	0.00760	0.00010	0.00010	0.00870	0.00010	0.00010	0.00850	0.00010	0.00010	0.00750	0.00870	0.00010	0.00780	0.00010	0.00010
V15	177.14	1.79		0.00720	0.00010	0.00100	0.00700	0.00010	0.00460	0.00660	0.00010	0.00010	0.00910	0.00010	0.00010	0.00100	0.00740	0.00010	0.00640	0.00630	0.00010	0.00010	0.00740	0.00010
V16	125.02	1.74		0.01650	0.02010	0.01800	0.01510	0.02120	0.02050	0.01570	0.01890	0.01940	0.01560	0.01750	0.02650	0.01800	0.01860	0.01840	0.01550	0.02150	0.02410	0.01780	0.01940	0.02110
V17	288.20	1.74		0.00940	0.01320	0.01380	0.00970	0.01400	0.01560	0.01010	0.01220	0.01400	0.00730	0.01250	0.01640	0.01010	0.01000	0.01210	0.00960	0.01130	0.01330	0.01040	0.01390	0.01460
V18	204.14	1.72		0.01590	0.00010	0.00100	0.00010	0.00010	0.00010	0.00010	0.00010	0.00010	0.00010	0.00010	0.00010	0.00010	0.00120	0.00010	0.00010	0.00010	0.00010	0.00010	0.00010	0.00010
V19	144.99	1.50		0.00010	0.00010	0.00010	0.01820	0.00830	0.00010	0.01330	0.00820	0.00010	0.02170	0.00010	0.00010	0.01970	0.00010	0.00010	0.02430	0.00010	0.00010	0.00010	0.00010	
V20	162.64	1.49		0.00010	0.00580	0.00530	0.00010	0.00590	0.00580	0.00010	0.00580	0.00010	0.00580	0.00570	0.00010	0.00580	0.00010	0.00580	0.00550	0.00010	0.00580	0.00630	0.00610	0.00060
V21	138.00	1.48		0.00920	0.01210	0.01130	0.00930	0.01290	0.01240	0.01030	0.01230	0.01350	0.01050	0.01100	0.01690	0.00840	0.01020	0.00870	0.00900	0.01190	0.01440	0.01110	0.01150	0.01440
V22	755.31	1.46		0.01170	0.01220	0.01200	0.00370	0.00640	0.00490	0.01450	0.01310	0.00850	0.01030	0.01520	0.00970	0.00010	0.00010	0.01500	0.01350	0.00880	0.00920	0.00850	0.00430	
V23	128.00	1.45		0.00430	0.00180	0.00010	0.01670	0.00640	0.00240	0.00740	0.00610	0.00010	0.01520	0.00340	0.00010	0.00530	0.00610	0.00370	0.00930	0.00550	0.00210	0.01210	0.00300	0.00240
V24	175.44	1.34		0.00200	0.00190	0.00170	0.01280	0.00010	0.01900	0.00180	0.00170	0.01810	0.00100	0.02220	0.00010	0.00010	0.00010	0.00010	0.02000	0.00210	0.00230	0.00210	0.00010	
V25	307.24	1.34		0.00440	0.00530	0.00500	0.00400	0.00010	0.00010	0.00490	0.00510	0.00010	0.00430	0.00010	0.00010	0.00390	0.00400	0.00370	0.00440	0.00490	0.00520	0.00510	0.00010	
V26	145.99	1.25		0.01070	0.00620	0.00510	0.01140	0.00740	0.00520	0.01190	0.01000	0.00710	0.01900	0.00810	0.00360	0.00960	0.00810	0.00630	0.01150	0.01060	0.00860	0.01290	0.00910	0.00760
V27	293.20	1.24		0.00010	0.00010	0.00260	0.00010	0.00010	0.00290	0.00010	0.00010	0.00010	0.00010	0.00010	0.00010	0.00010	0.00010	0.00010	0.00010	0.00010	0.00010	0.00010	0.00320	0.00340
V28	126.97	1.23		0.00850	0.00430	0.00010	0.00680	0.00510	0.00010	0.00660	0.00450	0.00010	0.00720	0.00360	0.00040	0.00650	0.00700	0.00380	0.00610	0.00690	0.00470	0.00730	0.00380	0.00400
V29	756.29	1.23		0.00410	0.00440	0.00440	0.00010	0.00010	0.00010	0.00530	0.00470	0.00290	0.00010	0.00550	0.00350	0.00010	0.00010	0.00010	0.00560	0.00480	0.00260	0.00310	0.00010	
V30	456.09	1.20		0.01440	0.01790	0.01790	0.01090	0.01810	0.01750	0.01540	0.01820	0.01610	0.00970	0.01720	0.01640	0.01380	0.01220	0.01770	0.01460	0.01730	0.01630	0.01450	0.02140	0.01900
V31	202.14	1.17		0.00740	0.00100	0.00010	0.00010	0.00010	0.00010	0.00010	0.00010	0.00010	0.00010	0.00010	0.00010	0.00010	0.00010	0.00010	0.00010	0.00010	0.00010	0.00010	0.00010	
V32	160.13	1.15		0.00960	0.00700	0.00440	0.00720	0.00630	0.00446	0.00770	0.00780	0.00500	0.00970	0.00690	0.00010	0.01030	0.00010	0.00530	0.00970	0.00900	0.00570	0.00990	0.00710	0.00560
V33	124.01	1.15		0.00800	0.01020	0.00890	0.00730	0.00960	0.00970	0.00710	0.00880	0.00920	0.00710	0.00850	0.01310	0.00810	0.00790	0.00830	0.00730	0.01050	0.01210	0.00800	0.00970	0.01040
V34	479.57	1.14		0.00830	0.01010	0.02060	0.00010	0.00010	0.00910	0.00880	0.00010	0.01390	0.00010	0.01020	0.01940	0.03020	0.02440	0.03290	0.00770	0.00010	0.01480	0.00010	0.00760	0.00860
V35	220.15	1.10		0.00340	0.00010	0.00010	0.00010	0.00010	0.00010	0.00250	0.00010	0.00010	0.00010	0.00010	0.00010	0.00010	0.00010	0.00010	0.00010	0.00010	0.00010	0.00010	0.00010	
V36	304.16	1.06		0.00720	0.00970	0.00970	0.00680	0.00890	0.00980	0.00810	0.00910	0.01010	0.00690	0.00880	0.01010	0.00660	0.00640	0.00680	0.00730	0.00790	0.00860	0.00810	0.00970	0.01070
V37	286.15	1.02		0.00710	0.00920	0.01010	0.00600	0.00820	0.00930	0.00850	0.00910	0.00980	0.00640	0.00970	0.01060	0.00940	0.00840	0.00920	0.00800	0.00800	0.00910	0.00770	0.00980	0.00920
V38	354.53	1.01		0.00190	0.00010	0.00010</																		