

Prediction of flavor potential of *Ocimum basilicum* L. side-stream phytoconstituents, using LC-MS analysis and *in silico* techniques

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Table S1. Taste prediction results of *Ocimum basilicum* side-stream characterized phytochemicals, derived from Virtuous Multitaste tool (<https://virtuous.isi.gr/#/multitaste>) (accessed on 22 May 2024).

Compound	.smi files	%Bitter	%Sweet	%Umami	%Other (Sour and Salty)
1-octen-yl pentosyl glucoside	<chem>C=CC(CCCCC)OC1OC(CO)C(O)C(O)C1O</chem>	48	24	5	22
3-(3,4-dihydroxyphenyl) lactic acid glucoside	<chem>O=C([O-])C(O)CC1=CC(O)=C(O)C=C1</chem>	33	13	39	16
Caffeic acid	<chem>O=C(O)/C=C/C1=CC(O)=C(O)C=C1</chem>	42	33	16	9
Caffeoyl-dihydroxyphenyllactoyltartaric acid	<chem>O=C(/C=C/C1=CC(O)=C(O)C=C1)OC(C(=O)O)C(O)C(=O)O</chem>	20	21	38	21
Caffeoylferuloyltartaric acid (cichoric acid methyl ether)	<chem>COC1=C(O)C=CC(/C=C/C(=O)C(O)(C(=O)O)C(=O)O)C(=O)/C=C/C2=CC(O)=C(O)C=C2)=C1</chem>	55	25	4	16
Caftaric acid (Caffeoyl-tartaric acid)	<chem>O=C(/C=C/C1=CC(O)=C(O)C=C1)OC(C(=O)O)C(O)C(=O)O</chem>	20	21	38	21
Chicoric acid	<chem>O=C(/C=C/C1=CC(O)=C(O)C=C1)OC(C(=O)O)C(OC(=O)/C=C/C1=CC(O)=C(O)C=C1)C(=O)O</chem>	36	13	33	19
Chlorogenic acid	<chem>O=C(/C=C/C1=CC(O)=C(O)C=C1)OC1CC(O)(C(=O)O)CC(O)C1O</chem>	44	6	26	23
Dihydroxy dimethoxyflavone	<chem>COC1=C(OC)C=C(C2=C(O)C(=O)C3=C(C=C(O)C=C3)O2)C=C1</chem>	41	33	0	26
Dihydroxybenzoic acid-O-pentosyl pentoside	<chem>O=C(/C=C/C1=CC(O)=C(O)C=C1)OC(CCC1=CC(OC2OC(C(O)C(O)C(O)C2O)=C(O)C=C1)C(=O)[O-])</chem>	41	6	19	34
Dihydroxy-octadecadienoic acid	<chem>CCCCC(C=CC=CC(CCCC(CCC(=O)O)O)O</chem>	39	21	22	18
Dihydroxy-octadecatrienoic acid	<chem>CCC=CCC=CCC=CC(C(CCC(CCC(=O)O)O)O</chem>	57	15	4	24
Dihydroxy-oleanenoic acid	<chem>CC1(CCC2(CCC3(C(=CCC4C3(CCC5C4(CCC(C5(C)C)O)C)C)C2C1)CO)C(=O)O)C</chem>	81	8	1	9
Ethyl caffeate	<chem>CCOC(=O)/C=C/C1=CC(O)=C(O)C=C1</chem>	78	17	3	2
Ethyl protocatechuate	<chem>CCOC(=O)C1=CC(O)=C(O)C=C1</chem>	80	6	8	5
Fertaric acid (feruloyltartaric acid)	<chem>COC1=CC(/C=C/C(=O)OC(C(=O)O)C(O)C(=O)O)=CC=C1O</chem>	38	12	22	27
Ferulic acid	<chem>COC1=C(O)C=CC(/C=C/C(=O)O)=C1</chem>	54	19	11	17
Gallic acid	<chem>O=C(O)C1=CC(O)=C(O)C(O)=C1</chem>	79	5	7	8

Galloylglucose	<chem>CO[C@H]1O[C@@H](OC(=O)C2=CC(O)=C(O)C(O)=C2)[C@H](O)[C@@H](O)[C@H]1O</chem>	23	8	35	34
Hydroxy jasmonic acid-O-glucoside	<chem>CCC1OC(OCC/C=C/CC2C(=O)CCC2CC(=O)O)C(O)C(O)C1O</chem>	47	19	9	25
Hydroxy-octadecatrienoic acid		57	13	23	7
Hydroxy-oxo-phytodienoic acid	<chem>CC/C=C/CC1C(=O)C=CC1CCCCCCCC(=O)O</chem>	25	41	4	29
Isocitric acid	<chem>O=C(O)CC(C(=O)O)C(O)C(=O)O</chem>	2	1	83	14
Isoquercetin	<chem>O=C1C(OC2OC(CO)C(O)C(O)C2O)=C(C2=CC(O)=CC=C2)OC2=CC(O)=CC(O)=C12</chem>	86	8	0	5
Lithospermic acid A	<chem>O=C(/C=C/C1=C2C(=C(O)C=C1)OC(C1=CC(O)=C(O)C=C1)C2C(=O)O)OC(CC1=CC(O)=C(O)C=C1)C(=O)O</chem>	53	7	15	25
Methyl gallate	<chem>COC(=O)C1=CC(O)=C(O)C(O)=C1</chem>	59	11	17	16
Nepetoidin glucoside	<chem>COC1=C(O)C2=C(C=C1O)OC(C1=CC(O)=C(OC3OC(CO)C(O)C(O)C3O)C=C1)=CC2=O</chem>	55	26	0	19
O-caffeoyl rosmarinic acid (isomelitrac acid A)	<chem>O=C(/C=C/C1=CC(O/C(=C/C2=CC(O)=C(O)C=C2)C(=O)O)=C(O)C=C1)OC(CC1=CC(O)=C(O)C=C1)C(=O)O</chem>	48	9	23	25
Palmitic acid	<chem>CCCCCCCCCCCCCCCC(=O)O</chem>	58	19	3	20
p-Coumaric acid	<chem>O=C(O)/C=C/C1=CC=C(O)C=C1</chem>	41	13	27	19
p-Hydroxybenzoic acid	<chem>O=C(O)C1=CC=C(O)C=C1</chem>	45	22	12	21
Protocatechuic acid	<chem>C1=CC(=C(C=C1C(=O)O)O)O</chem>	48	16	14	22
Quercetin 3-O-glucoside	<chem>O=C1C(OC2OC(CO)C(O)C(O)C2O)=C(C2=CC(O)=C([O-])C=C2)OC2=CC(O)=CC(O)=C12</chem>	47	21	4	27
Quercetin-3-O-apiosyl (1-2) galactoside	<chem>O=C1C(OC2OC(CO)C(O)C(O)C2OC2OCC(O)(CO)C2O)=C(C2=CC(O)=C(O)C=C2)OC2=CC(O)=CC(O)=C12</chem>	19	15	4	62
Quercetin-O-pentosyl-glucoside	<chem>O=C1C(OC2CC(O)C(O)C(O)O2)=C(C2=CC(O)=C(O)C=C2)OC2=CC(OC3OC(CO)C(O)C(O)C3O)=CC(O)=C12</chem>	16	73	8	3
Rosmarinic acid	<chem>O=C(/C=C/C1=CC(O)=C(O)C=C1)OC(CC1=CC(O)=C(O)C=C1)C(=O)O</chem>	40	11	26	23
Rosmarinic acid glucoside A	<chem>C1=CC(=C(C=C1CC(C(=O)O)OC(=O)C=CC2=CC(=C(C=C2)O)OC3C(C(C(C(O3)CO)O)O)O)O</chem>	40	5	35	20
Rosmarinic acid glucoside B	<chem>C1=CC(=C(C=C1CC(C(=O)[O-]</chem>	41	6	34	19

	<chem>]]OC(=O)C=CC2=CC(=C(C=C2)O)OC3C(C(C(C(O3)C(O)O)O)O)O</chem>				
Rosmarinic acid-O-glucoside	<chem>O=C(/C=C/C1=CC(O)=C(O)C=C1)OC(CC1=CC(OC2OC(C(O)C(O)C(O)C2O)=C(O)C=C1)C(=O)[O-])</chem>	41	6	19	34
Rutin	<chem>CC1OC(OCC2OC(OC3=C(C4=CC(O)=C(O)C=C4)OC4=C(C(O)=CC(O)=C4C3=O)C(O)C(O)C2O)C(O)C(O)C1O</chem>	11	7	2	80
Sagerinic acid	<chem>O=C(O)C(CC1=CC(O)=C(O)C=C1)OC(=O)C1C(C(=O)OC(CC2=CC(O)=C(O)C=C2)C(=O)O)C(C2=CC(O)=C(O)C=C2)C1C1=CC(O)=C(O)C=C1</chem>	52	13	22	14
Salvialinic acid (danshensu)	<chem>C1=CC(=C(C=C1C[C@H](C(=O)O)O)O)O</chem>	33	39	16	13
Salvianolic acid A	<chem>C1=CC(=C(C=C1CC(C(=O)O)OC(=O)C=CC2=C(C(=C(C=C2)O)O)C=CC3=CC(=C(C=C3)O)O)O)O</chem>	55	3	13	29
Salvianolic acid B	<chem>O=C(/C=C/C1=C2C(=C(O)C=C1)OC(C1=CC(O)=C(O)C=C1)C2C(=O)OC(CC1=CC(O)=C(O)C=C1)C(=O)O)OC(CC1=CC(O)=C(O)C=C1)C(=O)O</chem>	62	6	13	19
Salvianolic acid C	<chem>O=C(/C=C/C1=C2C=C(C3=C(C(O)=C(O)C=C3)OC2=C(O)C=C1)OC(CC1=CC(O)=C(O)C=C1)C(=O)O</chem>	64	7	9	19
Salvianolic acid F	<chem>O=C(O)/C=C/C1=C(/C=C/C2=CC(O)=C(O)C=C2)C(O)=C(O)C=C1</chem>	78	5	4	13
Salvianolic acid G	<chem>O=C(O)C1CC2=C3C(=CC4=C(OC3=C(O)C=C2)C(O)=C(O)C=C4)C1=O</chem>	77	14	1	8
Salvianolic acid H/I	<chem>O=C(/C=C/C1=CC(O/C(=C/C2=CC(O)=C(O)C=C2)C(=O)O)=C(O)C=C1)OC(CC1=CC(O)=C(O)C=C1)C(=O)O</chem>	42	9	23	25
Salvianolic acid K	<chem>O=C(/C=C/C1=CC(O)=C(OC(C(=O)O)C(O)C2=CC(O)=C(O)C=C2)C=C1)OC(CC1=CC(O)=C(O)C=C1)C(=O)O</chem>	53	5	15	27
Salvigenin (5-Hydroxy-6,7,4'-trimethoxyflavone)	<chem>COC1=CC=C(C2=CC(=O)C3=C(O)C(OC)=C(OC)C=C3O2)C=C1</chem>	62	14	1	23
Trihydroxy-octadecendic acid	<chem>O=C(O)/C=C/CCCCCCCCCCCCCCCC(O)(O)O</chem>	21	26	39	14
Vanillic acid	<chem>COC1=CC(C(=O)O)=CC=C1O</chem>	58	16	16	11

Table S2. The glide score (gscore) and the interaction pattern of the co-crystallized ligand strychnine and examined phytochemicals into *h*TASR46 binding site.

Compound	Glide gscore (kcal·mol ⁻¹)	Interaction Pattern
Strychnine	-5.44	HB(x2) Glu265 , HB Thr180 , p-c Trp88 , p-p(x2) Trp88
Caffeoylferuloyltartaric acid (cichoric acid methyl ether)	-7.21	HB(x4) Glu265 , HB Asn176, HB Ala84, p-p Trp88
Dihydroxy-octadecatrienoic acid	-5.22	HB(x3) Glu265 , HB Thr180 , HB Asn65, HB & SB Lys156, p-p Trp66
Dihydroxy-oleanenoic acid	-3.86	HB Thr180 , HB Asn65
Ethyl caffeate	-4.84	HB Ala268, HB Ser248
Ethyl protocatechuate	-5.14	HB(x2) Glu265
Ferulic acid	-5.74	HB Glu265 , HB Trp66, p-p Trp88
Gallic acid	-5.73	HB(x2) Glu265 , HB Asn92, HB Trp88
Hydroxy-octadecatrienoic acid	NB	-
Isoquercetin	-6.48	HB(x2) Glu265 , HB Thr180 , HB Lys156, HB Asn65
Lithospermic acid A	-5.70	HB Glu265 , HB Thr180 , HB Lys156, HB Val61, p-p Trp88
Methyl gallate	-5.27	HB(x2) Glu265 , p-p Trp88
Nepetoidin glucoside	-4.36	HB(x2) Glu265 , HB Thr180 , HB(x2) Lys156
Palmitic acid	NB	-
Sagerinic acid	-6.81	HB Ala268, HB(x2) Glu265 , HB Thr180 , HB Lys156, HB Arg81, HB Asn65, p-p Tyr85
Salvianolic acid A	-6.32	HB Glu265 , HB Ser248, HB Asn176, HB Lys156, HB Val61, p-p Trp88
Salvianolic acid B	-7.26	HB Glu265 , HB Thr69, HB(x2) Asn65, p-p Tyr85
Salvianolic acid C	-7.14	HB(x2) Glu265 , HB Asn176, HB(x2) Lys156, HB(x2) Thr69, HB Asn65, HB Val61, p-p(x2) Trp88
Salvianolic acid F	-6.31	HB Glu265 , HB Thr180 , HB Ala84, HB Trp66, HB(x2) Asn65, p-p(x2) Trp88
Salvianolic acid G	-5.63	HB Glu265 , HB Ser248, p-p(x2) Trp88
Salvianolic acid K	-6.38	HB(x2) Glu265 , HB(x2) Asn176, HB Lys156, HB Asn92, HB Arg81, HB Thr69
Salvigenin (5-Hydroxy-6,7,4'- trimethoxyflavone)	-4.57	p-p Phe252, p-p Tyr85
Vanillic acid	-5.16	HB Glu265

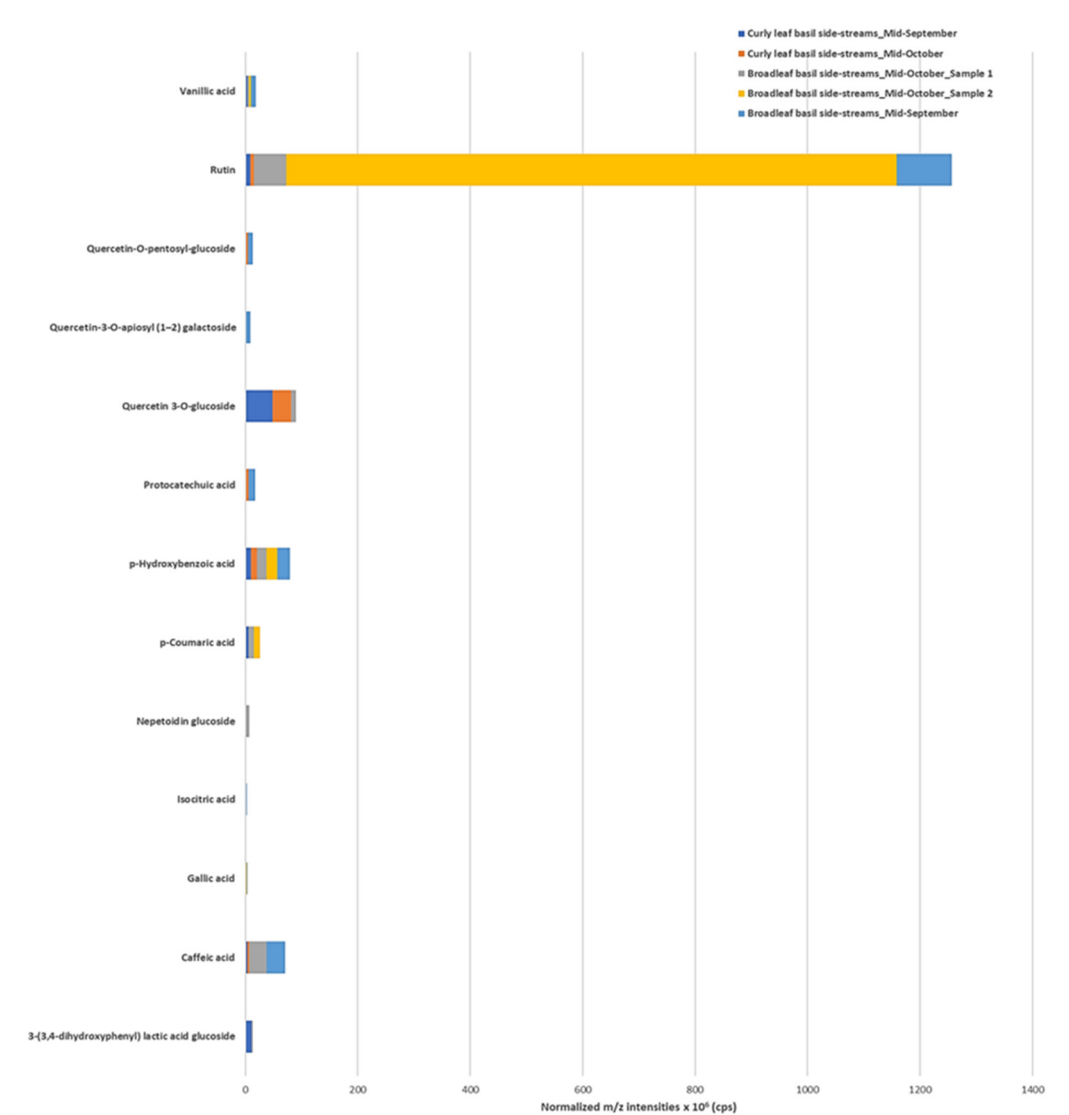


Figure S1. Annotated compounds with low normalized contents in basil side-stream extracts.

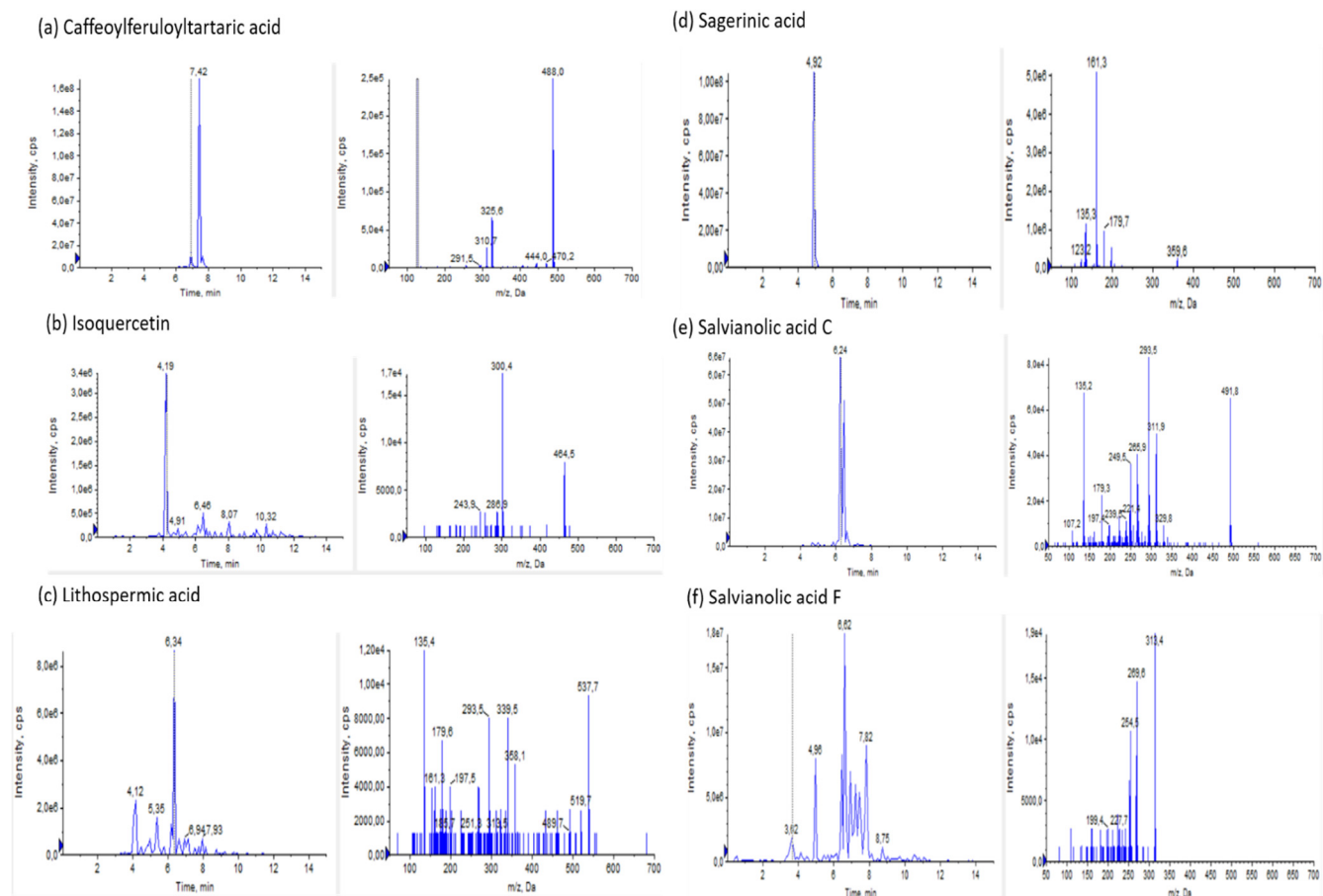


Figure S2. LC-MS/MS spectra of the six potential bitterants.