

Supplementary table 1. The database of all 301 selected flavor compounds.

pubchem_ cid	cas	canonical_smiles	chemical_name	flavor
11039	547-63-7	<chem>O=C(OC)C(C)C</chem>	methyl 2-methylpropanoate	aromatic
7342	97-62-1	<chem>O=C(OCC)C(C)C</chem>	ethyl 2-methylpropanoate	aromatic
13357	868-57-5	<chem>O=C(OC)C(CC)C</chem>	methyl 2-methylbutanoate	aromatic
24020	7452-79- 1/53956-13-1	<chem>O=C(OCC)C(CC) C</chem>	ethyl 2-methylbutanoate	aromatic
6560	78-83-1	<chem>OCC(C)C</chem>	2-methylpropan-1-ol	aromatic
31276	123-92-2	<chem>O=C(OCCC(C)C) C</chem>	3-methylbutyl acetate	aromatic
162239	37064-20-3	<chem>O=C(OCCC)C(CC))C</chem>	propyl 2-methylbutanoate	aromatic
31265	123-66-0	<chem>O=C(OCC)CCCC C</chem>	ethyl hexanoate	aromatic
522834	85213-22-5	<chem>O=C(C)C1=NCCC 1</chem>	2-acetyl-1-pyrroline	other
5352367	19883-27- 3/51447-08- 6/16356-11-9	<chem>C(C=CCCCC)= CC=C</chem>	(3E,5Z)-undeca-1,3,5-triene	aromatic
176	64-19-7	<chem>O=C(O)C</chem>	acetic acid	other
18635	3268-49-3	<chem>S(CCC=O)C</chem>	3-(methylsulfanyl)propanal	sulfury
1032	29102	<chem>O=C(O)CC</chem>	propanoic acid	other
6549	78-70-6	<chem>OC(C=C)(CCC=C (C)C)C</chem>	linalool	aromatic
6590	79-31-2	<chem>O=C(O)C(C)C</chem>	2-methylpropanoic acid	other
264	203-532-3	<chem>O=C(O)CCC</chem>	butanoic acid	other
10448	505-10-2	<chem>S(CCCO)C</chem>	3-(methylsulfanyl)propan-1-ol	sulfury
5366074	23696-85- 7/23726-93-4	<chem>O=C(C=CC)C1=C (C)C=CCC1(C)C</chem>	(E)-damascenone	aromatic
637566	106-24-1	<chem>OCC=C(CCC=C(C)C)C</chem>	geraniol	aromatic
6054	22258	<chem>OCCc1ccccc1</chem>	2-phenylethan-1-ol	aromatic
638014	79-77-6	<chem>O=C(C=CC=1C(C)C)CCCC=1C)C</chem>	ionone	aromatic
33931	27538-10-9	<chem>O=C1C(O)=C(C) OC1CC</chem>	2-Ethyl-4-hydroxy-5- methylfuran-3(2H)-one	other
62835	28664-35-9	<chem>O=C1C(O)=C(C)C (C)O1</chem>	sotolon	other
332	7786-61- 0/31853-85-7	<chem>O(C)c1c(O)ccc(C= C)c1</chem>	2-methoxy-4-vinylphenol	other
11952	613-89-8	<chem>O=C(CN)c1ccccc1</chem>	2-aminoacetophenone	other
61199	698-10-2	<chem>O=C1C(O)=C(C)C (CC)O1</chem>	abhexone	other

999	103-82-2	<chem>O=C(O)Cc1ccccc1</chem>	phenylacetic acid	aromatic
1183	121-33-5	<chem>O=Cc1cc(OC)c(O)cc1</chem>	vanillin	aromatic
8103	111-27-3	<chem>OCCCCC</chem>	1-hexanol	aromatic
5281167	928-96-1	<chem>OCCC=CCC</chem>	Z-3-hexenol	other
31260	123-51-3	<chem>OCC(C)C</chem>	3-methyl-1-butanol	aromatic
8723	137-32-6	<chem>OCCC(C)C</chem>	2-methyl-1-butanol	aromatic
6276	71-41-0	<chem>OCC(CC)C</chem>	1-pentanol	aromatic
5364919	1576-95-0/1576-96-1	<chem>OCCCC</chem>	Z-2-penten-1-ol	aromatic
8109	111-35-3	<chem>O(CCCO)CC</chem>	3-ethoxy-1-propanol	aromatic
7720	104-76-7	<chem>OCC(CCCC)CC</chem>	2-ethyl-1-hexanol	aromatic
957	111-87-5	<chem>OCCCCCCCC</chem>	1-octanol	aromatic
263	71-36-3	<chem>OCCCC</chem>	1-butanol	aromatic
11508	589-35-5	<chem>OCCC(CC)C</chem>	3-methyl-1-pentanol	aromatic
7361	98-00-0	<chem>OCc1ccccc1</chem>	Furfuryl alcohol	other
244	100-51-6	<chem>OCc1ccccc1</chem>	Benzyl alcohol	aromatic
17100	98-55-5	<chem>OC(C)(C)C1CC=C(C)CC1</chem>	terpineol	aromatic
8842	106-22-9	<chem>OCCC(CCC=C(C)C)C</chem>	citronellol	aromatic
7762	105-54-4	<chem>O=C(OCC)CCC</chem>	Ethyl butyrate	aromatic
7945	108-64-5	<chem>O=C(OCC)CC(C)C</chem>	Ethyl 3-methylbutyrate	aromatic
10882	539-82-2	<chem>O=C(OCC)CCCC</chem>	Ethyl pentanoate	aromatic
7344	97-64-3	<chem>O=C(OCC)C(O)C</chem>	Ethyl lactate	aromatic
7799	106-32-1	<chem>O=C(OCC)CCCCC</chem>	Ethyl octanoate	aromatic
62572	5405-41-4	<chem>O=C(OCC)CC(O)C</chem>	Ethyl 3-hydroxybutyrate	aromatic
8048	110-38-3	<chem>O=C(OCC)CCCCC</chem>	Ethyl decanoate	aromatic
31249	123-25-1	<chem>O=C(OCC)CCC(=O)OCC</chem>	Diethyl succinate	aromatic
7590	101-97-3	<chem>O=C(OCC)Cc1ccccc1</chem>	Ethyl phenylacetate	aromatic
7654	103-45-7	<chem>O=C(OCCc1ccccc1)C</chem>	2-phenylethyl acetate	aromatic
24197	2065419	<chem>O=C(OCC)C(O)CC(=O)OCC</chem>	Diethyl malate	other
70610	1070-34-4	<chem>O=C(OCC)CCC(=O)O</chem>	Monoethyl succinate	aromatic
10430	503-74-2/35915-22-1	<chem>O=C(O)CC(C)C</chem>	Isovaleric acid	other

8892	142-62-1	<chem>O=C(O)CCCCC</chem>	Hexanoic acid	other
5365909	3142-72-1/16957-70-3	<chem>O=C(O)C(=CCC)C</chem>	2-methyl-2-Pentenoic acid	aromatic
379	124-07-2	<chem>O=C(O)CCCCCC</chem> <chem>C</chem>	Octanoic acid	other
2969	334-48-5	<chem>O=C(O)CCCCCC</chem> <chem>CCC</chem>	Decanoic acid	other
243	65-85-0	<chem>O=C(O)c1ccccc1</chem>	Benzoic acid	other
7976	109-08-0	<chem>Cc1nccnc1</chem>	2-methylpyrazine	other
14296	1124-11-4	<chem>Cc1c(C)nc(C)c(C)n1</chem>	2,3,5,6-tetramethylpyrazine	other
41285	55013-32-6/55013-32-6	<chem>O=C1OC(CCCC)C(C)C1</chem>	cis-oak lactone	aromatic
7710	104-61-0	<chem>O=C1OC(CCCCC)CC1</chem>	nonalactone	aromatic
19309	3658-77-3	<chem>O=C1C(O)=C(C)OC1C</chem>	Furaneol	other
62465	2785-89-9/29760-89-2	<chem>O(C)c1c(O)ccc(C)C)c1</chem>	4-ethylguaiaicol	other
31242	123-07-9	<chem>Oc1ccc(CC)cc1</chem>	4-ethylphenol	other
7041	33512	<chem>O(C)c1c(O)c(OC)ccc1</chem>	2,6-dimethoxyphenol	other
10393	501-94-0	<chem>OCCc1ccc(O)cc1</chem>	tyrosol	aromatic
1549106	4501-31-9	<chem>O=C(O)C=Cc1ccc(O)cc1</chem>	cis-p-coumaric acid	bitter
12304324		<chem>O=C1C(OC2C(O)C(O)C(O)C(CO)O2)=C(c2cc(O)c(O)cc2)Oc2c1c(O)cc(O)c2</chem>	quercetin-3-O-glucopyranoside	-D- bitter
5280537	65646-26-6/66648-43-9	<chem>O=C(NCCc1ccc(O)cc1)C=Cc1cc(OC)c(O)cc1</chem>	trans-N-feruloyltyramine	bitter
23251204		<chem>O=C(C=Cc1ccc(O)cc1)c1c(OC)cc(O)c2c1OC(C)(C)C(O)C2</chem>	xanthohumol L	bitter
12986068		<chem>O=C(C=Cc1ccc(O)cc1)c1c(OC)cc(O)c2c1OC(C(O)(C)C)C2</chem>	xanthohumol I	bitter
5280343	117-39-5	<chem>O=C1C(O)=C(c2cc(O)c(O)cc2)Oc2c1c(O)cc(O)c2</chem>	quercetin	bitter

91064206		<chem>O(C)c1cc(O)c(CC=C(C)C)c(O)c1</chem>	1-methoxy-4-prenylphloroglucinol	bitter
5319562	19367-38-5/3943-97-3	<chem>O=C(OC)C=Cc1cc(O)cc1</chem>	trans-p-coumaric acid methyl ester	bitter
12719326		<chem>O=C(OCC)C=Cc1ccc(O)cc1</chem>	cis-p-coumaric acid ethyl ester	bitter
676946	394257	<chem>O=C(OCC)C=Cc1ccc(O)cc1</chem>	trans-p-coumaric acid ethyl ester	bitter
513197		<chem>O(C)c1c2C(=O)C(C3ccc(O)cc3)Oc2c(CC=C(C)C)c(O)c1</chem>	isoxanthohumol	bitter
9799506	189308-10-9	<chem>O=C(C=Cc1ccc(O)cc1)c1c(O)c2c(OC(C)(C)C(O)C2)c1OC</chem>	xanthohumol B	bitter
10317069	274675-25-1	<chem>O=C(C=Cc1ccc(O)cc1)c1c(O)c(CC(O)C(=C)C)c(O)cc1OC</chem>	xanthohumol D	bitter
6443339	115063-39-3	<chem>O=C(C=Cc1ccc(O)cc1)c1c(O)c(CC=C(C)C)c(O)cc1OC</chem>	desmethylxanthohumol	bitter
1.22E+08		<chem>O=C(C=Cc1ccc(O)cc1)c1c(OC)c(CC=C(C)C)c(O)c2c1OC(C)(C)CC2</chem>	dihydroxanthohumol F	bitter
1.22E+08		<chem>O=C(C=Cc1ccc(O)cc1)c1c(O)c(CCC(OC)(C)C)c(O)cc1OC</chem>	xanthohumol M	bitter
1.22E+08		<chem>O(C(Cc1c(O)cc(OC)c2C(=O)CC(c3ccc(O)cc3)Oc12)(C)C</chem>	isoxanthohumol M	bitter
155094	68236-13-5	<chem>O=C1c2c(O)c(CC=C(C)C)c(O)cc2OC(c2ccc(O)cc2)C1</chem>	6-prenylnaringenin	bitter
480764	53846-50-7	<chem>O=C1c2c(O)cc(O)c(CC=C(C)C)c2OC(c2ccc(O)cc2)C1</chem>	8-prenylnaringenin	bitter
639665	6754-58-1	<chem>O=C(C=Cc1ccc(O)cc1)c1c(O)c(CC=C(C)C)c(O)cc1OC</chem>	xanthohumol	bitter

11046840		<chem>O=C(C=Cc1ccc(O)cc1)c1c(O)c2c(OC(C)(C)CC2)cc1OC</chem>	dihydroxanthohumol C	bitter
10338075	189299-05-6	<chem>O=C(C=Cc1ccc(O)cc1)c1c(O)c2c(OC(C)(C)C=C2)cc1OC</chem>	xanthohumol C	bitter
1.22E+08		<chem>O(C)C=1C(=C(O)C=Cc2ccc(O)cc2)C(=O)C(CC=C(C)C)(CC=C(C)C)C(=O)C=1</chem>	hydroxytunicatachalcone	bitter
23250008	189299-04-5	<chem>O=C(C=Cc1ccc(O)cc1)c1c(OC)c(CC=C(C)C)c(O)c(CC=C(C)C)c1O</chem>	prenylxanthohumol	bitter
1.22E+08		<chem>O=C1C(CC=C(C)C)(CC=C(C)C)C(O)=C(CC=C(C)C)C=2OC(c3ccc(O)c3)CC(=O)C1=2</chem>	isoxantholupon	bitter
1.22E+08		<chem>O=C(C=Cc1ccc(O)cc1)c1c(O)c(CCC(=C)C)c(O)cc1OC</chem>	xanthohumol N	bitter
1.22E+08		<chem>O=C(C=Cc1ccc(O)cc1)c1c(O)c(CCC(OCC)(C)C)c(O)c1OC</chem>	xanthohumol P	bitter
1.22E+08		<chem>O(C(CCCc1c(O)cc(OC)c2C(=O)CC(c3ccc(O)cc3)Oc12)(C)C)CC</chem>	isoxanthohumol P	bitter
7797	106-30-9	<chem>O=C(OCC)CCCCC</chem>	Ethyl heptanoate	aromatic
7165	93-89-0	<chem>O=C(OCC)c1ccccc1</chem>	Ethyl benzoate	aromatic
5365910	1189-09-9	<chem>O=C(OC)C=C(CCC=C(C)C)C</chem>	Methyl geranate	aromatic
7800	106-33-2	<chem>O=C(OCC)CCCCCCCC</chem>	Ethyl laurate	aromatic
7501	100-42-5	<chem>C(=C)c1ccccc1</chem>	Styrene	aromatic
10722	529-20-4/1334-78-7	<chem>O=Cc1c(C)cccc1</chem>	o-Tolualdehyde	aromatic

5284503	544-12-7/928-97-2	<chem>OCCC=CCC</chem>	3-Hexen-1-ol	other
5281520	6753-98-6	<chem>CC1(C)C=CCC(C)=CCCC(C)=CC1</chem>	Humulene	aromatic
14896	25719-60-2	<chem>C=C1C2C(C)(C)C(C2)CC1</chem>	Pinene	other
240	100-52-7	<chem>O=Cc1ccccc1</chem>	Benzaldehyde	other
8857	141-78-6	<chem>O=C(OCC)C</chem>	Ethyl acetate	aromatic
1031	8/142583-61-7/62309-51-7	<chem>OCCC</chem>	n-Propanol	aromatic
5283324	2363-89-5	<chem>O=CC=CCCCC</chem>	E-2-Octenal	other
643731	557-48-2/26370-28-5	<chem>O=CC=CCCC=C</chem> <chem>CC</chem>	E,Z-2,6-Nonadienal	other
5283335	2463-53-8/18829-56-6	<chem>O=CC=CCCCC</chem> <chem>C</chem>	E-2-Nonenal	other
5283349	2363-88-4/25152-84-5/30551-18-9	<chem>O=CC=CC=CCC</chem> <chem>CCC</chem>	E,E-2,4-Decadienal	aromatic
650	431-03-8	<chem>O=C(C(=O)C)C</chem>	Diacetyl	other
1068	75-18-3	<chem>S(C)C</chem>	Dimethyl sulfide	sulfury
7997	109-60-4	<chem>O=C(OCCC)C</chem>	Propyl acetate	aromatic
8038	110-19-0	<chem>O=C(OCC(C)C)C</chem>	Isobutyl acetate	aromatic
12348	628-63-7	<chem>O=C(OCCCC)C</chem>	Amyl acetate	aromatic
6184	66-25-1	<chem>O=CCCCCC</chem>	Hexanal	other
11552	590-86-3/26140-47-6	<chem>O=CCC(C)C</chem>	3-Methyl butanal	other
527	123-38-6	<chem>O=CCC</chem>	Propanal	aromatic
7362	98-01-1/8030-97-5	<chem>O=Cc1occc1</chem>	Furfural	other
7284	96-17-3	<chem>O=CC(CC)C</chem>	2-Methylbutanal	other
6561	78-84-2	<chem>O=CC(C)C</chem>	2-Methylpropanal	aromatic
998	122-78-1	<chem>O=CCc1ccccc1</chem>	Phenylacetaldehyde	aromatic
31289	124-19-6	<chem>O=CCCCCCCC</chem>	Nonanal	aromatic
61743	14436-32-9	<chem>O=C(O)CCCCC</chem> <chem>CC=C</chem>	9-Decenoic acid	other
180	67-64-1	<chem>O=C(C)C</chem>	Acetone	aromatic
179	513-86-0	<chem>O=C(C(O)C)C</chem>	Acetoin	other
311	77-92-9	<chem>O=C(O)C(O)(CC(=O)O)CC(=O)O</chem>	Citric acid	other
612	50-21-5	<chem>O=C(O)C(O)C</chem>	Lactic acid	other
7991	109-52-4	<chem>O=C(O)CCCC</chem>	Pentanoic acid	other
1110	110-15-6	<chem>O=C(O)CCC(=O)O</chem>	Succinic acid	other

875	526-83-0	<chem>O=C(O)C(O)C(O)C(=O)O</chem>	Tartaric acid	other
44201359		<chem>O=C(C(C)C)C1=C(O)C(O)(C(=O)CC=C(C)C)C1=O</chem>	trans-isocohumulone	bitter
58473841	68127-23-1	<chem>O=C(C(C)C)C1=C(O)C(O)(C(=O)CC=C(C)C)C1=O</chem>	cis-isocohumulone	bitter
11175902	467-72-1	<chem>O=C(CC(C)C)C1=C(O)C(O)(C(=O)C=C(C)C)C1=O</chem>	trans-isohumulone	bitter
21594782	1534-03-8	<chem>O=C(CC(C)C)C1=C(O)C(O)(C(=O)C=C(C)C)C1=O</chem>	cis-isohumulone	bitter
91753956		<chem>[Si](OC1=C(C(=O)C(CC)C)C(=O)C(CC=C(C)C)C1(O[Si](C)(C)C)C(=O)CC=C(C)C)(C)C</chem>	trans-isoadhumulone	bitter
6431604		<chem>[Si](OC1=C(C(=O)C(CC)C)C(=O)C(CC=C(C)C)C1(O[Si](C)(C)C)CC=C(C)C)(C)C</chem>	cis-isoadhumulone	bitter
12314502		<chem>O=C(CC)C=1C(=O)C(O)(CC=C(C)C)C(O)=C(CC=C(C)C)C=1O</chem>	posthumulone	bitter
196915	511-25-1/142628-20-4	<chem>O=C(C(C)C)C=1C(=O)C(O)(CC=C(C)C)C(O)=C(CC=C(C)C)C=1O</chem>	cohumulone	bitter
442911	26472-41-3	<chem>O=C(CC(C)C)C=1C(=O)C(O)(CC=C(C)C)C(O)=C(CC=C(C)C)C=1O</chem>	humulone	bitter
193681	31769-65-0	<chem>O=C(C(CC)C)C=1C(=O)C(O)(CC=C(C)C)C(O)=C(CC</chem>	adhumulone	bitter

90473758		<chem>=C(C)C=C1O</chem> <chem>O=C(CCC(C)C)C</chem> <chem>=1C(=O)C(O)(CC</chem> <chem>=C(C)C)C(O)=C(</chem> <chem>CC=C(C)C)C=1O</chem> <chem>O=C(CCCCC)C=1</chem>	prehumulone	bitter
1.02E+08		<chem>C(=O)C(O)(CC=C</chem> <chem>(C)C)C(O)=C(CC</chem> <chem>=C(C)C)C=1O</chem> <chem>O=C(CC)C=1C(=</chem> <chem>O)C(CC=C(C)C)(</chem>	adprehumulone	bitter
1.02E+08		<chem>CC=C(C)C)C(O)=</chem> <chem>C(CC=C(C)C)C=1</chem> <chem>O</chem> <chem>O=C(C(C)C)C=1C</chem> <chem>(=O)C(CC=C(C)C</chem>	postlupulone	bitter
373677	468-27-9	<chem>)(CC=C(C)C)C(O)</chem> <chem>=C(CC=C(C)C)C=</chem> <chem>1O</chem> <chem>O=C(CC(C)C)C=1</chem> <chem>C(=O)C(CC=C(C)</chem>	colupulone	bitter
68051	468-28-0	<chem>C)(CC=C(C)C)C(</chem> <chem>O)=C(CC=C(C)C)</chem> <chem>C=1O</chem> <chem>O=C(C(CC)C)C=1</chem> <chem>C(=O)C(CC=C(C)</chem>	lupulone	bitter
9909740	28374-71-2	<chem>C)(CC=C(C)C)C(</chem> <chem>O)=C(CC=C(C)C)</chem> <chem>C=1O</chem> <chem>O=C(CCC(C)C)C</chem> <chem>=1C(=O)C(CC=C(</chem>	adlupulone	bitter
1.02E+08		<chem>C)C)(CC=C(C)C)</chem> <chem>C(O)=C(CC=C(C)</chem> <chem>C)C=1O</chem> <chem>O=C(CC(CC)C)C</chem> <chem>=1C(=O)C(CC=C(</chem>	prelupulone	bitter
1.01E+08		<chem>C)C)(CC=C(C)C)</chem> <chem>C(O)=C(CC=C(C)</chem> <chem>C)C=1O</chem> <chem>O=C(CC=C(C)C)</chem> <chem>C1(O)C(=O)C(C(=</chem>	adprelupulone	bitter
534962	26110-47-4	<chem>O)CC(C)C)=C(O)</chem> <chem>C1(O)CC=C(C)C</chem> <chem>O=C(C(C)C)C1=C</chem>	humulinone	bitter
1.02E+08		<chem>O=C(C(C)C)C1=C</chem>	tricyclohumol	bitter

1.02E+08	<chem>(O)C2(O)C3(O)C(C(C)(C)C(C(O)(C)C)C3)CC2C1=O</chem> <chem>O=C(CC(C)C)C1=C(O)C2(O)C3(O)C(C(C)(C)C(C(O)(C)C)C3)CC2C1=O</chem>	tricyclohumol	bitter
1.02E+08	<chem>O=C(C(C)C)C1=C(O)C2(O)C3(O)C(C(C)(C)C(C(=C)C)C3)CC2C1=O</chem> <chem>O=C(CC(C)C)C1=C(O)C2(O)C3(O)C(C(C)(C)C(C(=C)C)C3)CC2C1=O</chem>	tricyclohumene	bitter
1.02E+08	<chem>O=C(C(C)C)C1=C(O)C2(O)C3(O)C(C(C)(C)C(C(=C)C)C3)CC2C1=O</chem> <chem>O=C(C(C)C)C1=C(O)C2(O)C3(O)C(C(C)(C)C(C(=C)C)C3)CC2C1=O</chem>	tricyclohumene	bitter
1.02E+08	<chem>O=C(CC(C)C)C1=C(O)C2(O)C3(O)C(C(C)(C)C(=C(C)C)C3)CC2C1=O</chem> <chem>O=C(CC(C)C)C1=C(O)C2(O)C3(O)C(C(C)(C)C(=C(C)C)C3)CC2C1=O</chem>	isotricyclohumene	bitter
1.02E+08	<chem>O=C(CC(C)C)C1=C(O)C2(O)C3(O)C(C(C)(C)C(=C(C)C)C3)CC2C1=O</chem> <chem>O=C1C2=C(C(C)C)C)OC(C)(C)C3C2(O)C2(O)C(O)(C(C(O)(C)C)CC12)C3</chem>	isotricyclohumene	bitter
1.02E+08	<chem>O=C1C2=C(C(C)C)C)OC(C)(C)C3C2(O)C2(O)C(O)(C(C(O)(C)C)CC12)C3</chem> <chem>O=C1C2=C(C(C)C)C)OC(C)(C)C3C2(O)C2(O)C(O)(C(C(O)(C)C)CC12)C3</chem>	tetracyclohumol	bitter
1.02E+08	<chem>O=C1C2=C(C(C)C)C)OC(C)(C)C3C2(O)C2(O)C(O)(C(C(O)(C)C)CC12)C3</chem> <chem>O=C1C2=C(C(C)C)C)OC(C)(C)C3C2(O)C2(O)C(O)(C(C(O)(C)C)CC12)C3</chem>	tetracyclohumol	bitter
1.02E+08	<chem>O=C1C2=C(C(C)C)C)OC(C)(C)C3C2(O)C2(O)C(O)(C(C(O)(C)C)CC12)C3</chem> <chem>O=C1C2=C(C(C)C)C)OC(C)(C)C3C2(O)C2(O)C(O)(C(C(O)(C)C)CC12)C3</chem>	epitetracyclohumol	bitter
1.02E+08	<chem>O=C1C2=C(C(C)C)C)OC(C)(C)C3C2(O)C2(O)C(O)(C(C(O)(C)C)CC12)C3</chem> <chem>O=C1C2=C(C(C)C)C)OC(C)(C)C3C2(O)C2(O)C(O)(C(C(O)(C)C)CC12)C3</chem>	epitetracyclohumol	bitter
530272	<chem>[Si](OC=1C(C(=O)C(C)C)=C(O[Si](</chem>	cis-cohumulinic acid	bitter

15558357		<chem>C(C)C(C)C(O[Si](C)(C)C)C=1CC=C(C)C(C)(C)C</chem>	trans-humulonic acid	bitter
		<chem>O=C(C(CC)C)C1C(=O)C(=O)C(CC=C(C)C)C1=O</chem>		
530273		<chem>[Si](OC=1C(C(=O)CC(C)C)=C(O[Si](C)(C)C)C(O[Si](C)(C)C)C=1CC=C(C)C(C)(C)C</chem>	cis-humulonic acid	bitter
12310637	1891-42-5	<chem>O=C1C(CC=C(C)C)C(C)(CC=C(C)C)C(=O)C(O)=C1O</chem>	hulupinic acid	bitter
643820	106-25-2	<chem>OCC=C(CCC=C(C)C)C</chem>	Nerol	aromatic
638011	141-27-5/5392-40-5	<chem>O=CC=C(CCC=C(C)C)C</chem>	Geranial	aromatic
643779	106-26-3	<chem>O=CC=C(CCC=C(C)C)C</chem>	Neral	aromatic
5275520	459-80-3/4698-08-2	<chem>O=C(O)C=C(CCC=C(C)C)C</chem>	Geranic Acid	aromatic
7462		<chem>C(C)(C)C1=CC=C(C)CC1</chem>	Terpinene	aromatic
7461	99-85-4	<chem>C(C)(C)C1=CCC(C)=CC1</chem>	Terpinene	aromatic
440917	5989-27-5	<chem>C(=C)(C)C1CC=C(C)CC1</chem>	(+)-limonene	aromatic
11463	586-62-9	<chem>C(C)(C)=C1CC=C(C)CC1</chem>	Terpinolene	aromatic
31253	123-35-3	<chem>C(C=C)(=C)CCC=C(C)C</chem>	Myrcene	aromatic
8785	140-11-4	<chem>O=C(OCc1ccccc1)C</chem>	Benzyl acetate	aromatic
369312	18457-55-1	<chem>OCC1=CCC(C(=C)C)CC1</chem>	(S)-(-)-perillyl alcohol	aromatic
445070	106-28-5/4602-84-0	<chem>OCC=C(CCC=C(C)C)C</chem>	farnesol	aromatic
11196	26370-28-5	<chem>O=CC=CCCC=C</chem>	2,6-Nonadienal	aromatic
7150	93-58-3	<chem>O=C(OC)c1ccccc1</chem>	Methyl benzoate	aromatic
65040	554-01-8	<chem>O=C1N=CC(C)=C(N)N1</chem>	5-Methylcytosine	aromatic

6175	65-46-3	<chem>O=C1N(C2C(O)C(O)C(CO)O2)C=C(C(N)=N1)</chem>	Cytidine	aromatic
6180	1115-47-5	<chem>S(CCC(NC(=O)C)C(=O)O)C</chem>	n-Acetyl-methionine	sulfury
5789	50-89-5	<chem>O=C1N(C2OC(C)C(O)C2)C=C(C)C(=O)N1</chem>	Thymidine	aromatic
1130	70-16-6/59-43-8	<chem>OCCc1c(C)[n+](C)c2c(N)nc(C)nc2cs1</chem>	Thiamine	bitter
10972	543-24-8	<chem>O=C(O)CNC(=O)C</chem>	Acetylglycine	aromatic
239	107-95-9	<chem>O=C(O)CCN</chem>	Alanine	aromatic
16617	2198-61-0	<chem>O=C(OCCCC(C)C)CCCC</chem>	Isopentyl hexanoate	aromatic
8050	110-42-9	<chem>O=C(OC)CCCCCCCC</chem>	Methyl decanoate/methyl caprate	aromatic
31284	124-10-7	<chem>O=C(OC)CCCCCCCCC</chem>	Methyl tetradecanoate	aromatic
562667	72109-82-1	<chem>O=C(OCCCCCCC)Cc1ccccc1</chem>	Nonyl phenylacetate	aromatic
550967	562-13-0	<chem>O=C1C(C)(C)C(=O)CCC1</chem>	2,2-Dimethyl-1,3-cyclohexanedione	other
75725	2566-34-9	<chem>O=C(O)C(NC)(C)C</chem>	n-Methyl-a-aminoisobutyric acid	aromatic
643798	498-23-7/7407-59-2	<chem>O=C(O)C(=CC(=O)O)C</chem>	Citraconic acid	other
162350	29702-25-8	<chem>O=C1c2c(O)c(c(O)cc2OC(c2ccc(O)c2)=C1)C1C(O)C(O)C(O)C(CO)O1</chem>	Apigenin-6-C-glucoside	aromatic
439312		<chem>OCC1(O)C(O)C(O)C(O)C(O)CO1</chem>	Tagatose	aromatic
439531	470-55-3	<chem>O(CC1C(O)C(O)C(O)C(OC2(CO)C(O)C(O)C(CO)O2)O1)C1C(O)C(O)C(O)C(COC2C(O)C(O)C(O)C(CO)O2)O1</chem>	Stachyose	aromatic
5988	57-50-1	<chem>O(C1(CO)C(O)C(O)C(CO)O1)C1C(O)C(O)C(O)C(CO)O1</chem>	Sucrose	aromatic

7427	99-20-7	<chem>O=C1C(O)C(O)C(O)C(CO)O1C1C(O)C(O)C(O)C(CO)O1</chem>	Trehalose	aromatic
5460935	547-25-1	<chem>O=C(C(OC1C(O)C(O)C(O)C(CO)O1)C(O)C(O)CO)C</chem>	Turanose	aromatic
564550	7779-23-9	<chem>O=C(OC(C=C)(C)C)C</chem>	Linalyl hexanoate	aromatic
538753		<chem>O=C1C(N)=NON1</chem>	Furazan-3-ol, 4-amino	aromatic
637511	104-55-2/14371-10-9	<chem>O=CC=Cc1ccccc1</chem>	Cinnamaldehyde	aromatic
237332	67-47-0	<chem>O=Cc1oc(CO)cc1</chem>	Hydroxymethylfurfural	other
6088	61-49-4	<chem>N(CCc1c2c([nH]c1)cccc2)C</chem>	N-Methyltryptamine	other
12489	636-41-9	<chem>Cc1[nH]ccc1</chem>	2-Methylpyrrole	sulfury
7963	108-89-4	<chem>Cc1ccncc1</chem>	4-Methylpyridine	other
9061	154-02-9	<chem>OCCc1c2c([nH]c1)ccc(O)c2</chem>	5-Hydroxytryptophol	sulfury
1712448	2001-93-6	<chem>S=C1NC(=S)C=C</chem>	Dithiouracil	sulfury
14284	1122-58-3	<chem>N(C)(C)c1ccncc1</chem>	4-Dimethylaminopyridine	sulfury
12709	687-48-9	<chem>O=C(OCC)N(C)C</chem>	Ethyl dimethylcarbamate	sulfury
6262	70-26-8	<chem>O=C(O)C(N)CCC</chem>	Ornithine	sulfury
7405	98-79-3	<chem>O=C(O)C1NC(=O)CC1</chem>	Pyroglutamic acid	aromatic
91692231		<chem>O=C(O)C(N)C(=O)C1=CC=CC=C1</chem>	Sarcosine, N-(3-phenylpropionyl)	aromatic
967	65-86-1	<chem>O=C(O)C=1NC(=O)NC(=O)C=1</chem>	Orotic acid	sulfury
938	59-67-6	<chem>O=C(O)c1cnccc1</chem>	Niacin	other
6322	74-79-3	<chem>O=C(O)C(N)CCC</chem>	Arginine	aromatic
6267	70-47-3	<chem>N=C(N)N</chem>	Asparagine	aromatic
83814	576-19-2	<chem>O=C(O)C(N)CCC</chem>	Biocytin	aromatic
		<chem>CNC(=O)CCCC</chem>		
		<chem>1SCC2NC(=O)NC</chem>		

6306	73-32-5	<chem>O=C(O)C(N)C(CC)C</chem>	Isoleucine	sulfury
5962	56-87-1	<chem>O=C(O)C(N)CCC(N)C</chem>	Lysine	other
6137	63-68-3	<chem>S(CCC(N)C(=O)O)C</chem>	Methionine	other
6305	73-22-3	<chem>O=C(O)C(N)Cc1c2c([nH]c1)cccc2</chem>	Tryptophan	sulfury
6613	79-83-4	<chem>O=C(NCCC(=O)O)C(O)C(CO)(C)C</chem>	Pantothenic acid	sulfury
21889526		<chem>O=C([O-])C(N)CC</chem>	Aminobutyrate	other
978	150-13-0	<chem>O=C(O)c1ccc(N)cc1</chem>	para-aminobenzoic acid	sulfury
121709	30434-54-9	<chem>O=C(OCC(C)C)C=C(C)C</chem>	Isobutyl 3-methyl-2-butenolate	sulfury
79582	1300784	<chem>O=C(OCC(C)C)CCCCC</chem>	Isobutyl caprylate	other
560572	51534-66-8	<chem>S(C(C(=O)OC)CC)C</chem>	Methyl 2-(methylthio)butyrate	sulfury
65425	53053-51-3	<chem>S(CCCC(=O)OC)C</chem>	Methyl-4-(methylthio)butyrate	sulfury
20831779	827024-53-3	<chem>S(C(=O)C(OC(=O)CC)C)C</chem>	Methylthio-2-(propanoyloxy)propanoate	sulfury
573623		<chem>O=C(CCCCCCCC)CCCCCCCCC)c1occc1</chem>	Furan, 2-nonadecanoyl	other
76662	3194-15-8	<chem>O=C(CC)c1occc1</chem>	2-Propionylfuran	other
11427	583-91-5	<chem>S(CCC(O)C(=O)O)C</chem>	2-Hydroxy-4-(methylthio)butyric acid	sulfury
444972	110-17-8	<chem>O=C(O)C=CC(=O)O</chem>	Fumaric acid	sulfury
533935	55021-77-7	<chem>S(CCCCN)C</chem>	4-(methylthio)-1-butanamine	sulfury
7222	95-16-9	<chem>s1c2c(nc1)cccc2</chem>	Benzothiazole	sulfury
16592	2179-60-4	<chem>S(SC)CCC</chem>	Methyl propyl disulfide	sulfury
96757	1999-34-4/554-94-9	<chem>S(CCC(NC(=O)C)N)C(=O)O</chem>	Glycyl-methionine	aromatic
435728		<chem>O=C(O)C(NC(=O)C(N)C(CC)C)Cc1cccc1</chem>	Isoleucyl-phenylalanine	sulfury
151004	2418-74-8	<chem>O=C(O)C(NC(=O)C1NCCC1)CCCN=C(N)N</chem>	Prolyl-arginine	sulfury
18218234		<chem>SCC(NC(=O)C1NCCC1)C(=O)O</chem>	Prolyl-cysteine	sulfury

19762195		SCC(NC(=O)C(N) Cc1c2c([nH]c1)cc cc2)C(=O)O	Tryptophyl-cysteine	sulfury
8468	121-34-6	O=C(O)c1cc(OC)c (O)cc1	Vanillic acid	sulfury
439176	2457-80-9	S(CC1C(O)C(O)C (n2c3ncnc(N)c3nc 2)O1)C	5-Methylthioadenosine	sulfury
190	73-24-5	Nc1ncnc2nc[nH]c 12	Adenine	other
60961	58-61-7	OCC1C(O)C(O)C(n2c3ncnc(N)c3nc2)O1	Adenosine	sulfury
1.35E+08	58-63-9	O=C1NC=Nc2n(C 3C(O)C(O)C(CO) O3)cnc12	Inosine	aromatic
1044	120-73-0	[nH]1c2c(nc1)ncn c2	Purine	sulfury
439193	499-40-1	O(CC1C(O)C(O)C (O)C(O)O1)C1C(O)C(O)C(O)C(CO)O1	Isomaltose	aromatic
5282108	127-41-3	O=C(C=CC1C(C) =CCCC1(C)C)C	Ionone	aromatic
25913	13360-61- 7/27251-68-9	C(=C)CCCCCCC CCCCC	1-Pentadecene	aromatic
124886	70-18-8	SCC(NC(=O)CCC (N)C(=O)O)C(=O) NCC(=O)O	Glutathione	aromatic
74839	2018-61- 3/2901-75-9	O=C(O)C(NC(=O) C)Cc1ccccc1	n-Acetyl-phenylalanine	aromatic
22880	6384-92-5	O=C(O)C(NC)CC(=O)O	n-methyl-D-aspartate	other
44423663		O=C(O)C(NC(=O) CCCCCCCC=CC CCCCCCC)C	n-Oleoyl-alanine	aromatic
99289	28954-12-3	O=C(O)C(N)C(O) C	Allothreonine	aromatic
6287	72-18-4	O=C(O)C(N)C(C) C	Valine	aromatic
4649	65-49-6	O=C(O)c1c(O)cc(N)cc1	4-Aminosalicylic acid	aromatic
409323	5782-80-9	O=C(O)C(N)CCC CCCCCCCCCCC	2-Amino-octadecanoic acid	aromatic

7012	90-27-7	CC O=C(O)C(CC)c1c cccc1	2-Phenylbutyric acid	aromatic
44256507		O=C(O)CCCCC CCCC=CCC1C(C CCCC)O1	Alchornoic acid	aromatic
637517	112-79- 8/2027-47-6	O=C(O)CCCCC CC=CCCCCCCC C	Elaidic acid	aromatic
86289532	103597-60-0	P(=O)(OCC(OC(= O)CCCC=CCC=C CC=CCC=CCCC CC)COC=CCCCC CCCCCCCCCCCC C)(OCC[N+])[O-]	GPE (p-18:0/20:4)	aromatic
8094	111-14-8	O=C(O)CCCCC P(=O)(OCC(O)CO C(=O)CCCCCCC	Heptanoic acid	other
11005824		C=CCC=CCCCC C)(OCC[N+](C)(C)C)[O-]	LysoPC (18:2)	aromatic
24779469		P(=O)(OCC(O)CO C(=O)CCCCCCC C=CCC=CCC=CC C)(OCC[N+](C)(C)C)[O-]	LysoPC (18:3)	aromatic
5281120	506-37-6	O=C(O)CCCCC CCCCCCCC=CC CCCCCCC	Nervonic acid	aromatic
445639	112-80-1	O=C(O)CCCCC CC=CCCCCCCC C	Oleic acid	other
24779471		P(=O)(OC[C@H](O)COC(=O)CCCC CCC/C=C/C=C/C/ =C/C=C/CC)(OCC [N+](C)(C)C)[O-]	PC (18:4)	aromatic
49859598		P(=O)(OCC(OC(= O)CCCCCCCCCCC CCCC)COC(=O) CCCCCCCCCCCC CCCC)(OCC(O)C OP(=O)(O)O)O	PGP (32:0)	aromatic
70		O=C(O)C(=O)CC(Ketoisocaproate	aromatic

439939	13095-48-2	C)C O=C(O)C(O)CCC(=O)O	1-2-Hydroxyglutaric acid	aromatic
71	3184-35-8	O=C(O)C(=O)CC CC(=O)O	Oxoadipic acid	aromatic
439197	131-48-6	O=C(NC1C(C(O) C(O)CO)OC(O)(C (=O)O)CC1O)C	N-Acetyl-Neuraminic Acid	aromatic
12101	620-17-7	Oc1cc(CC)ccc1	3-Ethylphenol	aromatic
736186	25522-33- 2/537-73-5	O=C(O)C=Cc1cc(O)c(OC)cc1	Isoferulic acid	aromatic
9260786		O=C(Nc1ccc(CC#N)cc1)c1oc(COc2ccccc2)cc1	n-[4-(cyanomethyl)phenyl]-5-(phenoxyethyl)furan-2-carboxamide	aromatic
8742	138-59-0	O=C(O)C1=CC(O)C(O)C(O)C1	Shikimate	aromatic
27476	15763-06-1	OCC1C(O)C(O)C(n2c3N=CN(C)C(=N)c3nc2)O1	1-Methyladenosine	aromatic
94154	488-82-4	OC(C(O)CO)C(O)CO	Arabitol	aromatic
2723872	57-48-7	OCC1(O)C(O)C(O)C(O)C(O)CO1	Fructose	aromatic
11850	608-66-2	OC(C(O)C(O)CO)C(O)CO	Galactitol	aromatic
5961	56-85-9	O=C(O)C(N)CCC(=O)N	Glutamine	other
444266	110-16-7	O=C(O)C=CC(=O)O	Maleic acid	aromatic
1.32E+08	34393-18-5	O=C(O)C(NCC1(O)C(O)C(O)C(CO)O1)CC(C)C	n-(1-deoxy-1-fructosyl)leucine	aromatic
91482	2370-61-8	O=C(O)C(N)Cc1c(O)cccc1	o-Tyrosine	other
1174	66-22-8	O=C1NC(=O)C=C N1	Uracil	sulfury
5950	56-41-7	O=C(O)C(N)C	Alanine	sulfury
69522	644-90-6	O=C(O)C(N)CCC CCC	Aminooctanoic acid	aromatic
865	583-93- 7/922-54-3	O=C(O)C(N)CCC C(N)C(=O)O	Diaminopimelic acid	aromatic
5610	51-67-2	Oc1ccc(CCN)cc1	Tyramine	other
6057	60-18-4	O=C(O)C(N)Cc1c(O)cc1	Tyrosine	aromatic

81596		<chem>O=C(O)CCOc1ccc</chem> <chem>cc1</chem>	3-Phenoxypropionic acid	sulfury
83697	13748-90-8	<chem>O=C(O)C(O)CC(C</chem> <chem>)C</chem>	Hydroxyisocaproic acid	sulfury
9547167		<chem>P(=O)(OCC(OC(=</chem> <chem>O)CCCCCCCC=C</chem> <chem>CC=CCCCC)CO</chem> <chem>C(=O)CCCCCCC</chem> <chem>CCCCCCCC)(O</chem> <chem>O</chem>	PA (34:2)	other
79101	118203-80- 8/704-15-4	<chem>O=C(CN)N1C(C(</chem> <chem>=O)O)CCC1</chem>	Glycylproline	aromatic
5280805	153-18-4	<chem>O=C1C(OC2C(O)</chem> <chem>C(O)C(O)C(COC3</chem> <chem>C(O)C(O)C(O)C(</chem> <chem>C)O3)O2)=C(c2cc</chem> <chem>(O)c(O)cc2)Oc2c1</chem> <chem>c(O)cc(O)c2</chem>	Rutin	sulfury
1.3508	118-00-3	<chem>O=C1NC(N)=Nc2</chem> <chem>n(C3C(O)C(O)C(</chem> <chem>CO)O3)cnc12</chem>	Guanosine	sulfury
