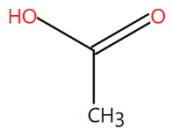
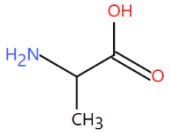
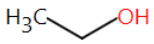
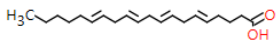
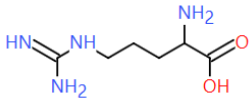
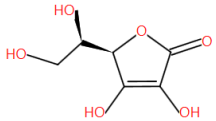
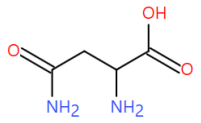
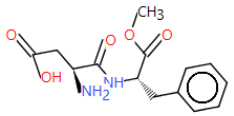
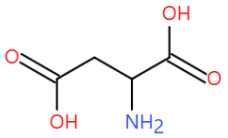
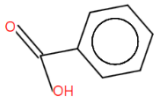
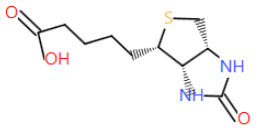
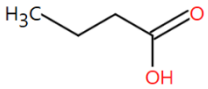
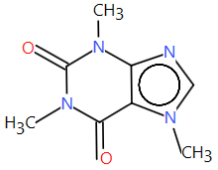
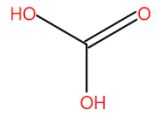
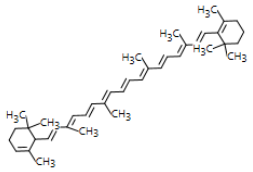
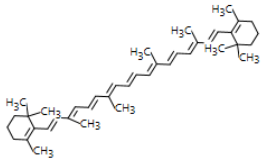
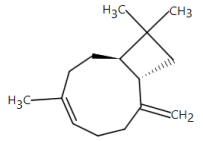
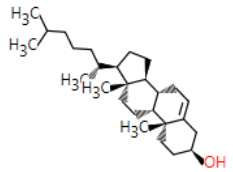
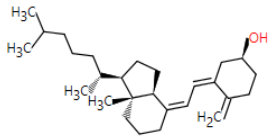
Appendix II. R22 Inventory

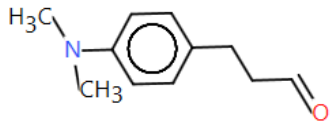
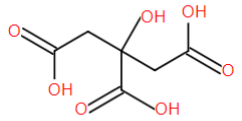
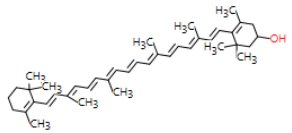
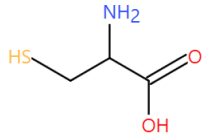
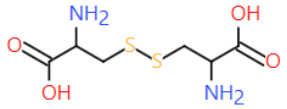
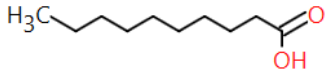
List with 122 predefined chemicals included in the definition of the question R22:

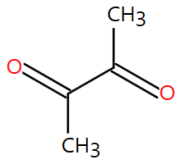
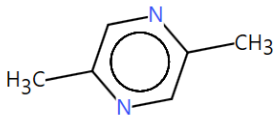
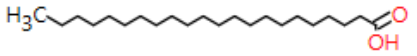
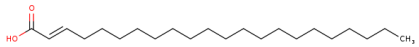
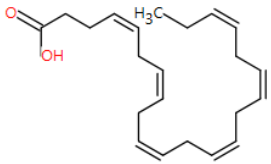
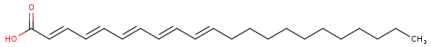
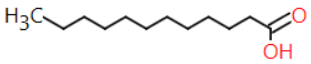
"Is the substance a *common component of food (C)* or *structurally closely related (K)* to a *common component of food (C)?"*

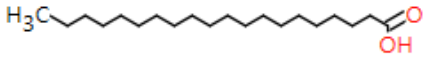
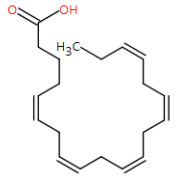
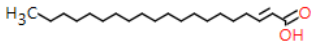
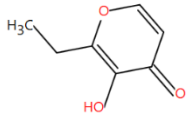
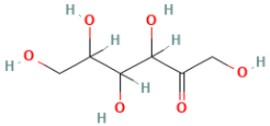
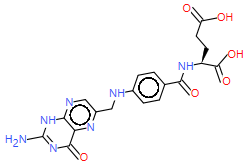
#	CAS #	EC #	Chemical name	SMILES	Structure	Reference source
1	758-12-3	2120591	acetic [2H]acid	CC(O)=O		[1]
2	302-72-7	2061264	2-aminopropanoic acid alanine	CC(N)C(O)=O		[2]
3	64-17-5	2005786	Ethanol	CCO		[3]
4	506-32-1	2080334	5,8,11,14-EICOSATETRAENOIC ACID	CCCCCC=CCC=CCC=CCC=CCCCC(O)=O		[4]
5	7200-25-1		Arginine; DL-arginine	NC(CCCNC(N)=N)C(O)=O		[5]
6	89-65-6	2019280	Isoascorbic acid	OC[C@@H](O)[C@H]1OC(=O)C(O)=C1O		[6]

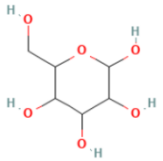
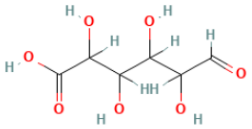
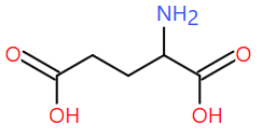
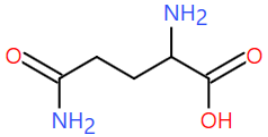
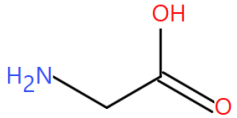
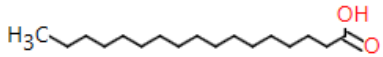
7	70-47-3	2007359	2-Amino-3-carbamoylpropanoic acid; L-Asparagine;	NC(CC(N)=O)C(O)=O		[7]
8	22839-47-0	2452613	Aspartame	COC(=O)[C@H](Cc1ccccc1)NC(=O)[C@@H](N)CC(O)=O		[8]
9	617-45-8	2105133	(r)-2-amino-succinic acid; DL-Aspartic acid	NC(CC(O)=O)C(O)=O		[9]
10	65-85-0	2006182	benzoic acid / benzoate	OC(=O)c1ccccc1		[10]
11	58-85-5	2003993	(3as,4s,6ar)-hexahydro-2-oxo-1h-thieno[3,4-d]imidazole-4-pentanoic acid /Biotin	OC(=O)CCCC[C@@H]1SC[C@@H]2NC(=O)N[C@H]12		[11]
12	107-92-6	2035323	"butyric acid;n-butyric acid;butanoic acid";	CCCC(O)=O		[12]
13	58-08-2	2003621	1,3,7-trimethyl-2,3,6,7-tetrahydro-1H-purine-2,6-dione; Caffeine	CN1C(=O)N(C)c2ncn(C)c2C1=O		[13]

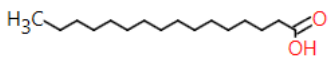
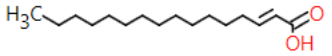
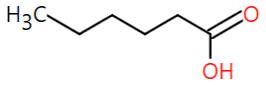
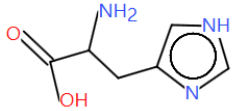
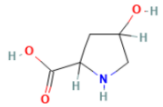
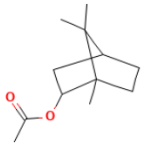
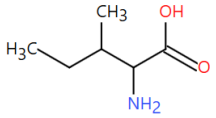
14	463-79-6		Carbonic acid	OC(O)=O		[14]
15	7488-99-5		alpha-Carotene	CC(C=CC=C(C)C=CC1C(C)=CCCC1(C)C)=CC=CC=C(C)C=CC=C(C)C=CC1=C(C)CCCC1(C)C		[15]
16	7235-40-7	2306366	beta.-Carotene	C\C(\C=C\C=C(/C)\C=C\C1=C(C)CCCC1(C)C)=C/C=C/C=C(\C)/C=C/C=C(\C)/C=C/C1=C(C)CCCC1(C)C		[16]
17	87-44-5	2017461	(1R,4E,9S)-4,11,11-Trimethyl-8-methylenebicyclo[7.2.0]undec-4-ene; caryophyllene	C\C1CC[C@@H]2[C@H](CC2(C)C)C(=C)CC\C=1		[17]
18	57-88-5	2003532	Cholesterol	CC(C)CCC[C@@H](C)[C@H]1CC[C@H]2[C@@H]3CC=C4C[C@@H](O)CC[C@]4(C)[C@H]3CC[C@]12C		[18]
19	1406-16-2	2157972	Vitamin D	CC(C)CCC[C@@H](C)[C@H]1CC[C@H]2C(/CCC[C@]12C)=C/C=C1/C[C@@H](O)CCC1=C		[19]

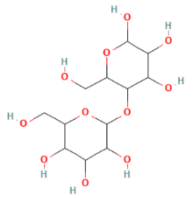
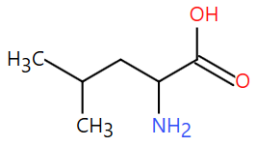
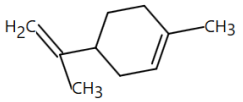
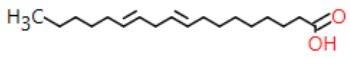
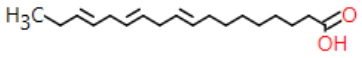
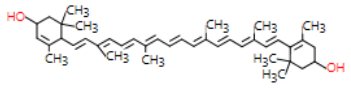
20	377084-04-3		3-[4-(Dimethylamino)phenyl]propanal	CN(C)c1ccc(CCC=O)cc1		N/A
21	77-92-9	2010691	1,2,3-Propanetricarboxylic acid, Citric_acid	OC(=O)CC(O)(CC(O)=O)C(O)=O		[20]
22	472-70-8		Cryptoxanthin	CC(C=CC=C(C)C=CC1=C(C)CCCC1(C)C)=CC=CC=C(C)C=CC=C(C)C=CC1=C(C)CC(O)CC1(C)C		[21]
23	3374-22-9	2221602	2-amino-3-sulfanylpropanoic acid cysteine DL-Cysteine	NC(CS)C(O)=O		[22]
24	923-32-0		cystine Cystine DL-form DL-cystine	NC(CSSCC(N)C(O)=O)C(O)=O		[23]
25	334-48-5	2063764	capric acid Decanoic acid	CCCCCCCCCC(O)=O		[24]

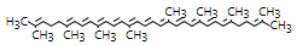
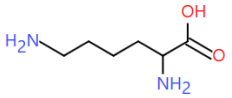
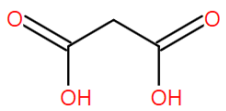
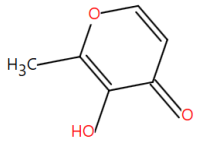
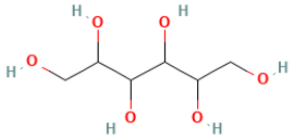
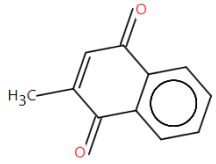
26	431-03-8	2070698	2,3-Butanedion; Diacetyl	CC(=O)C(C)=O		[25]
27	123-32-0	2046183	2,5-Dimethyl-pyrazine	Cc1cnc(C)cn1		[26]
28	112-85-6	2040108	Docosanoic acid	CCCCCCCCCCCCCCCCCCCCCC(O)=O		[27]
29	25378-26-1		Docosenoic acid	CCCCCCCCCCCCCCCCCC\C=C\C(=O)O		
30	6217-54-5		(4Z,7Z,10Z,13Z,16Z,19Z)-4,7,10,13,16,19-docosahexaenoic acid;	CC\C=C/C\C=C/C\C=C/C\C=C/C\C=C/C\C=C/C\C=C/CCC(O)=O		[28]
31	25448-00-4		Docosapentaenoic acid	CCCCCCCCCCC\C=C\C=C\C=C\C=C\C=C\C(=O)O		[29]
32	143-07-7	2055821	Dodecanoic acid; Lauric acid, pure	CCCCCCCCCCCC(O)=O		[30]

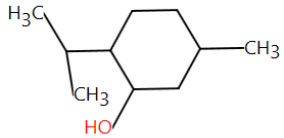
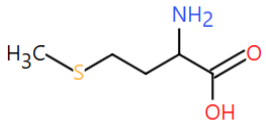
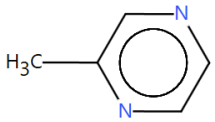
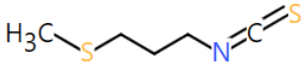
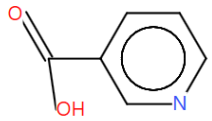
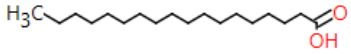
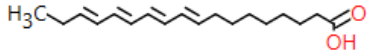
33	506-30-9	2080313	Eicosanoic acid; icosanoic acid	CCCCCCCCCCCCCCCCCC(O)=O		[31]
34	10417-94-4		5,8,11,14,17-Eicosapentaenoic acid, (5Z,8Z,11Z,14Z,17Z)-Eicosapentaenoic acid	CC\C=C/C\C=C/C\C=C/C\C=C/C\C=C/CCCC(O)=O		[32]
35	26764-41-0; 29204-02-2		2-Eicosenoic acid	CCCCCCCCCCCCCCCCC=CC(O)=O		ID
36	4940-11-8	2255825	2-ethyl-3-hydroxy-4-pyrone	CCC1OC=CC(=O)C=1O		[33]
37	87-79-6; 139686-85-4		1,3,4,5,6-pentahydroxyhexan-2-one	C(C(C(C(C(=O)CO)O)O)O)O		ID Food: [34]
38	59-30-3	2004190	(2S)-2-[(4-{[(2-amino-4-oxo-1,4-dihydropteridin-6-yl)methyl]amino}phenyl)formamido]pentanedioic acid Folic acid	NC1Nc2ncc(CNc3ccc(cc3)C(=O)N[C@@H](CCC(O)=O)C(O)=O)nc2C(=O)N=1		[35]

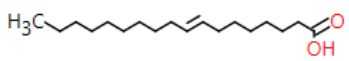
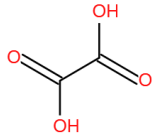
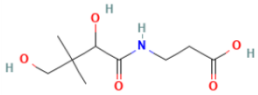
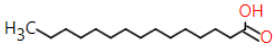
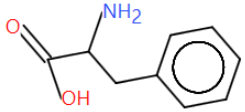
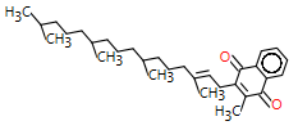
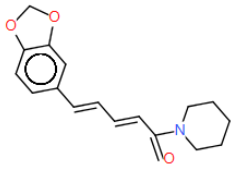
39			Hexopyranose; D-(+)-Mannose	C(C1C(C(C(C(O1)O)O)O)O)O		ID Food: [36]
40	685-73-4		Galacturonic acid, D-2,3,4,5-tetrahydroxy-6-oxohexanoic acid; Hexuronic acid	C(=O)C(C(C(C(C(=O)O)O)O)O)O		ID Food: [37]
41	56-86-0	2002937	(s)-2-amino-pentanedioic acid DL-Glutamic acid	NC(CCC(O)=O)C(O)=O		[38]
42	6899-04-3	2300060	DL-Glutamine glutamine	NC(CCC(N)=O)C(O)=O		[39]
43	56-40-6	2002722	Amino-acetic acid Glycine	NCC(O)=O		[40]
44	506-12-7	2080271	Heptadecanoic acid Margaric acid	CCCCCCCCCCCCCCCC(O)=O		[41]

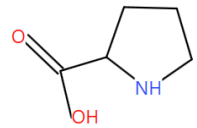
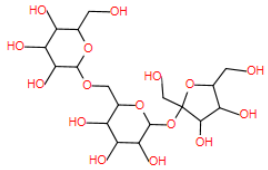
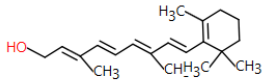
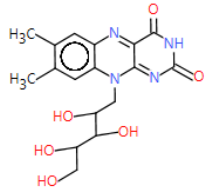
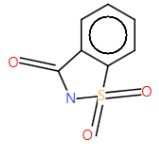
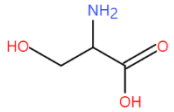
45	57-10-3	2003129	Hexadecanoic acid PALMITICACID	CCCCCCCCCCCCCC(O)=O		[42]
46	25447-95-4		Hexadecenoic acid	CCCCCCCCCCCCCC=CC(O)=O		[43]
47	142-62-1	2055507	"caproic acid;hexanoic acid;capronic acid; HEXANOIC ACID	CCCCCC(O)=O		[44]
48	4998-57-6	2256609	DL-Histidine Histidine	NC(Cc1c[nH]cn1)C(O)=O		[45]
49	51-35-4		4-hydroxyproline	C1C(CNC1C(=O)O)O		ID Food: [46]
50	125-12-2/76-49-3		BORNYL ACETATE Isobornyl acetate Borneol, acetate	CC(=O)OC1CC2CCC1(C2(C)C)C		ID Food: [47]
51	443-79-8	2071398	DL-allo-isoleucine DL-Isoleucine isoleucine	CCC(C)C(N)C(O)=O		[48]

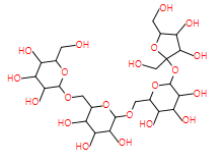
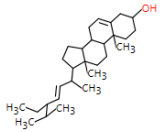
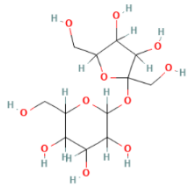
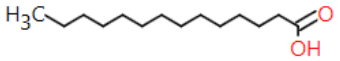
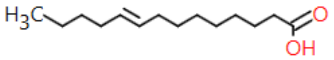
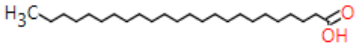
52			cellobiose maltose D-(+)-Cellobiose	C(C1C(C(C(C(O1)O C2C(OC(C(C2O)O)O)CO)O)O)O)O		ID Food: [49]
53	328-39-2	2063282	(r)-2-amino-4-methyl-pentanoic acid;leucine;dl-leucine"	CC(C)CC(N)C(O)=O		[50]
54	7705-14-8	2317320	(±)-1-methyl-4-(1-methylvinyl)cyclohexene; Limonene	CC(=C)C1CCC(C)=CC1		[51]
55	2197-37-7		9,12-Octadecadienoic acid	CCCCCC=CCC=CCCCCCCC(O)=O		[52]
56	1955-33-5	2177920	9,12,15-Octadecatrienoic acid	CCC=CCC=CCC=CCCCCCCC(O)=O		[53]
57	127-40-2		Lutein Xanthophyll	CC(C=CC=C(C)C=CC1C(C)=CC(O)CC1(C)C)=CC=CC=C(C)C=CC=C(C)C=CC1=C(C)CC(O)CC1(C)C		[54]

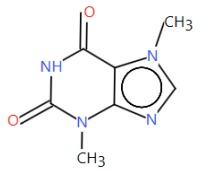
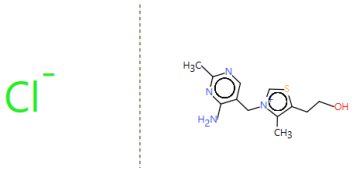
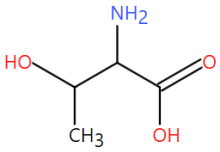
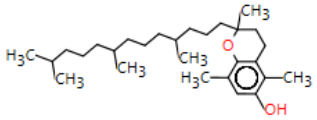
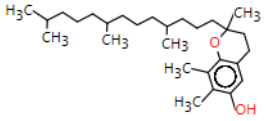
58	502-65-8		Lycopene	CC(C)=CCCC(C)=CC=CC(C)=CC=CC=C(C)C=CC=C(C)C=CC=C(C)CCC=C(C)C		[55]
59	70-54-2	2007406	2,6-Diaminohexanoic acid; DL-lysine; Lysine	NCCCCC(N)C(O)=O		[56]
60	141-82-2	2055030	Malonic acid;propanedioic acid	OC(=O)CC(O)=O		[57]
61	118-71-8	2042718	2-ethyl-3-hydroxy-4-pyrone; Maltol	CC1OC=CC(=O)C=1O		[58]
62			Hexitol	OCC(O)C(O)C(O)C(O)CO		ID Food: [59]
63	58-27-5	2003726	1,4-Naphthalenedione, 2-methyl-; Menadione	CC1=CC(=O)c2ccccc2C1=O		[60] Not allowed for human

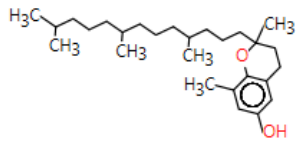
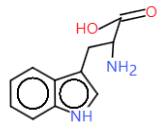
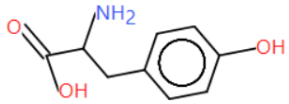
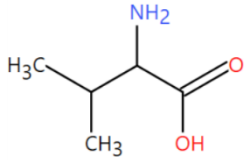
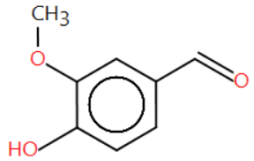
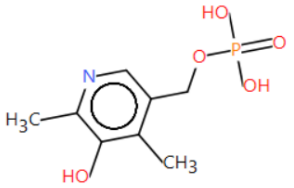
64	89-78-1	2019390	5-methyl-2-(propan-2-yl)cyclohexanol; D,L-Menthol	CC(C)C1CCC(C)CC1O		[61]
65	59-51-8	2004321	2-amino-4-methylsulfanyl-butyric acid DL-Methionin	CSCCC(N)C(O)=O		[62]
66	109-08-0	2036458	2-Methyl-pyrazine	Cc1cnccn1		[63]
67	505-79-3	2080203	1-isothiocyanato-3-(methylsulfanyl)propane	CSCCCN=C=S		[64]
68	59-67-6	2004410	"3-carboxylpyridine (nicotinic acid) (niacin);	OC(=O)c1cccnc1		[65]
69	57-11-4	2003134	heptadecane-1-carboxylic acid Octadecanoic acid stearic acid	CCCCCCCCCCCCCCCCCC(O)=O		[66]
70	18841-21-9		Parinaric acid, (E)-	CCC=CC=CC=CC=CCCCCCCCC(O)=O		[67]

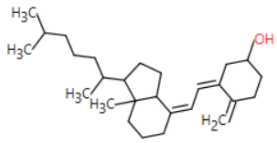
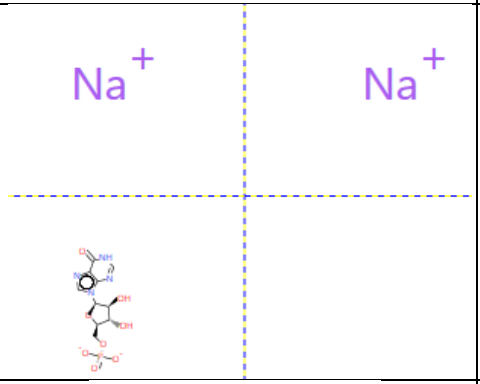
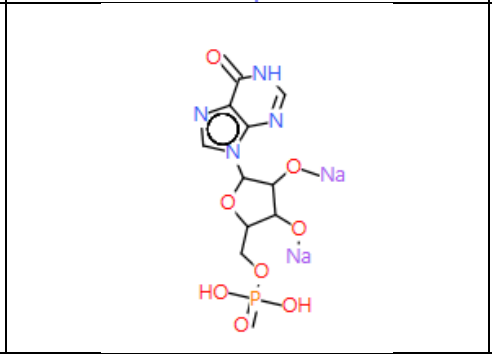
71	693-72-1		11-Octadecenoic acid, (E)- VACCENIC ACID	CCCCCCCCCC=CCCCCCCC(O)=O		[68]
72	2065-73-8	2181811	ethane(~2~H_2_)dioic acid;oxalic [2H]acid;Oxalic acid-d2	OC(=O)C(O)=O		[69]
73	599-54-2		DL-Pantothenic acid	CC(C)(CO)C(O)C(=O)NCCC(O)=O		ID Food: [70]
74	1002-84-2	2136931	Pentadecanoic acid	CCCCCCCCCCCCCCC(O)=O		[71]
75	150-30-1	2057567	"(dl)-phenylalanine;phenylalanine; DL-Phenylalanine	NC(Cc1ccccc1)C(O)=O		[72]
76	81818-54-4	2798339	2-methyl-3-(3,7,11,15-tetramethylhexadec-2-en-1-yl)naphthalene-1,4-dione	CC(C)CCCC(C)CCCC(C)CCCC(C)=CCC1=C(C)C(=O)c2ccccc2C1=O		[73]
77	94-62-2		Bioperine;1-Piperoylpiperidine	O=C(C=CC=Cc1ccc2c(c1)OCO2)N1CCCCC1		[74]

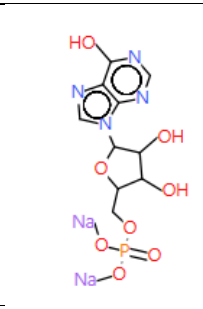
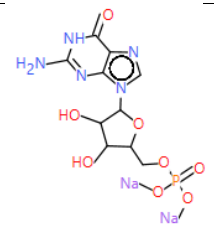
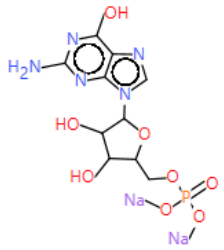
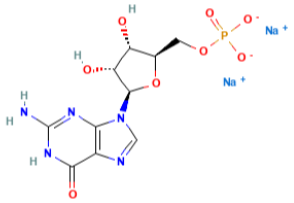
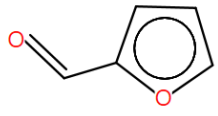
78	609-36-9	2101893	(S)-Pyrrolidine-2-carboxylic acid DL-Proline	OC(=O)C1CCCN1		[75]
79	512-69-6		α-D-Glucopyranoside, β-D-fructofuranosyl O-α-D-galactopyranosyl-(1>6)-; Raffinose	OCC1C(O)C(O)C(O)C(OCC2C(O)C(O)C(O)C(OC3(CO)C(O)C(O)C(CO)O3)O2)O1		[76]
80	68-26-8		Vitamin A; Retinol	CC1CCCC(C)(C)C=1C=CC(C)=CC=CC(C)=CCO		[77]
81	83-88-5		(-)-riboflavin Riboflavin	Cc1cc2c(cc1C)N=C1C(=O)NC(=O)N=C1N2CC(O)C(O)C(O)CO		[78]
82	81-07-2	2013210	1,1-diox-1,2-benzisothiazol-3-one Saccharin	O=C1c2ccccc2S(=O)(=O)N1		[79]
83	302-84-1	2061306	(R)-2-Amino-3-hydroxy-propionic acid D,L-Serine	NC(CO)C(O)=O		[80]

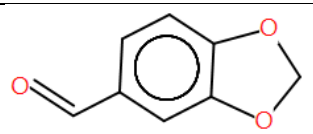
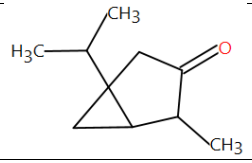
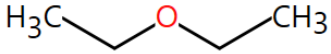
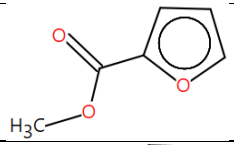
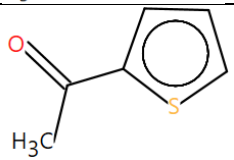
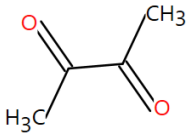
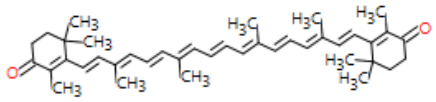
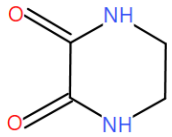
84	470-55-3	2074273	hex-2-ulofuranosyl hexopyranosyl-(1->6)hexopyranosyl-(1->6)hexopyranoside	OCC1C(O)C(O)C(O)C(OCC2C(O)C(O)C(O)C(OCC3C(O)C(O)C(O)C(OC4(CO)C(O)C(O)C(CO)O4)O3)O2)O1		[81]
85	83-48-7		(3-beta)-Stigmasta-5,22-dien-3-ol	CCC(C=CC(C)C1CCC2C3CC=C4CC(O)CCC4(C)C3CCC12C)C(C)C		[82]
86	79324-70-2; 57-50-1		.alpha.-D-Glucopyranoside, .beta.-D-fructofuranosyl Sucrose	OCC1C(O)C(O)C(O)C(OC2(CO)C(O)C(O)C(CO)O2)O1		ID [83]
87	544-63-8	2088752	myristic acid Tetradecanoic acid	CCCCCCCCCCCCCC(O)=O		[84]
88	544-64-9	2088768	(9Z)-tetradec-9-enoic acid	CCCCC=CCCCCCCCC(O)=O		[85]
89	557-59-5	2091807	Tetracosanoic acid	CCCCCCCCCCCCCCCCCCCCCCC(O)=O		[86]

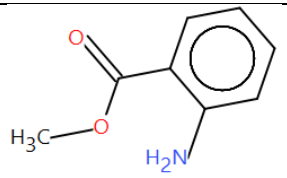
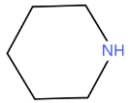
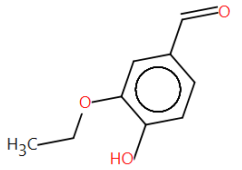
90	83-67-0	2014942	1H-Purine-2,6-dione,_3,7-dihydro-3,7-dimethyl-; Theobromine	CN1C=NC2=C1C(=O)NC(=O)N2C		[87]
91	59-43-8	2004253	3-[(4-Amino-2-methyl-5-pyrimidinyl)methyl]-5-(2-hydroxyethyl)-4-methylthiazolium chloride; Thiamine	[Cl-].Cc1ncc(C[n+]2csc(CCO)c2C)c(N)n1		[88]
92	144-98-9	2056453	allo-DL-threonine DL-Allothreonine threonine	CC(O)C(N)C(O)=O		L-threonine: [89]
93	110-02-1	2037294	Thiophene	C1=CC=CS1		[90]
94	1406-66-2		dl-Tocopherol mixture dl-Tocopherol mixture, natural (alpha, beta, gamma and delta) mixed tocopherols Tocopherols	CC(C)CCCC(C)CCCC(C)CCCC1(C)CCc2c(C)c(O)cc(C)c2O1		[92]
95	7616-22-0	2315234	2,7,8-trimethyl-2-(4,8,12-trimethyltridecyl)-3,4-dihydro-2H-chromen-6-ol; gamma-Tocopherol	CC(C)CCCC(C)CCCC(C)CCCC1(C)CCc2cc(O)c(C)c(C)c2O1		[93]

96	119-13-1	2042990	2,8-dimethyl-2-(4,8,12-trimethyltridecyl)-3,4-dihydro-2H-chromen-6-ol; d-Tocopherol	CC(C)CCCC(C)CCCC(C)CCCC1(C)CCc2cc(O)cc(C)c2O1		[94]
97	54-12-6		(R)-2-Amino-3-(1H-indol-3-yl)-propionic acid DL-Tryptophan	NC(CC1=CNc2ccccc12)C(O)=O		[95]
98	556-03-6	2091131	DL-Tyrosine tyrosine	NC(Cc1ccc(O)cc1)C(O)=O		[96]
99	516-06-3	2082200	(s)-2-amino-3-methyl-butyric acid; DL-Valine	CC(C)C(N)C(O)=O		[97]
100	121-33-5	2044652	4-hydroxy-3-methoxy-benzaldehyde; vanilin	COc1cc(C=O)ccc1O		[98]
101	883-84-1		4-Deoxypyridoxine 5'-phosphate	Cc1c(COP(O)(O)=O)cnc(C)c1O		[99]

102	67-97-0		9,10-Secocholesta-5,7,10(19)-trien-3-ol, (3 ,5Z,7E)-Cholecalciferol Vitamin D3	CC(C)CCCC(C)C1CCC2C(=CC=C3CC(O)CCC3=C)CCCC12C		[100]
103	7732-18-5	2317912	Water	O		[101]
104	7647-14-5	2315983	Sodium chloride (NaCl)	[Na+].[Cl-]		[102]
105	4691-65-0	2251464	Inosine 5'-monophosphate disodium salt hydrate	[Na+].[Na+].O[C@@H]1[C@@H](COP([O-])([O-])=O)O[C@H]([C@@H]1O)n1cnc2C(=O)NC=Nc21		[103]
106	4691-65-0	2251464	Inosine 5'-monophosphate disodium salt hydrate	OC1C(COP(=O)([O][Na])[O][Na])OC(C1O)n1cnc2C(=O)NC=Nc12		[103]

107	4691-65-0	2251464	Inosine 5'-monophosphate disodium salt hydrate	OC1C(COP(=O)(O[Na])O[Na])OC(C1O)n1cnc2c(O)ncnc12		[103]
108	5550-12-9	226-914-1	Disodium guanylate	NC1NC(=O)c2ncn(C3OC(COP(=O)(O[Na])O[Na])C(O)C3O)c2N=1		[103]
109	5550-12-9	226-914-1	Disodium guanylate	Nc1nc(O)c2ncn(C3OC(COP(=O)(O[Na])O[Na])C(O)C3O)c2n1		[103]
110	5550-12-9	226-914-1	Disodium guanylate	C1=NC2=C(N1C3C(C(C(O3)COP(=O)([O-])[O-])O)O)N=C(NC2=O)N.[Na+].[Na+]		[104]
111	98-01-1	2026-27-7	Furfural	O=Cc1ccco1		[105]

112	120-57-0	2044-09-7	Piperonal	O=Cc1ccc2OCOc2c1		[106]
113	546-80-5	2089-12-2	Thujanone	CC(C)C12CC1C(C)C(=O)C2		[107]
114	60-29-7	2004-67-2	Diethylether	CCOCC		[108]
115	611-13-2	2102-54-6	Methyl-2-furoate	COC(=O)c1ccco1		[109]
116	88-15-3	2018-04-6	2-Acetyl thiophene	CC(=O)c1cccs1		[110]
117	431-03-8	2070-69-8	Diacetyl	CC(=O)C(C)=O		[111]
118	514-78-3	2081-87-2	Canthaxanthin	C\C(\C=C\C=C(/C)\C=C\C1=C(C)C(=O)CCC1(C)C)=C/C=C/C=C(\C)/C=C/C=C(\C)/C=C/C1=C(C)C(=O)CCC1(C)C		[112]
119	29990-68-9		Diketopiperazine	O=C1NCCNC1=O		[113]

120	134-20-3	2051-32-4	2-Amino-benzoic acid methyl ester	COC(=O)c1ccccc1N		[114]
121	110-89-4	110-89-4	2038-13-0	C1CCNCC1		[115]
122	121-32-4	2044-64-7	Ethylvanillin	CCOc1cc(C=O)ccc1O		[116]

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